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Supporting Information for "Additivity of Diene Substituent Gibbs Free Energy Contributions for Diels–Alder Reactions Between Me2C=CMe2 and Substituted Cyclopentadienes"

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Electronic Supporting Information for:

Additivity of Diene Substituent Gibbs Free Energy Contributions for Diels–Alder Reactions Between $Me_2C=CMe_2$ and Substituted Cyclopentadienes

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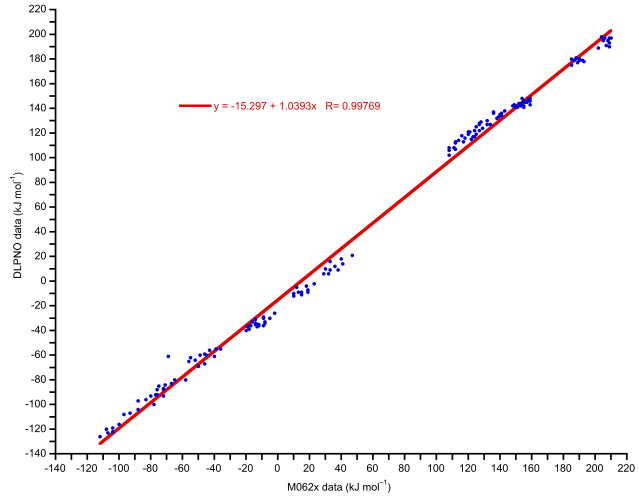
Information 1. Example calculation for determining $\Delta G^{\ddagger}_{\mathrm{ASC1}}$.

$$
\begin{aligned}
\Delta G^{\ddagger}_{\mathrm{ASC1}} = (1/32)\{&[\Delta G^{\ddagger}_{298}\,(\mathbf{1} + c\text{-}1\text{-}C_5H_5R) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + c\text{-}C_5H_6)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,2\text{-}c\text{-}C_5H_4R_2) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 2\text{-}c\text{-}C_5H_5R)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,3\text{-}c\text{-}C_5H_4R_2) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 3^{*}\text{-}c\text{-}C_5H_5R)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,4\text{-}c\text{-}C_5H_4R_2) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 4^{*}\text{-}c\text{-}C_5H_5R)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,5a\text{-}c\text{-}C_5H_4R_2) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 5a\text{-}c\text{-}C_5H_5R)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,5b\text{-}c\text{-}C_5H_4R_2) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 5b\text{-}c\text{-}C_5H_5R)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,2,3\text{-}c\text{-}C_5H_3R_3) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 2,3\text{-}c\text{-}C_5H_4R_2)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,2,4\text{-}c\text{-}C_5H_3R_3) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 2,4\text{-}c\text{-}C_5H_4R_2)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,2,5a\text{-}c\text{-}C_5H_3R_3) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 2,5a\text{-}c\text{-}C_5H_4R_2)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,2,5b\text{-}c\text{-}C_5H_3R_3) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 2,5b\text{-}c\text{-}C_5H_4R_2)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,3,4\text{-}c\text{-}C_5H_3R_3) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 3,4^{*}\text{-}c\text{-}C_5H_4R_2)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,3,5a\text{-}c\text{-}C_5H_3R_3) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 3,5a^{*}\text{-}c\text{-}C_5H_4R_2)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,3,5b\text{-}c\text{-}C_5H_3R_3) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 3,5b^{*}\text{-}c\text{-}C_5H_4R_2)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,4,5a\text{-}c\text{-}C_5H_3R_3) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 4,5a^{*}\text{-}c\text{-}C_5H_4R_2)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,4,5b\text{-}c\text{-}C_5H_3R_3) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 4,5b^{*}\text{-}c\text{-}C_5H_4R_2)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,5a,5b\text{-}c\text{-}C_5H_3R_3) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 5a,5b\text{-}c\text{-}C_5H_4R_2)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,2,3,4\text{-}c\text{-}C_5H_2R_4) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 2,3,4^{*}\text{-}c\text{-}C_5H_3R_3)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,2,3,5a\text{-}c\text{-}C_5H_2R_4) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 2,3,5a\text{-}c\text{-}C_5H_3R_3)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,2,3,5b\text{-}c\text{-}C_5H_2R_4) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 2,3,5b\text{-}c\text{-}C_5H_3R_3)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,2,4,5a\text{-}c\text{-}C_5H_2R_4) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 2,4,5a^{*}\text{-}c\text{-}C_5H_3R_3)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,2,4,5b\text{-}c\text{-}C_5H_2R_4) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 2,4,5b^{*}\text{-}c\text{-}C_5H_3R_3)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,2,5a,5b\text{-}c\text{-}C_5H_2R_4) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 2,5a,5b\text{-}c\text{-}C_5H_3R_3)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,3,4,5a\text{-}c\text{-}C_5H_2R_4) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 3,4,5a^{*}\text{-}c\text{-}C_5H_3R_3)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,3,4,5b\text{-}c\text{-}C_5H_2R_4) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 3,4,5b^{*}\text{-}c\text{-}C_5H_3R_3)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,3,5a,5b\text{-}c\text{-}C_5H_2R_4) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 3,5a,5b^{*}\text{-}c\text{-}C_5H_3R_3)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,4,5a,5b\text{-}c\text{-}C_5H_2R_4) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 4,5a,5b^{*}\text{-}c\text{-}C_5H_3R_3)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,2,3,4,5a\text{-}c\text{-}C_5HR_5) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 2,3,4,5a\text{-}c\text{-}C_5H_2R_4)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,2,3,4,5b\text{-}c\text{-}C_5HR_5) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 2,3,4,5b\text{-}c\text{-}C_5H_2R_4)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,2,3,5a,5b\text{-}c\text{-}C_5HR_5) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 2,3,5a,5b\text{-}c\text{-}C_5H_2R_4)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,2,4,5a,5b\text{-}c\text{-}C_5HR_5) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 2,4,5a,5b\text{-}c\text{-}C_5H_2R_4)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,3,4,5a,5b\text{-}c\text{-}C_5HR_5) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 3,4,5a,5b^{*}\text{-}c\text{-}C_5H_2R_4)] \\
&+ [\Delta G^{\ddagger}_{298}\,(\mathbf{1} + 1,2,3,4,5a,5b\text{-}c\text{-}C_5R_6) - \Delta G^{\ddagger}_{298}\,(\mathbf{1} + 2,3,4,5a,5b\text{-}c\text{-}C_5HR_5)]\}
\end{aligned}
$$

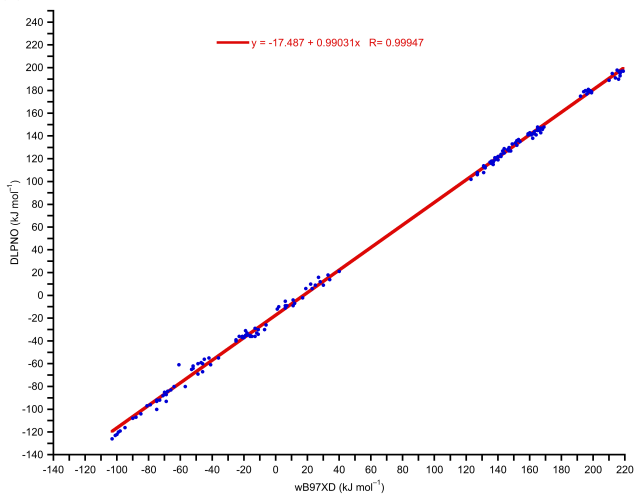
Components marked with asterisks are symmetry-identical to another component. The calculation utilizes the combinations that differ by the presence of 1-substitution; left and right terms have identical substitution patterns save for this position. Overall reaction energy $\Delta G_{\mathrm{ASC\#}}$ values were obtained analogously.

Figure S1. Scatter plots and least-squares line fits for transition state barrier and product Gibbs free energy data for Diels–Alder reactions **1** + *c*-$C_5H_xR_{6-x}$ (R = CH_3, F). (a) DLPNO–CCSD(T) vs M06-2x; (b) DLPNO–CCSD(T) vs M06-2x+GD3; (c) DLPNO–CCSD(T) vs wB97X-D.

(a)



(b)



(c)

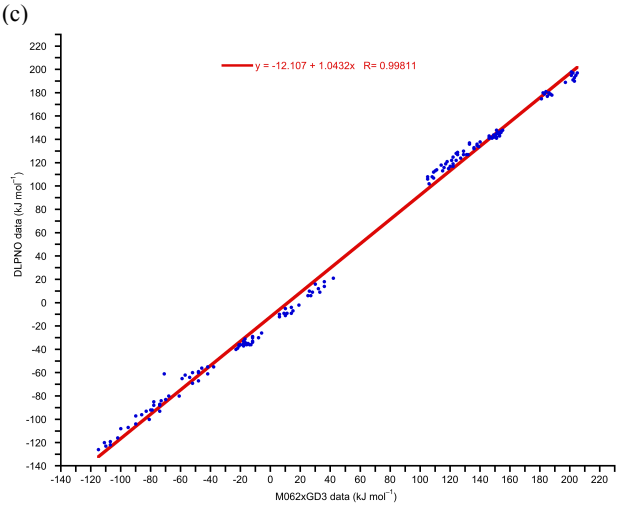


Table S1. C···C forming distances (M06-2X+GD3/6-311+G(d,p), pm) in transition states for Diels–Alder reactions **1** + *c*-$C_5R^1R^2R^3R^4R^{5a}R^{5b}$ (R = H, CH_3, CF_3, F). The row "1 not 2" is the average absolute Δ value for cases where the 1 position is substituted and the 2 position is not; the row "2 not 1" is the average absolute Δ value for cases where the 2 position is substituted and the 1 position is not.

	CH_3				CF_3				F		
	C···C^1	C···C^4	Δ		C···C^1	C···C^4	Δ		C···C^1	C···C^4	Δ
Parent	223.4	223.3	0.1		223.4	223.3	0.1		223.4	223.3	0.1
1	232.2	215.9	16.3		237.3	215.1	22.2		222.8	225.6	-2.8
2	225.2	220.8	4.4		220.1	225.7	-5.6		227.8	219.1	8.7
5a	220.0	228.7	-8.7		216.3	236.4	-20.1		226.9	227.0	-0.1
5b	223.6	223.5	0.1		223.6	223.7	-0.1		226.5	226.5	0.0
12	234.3	216.0	18.3		241.4	215.4	26.0		226.5	224.2	2.3
13	229.8	218.3	11.5		240.1	211.8	28.3		218.8	230.4	-11.6
14	225.5	225.4	0.1		229.2	229.1	0.1		224.9	225.0	-0.1
15a	230.7	219.7	11.0		249.0	211.4	37.6		225.4	230.7	-5.3
15b	232.0	217.4	14.6		242.3	211.8	30.5		224.6	228.9	-4.3
23	222.0	222.0	0.0		220.3	224.4	-4.1		222.5	222.5	0.0
25a	223.8	224.5	-0.7		213.6	239.6	-26.0		233.0	221.2	11.8
25b	225.8	220.7	5.1		219.7	227.5	-7.8		233.3	219.0	14.3
5a5b	219.0	230.1	-11.1		213.3	238.2	-24.9		228.9	229.0	-0.1
123	231.1	218.1	13.0		242.2	211.5	30.7		221.5	228.0	-6.5
124	227.6	224.3	3.3		227.6	232.1	-4.5		229.3	223.0	6.3
125a	242.2	212.0	30.2		248.8	213.2	35.6		230.4	228.3	2.1
125b	234.0	216.5	17.5		247.4	211.9	35.5		230.2	225.3	4.9
135a	237.2	215.0	22.2		252.1	209.6	42.5		220.3	237.2	-16.9
135b	229.6	218.7	10.9		246.5	208.3	38.2		218.5	235.1	-16.6
145a	222.5	231.4	-8.9		228.0	237.0	-9.0		228.9	229.1	-0.2
145b	225.4	225.4	0.0		229.3	229.5	-0.2		227.2	227.2	0.0
15a5b	229.8	220.1	9.7		250.8	207.5	43.3		224.7	234.3	-9.6
235a	227.7	219.4	8.3		210.4	244.1	-33.7		226.1	226.2	-0.1
235b	222.2	222.3	-0.1		221.0	225.9	-4.9		224.7	224.6	0.1
25a5b	223.6	225.2	-1.6		210.0	243.4	-33.4		239.4	218.3	21.1
1234	224.6	224.6	0.0		231.6	228.1	3.5		226.5	226.6	-0.1
1235a	238.9	213.0	25.9		258.2	208.9	49.3		224.1	233.6	-9.5
1235b	230.5	216.9	13.6		252.1	206.4	45.7		222.4	230.8	-8.4
1245a	224.9	230.2	-5.3		231.5	239.9	-8.4		234.7	226.1	8.6
1245b	227.5	224.4	3.1		229.7	232.2	-2.5		233.0	223.1	9.9
125a5b	243.3	210.8	32.5		254.1	208.3	45.8		232.0	229.1	2.9
135a5b	226.5	223.2	3.3		256.0	205.1	50.9		217.2	243.4	-26.2
145a5b	220.5	231.9	-11.4		222.8	236.9	-14.1		229.9	230.1	-0.2
235a5b	218.2	229.7	-11.5		205.6	251.3	-45.7		227.4	227.5	-0.1
12345a	221.8	231.4	-9.6		242.0	234.4	7.6		230.7	230.8	-0.1
12345b	224.7	224.7	0.0		233.1	229.7	3.4		228.1	228.0	0.1
1235a5b	239.4	212.5	26.9		270.6	199.6	71.0		222.6	237.3	-14.7
1245a5b	223.1	230.9	-7.8		222.4	241.5	-19.1		237.8	224.5	13.3
12345a5b	221.0	231.8	-10.8		230.1	238.1	-8.0		231.2	231.3	-0.1
1 not 2			10.0				26.4				7.8
2 not 1			3.8				21.9				6.0

Table S2. $\Delta G^{\ddagger}_{ASC\#}/\Delta G_{ASC\#}$ values with standard deviations (σ) vs model for Diels–Alder reactions **1** + *c*-$C_5R^1R^2R^3R^4R^{5a}R^{5b}$. Values were rounded to the nearest kJ/mol.

R = CH_3	**M06-2x+GD3**		**M06-2X**		**wB97XD**		**DLPNO–CCSD(T)// M06-2X+GD3**	
$\Delta G^{\ddagger}_{ASC1}/\Delta G_{ASC1}$	1(3)	5(1)	2(3)	5(1)	1(3)	6(1)	–1(3)	2(1)
$\Delta G^{\ddagger}_{ASC2}/\Delta G_{ASC2}$	0(2)	–3(2)	1(2)	–2(2)	0(3)	–4(2)	–1(2)	–4(2)
$\Delta G^{\ddagger}_{ASC5a}/\Delta G_{ASC5a}$	42(8)	37(10)	43(8)	38(11)	41(9)	34(11)	42(7)	36(10)
$\Delta G^{\ddagger}_{ASC5b}/\Delta G_{ASC5b}$	10(8)	10(11)	11(8)	10(11)	11(9)	9(11)	9(7)	10(10)

R = CF_3	**M06-2x+GD3**		**M06-2X**		**wB97XD**	
$\Delta G^{\ddagger}_{ASC1}/\Delta G_{ASC1}$	–6(10)	–8(6)	–5(10)	–7(6)	–2(14)	0(9)
$\Delta G^{\ddagger}_{ASC2}/\Delta G_{ASC2}$	–11(4)	–12(6)	–11(4)	–11(6)	–10(5)	–12(8)
$\Delta G^{\ddagger}_{ASC5a}/\Delta G_{ASC5a}$	59(20)	60(28)	60(20)	61(28)	66(25)	66(33)
$\Delta G^{\ddagger}_{ASC5b}/\Delta G_{ASC5b}$	11(20)	22(29)	11(20)	23(28)	16(25)	30(33)

R = F	**M06-2x+GD3**		**M06-2X**		**wB97XD**		**DLPNO–CCSD(T)// M06-2X+GD3**	
$\Delta G^{\ddagger}_{ASC1}/\Delta G_{ASC1}$	–12(3)	–26(6)	–12(3)	–26(6)	–10(3)	–23(5)	–12(3)	–28(5)
$\Delta G^{\ddagger}_{ASC2}/\Delta G_{ASC2}$	–2(4)	–4(7)	–2(4)	–4(7)	–2(4)	–4(6)	–3(3)	–5(6)
$\Delta G^{\ddagger}_{ASC5a}/\Delta G_{ASC5a}$	–10(9)	–22(12)	–10(9)	–22(12)	–5(10)	–18(12)	–4(9)	–16(11)
$\Delta G^{\ddagger}_{ASC5b}/\Delta G_{ASC5b}$	–3(9)	–17(12)	–2(9)	–17(12)	–2(10)	–14(12)	–2(9)	–12(11)

Table S3. Raw molecular energies (hartree) of components, corrected relative free energy barrier heights $\Delta G^{\ddagger}_{298}$ and reaction free energies ΔG_{298} , and subtractions used to derive $\Delta G^{\ddagger}_{ASC\#}$ and $\Delta G_{ASC\#}$ values (kJ mol^{-1}) using various model chemistries for Diels–Alder reactions **1** + *c*–$C_5H_x(CH_3)_{6-x}$.

						DLPNO-CCSD(T)/	DLPNO-CCSD(T)/
		M062X				6-311+G(d,p)//	aug-ccPVTZ//
6-311+G(d,p)	Equivalencies	ΔG_{298} corr	M062X	wB97XD	M062XGD3	M062XGD3	M062XGD3
Me_2CCMe_2		0.132537	-235.788686	-235.841397	-235.789114	-235.247231	-235.422880
123455$C_5(CH_3)_6$		0.222647	-429.904555	-429.983850	-429.905889	-428.919559	-429.229105
CC + 12345a5b ts		0.384508	-665.643073	-665.772345	-665.647053	-664.123646	-664.609332
CC + 12345a5b		0.391270	-665.714665	-665.849961	-665.718525	-664.199513	-664.683625
Barrier		**-77**	**209**	**216**	**203**	**190**	**189**
Reaction		**-95**	**38**	**30**	**33**	**9**	**12**
12345$C_5H(CH_3)_5$		0.195679	-390.597493	-390.668184	-390.598528	-389.701029	-389.981784
CC + 12345a ts		0.356998	-626.341490	-626.462501	-626.344963	-624.909181	-625.366251
CC + 12345a		0.365147	-626.415863	-626.542302	-626.419213	-624.988633	-625.443373
Barrier		**-76**	**193**	**199**	**188**	**178**	**176**
Reaction		**-97**	**19**	**11**	**14**	**-9**	**-5**
12345$C_5H(CH_3)_5$		0.195679	-390.597493	-390.668184	-390.598528	-389.701029	
CC + 12345b ts		0.356702	-626.354205	-626.474647	-626.357691	-624.922213	
CC + 12345b		0.364960	-626.426489	-626.552101	-626.429866	-624.998590	
Barrier		**-75**	**159**	**167**	**153**	**143**	
Reaction		**-96**	**-9**	**-15**	**-14**	**-36**	
12355$C_5H(CH_3)_5$		0.196841	-390.595760	-390.665684	-390.596794	-389.700979	-389.980821
CC + 1235a5b ts	CC + 2345a5b ts	0.357784	-626.333934	-626.453899	-626.337403	-624.903721	-625.360479
CC + 1235a5b	CC + 2345a5b	0.363478	-626.406196	-626.532340	-626.409552	-624.980061	-625.435294
Barrier		**-75**	**207**	**214**	**202**	**191**	**188**
Reaction		**-90**	**32**	**23**	**27**	**6**	**7**
12455$C_5H(CH_3)_5$		0.197066	-390.596321	-390.666215	-390.597365	-389.701415	-389.981259
CC + 1245a5b ts	CC + 1345a5b ts	0.358767	-626.334726	-626.454293	-626.338197	-624.904407	
CC + 1245a5b	CC + 1345a5b	0.365027	-626.404722	-626.530145	-626.408057	-624.978839	-625.433655
Barrier		**-77**	**209**	**217**	**203**	**193**	
Reaction		**-93**	**41**	**34**	**36**	**14**	**16**
1234$C_3H_2(CH_3)_4$		0.168696	-351.291815	-351.353563	-351.292596	-350.484124	-350.736502
CC + 1234 ts		0.329067	-587.049211	-587.160255	-587.052127	-585.705425	-586.132818
CC + 1234		0.338523	-587.121219	-587.237110	-587.124090	-585.782243	-586.207628
Barrier		**-73**	**155**	**164**	**151**	**141**	**143**
Reaction		**-98**	**-9**	**-13**	**-13**	**-36**	**-29**
1235$C_3H_2(CH_3)_4$		0.170074	-351.289390	-351.350705	-351.290169	-350.482959	
CC + 1235a ts	CC + 2345a ts	0.330510	-587.033813	-587.145265	-587.036815	-585.690647	
CC + 1235a	CC + 2345a	0.337746	-587.107681	-587.224988	-587.110568	-585.769409	
Barrier		**-73**	**189**	**196**	**185**	**177**	
Reaction		**-92**	**15**	**6**	**10**	**-11**	
1235$C_3H_2(CH_3)_4$		0.170074	-351.289390	-351.350705	-351.290169	-350.482959	
CC + 1235b ts	CC + 2345b ts	0.329255	-587.045506	-587.156629	-587.048536	-585.702925	
CC + 1235b	CC + 2345b	0.338012	-587.118581	-587.235182	-587.121497	-585.779856	
Barrier		**-70**	**155**	**163**	**151**	**142**	
Reaction		**-93**	**-13**	**-20**	**-18**	**-37**	
1245$C_3H_2(CH_3)_4$		0.170250	-351.289130	-351.350490	-351.289907	-350.482830	
CC + 1245a ts	CC + 1345a ts	0.331291	-587.033238	-587.144707	-587.036223	-585.6903332	
CC + 1245a	CC + 1345a	0.338600	-587.106358	-587.223081	-587.109227	-585.768707	
Barrier		**-75**	**192**	**199**	**187**	**179**	
Reaction		**-94**	**19**	**12**	**15**	**-7**	
1245$C_3H_2(CH_3)_4$		0.170250	-351.289130	-351.350490	-351.289907	-350.482830	
CC + 1245b ts	CC + 1345b ts	0.331235	-587.045743	-587.156389	-587.048716	-585.702952	
CC + 1245b	CC + 1345b	0.338799	-587.116776	-587.232569	-587.119646	-585.778498	
Barrier		**-75**	**159**	**168**	**154**	**146**	
Reaction		**-95**	**-8**	**-12**	**-12**	**-33**	

Table S3. continued

						DLPNO-CCSD(T)/	DLPNO-CCSD(T)/
		M062X				6-311+G(d,p)//	aug-ccPVTZ//
6-311+G(d,p)	Equivalencies	ΔG_{298} corr	M062X	wB97XD	M062XGD3	M062XGD3	M062XGD3
1255$C_3H_2(CH_3)_4$		0.171228	-351.286582	-351.347051	-351.287366	-350.481910	
CC + 125a5b ts	CC + 345a5b ts	0.331686	-587.026401	-587.136543	-587.029350	-585.685183	
CC + 125a5b	CC + 345a5b	0.337499	-587.096559	-587.212580	-587.099422	-585.759392	
Barrier		**-73**	**202**	**210**	**197**	**189**	
Reaction		**-89**	**33**	**25**	**28**	**9**	
1355$C_3H_2(CH_3)_4$		0.171373	-351.287496	-351.348012	-351.288260	-350.482852	
CC + 135a5b ts	CC + 245a5b ts	0.332250	-587.024567	-587.134275	-587.027517	-585.683278	
CC + 135a5b	CC + 245a5b	0.337548	-587.096025	-587.212317	-587.098876	-585.759299	
Barrier		**-74**	**210**	**219**	**205**	**197**	
Reaction		**-88**	**36**	**28**	**32**	**12**	
1455$C_3H_2(CH_3)_4$		0.171468	-351.288463	-351.348812	-351.289254	-350.483388	
CC + 145a5b ts		0.332777	-587.026519	-587.136223	-587.029490	-585.685195	
CC + 145a5b		0.338335	-587.093693	-587.209265	-587.096542	-585.757036	
Barrier		**-76**	**208**	**217**	**204**	**195**	
Reaction		**-90**	**47**	**40**	**42**	**21**	
2355$C_3H_2(CH_3)_4$		0.171016	-351.286420	-351.346964	-351.287175	-350.481994	-350.731900
CC + 235a5b ts		0.331013	-587.022807	-587.132834	-587.025761	-585.681637	-586.109515
CC + 235a5b		0.336752	-587.097240	-587.214199	-587.100107	-585.760100	-586.186379
Barrier		**-72**	**209**	**218**	**205**	**197**	**191**
Reaction		**-87**	**29**	**19**	**25**	**6**	**4**
123$C_3H_3(CH_3)_3$		0.142969	-311.984415	-312.036719	-311.984983	-311.266728	-311.489779
CC + 123 ts	CC + 234 ts	0.302925	-547.741685	-547.843329	-547.744230	-546.487179	-546.885824
CC + 123	CC + 234	0.311821	-547.813865	-547.920620	-547.816316	-546.563826	-546.960506
Barrier		**-72**	**154**	**163**	**150**	**142**	**142**
Reaction		**-95**	**-12**	**-16**	**-16**	**-36**	**-30**
124$C_3H_3(CH_3)_3$		0.143300	-311.983425	-312.035878	-311.983977	-311.266093	
CC + 124 ts	CC + 134 ts	0.304097	-547.740766	-547.842213	-547.743300	-546.486423	
CC + 124	CC + 134	0.312227	-547.811687	-547.917891	-547.814097	-546.562544	
Barrier		**-74**	**156**	**166**	**152**	**145**	
Reaction		**-96**	**-8**	**-11**	**-12**	**-34**	
125$C_3H_3(CH_3)_3$		0.144384	-311.980141	-312.032100	-311.980703	-311.263997	
CC + 125a ts	CC + 345a ts	0.304744	-547.726252	-547.828107	-547.728812	-546.472400	
CC + 125a	CC + 345a	0.311575	-547.798526	-547.905823	-547.800965	-546.549499	
Barrier		**-73**	**185**	**192**	**181**	**175**	
Reaction		**-91**	**13**	**6**	**9**	**-9**	
125$C_3H_3(CH_3)_3$		0.144384	-311.980141	-312.032100	-311.980703	-311.263997	
CC + 125b ts	CC + 345b ts	0.304001	-547.737509	-547.838773	-547.740067	-546.484071	
CC + 125b	CC + 345b	0.311985	-547.809148	-547.915653	-547.811591	-546.559657	
Barrier		**-71**	**153**	**162**	**149**	**142**	
Reaction		**-92**	**-14**	**-19**	**-18**	**-35**	
135$C_3H_3(CH_3)_3$		0.144586	-311.981031	-312.033019	-311.981570	-311.264886	
CC + 135a ts	CC + 245a ts	0.304449	-547.724652	-547.826582	-547.727194	-546.471141	
CC + 135a	CC + 245a	0.311124	-547.798006	-547.905621	-547.800432	-546.549473	
Barrier		**-72**	**190**	**197**	**186**	**179**	
Reaction		**-89**	**15**	**7**	**11**	**-9**	
135$C_3H_3(CH_3)_3$		0.144586	-311.981031	-312.033019	-311.981570	-311.264886	
BN + 135b ts	CC + 245b ts	0.304084	-547.736400	-547.837691	-547.738936	-546.483236	
BN + 135b	CC + 245b	0.311576	-547.808802	-547.915560	-547.811231	-546.559725	
Barrier		**-71**	**158**	**167**	**154**	**147**	
Reaction		**-90**	**-12**	**-18**	**-16**	**-35**	

Table S3. continued

						DLPNO-CCSD(T)/	DLPNO-CCSD(T)/
		M062X				6-311+G(d,p)//	aug-ccPVTZ//
6-311+G(d,p)	Equivalencies	ΔG_{298} corr	M062X	wB97XD	M062XGD3	M062XGD3	M062XGD3
$145C_3H_3(CH_3)_3$		0.144673	-311.981197	-312.033084	-311.981752	-311.264789	
CC + 145a ts		0.304914	-547.725098	-547.826842	-547.727659	-546.471434	
CC + 145a		0.311893	-547.795739	-547.902752	-547.798167	-546.547504	
Barrier		**-73**	**190**	**198**	**186**	**179**	
Reaction		**-91**	**23**	**17**	**19**	**-2**	
$145C_3H_3(CH_3)_3$		0.144673	-311.981197	-312.033084	-311.981752	-311.264789	
CC + 145b ts		0.305054	-547.737151	-547.837993	-547.739680	-546.483528	
CC + 145b		0.312553	-547.806103	-547.912053	-547.808508	-546.557192	
Barrier		**-73**	**159**	**169**	**155**	**148**	
Reaction		**-93**	**-2**	**-6**	**-6**	**-26**	
$155C_3H_3(CH_3)_3$		0.145743	-311.978743	-312.029701	-311.979292	-311.263944	
CC + 15a5b ts	CC + 45a5b ts	0.306094	-547.717104	-547.817998	-547.719617	-546.464667	
CC + 15a5b	CC + 45a5b	0.311525	-547.785515	-547.891688	-547.787916	-546.537736	
Barrier		**-73**	**205**	**212**	**201**	**195**	
Reaction		**-87**	**40**	**33**	**36**	**18**	
$235C_3H_3(CH_3)_3$		0.144494	-311.980933	-312.032897	-311.981476	-311.264735	-311.486504
CC + 235a ts		0.303878	-547.724047	-547.825700	-547.726582	-546.470123	-546.869405
CC + 235a		0.310362	-547.799076	-547.907314	-547.801520	-546.549832	-546.947066
Barrier		**-70**	**190**	**198**	**186**	**180**	**175**
Reaction		**-88**	**10**	**1**	**6**	**-12**	**-11**
$235C_3H_3(CH_3)_3$		0.144494	-311.980933	-312.032897	-311.981476	-311.264735	
CC + 235b ts		0.302929	-547.735852	-547.837422	-547.738404	-546.482550	
CC + 235b		0.310909	-547.810298	-547.917872	-547.812773	-546.560793	
Barrier		**-68**	**157**	**165**	**153**	**145**	
Reaction		**-89**	**-18**	**-25**	**-22**	**-39**	
$255C_3H_3(CH_3)_3$		0.145394	-311.977240	-312.028347	-311.977761	-311.263030	
CC + 25a5b ts	CC + 35a5b ts	0.305019	-547.714408	-547.814482	-547.716901	-546.462333	
CC + 25a5b	CC + 35a5b	0.310827	-547.787512	-547.894324	-547.789912	-546.539486	
Barrier		**-71**	**206**	**216**	**202**	**197**	
Reaction		**-86**	**30**	**22**	**26**	**10**	
$12C_3H_4(CH_3)_2$		0.117527	-272.675229	-272.718229	-272.675611	-272.047887	
CC + 12 ts	CC + 34 ts	0.277378	-508.433716	-508.525647	-508.435843	-507.268549	
CC + 12	CC + 34	0.285760	-508.504631	-508.601430	-508.506657	-507.344074	
Barrier		**-72**	**151**	**161**	**148**	**141**	
Reaction		**-94**	**-13**	**-16**	**-16**	**-35**	
$13C_3H_4(CH_3)_2$		0.117771	-272.676078	-272.719085	-272.676436	-272.048782	
CC + 13 ts	CC + 24 ts	0.277070	-508.432533	-508.524488	-508.434648	-507.267693	
CC + 13	CC + 24	0.285215	-508.504239	-508.601321	-508.506250	-507.344148	
Barrier		**-70**	**155**	**165**	**151**	**145**	
Reaction		**-92**	**-12**	**-16**	**-15**	**-35**	
$14C_3H_4(CH_3)_2$		0.118390	-272.675545	-272.718550	-272.675904	-272.048160	-272.241165
CC + 14 ts		0.278153	-508.432166	-508.523899	-508.434276	-507.267213	-507.636335
CC + 14		0.285813	-508.501105	-508.597623	-508.503087	-507.341673	-507.708187
Barrier		**-71**	**156**	**166**	**152**	**145**	**144**
Reaction		**-92**	**-5**	**-7**	**-8**	**-30**	**-24**
$15C_3H_4(CH_3)_2$		0.118982	-272.672266	-272.714798	-272.672628	-272.046103	
CC + 15a ts	CC + 45a ts	0.278663	-508.417024	-508.509584	-508.419166	-507.252468	
CC + 15a	CC + 45a	0.285131	-508.487878	-508.585505	-508.489902	-507.328517	
Barrier		**-71**	**187**	**194**	**183**	**179**	
Reaction		**-88**	**18**	**11**	**14**	**-4**	

Table S3. continued

						DLPNO-CCSD(T)/	DLPNO-CCSD(T)/
		M062X				6-311+G(d,p)//	aug-ccPVTZ//
6-311+G(d,p)	Equivalencies	ΔG_{298} corr	M062X	wB97XD	M062XGD3	M062XGD3	M062XGD3
$15C_3H_4(CH_3)_2$		0.118982	-272.672266	-272.714798	-272.672628	-272.046103	
CC + 15b ts	CC + 45b ts	0.278369	-508.428722	-508.520177	-508.430853	-507.264641	
CC + 15b	CC + 45b	0.285576	-508.498416	-508.595126	-508.500418	-507.338592	
Barrier		-70	155	165	152	146	
Reaction		-89	-9	-13	-12	-29	
$23C_3H_4(CH_3)_2$		0.117527	-272.675229	-272.718230	-272.675611	-272.047893	-272.241390
CC + 23 ts		0.276335	-508.433128	-508.525158	-508.435250	-507.267858	-507.637955
CC + 23		0.284800	-508.506143	-508.603790	-508.508196	-507.345161	-507.713113
Barrier		-69	150	159	146	141	138
Reaction		-91	-20	-25	-23	-40	-37
$25C_3H_4(CH_3)_2$		0.118798	-272.671723	-272.714353	-272.672070	-272.045922	
CC + 25a ts	CC + 35a ts	0.278226	-508.415712	-508.507592	-508.417824	-507.251197	
CC + 25a	CC + 35a	0.284465	-508.489876	-508.588099	-508.491894	-507.329986	
Barrier		-71	188	197	184	181	
Reaction		-87	10	2	6	-10	
$25C_3H_4(CH_3)_2$		0.118798	-272.671723	-272.714353	-272.672070	-272.045922	
CC + 25b ts	CC + 35b ts	0.277268	-508.427182	-508.518828	-508.429305	-507.263303	
CC + 25b	CC + 35b	0.284976	-508.500832	-508.598306	-508.502856	-507.340637	
Barrier		-68	155	165	152	146	
Reaction		-88	-18	-23	-21	-36	
$55C_3H_4(CH_3)_2$		0.119741	-272.668511	-272.710117	-272.668845	-272.044287	
CC + 5a5b ts		0.279623	-508.406718	-508.496919	-508.408776	-507.243635	
CC + 5a5b		0.284731	-508.476898	-508.573698	-508.478872	-507.317967	
Barrier		-72	204	215	201	198	
Reaction		-85	33	27	30	16	
$1C_5H_5(CH_3)$		0.092112	-233.367377	-233.401001	-233.367588	-232.830168	
CC + 1 ts	CC + 4 ts	0.251559	-469.124871	-469.207104	-469.126616	-468.049290	
CC + 1	CC + 4	0.259186	-469.194070	-469.281223	-469.195701	-468.123444	
Barrier		-71	153	163	150	144	
Reaction		-91	-9	-11	-12	-30	
$2C_5H_5(CH_3)$		0.092222	-233.367679	-233.401275	-233.367887	-232.830611	-232.994636
CC + 2 ts	CC + 3 ts	0.250730	-469.124502	-469.206729	-469.126236	-468.048832	-468.389549
CC + 2	CC + 3	0.258758	-469.196918	-469.284616	-469.198566	-468.125534	-468.463902
Barrier		-68	152	163	149	144	142
Reaction		-89	-17	-21	-20	-36	-33
$5C_5H_5(CH_3)$		0.093122	-233.363018	-233.396219	-233.363207	-232.827335	
CC + 5a ts		0.252527	-469.108053	-469.190210	-469.109798	-468.032807	
CC + 5a		0.258284	-469.179657	-469.267966	-469.181297	-468.109093	
Barrier		-71	185	195	182	180	
Reaction		-86	12	6	10	-5	
$5C_5H_5(CH_3)$		0.093122	-233.363018	-233.396219	-233.363207	-232.827335	-232.990342
CC + 5b ts		0.251955	-469.119303	-469.201063	-469.121023	-468.044562	-468.385178
CC + 5b		0.258897	-469.190464	-469.277929	-469.192083	-468.119615	-468.458095
Barrier		-69	154	165	151	148	143
Reaction		-87	-14	-19	-17	-31	-31
C_5H_6		0.067204	-194.059034	-194.083259	-194.059115	-193.612139	-193.746873
CC + C_5H_6 ts		0.225256	-429.816625	-429.889108	-429.818003	-428.830405	-429.142071
CC + C_5H_6		0.232680	-429.886742	-429.964550	-429.888032	-428.904933	-429.214192
Barrier		-67	149	160	146	143	140
Reaction		-86	-16	-18	-18	-33	-30

Table S3. continued

M062xGD3 values											
Change by Placing CH_3 at Position 1			Change by Placing CH_3 at Position 2			Change by Placing CH_3 at Position 5a			Change by Placing CH_3 at Position 5b		
Subst. Pattern	$\Delta G^{\ddagger}_{ASC1}$	ΔG_{ASC1}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC2}$	ΔG_{ASC2}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5a}$	ΔG_{ASC5a}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5b}$	ΔG_{ASC5b}
1-0	3	6	2-0	3	-2	5a-0	36	28	5b-0	5	1
12-2	-1	3	12-1	-2	-5	15a-1	33	26	15b-1	2	0
13-3	2	5	23-3	-3	-3	25a-2	35	26	25b-2	3	-1
14-4	3	3	24-4	2	-3	35a-3	35	26	35b-3	3	-1
15a-5a	1	5	25a-5a	2	-3	45a-4	33	26	45b-4	2	0
15b-5b	0	5	25b-5b	1	-4	5a5b-5b	50	47	5a5b-5a	19	21
123-23	4	7	123-13	-1	0	125a-12	33	26	125b-12	2	-1
124-24	1	3	124-14	0	-4	135a-13	35	26	135b-13	3	-1
125a-25a	-4	3	125a-15a	-2	-5	145a-14	34	28	145b-14	3	2
125b-25b	-3	3	125b-15b	-2	-5	15a5b-15b	50	48	15a5b-15a	18	22
134-34	5	4	234-34	3	1	235a-23	40	29	235b-23	6	1
135a-35a	1	5	235a-35a	2	0	245a-24	35	26	245b-24	3	-1
135b-35b	2	5	235b-35b	1	-1	25a5b-25b	51	47	25a5b-25a	18	20
145a-45a	3	5	245a-45a	3	-3	345a-34	33	26	345b-34	2	-1
145b-45b	3	6	245b-45b	3	-4	35a5b-35b	51	47	35a5b-35a	18	20
15a5b-5a5b	0	6	25a5b-5a5b	1	-4	45a5b-45b	50	48	45a5b-45a	18	22
1234-234	0	2	1234-134	-2	-1	1235a-123	34	26	1235b-123	0	-2
1235a-235a	-1	4	1235a-135a	-1	-1	1245a-124	35	27	1245b-124	2	0
1235b-235b	-2	4	1235b-135b	-3	-2	125a5b-125b	48	46	125a5b-125a	16	19
1245a-245a	1	4	1245a-145a	1	-5	1345a-134	35	27	1345b-134	2	0
1245b-245b	0	4	1245b-145b	-1	-6	135a5b-135b	51	48	135a5b-135a	19	21
125a5b-25a5b	-5	2	125a5b-15a5b	-4	-8	145a5b-145b	49	48	145a5b-145a	18	23
1345a-345a	6	6	2345a-345a	4	1	2345a-234	34	26	2345b-234	0	-2
1345b-345b	5	6	2345b-345b	1	0	235a5b-235b	52	46	235a5b-235a	19	18
135a5b-35a5b	3	6	235a5b-35a5b	2	-1	245a5b-245b	51	48	245a5b-245a	19	21
145a5b-45a5b	3	6	245a5b-45a5b	4	-4	345a5b-345b	48	46	345a5b-345a	16	19
12345a-2345a	3	4	12345a-1345a	0	-1	12345a-1234	37	27	12345b-1234	3	-1
12345b-2345b	3	4	12345b-1345b	-1	-2	1235a5b-1235b	51	45	1235a5b-1235a	17	17
1235a5b-235a5b	-3	3	1235a5b-135a5b	-3	-4	1245a5b-1245b	49	48	1245a5b-1245a	16	22
1245a5b-245a5b	-2	4	1245a5b-145a5b	-1	-6	1345a5b-1345b	49	48	1345a5b-1345a	16	22
1345a5b-345a5b	6	8	2345a5b-345a5b	5	-1	2345a5b-2345b	51	45	2345a5b-2345a	17	17
12345a5b-2345a5b	1	6	12345a5b-1345a5b	0	-3	12345a5b-12345b	49	47	12345a5b-12345a	15	19
Avg(StdDev)	1 (3)	5 (1)	Avg(StdDev)	0 (2)	–3(2)	Avg(StdDev)	42 (8)	37 (11)	Avg(StdDev)	10 (8)	10 (11)

M062x values											
Change by Placing CH_3 at Position 1			Change by Placing CH_3 at Position 2			Change by Placing CH_3 at Position 5a			Change by Placing CH_3 at Position 5b		
Subst. Pattern	$\Delta G^{\ddagger}_{ASC1}$	ΔG_{ASC1}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC2}$	ΔG_{ASC2}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5a}$	ΔG_{ASC5a}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5b}$	ΔG_{ASC5b}
1-0	4	7	2-0	3	-1	5a-0	37	28	5b-0	5	1
12-2	-1	4	12-1	-2	-4	15a-1	34	27	15b-1	3	0
13-3	3	5	23-3	-2	-2	25a-2	36	27	25b-2	3	-1
14-4	3	4	24-4	2	-3	35a-3	36	27	35b-3	3	-1
15a-5a	1	5	25a-5a	3	-3	45a-4	34	27	45b-4	3	0
15b-5b	1	6	25b-5b	1	-3	5a5b-5b	50	48	5a5b-5a	19	21
123-23	5	8	123-13	0	0	125a-12	34	26	125b-12	2	-1
124-24	2	4	124-14	1	-3	135a-13	35	27	135b-13	3	0
125a-25a	-3	3	125a-15a	-2	-5	145a-14	35	28	145b-14	3	3
125b-25b	-2	4	125b-15b	-2	-5	15a5b-15b	50	49	15a5b-15a	19	22
134-34	5	5	234-34	3	1	235a-23	40	30	235b-23	7	2
135a-35a	2	5	235a-35a	2	1	245a-24	35	27	245b-24	3	0
135b-35b	3	6	235b-35b	1	0	25a5b-25b	51	48	25a5b-25a	18	20
145a-45a	4	6	245a-45a	3	-3	345a-34	34	26	345b-34	2	-1
145b-45b	4	7	245b-45b	3	-3	35a5b-35b	51	48	35a5b-35a	18	20
15a5b-5a5b	1	6	25a5b-5a5b	2	-4	45a5b-45b	50	49	45a5b-45a	19	22
1234-234	1	3	1234-134	-1	-1	1235a-123	35	26	1235b-123	1	-2
1235a-235a	-1	4	1235a-135a	-1	0	1245a-124	35	27	1245b-124	2	1
1235b-235b	-1	4	1235b-135b	-3	-1	125a5b-125b	48	46	125a5b-125a	17	20
1245a-245a	2	4	1245a-145a	2	-4	1345a-134	35	27	1345b-134	2	1
1245b-245b	1	4	1245b-145b	0	-5	135a5b-135b	52	48	135a5b-135a	20	21
125a5b-25a5b	-5	3	125a5b-15a5b	-4	-7	145a5b-145b	49	49	145a5b-145a	18	24
1345a-345a	7	6	2345a-345a	5	2	2345a-234	35	26	2345b-234	1	-2
1345b-345b	6	6	2345b-345b	2	0	235a5b-235b	53	47	235a5b-235a	19	19
135a5b-35a5b	4	7	235a5b-35a5b	3	-1	245a5b-245b	52	48	245a5b-245a	20	21
145a5b-45a5b	3	7	245a5b-45a5b	5	-4	345a5b-345b	48	46	345a5b-345a	17	20
12345a-2345a	3	5	12345a-1345a	1	0	12345a-1234	38	28	12345b-1234	4	0
12345b-2345b	3	4	12345b-1345b	0	-2	1235a5b-1235b	52	46	1235a5b-1235a	18	18
1235a5b-235a5b	-2	3	1235a5b-135a5b	-3	-4	1245a5b-1245b	50	49	1245a5b-1245a	17	22
1245a5b-245a5b	-1	5	1245a5b-145a5b	0	-5	1345a5b-1345b	50	49	1345a5b-1345a	17	22
1345a5b-345a5b	7	9	2345a5b-345a5b	6	0	2345a5b-2345b	52	46	2345a5b-2345a	18	18
12345a5b-2345a5b	2	6	12345a5b-1345a5b	0	-3	12345a5b-12345b	50	48	12345a5b-12345a	16	19
Avg(StdDev)	2 (3)	5 (1)	Avg(StdDev)	1 (2)	–2 (2)	Avg(StdDev)	43 (8)	38 (11)	Avg(StdDev)	11 (8)	10 (11)

Table S3. continued

wB9XD values											
Change by Placing CH_3 at Position 1			Change by Placing CH_3 at Position 2			Change by Placing CH_3 at Position 5a			Change by Placing CH_3 at Position 5b		
Subst. Pattern	$\Delta G^{\ddagger}_{ASC1}$	ΔG_{ASC1}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC2}$	ΔG_{ASC2}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5a}$	ΔG_{ASC5a}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5b}$	ΔG_{ASC5b}
1-0	3	7	2-0	2	-3	5a-0	35	24	5b-0	5	0
12-2	-2	5	12-1	-2	-5	15a-1	30	23	15b-1	2	-2
13-3	2	5	23-3	-3	-4	25a-2	34	23	25b-2	2	-3
14-4	3	4	24-4	1	-4	35a-3	34	23	35b-3	2	-3
15a-5a	-1	5	25a-5a	2	-4	45a-4	30	23	45b-4	2	-2
15b-5b	0	6	25b-5b	0	-5	5a5b-5b	50	46	5a5b-5a	20	21
123-23	4	9	123-13	-1	-1	125a-12	31	22	125b-12	1	-3
124-24	1	4	124-14	0	-4	135a-13	33	23	135b-13	2	-2
125a-25a	-5	4	125a-15a	-1	-5	145a-14	32	24	145b-14	3	1
125b-25b	-3	5	125b-15b	-3	-6	15a5b-15b	47	46	15a5b-15a	19	22
134-34	5	5	234-34	2	0	235a-23	39	26	235b-23	5	-1
135a-35a	0	5	235a-35a	1	-1	245a-24	33	23	245b-24	2	-2
135b-35b	2	6	235b-35b	0	-2	25a5b-25b	51	45	25a5b-25a	19	20
145a-45a	4	6	245a-45a	4	-4	345a-34	31	22	345b-34	1	-3
145b-45b	4	7	245b-45b	2	-5	35a5b-35b	51	45	35a5b-35a	19	20
15a5b-5a5b	-3	6	25a5b-5a5b	1	-5	45a5b-45b	47	46	45a5b-45a	19	22
1234-234	1	3	1234-134	-2	-2	1235a-123	33	22	1235b-123	0	-4
1235a-235a	-2	5	1235a-135a	-1	-1	1245a-124	32	23	1245b-124	2	-1
1235b-235b	-2	5	1235b-135b	-4	-3	125a5b-125b	47	44	125a5b-125a	17	19
1245a-245a	1	5	1245a-145a	1	-5	1345a-134	32	23	1345b-134	2	-1
1245b-245b	1	5	1245b-145b	-1	-6	135a5b-135b	52	46	135a5b-135a	22	21
125a5b-25a5b	-7	3	125a5b-15a5b	-3	-8	145a5b-145b	48	46	145a5b-145a	19	23
1345a-345a	6	6	2345a-345a	4	0	2345a-234	33	22	2345b-234	0	-4
1345b-345b	6	6	2345b-345b	1	-2	235a5b-235b	53	45	235a5b-235a	20	19
135a5b-35a5b	3	6	235a5b-35a5b	2	-3	245a5b-245b	52	46	245a5b-245a	22	21
145a5b-45a5b	5	7	245a5b-45a5b	7	-5	345a5b-345b	47	44	345a5b-345a	17	19
12345a-2345a	3	5	12345a-1345a	0	-1	12345a-1234	35	24	12345b-1234	2	-2
12345b-2345b	3	5	12345b-1345b	-1	-3	1235a5b-1235b	51	43	1235a5b-1235a	18	17
1235a5b-235a5b	-4	4	1235a5b-135a5b	-5	-5	1245a5b-1245b	49	46	1245a5b-1245a	18	22
1245a5b-245a5b	-3	6	1245a5b-145a5b	-1	-6	1345a5b-1345b	49	46	1345a5b-1345a	18	22
1345a5b-345a5b	7	9	2345a5b-345a5b	5	-2	2345a5b-2345b	51	43	2345a5b-2345a	18	17
12345a5b-2345a5b	2	7	12345a5b-1345a5b	-1	-4	12345a5b-12345b	49	45	12345a5b-12345a	17	19
Avg(StdDev)	1 (3)	6 (1)	Avg(StdDev)	0 (3)	–4 (2)	Avg(StdDev)	41 (9)	34 (11)	Avg(StdDev)	11 (9)	9 (11)

DLPNO-CCSD(T)//M062x+GD3 values											
Change by Placing CH_3 at Position 1			Change by Placing CH_3 at Position 2			Change by Placing CH_3 at Position 5a			Change by Placing CH_3 at Position 5b		
Subst. Pattern	$\Delta G^{\ddagger}_{ASC1}$	ΔG_{ASC1}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC2}$	ΔG_{ASC2}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5a}$	ΔG_{ASC5a}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5b}$	ΔG_{ASC5b}
1-0	1	3	2-0	1	-3	5a-0	37	28	5b-0	5	2
12-2	-3	1	12-1	-3	-5	15a-1	34	26	15b-1	1	1
13-3	0	1	23-3	-4	-4	25a-2	36	26	25b-2	2	0
14-4	1	0	24-4	0	-5	35a-3	36	26	35b-3	2	0
15a-5a	-2	1	25a-5a	1	-5	45a-4	34	26	45b-4	1	1
15b-5b	-2	2	25b-5b	-1	-5	5a5b-5b	50	47	5a5b-5a	17	21
123-23	2	5	123-13	-2	-1	125a-12	34	25	125b-12	1	0
124-24	0	1	124-14	-1	-4	135a-13	35	26	135b-13	2	0
125a-25a	-6	0	125a-15a	-4	-5	145a-14	34	28	145b-14	2	4
125b-25b	-4	1	125b-15b	-3	-6	15a5b-15b	49	47	15a5b-15a	17	22
134-34	3	1	234-34	1	-1	235a-23	40	28	235b-23	5	1
135a-35a	-1	1	235a-35a	0	-2	245a-24	35	26	245b-24	2	0
135b-35b	0	2	235b-35b	-1	-3	25a5b-25b	50	46	25a5b-25a	16	19
145a-45a	1	2	245a-45a	1	-5	345a-34	34	25	345b-34	1	0
145b-45b	2	4	245b-45b	1	-5	35a5b-35b	50	46	35a5b-35a	16	19
15a5b-5a5b	-2	2	25a5b-5a5b	-1	-6	45a5b-45b	49	47	45a5b-45a	17	22
1234-234	-1	0	1234-134	-4	-2	1235a-123	35	25	1235b-123	-1	-2
1235a-235a	-3	1	1235a-135a	-2	-2	1245a-124	34	26	1245b-124	1	1
1235b-235b	-4	2	1235b-135b	-5	-3	125a5b-125b	46	44	125a5b-125a	14	19
1245a-245a	0	1	1245a-145a	0	-5	1345a-134	34	26	1345b-134	1	1
1245b-245b	-1	2	1245b-145b	-2	-7	135a5b-135b	51	46	135a5b-135a	18	20
125a5b-25a5b	-8	0	125a5b-15a5b	-6	-8	145a5b-145b	47	47	145a5b-145a	16	23
1345a-345a	4	2	2345a-345a	2	-1	2345a-234	35	25	2345b-234	-1	-2
1345b-345b	3	2	2345b-345b	-1	-2	235a5b-235b	52	45	235a5b-235a	17	18
135a5b-35a5b	0	2	235a5b-35a5b	0	-4	245a5b-245b	51	46	245a5b-245a	18	20
145a5b-45a5b	0	3	245a5b-45a5b	2	-6	345a5b-345b	46	44	345a5b-345a	14	19
12345a-2345a	1	2	12345a-1345a	-1	-2	12345a-1234	37	27	12345b-1234	2	0
12345b-2345b	2	2	12345b-1345b	-3	-3	1235a5b-1235b	50	43	1235a5b-1235a	14	17
1235a5b-235a5b	-6	0	1235a5b-135a5b	-6	-6	1245a5b-1245b	47	46	1245a5b-1245a	14	21
1245a5b-245a5b	-5	2	1245a5b-145a5b	-2	-7	1345a5b-1345b	47	46	1345a5b-1345a	14	21
1345a5b-345a5b	4	5	2345a5b-345a5b	3	-3	2345a5b-2345b	50	43	2345a5b-2345a	14	17
12345a5b-2345a5b	-1	3	12345a5b-1345a5b	-2	-5	12345a5b-12345b	47	44	12345a5b-12345a	12	18
Avg(StdDev)	–1 (3)	2 (1)	Avg(StdDev)	–1 (2)	–4 (2)	Avg(StdDev)	42 (7)	36 (10)	Avg(StdDev)	9 (7)	10 (10)

Table S4. Corrected relative free energy barrier heights $\Delta G^{\ddagger}$ and reaction free energies ΔG from Table S3, and $\Delta G^{\ddagger}/\Delta G$ values derived by summing $\Delta G^{\ddagger}_{ASC\#}/\Delta G_{ASC\#}$ values (marked with "(p)") (kJ mol^{-1}) using various model chemistries for Diels–Alder reactions **1** + *c*–$C_5H_x(CH_3)_{6-x}$.

M062x values								
Change by Placing CH_3 at Position 1			**Change by Placing CH_3 at Position 2**					
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**2**	**5**		**1**	**-2**			
Change by Placing CH_3 at Position 5a			**Change by Placing CH_3 at Position 5b**					
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**43**	**37**		**11**	**10**			
wB97XD values								
Change by Placing CH_3 at Position 1			**Change by Placing CH_3 at Position 2**					
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**1**	**6**		**0**	**-4**			
Change by Placing CH_3 at Position 5a			**Change by Placing CH_3 at Position 5b**					
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**41**	**34**		**11**	**9**			
M062x+GD3 values								
Change by Placing CH_3 at Position 1			**Change by Placing CH_3 at Position 2**					
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**1**	**5**		**0**	**-3**			
Change by Placing CH_3 at Position 5a			**Change by Placing CH_3 at Position 5b**					
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**42**	**37**		**10**	**10**			
DLPNO-CCSD(T)//M062x+GD3 values								
Change by Placing CH_3 at Position 1			**Change by Placing CH_3 at Position 2**					
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**-1**	**2**		**-1**	**-4**			
Change by Placing CH_3 at Position 5a			**Change by Placing CH_3 at Position 5b**					
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**42**	**36**		**9**	**10**			
						(p)	**(p)**	**(p)**
	M062X	**wB97XD**	**M062XGD3**	**DLPNO-CCSD(T)**	**M062X**	**wB97XD**	**M062XGD3**	**DLPNO-CCSD(T)**
CC + C_5H_6 ts	149	160	146	143				
CC + C_5H_6	-16	-18	-18	-33				
CC + 12345a5b ts	209	216	203	190	209	214	200	190
CC + 12345a5b	38	30	33	9	37	29	33	9
CC + 12345a ts	193	199	188	178	198	203	190	181
CC + 12345a	19	11	14	-9	27	20	23	-1
CC + 12345b ts	159	167	153	143	166	173	158	148
CC + 12345b	-9	-15	-14	-36	0	-5	-4	-27
CC + 1235a5b ts	207	214	202	191	207	213	199	191
CC + 1235a5b	32	23	27	6	32	23	28	7
CC + 1245a5b ts	209	217	203	193	208	214	200	191
CC + 1245a5b	41	34	36	14	39	33	36	13
CC + 1234 ts	155	164	151	141	155	163	149	142
CC + 1234	-9	-13	-13	-36	-10	-15	-14	-34
CC + 1235a ts	189	196	185	177	196	202	189	182
CC + 1235a	15	6	10	-11	22	14	18	-3
CC + 1235b ts	155	163	151	142	164	172	157	149
CC + 1235b	-13	-20	-18	-37	-5	-11	-9	-29
CC + 1245a ts	192	199	187	179	197	203	190	182
CC + 1245a	19	12	15	-7	29	24	26	3
CC + 1245b ts	159	168	154	146	165	173	158	149
CC + 1245b	-8	-12	-12	-33	2	-1	-1	-23
CC + 125a5b ts	202	210	197	189	206	213	199	192
CC + 125a5b	33	25	28	9	34	27	31	11
CC + 135a5b ts	210	219	205	197	206	213	199	192
CC + 135a5b	36	28	32	12	34	27	31	11
CC + 145a5b ts	208	217	204	195	207	214	200	192
CC + 145a5b	47	40	42	21	41	37	39	17
CC + 235a5b ts	209	218	205	197	205	212	198	192
CC + 235a5b	29	19	25	6	27	17	23	5
CC + 123 ts	154	163	150	142	153	162	148	142
CC + 123	-12	-16	-16	-36	-15	-18	-18	-37
CC + 124 ts	156	166	152	145	154	163	149	143
CC + 124	-8	-11	-12	-34	-8	-11	-11	-30

Table S4. continued

					(p)	(p)	(p)	(p)
				DLPNO-				DLPNO-
	M062X	wB97XD	M062XGD3	CCSD(T)	M062X	wB97XD	M062XGD3	CCSD(T)
CC + 125a ts	185	192	181	175	195	202	189	183
CC + 125a	13	6	9	-9	24	18	21	1
CC + 125b ts	153	162	149	142	163	172	157	150
CC + 125b	-14	-19	-18	-35	-3	-7	-6	-25
CC + 135a ts	190	197	186	179	195	202	189	183
CC + 135a	15	7	11	-9	24	18	21	1
CC + 135b ts	158	167	154	147	163	172	157	150
CC + 135b	-12	-18	-16	-35	-3	-7	-6	-25
CC + 145a ts	190	198	186	179	196	203	190	183
CC + 145a	23	17	19	-2	31	28	29	7
CC + 145b ts	159	169	155	148	164	173	158	150
CC + 145b	-2	-6	-6	-26	4	3	2	-19
CC + 15a5b ts	205	212	201	195	205	213	199	193
CC + 15a5b	40	33	36	18	36	31	34	15
CC + 235a ts	190	198	186	180	194	201	188	183
CC + 235a	10	1	6	-12	17	8	13	-5
CC + 235b ts	157	165	153	145	162	171	156	150
CC + 235b	-18	-25	-22	-39	-10	-17	-14	-31
CC + 25a5b ts	206	216	202	197	204	212	198	193
CC + 25a5b	30	22	26	10	29	21	26	9
CC + 12 ts	151	161	148	141	152	162	148	143
CC + 12	-13	-16	-16	-35	-13	-14	-15	-33
CC + 13 ts	155	165	151	145	152	162	148	143
CC + 13	-12	-16	-15	-35	-13	-14	-15	-33
CC + 14 ts	156	166	152	145	153	163	149	144
CC + 14	-5	-7	-8	-30	-6	-7	-8	-26
CC + 15a ts	187	194	183	179	194	202	189	184
CC + 15a	18	11	14	-4	26	22	24	5
CC + 15b ts	155	165	152	146	162	172	157	151
CC + 15b	-9	-13	-12	-29	-1	-3	-3	-21
CC + 23 ts	150	159	146	141	151	161	147	143
CC + 23	-20	-25	-23	-40	-20	-24	-23	-39
CC + 25a ts	188	197	184	181	193	201	188	184
CC + 25a	10	2	6	-10	19	12	16	-1
CC + 25b ts	155	165	152	146	161	171	156	151
CC + 25b	-18	-23	-21	-36	-8	-13	-11	-27
CC + 5a5b ts	204	215	201	198	203	212	198	194
CC + 5a5b	33	27	30	16	31	25	29	13
CC + 1 ts	153	163	150	144	151	162	148	145
CC + 1	-9	-11	-12	-30	-11	-13	-13	-28
CC + 2 ts	152	163	149	144	150	161	147	144
CC + 2	-17	-21	-20	-36	-18	-20	-20	-35
CC + 5a ts	185	195	182	180	192	201	188	185
CC + 5a	12	6	10	-5	21	16	19	3
CC + 5b ts	154	165	151	148	160	171	156	152
CC + 5b	-14	-19	-17	-31	-6	-9	-8	-23

Figure S2. DLPNO-CCSD(T)/6-311+G(d,p) model chemistry-predicted transition state free energy barriers $\Delta G^{\ddagger}_{298}$ (red dots) and reaction free energies ΔG_{298} (blue squares) vs. $\Delta G^{\ddagger}_{298}/\Delta G_{298}$ values predicted by summing $\Delta G^{\ddagger}_{ASC\#}/\Delta G_{ASC\#}$ values (from Table S4, kJ mol^{-1}) for Diels–Alder reactions **1** + *c*-$C_5H_x(CH_3)_{6-x}$.

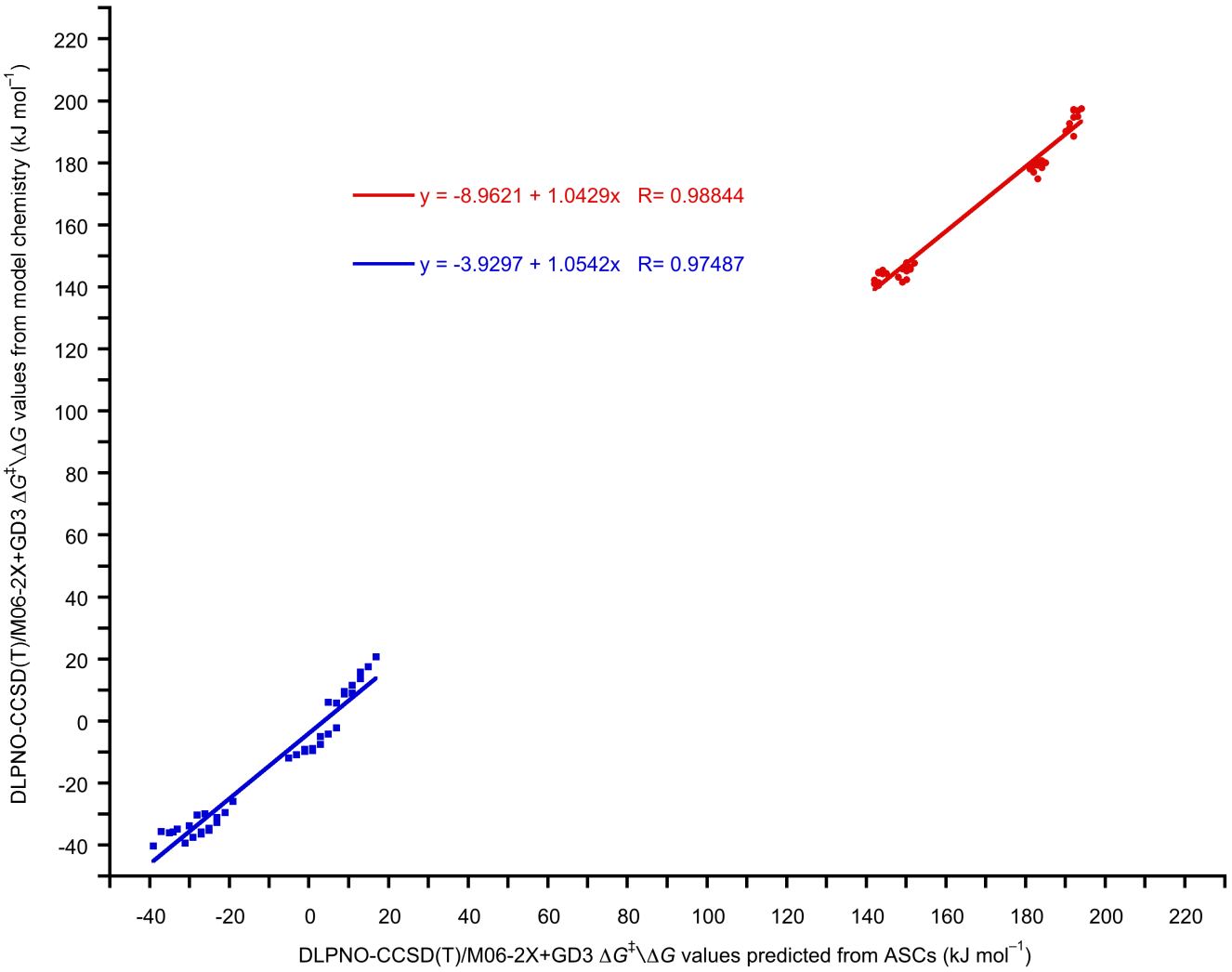


Table S5. Raw molecular energies (hartree) of components, corrected relative free energy barrier heights $\Delta G^{\ddagger}_{298}$ and reaction free energies ΔG_{298}, and subtractions used to derive $\Delta G^{\ddagger}_{ASC\#}$ and $\Delta G_{ASC\#}$ values (kJ mol^{-1}) using various model chemistries for Diels–Alder reactions **1** + *c*–$C_5H_xF_{6-x}$.

						DLPNO-CCSD(T)/	DLPNO-CCSD(T)/
		M062X				6-311+G(d,p)//	aug-ccPVTZ//
6-311+G(d,p)	Equivalencies	ΔG_{298} corr	M062X	wB97XD	M062XGD3	M062XGD3	M062XGD3
Me_2CCMe_2		0.132537	-235.788686	-235.841397	-235.789114	-235.247231	-235.422880
123455C_5F_6		0.012172	-789.460075	-789.486915	-789.460217	-788.043470	-788.551764
CC + 12345a5b ts		0.170884	-1025.232782	-1025.304758	-1025.234506	-1023.275583	-1023.960754
CC + 12345a5b		0.178473	-1025.325340	-1025.401359	-1025.326964	-1023.372413	-1024.056851
Barrier		**-69**	**111**	**131**	**108**	**108**	**105**
Reaction		**-89**	**-112**	**-103**	**-115**	**-126**	**-127**
12345C_5HF_5		0.021312	-690.219396	-690.246498	-690.219538	-688.962930	
CC + 12345a ts		0.180225	-925.993376	-926.065768	-925.995067	-924.196216	
CC + 12345a		0.187732	-926.082896	-926.160095	-926.084491	-924.291050	
Barrier		**-69**	**108**	**127**	**105**	**106**	
Reaction		**-89**	**-107**	**-101**	**-110**	**-123**	
12345C_5HF_5		0.021312	-690.219396	-690.246498	-690.219538	-688.962930	-689.409033
CC + 12345b ts		0.179405	-925.992330	-926.066638	-925.993995	-924.196949	-924.819711
CC + 12345b		0.187351	-926.081357	-926.159387	-926.082923	-924.290088	-924.911611
Barrier		**-67**	**108**	**123**	**106**	**102**	**99**
Reaction		**-88**	**-104**	**-100**	**-107**	**-122**	**-121**
12355C_5HF_5		0.021361	-690.237610	-690.263439	-690.237749	-688.982079	-689.428138
CC + 1235a5b ts	CC + 2345a5b ts	0.179956	-926.005206	-926.076807	-926.006880	-924.209090	-924.833167
CC + 1235a5b	CC + 2345a5b	0.187557	-926.090611	-926.167188	-926.092184	-924.298536	-924.920641
Barrier		**-68**	**124**	**142**	**121**	**122**	**115**
Reaction		**-88**	**-80**	**-75**	**-83**	**-93**	**-94**
12455C_5HF_5		0.021186	-690.233729	-690.259651	-690.233867	-688.978673	
CC + 1245a5b ts	CC + 1345a5b ts	0.179951	-926.006109	-926.077122	-926.007791	-924.209570	
CC + 1245a5b	CC + 1345a5b	0.187302	-926.097233	-926.172462	-926.098815	-924.305308	
Barrier		**-69**	**112**	**132**	**109**	**112**	
Reaction		**-88**	**-108**	**-99**	**-111**	**-120**	
1234$C_3H_2F_4$		0.030270	-590.994825	-591.021628	-590.994964	-589.898085	-590.282220
CC + 1234 ts		0.189023	-826.763314	-826.836980	-826.764932	-825.127905	-825.688777
CC + 1234		0.196540	-826.846982	-826.925249	-826.848514	-825.217090	-825.776494
Barrier		**-69**	**122**	**137**	**119**	**115**	**112**
Reaction		**-89**	**-78**	**-75**	**-81**	**-100**	**-99**
1235$C_3H_2F_4$		0.030533	-590.993990	-591.020131	-590.994124	-589.898934	
CC + 1235a ts	CC + 2345a ts	0.189287	-826.763788	-826.835979	-826.765424	-825.128171	
CC + 1235a	CC + 2345a	0.196841	-826.845461	-826.923165	-826.847001	-825.214923	
Barrier		**-69**	**118**	**136**	**116**	**116**	
Reaction		**-89**	**-76**	**-73**	**-79**	**-92**	
1235$C_3H_2F_4$		0.030533	-590.993990	-591.020131	-590.994124	-589.898934	
CC + 1235b ts	CC + 2345b ts	0.189055	-826.761301	-826.835418	-826.762914	-825.127518	
CC + 1235b	CC + 2345b	0.196457	-826.843300	-826.921800	-826.844812	-825.213198	
Barrier		**-68**	**124**	**137**	**122**	**117**	
Reaction		**-88**	**-72**	**-71**	**-74**	**-88**	
1245$C_3H_2F_4$		0.030317	-590.992086	-591.018285	-590.992219	-589.897244	
CC + 1245a ts	CC + 1345a ts	0.189185	-826.765992	-826.837537	-826.767626	-825.129706	
CC + 1245a	CC + 1345a	0.196569	-826.854080	-826.930587	-826.855618	-825.223432	
Barrier		**-69**	**108**	**127**	**105**	**108**	
Reaction		**-89**	**-104**	**-98**	**-107**	**-119**	
1245$C_3H_2F_4$		0.030317	-590.992086	-591.018285	-590.992219	-589.897244	
CC + 1245b ts	CC + 1345b ts	0.188781	-826.764122	-826.837396	-826.765742	-825.129647	
CC + 1245b	CC + 1345b	0.196239	-826.852129	-826.929360	-826.853653	-825.222043	
Barrier		**-68**	**112**	**127**	**109**	**107**	
Reaction		**-88**	**-100**	**-95**	**-102**	**-116**	

Table S5. continued

						DLPNO-CCSD(T)/	DLPNO-CCSD(T)/
		M062X				6-311+G(d,p)//	aug-ccPVTZ//
6-311+G(d,p)	Equivalencies	ΔG_{298} corr	M062X	wB97XD	M062XGD3	M062XGD3	M062XGD3
$1255C_3H_2F_4$		0.030419	-591.002900	-591.028225	-591.003032	-589.910115	
CC + 125a5b ts	CC + 345a5b ts	0.188743	-826.771415	-826.842550	-826.773045	-825.137181	
CC + 125a5b	CC + 345a5b	0.196560	-826.858572	-826.934101	-826.860099	-825.227945	
Barrier		**-68**	**121**	**139**	**118**	**121**	
Reaction		**-88**	**-88**	**-81**	**-90**	**-97**	
$1355C_3H_2F_4$		0.030339	-591.010797	-591.035721	-591.010930	-589.916776	-590.300513
CC + 135a5b ts	CC + 245a5b ts	0.189236	-826.778202	-826.848789	-826.779832	-825.142719	-825.703865
CC + 135a5b	CC + 245a5b	0.196404	-826.861846	-826.937516	-826.863375	-825.230925	-825.790749
Barrier		**-69**	**125**	**144**	**122**	**125**	**120**
Reaction		**-88**	**-76**	**-71**	**-78**	**-88**	**-89**
$1455C_3H_2F_4$		0.030355	-591.002399	-591.027363	-591.002530	-589.909465	
CC + 145a5b ts		0.188934	-826.772758	-826.842894	-826.774393	-825.137926	
CC + 145a5b		0.196239	-826.861414	-826.936223	-826.862950	-825.231305	
Barrier		**-68**	**116**	**136**	**114**	**118**	
Reaction		**-88**	**-97**	**-90**	**-100**	**-108**	
$2355C_3H_2F_4$		0.030405	-591.012790	-591.037669	-591.012925	-589.918687	
CC + 235a5b ts		0.188589	-826.772758	-826.842894	-826.774393	-825.139120	
CC + 235a5b		0.196747	-826.861414	-826.936223	-826.862950	-825.223044	
Barrier		**-67**	**143**	**162**	**140**	**138**	
Reaction		**-89**	**-69**	**-61**	**-71**	**-61**	
$123C_3H_3F_3$		0.039445	-491.766518	-491.792408	-491.766646	-490.831544	-491.153715
CC + 123 ts	CC + 234 ts	0.198061	-727.530075	-727.603643	-727.531636	-726.056643	-726.555469
CC + 123	CC + 234	0.205618	-727.606207	-727.684861	-727.607682	-726.137878	-726.634827
Barrier		**-68**	**134**	**148**	**132**	**127**	**124**
Reaction		**-88**	**-46**	**-46**	**-48**	**-67**	**-65**
$124C_3H_3F_3$		0.039237	-491.767229	-491.793189	-491.767356	-490.832147	
CC + 124 ts	CC + 134 ts	0.197888	-727.534553	-727.607361	-727.536115	-726.060244	
CC + 124	CC + 134	0.205391	-727.616923	-727.694518	-727.618399	-726.148399	
Barrier		**-69**	**125**	**140**	**122**	**119**	
Reaction		**-88**	**-72**	**-69**	**-74**	**-93**	
$125C_3H_3F_3$		0.039548	-491.758513	-491.784166	-491.758635	-490.826136	
CC + 125a ts	CC + 345a ts	0.198075	-727.529818	-727.601557	-727.531396	-726.056024	
CC + 125a	CC + 345a	0.205841	-727.612662	-727.689492	-727.614143	-726.143756	
Barrier		**-68**	**114**	**131**	**111**	**114**	
Reaction		**-89**	**-83**	**-79**	**-86**	**-96**	
$125C_3H_3F_3$		0.039548	-491.758513	-491.784166	-491.758635	-490.826136	
CC + 125b ts	CC + 345b ts	0.197877	-727.526300	-727.599907	-727.527865	-726.054554	
CC + 125b	CC + 345b	0.205500	-727.610114	-727.687672	-727.611581	-726.141669	
Barrier		**-68**	**123**	**135**	**120**	**117**	
Reaction		**-88**	**-77**	**-75**	**-80**	**-92**	
$135C_3H_3F_3$		0.039506	-491.766145	-491.791419	-491.766270	-490.832737	
CC + 135a ts	CC + 245a ts	0.198566	-727.535699	-727.606966	-727.537278	-726.061099	
CC + 135a	CC + 245a	0.205679	-727.615903	-727.692901	-727.617386	-726.146728	
Barrier		**-70**	**120**	**138**	**117**	**119**	
Reaction		**-88**	**-72**	**-69**	**-74**	**-87**	
$135C_3H_3F_3$		0.039506	-491.766145	-491.791419	-491.766270	-490.832737	
BN + 135b ts	CC + 245b ts	0.198238	-727.532671	-727.605631	-727.534237	-726.059834	
BN + 135b	CC + 245b	0.205248	-727.613638	-727.691348	-727.615106	-726.144896	
Barrier		**-69**	**127**	**140**	**124**	**122**	
Reaction		**-87**	**-67**	**-66**	**-70**	**-83**	

Table S5. continued

						DLPNO-CCSD(T)/	DLPNO-CCSD(T)/
		M062X				6-311+G(d,p)//	aug-ccPVTZ//
6-311+G(d,p)	Equivalencies	ΔG_{298} corr	M062X	wB97XD	M062XGD3	M062XGD3	M062XGD3
$145C_3H_3F_3$		0.039427	-491.760024	-491.785327	-491.760144	-490.827330	
CC + 145a ts		0.198234	-727.532218	-727.603017	-727.533791	-726.057708	
CC + 145a		0.205491	-727.617572	-727.693680	-727.619051	-726.148967	
Barrier		**-69**	**112**	**131**	**110**	**113**	
Reaction		**-88**	**-93**	**-88**	**-95**	**-107**	
$145C_3H_3F_3$		0.039427	-491.760024	-491.785327	-491.760144	-490.827330	
CC + 145b ts		0.197750	-727.529767	-727.602228	-727.531339	-726.057152	
CC + 145b		0.205135	-727.6153527	-727.692135	-727.616830	-726.147311	
Barrier		**-68**	**117**	**132**	**115**	**113**	
Reaction		**-87**	**-88**	**-85**	**-90**	**-104**	
$155C_3H_3F_3$		0.039576	-491.771041	-491.795419	-491.771164	-490.840272	
CC + 15a5b ts	CC + 45a5b ts	0.198440	-727.537634	-727.607655	-727.539217	-726.064958	
CC + 15a5b	CC + 45a5b	0.205550	-727.621768	-727.696804	-727.623249	-726.153137	
Barrier		**-69**	**127**	**146**	**124**	**128**	
Reaction		**-88**	**-75**	**-70**	**-78**	**-85**	
$235C_3H_3F_3$		0.039608	-491.766259	-491.791496	-491.766388	-490.832960	-491.154481
CC + 235a ts		0.198104	-727.530625	-727.602704	-727.532203	-726.056707	-726.555383
CC + 235a		0.206029	-727.606153	-727.684329	-727.607638	-726.137027	-726.634131
Barrier		**-68**	**132**	**147**	**129**	**130**	**126**
Reaction		**-89**	**-45**	**-46**	**-48**	**-60**	**-60**
$235C_3H_3F_3$		0.039608	-491.766259	-491.791496	-491.766388	-490.832960	
CC + 235b ts		0.197917	-727.526931	-727.601033	-727.528488	-726.055016	
CC + 235b		0.205612	-727.603430	-727.682404	-727.604886	-726.134668	
Barrier		**-68**	**141**	**151**	**139**	**134**	
Reaction		**-88**	**-39**	**-42**	**-42**	**-55**	
$255C_3H_3F_3$		0.039432	-491.777754	-491.802175	-491.777881	-490.846386	
CC + 25a5b ts	CC + 35a5b ts	0.197817	-727.540580	-727.611497	-727.542153	-726.067634	
CC + 25a5b	CC + 35a5b	0.205750	-727.621664	-727.697644	-727.623138	-726.152217	
Barrier		**-68**	**136**	**152**	**133**	**136**	
Reaction		**-89**	**-56**	**-53**	**-59**	**-65**	
$12C_3H_4F_2$		0.048419	-392.530957	-392.556383	-392.531070	-391.758615	
CC + 12 ts	CC + 34 ts	0.207136	-628.294961	-628.368005	-628.296464	-626.983509	
CC + 12	CC + 34	0.214614	-628.372189	-628.450018	-628.373605	-627.065663	
Barrier		**-69**	**134**	**147**	**131**	**127**	
Reaction		**-88**	**-50**	**-49**	**-52**	**-69**	
$13C_3H_4F_2$		0.048344	-392.538195	-392.563303	-392.538310	-391.764997	-392.024710
CC + 13 ts	CC + 24 ts	0.207331	-628.300671	-628.373305	-628.302174	-626.988500	-627.425031
CC + 13	CC + 24	0.214345	-628.375638	-628.453651	-628.377055	-627.068855	-627.503211
Barrier		**-69**	**138**	**152**	**136**	**132**	**129**
Reaction		**-88**	**-40**	**-41**	**-42**	**-61**	**-58**
$14C_3H_4F_2$		0.048297	-392.535063	-392.560202	-392.535174	-391.762180	
CC + 14 ts		0.207068	-628.299827	-628.371980	-628.301327	-626.987453	
CC + 14		0.214224	-628.379380	-628.456640	-628.380796	-627.073089	
Barrier		**-69**	**132**	**147**	**129**	**127**	
Reaction		**-88**	**-58**	**-57**	**-61**	**-80**	
$15C_3H_4F_2$		0.048659	-392.525869	-392.550648	-392.525978	-391.755607	
CC + 15a ts	CC + 45a ts	0.207551	-628.295163	-628.366022	-628.296680	-626.983188	
CC + 15a	CC + 45a	0.214807	-628.375057	-628.451508	-628.376478	-627.068377	
Barrier		**-69**	**120**	**138**	**118**	**121**	
Reaction		**-88**	**-71**	**-68**	**-73**	**-84**	

Table S5. continued

6-311+G(d,p)	Equivalencies	M062X ΔG_{298} corr	M062X	wB97XD	M062XGD3	DLPNO-CCSD(T)/ 6-311+G(d,p)// M062XGD3	DLPNO-CCSD(T)/ aug-ccPVTZ// M062XGD3
$15C_3H_4F_2$		0.048659	-392.525869	-392.550648	-392.525978	-391.755607	
CC + 15b ts	CC + 45b ts	0.207257	-628.291434	-628.363981	-628.292950	-626.981499	
CC + 15b	CC + 45b	0.214397	-628.372585	-628.449720	-628.374004	-627.066370	
Barrier		**-68**	**129**	**142**	**127**	**124**	
Reaction		**-87**	**-65**	**-64**	**-68**	**-80**	
$23C_3H_4F_2$		0.048522	-392.535629	-392.560646	-392.535747	-391.762790	
CC + 23 ts		0.207266	-628.293387	-628.366925	-628.294888	-626.982128	
CC + 23		0.214742	-628.363466	-628.442502	-628.364882	-627.056779	
Barrier		**-69**	**150**	**161**	**147**	**142**	
Reaction		**-88**	**-14**	**-18**	**-17**	**-34**	
$25C_3H_4F_2$		0.048608	-392.530480	-392.555284	-392.530594	-391.759905	
CC + 25a ts	CC + 35a ts	0.207160	-628.296664	-628.368208	-628.298183	-626.984706	
CC + 25a	CC + 35a	0.215045	-628.372882	-628.450210	-628.374306	-627.065542	
Barrier		**-68**	**127**	**143**	**125**	**127**	
Reaction		**-89**	**-52**	**-52**	**-54**	**-64**	
$25C_3H_4F_2$		0.048608	-392.530480	-392.555284	-392.530594	-391.759905	
CC + 25b ts	CC + 35b ts	0.206916	-628.292123	-628.365547	-628.293630	-626.982250	
CC + 25b	CC + 35b	0.214636	-628.370023	-628.448086	-628.371432	-627.063094	
Barrier		**-68**	**139**	**149**	**136**	**133**	
Reaction		**-88**	**-46**	**-47**	**-48**	**-59**	
$55C_3H_4F_2$		0.048653	-392.537643	-392.561555	-392.537759	-391.769493	-392.027940
CC + 5a5b ts		0.206551	-628.299939	-628.370110	-628.301466	-626.989723	-627.425863
CC + 5a5b		0.214870	-628.380915	-628.456282	-628.382339	-627.073912	-627.508919
Barrier		**-67**	**136**	**153**	**133**	**137**	**132**
Reaction		**-88**	**-55**	**-52**	**-57**	**-62**	**-64**
$1C_5H_5F$		0.057465	-293.297989	-293.322637	-293.298086	-292.687911	
CC + 1 ts	CC + 4 ts	0.216211	-529.059393	-529.131679	-529.060833	-527.909962	
CC + 1	CC + 4	0.223447	-529.133778	-529.211312	-529.135132	-527.989686	
Barrier		**-69**	**140**	**154**	**138**	**135**	
Reaction		**-88**	**-36**	**-36**	**-38**	**-55**	
$2C_5H_5F$		0.057436	-293.299642	-293.324272	-293.299744	-292.689545	-292.886863
CC + 2 ts	CC + 3 ts	0.216175	-529.058194	-529.131127	-529.059636	-527.909049	-528.283113
CC + 2	CC + 3	0.223725	-529.129160	-529.207419	-529.130516	-527.984463	-528.356421
Barrier		**-69**	**148**	**159**	**146**	**142**	**139**
Reaction		**-89**	**-19**	**-21**	**-21**	**-37**	**-34**
$5C_5H_5F$		0.057733	-293.289914	-293.314266	-293.290011	-292.682482	-292.878678
CC + 5a ts		0.216169	-529.055819	-529.126883	-529.057275	-527.906543	-528.280570
CC + 5a		0.224120	-529.131269	-529.208077	-529.132630	-527.986576	-528.358619
Barrier		**-68**	**128**	**144**	**125**	**129**	**123**
Reaction		**-89**	**-49**	**-49**	**-52**	**-60**	**-61**
$5C_5H_5F$		0.057733	-293.289914	-293.314266	-293.290011	-292.682482	
CC + 5b ts		0.216009	-529.050745	-529.123552	-529.052203	-527.903777	
CC + 5b		0.223652	-529.128527	-529.206038	-529.129886	-527.984290	
Barrier		**-68**	**141**	**152**	**138**	**136**	
Reaction		**-88**	**-43**	**-45**	**-46**	**-56**	

Table S5. continued

M062xGD3 values										
Change by Placing CH_3 at Position 1			Change by Placing CH_3 at Position 2			Change by Placing CH_3 at Position 5a			Change by Placing CH_3 at Position 5b		
Subst. Pattern	$\Delta G^{\ddagger}_{ASC1}$	ΔG_{ASC1}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC2}$	ΔG_{ASC2}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5a}$	ΔG_{ASC5a}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5b}$	ΔG_{ASC5b}
1-0	-8	-20	2-0	-1	-3	5a-0	-21	-34	5b-0	-8	-28
12-2	-15	-31	12-1	-7	-14	15a-1	-21	-35	15b-1	-11	-29
13-3	-10	-22	23-3	2	4	25a-2	-21	-34	25b-2	-9	-27
14-4	-9	-23	24-4	-2	-4	35a-3	-21	-34	35b-3	-9	-27
15a-5a	-8	-21	25a-5a	-1	-3	45a-4	-21	-35	45b-4	-11	-29
15b-5b	-12	-22	25b-5b	-2	-2	5a5b-5b	-5	-12	5a5b-5a	8	-6
123-23	-16	-31	123-13	-4	-6	125a-12	-20	-34	125b-12	-11	-28
124-24	-14	-32	124-14	-7	-14	135a-13	-19	-32	135b-13	-11	-27
125a-25a	-14	-31	125a-15a	-6	-13	145a-14	-20	-35	145b-14	-14	-30
125b-25b	-16	-32	125b-15b	-7	-12	15a5b-15b	-2	-10	15a5b-15a	7	-5
134-34	-9	-22	234-34	1	4	235a-23	-18	-31	235b-23	-9	-25
135a-35a	-8	-20	235a-35a	5	6	245a-24	-19	-32	245b-24	-11	-27
135b-35b	-12	-22	235b-35b	2	6	25a5b-25b	-3	-11	25a5b-25a	8	-4
145a-45a	-8	-22	245a-45a	0	-2	345a-34	-20	-34	345b-34	-11	-28
145b-45b	-12	-23	245b-45b	-2	-2	35a5b-35b	-3	-11	35a5b-35a	8	-4
15a5b-5a5b	-9	-20	25a5b-5a5b	0	-2	45a5b-45b	-2	-10	45a5b-45a	7	-5
1234-234	-13	-33	1234-134	-3	-6	1235a-123	-16	-31	1235b-123	-10	-26
1235a-235a	-14	-31	1235a-135a	-2	-4	1245a-124	-17	-32	1245b-124	-13	-28
1235b-235b	-17	-32	1235b-135b	-3	-4	125a5b-125b	-2	-10	125a5b-125a	7	-4
1245a-245a	-12	-32	1245a-145a	-4	-11	1345a-134	-17	-32	1345b-134	-13	-28
1245b-245b	-15	-33	1245b-145b	-6	-12	135a5b-135b	-2	-9	135a5b-135a	5	-4
125a5b-25a5b	-15	-31	125a5b-15a5b	-7	-13	145a5b-145b	-1	-9	145a5b-145a	4	-4
1345a-345a	-6	-21	2345a-345a	4	7	2345a-234	-16	-31	2345b-234	-10	-26
1345b-345b	-11	-22	2345b-345b	2	6	235a5b-235b	1	-29	235a5b-235a	11	-23
135a5b-35a5b	-11	-20	235a5b-35a5b	7	-12	245a5b-245b	-2	-9	245a5b-245a	5	-4
145a5b-45a5b	-11	-22	245a5b-45a5b	-2	-1	345a5b-345b	-2	-10	345a5b-345a	7	-4
12345a-2345a	-11	-31	12345a-1345a	0	-4	12345a-1234	-14	-30	12345b-1234	-14	-26
12345b-2345b	-16	-33	12345b-1345b	-3	-5	1235a5b-1235b	-1	-9	1235a5b-1235a	5	-4
1235a5b-235a5b	-19	-12	1235a5b-135a5b	-1	-5	1245a5b-1245b	0	-9	1245a5b-1245a	4	-4
1245a5b-245a5b	-14	-33	1245a5b-145a5b	-5	-11	1345a5b-1345b	0	-9	1345a5b-1345a	4	-4
1345a5b-345a5b	-9	-21	2345a5b-345a5b	3	7	2345a5b-2345b	-1	-9	2345a5b-2345a	5	-4
12345a5b-2345a5b	-13	-32	12345a5b-1345a5b	-1	-4	12345a5b-12345b	2	-8	12345a5b-12345a	3	-5
Avg(StdDev)	–12 (3)	–26 (6)	Avg(StdDev)	–2 (4)	–4 (7)	Avg(StdDev)	–10 (9)	–22 (12)	Avg(StdDev)	–3 (9)	–17 (12)

M062x values										
Change by Placing CH_3 at Position 1			Change by Placing CH_3 at Position 2			Change by Placing CH_3 at Position 5a			Change by Placing CH_3 at Position 5b		
Subst. Pattern	$\Delta G^{\ddagger}_{ASC1}$	ΔG_{ASC1}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC2}$	ΔG_{ASC2}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5a}$	ΔG_{ASC5a}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5b}$	ΔG_{ASC5b}
1-0	-8	-20	2-0	-1	-3	5a-0	-21	-33	5b-0	-8	-27
12-2	-14	-31	12-1	-7	-14	15a-1	-20	-35	15b-1	-11	-29
13-3	-10	-22	23-3	2	4	25a-2	-21	-33	25b-2	-9	-27
14-4	-9	-23	24-4	-2	-4	35a-3	-21	-33	35b-3	-9	-27
15a-5a	-8	-21	25a-5a	0	-3	45a-4	-20	-35	45b-4	-11	-29
15b-5b	-12	-22	25b-5b	-2	-2	5a5b-5b	-5	-11	5a5b-5a	8	-5
123-23	-16	-31	123-13	-4	-5	125a-12	-20	-34	125b-12	-11	-28
124-24	-14	-32	124-14	-7	-14	135a-13	-18	-32	135b-13	-11	-27
125a-25a	-14	-31	125a-15a	-6	-13	145a-14	-19	-34	145b-14	-14	-29
125b-25b	-16	-32	125b-15b	-7	-12	15a5b-15b	-2	-10	15a5b-15a	7	-4
134-34	-9	-22	234-34	1	4	235a-23	-18	-31	235b-23	-9	-25
135a-35a	-8	-20	235a-35a	5	7	245a-24	-18	-32	245b-24	-11	-27
135b-35b	-12	-22	235b-35b	3	6	25a5b-25b	-3	-11	25a5b-25a	8	-4
145a-45a	-8	-22	245a-45a	0	-1	345a-34	-20	-34	345b-34	-11	-28
145b-45b	-12	-23	245b-45b	-2	-2	35a5b-35b	-3	-11	35a5b-35a	8	-4
15a5b-5a5b	-9	-20	25a5b-5a5b	0	-1	45a5b-45b	-2	-10	45a5b-45a	7	-4
1234-234	-13	-32	1234-134	-3	-6	1235a-123	-16	-31	1235b-123	-10	-26
1235a-235a	-14	-31	1235a-135a	-1	-4	1245a-124	-17	-32	1245b-124	-13	-28
1235b-235b	-17	-32	1235b-135b	-3	-4	125a5b-125b	-2	-10	125a5b-125a	7	-4
1245a-245a	-12	-32	1245a-145a	-4	-11	1345a-134	-17	-32	1345b-134	-13	-28
1245b-245b	-15	-32	1245b-145b	-6	-12	135a5b-135b	-2	-8	135a5b-135a	5	-4
125a5b-25a5b	-15	-31	125a5b-15a5b	-6	-13	145a5b-145b	-1	-9	145a5b-145a	4	-4
1345a-345a	-6	-21	2345a-345a	5	7	2345a-234	-16	-31	2345b-234	-10	-26
1345b-345b	-11	-22	2345b-345b	2	6	235a5b-235b	2	-29	235a5b-235a	11	-23
135a5b-35a5b	-11	-19	235a5b-35a5b	7	-12	245a5b-245b	-2	-8	245a5b-245a	5	-4
145a5b-45a5b	-11	-22	245a5b-45a5b	-2	-1	345a5b-345b	-2	-10	345a5b-345a	7	-4
12345a-2345a	-11	-31	12345a-1345a	0	-4	12345a-1234	-14	-29	12345b-1234	-13	-26
12345b-2345b	-16	-33	12345b-1345b	-3	-5	1235a5b-1235b	-1	-9	1235a5b-1235a	5	-4
1235a5b-235a5b	-19	-12	1235a5b-135a5b	-1	-5	1245a5b-1245b	0	-9	1245a5b-1245a	4	-4
1245a5b-245a5b	-13	-33	1245a5b-145a5b	-5	-11	1345a5b-1345b	0	-9	1345a5b-1345a	4	-4
1345a5b-345a5b	-9	-21	2345a5b-345a5b	3	7	2345a5b-2345b	-1	-9	2345a5b-2345a	5	-4
12345a5b-2345a5b	-13	-32	12345a5b-1345a5b	-1	-4	12345a5b-12345b	2	-8	12345a5b-12345a	3	-5
Avg(StdDev)	–12 (3)	–26 (6)	Avg(StdDev)	–2 (4)	–4 (7)	Avg(StdDev)	–10 (9)	–22 (12)	Avg(StdDev)	–2 (9)	–17 (12)

Table S5. continued

wB9XD values										
Change by Placing CH_3 at Position 1			Change by Placing CH_3 at Position 2			Change by Placing CH_3 at Position 5a			Change by Placing CH_3 at Position 5b	
Subst. Pattern	$\Delta G^{\ddagger}_{ASC1}$	ΔG_{ASC1}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC2}$	ΔG_{ASC2}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5a}$	ΔG_{ASC5a}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5b}$	ΔG_{ASC5b}
1-0	-7	-18	2-0	-1	-3	5a-0	-17	-30	5b-0	-8	-26
12-2	-13	-28	12-1	-7	-12	15a-1	-16	-32	15b-1	-12	-28
13-3	-8	-20	23-3	2	3	25a-2	-16	-31	25b-2	-10	-26
14-4	-7	-21	24-4	-2	-4	35a-3	-16	-31	35b-3	-10	-26
15a-5a	-6	-19	25a-5a	-1	-3	45a-4	-16	-32	45b-4	-12	-28
15b-5b	-10	-20	25b-5b	-2	-2	5a5b-5b	1	-7	5a5b-5a	9	-3
123-23	-13	-28	123-13	-4	-5	125a-12	-16	-30	125b-12	-12	-27
124-24	-12	-28	124-14	-7	-12	135a-13	-14	-29	135b-13	-12	-26
125a-25a	-12	-28	125a-15a	-6	-11	145a-14	-15	-31	145b-14	-15	-28
125b-25b	-14	-28	125b-15b	-7	-11	15a5b-15b	4	-5	15a5b-15a	8	-2
134-34	-7	-20	234-34	1	3	235a-23	-14	-28	235b-23	-10	-24
135a-35a	-6	-18	235a-35a	4	5	245a-24	-14	-29	245b-24	-12	-26
135b-35b	-9	-19	235b-35b	2	5	25a5b-25b	3	-6	25a5b-25a	9	-2
145a-45a	-6	-20	245a-45a	0	-2	345a-34	-16	-30	345b-34	-12	-27
145b-45b	-10	-20	245b-45b	-2	-2	35a5b-35b	3	-6	35a5b-35a	9	-2
15a5b-5a5b	-7	-18	25a5b-5a5b	-1	-2	45a5b-45b	4	-5	45a5b-45a	8	-2
1234-234	-10	-29	1234-134	-3	-6	1235a-123	-12	-27	1235b-123	-11	-25
1235a-235a	-12	-27	1235a-135a	-2	-4	1245a-124	-13	-29	1245b-124	-13	-26
1235b-235b	-15	-28	1235b-135b	-3	-4	125a5b-125b	4	-6	125a5b-125a	8	-2
1245a-245a	-10	-28	1245a-145a	-4	-10	1345a-134	-13	-29	1345b-134	-13	-26
1245b-245b	-14	-29	1245b-145b	-5	-11	135a5b-135b	3	-4	135a5b-135a	6	-1
125a5b-25a5b	-13	-28	125a5b-15a5b	-7	-11	145a5b-145b	4	-5	145a5b-145a	5	-2
1345a-345a	-4	-18	2345a-345a	5	6	2345a-234	-12	-27	2345b-234	-11	-25
1345b-345b	-8	-20	2345b-345b	2	5	235a5b-235b	11	-19	235a5b-235a	15	-15
135a5b-35a5b	-8	-17	235a5b-35a5b	10	-8	245a5b-245b	3	-4	245a5b-245a	6	-1
145a5b-45a5b	-9	-20	245a5b-45a5b	-2	-1	345a5b-345b	4	-6	345a5b-345a	8	-2
12345a-2345a	-9	-27	12345a-1345a	0	-3	12345a-1234	-10	-26	12345b-1234	-14	-25
12345b-2345b	-14	-29	12345b-1345b	-4	-4	1235a5b-1235b	5	-5	1235a5b-1235a	6	-2
1235a5b-235a5b	-20	-14	1235a5b-135a5b	-2	-5	1245a5b-1245b	5	-4	1245a5b-1245a	4	-2
1245a5b-245a5b	-12	-29	1245a5b-145a5b	-5	-10	1345a5b-1345b	5	-4	1345a5b-1345a	4	-2
1345a5b-345a5b	-7	-18	2345a5b-345a5b	3	6	2345a5b-2345b	5	-5	2345a5b-2345a	6	-2
12345a5b-2345a5b	-11	-28	12345a5b-1345a5b	-1	-4	12345a5b-12345b	8	-3	12345a5b-12345a	3	-3
Avg(StdDev)	–10 (3)	–23 (5)	Avg(StdDev)	–2 (4)	–4 (6)	Avg(StdDev)	–5 (10)	–18 (12)	Avg(StdDev)	–2 (10)	–14 (12)

DLPNO-CCSD(T)//M062x+GD3 values										
Change by Placing CH_3 at Position 1			Change by Placing CH_3 at Position 2			Change by Placing CH_3 at Position 5a			Change by Placing CH_3 at Position 5b	
Subst. Pattern	$\Delta G^{\ddagger}_{ASC1}$	ΔG_{ASC1}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC2}$	ΔG_{ASC2}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5a}$	ΔG_{ASC5a}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5b}$	ΔG_{ASC5b}
1-0	-8	-22	2-0	-1	-3	5a-0	-14	-27	5b-0	-7	-23
12-2	-14	-32	12-1	-8	-13	15a-1	-14	-28	15b-1	-10	-24
13-3	-10	-24	23-3	0	2	25a-2	-14	-28	25b-2	-9	-22
14-4	-8	-24	24-4	-3	-5	35a-3	-14	-28	35b-3	-9	-22
15a-5a	-8	-23	25a-5a	-2	-4	45a-4	-14	-28	45b-4	-10	-24
15b-5b	-11	-24	25b-5b	-3	-3	5a5b-5b	2	-6	5a5b-5a	9	-1
123-23	-15	-33	123-13	-5	-6	125a-12	-14	-27	125b-12	-10	-23
124-24	-13	-32	124-14	-8	-13	135a-13	-13	-26	135b-13	-10	-22
125a-25a	-13	-32	125a-15a	-7	-12	145a-14	-13	-28	145b-14	-13	-24
125b-25b	-16	-33	125b-15b	-7	-12	15a5b-15b	4	-5	15a5b-15a	8	-1
134-34	-9	-24	234-34	-1	2	235a-23	-12	-26	235b-23	-8	-21
135a-35a	-8	-23	235a-35a	3	4	245a-24	-13	-26	245b-24	-10	-22
135b-35b	-11	-24	235b-35b	1	4	25a5b-25b	3	-6	25a5b-25a	9	-1
145a-45a	-8	-24	245a-45a	-2	-3	345a-34	-14	-27	345b-34	-10	-23
145b-45b	-11	-24	245b-45b	-3	-4	35a5b-35b	3	-6	35a5b-35a	9	-1
15a5b-5a5b	-9	-23	25a5b-5a5b	-1	-3	45a5b-45b	4	-5	45a5b-45a	8	-1
1234-234	-12	-33	1234-134	-4	-7	1235a-123	-11	-25	1235b-123	-9	-21
1235a-235a	-14	-32	1235a-135a	-3	-5	1245a-124	-11	-26	1245b-124	-12	-23
1235b-235b	-17	-33	1235b-135b	-4	-5	125a5b-125b	4	-6	125a5b-125a	7	-1
1245a-245a	-11	-32	1245a-145a	-5	-11	1345a-134	-11	-26	1345b-134	-12	-23
1245b-245b	-15	-33	1245b-145b	-6	-12	135a5b-135b	3	-4	135a5b-135a	6	-1
125a5b-25a5b	-15	-32	125a5b-15a5b	-8	-13	145a5b-145b	4	-4	145a5b-145a	4	-1
1345a-345a	-6	-23	2345a-345a	2	4	2345a-234	-11	-25	2345b-234	-9	-21
1345b-345b	-10	-24	2345b-345b	0	3	235a5b-235b	4	-6	235a5b-235a	8	-1
135a5b-35a5b	-11	-23	235a5b-35a5b	2	4	245a5b-245b	3	-4	245a5b-245a	6	-1
145a5b-45a5b	-11	-24	245a5b-45a5b	-3	-3	345a5b-345b	4	-6	345a5b-345a	7	-1
12345a-2345a	-10	-32	12345a-1345a	-2	-5	12345a-1234	-9	-24	12345b-1234	-13	-22
12345b-2345b	-15	-34	12345b-1345b	-5	-6	1235a5b-1235b	4	-5	1235a5b-1235a	5	-2
1235a5b-235a5b	-16	-32	1235a5b-135a5b	-4	-6	1245a5b-1245b	5	-4	1245a5b-1245a	4	-2
1245a5b-245a5b	-13	-33	1245a5b-145a5b	-6	-12	1345a5b-1345b	5	-4	1345a5b-1345a	4	-2
1345a5b-345a5b	-9	-23	2345a5b-345a5b	1	4	2345a5b-2345b	4	-5	2345a5b-2345a	5	-2
12345a5b-2345a5b	-13	-33	12345a5b-1345a5b	-3	-6	12345a5b-12345b	7	-4	12345a5b-12345a	3	-2
Avg(StdDev)	–12 (3)	–28 (5)	Avg(StdDev)	–3 (3)	–5 (6)	Avg(StdDev)	–4 (9)	–16 (11)	Avg(StdDev)	–2 (9)	–12 (11)

Table S6. Corrected relative free energy barrier heights $\Delta G^{\ddagger}$ and reaction free energies ΔG from Table S5, and $\Delta G^{\ddagger}/\Delta G$ values derived by summing $\Delta G^{\ddagger}_{ASC\#}/\Delta G_{ASC\#}$ values (marked with "(p)") (kJ mol^{-1}) using various model chemistries for Diels–Alder reactions **1** + *c*–$C_5H_xF_{6-x}$.

M062x values								
Change by Placing F at Position 1			**Change by Placing F at Position 2**					
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**-12**	**-26**		**-2**	**-4**			
Change by Placing F at Position 5a			**Change by Placing F at Position 5b**					
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**-10**	**-22**		**-2**	**-17**			
wB97XD values								
Change by Placing F at Position 1			**Change by Placing F at Position 2**					
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**-10**	**-23**		**-2**	**-4**			
Change by Placing F at Position 5a			**Change by Placing F at Position 5b**					
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**-5**	**-18**		**-2**	**-14**			
M062x+GD3 values								
Change by Placing F at Position 1			**Change by Placing F at Position 2**					
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**-12**	**-26**		**-2**	**-4**			
Change by Placing F at Position 5a			**Change by Placing F at Position 5b**					
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**-10**	**-22**		**-3**	**-17**			
DLPNO-CCSD(T)//M062x+GD3 values								
Change by Placing F at Position 1			**Change by Placing F at Position 2**					
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**-12**	**-28**		**-3**	**-5**			
Change by Placing F at Position 5a			**Change by Placing F at Position 5b**					
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**-4**	**-16**		**-2**	**-12**			
					(p)	**(p)**	**(p)**	**(p)**
	M062X	**wB97XD**	**M062XGD3**	**DLPNO-CCSD(T)**	**M062X**	**wB97XD**	**M062XGD3**	**DLPNO-CCSD(T)**
CC + C_5H_6 ts	149	160	146	143				
CC + C_5H_6	-16	-18	-18	-33				
CC + 12345a5b ts	111	131	108	108	109	129	105	107
CC + 12345a5b	-112	-103	-115	-126	-115	-104	-117	-127
CC + 12345a ts	108	127	105	106	111	131	108	109
CC + 12345a	-107	-101	-110	-123	-98	-90	-100	-115
CC + 12345b ts	108	123	106	102	119	134	115	111
CC + 12345b	-104	-100	-107	-122	-93	-86	-95	-111
CC + 1235a5b ts	124	142	121	122	121	139	117	119
CC + 1235a5b	-80	-75	-83	-93	-89	-81	-91	-99
CC + 1245a5b ts	112	132	109	112	111	131	107	110
CC + 1245a5b	-108	-99	-111	-120	-111	-100	-113	-122
CC + 1234 ts	122	137	119	115	121	134	118	113
CC + 1234	-78	-75	-81	-100	-76	-75	-78	-97
CC + 1235a ts	118	136	116	116	123	141	120	121
CC + 1235a	-76	-73	-79	-92	-72	-67	-74	-87
CC + 1235b ts	124	137	122	117	131	144	127	123
CC + 1235b	-72	-71	-74	-88	-67	-63	-69	-83
CC + 1245a ts	108	127	105	108	113	133	110	112
CC + 1245a	-104	-98	-107	-119	-94	-86	-96	-110
CC + 1245b ts	112	127	109	107	121	136	117	114
CC + 1245b	-100	-95	-102	-116	-89	-82	-91	-106
CC + 125a5b ts	121	139	118	121	123	141	119	122
CC + 125a5b	-88	-81	-90	-97	-85	-77	-87	-94
CC + 135a5b ts	125	144	122	125	123	141	119	122
CC + 135a5b	-76	-71	-78	-88	-85	-77	-87	-94
CC + 145a5b ts	116	136	114	118	113	133	109	113
CC + 145a5b	-97	-90	-100	-108	-107	-96	-109	-117
CC + 235a5b ts	143	162	140	138	133	149	129	131
CC + 235a5b	-69	-61	-71	-61	-63	-58	-65	-71
CC + 123 ts	134	148	132	127	133	146	130	126
CC + 123	-46	-46	-48	-67	-50	-49	-52	-70
CC + 124 ts	125	140	122	119	123	136	120	116
CC + 124	-72	-69	-74	-93	-72	-71	-74	-92

Table S6. continued

					(p)	(p)	(p)	(p)
	M062X	wB97XD	M062XGD3	DLPNO-CCSD(T)	M062X	wB97XD	M062XGD3	DLPNO-CCSD(T)
CC + 125a ts	114	131	111	114	125	143	122	124
CC + 125a	-83	-79	-86	-96	-68	-63	-70	-82
CC + 125b ts	123	135	120	117	133	146	129	126
CC + 125b	-77	-75	-80	-92	-63	-59	-65	-78
CC + 135a ts	120	138	117	119	125	143	122	124
CC + 135a	-72	-69	-74	-87	-68	-63	-70	-82
CC + 135b ts	127	140	124	122	133	146	129	126
CC + 135b	-67	-66	-70	-83	-63	-59	-65	-78
CC + 145a ts	112	131	110	113	115	135	112	115
CC + 145a	-93	-88	-95	-107	-90	-82	-92	-105
CC + 145b ts	117	132	115	113	123	138	119	117
CC + 145b	-88	-85	-90	-104	-85	-78	-87	-101
CC + 15a5b ts	127	146	124	128	125	143	121	125
CC + 15a5b	-75	-70	-78	-85	-81	-73	-83	-89
CC + 235a ts	132	147	129	130	135	151	132	133
CC + 235a	-45	-46	-48	-60	-46	-44	-48	-59
CC + 235b ts	141	151	139	134	143	154	139	135
CC + 235b	-39	-42	-42	-55	-41	-40	-43	-55
CC + 25a5b ts	136	152	133	136	135	151	131	134
CC + 25a5b	-56	-53	-59	-65	-59	-54	-61	-66
CC + 12 ts	134	147	131	127	135	148	132	129
CC + 12	-50	-49	-52	-69	-46	-45	-48	-65
CC + 13 ts	138	152	136	132	135	148	132	129
CC + 13	-40	-41	-42	-61	-46	-45	-48	-65
CC + 14 ts	132	147	129	127	125	138	122	119
CC + 14	-58	-57	-61	-80	-68	-67	-70	-87
CC + 15a ts	120	138	118	121	127	145	124	127
CC + 15a	-71	-68	-73	-84	-64	-59	-66	-77
CC + 15b ts	129	142	127	124	135	148	131	129
CC + 15b	-65	-64	-68	-80	-59	-55	-61	-73
CC + 23 ts	150	161	147	142	145	156	142	138
CC + 23	-14	-18	-17	-34	-24	-26	-26	-42
CC + 25a ts	127	143	125	127	137	153	134	136
CC + 25a	-52	-52	-54	-64	-42	-40	-44	-54
CC + 25b ts	139	149	136	133	145	156	141	138
CC + 25b	-46	-47	-48	-59	-37	-36	-39	-50
CC + 5a5b ts	136	153	133	137	137	153	133	137
CC + 5a5b	-55	-52	-57	-62	-55	-50	-57	-61
CC + 1 ts	140	154	138	135	137	148	134	131
CC + 1	-36	-36	-38	-55	-42	-44	-44	-59
CC + 2 ts	148	159	146	142	147	158	144	141
CC + 2	-19	-21	-21	-37	-20	-22	-22	-37
CC + 5a ts	128	144	125	129	139	155	136	139
CC + 5a	-49	-49	-52	-60	-38	-36	-40	-49
CC + 5b ts	141	152	138	136	147	158	143	141
CC + 5b	-43	-45	-46	-56	-33	-32	-35	-45

Figure S3. DLPNO-CCSD(T)/6-311+G(d,p) model chemistry-predicted transition state free energy barriers $\Delta G^{\ddagger}_{298}$ (red dots) and reaction free energies ΔG_{298} (blue squares) vs. $\Delta G^{\ddagger}_{298}/\Delta G_{298}$ values predicted by summing $\Delta G^{\ddagger}_{ASC\#}/\Delta G_{ASC\#}$ values (from Table S6, kJ mol^{-1}) for Diels–Alder reactions **1** + *c*-$C_5H_xF_{6-x}$.

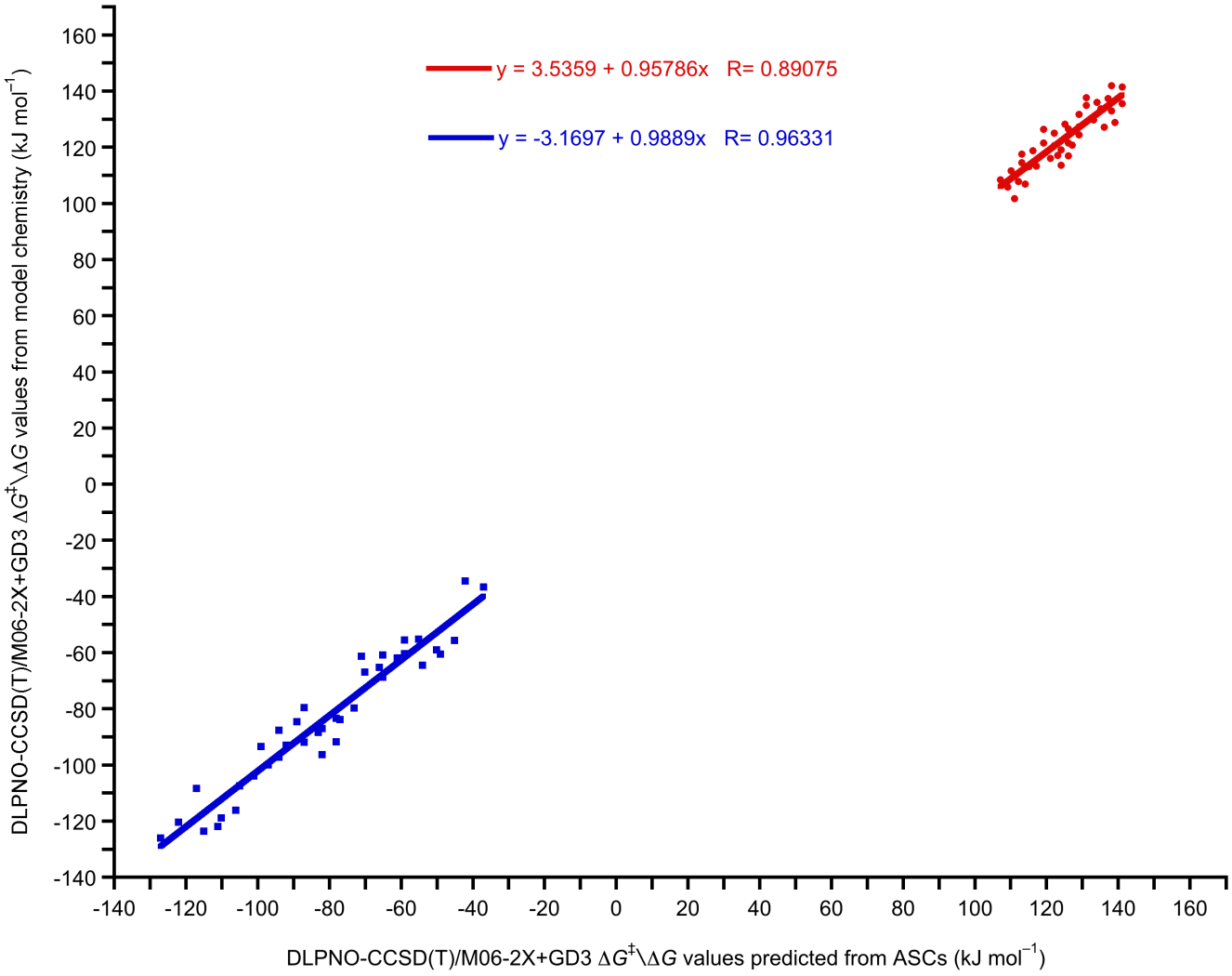


Table S7. Raw molecular energies (hartree) of components, corrected relative free energy barrier heights $\Delta G^{\ddagger}_{298}$ and reaction free energies ΔG_{298}, and subtractions used to derive $\Delta G^{\ddagger}_{ASC\#}$ and $\Delta G_{ASC\#}$ values (kJ mol^{-1}) using various model chemistries for Diels–Alder reactions **1** + *c*–$C_5H_x(CF_3)_{6-x}$.

						DLPNO-CCSD(T)/
		M062X				6-311+G(d,p)//
6-311+G(d,p)	Equivalencies	ΔG_{298} corr	M062X	wB97XD	M062XGD3	M062XGD3
Me_2CCMe_2		0.132537	-235.788686	-235.841397	-235.789114	-235.247231
123455$C_5(CF_3)_6$		0.070113	-2216.308860	-2216.365098	-2216.310919	
CC + 12345a5b ts		0.235781	-2452.056891	-2452.154117	-2452.062216	
CC + 12345a5b		0.241983	-2452.122922	-2452.223190	-2452.128140	
Barrier		**-87**	**194**	**225**	**186**	
Reaction		**-103**	**37**	**59**	**29**	
12345$C_5H(CF_3)_5$		0.068493	-1879.283272	-1879.339003	-1879.284843	
CC + 12345a ts		0.231527	-2115.033891	-2115.133574	-2115.038525	
CC + 12345a		0.240915	-2115.112484	-2115.214865	-2115.116995	
Barrier		**-80**	**180**	**203**	**173**	
Reaction		**-105**	**-2**	**14**	**-8**	
12345$C_5H(CF_3)_5$		0.068493	-1879.283272	-1879.339003	-1879.284843	
CC + 12345b ts		0.232167	-2115.060357	-2115.159762	-2115.064924	
CC + 12345b		0.238987	-2115.130419	-2115.232369	-2115.134876	
Barrier		**-82**	**112**	**136**	**105**	
Reaction		**-100**	**-54**	**-37**	**-60**	
12355$C_5H(CF_3)_5$		0.068336	-1879.284422	-1879.338106	-1879.286038	
CC + 1235a5b ts	CC + 2345a5b ts	0.231063	-2115.030461	-2115.129450	-2115.034989	
CC + 1235a5b	CC + 2345a5b	0.236505	-2115.095300	-2115.196930	-2115.099738	
Barrier		**-79**	**191**	**211**	**185**	
Reaction		**-94**	**35**	**48**	**29**	
12455$C_5H(CF_3)_5$		0.068685	-1879.282105	-1879.334860	-1879.283723	
CC + 1245a5b ts	CC + 1345a5b ts	0.232380	-2115.020637	-2115.116105	-2115.025204	
CC + 1245a5b	CC + 1345a5b	0.239357	-2115.090279	-2115.188948	-2115.094719	
Barrier		**-82**	**213**	**240**	**207**	
Reaction		**-100**	**49**	**67**	**43**	
1234$C_3H_2(CF_3)_4$		0.066882	-1542.247387	-1542.297395	-1542.248552	
CC + 1234 ts		0.229815	-1778.019115	-1778.114968	-1778.022968	
CC + 1234		0.237451	-1778.091029	-1778.189894	-1778.094772	
Barrier		**-80**	**124**	**142**	**118**	
Reaction		**-100**	**-44**	**-34**	**-50**	
1235$C_3H_2(CF_3)_4$		0.067358	-1542.249964	-1542.299793	-1542.251151	
CC + 1235a ts	CC + 2345a ts	0.228996	-1778.004392	-1778.102135	-1778.008262	
CC + 1235a	CC + 2345a	0.236387	-1778.077121	-1778.179418	-1778.080888	
Barrier		**-76**	**166**	**179**	**160**	
Reaction		**-96**	**-5**	**-5**	**-11**	
1235$C_3H_2(CF_3)_4$		0.067358	-1542.249964	-1542.299793	-1542.251151	
CC + 1235b ts	CC + 2345b ts	0.228347	-1778.022449	-1778.121796	-1778.026284	
CC + 1235b	CC + 2345b	0.234657	-1778.090906	-1778.193265	-1778.094633	
Barrier		**-75**	**117**	**126**	**111**	
Reaction		**-91**	**-46**	**-45**	**-51**	
1245$C_3H_2(CF_3)_4$		0.066888	-1542.252245	-1542.302708	-1542.253439	
CC + 1245a ts	CC + 1345a ts	0.228932	-1778.001198	-1778.099324	-1778.005126	
CC + 1245a	CC + 1345a	0.237019	-1778.079887	-1778.180831	-1778.083682	
Barrier		**-77**	**182**	**195**	**176**	
Reaction		**-99**	**-4**	**2**	**-9**	
1245$C_3H_2(CF_3)_4$		0.066888	-1542.252245	-1542.302708	-1542.253439	
CC + 1245b ts	CC + 1345b ts	0.228752	-1778.021478	-1778.117995	-1778.025308	
CC + 1245b	CC + 1345b	0.237355	-1778.093649	-1778.192625	-1778.097378	
Barrier		**-77**	**128**	**146**	**122**	
Reaction		**-100**	**-39**	**-28**	**-44**	

Table S7. continued

						DLPNO-CCSD(T)/
		M062X				6-311+G(d,p)//
6-311+G(d,p)	Equivalencies	ΔG_{298} corr	M062X	wB97XD	M062XGD3	M062XGD3
1255$C_3H_2(CF_3)_4$		0.067392	-1542.242788	-1542.290175	-1542.244008	
CC + 125a5b ts	CC + 345a5b ts	0.230992	-1777.986838	-1778.079181	-1777.990625	
CC + 125a5b	CC + 345a5b	0.236293	-1778.049920	-1778.145901	-1778.053625	
Barrier		**-82**	**199**	**219**	**193**	
Reaction		**-95**	**47**	**58**	**42**	
1355$C_3H_2(CF_3)_4$		0.065623	-1542.249525	-1542.299085	-1542.250722	
CC + 135a5b ts	CC + 245a5b ts	0.229682	-1777.991254	-1778.085686	-1777.995064	
CC + 135a5b	CC + 245a5b	0.235316	-1778.052531	-1778.150117	-1778.056255	
Barrier		**-83**	**206**	**227**	**200**	
Reaction		**-98**	**60**	**72**	**54**	
1455$C_3H_2(CF_3)_4$		0.067303	-1542.243140	-1542.289855	-1542.244351	
CC + 145a5b ts		0.231504	-1777.979523	-1778.068868	-1777.983344	
CC + 145a5b		0.238454	-1778.042373	-1778.134879	-1778.046092	
Barrier		**-83**	**220**	**247**	**215**	
Reaction		**-101**	**74**	**92**	**68**	
2355$C_3H_2(CF_3)_4$		0.066841	-1542.250091	-1542.300038	-1542.251294	
CC + 235a5b ts		0.229301	-1777.987102	-1778.082072	-1777.990875	
CC + 235a5b		0.234971	-1778.053438	-1778.153113	-1778.057124	
Barrier		**-79**	**214**	**234**	**209**	
Reaction		**-93**	**55**	**63**	**50**	
123$C_3H_3(CF_3)_3$		0.066477	-1205.206106	-1205.249961	-1205.206945	
CC + 123 ts	CC + 234 ts	0.228093	-1440.974368	-1441.066231	-1440.977522	
CC + 123	CC + 234	0.234531	-1441.044144	-1441.147461	-1441.047200	
Barrier		**-76**	**130**	**142**	**125**	
Reaction		**-93**	**-36**	**-54**	**-41**	
124$C_3H_3(CF_3)_3$		0.063949	-1205.209940	-1205.255867	-1205.210783	
CC + 124 ts	CC + 134 ts	0.227618	-1440.977824	-1441.070290	-1440.981003	
CC + 124	CC + 134	0.235125	-1441.051971	-1441.147461	-1441.055040	
Barrier		**-82**	**136**	**153**	**131**	
Reaction		**-101**	**-39**	**-30**	**-43**	
125$C_3H_3(CF_3)_3$		0.066251	-1205.206441	-1205.250125	-1205.207284	
CC + 125a ts	CC + 345a ts	0.228385	-1440.957341	-1441.049335	-1440.960543	
CC + 125a	CC + 345a	0.235381	-1441.032198	-1441.128409	-1441.035297	
Barrier		**-78**	**177**	**188**	**172**	
Reaction		**-96**	**-1**	**-1**	**-6**	
125$C_3H_3(CF_3)_3$		0.066251	-1205.206441	-1205.250125	-1205.207284	
CC + 125b ts	CC + 345b ts	0.227169	-1440.973943	-1441.067171	-1440.977089	
CC + 125b	CC + 345b	0.234317	-1441.045102	-1441.140833	-1441.048145	
Barrier		**-75**	**130**	**138**	**125**	
Reaction		**-93**	**-38**	**-36**	**-43**	
135$C_3H_3(CF_3)_3$		0.065591	-1205.212903	-1205.258108	-1205.213735	
CC + 135a ts	CC + 245a ts	0.226951	-1440.963540	-1441.057447	-1440.966739	
CC + 135a	CC + 245a	0.234226	-1441.036596	-1441.134665	-1441.039703	
Barrier		**-76**	**176**	**186**	**170**	
Reaction		**-95**	**3**	**2**	**-2**	
135$C_3H_3(CF_3)_3$		0.065591	-1205.212903	-1205.258108	-1205.213735	
BN + 135b ts	CC + 245b ts	0.226857	-1440.980361	-1441.075047	-1440.983503	
BN + 135b	CC + 245b	0.234078	-1441.049135	-1441.146464	-1441.052180	
Barrier		**-75**	**131**	**140**	**126**	
Reaction		**-94**	**-30**	**-29**	**-35**	

Table S7. continued

						DLPNO-CCSD(T)/
		M062X				6-311+G(d,p)//
6-311+G(d,p)	Equivalencies	ΔG_{298} corr	M062X	wB97XD	M062XGD3	M062XGD3
145$C_3H_3(CF_3)_3$		0.067157	-1205.211610	-1205.255414	-1205.212459	
CC + 145a ts		0.227973	-1440.956818	-1441.048081	-1440.960061	
CC + 145a		0.236435	-1441.032958	-1441.127714	-1441.036063	
Barrier		**-74**	**188**	**202**	**183**	
Reaction		**-96**	**11**	**15**	**6**	
145$C_3H_3(CF_3)_3$		0.067157	-1205.211610	-1205.255414	-1205.212459	
CC + 145b ts		0.229220	-1440.975175	-1441.065241	-1440.978321	
CC + 145b		0.236693	-1441.045674	-1441.138030	-1441.048712	
Barrier		**-78**	**143**	**160**	**139**	
Reaction		**-97**	**-22**	**-11**	**-27**	
155$C_3H_3(CF_3)_3$		0.066877	-1205.202584	-1205.243753	-1205.203439	
CC + 15a5b ts	CC + 45a5b ts	0.229732	-1440.938455	-1441.024831	-1440.941567	
CC + 15a5b	CC + 45a5b	0.235984	-1441.000398	-1441.090193	-1441.003427	
Barrier		**-80**	**218**	**238**	**213**	
Reaction		**-96**	**72**	**83**	**67**	
235$C_3H_3(CF_3)_3$		0.066120	-1205.210555	-1205.255355	-1205.211384	
CC + 235a ts		0.227101	-1440.958746	-1441.051682	-1440.961913	
CC + 235a		0.233239	-1441.029467	-1441.129634	-1441.032538	
Barrier		**-75**	**181**	**193**	**176**	
Reaction		**-91**	**11**	**4**	**7**	
235$C_3H_3(CF_3)_3$		0.066120	-1205.210555	-1205.255355	-1205.211384	
CC + 235b ts		0.226165	-1440.975577	-1441.069764	-1440.978710	
CC + 235b		0.232033	-1441.044282	-1441.144571	-1441.047320	
Barrier		**-72**	**134**	**143**	**129**	
Reaction		**-88**	**-31**	**-38**	**-35**	
255$C_3H_3(CF_3)_3$		0.066008	-1205.206087	-1205.248857	-1205.206915	
CC + 25a5b ts	CC + 35a5b ts	0.229368	-1440.939242	-1441.026192	-1440.942344	
CC + 25a5b	CC + 35a5b	0.233699	-1441.006084	-1441.099103	-1441.009079	
Barrier		**-81**	**227**	**249**	**222**	
Reaction		**-92**	**63**	**69**	**58**	
12$C_3H_4(CF_3)_2$		0.064671	-868.159619	-868.197620	-868.160172	-866.562545
CC + 12 ts	CC + 34 ts	0.226661	-1103.924808	-1104.011865	-1103.927342	-1101.789945
CC + 12	CC + 34	0.234064	-1103.997267	-1104.086899	-1103.999695	-1101.866325
Barrier		**-77**	**139**	**149**	**135**	**129**
Reaction		**-97**	**-32**	**-29**	**-36**	**-52**
13$C_3H_4(CF_3)_2$		0.064914	-868.166654	-868.205730	-868.167192	-866.568749
CC + 13 ts	CC + 24 ts	0.226210	-1103.930765	-1104.018249	-1103.933284	-1101.794581
CC + 13	CC + 24	0.233496	-1104.001289	-1104.092481	-1104.003721	-1101.870106
Barrier		**-76**	**140**	**151**	**136**	**132**
Reaction		**-95**	**-26**	**-24**	**-30**	**-47**
14$C_3H_4(CF_3)_2$		0.065005	-868.167505	-868.206543	-868.168003	-866.569367
CC + 14 ts		0.227274	-1103.928871	-1104.014937	-1103.931420	-1101.793232
CC + 14		0.234572	-1104.002780	-1104.091629	-1104.005215	-1101.871410
Barrier		**-78**	**150**	**165**	**146**	**139**
Reaction		**-97**	**-25**	**-17**	**-29**	**-47**
15$C_3H_4(CF_3)_2$		0.066705	-868.163977	-868.201242	-868.164519	-866.567047
CC + 15a ts	CC + 45a ts	0.226976	-1103.909697	-1103.995752	-1103.912265	-1101.775109
CC + 15a	CC + 45a	0.234488	-1103.983262	-1104.073110	-1103.985732	-1101.852630
Barrier		**-73**	**186**	**196**	**181**	**176**
Reaction		**-93**	**12**	**13**	**8**	**-8**

Table S7. continued

						DLPNO-CCSD(T)/
		M062X				6-311+G(d,p)//
6-311+G(d,p)	Equivalencies	ΔG_{298} corr	M062X	wB97XD	M062XGD3	M062XGD3
$15C_3H_4(CF_3)_2$		0.066705	-868.163977	-868.201242	-868.164519	-866.567047
CC + 15b ts	CC + 45b ts	0.227037	-1103.926414	-1104.012693	-1103.928913	-1101.792377
CC + 15b	CC + 45b	0.234228	-1103.995263	-1104.084381	-1103.997661	-1101.864491
Barrier		**-73**	**142**	**152**	**138**	**130**
Reaction		**-92**	**-20**	**-18**	**-24**	**-40**
$23C_3H_4(CF_3)_2$		0.067752	-868.162521	-868.200331	-868.163061	-866.565253
CC + 23 ts		0.226179	-1103.925367	-1104.011946	-1103.927860	-1101.789889
CC + 23		0.232713	-1103.992971	-1104.085591	-1103.995385	-1101.863030
Barrier		**-68**	**136**	**146**	**132**	**127**
Reaction		**-85**	**-25**	**-30**	**-28**	**-48**
$25C_3H_4(CF_3)_2$		0.065857	-868.164545	-868.202598	-868.165062	-866.567718
CC + 25a ts	CC + 35a ts	0.226843	-1103.909925	-1103.995655	-1103.912476	-1101.773196
CC + 25a	CC + 35a	0.233195	-1103.982460	-1104.075645	-1103.984901	-1101.850562
Barrier		**-75**	**188**	**202**	**184**	**184**
Reaction		**-91**	**15**	**8**	**11**	**-2**
$25C_3H_4(CF_3)_2$		0.065857	-868.164545	-868.202598	-868.165062	-866.567718
CC + 25b ts	CC + 35b ts	0.225236	-1103.926494	-1104.013534	-1103.928982	-1101.791779
CC + 25b	CC + 35b	0.232090	-1103.996998	-1104.089817	-1103.999394	-1101.866492
Barrier		**-70**	**141**	**150**	**137**	**131**
Reaction		**-88**	**-26**	**-32**	**-30**	**-47**
$55C_3H_4(CF_3)_2$		0.066988	-868.156876	-868.191554	-868.157389	-866.561924
CC + 5a5b ts		0.229140	-1103.884621	-1103.963879	-1103.887064	-1101.749236
CC + 5a5b		0.233216	-1103.951720	-1104.037356	-1103.954091	-1101.819334
Barrier		**-78**	**238**	**259**	**234**	**235**
Reaction		**-88**	**72**	**77**	**69**	**62**
$1C_5H_5(CF_3)$		0.065879	-531.115003	-531.146518	-531.115304	-530.092154
CC + 1 ts	CC + 4 ts	0.226197	-766.875188	-766.954957	-766.877130	-765.313899
CC + 1	CC + 4	0.233679	-766.946021	-767.029243	-766.947863	-765.389070
Barrier		**-73**	**148**	**159**	**145**	**140**
Reaction		**-93**	**-19**	**-16**	**-21**	**-38**
$2C_5H_5(CF_3)$		0.065666	-531.113769	-531.145196	-531.114052	-530.091209
CC + 2 ts	CC + 3 ts	0.225156	-766.874436	-766.954200	-766.876348	-765.312786
CC + 2	CC + 3	0.232624	-766.944573	-767.030069	-766.946407	-765.387745
Barrier		**-71**	**144**	**156**	**141**	**138**
Reaction		**-90**	**-20**	**-24**	**-23**	**-39**
$5C_5H_5(CF_3)$		0.066794	-531.113098	-531.143524	-531.113362	-530.091389
CC + 5a ts		0.226846	-766.853818	-766.932040	-766.855781	-765.292106
CC + 5a		0.233079	-766.927072	-767.012186	-766.928936	-765.369502
Barrier		**-72**	**198**	**211**	**195**	**194**
Reaction		**-89**	**22**	**17**	**19**	**8**
$5C_5H_5(CF_3)$		0.066794	-531.113098	-531.143524	-531.113362	-530.091389
CC + 5b ts		0.225562	-766.870991	-766.950157	-766.872884	-765.310501
CC + 5b		0.232278	-766.940933	-767.025727	-766.942727	-765.384176
Barrier		**-69**	**150**	**160**	**147**	**143**
Reaction		**-87**	**-16**	**-21**	**-19**	**-33**

Table S7. continued

M062xGD3 values											
Change by Placing CH_3 at Position 1			Change by Placing CH_3 at Position 2			Change by Placing CH_3 at Position 5a			Change by Placing CH_3 at Position 5b		
Subst. Pattern	$\Delta G^{\ddagger}_{ASC1}$	ΔG_{ASC1}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC2}$	ΔG_{ASC2}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5a}$	ΔG_{ASC5a}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5b}$	ΔG_{ASC5b}
1-0	-2	-3	2-0	-5	-5	5a-0	48	37	5b-0	0	-1
12-2	-6	-12	12-1	-10	-14	15a-1	37	30	15b-1	-7	-2
13-3	-5	-7	23-3	-9	-5	25a-2	43	34	25b-2	-5	-7
14-4	1	-8	24-4	-9	-8	35a-3	43	34	35b-3	-5	-7
15a-5a	-13	-11	25a-5a	-11	-8	45a-4	37	30	45b-4	-7	-2
15b-5b	-9	-5	25b-5b	-10	-11	5a5b-5b	87	88	5a5b-5a	39	49
123-23	-7	-13	123-13	-11	-11	125a-12	37	30	125b-12	-10	-7
124-24	-5	-13	124-14	-14	-14	135a-13	35	28	135b-13	-10	-5
125a-25a	-12	-17	125a-15a	-10	-14	145a-14	38	35	145b-14	-7	2
125b-25b	-11	-12	125b-15b	-13	-19	15a5b-15b	76	91	15a5b-15a	32	59
134-34	-4	-8	234-34	-10	-5	235a-23	44	35	235b-23	-2	-7
135a-35a	-14	-13	235a-35a	-8	-4	245a-24	35	28	245b-24	-10	-5
135b-35b	-10	-5	235b-35b	-7	-5	25a5b-25b	85	88	25a5b-25a	38	47
145a-45a	2	-2	245a-45a	-11	-10	345a-34	37	30	345b-34	-10	-7
145b-45b	1	-3	245b-45b	-12	-11	35a5b-35b	85	88	35a5b-35a	38	47
15a5b-5a5b	-20	-1	25a5b-5a5b	-12	-11	45a5b-45b	76	91	45a5b-45a	32	59
1234-234	-7	-9	1234-134	-13	-7	1235a-123	35	30	1235b-123	-14	-10
1235a-235a	-16	-18	1235a-135a	-10	-9	1245a-124	44	34	1245b-124	-9	-1
1235b-235b	-18	-16	1235b-135b	-15	-16	125a5b-125b	68	84	125a5b-125a	21	48
1245a-245a	5	-7	1245a-145a	-8	-15	1345a-134	44	34	1345b-134	-9	-1
1245b-245b	-4	-9	1245b-145b	-16	-18	135a5b-135b	74	90	135a5b-135a	30	56
125a5b-25a5b	-29	-16	125a5b-15a5b	-20	-26	145a5b-145b	76	95	145a5b-145a	31	62
1345a-345a	4	-3	2345a-345a	-11	-5	2345a-234	35	30	2345b-234	-14	-10
1345b-345b	-3	-2	2345b-345b	-14	-9	235a5b-235b	79	85	235a5b-235a	33	43
135a5b-35a5b	-22	-4	235a5b-35a5b	-13	-8	245a5b-245b	74	90	245a5b-245a	30	56
145a5b-45a5b	1	1	245a5b-45a5b	-13	-13	345a5b-345b	68	84	345a5b-345a	21	48
12345a-2345a	13	3	12345a-1345a	-3	1	12345a-1234	55	42	12345b-1234	-13	-10
12345b-2345b	-6	-9	12345b-1345b	-17	-16	1235a5b-1235b	73	80	1235a5b-1235a	24	40
1235a5b-235a5b	-24	-21	1235a5b-135a5b	-16	-25	1245a5b-1245b	85	87	1245a5b-1245a	31	52
1245a5b-245a5b	7	-12	1245a5b-145a5b	-8	-26	1345a5b-1345b	85	87	1345a5b-1345a	31	52
1345a5b-345a5b	14	1	2345a5b-345a5b	-8	-13	2345a5b-2345b	73	80	2345a5b-2345a	24	40
12345a5b-2345a5b	2	0	12345a5b-1345a5b	-21	-13	12345a5b-12345b	81	90	12345a5b-12345a	13	38
Avg(StdDev)	–6 (10)	–8 (6)	Avg(StdDev)	–11 (4)	–12 (6)	Avg(StdDev)	59 (20)	60 (28)	Avg(StdDev)	11 (20)	22 (29)

M062x values											
Change by Placing CH_3 at Position 1			Change by Placing CH_3 at Position 2			Change by Placing CH_3 at Position 5a			Change by Placing CH_3 at Position 5b		
Subst. Pattern	$\Delta G^{\ddagger}_{ASC1}$	ΔG_{ASC1}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC2}$	ΔG_{ASC2}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5a}$	ΔG_{ASC5a}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5b}$	ΔG_{ASC5b}
1-0	-1	-3	2-0	-4	-4	5a-0	50	38	5b-0	1	0
12-2	-5	-12	12-1	-9	-13	15a-1	38	31	15b-1	-6	-1
13-3	-4	-6	23-3	-9	-4	25a-2	44	35	25b-2	-4	-6
14-4	2	-7	24-4	-8	-7	35a-3	44	35	35b-3	-4	-6
15a-5a	-13	-10	25a-5a	-10	-8	45a-4	38	31	45b-4	-6	-1
15b-5b	-8	-4	25b-5b	-9	-10	5a5b-5b	88	89	5a5b-5a	40	50
123-23	-6	-12	123-13	-10	-10	125a-12	38	31	125b-12	-9	-6
124-24	-4	-13	124-14	-13	-14	135a-13	36	29	135b-13	-9	-4
125a-25a	-11	-16	125a-15a	-9	-13	145a-14	39	36	145b-14	-6	3
125b-25b	-11	-11	125b-15b	-12	-18	15a5b-15b	76	92	15a5b-15a	33	60
134-34	-3	-7	234-34	-9	-5	235a-23	45	36	235b-23	-1	-6
135a-35a	-13	-12	235a-35a	-7	-3	245a-24	36	29	245b-24	-9	-4
135b-35b	-10	-4	235b-35b	-6	-4	25a5b-25b	86	89	25a5b-25a	38	48
145a-45a	3	-1	245a-45a	-10	-9	345a-34	38	31	345b-34	-9	-6
145b-45b	2	-2	245b-45b	-11	-10	35a5b-35b	86	89	35a5b-35a	38	48
15a5b-5a5b	-19	0	25a5b-5a5b	-11	-10	45a5b-45b	76	92	45a5b-45a	33	60
1234-234	-6	-8	1234-134	-12	-6	1235a-123	36	31	1235b-123	-13	-10
1235a-235a	-15	-17	1235a-135a	-9	-8	1245a-124	45	35	1245b-124	-8	0
1235b-235b	-17	-15	1235b-135b	-14	-15	125a5b-125b	69	85	125a5b-125a	22	48
1245a-245a	6	-6	1245a-145a	-7	-14	1345a-134	45	35	1345b-134	-8	0
1245b-245b	-3	-8	1245b-145b	-15	-17	135a5b-135b	75	90	135a5b-135a	30	57
125a5b-25a5b	-28	-16	125a5b-15a5b	-20	-25	145a5b-145b	77	96	145a5b-145a	32	63
1345a-345a	5	-2	2345a-345a	-11	-4	2345a-234	36	31	2345b-234	-13	-10
1345b-345b	-2	-1	2345b-345b	-13	-8	235a5b-235b	80	86	235a5b-235a	33	44
135a5b-35a5b	-21	-3	235a5b-35a5b	-12	-8	245a5b-245b	75	90	245a5b-245a	30	57
145a5b-45a5b	2	2	245a5b-45a5b	-12	-12	345a5b-345b	69	85	345a5b-345a	22	48
12345a-2345a	14	4	12345a-1345a	-2	2	12345a-1234	56	43	12345b-1234	-12	-9
12345b-2345b	-5	-8	12345b-1345b	-16	-15	1235a5b-1235b	74	81	1235a5b-1235a	25	40
1235a5b-235a5b	-23	-20	1235a5b-135a5b	-15	-25	1245a5b-1245b	85	88	1245a5b-1245a	32	53
1245a5b-245a5b	7	-11	1245a5b-145a5b	-7	-25	1345a5b-1345b	85	88	1345a5b-1345a	32	53
1345a5b-345a5b	15	2	2345a5b-345a5b	-8	-12	2345a5b-2345b	74	81	2345a5b-2345a	25	40
12345a5b-2345a5b	2	1	12345a5b-1345a5b	-20	-12	12345a5b-12345b	82	90	12345a5b-12345a	14	38
Avg(StdDev)	–5 (10)	–7 (6)	Avg(StdDev)	–11 (4)	–11 (6)	Avg(StdDev)	60 (20)	61 (28)	Avg(StdDev)	11 (20)	23 (28)

Table S7. continued

wB9XD values											
Change by Placing CH_3 at Position 1			Change by Placing CH_3 at Position 2			Change by Placing CH_3 at Position 5a			Change by Placing CH_3 at Position 5b		
Subst. Pattern	$\Delta G^{\ddagger}_{ASC1}$	ΔG_{ASC1}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC2}$	ΔG_{ASC2}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5a}$	ΔG_{ASC5a}	Subst. Pattern	$\Delta G^{\ddagger}_{ASC5b}$	ΔG_{ASC5b}
1-0	-1	2	2-0	-5	-6	5a-0	51	35	5b-0	0	-2
12-2	-7	-5	12-1	-11	-13	15a-1	36	28	15b-1	-8	-2
13-3	-4	-1	23-3	-10	-6	25a-2	46	32	25b-2	-5	-8
14-4	5	-2	24-4	-8	-9	35a-3	46	32	35b-3	-5	-8
15a-5a	-15	-4	25a-5a	-9	-9	45a-4	36	28	45b-4	-8	-2
15b-5b	-9	3	25b-5b	-10	-11	5a5b-5b	99	98	5a5b-5a	48	60
123-23	-4	-24	123-13	-9	-30	125a-12	40	28	125b-12	-10	-7
124-24	1	-6	124-14	-12	-13	135a-13	35	27	135b-13	-12	-4
125a-25a	-13	-9	125a-15a	-7	-13	145a-14	37	33	145b-14	-4	6
125b-25b	-12	-4	125b-15b	-13	-18	15a5b-15b	86	101	15a5b-15a	42	70
134-34	4	-1	234-34	-6	-25	235a-23	47	34	235b-23	-3	-8
135a-35a	-16	-6	235a-35a	-9	-4	245a-24	35	27	245b-24	-12	-4
135b-35b	-11	3	235b-35b	-7	-6	25a5b-25b	99	101	25a5b-25a	48	61
145a-45a	6	3	245a-45a	-10	-10	345a-34	40	28	345b-34	-10	-7
145b-45b	9	7	245b-45b	-12	-11	35a5b-35b	99	101	35a5b-35a	48	61
15a5b-5a5b	-21	6	25a5b-5a5b	-10	-8	45a5b-45b	86	101	45a5b-45a	42	70
1234-234	0	20	1234-134	-10	-4	1235a-123	37	49	1235b-123	-17	9
1235a-235a	-14	-9	1235a-135a	-7	-7	1245a-124	42	33	1245b-124	-7	3
1235b-235b	-17	-8	1235b-135b	-14	-17	125a5b-125b	81	94	125a5b-125a	31	59
1245a-245a	9	0	1245a-145a	-7	-13	1345a-134	42	33	1345b-134	-7	3
1245b-245b	6	1	1245b-145b	-15	-17	135a5b-135b	87	101	135a5b-135a	41	70
125a5b-25a5b	-30	-11	125a5b-15a5b	-19	-25	145a5b-145b	87	103	145a5b-145a	45	77
1345a-345a	7	3	2345a-345a	-10	-4	2345a-234	37	49	2345b-234	-17	9
1345b-345b	7	8	2345b-345b	-13	-9	235a5b-235b	91	101	235a5b-235a	41	58
135a5b-35a5b	-22	3	235a5b-35a5b	-15	-6	245a5b-245b	87	101	245a5b-245a	41	70
145a5b-45a5b	9	9	245a5b-45a5b	-11	-11	345a5b-345b	81	94	345a5b-345a	31	59
12345a-2345a	24	19	12345a-1345a	8	12	12345a-1234	61	49	12345b-1234	-6	-2
12345b-2345b	10	9	12345b-1345b	-10	-9	1235a5b-1235b	85	93	1235a5b-1235a	32	52
1235a5b-235a5b	-24	-15	1235a5b-135a5b	-16	-24	1245a5b-1245b	94	95	1245a5b-1245a	45	65
1245a5b-245a5b	13	-5	1245a5b-145a5b	-7	-25	1345a5b-1345b	94	95	1345a5b-1345a	45	65
1345a5b-345a5b	21	9	2345a5b-345a5b	-8	-10	2345a5b-2345b	85	93	2345a5b-2345a	32	52
12345a5b-2345a5b	14	12	12345a5b-1345a5b	-15	-7	12345a5b-12345b	89	96	12345a5b-12345a	21	45
Avg(StdDev)	–2 (14)	0 (9)	Avg(StdDev)	–10 (5)	–12 (8)	Avg(StdDev)	66 (25)	66 (33)	Avg(StdDev)	16 (25)	30 (33)

Table S8. Corrected relative free energy barrier heights $\Delta G^{\ddagger}$ and reaction free energies ΔG from Table S3, and $\Delta G^{\ddagger}/\Delta G$ values derived by summing $\Delta G^{\ddagger}_{ASC\#}/\Delta G_{ASC\#}$ values (marked with "(p)") (kJ mol^{-1}) using various model chemistries for Diels–Alder reactions **1** + *c*–$C_5H_x(CF_3)_{6-x}$.

M062x values						
Change by Placing CF_3 at Position 1			**Change by Placing CF_3 at Position 2**			
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**-5**	**-7**		**-11**	**-11**	
Change by Placing CF_3 at Position 5a			**Change by Placing CF_3 at Position 5b**			
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**60**	**61**		**11**	**23**	
wB97XD values						
Change by Placing CF_3 at Position 1			**Change by Placing CF_3 at Position 2**			
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**-2**	**0**		**-10**	**-12**	
Change by Placing CF_3 at Position 5a			**Change by Placing CF_3 at Position 5b**			
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**66**	**66**		**16**	**30**	
M062x+GD3 values						
Change by Placing CF_3 at Position 1			**Change by Placing CF_3 at Position 2**			
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**-6**	**-8**		**-11**	**-12**	
Change by Placing CF_3 at Position 5a			**Change by Placing CF_3 at Position 5b**			
$\Delta G^{\ddagger}_{ASC\#}$ / $\Delta G_{ASC\#}$	**59**	**60**		**11**	**22**	
				(p)	**(p)**	**(p)**
	M062X	**wB97XD**	**M062XGD3**	**M062X**	**wB97XD**	**M062XGD3**
CC + C_5H_6 ts	149	160	146			
CC + C_5H_6	-16	-18	-18			
CC + 12345a5b ts	194	225	186	188	218	182
CC + 12345a5b	37	59	29	32	54	24
CC + 12345a ts	180	203	173	177	202	171
CC + 12345a	-2	14	-8	9	24	2
CC + 12345b ts	112	136	105	128	152	123
CC + 12345b	-54	-37	-60	-29	-12	-36
CC + 1235a5b ts	191	211	185	193	220	188
CC + 1235a5b	35	48	29	39	54	32
CC + 1245a5b ts	213	240	207	199	228	193
CC + 1245a5b	49	67	43	43	66	36
CC + 1234 ts	124	142	118	117	133	113
CC + 1234	-44	-34	-50	-52	-49	-57
CC + 1235a ts	166	179	160	182	204	177
CC + 1235a	-5	-5	-11	16	24	10
CC + 1235b ts	117	126	111	133	154	129
CC + 1235b	-46	-45	-51	-22	-12	-28
CC + 1245a ts	182	195	176	188	212	182
CC + 1245a	-4	2	-9	20	36	14
CC + 1245b ts	128	146	122	139	162	134
CC + 1245b	-39	-28	-44	-18	0	-24
CC + 125a5b ts	199	219	193	204	230	199
CC + 125a5b	47	58	42	50	66	44
CC + 135a5b ts	206	227	200	204	230	199
CC + 135a5b	60	72	54	50	66	44
CC + 145a5b ts	220	247	215	210	238	204
CC + 145a5b	74	92	68	54	78	48
CC + 235a5b ts	214	234	209	198	222	194
CC + 235a5b	55	63	50	46	54	40
CC + 123 ts	130	142	125	122	137	118
CC + 123	-36	-54	-41	-45	-41	-49
CC + 124 ts	136	153	131	128	143	124
CC + 124	-39	-30	-43	-41	-37	-45
CC + 125a ts	177	188	172	193	214	188
CC + 125a	-1	-1	-6	27	36	22
CC + 125b ts	130	138	125	144	164	140
CC + 125b	-38	-36	-43	-11	0	-16
CC + 135a ts	176	186	170	193	214	188
CC + 135a	3	2	-2	27	36	22

Table S8. continued

				(p)	(p)	(p)
	M062X	**wB97XD**	**M062XGD3**	**M062X**	**wB97XD**	**M062XGD3**
CC + 135b ts	131	140	126	144	164	140
CC + 135b	-30	-29	-35	-11	0	-16
CC + 145a ts	188	202	183	199	222	193
CC + 145a	11	15	6	31	48	26
CC + 145b ts	143	160	139	150	172	145
CC + 145b	-22	-11	-27	-7	12	-12
CC + 15a5b ts	218	238	213	215	240	210
CC + 15a5b	72	83	67	61	78	56
CC + 235a ts	181	193	176	187	206	183
CC + 235a	11	4	7	23	24	18
CC + 235b ts	134	143	129	138	156	135
CC + 235b	-31	-38	-35	-15	-12	-20
CC + 25a5b ts	227	249	222	209	232	205
CC + 25a5b	63	69	58	57	66	52
CC + 12 ts	139	149	135	133	147	129
CC + 12	-32	-29	-36	-34	-29	-37
CC + 13 ts	140	151	136	133	147	129
CC + 13	-26	-24	-30	-34	-29	-37
CC + 14 ts	150	165	146	139	153	135
CC + 14	-25	-17	-29	-30	-25	-33
CC + 15a ts	186	196	181	204	224	199
CC + 15a	12	13	8	38	48	34
CC + 15b ts	142	152	138	155	174	151
CC + 15b	-20	-18	-24	0	12	-4
CC + 23 ts	136	146	132	127	139	124
CC + 23	-25	-30	-28	-38	-41	-41
CC + 25a ts	188	202	184	198	216	194
CC + 25a	15	8	11	34	36	30
CC + 25b ts	141	150	137	149	166	146
CC + 25b	-26	-32	-30	-4	0	-8
CC + 5a5b ts	238	259	234	220	242	216
CC + 5a5b	72	77	69	68	78	64
CC + 1 ts	148	159	145	144	155	141
CC + 1	-19	-16	-21	-23	-25	-25
CC + 2 ts	144	156	141	138	149	135
CC + 2	-20	-24	-23	-27	-29	-29
CC + 5a ts	198	211	195	209	226	205
CC + 5a	22	17	19	45	48	42
CC + 5b ts	150	160	147	160	176	157
CC + 5b	-16	-21	-19	7	12	4

Figure S4. M06-2X+GD3/6-311+G(d,p) model chemistry-predicted transition state free energy barriers $\Delta G^{\ddagger}_{298}$ (red dots) and reaction free energies ΔG_{298} (blue squares) vs. $\Delta G^{\ddagger}_{298}/\Delta G_{298}$ values predicted by summing $\Delta G^{\ddagger}_{ASC\#}/\Delta G_{ASC\#}$ values (from Table S8, kJ mol^{-1}) for Diels–Alder reactions **1** + *c*-$C_5H_x(CF_3)_{6-x}$.

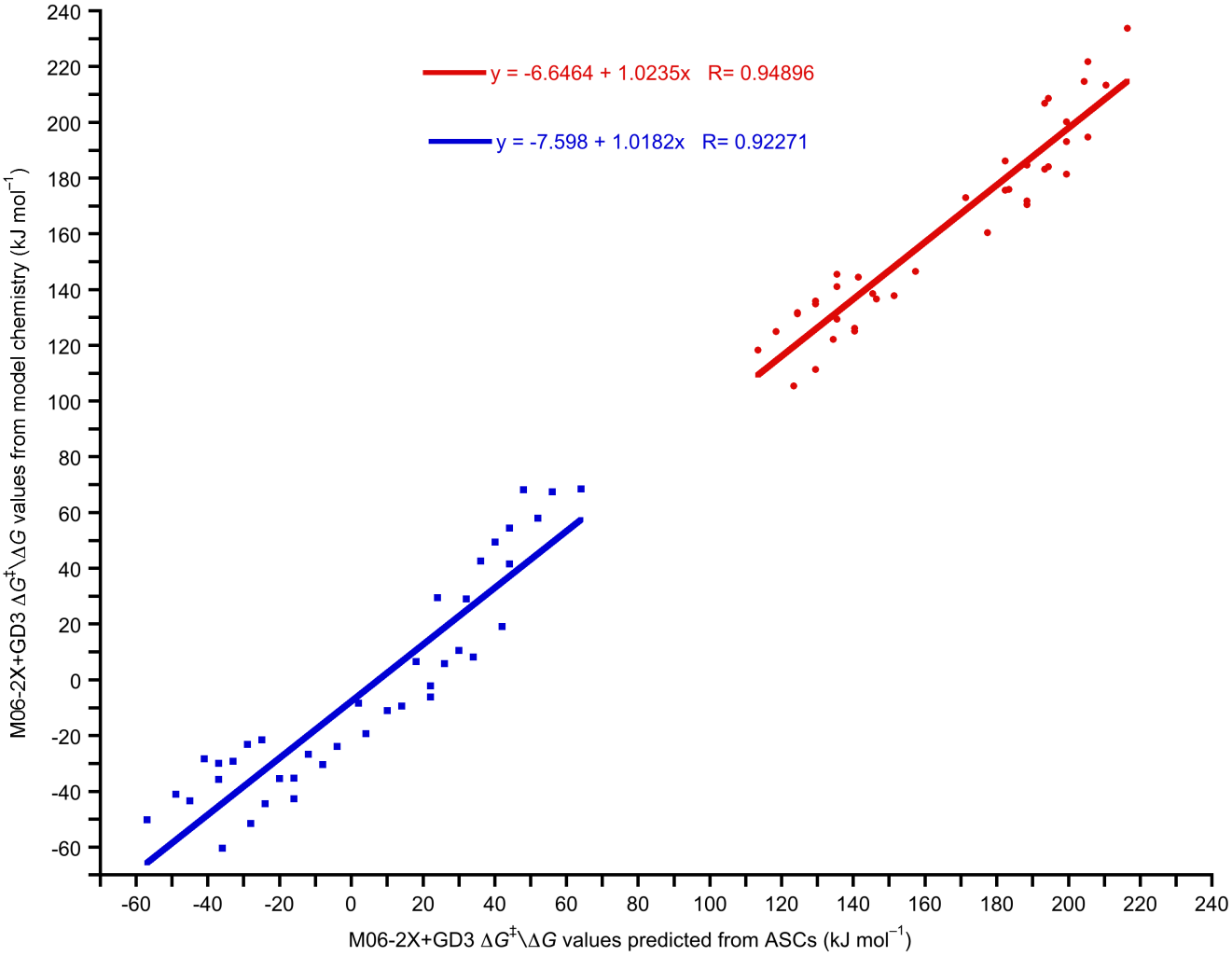


Table S9. Raw molecular energies (hartree) of components, corrected relative barrier heights $\Delta G^{\ddagger}$ and reaction energies $\Delta G^{\ddagger}$, and $\Delta G^{\ddagger}/\Delta G$ values derived by summing $\Delta G^{\ddagger}_{ASC\#}/\Delta G_{ASC\#}$ values (marked with "(p)") (M062x+GD3/6-311+G(d,p), kJ mol^{-1}) for Diels–Alder reactions **1** + randomly substituted cyclopentadienes *c*-$C_5H_a(CH_3)_b(F)_c(CF_3)_d$ (a+b+c+d=6)

6-311+G(d,p) basis set	M062XGD3	M062XGD3			M062XGD3	M062XGD3
	ΔG_{298} corr				ΔG_{298} corr	
Me_2CCMe_2	0.132527	-235.789114		Me_2CCMe_2	0.132527	-235.789114
5-CH_3-3-F-2-CF_3-C_5H_3	0.083293	-669.655014		5-CH_3-1-F-5-CF_3-C_5H_3	0.084533	-669.656604
CC + 5a32 ts	0.243541	-905.406997		CC + 5b15a ts	0.246014	-905.391931
CC + 5a32	0.249013	-905.478747		CC + 5b15a	0.251219	-905.464561
Barrier	**-73**	**170**		**Barrier**	**-76**	**217**
Reaction	**-87**	**-4**		**Reaction**	**-90**	**40**
4-CH_3-3-F-5-CF_3-C_5H_3	0.083744	-669.663194		3-CH_3-5-F-1-CF_3-C_5H_3	0.082746	-669.652566
CC + 435b ts	0.243003	-905.424745		CC + 35a1 ts	0.242619	-905.421521
CC + 435b	0.250445	-905.493417		CC + 35a1	0.251089	-905.500470
Barrier	**-70**	**143**		**Barrier**	**-72**	**125**
Reaction	**-90**	**-18**		**Reaction**	**-94**	**-60**
2-CH_3-4-F-C_5H_4	0.083204	-332.607561		3-F-5-CF_3-C_5H_4	0.057657	-630.353003
CC + 240 ts	0.241890	-568.369485		CC + 035a ts	0.217689	-866.095228
CC + 240	0.249460	-568.446174		CC + 035a	0.224120	-866.169699
Barrier	**-69**	**140**		**Barrier**	**-72**	**195**
Reaction	**-89**	**-41**		**Reaction**	**-89**	**17**
1-CH_3-2-F-4-CF_3-C_5H_3	0.082225	-669.663586		2-CH_3-5bF-1-CF_3-C_5H_3	0.082422	-669.652243
CC + 124 ts	0.243323	-905.426216		CC + 25b1 ts	0.242295	-905.420539
CC + 124	0.251378	-905.497669		CC + 25b1	0.251235	-905.498067
Barrier	**-75**	**145**		**Barrier**	**-72**	**126**
Reaction	**-96**	**-22**		**Reaction**	**-95**	**-54**
3-CH_3-5-F-4-CF_3-C_5H_3	0.082457	-669.652242		4-F-2-CF_3-C_5H_4	0.056700	-630.351875
CC + 35b4 ts	0.242218	-905.420539		CC + 042 ts	0.215894	-866.117760
CC + 35b4	0.251234	-905.498067		CC + 042	0.223148	-866.191694
Barrier	**-72**	**126**		**Barrier**	**-70**	**131**
Reaction	**-95**	**-54**		**Reaction**	**-89**	**-44**
1-CH_3-5-F-3-CF_3-C_5H_3	0.082486	-669.653607		5-CH_3-3-CF_3-C_5H_4	0.092335	-570.418366
CC + 15a3 ts	0.243278	-905.424592		CC + 5b03 ts	0.251810	-806.179947
CC + 15a3	0.250482	-905.498019		CC + 5b03	0.258701	-806.251219
Barrier	**-74**	**122**		**Barrier**	**-71**	**143**
Reaction	**-93**	**-52**		**Reaction**	**-89**	**-26**
4-CH_3-1-F-5-CF_3-C_5H_3	0.083583	-669.657973				
CC + 415b ts	0.243136	-905.421974				
CC + 415b	0.250050	-905.494271				
Barrier	**-71**	**137**				
Reaction	**-89**	**-35**				

Table S10. Mathematics and comparison of relative barrier heights $\Delta G^{\ddagger}$ and reaction energies $\Delta G^{\ddagger}$, and $\Delta G^{\ddagger}/\Delta G$ values derived by summing $\Delta G^{\ddagger}_{ASC\#}/\Delta G_{ASC\#}$ values (M062x+GD3/6-311+G(d,p), kJ mol^{-1}) for Diels–Alder reactions **1** + randomly substituted cyclopentadienes *c*-$C_5H_a(CH_3)_b(F)_c(CF_3)_d$ (a+b+c+d=6)

Cage ring			Parent	$\Delta G^{\ddagger}_{ASC}/\Delta G_{ASC}$				
		M062xGD3	M062xGD3	CH_3	CF_3	F	Sum	Δ
5a-CH_3-3-F-2-CF_3-C_5H_3	TS	170	146	42	-11	-2	175	-5
	Product	-4	-18	37	-12	-4	3	-7
4-CH_3-3-F-5b-CF_3-C_5H_3	TS	143	146	1	11	-2	156	-13
	Product	-18	-18	5	22	-4	5	-23
2-CH_3-4-F-C_5H_4	TS	140	146	0		-12	134	6
	Product	-41	-18	-3		-26	-47	6
1-CH_3-2-F-4-CF_3-C_5H_3	TS	145	146	1	-6	-2	139	6
	Product	-22	-18	5	-8	-4	-25	3
3-CH_3-5b-F-4-CF_3-C_5H_3	TS	126	146	0	-6	-3	137	-11
	Product	-54	-18	-3	-8	-17	-46	-8
1-CH_3-5a-F-3-CF_3-C_5H_3	TS	122	146	1	-11	-10	126	-4
	Product	-52	-18	5	-12	-22	-47	-5
4-CH_3-1-F-5b-CF_3-C_5H_3	TS	137	146	1	11	-12	146	-9
	Product	-35	-18	5	22	-26	-17	-18
5b-CH_3-1-F-5a-CF_3-C_5H_3	TS	217	146	10	59	-12	203	14
	Product	40	-18	10	60	-26	26	14
3-CH_3-5a-F-1-CF_3-C_5H_3	TS	125	146	0	-6	-10	130	-5
	Product	-60	-18	-3	-8	-22	-51	-9
3-F-5a-CF_3-C_5H_4	TS	195	146		59	-2	203	-8
	Product	17	-18		60	-4	38	-21
2-CH_3-5b-F-1-CF_3-C_5H_3	TS	126	146	0	-6	-3	137	-11
	Product	-54	-18	-3	-8	-17	-46	-8
4-F-2-CF_3-C_5H_4	TS	131	146		-11	-12	123	8
	Product	-44	-18		-12	-26	-56	12
5b-CH_3-3-CF_3-C_5H_4	TS	143	146	10	-11		145	-2
	Product	-26	-18	10	-12		-20	-6
RMS Dev								9
RMS Dev								13
Avg Signed Dev								-3
Avg Signed Dev								-5
Avg Unsign Dev								8
Avg Unsign Dev								11

Table S11. Cartesian coordinates for cyclopentadiene *c*-C_5H_6; substituted cyclopentadienes *c*-$C_5H_xR_{6-x}$ including randomly substituted cyclopentadienes *c*-$C_5H_a(CH_3)_b(F)_c(CF_3)_d$ (a+b+c+d=6); $Me_2C{=}CMe_2$, **1**; **1** + C_5H_6 TS; **1** + C_5H_6 (parent Diels–Alder reaction)

11
c-C_5H_6

C	-0.001231	-0.068175	-0.008978
C	1.157703	-1.013587	-0.138848
C	0.694121	-2.263424	-0.301437
H	1.293288	-3.156124	-0.421808
C	-0.775383	-2.238216	-0.291416
C	-1.193569	-0.973254	-0.122813
H	-2.218461	-0.632902	-0.073290
H	-1.406399	-3.109815	-0.403398
H	2.194244	-0.708596	-0.103382
H	0.014482	0.467473	0.947784
H	0.006540	0.697059	-0.794419

14
c-1–$C_5H_5(CH_3)$ = *c*-4–$C_5H_5(CH_3)$

C	-0.025957	-0.077323	0.000704
C	0.853725	-1.300497	0.014979
C	0.067156	-2.391542	0.023891
H	0.414296	-3.417199	0.034911
C	-1.344192	-1.983261	0.016408
C	-1.417890	-0.642940	0.002931
H	-2.317357	-0.043539	-0.005203
H	-2.182313	-2.667630	0.021160
C	2.346568	-1.234694	0.017956
H	2.716102	-0.692552	0.893430
H	2.781120	-2.235099	0.028938
H	2.720381	-0.710011	-0.866295
H	0.160107	0.559954	0.873888
H	0.164382	0.542513	-0.884037

14
c-2–$C_5H_5(CH_3)$ = *c*-3–$C_5H_5(CH_3)$

C	-0.046940	0.037165	-0.000399
C	-1.486107	-0.389086	0.005006
C	-2.283750	0.693282	0.005223
C	-3.779317	0.737115	0.009817
H	-4.149736	1.269248	0.890299
H	-4.155253	1.265594	-0.870527
H	-4.201754	-0.268220	0.013228
C	-1.431748	1.897559	0.000017
C	-0.139674	1.536336	-0.003269
H	0.716797	2.196311	-0.007344
H	-1.814706	2.910892	-0.000921
H	-1.813421	-1.420483	0.008203
H	0.495909	-0.333002	0.877546
H	0.490407	-0.336708	-0.880156

14
c-5–$C_5H_5(CH_3)$

C	0.046215	0.000173	-0.058910
C	0.915070	1.176506	-0.413890
C	2.092143	0.743176	-0.891257
H	2.913644	1.361092	-1.228858
C	2.097184	-0.728379	-0.891625
C	0.923108	-1.170001	-0.414477
H	0.617558	-2.201465	-0.297406
H	2.922898	-1.340483	-1.229534
H	0.602461	2.205793	-0.296302
H	-0.135566	-0.000721	1.025432
C	-1.304851	-0.004273	-0.787112
H	-1.890724	0.878232	-0.522614
H	-1.146132	-0.003459	-1.867441
H	-1.884664	-0.890903	-0.523057

17
c-1,2–$C_5H_4(CH_3)_2$ = *c*-3,4–$C_5H_4(CH_3)_2$

C	0.000000	0.000000	0.000000
C	-1.444765	-0.428369	0.000011
C	-1.503047	-1.775654	0.000034
C	-2.706977	-2.665620	0.000027
H	-2.707058	-3.315030	-0.879995
H	-2.707270	-3.314719	0.880280
H	-3.636795	-2.097005	-0.000168
C	-0.126766	-2.308312	0.000095
C	0.754282	-1.298271	0.000130

H	1.832495	-1.376620	0.000158
H	0.110085	-3.365666	0.000098
C	-2.561622	0.566116	0.000110
H	-2.508613	1.215558	-0.879050
H	-3.538062	0.081277	-0.001020
H	-2.509887	1.214008	0.880500
H	0.238570	0.610961	-0.879393
H	0.238618	0.611535	0.878956

17

c-1,3–$C_5H_4(CH_3)_2$ = *c*-2,4–$C_5H_4(CH_3)_2$

C	0.000000	-0.000000	0.000000
C	0.411494	1.449997	-0.000044
C	-0.699211	2.206057	-0.000106
H	-0.726171	3.290012	-0.000031
C	-1.897917	1.346849	0.000011
C	-1.500890	0.062895	-0.000276
H	-2.147498	-0.804644	-0.000402
C	-3.296046	1.879215	0.000003
H	-3.474289	2.502174	-0.880886
H	-4.025580	1.068582	0.001025
H	-3.473578	2.503899	0.879821
C	1.838067	1.894801	-0.000074
H	2.367684	1.519293	-0.880674
H	1.908486	2.983331	0.001167
H	2.368555	1.517094	0.879036
H	0.394138	-0.525457	-0.878463
H	0.392878	-0.523810	0.880132

17

c-1,4–$C_5H_4(CH_3)_2$

C	0.097243	-0.017519	0.000000
C	1.219936	0.988829	0.000000
C	2.385080	0.318665	0.000000
H	3.369428	0.770520	0.000000
C	2.125641	-1.127843	-0.000000
C	0.800219	-1.351310	-0.000000
C	0.078143	-2.659358	-0.000000
H	0.782296	-3.492610	-0.000000
H	-0.564986	-2.757048	0.879882
H	-0.564986	-2.757048	-0.879882
H	2.891599	-1.893625	-0.000000
C	0.997456	2.466288	0.000000
H	0.428365	2.781396	0.879882
H	1.947299	3.002886	0.000000
H	0.428365	2.781396	-0.879882
H	-0.548976	0.098384	0.879275
H	-0.548976	0.098384	-0.879275

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c-1,5–$C_5H_4(CH_3)_2$ = *c*-4,5–$C_5H_4(CH_3)_2$

C	0.075387	-0.026639	-0.017245
C	1.205889	0.977273	-0.028623
C	2.375838	0.315406	-0.047621
H	3.358451	0.770609	-0.062324
C	2.121636	-1.132734	-0.048756
C	0.797438	-1.347343	-0.029750
H	0.293648	-2.304901	-0.031128
H	2.892734	-1.891838	-0.063340
C	0.976679	2.453380	-0.036666
H	0.372243	2.765279	0.820345
H	1.922434	2.995731	-0.003293
H	0.439064	2.763585	-0.938663
H	-0.485010	0.077400	0.923052
C	-0.893249	0.147345	-1.194432
H	-0.348508	0.069396	-2.138199
H	-1.667217	-0.622330	-1.178435
H	-1.384020	1.122500	-1.156403

17

c-2,3–$C_5H_4(CH_3)_2$

C	-0.049900	0.048581	-0.001669
C	0.358334	1.499210	-0.009404
C	-0.750103	2.267127	0.009572
C	-0.861027	3.760233	0.010749
H	0.115592	4.243737	-0.007796
H	-1.426485	4.106028	-0.859237
H	-1.393716	4.107179	0.900731
C	-1.934573	1.387022	0.030679

C	-1.550187	0.103025	0.024563
H	-2.191431	-0.767223	0.036127
H	-2.955146	1.750649	0.048325
C	1.795127	1.913421	-0.034634
H	2.300270	1.523523	-0.923657
H	1.905986	2.997972	-0.036059
H	2.331400	1.522726	0.835608
H	0.324331	-0.479596	-0.887385
H	0.355221	-0.478976	0.870723

17

c-2,5–$C_5H_4(CH_3)_2$ = *c*-3,5–$C_5H_4(CH_3)_2$

C	-0.011044	-0.038611	-0.056772
C	0.686210	-1.321029	-0.421049
C	-0.213010	-2.272311	-0.724351
C	0.040104	-3.686288	-1.142273
H	1.109066	-3.895355	-1.194525
H	-0.413799	-4.387183	-0.436240
H	-0.398783	-3.885413	-2.123853
C	-1.563719	-1.691554	-0.583802
C	-1.462669	-0.410475	-0.201517
H	-2.276592	0.280584	-0.024154
H	-2.480810	-2.237327	-0.770561
H	1.763515	-1.432466	-0.437093
H	0.194683	0.206048	0.995091
C	0.399872	1.154027	-0.930591
H	0.198955	0.933024	-1.981003
H	-0.157292	2.051140	-0.652519
H	1.465223	1.366145	-0.819919

17

c-5,5–$C_5H_4(CH_3)_2$

C	-0.019274	-0.042080	-0.015054
C	0.677760	-1.326796	-0.393083
C	-0.221140	-2.251952	-0.758033
H	-0.007689	-3.263341	-1.077898
C	-1.571784	-1.671602	-0.655828
C	-1.468921	-0.404422	-0.230576
H	-2.280587	0.290862	-0.054645
H	-2.487750	-2.197765	-0.890209
H	1.754184	-1.442626	-0.360333
C	0.249191	0.323651	1.454942
H	1.312619	0.523792	1.608836
H	-0.309726	1.221230	1.731684
H	-0.051371	-0.491852	2.115534
C	0.407473	1.113453	-0.936678
H	0.219218	0.861573	-1.982100
H	-0.148984	2.021437	-0.690651
H	1.473103	1.323599	-0.814616

20

c-1,2,3–$C_5H_3(CH_3)_3$ = *c*-2,3,4–$C_5H_3(CH_3)_3$

C	-0.018624	-0.026354	0.010535
C	-1.421590	0.486010	0.085207
C	-1.860980	1.748622	0.256083
C	-1.063579	3.005604	0.420828
H	0.008952	2.814531	0.390560
H	-1.300368	3.724258	-0.369420
H	-1.292737	3.490887	1.374249
C	-3.343861	1.749612	0.262660
C	-3.783640	0.492339	0.096319
H	-4.817965	0.176686	0.058572
C	-2.609668	-0.432974	-0.032610
H	-2.600477	-1.199777	0.751979
H	-2.608054	-0.966499	-0.991255
C	-4.159706	2.992798	0.432575
H	-3.935695	3.482484	1.384808
H	-3.943220	3.715915	-0.359231
H	-5.226116	2.766287	0.406859
H	0.165099	-0.527377	-0.944883
H	0.714434	0.773939	0.114543
H	0.172626	-0.760893	0.798873

20

c-1,2,4–$C_5H_3(CH_3)_3$ = *c*-1,3,4–$C_5H_3(CH_3)_3$

C	0.040708	-0.019702	-0.001701
C	-1.364945	0.486674	0.061603
C	-1.813279	1.747409	0.222061
C	-1.027443	3.011253	0.384325

H	0.047384	2.831511	0.362666
H	-1.268603	3.720591	-0.412621
H	-1.270702	3.497611	1.333389
C	-3.289098	1.730926	0.218238
C	-3.742298	0.477928	0.057827
C	-5.156142	-0.001306	-0.005025
H	-5.361744	-0.502496	-0.955747
H	-5.364556	-0.723602	0.790076
H	-5.854875	0.830043	0.099095
C	-2.550890	-0.437066	-0.057623
H	-2.552007	-1.199585	0.731762
H	-2.550121	-0.976785	-1.013273
H	-3.905156	2.616511	0.330583
H	0.234992	-0.523454	-0.953801
H	0.767988	0.785723	0.103900
H	0.232127	-0.749562	0.791169

20

c-1,2,5–$C_5H_3(CH_3)_3$ = *c*-3,4,5–$C_5H_3(CH_3)_3$

C	0.041531	-0.088981	0.133797
C	-1.362570	0.420320	0.199798
C	-1.802811	1.680492	0.386962
C	-1.011769	2.937938	0.572530
H	0.062190	2.754763	0.540463
H	-1.255367	3.666527	-0.205964
H	-1.246742	3.402733	1.534372
C	-3.279224	1.667131	0.392698
C	-3.722635	0.416083	0.211530
H	-4.753250	0.088248	0.175211
C	-2.546788	-0.511395	0.072371
C	-2.540993	-1.638213	1.113483
H	-1.666318	-2.280865	0.989832
H	-2.519345	-1.213407	2.119902
H	-3.433565	-2.260164	1.020607
H	-2.547792	-0.957384	-0.932784
H	-3.889258	2.552820	0.526025
H	0.206380	-0.667979	-0.779994
H	0.769937	0.721911	0.152728
H	0.259128	-0.753094	0.977128

20

c-1,3,5–$C_5H_3(CH_3)_3$ = *c*-2,4,5–$C_5H_3(CH_3)_3$

C	0.024346	-0.055191	0.022294
C	-1.387057	0.430614	0.079426
C	-1.830992	1.684987	0.261330
H	-1.210213	2.565113	0.388121
C	-3.306491	1.702498	0.268911
C	-3.744752	0.445571	0.088984
H	-4.779290	0.127032	0.052579
C	-2.577257	-0.493934	-0.047515
C	-2.572876	-1.617802	0.996674
H	-1.702563	-2.266576	0.872745
H	-2.547324	-1.190330	2.001855
H	-3.469675	-2.233993	0.907662
H	-2.573623	-0.942194	-1.051519
C	-4.116889	2.946601	0.451232
H	-3.877628	3.429645	1.402737
H	-3.902366	3.668926	-0.341373
H	-5.184796	2.726173	0.435730
H	0.220095	-0.593411	-0.909961
H	0.727537	0.775737	0.091874
H	0.234991	-0.748374	0.843223

20

c-1,4,5–$C_5H_3(CH_3)_3$

C	0.036784	-0.047974	0.029532
C	-1.377672	0.429802	0.084982
C	-1.829721	1.682329	0.263350
H	-1.212155	2.563559	0.387592
C	-3.299589	1.682014	0.263396
C	-3.751113	0.429294	0.085056
C	-5.165368	-0.049086	0.029694
H	-5.365508	-0.590693	-0.899913
H	-5.384685	-0.734974	0.854537
H	-5.862170	0.787858	0.093382
C	-2.564198	-0.498549	-0.044437
C	-2.563926	-1.619953	1.001713
H	-1.680769	-2.253894	0.897043
H	-2.563986	-1.189477	2.006339

H	-3.446817	-2.254271	0.897098
H	-2.564133	-0.947600	-1.048547
H	-3.917524	2.562981	0.387676
H	0.237098	-0.589495	-0.900087
H	0.733233	0.789269	0.093177
H	0.256446	-0.733767	0.854361

20

c-1,5,5–$C_5H_3(CH_3)_3$ = *c*-4,5,5–$C_5H_3(CH_3)_3$

C	0.012316	-0.054988	-0.009540
C	-1.406079	0.398077	0.096425
C	-1.865991	1.641881	0.311729
H	-1.255296	2.526540	0.444218
C	-3.336350	1.623702	0.341105
C	-3.762320	0.368282	0.143388
H	-4.788850	0.024766	0.109322
C	-2.581826	-0.554945	-0.034901
C	-2.547746	-1.626336	1.066930
H	-1.667935	-2.265951	0.953697
H	-2.517037	-1.160877	2.054466
H	-3.435489	-2.261054	1.009141
C	-2.602561	-1.215631	-1.422755
H	-1.723242	-1.851495	-1.558666
H	-3.491471	-1.841571	-1.533805
H	-2.610917	-0.457572	-2.208948
H	-3.959174	2.494575	0.498477
H	0.209087	-0.517038	-0.982454
H	0.699277	0.783172	0.113593
H	0.247324	-0.803503	0.754181

20

c-2,3,5–$C_5H_3(CH_3)_3$

C	-0.000041	-0.019370	0.050340
C	-0.389660	1.368400	-0.351942
C	-1.610807	1.828389	-0.668547
H	-2.528455	1.252590	-0.676979
C	-1.544398	3.292571	-1.007011
C	-0.081039	3.593690	-0.831881
C	0.579698	2.486962	-0.455535
C	2.040373	2.335025	-0.167597
H	2.204208	1.991596	0.857976
H	2.495774	1.594246	-0.831325
H	2.565489	3.281481	-0.299734
H	0.351069	4.575313	-0.984848
C	-2.455329	4.162606	-0.130936
H	-3.503174	3.884775	-0.263436
H	-2.193694	4.033138	0.921491
H	-2.347818	5.218921	-0.386611
H	-1.823979	3.437670	-2.060240
H	0.732357	-0.438269	-0.645941
H	0.459825	-0.025568	1.042837
H	-0.868266	-0.678735	0.071146

20

c-2,5,5–$C_5H_3(CH_3)_3$ = *c*-3,5,5–$C_5H_3(CH_3)_3$

C	-0.006677	-0.030956	0.003015
C	-0.486191	1.385927	-0.008111
C	-1.748754	1.838496	0.040945
H	-2.645323	1.231572	0.097966
C	-1.779865	3.347413	0.006361
C	-0.308352	3.679404	-0.071360
C	0.417902	2.554246	-0.078908
H	1.497954	2.483991	-0.128443
H	0.063702	4.696031	-0.113298
C	-2.409529	3.924462	1.285388
H	-3.458238	3.625503	1.360864
H	-1.880902	3.564690	2.170335
H	-2.367591	5.016815	1.273583
C	-2.528999	3.864277	-1.233404
H	-3.579473	3.564455	-1.194989
H	-2.488580	4.955853	-1.277699
H	-2.085663	3.461528	-2.146235
H	0.651313	-0.211367	0.857653
H	-0.842748	-0.728752	0.059340
H	0.567942	-0.253389	-0.900446

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c-1,2,3,4–$C_5H_2(CH_3)_4$

C	0.109188	0.203098	0.143951

C	0.144270	1.642674	-0.267670
C	-0.584442	2.264273	-1.213573
C	-1.633127	1.709697	-2.123998
H	-2.590346	2.219841	-1.977377
H	-1.355147	1.847904	-3.173587
H	-1.794435	0.644013	-1.959213
C	-0.183361	3.715183	-1.250759
C	0.879022	3.832288	-0.190090
C	1.058470	2.622185	0.371682
C	2.001454	2.230560	1.467333
H	2.593797	3.076448	1.815776
H	1.456885	1.824326	2.324988
H	2.691915	1.452130	1.129013
C	1.559201	5.130099	0.108591
H	2.070717	5.518596	-0.777655
H	0.835641	5.890577	0.418669
H	2.298826	5.029674	0.903402
H	0.199480	4.002661	-2.238604
H	-1.035760	4.374784	-1.042458
H	1.087953	-0.266428	0.007141
H	-0.147024	0.105666	1.203203
H	-0.619989	-0.366807	-0.431651

23

c-1,2,3,5–$C_5H_2(CH_3)_4$ = *c*-2,3,4,5–$C_5H_2(CH_3)_4$

C	0.085465	0.009718	-0.043966
C	-0.888859	0.668514	-0.969382
C	-1.279493	1.951986	-0.979712
H	-0.949111	2.728882	-0.301108
C	-2.275939	2.174218	-2.082498
C	-2.393041	0.804706	-2.711853
C	-3.309557	0.551056	-3.865466
H	-3.202487	-0.460897	-4.256734
H	-4.356295	0.687107	-3.573118
H	-3.112940	1.250703	-4.683545
C	-1.588550	-0.055968	-2.058637
C	-1.373036	-1.516522	-2.310379
H	-0.320646	-1.725010	-2.524950
H	-1.643520	-2.107874	-1.430443
H	-1.965933	-1.876500	-3.151025
C	-3.619938	2.720816	-1.584184
H	-3.489165	3.686623	-1.091836
H	-4.321226	2.855119	-2.411205
H	-4.059916	2.024712	-0.865909
H	-1.861767	2.874105	-2.822714
H	0.474964	0.721816	0.684262
H	-0.384910	-0.815100	0.499270
H	0.929692	-0.410977	-0.598181

23

c-1,2,4,5–$C_5H_2(CH_3)_4$ = *c*-1,3,4,5–$C_5H_2(CH_3)_4$

C	-0.150715	0.053475	0.017941
C	-1.148404	0.910827	0.726043
C	-1.573173	0.670268	2.155931
C	-2.584658	1.765216	2.411214
C	-3.280547	1.897921	3.728042
H	-3.897209	2.795993	3.772399
H	-3.930853	1.038015	3.921393
H	-2.559794	1.945018	4.550368
C	-2.719199	2.510316	1.297053
C	-3.600445	3.696633	1.058020
H	-4.288926	3.504205	0.230065
H	-4.192931	3.951107	1.936796
H	-3.004307	4.572013	0.784486
C	-1.822183	1.971581	0.256347
H	-1.732614	2.388185	-0.741220
C	-2.141685	-0.736330	2.379425
H	-1.394405	-1.502530	2.161045
H	-2.464929	-0.868666	3.414260
H	-3.002875	-0.895861	1.725360
H	-0.706605	0.812431	2.818553
H	-0.509105	-0.976984	-0.074590
H	0.047266	0.433028	-0.985464
H	0.797412	0.015487	0.563050

23

c-1,2,5,5–$C_5H_2(CH_3)_4$ = *c*-3,4,5,5–$C_5H_2(CH_3)_4$

C	-0.075489	-0.053414	0.040857
C	0.427098	-1.472855	0.120139

H	1.480166	-1.725791	0.135419
C	-0.609253	-2.318464	0.165758
H	-0.556889	-3.399233	0.225719
C	-1.874386	-1.558193	0.122095
C	-3.212166	-2.229573	0.157698
H	-4.032475	-1.513188	0.116909
H	-3.320977	-2.917548	-0.685656
H	-3.323167	-2.819996	1.071741
C	-1.583632	-0.244782	0.049651
C	-2.516430	0.920393	-0.016037
H	-3.559952	0.605825	0.000067
H	-2.359077	1.600190	0.827942
H	-2.356864	1.502885	-0.929506
C	0.388461	0.760639	1.259366
H	1.479286	0.825338	1.283409
H	-0.007848	1.778967	1.215354
H	0.047554	0.292912	2.185655
C	0.391488	0.621033	-1.259046
H	1.482377	0.682826	-1.287478
H	0.052744	0.053741	-2.128775
H	-0.004792	1.637932	-1.328814

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c-1,3,5,5–$C_5H_2(CH_3)_4$ = *c*-2,4,5,5–$C_5H_2(CH_3)_4$

C	-0.034232	-0.045321	-0.001274
C	1.429127	0.218902	-0.163869
C	2.409644	-0.662789	-0.412749
H	2.295356	-1.733442	-0.538784
C	3.743235	0.037358	-0.500272
C	3.357284	1.487072	-0.256754
C	4.356886	2.595800	-0.246327
H	3.874109	3.554602	-0.053305
H	5.117837	2.435580	0.524384
H	4.881371	2.664537	-1.204929
C	2.030680	1.563207	-0.067601
H	1.469175	2.470328	0.127629
C	4.707324	-0.463951	0.586786
H	4.919276	-1.526884	0.446265
H	5.656543	0.077603	0.541596
H	4.272339	-0.325595	1.579065
C	4.372739	-0.136189	-1.891695
H	5.319199	0.407962	-1.958612
H	4.576780	-1.191821	-2.087859
H	3.699323	0.236495	-2.666677
H	-0.256951	-1.107121	-0.111797
H	-0.380018	0.279129	0.984222
H	-0.613492	0.508213	-0.745647

23

c-1,4,5,5–$C_5H_2(CH_3)_4$

C	-0.072064	0.059152	-0.040405
C	-1.535946	0.355000	-0.042232
C	-2.092554	1.757086	-0.217852
C	-3.592734	1.530906	-0.148307
C	-4.585594	2.639665	-0.272425
H	-5.604321	2.257213	-0.195521
H	-4.445308	3.390665	0.511874
H	-4.488955	3.156432	-1.232832
C	-3.830032	0.222011	0.035268
H	-4.808443	-0.234742	0.122551
C	-2.556232	-0.506230	0.100973
H	-2.462508	-1.576016	0.243477
C	-1.624679	2.678324	0.919018
H	-0.537958	2.796304	0.896268
H	-2.070074	3.671642	0.817389
H	-1.910558	2.265434	1.889338
C	-1.689169	2.339652	-1.580899
H	-0.603490	2.451635	-1.645503
H	-2.021238	1.685797	-2.390798
H	-2.135340	3.327436	-1.724507
H	0.443273	0.599160	0.760600
H	0.107029	-1.007487	0.101682
H	0.396925	0.359014	-0.983217

23

c-2,3,5,5–$C_5H_2(CH_3)_4$

C	-0.010405	0.013507	0.081988
C	-1.506156	0.001162	0.038078
C	-2.328547	-1.058352	0.047164

H	-2.032137	-2.100610	0.088841
C	-3.770465	-0.616024	-0.009505
C	-3.623237	0.885463	-0.052540
H	-4.470635	1.560490	-0.098946
C	-2.329053	1.236640	-0.025293
C	-1.741629	2.612723	-0.051331
H	-1.085028	2.742458	-0.916626
H	-2.523908	3.370904	-0.098446
H	-1.137120	2.797959	0.841389
C	-4.466020	-1.144223	-1.275190
H	-4.509267	-2.236561	-1.259920
H	-5.489579	-0.764747	-1.335413
H	-3.925181	-0.829895	-2.170086
C	-4.540622	-1.064716	1.243603
H	-5.565242	-0.684110	1.219171
H	-4.584929	-2.155923	1.294666
H	-4.053055	-0.693613	2.147323
H	0.387800	-1.000660	0.125782
H	0.403754	0.507233	-0.801979
H	0.351688	0.562704	0.956038

26

c-1,2,3,4,5–$C_5H(CH_3)_5$

C	-0.003517	0.002477	-0.022157
C	-0.516835	1.406828	-0.007345
C	-1.786839	1.851566	-0.001807
C	-3.056859	1.057663	0.002990
H	-2.865442	-0.015246	0.007085
H	-3.664158	1.296245	0.881307
H	-3.664270	1.287444	-0.877611
C	-1.786076	3.335840	-0.002386
C	-0.515614	3.779266	-0.008274
C	-0.000847	5.183075	-0.024172
H	0.721703	5.344990	0.781785
H	0.514627	5.405036	-0.964792
H	-0.802759	5.912280	0.094151
C	0.418109	2.592563	-0.015832
C	1.373450	2.591605	-1.215592
H	2.016166	1.708391	-1.206217
H	0.799122	2.591530	-2.145823
H	2.017059	3.474176	-1.206912
H	1.012752	2.592621	0.909954
C	-3.055275	4.131058	0.001832
H	-3.663123	3.900943	-0.878379
H	-3.662619	3.894064	0.880549
H	-2.862747	5.203772	0.004713
H	0.718830	-0.159575	0.783954
H	-0.806189	-0.725808	0.096678
H	0.511767	-0.220726	-0.962587

26

c-1,2,3,5,5–$C_5H(CH_3)_5$ = *c*-2,3,4,5,5–$C_5H(CH_3)_2$

C	0.013057	-0.018170	0.000823
C	1.265923	0.800582	0.000485
C	2.534770	0.368595	0.000826
H	2.864210	-0.664333	0.001412
C	3.487519	1.535679	0.000245
C	2.538729	2.722872	-0.000466
C	1.265765	2.284247	-0.000324
C	-0.003866	3.078827	-0.000846
H	-0.610700	2.843902	-0.880442
H	-0.611043	2.844491	0.878670
H	0.186511	4.151817	-0.001163
C	3.048595	4.127171	-0.001167
H	3.670811	4.321120	0.878857
H	3.671327	4.320050	-0.881060
H	2.236748	4.854573	-0.001852
C	4.366935	1.529391	-1.260323
H	4.988065	0.630355	-1.287802
H	3.747486	1.550443	-2.159751
H	5.032046	2.397625	-1.272957
C	4.366806	1.530794	1.260907
H	3.747266	1.552824	2.160249
H	4.987952	0.631801	1.289437
H	5.031895	2.399059	1.272649
H	0.243524	-1.083994	0.001479
H	-0.599242	0.201448	0.880378
H	-0.599032	0.200410	-0.879137

26

c-1,2,4,5,5–$C_5H(CH_3)_5$ = *c*-1,3,4,5,5–$C_5H(CH_3)_2$

C	-0.018907	-0.004731	0.000698
C	-0.493026	1.411502	0.000112
C	-1.755377	1.863629	0.000077
H	-2.648650	1.248029	0.000490
C	-1.771075	3.337923	-0.000604
C	-0.500274	3.783386	-0.000988
C	0.000922	5.191531	-0.001705
H	0.620508	5.393302	0.878392
H	0.620465	5.392413	-0.882035
H	-0.817899	5.911201	-0.002052
C	0.451869	2.598914	-0.000577
C	1.329262	2.595228	-1.261589
H	1.972977	1.711546	-1.281871
H	0.708076	2.595228	-2.160480
H	1.975024	3.477178	-1.284074
C	1.329641	2.596413	1.260174
H	0.708726	2.597245	2.159252
H	1.973376	1.712761	1.281088
H	1.975396	3.478395	1.281639
C	-3.046553	4.122043	-0.000797
H	-3.648756	3.877750	-0.880697
H	-3.648777	3.878132	0.879193
H	-2.868753	5.197296	-0.001025
H	0.595674	-0.218934	0.881054
H	-0.863063	-0.695666	0.001223
H	0.595277	-0.219793	-0.879726

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c-1,2,3,4,5,5–$C_5(CH_3)_6$

C	-0.061985	-0.085772	-0.046585
C	0.535171	0.954890	-0.938099
C	0.431756	2.294008	-0.863098
C	-0.312747	3.122896	0.138243
H	-0.816123	2.507594	0.883519
H	0.365211	3.801970	0.663984
H	-1.068515	3.743136	-0.352999
C	1.199554	2.907563	-1.973050
C	1.763204	1.936365	-2.713640
C	2.625804	2.060315	-3.928141
H	3.610407	1.610349	-3.763171
H	2.179590	1.546951	-4.786282
H	2.781060	3.101932	-4.209595
C	1.397792	0.584089	-2.130136
C	0.602092	-0.253421	-3.142992
H	0.297054	-1.206317	-2.701950
H	-0.293175	0.284242	-3.464666
H	1.210560	-0.475953	-4.023784
C	2.654794	-0.177211	-1.682018
H	3.224334	0.415175	-0.961769
H	2.385006	-1.128593	-1.215487
H	3.298365	-0.398804	-2.537763
C	1.276383	4.392235	-2.157146
H	0.278547	4.821096	-2.289566
H	1.716164	4.872349	-1.277775
H	1.877060	4.665356	-3.024329
H	0.713454	-0.707413	0.413127
H	-0.649323	0.358744	0.756995
H	-0.720320	-0.758095	-0.606658

14

c-1–$C_5H_5(CF_3)$ = *c*-4–$C_5H_5(CF_3)$

C	0.000000	0.000000	0.000000
C	0.858598	-1.228604	0.000066
C	0.092258	-2.329368	0.000037
C	-1.316724	-1.920248	0.000129
C	-1.384453	-0.578739	0.000091
H	-2.283363	0.021512	0.000147
H	-2.152697	-2.605601	0.000003
H	0.452582	-3.349105	0.000047
C	2.340586	-1.183633	0.000020
F	2.821080	-0.533872	1.077527
F	2.887389	-2.405268	-0.002631
F	2.820763	-0.529270	-1.074749
H	0.185430	0.626023	0.880487
H	0.185469	0.625583	-0.880800

14

c-2–$C_5H_5(CF_3)$ = *c*-3–$C_5H_5(CF_3)$

C	0.000000	-0.000000	0.000000
C	-1.435814	-0.429976	-0.000139
C	-2.206757	0.666300	-0.000248
C	-1.373467	1.875929	-0.000156
C	-0.086132	1.499153	-0.000065
H	0.774204	2.153158	-0.000026
H	-1.759990	2.885821	-0.000110
C	-3.694529	0.692921	-0.000078
F	-4.176970	1.335104	1.077774
F	-4.177225	1.339382	-1.075240
F	-4.224843	-0.535894	-0.002463
H	-1.779380	-1.454453	-0.000119
H	0.533853	-0.381105	0.878455
H	0.534031	-0.381259	-0.878264

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c-5–$C_5H_5(CF_3)$

C	0.000000	0.000000	0.000000
C	0.856904	1.183021	-0.368600
C	2.033159	0.736379	-0.828546
C	2.033109	-0.736452	-0.828564
C	0.856873	-1.183045	-0.368521
H	0.538221	-2.208992	-0.254141
H	2.861588	-1.349791	-1.155640
H	2.861745	1.349670	-1.155428
H	0.538247	2.208987	-0.254396
H	-0.215706	0.000022	1.076328
C	-1.344138	-0.000023	-0.690847
F	-2.065780	1.079788	-0.347749
F	-1.239657	0.000333	-2.022806
F	-2.065478	-1.080188	-0.348347

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c-1,2–$C_5H_4(CF_3)_2$ = *c*-3,4–$C_5H_4(CF_3)_2$

C	-0.008065	0.000998	-0.000002
C	-1.426845	0.487318	0.000106
C	-1.424135	1.830842	0.001762
C	-2.584442	2.774402	0.002522
F	-3.762282	2.154955	0.001351
F	-2.541890	3.571855	1.080718
F	-2.541144	3.574508	-1.073675
C	-0.042722	2.323114	0.002847
C	0.785851	1.268380	0.001835
H	1.865911	1.299671	0.002247
H	0.224483	3.370688	0.004230
C	-2.587739	-0.460805	-0.001464
F	-3.366246	-0.324728	1.077529
F	-3.365498	-0.322070	-1.080658
F	-2.139105	-1.728638	-0.002870
H	0.199125	-0.623534	0.876934
H	0.199733	-0.621372	-0.878330

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c-1,3–$C_5H_4(CF_3)_2$ = *c*-2,4–$C_5H_4(CF_3)_2$

C	0.000508	0.000460	-0.000012
C	-0.395795	-1.445993	-0.000012
C	0.689829	-2.230552	-0.000012
H	0.706512	-3.311904	-0.000012
C	1.870581	-1.359871	-0.000012
C	1.496770	-0.072477	-0.000012
H	2.155181	0.784431	-0.000012
C	3.269018	-1.873976	-0.000012
F	3.509088	-2.638771	1.076419
F	3.509088	-2.638771	-1.076442
F	4.166400	-0.883555	-0.000012
C	-1.810861	-1.899321	-0.000012
F	-2.474237	-1.442316	-1.076355
F	-1.913765	-3.231364	-0.000012
F	-2.474237	-1.442316	1.076331
H	-0.381667	0.529773	-0.880502
H	-0.381667	0.529773	0.880479

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c-1,4–$C_5H_4(CF_3)_2$

C	0.014578	0.002185	-0.000214
C	0.006545	1.416680	-0.457721
C	0.004125	1.843328	-1.728938
H	0.007631	1.216023	-2.609265

C	-0.004125	3.309952	-1.728938
C	-0.006545	3.736600	-0.457721
C	-0.014578	5.151095	-0.000214
F	1.060276	5.429351	0.757043
F	-0.019007	6.011039	-1.023461
F	-1.092937	5.417426	0.756294
C	-0.000000	2.576640	0.491205
H	0.882746	2.581636	1.140938
H	-0.882746	2.571644	1.140938
H	-0.007631	3.937257	-2.609265
F	-1.060276	-0.276071	0.757043
F	0.019007	-0.857759	-1.023461
F	1.092937	-0.264146	0.756294

17

c-1,5–$C_5H_4(CF_3)_2$ = *c*-4,5–$C_5H_4(CF_3)_2$

C	-0.029794	-0.072566	0.033907
C	-0.742339	0.157712	1.341939
C	-1.042543	-1.021872	1.900605
H	-1.524680	-1.154719	2.859529
C	-0.597011	-2.104431	1.012825
C	-0.021462	-1.575652	-0.074807
H	0.399649	-2.100586	-0.920027
H	-0.720669	-3.157257	1.223083
C	-1.019112	1.497444	1.929942
F	-2.020891	2.132043	1.304724
F	-1.360997	1.401958	3.221568
F	0.057299	2.296773	1.853404
C	-0.675790	0.592103	-1.166738
F	-0.046713	0.229370	-2.295850
F	-1.961426	0.259396	-1.299162
F	-0.604921	1.924386	-1.082960
H	0.994434	0.319007	0.083375

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c-2,3–$C_5H_4(CF_3)_2$

C	-0.034145	-0.000969	0.000145
C	-0.032503	-1.175926	0.927996
C	-0.005008	-0.736949	2.193725
C	0.057901	-1.613240	3.403008
F	-0.228899	-2.884624	3.093801
F	1.277300	-1.608164	3.958009
F	-0.807233	-1.219268	4.345094
C	0.007316	0.737146	2.192759
C	-0.006412	1.174909	0.926414
H	-0.004028	2.209637	0.615161
C	-0.016645	1.614212	3.402842
F	-1.218087	1.611383	3.995374
F	0.876816	1.219005	4.317860
F	0.262672	2.884895	3.084213
H	-0.044769	-2.210956	0.618004
H	0.834415	-0.014031	-0.668614
H	-0.921559	0.011461	-0.643149

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c-2,5–$C_5H_4(CF_3)_2$ = *c*-3,5–$C_5H_4(CF_3)_2$

C	-0.034114	0.025243	0.096044
C	-1.411106	0.251131	0.659368
C	-1.519575	1.545160	0.977441
C	-2.728940	2.210786	1.540752
F	-2.462508	2.782337	2.724498
F	-3.167386	3.186935	0.729744
F	-3.737336	1.353468	1.721775
C	-0.262152	2.255606	0.693012
C	0.618903	1.379842	0.195318
H	1.637363	1.573569	-0.108264
H	-0.102863	3.310383	0.869272
H	-2.164981	-0.515228	0.766914
C	0.729657	-1.063193	0.819934
F	1.955303	-1.216061	0.298291
F	0.876896	-0.802177	2.120828
F	0.100537	-2.242898	0.715060
H	-0.100984	-0.296974	-0.951250

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c-5,5–$C_5H_4(CF_3)_2$

C	-0.059324	0.019948	0.023594
C	-1.350521	-0.766393	0.117735
C	-2.294759	0.021594	0.640725

C	-1.728042	1.352499	0.927975
C	-0.437840	1.376889	0.580313
H	0.263949	2.194384	0.659312
H	-2.283060	2.176023	1.355542
H	-3.321089	-0.261450	0.829371
H	-1.434853	-1.794922	-0.201720
C	1.026296	-0.629533	0.889733
F	2.158000	0.081712	0.888183
F	0.616067	-0.723760	2.156577
F	1.324661	-1.864243	0.473879
C	0.384194	0.147378	-1.438509
F	1.476801	0.906900	-1.564304
F	0.654405	-1.042633	-1.983848
F	-0.579869	0.711343	-2.169677

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c-1,2,3–$C_5H_3(CF_3)_3$ = *c*-2,3,4–$C_5H_3(CF_3)_3$

C	-0.120572	0.029327	-0.055847
C	-0.084606	1.188084	-0.993466
C	-0.046778	0.739602	-2.255955
C	0.003697	1.616659	-3.469234
F	1.213506	1.619653	-4.038455
F	-0.877857	1.222232	-4.394479
F	-0.284302	2.883995	-3.146620
C	-0.054607	-0.733716	-2.249014
C	-0.104022	-1.153672	-0.974017
C	-0.148489	-2.558174	-0.445737
F	1.026520	-3.182978	-0.565030
F	-0.449993	-2.536640	0.863896
F	-1.074089	-3.304038	-1.052197
C	-0.052679	-1.588928	-3.485767
F	0.407061	-2.815107	-3.235281
F	-1.283939	-1.708523	-3.990806
F	0.722879	-1.050420	-4.431431
H	-0.093320	2.225362	-0.691151
H	0.736496	0.023892	0.628333
H	-1.017955	0.034273	0.573548

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c-1,2,4–$C_5H_3(CF_3)_3$ = *c*-1,3,4–$C_5H_3(CF_3)_3$

C	0.039008	0.012257	-0.057851
C	0.047965	1.163067	-1.011953
C	-0.065127	0.733039	-2.275510
H	-0.089615	1.339430	-3.169764
C	-0.165199	-0.729433	-2.250647
C	-0.098531	-1.159699	-0.979799
C	-0.175715	-2.564399	-0.466160
F	0.438525	-2.654129	0.723465
F	-1.443985	-2.951674	-0.282549
F	0.403868	-3.439947	-1.287222
C	-0.312238	-1.556508	-3.496536
F	0.860359	-2.055945	-3.898557
F	-1.155155	-2.575609	-3.325343
F	-0.787085	-0.801224	-4.496860
C	0.172196	2.578867	-0.568994
F	1.316013	2.779664	0.104431
F	0.152545	3.427853	-1.598693
F	-0.827531	2.918684	0.260043
H	0.960904	-0.046312	0.532248
H	-0.792918	0.068448	0.654895

20

c-1,2,5–$C_5H_3(CF_3)_3$ = *c*-3,4,5–$C_5H_3(CF_3)_3$

C	-0.011661	0.024163	-0.070359
C	0.041426	1.185387	-1.024668
C	0.004107	0.732887	-2.282852
H	0.027524	1.317836	-3.190614
C	-0.067479	-0.735236	-2.257450
C	-0.079521	-1.169935	-0.988380
C	-0.198958	-2.577294	-0.487897
F	0.995269	-3.120533	-0.233083
F	-0.904184	-2.604370	0.652513
F	-0.824544	-3.365268	-1.364228
C	-0.131900	-1.561448	-3.514998
F	0.668624	-2.625511	-3.460752
F	-1.373181	-1.987052	-3.764194
F	0.252925	-0.822500	-4.565770
H	0.116201	2.212469	-0.698512
C	1.189026	0.016010	0.865100

F	1.130801	-0.995902	1.732975
F	2.339528	-0.084579	0.197338
F	1.227186	1.153686	1.572965
H	-0.901949	0.067240	0.569132

20

c-1,3,5–$C_5H_3(CF_3)_3$ = *c*-2,4,5–$C_5H_3(CF_3)_3$

C	-0.040668	0.014531	-0.085855
C	-0.021259	1.199385	-1.013750
C	-0.085272	0.756837	-2.273482
C	-0.119786	1.598913	-3.505208
F	0.903764	1.305971	-4.318333
F	-1.245588	1.385915	-4.201986
F	-0.057107	2.900935	-3.219319
C	-0.129735	-0.711229	-2.298808
C	-0.082906	-1.154642	-1.037669
C	-0.113642	-2.585506	-0.616236
F	1.082457	-3.010685	-0.191386
F	-0.980823	-2.773364	0.389570
F	-0.481546	-3.379666	-1.627363
H	-0.201203	-1.320008	-3.189982
H	0.032299	2.226723	-0.683037
C	1.136926	0.014458	0.874223
F	1.058968	-1.004717	1.732482
F	2.303684	-0.072958	0.234502
F	1.149216	1.147120	1.591082
H	-0.943733	0.031971	0.538189

20

c-1,4,5–$C_5H_3(CF_3)_3$

C	0.029628	-0.000227	-0.075235
C	-0.089404	1.168515	-1.023238
C	-0.217586	0.728555	-2.280891
H	-0.283795	1.351553	-3.161788
C	-0.220645	-0.737671	-2.277665
C	-0.094290	-1.172623	-1.018086
C	-0.031832	-2.607397	-0.606352
F	0.945055	-2.813539	0.287460
F	-1.175077	-3.027553	-0.052787
F	0.208028	-3.396109	-1.661195
H	-0.289462	-1.364257	-3.155813
C	-0.020955	2.604814	-0.617820
F	0.956791	2.810808	0.275084
F	0.222184	3.387868	-1.676123
F	-1.162432	3.032169	-0.066120
H	1.014644	-0.001217	0.409325
C	-0.995632	0.004388	1.049988
F	-2.244930	0.005969	0.583688
F	-0.846086	-1.071154	1.828132
F	-0.841592	1.082711	1.823392

20

c-1,5,5–$C_5H_3(CF_3)_3$ = *c*-4,5,5–$C_5H_3(CF_3)_3$

C	-0.003524	0.012506	0.014313
C	-0.567293	-0.006501	1.424919
C	0.431718	0.047462	2.308429
H	0.331297	0.055523	3.384231
C	1.712722	0.094072	1.591000
C	1.495044	0.069994	0.271374
C	2.583482	0.059181	-0.753904
F	2.696554	-1.132104	-1.356180
F	2.388155	0.970411	-1.712122
F	3.765593	0.322668	-0.180860
H	2.688352	0.138563	2.055102
H	-1.629973	-0.045671	1.614470
C	-0.417711	-1.271802	-0.722674
F	0.057471	-1.320030	-1.964244
F	0.035644	-2.342370	-0.069053
F	-1.749245	-1.371035	-0.792185
C	-0.541848	1.267743	-0.704893
F	-0.025149	2.366694	-0.153321
F	-0.261087	1.286991	-2.003324
F	-1.872556	1.342832	-0.583409

20

c-2,3,5–$C_5H_3(CF_3)_3$

C	-0.066028	0.054318	-0.055124
C	-1.566210	0.108452	-0.130208
C	-1.950035	1.389051	-0.122959

C	-3.373596	1.853659	-0.104841
F	-3.723627	2.307799	1.104379
F	-3.576247	2.843387	-0.979269
F	-4.207209	0.854595	-0.412588
C	-0.756332	2.258688	-0.082317
C	0.344243	1.500302	-0.055966
H	1.367519	1.846589	-0.034968
C	-0.760772	3.756045	-0.116042
F	0.448519	4.244186	0.181234
F	-1.093236	4.218510	-1.325283
F	-1.633877	4.261087	0.761871
H	-2.209477	-0.758987	-0.165398
H	0.250209	-0.434178	0.875865
C	0.561407	-0.741796	-1.182898
F	1.896190	-0.743392	-1.078049
F	0.150717	-2.015624	-1.150449
F	0.249892	-0.246092	-2.381466

20

c-2,5,5–$C_5H_3(CF_3)_3$ = *c*-3,5,5–$C_5H_3(CF_3)_3$

C	0.064689	-0.015447	0.027837
C	1.331342	-0.048469	-0.799389
C	2.369154	0.009337	0.036458
C	3.809790	0.002939	-0.356172
F	3.966890	-0.068964	-1.679090
F	4.428226	1.112404	0.071398
F	4.451347	-1.038708	0.191065
C	1.910803	0.083122	1.435426
C	0.575720	0.070095	1.451821
H	-0.081762	0.111247	2.308027
H	2.568722	0.137889	2.291623
H	1.348013	-0.108749	-1.878153
C	-0.763568	1.229760	-0.321156
F	-1.161740	1.218645	-1.595012
F	-1.850075	1.330085	0.447039
F	-0.035510	2.332278	-0.136701
C	-0.736975	-1.308961	-0.178105
F	-1.134979	-1.448731	-1.444351
F	0.014245	-2.368392	0.126839
F	-1.821283	-1.345716	0.598828

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c-1,2,3,4–$C_5H_2(CF_3)_4$

C	-0.000396	0.000767	0.000636
C	-0.895909	-1.208854	-0.069437
C	-0.511395	-2.494817	-0.125671
C	0.877757	-3.071688	-0.156721
F	0.810917	-4.372754	-0.481654
F	1.655152	-2.475523	-1.060073
F	1.481190	-2.993945	1.030908
C	-1.711349	-3.380950	-0.150756
C	-2.844931	-2.411805	-0.111958
C	-2.369524	-1.155786	-0.081500
C	-3.175484	0.117043	-0.069428
F	-4.410190	-0.089947	-0.526287
F	-3.272940	0.622695	1.160786
F	-2.604789	1.037846	-0.851378
C	-4.271602	-2.889323	-0.116467
F	-4.866283	-2.686471	-1.293580
F	-4.297666	-4.211324	0.117035
F	-5.006094	-2.304158	0.829029
H	-1.739861	-4.008414	-1.049918
H	-1.730078	-4.069051	0.703179
F	0.140407	0.573938	-1.195349
F	-0.507709	0.909644	0.838132
F	1.213395	-0.323370	0.445192

23

c-1,2,3,5–$C_5H_2(CF_3)_4$ = *c*-2,3,4,5–$C_5H_2(CF_3)_4$

C	-0.000151	0.000134	0.000147
C	-0.899618	-1.010237	-0.669961
C	-2.119017	-0.781314	-1.179492
C	-2.855019	0.525715	-1.295116
F	-3.583385	0.788514	-0.209505
F	-2.024263	1.548885	-1.496284
F	-3.689203	0.481220	-2.343882
C	-2.674116	-2.066657	-1.735628
C	-1.562087	-3.046376	-1.506627
C	-0.549944	-2.429933	-0.889416

C	0.740004	-3.103381	-0.519007
F	0.819740	-4.303309	-1.105759
F	1.792170	-2.383452	-0.921151
F	0.849755	-3.296081	0.796138
H	-1.606593	-4.088409	-1.788794
C	-3.949322	-2.528779	-1.034056
F	-4.950683	-1.669801	-1.216950
F	-4.331920	-3.714885	-1.522131
F	-3.763097	-2.667719	0.279019
H	-2.919711	-1.966981	-2.799201
F	-0.705547	0.918337	0.659094
F	0.797710	-0.602499	0.884101
F	0.772303	0.624745	-0.889929

23

c-1,2,4,5–$C_5H_2(CF_3)_4$ = *c*-1,3,4,5–$C_5H_2(CF_3)_4$

C	-0.000152	0.000540	-0.002743
C	1.451425	0.352687	-0.082616
C	2.437832	-0.508155	-0.351983
C	3.713176	0.217936	-0.332379
C	3.495095	1.507375	-0.035966
C	4.516333	2.591801	0.162763
F	5.685550	2.090252	0.562722
F	4.729680	3.286196	-0.955931
F	4.101591	3.448288	1.104562
C	2.013600	1.731545	0.146354
C	1.443786	2.775719	-0.812752
F	0.137073	2.938303	-0.598997
F	2.034587	3.958194	-0.635763
F	1.616131	2.415278	-2.084571
H	1.796997	2.088877	1.160764
C	5.030795	-0.466775	-0.591853
F	5.824315	0.257613	-1.377904
F	5.684222	-0.722805	0.542831
F	4.815301	-1.639456	-1.203108
H	2.336340	-1.567491	-0.540881
F	-0.668434	0.368982	-1.100125
F	-0.160801	-1.319249	0.136948
F	-0.582148	0.599639	1.043815

23

c-1,2,5,5–$C_5H_2(CF_3)_4$ = *c*-3,4,5,5–$C_5H_2(CF_3)_4$

C	-0.007684	-0.002877	0.016266
C	-1.342635	-0.060364	-0.685401
C	-2.216662	0.938633	-0.867387
C	-2.060602	2.359909	-0.399804
F	-2.530780	2.521897	0.840646
F	-0.776827	2.724164	-0.398907
F	-2.719128	3.203534	-1.196419
C	-3.436026	0.383667	-1.591486
C	-3.064183	-1.072404	-1.791894
C	-1.861199	-1.307174	-1.268043
H	-1.331378	-2.248103	-1.246688
H	-3.721465	-1.769585	-2.289833
C	-4.690866	0.477149	-0.702879
F	-4.967187	1.732256	-0.361771
F	-5.751565	-0.025272	-1.338823
F	-4.514294	-0.219406	0.419648
C	-3.694803	1.024874	-2.976979
F	-2.534896	1.264954	-3.588371
F	-4.395174	0.186014	-3.748377
F	-4.379028	2.160155	-2.913502
F	-0.069326	0.682155	1.156452
F	0.396651	-1.245625	0.314754
F	0.930676	0.546209	-0.755263

23

c-1,3,5,5–$C_5H_2(CF_3)_4$ = *c*-2,4,5,5–$C_5H_2(CF_3)_4$

C	0.000533	-0.000337	-0.009398
C	-1.125974	-0.979633	-0.137546
C	-2.414438	-0.626964	-0.167411
C	-3.235839	-1.833171	-0.332570
C	-2.462593	-2.915586	-0.404210
H	-2.768186	-3.945276	-0.522415
C	-1.010879	-2.491886	-0.278424
C	-0.252558	-2.907130	-1.553884
F	1.034447	-2.583606	-1.504866
F	-0.337988	-4.226633	-1.742013
F	-0.790519	-2.307211	-2.615791

C	-0.417176	-3.172266	0.975933
F	-0.991443	-2.676977	2.072083
F	-0.657800	-4.486793	0.949219
F	0.894776	-3.005803	1.081782
C	-4.728071	-1.807661	-0.405411
F	-5.141595	-1.052315	-1.430532
F	-5.236260	-3.029942	-0.561369
F	-5.249830	-1.280662	0.709269
H	-2.796782	0.381382	-0.085051
F	0.723281	0.078278	-1.131915
F	-0.478043	1.223300	0.242651
F	0.834461	-0.322148	0.982930

23

c-1,4,5,5–$C_5H_2(CF_3)_4$

C	0.050990	-0.011413	0.035915
C	-1.058446	-1.000846	-0.192583
C	-2.335017	-0.621733	-0.302182
C	-3.187243	-1.800470	-0.451363
C	-2.433817	-2.903980	-0.444619
C	-3.023479	-4.274114	-0.636964
F	-2.984458	-4.662895	-1.916487
F	-2.411838	-5.206188	0.091078
F	-4.315508	-4.260344	-0.278237
C	-0.962076	-2.524798	-0.275251
C	-0.146736	-3.002962	-1.500335
F	1.160808	-2.847091	-1.330180
F	-0.368848	-4.296412	-1.732280
F	-0.514987	-2.321818	-2.585276
C	-0.347413	-3.089335	1.027535
F	-1.184125	-2.894802	2.046648
F	-0.083941	-4.387860	0.941951
F	0.796517	-2.466676	1.310412
H	-4.263289	-1.782502	-0.552189
H	-2.684361	0.400964	-0.281488
F	1.180455	-0.348570	-0.583089
F	-0.320718	1.192794	-0.422179
F	0.326491	0.140745	1.336427

23

c-2,3,5,5–$C_5H_2(CF_3)_4$

C	-0.016989	0.064302	0.024837
C	0.388423	1.415067	-0.519217
C	-0.152202	2.363847	0.246729
C	-0.020931	3.837275	-0.000717
F	-1.157225	4.350434	-0.480106
F	0.276682	4.491224	1.124980
F	0.942515	4.085435	-0.891934
C	-0.931224	1.736834	1.337178
C	-0.870408	0.409208	1.223851
H	-1.333565	-0.326698	1.865739
C	-1.644734	2.467131	2.435823
F	-2.456191	1.643702	3.104840
F	-0.780757	2.984670	3.313323
F	-2.380218	3.470484	1.950266
H	1.010063	1.551128	-1.392797
C	-0.846034	-0.701534	-1.019841
F	-1.282374	-1.865842	-0.540378
F	-1.911571	0.019271	-1.370685
F	-0.139140	-0.945662	-2.122943
C	1.223997	-0.729025	0.467281
F	1.913787	-0.027659	1.367445
F	0.888586	-1.890926	1.027298
F	2.034791	-0.981996	-0.559613

26

c-1,2,3,4,5–$C_5H(CF_3)_5$

C	-0.062669	-0.059292	0.350926
C	-0.752691	-1.321578	-0.112106
C	-0.214642	-2.529574	-0.321059
C	-1.224892	-3.402945	-0.959729
C	-2.363354	-2.714150	-1.112082
C	-3.663270	-3.166015	-1.733014
F	-3.540392	-3.353915	-3.048047
F	-4.118445	-4.289981	-1.187103
F	-4.593060	-2.219041	-1.556596
C	-2.191265	-1.319960	-0.560701
H	-2.348551	-0.564345	-1.339261
C	-3.178747	-0.996461	0.590714

F	-3.691528	-2.115166	1.110595
F	-2.568441	-0.343767	1.582313
F	-4.182413	-0.234185	0.169773
C	-0.959269	-4.831152	-1.369319
F	-1.861827	-5.264941	-2.244527
F	0.243074	-4.930091	-1.942590
F	-0.986333	-5.642818	-0.313355
C	1.202042	-2.947706	-0.006504
F	1.734231	-2.166847	0.930984
F	1.223894	-4.200953	0.451072
F	1.976509	-2.885402	-1.088888
F	-0.822553	1.000586	0.038516
F	0.159229	-0.034274	1.659760
F	1.107081	0.099159	-0.273546

26

c-1,2,3,5,5–$C_5H(CF_3)_5$ = *c*-2,3,4,5,5–$C_5H(CF_3)_2$

C	-0.092753	0.072531	0.065209
C	-0.410507	-0.644791	1.369351
C	-1.498348	-1.406987	1.194360
C	-2.134544	-2.319611	2.219061
F	-3.036618	-1.664061	2.947472
F	-2.753100	-3.332627	1.609596
F	-1.226295	-2.841007	3.039911
C	-2.013515	-1.217110	-0.178990
C	-1.223947	-0.368856	-0.835092
H	-1.334979	-0.027334	-1.853862
C	-3.242538	-1.843362	-0.777723
F	-3.065105	-3.136526	-1.047519
F	-4.287367	-1.727381	0.045288
F	-3.554533	-1.233705	-1.925559
C	0.388859	-0.498951	2.642193
F	-0.411844	-0.470264	3.708023
F	1.255098	-1.500635	2.798123
F	1.080907	0.641518	2.632077
C	-0.099811	1.621060	0.158980
F	-0.407132	2.148603	-1.030008
F	-1.027127	2.013533	1.031276
F	1.068989	2.129443	0.522620
C	1.242124	-0.433591	-0.524606
F	1.161705	-1.737298	-0.786923
F	1.512959	0.204231	-1.663860
F	2.255886	-0.249134	0.312584

26

c-1,2,4,5,5–$C_5H(CF_3)_5$ = *c*-1,3,4,5,5–$C_5H(CF_3)_2$

C	0.191528	-0.214491	0.174275
C	1.200350	0.557500	-0.634934
C	1.760876	1.679141	-0.180361
H	1.550726	2.158942	0.765088
C	2.706435	2.187189	-1.176547
C	2.732937	1.378752	-2.243224
C	3.613270	1.585070	-3.455770
F	3.064756	2.436107	-4.323252
F	4.791749	2.090054	-3.080167
F	3.852896	0.442002	-4.092669
C	1.730717	0.240792	-2.031168
C	0.611915	0.332494	-3.104478
F	-0.134847	-0.763495	-3.134146
F	-0.175057	1.377682	-2.855357
F	1.140035	0.497776	-4.315818
C	2.380284	-1.165951	-2.068399
F	3.557141	-1.136295	-1.444377
F	1.601197	-2.046295	-1.442618
F	2.565071	-1.608924	-3.304985
C	3.491295	3.456163	-0.942017
F	3.576091	4.204894	-2.037455
F	2.880958	4.185457	0.001711
F	4.723710	3.193224	-0.509967
F	-0.749979	-0.771281	-0.584146
F	0.764671	-1.180284	0.898120
F	-0.412805	0.610695	1.038980

29

c-1,2,3,4,5,5–$C_5(CF_3)_6$

C	0.039312	0.002214	-0.019199
C	-1.061197	0.809229	0.653347
C	-1.069125	2.131346	0.857808
C	-2.236961	2.494564	1.697950

C	-2.969817	1.401626	1.939189
C	-4.326877	1.353241	2.625199
F	-4.228856	1.625251	3.924410
F	-5.167524	2.225184	2.069437
F	-4.883942	0.149716	2.496015
C	-2.292204	0.183949	1.310153
C	-1.869018	-0.836390	2.418143
F	-1.768246	-2.073460	1.956951
F	-0.684602	-0.472220	2.916066
F	-2.737558	-0.845878	3.424764
C	-3.216130	-0.464452	0.226858
F	-4.007223	0.478306	-0.291566
F	-2.504261	-0.979275	-0.771199
F	-3.978644	-1.427459	0.721027
C	-2.429971	3.883433	2.272815
F	-1.474309	4.114573	3.176576
F	-2.340133	4.812507	1.323239
F	-3.599222	4.026829	2.880672
C	-0.147843	3.167969	0.246611
F	-0.825845	3.863177	-0.670177
F	0.297526	4.018023	1.169736
F	0.901372	2.626891	-0.356303
F	-0.157573	-1.304998	0.148140
F	0.097063	0.246678	-1.326229
F	1.225554	0.282262	0.519519

11

c-1–C_5H_5F = *c*-4–C_5H_5F

C	0.000357	0.000158	-0.000133
H	1.095421	0.014289	0.020898
H	-0.339979	1.041071	0.021049
C	-0.546302	-0.763781	-1.175147
H	-0.356926	-0.499078	-2.204938
C	-1.283219	-1.794750	-0.730169
H	-1.800202	-2.517964	-1.346094
C	-1.296816	-1.813522	0.741306
C	-0.556313	-0.778054	1.145323
F	-0.297908	-0.416377	2.403595
H	-1.806653	-2.526499	1.371512

11

c-2–C_5H_5F = *c*-3–C_5H_5F

C	0.000980	0.001403	-0.000248
H	1.096649	0.021371	-0.014363
H	-0.333993	1.044784	-0.014505
C	-0.543959	-0.760289	-1.178013
H	-0.352775	-0.493221	-2.207546
C	-1.281760	-1.792361	-0.743904
H	-1.809548	-2.530779	-1.330616
C	-1.259359	-1.760643	0.717326
C	-0.532307	-0.743951	1.188995
H	-0.354899	-0.496275	2.223786
F	-1.913258	-2.675426	1.437336

11

c-5–C_5H_5F

C	0.001413	0.000824	-0.000008
H	1.094225	-0.117672	0.000098
C	-0.573442	-0.731399	-1.186286
H	-0.399404	-0.431868	-2.209531
C	-1.237778	-1.802831	-0.742909
H	-1.712263	-2.560416	-1.351841
C	-1.237951	-1.803426	0.741144
C	-0.573794	-0.732310	1.185547
H	-0.400064	-0.433572	2.209075
H	-1.712599	-2.561494	1.349352
F	-0.259224	1.358970	0.000469

11

c-1,2–$C_5H_4F_2$ = *c*-3,4–$C_5H_4F_2$

C	-0.000612	0.000324	-0.000004
C	0.548599	-1.385465	0.000064
C	1.883006	-1.343444	0.000045
C	2.330489	0.048655	-0.000066
C	1.249204	0.842152	-0.000063
H	1.240745	1.921795	-0.000118
H	3.369967	0.344650	-0.000112
F	2.719909	-2.377557	0.000091
F	-0.228943	-2.465049	0.000139

H	-0.620056	0.188160	-0.883416
H	-0.620016	0.188251	0.883418

11

c-1,3–$C_5H_4F_2$ = *c*-2,4–$C_5H_4F_2$

C	-0.000920	0.000529	0.000012
C	0.472578	-1.417118	-0.000628
C	1.803598	-1.513486	-0.001082
C	2.282118	-0.128788	-0.000473
C	1.293701	0.769482	-0.000005
H	1.386976	1.843394	0.000366
F	3.588906	0.130519	-0.000661
H	2.415908	-2.401504	-0.001636
F	-0.401939	-2.418809	-0.000806
H	-0.613753	0.204590	0.884036
H	-0.614172	0.205267	-0.883567

11

c-1,4–$C_5H_4F_2$

C	-0.000086	0.000038	0.000002
C	0.582070	-1.378834	0.000074
C	1.915733	-1.366005	0.000037
C	2.352383	0.046045	-0.000042
C	1.258791	0.809516	-0.000077
F	1.202560	2.141895	-0.000161
H	3.375717	0.389469	-0.000079
H	2.566545	-2.227152	0.000072
F	-0.216599	-2.446829	0.000160
H	-0.612689	0.189436	-0.886689
H	-0.612643	0.189543	0.886704

11

c-1,5–$C_5H_4F_2$ = *c*-4,5–$C_5H_4F_2$

C	0.000000	0.000000	0.000000
C	0.570839	-1.395154	0.032615
C	1.898377	-1.380712	-0.033581
C	2.313374	0.045379	-0.031675
C	1.246392	0.848109	0.035673
H	1.226713	1.927152	0.061734
H	3.345882	0.363173	-0.080924
H	2.554570	-2.236639	-0.077952
F	-0.241063	-2.443263	0.064318
H	-0.542155	0.149818	-0.942534
F	-0.882691	0.240093	1.030215

11

c-2,3–$C_5H_4F_2$

C	-0.002164	0.000628	0.000002
C	0.521760	-1.410152	0.000077
C	1.853008	-1.338903	0.000022
C	2.285321	0.059064	-0.000029
C	1.226690	0.869354	-0.000080
H	1.233347	1.947997	-0.000146
F	3.573547	0.378550	-0.000063
F	2.735923	-2.329861	0.000052
H	-0.081793	-2.304142	0.000144
H	-0.623827	0.192853	-0.880917
H	-0.623783	0.192958	0.880930

11

c-2,5–$C_5H_4F_2$ = *c*-3,5–$C_5H_4F_2$

C	-0.001751	0.000276	0.000718
C	0.540906	-1.412009	-0.036330
C	1.872003	-1.365801	0.036119
C	2.268386	0.056041	0.028191
C	1.222794	0.875652	-0.043607
H	1.216187	1.953481	-0.065907
F	3.551492	0.396669	0.090650
H	2.571824	-2.187937	0.086143
H	-0.094019	-2.285118	-0.073127
F	-0.900044	0.253691	-1.018482
H	-0.536161	0.155166	0.947163

11

c-5,5–$C_5H_4F_2$

C	0.000550	-0.000192	0.000001
C	0.535529	-1.418245	0.000064
C	1.864335	-1.359960	0.000045
C	2.306546	0.070083	-0.000006

C	1.242618	0.868318	-0.000057
H	1.197653	1.947095	-0.000123
H	3.341780	0.381853	-0.000026
H	2.542705	-2.201823	0.000077
H	-0.110703	-2.283196	0.000112
F	-0.784499	0.242603	1.086845
F	-0.784525	0.242493	-1.086848

11

c-1,2,3–$C_5H_3F_3$ = *c*-2,3,4–$C_5H_3F_3$

C	-0.001571	0.000758	0.000002
C	0.547992	-1.387258	0.000069
C	1.880767	-1.354690	0.000032
C	2.291770	0.051875	-0.000038
C	1.235200	0.864626	-0.000078
H	1.240687	1.942523	-0.000145
F	3.577487	0.372659	-0.000079
F	2.740397	-2.360142	0.000066
F	-0.233972	-2.459055	0.000148
H	-0.621242	0.175037	0.885244
H	-0.621286	0.174936	-0.885228

11

c-1,2,4–$C_5H_3F_3$ = *c*-1,3,4–$C_5H_3F_3$

C	-0.000514	0.000167	-0.000001
C	0.583370	-1.378934	0.000072
C	1.916296	-1.372607	0.000042
C	2.316829	0.041126	-0.000042
C	1.243306	0.832090	-0.000074
F	1.205178	2.161591	-0.000158
F	3.590844	0.414345	-0.000087
H	2.591439	-2.214179	0.000082
F	-0.215112	-2.442257	0.000157
H	-0.616440	0.175790	0.887340
H	-0.616489	0.175693	-0.887325

11

c-1,2,5–$C_5H_3F_3$ = *c*-3,4,5–$C_5H_3F_3$

C	-0.000632	0.000373	0.001344
C	0.543807	-1.400235	-0.039308
C	1.870954	-1.351427	0.022354
C	2.322014	0.054323	0.027871
C	1.251751	0.849241	-0.029783
H	1.225880	1.927860	-0.063049
H	3.363405	0.340855	0.070913
F	2.716204	-2.370136	0.078864
F	-0.247420	-2.461478	-0.054182
H	-0.546291	0.159565	0.939657
F	-0.867103	0.267645	-1.034724

11

c-1,3,5–$C_5H_3F_3$ = *c*-2,4,5–$C_5H_3F_3$

C	-0.000634	-0.000035	-0.001876
C	0.573011	-1.399015	0.025500
C	1.900140	-1.390590	-0.023746
C	2.274458	0.039391	-0.015908
C	1.231927	0.865157	0.035598
H	1.231102	1.942661	0.048012
F	3.555031	0.379636	-0.069100
H	2.584531	-2.223656	-0.059634
F	-0.239877	-2.440317	0.057332
H	-0.562842	0.147742	-0.931575
F	-0.868827	0.213077	1.045962

11

c-1,4,5–$C_5H_3F_3$

C	0.001132	-0.000367	-0.002342
C	0.582161	-1.391960	0.025667
C	1.909355	-1.370513	-0.024027
C	2.349672	0.053382	-0.023998
C	1.266287	0.820287	0.025670
F	1.192754	2.144535	0.048603
H	3.375011	0.388436	-0.063950
H	2.566502	-2.225952	-0.063599
F	-0.226143	-2.443486	0.048941
F	-0.841878	0.260427	1.049049
H	-0.552035	0.170699	-0.933251

11

c-1,5,5–$C_5H_3F_3$ = *c*-4,5,5–$C_5H_3F_3$

C	0.002124	-0.001040	0.000002
C	0.567933	-1.413352	0.000067
C	1.891839	-1.390879	0.000025
C	2.306726	0.045875	-0.000051
C	1.248071	0.854131	-0.000083
H	1.213979	1.932714	-0.000149
H	3.341824	0.357798	-0.000091
H	2.555895	-2.241456	0.000053
F	-0.257503	-2.442937	0.000149
F	-0.782373	0.211525	-1.086334
F	-0.782312	0.211647	1.086359

11

c-2,3,5–$C_5H_3F_3$

C	-0.002425	0.000706	-0.000757
C	0.514820	-1.418635	0.038375
C	1.838689	-1.342449	-0.019163
C	2.275527	0.070102	-0.019172
C	1.225747	0.880314	0.038040
H	1.209243	1.958039	0.063997
F	3.560441	0.373749	-0.073719
F	2.727757	-2.318519	-0.074026
H	-0.107294	-2.298816	0.064334
F	-0.876677	0.271342	1.033600
H	-0.547635	0.169108	-0.937102

11

c-2,5,5–$C_5H_3F_3$ = *c*-3,5,5–$C_5H_3F_3$

C	-0.000017	0.000163	0.000001
C	0.510375	-1.420565	0.000062
C	1.832980	-1.328678	0.000014
C	2.313280	0.079661	-0.000052
C	1.247545	0.872009	-0.000089
H	1.197713	1.950670	-0.000152
H	3.357605	0.357089	-0.000083
F	2.706256	-2.323704	0.000051
H	-0.119131	-2.295129	0.000130
F	-0.778044	0.261005	-1.085824
F	-0.777978	0.261126	1.085846

11

c-1,2,3,4–$C_5H_2F_4$

C	-0.001274	0.000385	0.000002
C	0.555159	-1.390214	0.000072
C	1.886351	-1.353601	0.000040
C	2.321118	0.052365	-0.000047
C	1.242999	0.834066	-0.000074
F	1.196541	2.159879	-0.000155
F	3.597880	0.391029	-0.000091
F	2.748972	-2.353931	0.000082
F	-0.231703	-2.458319	0.000154
H	-0.610157	0.188627	-0.889312
H	-0.610117	0.188730	0.889321

11

c-1,2,3,5–$C_5H_2F_4$ = *c*-2,3,4,5–$C_5H_2F_4$

C	-0.001365	0.000497	-0.001705
C	0.543184	-1.404870	0.030462
C	1.869243	-1.365777	-0.012691
C	2.282035	0.055387	-0.012346
C	1.234669	0.870286	0.029029
H	1.222243	1.947710	0.048772
F	3.564839	0.360028	-0.059279
F	2.739118	-2.354826	-0.058389
F	-0.254818	-2.456150	0.047658
H	-0.566619	0.157576	-0.927344
F	-0.853573	0.238925	1.052364

11

c-1,2,4,5–$C_5H_2F_4$ = *c*-1,3,4,5–$C_5H_2F_4$

C	0.000500	-0.000364	0.002450
C	0.584288	-1.395649	-0.017201
C	1.910747	-1.381425	0.017594
C	2.311538	0.045776	0.011250
C	1.247503	0.840573	-0.032584
F	1.194954	2.163897	-0.035134
F	3.583134	0.404029	0.061851
H	2.594659	-2.215539	0.047683

F	-0.226448	-2.439276	-0.045729
F	-0.839591	0.227062	-1.058731
H	-0.564636	0.169973	0.925757

11

c-1,2,5,5–$C_5H_2F_4$ = *c*-3,4,5,5–$C_5H_2F_4$

C	0.001580	-0.000499	0.000001
C	0.551142	-1.415563	0.000076
C	1.879174	-1.353801	0.000031
C	2.305353	0.070305	-0.000053
C	1.244798	0.864518	-0.000077
F	1.168864	2.180419	-0.000155
F	3.579836	0.418055	-0.000104
H	2.582432	-2.174508	0.000059
H	-0.091107	-2.282920	0.000146
F	-0.771761	0.246615	1.085619
F	-0.771809	0.246486	-1.085612

11

c-1,3,5,5–$C_5H_2F_4$ = *c*-2,4,5,5–$C_5H_2F_4$

C	0.001789	-0.000166	0.000001
C	0.524638	-1.412471	0.000068
C	1.848360	-1.311141	0.000020
C	2.352955	0.087797	-0.000057
C	1.270579	0.849538	-0.000086
F	1.167693	2.160243	-0.000161
H	3.391220	0.380054	-0.000092
F	2.718508	-2.305540	0.000063
H	-0.096939	-2.292315	0.000140
F	-0.760037	0.282471	1.085123
F	-0.760099	0.282343	-1.085109

11

c-1,4,5,5–$C_5H_2F_4$

C	0.003592	-0.001133	0.000002
C	0.580198	-1.405718	0.000071
C	1.903828	-1.373066	0.000032
C	2.346594	0.058638	-0.000057
C	1.272482	0.832788	-0.000081
F	1.182836	2.150342	-0.000160
H	3.375321	0.385030	-0.000102
H	2.568632	-2.223270	0.000065
F	-0.237578	-2.442670	0.000156
F	-0.764240	0.236432	1.086124
F	-0.764298	0.236304	-1.086106

11

c-2,3,5,5–$C_5H_2F_4$

C	-0.000899	0.000270	0.000001
C	0.509348	-1.427277	0.000069
C	1.829831	-1.345942	0.000024
C	2.270183	0.077966	-0.000050
C	1.226114	0.890538	-0.000079
H	1.190503	1.967819	-0.000141
F	3.554118	0.370738	-0.000094
F	2.724267	-2.312450	0.000053
H	-0.128333	-2.296258	0.000135
F	-0.783201	0.242230	1.085336
F	-0.783255	0.242109	-1.085321

11

c-1,2,3,4,5–C_5HF_5

C	-0.000064	0.000019	0.000061
C	0.554006	-1.403243	0.024770
C	1.879455	-1.358599	-0.003995
C	2.318300	0.060467	-0.004059
C	1.249428	0.845544	0.024468
F	1.183629	2.164475	0.034215
F	3.593948	0.381060	-0.044717
F	2.751310	-2.343439	-0.044968
F	-0.244872	-2.454785	0.034580
F	-0.819667	0.253752	1.070633
H	-0.573284	0.177100	-0.916614

11

c-1,2,3,5,5–C_5HF_5 = *c*-2,3,4,5,5–C_5HF_2

C	0.000843	-0.000505	0.000001
C	0.538236	-1.422788	0.000064
C	1.860845	-1.375355	0.000034

C	2.273803	0.056226	-0.000063
C	1.233830	0.876042	-0.000076
H	1.206501	1.953294	-0.000133
F	3.555515	0.350612	-0.000110
F	2.739835	-2.352808	0.000071
F	-0.273832	-2.456018	0.000143
F	-0.781186	0.215271	1.084718
F	-0.781238	0.215156	-1.084701

11

c-1,2,4,5,5–C_5HF_5 = *c*-1,3,4,5,5–C_5HF_2

C	0.002981	-0.000796	0.000001
C	0.552136	-1.409925	0.000066
C	1.875994	-1.344059	0.000028
C	2.353818	0.067446	-0.000060
C	1.277031	0.836147	-0.000084
F	1.182124	2.148595	-0.000161
H	3.392303	0.360533	-0.000102
F	2.732190	-2.346733	0.000068
F	-0.248531	-2.458306	0.000153
F	-0.759278	0.254287	1.085134
F	-0.759338	0.254164	-1.085118

11

c-1,2,3,4,5,5–C_5F_6

C	-0.001362	-0.002050	0.000000
C	-0.549287	-0.768482	-1.190497
C	-1.274806	-1.782573	-0.746876
C	-1.274834	-1.782541	0.746905
C	-0.549328	-0.768433	1.190510
F	-0.278669	-0.389879	2.420699
F	-1.931120	-2.700013	1.418268
F	-1.931068	-2.700073	-1.418223
F	-0.278588	-0.389977	-2.420692
F	-0.416576	1.281978	-0.000033
F	1.347965	0.020772	0.000023

17

c-C_5H_3-5a-CH_3-3-F-2-CF_3

C	-0.065142	0.108123	0.021907
C	-0.044357	0.523913	1.468498
H	0.602010	0.109679	2.227487
C	-0.951060	1.488791	1.628972
F	-1.257374	2.140765	2.745800
C	-1.629193	1.791074	0.363544
C	-2.690925	2.823578	0.199628
F	-2.247153	4.044081	0.531336
F	-3.124178	2.883809	-1.065744
F	-3.752506	2.567884	0.976667
C	-1.122660	0.992670	-0.582485
H	-1.407063	0.978107	-1.625830
C	1.293218	0.247672	-0.679219
H	1.638541	1.281787	-0.625913
H	2.036650	-0.390700	-0.199618
H	1.217626	-0.041828	-1.728838
H	-0.402052	-0.934743	-0.055482

17

c-C_5H_3-4-CH_3-3-F-5b-CF_3

C	-0.016473	-0.036610	-0.022113
C	0.263910	-1.280373	-0.797228
C	0.060530	-2.695640	-0.306235
C	0.454888	-3.568444	-1.475944
H	0.402060	-4.646896	-1.456044
C	0.869990	-2.786839	-2.477995
C	0.742945	-1.396143	-2.039636
F	1.088340	-0.384057	-2.837371
H	1.237409	-3.089462	-3.448237
H	0.707997	-2.902327	0.555513
C	-1.352124	-2.967195	0.160417
F	-1.658509	-2.230777	1.241805
F	-2.263696	-2.691369	-0.776745
F	-1.509217	-4.254830	0.506811
H	0.468066	-0.064069	0.956826
H	0.349341	0.833068	-0.567945
H	-1.088939	0.088390	0.148426

14

c-C_5H_4-2-CH_3-4-F

C	0.016291	0.029983	-0.288282
C	0.031024	-0.672275	-1.605395
F	-0.836234	-1.653602	-1.862923
C	0.975795	-0.199738	-2.420252
C	1.678376	0.877882	-1.691492
C	2.811490	1.652404	-2.284259
H	3.186334	2.395524	-1.579776
H	3.635259	0.986903	-2.556312
H	2.495082	2.167601	-3.195223
C	1.136334	1.017839	-0.469156
H	1.444319	1.725127	0.288316
H	1.192661	-0.534771	-3.424472
H	-0.950905	0.510595	-0.106400
H	0.195607	-0.669576	0.535232

17

c-C_5H_3-1-CH_3-2-F-4-CF_3

C	-0.062053	-0.056612	0.186168
C	1.415276	-0.106448	0.063416
C	2.306526	1.066401	0.362890
C	3.689109	0.535122	0.094788
C	4.949863	1.316936	0.245043
H	4.946921	2.193478	-0.408221
H	5.069712	1.672863	1.271677
H	5.813771	0.702639	-0.008528
C	3.544322	-0.738846	-0.291359
C	2.147720	-1.159848	-0.319303
H	1.793728	-2.141900	-0.599952
F	4.529870	-1.576704	-0.625027
H	2.067416	1.921902	-0.279127
H	2.192310	1.398252	1.401167
F	-0.595607	0.887808	-0.610734
F	-0.636092	-1.221104	-0.135514
F	-0.447551	0.248549	1.439048

17

c-C_5H_3-3-CH_3-5b-F-4-CF_3

C	0.149760	-0.089055	-0.180037
C	-0.948167	-1.084091	-0.056573
C	-1.970443	-1.249800	-1.154962
C	-2.820906	-2.389448	-0.657732
H	-3.638851	-2.805314	-1.228184
C	-2.419513	-2.723360	0.569410
C	-1.232413	-1.912408	0.959520
C	-0.568857	-2.093318	2.284449
H	0.369022	-1.550384	2.361761
H	-1.236072	-1.754796	3.082187
H	-0.381152	-3.157205	2.450905
H	-2.861824	-3.470338	1.216229
H	-2.573260	-0.337058	-1.244564
F	-1.406280	-1.488306	-2.392501
F	-0.266356	1.001438	-0.846343
F	0.612650	0.330221	1.009632
F	1.204696	-0.573268	-0.853355

17

c-C_5H_3-1-CH_3-5a-F-3-CF_3

C	0.080543	-0.126266	-0.037453
C	1.351515	0.683153	-0.023044
H	1.652083	1.372595	-0.798090
C	2.038661	0.320541	1.061143
C	1.262364	-0.636241	1.882577
H	1.607981	-1.055206	2.818407
C	0.087125	-0.865332	1.285499
C	-1.065486	-1.700203	1.724529
H	-1.973683	-1.093058	1.768227
H	-1.253370	-2.512497	1.016938
H	-0.883116	-2.131785	2.708404
C	3.402333	0.790575	1.435179
F	3.880307	1.696054	0.576554
F	3.405312	1.347632	2.656369
F	4.276353	-0.228844	1.474814
F	-1.063043	0.621518	-0.232466
H	0.135729	-0.858802	-0.855550

17

c-C_5H_3-4-CH_3-1-F-5b-CF_3

C	-0.170825	0.013504	-0.063631
C	-0.018430	-1.385983	-0.563015

C	-0.477985	-2.609896	0.211288
C	-0.130763	-3.728679	-0.731952
F	-0.377141	-4.993539	-0.403858
C	0.451252	-3.271275	-1.838502
C	0.515496	-1.804036	-1.720947
H	0.944103	-1.157122	-2.475208
H	0.817412	-3.866999	-2.661009
H	0.073979	-2.715101	1.152949
C	-1.947432	-2.570278	0.575085
F	-2.727552	-2.373145	-0.492241
F	-2.342264	-3.706888	1.159127
F	-2.197864	-1.574197	1.441912
H	0.339894	0.705598	-0.733888
H	-1.223438	0.303157	-0.006911
H	0.249054	0.127333	0.939141

17

c-C_5H_3-5b-CH_3-1-F-5a-CF_3

C	0.155790	0.286389	-0.128390
C	-0.777734	0.013575	-1.287480
H	-0.486632	-0.575810	-2.145052
C	-1.955512	0.609673	-1.062229
C	-1.941019	1.305230	0.237596
H	-2.745558	1.881605	0.668598
C	-0.738227	1.099806	0.772210
F	-0.272029	1.563120	1.927655
H	-2.807351	0.599600	-1.728091
C	0.568092	-1.019518	0.538471
F	-0.479493	-1.725433	0.972422
F	1.246431	-1.798287	-0.321044
F	1.369081	-0.806890	1.591437
C	1.407115	1.079944	-0.537347
H	1.096856	1.991618	-1.048113
H	1.992240	1.344983	0.344134
H	2.025691	0.488191	-1.212704

17

c-C_5H_3-5a-CH_3-2-F-3-CF_3

C	0.016884	0.193770	0.423124
C	1.221763	-0.708176	0.392413
H	1.284197	-1.660156	0.901847
C	2.174180	-0.152990	-0.365212
C	1.667439	1.127069	-0.872371
F	2.410229	1.896679	-1.661147
C	0.428112	1.358297	-0.437452
H	-0.186691	2.217278	-0.660187
C	3.523708	-0.707027	-0.668625
F	3.710007	-1.893899	-0.077760
F	3.701133	-0.881201	-1.985647
F	4.498663	0.109929	-0.246391
C	-1.259992	-0.508787	-0.058792
H	-1.127327	-0.869198	-1.080542
H	-1.498961	-1.358411	0.583271
H	-2.104028	0.182247	-0.042357
H	-0.131489	0.535662	1.456670

17

c-C_5H_3-3-CH_3-5a-F-1-CF_3

C	0.035578	-0.097710	-0.062986
C	1.408342	0.496160	-0.239802
H	2.234980	0.267186	0.418414
C	1.404543	1.352964	-1.268209
C	0.055119	1.327699	-1.894988
H	-0.241495	1.932167	-2.743232
C	-0.722125	0.460667	-1.245256
C	-2.142165	0.136348	-1.538251
F	-2.628283	0.892140	-2.532702
F	-2.306346	-1.143815	-1.895137
F	-2.921036	0.340306	-0.460644
C	2.513963	2.217952	-1.767905
H	3.427411	2.052848	-1.197281
H	2.717376	2.007544	-2.821229
H	2.243879	3.274576	-1.693018
F	0.030385	-1.476097	-0.010100
H	-0.422171	0.265467	0.866549

14

c-C_5H_4-3-F-5a-CF_3

C	0.156957	-0.460452	-0.083528

C	-0.899843	-0.757871	0.944509
H	-0.715348	-1.081204	1.956590
C	-2.076221	-0.555999	0.348080
C	-1.929283	-0.108376	-1.039948
H	-2.756506	0.112718	-1.699166
C	-0.620897	-0.030192	-1.304933
H	-0.151628	0.278561	-2.227581
F	-3.278381	-0.725037	0.888364
C	1.147673	0.590010	0.369375
F	0.565022	1.755748	0.659995
F	1.810073	0.188519	1.464635
F	2.063934	0.827080	-0.583371
H	0.749564	-1.355630	-0.310212

17

c-C_5H_3-2-CH_3-5b-F-1-CF_3

C	0.029841	0.042606	0.012055
C	0.890197	-1.135474	0.388312
H	1.688063	-1.505070	-0.239540
C	0.525321	-1.568019	1.595900
C	-0.645214	-0.788960	2.087503
C	-1.271175	-1.074604	3.412233
H	-0.579529	-0.804531	4.215220
H	-2.203019	-0.535616	3.560222
H	-1.461296	-2.147642	3.497310
C	-0.956401	0.120589	1.152113
C	-2.054860	1.122733	1.147702
F	-3.147969	0.680759	0.506738
F	-2.449938	1.470653	2.384283
F	-1.670935	2.250133	0.525815
H	0.983863	-2.366527	2.165198
H	0.633702	0.958365	-0.023048
F	-0.574254	-0.094546	-1.221990

14

c-C_5H_4-4-F-2-CF_3

C	0.134562	0.133400	0.151523
C	-0.056508	-1.019515	1.082527
F	0.872737	-1.964206	1.186280
C	-1.215650	-0.956918	1.742418
C	-1.876910	0.270024	1.275512
C	-3.209576	0.708862	1.775103
F	-4.152639	-0.217733	1.538462
F	-3.194902	0.909879	3.103026
F	-3.612274	1.847503	1.201228
C	-1.130230	0.913038	0.367087
H	-1.382474	1.835768	-0.133692
H	-1.599397	-1.655991	2.469801
H	1.028465	0.712085	0.407291
H	0.246229	-0.200999	-0.885276

17

c-C_5H_4-5b-CH_3-3-CF_3

C	-0.237868	0.052592	0.179193
C	-1.230112	-0.955220	-0.329073
H	-1.450574	-1.127520	-1.373809
C	-1.789032	-1.579834	0.715611
C	-1.234083	-1.059594	1.974126
H	-1.524559	-1.399909	2.958693
C	-0.333988	-0.113257	1.672377
H	0.247777	0.469015	2.374311
C	-2.825826	-2.645262	0.652650
F	-3.944542	-2.285093	1.305580
F	-3.176125	-2.940849	-0.604723
F	-2.400564	-3.783559	1.227615
H	0.767831	-0.238976	-0.155128
C	-0.526165	1.482566	-0.300722
H	-1.524592	1.789800	0.016097
H	0.200383	2.180754	0.118148
H	-0.472425	1.543607	-1.389005

18

$Me_2C=CMe_2$, **1**

C	-0.077860	-0.031385	-0.034224
C	-1.162878	-0.987009	-0.469300
C	-2.451628	-0.274280	-0.801949
H	-3.315147	-0.933440	-0.856500
H	-2.659668	0.480339	-0.037166
H	-2.364265	0.260668	-1.753995

C	-1.000735	-2.314347	-0.550028
C	0.265869	-3.033353	-0.152015
H	0.939229	-2.431093	0.453828
H	0.012302	-3.927665	0.425471
H	0.811451	-3.376862	-1.037761
C	-2.063523	-3.263726	-1.048863
H	-2.870271	-2.773144	-1.588938
H	-1.611288	-3.996400	-1.724332
H	-2.498205	-3.830326	-0.218064
H	0.919731	-0.464621	-0.051474
H	-0.071124	0.839971	-0.696224
H	-0.274175	0.344348	0.975976

29

1 + *c*-C_5H_6 TS

C	1.153826	-0.000441	-0.008883
C	0.745370	0.000008	2.187065
C	-1.142892	0.000288	0.029778
C	-0.661770	0.000592	2.210341
C	0.701348	1.275074	-0.345183
C	-0.701169	1.275482	-0.321709
C	0.001041	-0.937353	-0.236366
C	1.495008	1.254892	2.582913
C	1.506581	-1.260817	2.547103
C	-1.411882	-1.259573	2.595288
C	-1.396582	1.256262	2.630814
H	1.086507	2.151490	2.119186
H	1.452027	1.395265	3.671099
H	2.548343	1.181573	2.300353
H	1.115684	-2.161535	2.074907
H	2.560392	-1.169768	2.273842
H	1.465147	-1.424085	3.632038
H	-1.334765	-1.423081	3.678222
H	-2.474052	-1.167329	2.356998
H	-1.037826	-2.160604	2.110195
H	-1.315877	1.397616	3.716702
H	-1.003657	2.152067	2.152325
H	-2.459091	1.183461	2.384813
H	2.191531	-0.310747	-0.052877
H	-2.181674	-0.309383	0.020212
H	1.326113	2.150826	-0.462899
H	-1.329025	2.151560	-0.418675
H	-0.017087	-1.201663	-1.304182
H	0.010413	-1.861466	0.334088

29

1 + *c*-C_5H_6

C	0.000105	0.000133	-0.000026
H	0.081799	1.030322	-0.349581
C	0.130729	-1.118777	-1.050389
C	0.001750	-2.239910	-0.002180
H	0.084829	-3.269314	-0.353711
C	-1.407559	-1.920593	0.624363
C	-1.408905	-0.322422	0.625509
C	-1.556457	0.307128	2.015247
H	-0.800695	-0.041434	2.718413
H	-1.462320	1.394491	1.934813
H	-2.540984	0.093605	2.440928
C	-2.504575	0.297290	-0.254470
H	-2.415381	1.386837	-0.226173
H	-2.445122	-0.010813	-1.298649
H	-3.501289	0.041508	0.114451
C	-1.553377	-2.552508	2.013208
H	-1.457543	-3.639593	1.930976
H	-0.797776	-2.203861	2.716490
H	-2.538004	-2.341244	2.439776
C	-2.502576	-2.540905	-0.255989
H	-2.411654	-3.630350	-0.229090
H	-3.499541	-2.287175	0.113685
H	-2.444076	-2.231407	-1.299804
C	1.061989	-1.787202	0.987666
C	1.060845	-0.453002	0.989129
H	1.628318	0.199959	1.639937
H	1.630522	-2.440622	1.637087
H	-0.658023	-1.118615	-1.803023
H	1.104048	-1.117570	-1.541695

Table S12. Cartesian coordinates for Diels-Alder transition states and product norbornenes formed from **1** + *c*-$C_5H_x(CH_3)_{6-x}$

32
1 + 1-*c*-$C_5H_5(CH_3)$ TS = **1** + 4-*c*-$C_5H_5(CH_3)$ TS

C	-0.000705	0.000618	0.000050
C	-1.179266	0.383462	0.854283
C	-1.515573	-0.760925	1.580076
C	-0.444206	-1.661590	1.558255
C	0.609882	-1.082766	0.845161
H	1.515736	-1.609854	0.567891
H	-0.386315	-2.580979	2.126121
H	-2.421669	-0.876122	2.163220
C	-2.139196	1.472563	0.480102
H	-2.750872	1.766802	1.337144
H	-1.619721	2.357393	0.108168
H	-2.819751	1.136690	-0.308978
H	-0.389731	-0.461588	-0.919798
H	0.655960	0.816927	-0.292072
C	0.312756	1.269907	2.397049
C	1.364874	0.338384	2.300116
C	2.643866	0.742917	1.591639
H	3.213744	1.437613	2.222440
H	3.280426	-0.126222	1.409840
H	2.477239	1.242582	0.637681
C	1.636220	-0.599073	3.460146
H	2.108589	-0.050535	4.285456
H	0.730621	-1.062788	3.847111
H	2.319790	-1.397813	3.159897
C	-0.575094	1.269074	3.620950
H	-0.876672	0.266064	3.919323
H	-0.051868	1.724085	4.473113
H	-1.481207	1.854942	3.444414
C	0.482613	2.650255	1.797575
H	0.786603	2.641931	0.749429
H	-0.442495	3.224859	1.873583
H	1.253869	3.205681	2.347661

32
1 + 1-*c*-$C_5H_5(CH_3)$ = **1** + 4-*c*-$C_5H_5(CH_3)$

C	0.002095	0.004717	-0.002188
C	-1.244121	-0.233554	-0.958355
C	-1.859131	-1.562554	-0.537720
C	-1.034053	-2.539597	-0.913755
C	0.163935	-1.882668	-1.577790
C	0.997257	-1.163614	-0.455132
C	2.316271	-0.658594	-1.059327
H	2.174576	-0.000186	-1.916731
H	2.913425	-0.120947	-0.318414
H	2.907587	-1.515322	-1.394405
C	1.377539	-2.138999	0.664422
H	0.509133	-2.590342	1.143239
H	1.989570	-2.946829	0.251315
H	1.970478	-1.640145	1.436184
H	0.775598	-2.529190	-2.208658
C	-0.534605	-0.689148	-2.249189
H	-1.245623	-0.995913	-3.018349
H	0.146094	0.058641	-2.660093
H	-1.130995	-3.596755	-0.701415
H	-2.768948	-1.657402	0.043973
C	-2.222768	0.920079	-1.082349
H	-2.616239	1.218648	-0.105944
H	-1.756478	1.794479	-1.541398
H	-3.070070	0.625340	-1.706675
C	0.581129	1.410747	-0.221211
H	-0.125840	2.162569	0.138214
H	1.505931	1.541064	0.346100
H	0.796709	1.632610	-1.267657
C	-0.408644	-0.065749	1.473955
H	-1.141639	0.716553	1.692581
H	-0.851202	-1.023712	1.744830
H	0.452011	0.106773	2.126167

32
1 + 2-*c*-$C_5H_5(CH_3)$ TS = **1** + 3-*c*-$C_5H_5(CH_3)$ TS

C	0.001010	0.003069	-0.002012
C	-0.584924	1.351531	0.300633
C	-1.822926	1.136065	0.909764
C	-1.838924	-0.180855	1.400541
C	-0.616690	-0.790512	1.116364

H	-0.406817	-1.840531	1.286992
H	-2.615729	-0.595099	2.032074
C	-2.888158	2.170423	1.128717
H	-3.678133	2.078589	0.378190
H	-3.355399	2.065685	2.111191
H	-2.475375	3.178004	1.052614
H	-0.334566	2.252157	-0.250745
H	-0.426843	-0.355864	-0.949634
H	1.082875	-0.044552	-0.086539
C	0.725438	1.506957	2.125005
C	0.703802	0.180286	2.595220
C	1.927713	-0.699672	2.426262
H	2.704969	-0.401305	3.141993
H	1.684842	-1.745191	2.631017
H	2.373184	-0.649597	1.433236
C	-0.057523	-0.143493	3.864606
H	0.491087	0.222454	4.742543
H	-1.049408	0.305567	3.884434
H	-0.178167	-1.224193	3.977784
C	-0.028817	2.576445	2.885274
H	-1.037882	2.268403	3.157466
H	0.499668	2.825757	3.815144
H	-0.105466	3.492484	2.293772
C	1.965991	2.050552	1.445154
H	2.393413	1.374657	0.705168
H	1.752990	2.999847	0.948140
H	2.747307	2.242626	2.192475

32

1 + 2-*c*-$C_5H_5(CH_3)$ = **1** + 3-*c*-$C_5H_5(CH_3)$

C	0.009929	-0.006445	0.007690
C	-1.226968	-0.249642	-0.936295
C	-1.877580	-1.564928	-0.527549
C	-1.042879	-2.537608	-0.904790
C	0.159893	-1.886122	-1.567695
C	1.005768	-1.169296	-0.452879
C	2.318959	-0.654646	-1.061051
H	2.170478	-0.004508	-1.923501
H	2.908425	-0.103457	-0.323542
H	2.921095	-1.506409	-1.389490
C	1.395382	-2.146792	0.661470
H	0.530847	-2.610863	1.134971
H	2.015787	-2.945711	0.243765
H	1.982534	-1.647078	1.437180
H	0.763460	-2.535772	-2.203607
C	-0.536804	-0.687582	-2.240474
H	-1.249555	-0.996751	-3.005506
H	0.146166	0.053590	-2.656990
H	-1.149337	-3.595727	-0.696771
C	-3.164429	-1.659591	0.224082
H	-3.983321	-1.228025	-0.359755
H	-3.413418	-2.697391	0.452531
H	-3.113959	-1.099070	1.162426
H	-1.899746	0.610049	-0.982856
C	0.554289	1.409282	-0.232809
H	-0.192517	2.141388	0.087169
H	1.460812	1.590610	0.350539
H	0.783975	1.609299	-1.279834
C	-0.389375	-0.075920	1.485914
H	-1.145619	0.686362	1.699002
H	-0.800429	-1.045239	1.767154
H	0.469685	0.125680	2.132018

32

1 + 5a-*c*-$C_5H_5(CH_3)$ TS

C	-0.000121	-0.000189	-0.000073
C	0.714480	-0.712027	1.126252
C	0.901924	-2.025977	0.677088
C	0.856872	-2.029540	-0.720959
C	0.625068	-0.724293	-1.163420
H	0.445870	-0.453682	-2.199004
H	1.092513	-2.874762	-1.354076
H	1.178999	-2.866775	1.299070
H	0.576837	-0.445385	2.169734
H	-1.010245	-0.442625	0.057866
C	-0.224495	1.503370	-0.030257
H	0.652457	2.076219	-0.303889
H	-1.003296	1.734323	-0.761454

H	-0.576960	1.851923	0.944140
C	2.719042	0.072722	0.671055
C	2.706362	0.122899	-0.738646
C	2.696286	1.449705	-1.482507
H	3.683448	1.594027	-1.937639
H	1.968317	1.470229	-2.298654
H	2.520647	2.313837	-0.845414
C	3.492844	-0.907761	-1.527677
H	4.566204	-0.683265	-1.464684
H	3.346462	-1.926549	-1.176535
H	3.212230	-0.873183	-2.584187
C	3.565074	-0.988182	1.352309
H	3.487729	-1.965009	0.880417
H	4.621066	-0.688543	1.326138
H	3.279493	-1.098527	2.401763
C	2.687652	1.337539	1.513835
H	1.952263	2.073709	1.202855
H	2.479573	1.089357	2.557342
H	3.673257	1.819975	1.490272

32

1 + 5a-*c*-$C_5H_5(CH_3)$

C	-0.009064	0.001327	0.000627
C	1.253549	0.239352	0.914093
C	0.909154	-0.340560	2.278806
C	0.011034	0.472047	2.839477
C	-0.253320	1.602079	1.854322
C	-1.083348	0.972604	0.670788
C	-1.631865	2.060350	-0.266383
H	-0.875140	2.708079	-0.699300
H	-2.195536	1.610380	-1.088450
H	-2.324716	2.696387	0.291788
C	-2.326425	0.249765	1.213147
H	-2.085648	-0.548878	1.912757
H	-2.965798	0.968933	1.734451
H	-2.914263	-0.179053	0.396686
H	-0.715380	2.499642	2.270758
C	1.186796	1.744904	1.290390
H	1.853813	1.894198	2.142682
C	1.561050	2.843353	0.298884
H	1.001461	2.870546	-0.628264
H	1.437321	3.816282	0.783087
H	2.618752	2.742699	0.039038
H	-0.508684	0.325152	3.777680
H	1.269975	-1.284419	2.667168
H	2.181228	-0.119602	0.463370
C	0.302710	0.313198	-1.471745
H	1.066552	-0.382887	-1.829757
H	-0.585666	0.167034	-2.092499
H	0.671843	1.318650	-1.652001
C	-0.411836	-1.481705	0.017986
H	0.414845	-2.086814	-0.366958
H	-0.655492	-1.847414	1.014070
H	-1.275453	-1.657688	-0.629534

32

1 + 5b-*c*-$C_5H_5(CH_3)$ TS

C	-0.079274	0.039236	-0.131885
C	-0.038448	1.212191	-1.081977
C	0.772556	0.842014	-2.151234
C	0.858778	-0.559974	-2.183493
C	0.102105	-1.075222	-1.134613
H	0.081540	-2.123742	-0.856375
H	1.321921	-1.141712	-2.969728
H	1.158737	1.511431	-2.908758
H	-0.186687	2.236489	-0.756319
C	1.079354	0.087061	0.883642
H	0.970631	0.950657	1.543628
H	1.078904	-0.812589	1.503178
H	2.039302	0.157807	0.370561
H	-1.005271	-0.030523	0.433159
C	-2.045556	0.663475	-1.901503
C	-1.958575	-0.741297	-1.933710
C	-2.724015	-1.571515	-0.922130
H	-3.792056	-1.575217	-1.176591
H	-2.384597	-2.609835	-0.935842
H	-2.642795	-1.206888	0.101385
C	-1.826283	-1.444993	-3.267928

H	-2.785149	-1.427197	-3.802701
H	-1.081030	-0.983073	-3.913572
H	-1.545301	-2.491786	-3.126847
C	-2.004036	1.438272	-3.201791
H	-1.207191	1.103324	-3.864005
H	-2.953540	1.324765	-3.741487
H	-1.856314	2.504476	-3.011977
C	-2.905121	1.345717	-0.855602
H	-2.780838	0.944049	0.149539
H	-2.693441	2.416799	-0.817379
H	-3.965805	1.233196	-1.116045

32

1 + 5b-*c*-$C_5H_5(CH_3)$

C	0.009560	-0.006471	0.001509
C	-1.521435	-0.293023	0.237509
C	-1.652811	-0.954127	1.599355
C	-1.161292	-2.188692	1.489912
C	-0.696607	-2.364526	0.053936
C	0.599535	-1.488215	-0.129836
C	1.230608	-1.787275	-1.498007
H	0.541676	-1.657452	-2.332843
H	2.099782	-1.149629	-1.679700
H	1.577641	-2.824209	-1.514728
C	1.660352	-1.837739	0.920462
H	1.308462	-1.691273	1.940994
H	1.947267	-2.888378	0.812986
H	2.562576	-1.235329	0.782190
H	-0.565949	-3.394261	-0.285416
C	-1.748794	-1.509522	-0.689109
C	-3.163627	-2.067201	-0.755071
H	-3.187076	-2.975685	-1.362498
H	-3.551263	-2.308930	0.234943
H	-3.837787	-1.342148	-1.218388
H	-1.424297	-1.290198	-1.707661
H	-1.023225	-2.909411	2.285726
H	-1.995929	-0.465613	2.502381
H	-2.149951	0.583628	0.067074
C	0.182122	0.846074	-1.264635
H	-0.275329	1.826147	-1.102940
H	1.239408	1.012425	-1.487203
H	-0.280159	0.409226	-2.150023
C	0.606770	0.808389	1.154740
H	0.091461	1.771279	1.225463
H	0.512636	0.308720	2.118162
H	1.666529	1.015320	0.981169

35

1 + 1,2-*c*-$C_5H_4(CH_3)_2$ TS = **1** + 3,4-*c*-$C_5H_4(CH_3)_2$ TS

C	-0.176326	-0.012167	-0.100033
C	-0.042450	1.210786	-0.962977
C	0.758393	0.845872	-2.050712
C	0.785926	-0.554108	-2.137965
C	-0.026195	-1.092154	-1.135720
H	-0.073835	-2.149069	-0.898618
H	1.242804	-1.112761	-2.946015
C	1.399514	1.807752	-3.006207
H	2.245411	2.319835	-2.536937
H	1.769642	1.294644	-3.895740
H	0.694676	2.579376	-3.326932
C	-0.161071	2.609554	-0.438246
H	-0.459327	3.304024	-1.230150
H	-0.897772	2.674838	0.364282
H	0.796183	2.966137	-0.041533
H	0.699620	-0.055369	0.564954
H	-1.066935	-0.055158	0.522813
C	-2.105502	0.646903	-1.919406
C	-2.007545	-0.757031	-1.929013
C	-2.815429	-1.561352	-0.927468
H	-3.872735	-1.569399	-1.222829
H	-2.479232	-2.600803	-0.901273
H	-2.771312	-1.169856	0.088337
C	-1.876965	-1.482664	-3.254199
H	-2.837429	-1.476608	-3.785947
H	-1.133039	-1.032310	-3.909092
H	-1.593927	-2.526955	-3.095949
C	-1.985746	1.410174	-3.217533
H	-1.166956	1.051756	-3.841347

H	-2.909799	1.314370	-3.804127
H	-1.829746	2.476680	-3.031659
C	-3.004705	1.334536	-0.914698
H	-2.850206	1.003411	0.113360
H	-2.865566	2.417274	-0.942476
H	-4.057702	1.138110	-1.157649

35

1 + 1,2-*c*-$C_5H_4(CH_3)_2$ = **1** + 3,4-*c*-$C_5H_4(CH_3)_2$

C	-0.001803	-0.001790	-0.000653
C	-1.185567	0.478501	-0.946468
C	-2.448318	-0.234792	-0.454409
C	-2.326472	-1.524047	-0.779819
C	-0.989707	-1.701462	-1.477552
C	0.143893	-1.543725	-0.403031
C	1.496208	-1.894890	-1.042319
H	1.727622	-1.295452	-1.923009
H	2.316990	-1.775332	-0.330412
H	1.483562	-2.944006	-1.350793
C	-0.052702	-2.523024	0.759430
H	-1.016572	-2.402061	1.252742
H	0.003111	-3.549330	0.383500
H	0.733043	-2.405913	1.511195
H	-0.880509	-2.607108	-2.076228
C	-0.901947	-0.353540	-2.211613
H	-1.684813	-0.232484	-2.962499
H	0.070215	-0.145227	-2.663070
H	-3.005780	-2.324009	-0.509447
C	-3.536352	0.439816	0.316197
H	-4.010753	1.224602	-0.280715
H	-4.304569	-0.275588	0.614536
H	-3.142552	0.921924	1.216465
C	-1.322370	1.979047	-1.132933
H	-1.462156	2.495757	-0.178139
H	-0.441342	2.401766	-1.619923
H	-2.188573	2.203001	-1.761370
C	1.267464	0.817736	-0.278876
H	1.126805	1.846955	0.060927
H	2.119132	0.410112	0.271043
H	1.536320	0.851557	-1.335983
C	-0.339122	0.220844	1.479088
H	-0.527831	1.283260	1.662863
H	-1.216031	-0.338515	1.803297
H	0.500429	-0.072455	2.115549

35

1 + 1,3-*c*-$C_5H_4(CH_3)_2$ TS = **1** + 2,4-*c*-$C_5H_4(CH_3)_2$ TS

C	-0.184793	0.000374	-0.067509
C	-0.060331	1.210276	-0.955580
C	0.765461	0.821241	-2.012726
C	0.822104	-0.577900	-2.088441
C	-0.000631	-1.093967	-1.079543
H	-0.051044	-2.149625	-0.832258
C	1.520353	-1.375336	-3.151196
H	1.432137	-0.903968	-4.133683
H	2.586880	-1.468347	-2.927942
H	1.107662	-2.383461	-3.218506
H	1.195293	1.499312	-2.742478
C	-0.181898	2.613608	-0.440738
H	-0.329778	3.320657	-1.261429
H	-1.015396	2.716398	0.256139
H	0.728056	2.912266	0.089575
H	0.680270	-0.005547	0.612419
H	-1.085103	-0.047477	0.540949
C	-2.078283	0.662871	-1.908788
C	-1.978780	-0.742496	-1.933453
C	-2.801457	-1.558387	-0.954985
H	-3.855120	-1.555865	-1.263920
H	-2.470512	-2.599545	-0.939642
H	-2.768438	-1.180131	0.066370
C	-1.819432	-1.453579	-3.261765
H	-2.770131	-1.441164	-3.810982
H	-1.066761	-0.994641	-3.901020
H	-1.539989	-2.499909	-3.111337
C	-1.956525	1.439278	-3.201472
H	-1.131553	1.092077	-3.822247
H	-2.877707	1.348336	-3.793261
H	-1.801583	2.503378	-3.002898

C	-3.017195	1.322793	-0.919227
H	-2.854682	1.015865	0.115528
H	-2.927232	2.410002	-0.962922
H	-4.058699	1.075615	-1.164603

35

1 + 1,3-*c*-$C_5H_4(CH_3)_2$ = **1** + 2,4-*c*-$C_5H_4(CH_3)_2$

C	0.006183	0.001965	-0.002893
C	-1.186361	0.472929	-0.935827
C	-2.433716	-0.263317	-0.460902
C	-2.324446	-1.549301	-0.801654
C	-0.975754	-1.697812	-1.493435
C	0.145109	-1.542089	-0.402183
C	1.500666	-1.905431	-1.026765
H	1.732308	-1.324107	-1.919767
H	2.318000	-1.767279	-0.314421
H	1.492105	-2.961158	-1.312175
C	-0.069860	-2.511639	0.765292
H	-1.018112	-2.351118	1.277861
H	-0.056392	-3.541656	0.394594
H	0.731994	-2.418947	1.503161
H	-0.856180	-2.600927	-2.096680
C	-0.894226	-0.342616	-2.212123
H	-1.676496	-0.216790	-2.962872
H	0.077634	-0.125149	-2.659804
C	-3.247857	-2.688491	-0.520141
H	-3.577182	-3.155900	-1.453273
H	-2.746178	-3.465787	0.064171
H	-4.130332	-2.355972	0.029275
H	-3.228233	0.188628	0.123812
C	-1.350338	1.972542	-1.105408
H	-1.479588	2.473294	-0.141069
H	-0.487055	2.417269	-1.605337
H	-2.235030	2.184389	-1.711281
C	1.274471	0.817882	-0.297253
H	1.130787	1.852988	0.022311
H	2.127153	0.424147	0.261421
H	1.545099	0.832567	-1.354160
C	-0.320249	0.236927	1.477149
H	-0.457322	1.306786	1.660200
H	-1.227781	-0.274599	1.795786
H	0.501698	-0.097108	2.116531

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1 + 1,4-*c*-$C_5H_4(CH_3)_2$ TS

C	-0.150903	0.013482	-0.062248
C	-0.072939	1.209037	-0.973759
C	0.745043	0.817109	-2.040179
C	0.825930	-0.576707	-2.076760
C	0.061799	-1.115743	-1.034855
C	0.107605	-2.553166	-0.604735
H	1.065576	-2.783153	-0.127723
H	-0.679315	-2.783990	0.115211
H	-0.001100	-3.225036	-1.460308
H	1.301400	-1.159183	-2.857140
H	1.147555	1.490597	-2.787674
C	-0.192627	2.617688	-0.469190
H	-0.380950	3.316188	-1.288876
H	-0.998822	2.717950	0.259396
H	0.733694	2.931847	0.022133
H	0.720494	0.046398	0.609797
H	-1.043242	-0.054532	0.558473
C	-2.055156	0.657123	-1.896244
C	-1.973202	-0.750425	-1.932864
C	-2.829960	-1.552847	-0.974360
H	-3.891294	-1.417707	-1.221845
H	-2.615256	-2.619887	-1.055557
H	-2.709546	-1.262776	0.070933
C	-1.793999	-1.449289	-3.263663
H	-2.736680	-1.437431	-3.827305
H	-1.033266	-0.980906	-3.885723
H	-1.514629	-2.496515	-3.119958
C	-1.961862	1.440176	-3.188400
H	-1.153821	1.095992	-3.831597
H	-2.898424	1.348549	-3.754919
H	-1.805247	2.503814	-2.989612
C	-2.996111	1.304307	-0.900104
H	-2.840796	0.975473	0.128998

H	-2.905462	2.391716	-0.924464
H	-4.035480	1.061405	-1.158299

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1 + 1,4-*c*-$C_5H_4(CH_3)_2$

C	0.001058	0.003746	-0.003592
C	-0.865539	-1.040428	-0.824379
C	-1.113442	-2.216703	0.111290
C	0.037802	-2.867866	0.265876
C	1.097479	-2.150744	-0.560790
C	1.386765	-0.780034	0.182476
C	2.580575	-0.066328	-0.470490
H	2.471045	0.064489	-1.548295
H	2.734163	0.920148	-0.026835
H	3.493587	-0.641074	-0.296934
C	1.778429	-1.013934	1.647047
H	1.008047	-1.536221	2.213329
H	2.693363	-1.611957	1.694756
H	1.986123	-0.066006	2.151151
C	2.310429	-2.989795	-0.920998
H	2.947260	-2.483834	-1.649738
H	2.917457	-3.217701	-0.039584
H	1.989638	-3.938685	-1.358443
C	0.214512	-1.666274	-1.724212
H	-0.175265	-2.496402	-2.318192
H	0.708970	-0.948603	-2.383528
H	0.238622	-3.705292	0.924450
H	-2.053042	-2.409088	0.616731
C	-2.102844	-0.493570	-1.513600
H	-2.772825	0.000824	-0.803660
H	-1.843899	0.226131	-2.293081
H	-2.658590	-1.309565	-1.982595
C	0.144834	1.311369	-0.797551
H	-0.827728	1.803128	-0.877191
H	0.813836	2.006316	-0.284678
H	0.525984	1.164658	-1.809466
C	-0.684476	0.379126	1.316337
H	-1.652405	0.846086	1.111222
H	-0.858532	-0.480455	1.962691
H	-0.086959	1.106562	1.872787

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1 + 1,5a-*c*-$C_5H_4(CH_3)_2$ TS = **1** + 4,5a-*c*-$C_5H_4(CH_3)_2$ TS

C	0.000263	0.000171	0.000521
C	0.373774	0.746786	-1.264318
C	-0.774103	0.690273	-2.066942
C	-1.888341	0.427854	-1.268210
C	-1.467622	0.338911	0.066247
H	-2.109090	0.020906	0.882172
H	-2.916965	0.436223	-1.603372
H	-0.798787	0.933599	-3.122470
C	1.776016	0.801282	-1.791495
H	1.846416	1.494042	-2.634161
H	2.485699	1.121453	-1.026017
H	2.098304	-0.183175	-2.147039
H	-0.005254	-1.048095	-0.347279
C	0.881825	0.003159	1.238344
H	0.911733	0.949732	1.762017
H	0.517320	-0.748826	1.943108
H	1.905173	-0.273322	0.969568
C	-0.126679	2.812094	-0.365879
C	-1.188294	2.473936	0.501282
C	-0.991823	2.507220	2.011076
H	-1.516080	3.385125	2.406649
H	-1.420182	1.632711	2.509424
H	0.046226	2.600436	2.321858
C	-2.599035	2.928686	0.162928
H	-2.692979	4.007435	0.344633
H	-2.880552	2.739440	-0.869878
H	-3.325588	2.423973	0.806469
C	-0.440974	3.567746	-1.641435
H	-1.336439	3.207277	-2.142707
H	-0.594878	4.631355	-1.412782
H	0.390473	3.503355	-2.348653
C	1.237476	3.212413	0.167746
H	1.681769	2.507931	0.867457
H	1.941930	3.338242	-0.657033
H	1.166296	4.183291	0.675122

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1 + 1,5a-*c*-$C_5H_4(CH_3)_2$ = **1** + 4,5a-*c*-$C_5H_4(CH_3)_2$

C	0.002861	0.005112	0.001574
C	-1.125322	0.783016	-0.807979
C	-1.864093	-0.299103	-1.590958
C	-1.059717	-0.724847	-2.565583
C	0.240317	0.057931	-2.447743
C	0.972993	-0.487690	-1.167332
C	2.406822	0.060161	-1.082383
H	2.473939	1.144168	-1.060741
H	2.916276	-0.324565	-0.194656
H	2.971057	-0.284383	-1.953692
C	1.131813	-2.013798	-1.248393
H	0.181740	-2.538344	-1.336428
H	1.736503	-2.269206	-2.124171
H	1.653014	-2.399219	-0.367520
H	0.877600	0.060879	-3.334635
C	-0.358149	1.416805	-2.004998
H	-1.107678	1.698697	-2.749857
C	0.504146	2.662774	-1.819086
H	1.258546	2.615389	-1.042408
H	1.013635	2.891433	-2.759595
H	-0.144834	3.512978	-1.589630
H	-1.243486	-1.533630	-3.261345
H	-2.840833	-0.687380	-1.325726
C	-2.001524	1.716541	0.005304
H	-2.504426	1.186932	0.819853
H	-1.419432	2.530979	0.443150
H	-2.773086	2.158323	-0.631309
C	0.690993	0.895105	1.050461
H	-0.024792	1.157805	1.833742
H	1.504923	0.346649	1.532058
H	1.101648	1.823461	0.661953
C	-0.616071	-1.144931	0.814619
H	-1.335366	-0.742555	1.534219
H	-1.134982	-1.877031	0.198599
H	0.153750	-1.669054	1.387820

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1 + 1,5b-*c*-$C_5H_4(CH_3)_2$ TS = **1** + 4,5b-*c*-$C_5H_4(CH_3)_2$ TS

C	-0.072100	0.036365	-0.127767
C	-0.003729	1.250586	-1.027251
C	0.765396	0.880009	-2.129947
C	0.830077	-0.517876	-2.204568
C	0.068806	-1.052299	-1.163131
H	0.048302	-2.106715	-0.907593
H	1.272129	-1.083315	-3.014465
H	1.155841	1.568290	-2.870298
C	-0.114913	2.645713	-0.492204
H	-0.267759	3.366560	-1.299595
H	-0.939134	2.742046	0.217383
H	0.802923	2.931517	0.033844
C	1.096713	0.028390	0.875988
H	1.014763	0.877634	1.559771
H	1.083825	-0.885693	1.473508
H	2.052417	0.090746	0.353086
H	-0.996252	-0.018263	0.445118
C	-2.066452	0.658786	-1.908882
C	-1.943618	-0.744590	-1.925230
C	-2.714347	-1.565788	-0.909054
H	-3.778042	-1.585906	-1.180141
H	-2.363386	-2.600402	-0.897238
H	-2.652801	-1.178098	0.107423
C	-1.826193	-1.463822	-3.254396
H	-2.799234	-1.476300	-3.762601
H	-1.109214	-0.994430	-3.925455
H	-1.517009	-2.501951	-3.106002
C	-2.002000	1.427989	-3.208959
H	-1.195823	1.087792	-3.857213
H	-2.942710	1.317490	-3.765580
H	-1.856444	2.495362	-3.021905
C	-2.966088	1.317941	-0.884563
H	-2.761613	1.016443	0.144278
H	-2.885003	2.405407	-0.937361
H	-4.014482	1.062075	-1.087892

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1 + 1,5b-*c*-$C_5H_4(CH_3)_2$ = **1** + 4,5b-*c*-$C_5H_4(CH_3)_2$

C	0.000902	0.001837	0.004794
C	-1.472721	0.594866	-0.030512
C	-1.980635	0.372794	-1.449632
C	-1.331110	1.208781	-2.258080
C	-0.356953	1.995178	-1.397522
C	0.786277	1.006327	-0.964060
C	1.905464	1.797486	-0.269558
H	1.562004	2.378217	0.586726
H	2.704187	1.135289	0.074403
H	2.347718	2.495315	-0.986107
C	1.429458	0.332817	-2.182104
H	0.715266	-0.235097	-2.777238
H	1.871249	1.097015	-2.829150
H	2.232921	-0.343929	-1.878055
H	0.025148	2.922441	-1.829754
C	-1.167146	2.113776	-0.090082
C	-2.368372	3.048563	-0.108091
H	-2.043854	4.081307	-0.259103
H	-3.070735	2.792106	-0.902376
H	-2.900643	3.007923	0.846071
H	-0.525852	2.405864	0.744918
H	-1.400421	1.262405	-3.337109
H	-2.690863	-0.395858	-1.732181
C	-2.406346	0.128390	1.071608
H	-2.475682	-0.963044	1.101594
H	-2.071899	0.473807	2.052945
H	-3.413421	0.518916	0.903935
C	0.545058	-0.005407	1.441841
H	-0.008534	-0.731109	2.043027
H	1.594392	-0.310223	1.455161
H	0.472378	0.961673	1.941610
C	0.023756	-1.458524	-0.464778
H	-0.589600	-2.071909	0.202030
H	-0.355887	-1.584175	-1.477985
H	1.039602	-1.861914	-0.430800

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1 + 2,3-*c*-$C_5H_4(CH_3)_2$ TS

C	0.022221	0.002176	0.012654
C	-0.566568	1.348557	0.324312
C	-1.814169	1.119758	0.910346
C	-1.837569	-0.201179	1.400808
C	-0.604588	-0.795693	1.120257
H	-0.394903	-1.846712	1.293050
C	-2.943886	-0.792584	2.222640
H	-2.651324	-1.759290	2.635432
H	-3.228102	-0.140682	3.054994
H	-3.841442	-0.943855	1.615298
C	-2.892136	2.138122	1.133946
H	-3.791580	1.883570	0.565138
H	-3.186645	2.197347	2.186720
H	-2.565275	3.130143	0.818358
H	-0.322259	2.250593	-0.228040
H	-0.395443	-0.345247	-0.943449
H	1.104954	-0.043928	-0.059985
C	0.732576	1.522025	2.116427
C	0.707802	0.201757	2.607461
C	1.930999	-0.682458	2.461264
H	2.704893	-0.373254	3.176284
H	1.685111	-1.724117	2.681789
H	2.382035	-0.649639	1.469999
C	-0.065068	-0.107447	3.872525
H	0.482188	0.256273	4.752512
H	-1.051362	0.354110	3.888283
H	-0.200040	-1.185974	3.991102
C	-0.013960	2.608105	2.862393
H	-1.015711	2.302775	3.161250
H	0.530273	2.888309	3.774233
H	-0.109388	3.506500	2.246519
C	1.982421	2.054703	1.443038
H	2.421788	1.365939	0.722187
H	1.773446	2.993172	0.923653
H	2.753123	2.265352	2.196323

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1 + 2,3-*c*-$C_5H_4(CH_3)_2$

C	0.021777	0.001379	-0.017233
C	0.906839	0.302229	1.246394

C	2.335490	-0.140028	0.948752
C	2.334978	-1.479376	0.933937
C	0.905988	-1.927018	1.221734
C	0.021166	-1.597612	-0.034921
C	-1.371262	-2.219844	0.146378
H	-1.857748	-1.923163	1.076000
H	-2.036039	-1.954313	-0.679897
H	-1.279779	-3.309658	0.154944
C	0.609411	-2.210499	-1.310784
H	1.615483	-1.851419	-1.526115
H	0.655943	-3.299224	-1.206660
H	-0.020639	-1.991204	-2.177488
H	0.802969	-2.963796	1.551838
C	0.473106	-0.822939	2.202240
H	1.054775	-0.833363	3.124519
H	-0.590892	-0.825190	2.442516
C	3.440719	-2.438536	0.632379
H	3.614283	-3.104079	1.483934
H	3.185132	-3.075846	-0.219905
H	4.377312	-1.926678	0.406317
C	3.441965	0.824722	0.668475
H	3.616030	1.471133	1.534541
H	4.378169	0.317275	0.431137
H	3.186871	1.480924	-0.169502
H	0.804609	1.331529	1.599352
C	-1.370177	0.620512	0.177797
H	-1.277860	1.709800	0.210462
H	-2.035150	0.373828	-0.654142
H	-1.856896	0.303717	1.100635
C	0.610502	0.641891	-1.279230
H	0.657883	1.728008	-1.151039
H	1.616294	0.286879	-1.502470
H	-0.019718	0.442322	-2.150565

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1 + 2,5a-*c*-$C_5H_4(CH_3)_2$ TS = **1** + 3,5a-*c*-$C_5H_4(CH_3)_2$ TS

C	-0.012898	-0.008861	0.004264
C	-0.681301	-0.777075	-1.111107
C	-0.837286	-2.088220	-0.638424
C	-0.817147	-2.043124	0.762358
C	-0.645715	-0.717732	1.175153
H	-0.487119	-0.418679	2.206627
H	-1.038396	-2.881728	1.411422
C	-1.094214	-3.304945	-1.478709
H	-0.164119	-3.850793	-1.660765
H	-1.788487	-3.993275	-0.990061
H	-1.510797	-3.031948	-2.449766
H	-0.543477	-0.534567	-2.161647
H	1.011740	-0.419494	-0.009408
C	0.166397	1.500888	-0.015421
H	-0.737448	2.060274	0.187566
H	0.900691	1.784647	0.742997
H	0.558740	1.818371	-0.985340
C	-2.742221	-0.033759	-0.654065
C	-2.705988	0.068175	0.752639
C	-2.720288	1.423598	1.445402
H	-3.695999	1.552295	1.928441
H	-1.966273	1.503458	2.234191
H	-2.597179	2.267542	0.769731
C	-3.467945	-0.945027	1.589399
H	-4.544897	-0.735421	1.539936
H	-3.314274	-1.973145	1.269993
H	-3.168731	-0.872846	2.639123
C	-3.560377	-1.149106	-1.275839
H	-3.415277	-2.111532	-0.788775
H	-4.628598	-0.903885	-1.206001
H	-3.319216	-1.267203	-2.335195
C	-2.757834	1.193456	-1.549467
H	-2.041022	1.963284	-1.279578
H	-2.554013	0.907501	-2.584009
H	-3.757024	1.648208	-1.533855

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1 + 2,5a-*c*-$C_5H_4(CH_3)_2$ = **1** + 3,5a-*c*-$C_5H_4(CH_3)_2$

C	0.001282	-0.000344	0.001550
C	0.875333	0.306683	1.277669
C	2.300642	-0.123457	0.942100
C	2.298763	-1.459655	0.916054

C	0.886199	-1.927922	1.240540
C	-0.001457	-1.596935	-0.015957
C	-1.396593	-2.232497	0.097000
H	-1.960224	-1.934298	0.976107
H	-2.000511	-1.993004	-0.782863
H	-1.291259	-3.320621	0.130916
C	0.613676	-2.211618	-1.283049
H	1.629416	-1.869642	-1.474161
H	0.643396	-3.300652	-1.178812
H	0.005095	-1.983821	-2.162785
H	0.793062	-2.965824	1.568071
C	0.524673	-0.828347	2.277289
H	1.305321	-0.838923	3.041801
C	-0.789139	-0.845359	3.054774
H	-1.699576	-0.811906	2.468601
H	-0.828506	-1.750183	3.668262
H	-0.809409	0.009829	3.736466
H	3.127743	-2.101801	0.642630
C	3.416826	0.827087	0.658796
H	3.617104	1.454499	1.533081
H	4.333451	0.293014	0.401447
H	3.163599	1.501394	-0.164586
H	0.769620	1.335976	1.631982
C	-1.391222	0.640271	0.115671
H	-1.283280	1.728594	0.133051
H	-2.003727	0.388658	-0.754653
H	-1.945480	0.356300	1.005667
C	0.628321	0.629565	-1.252152
H	0.699453	1.714066	-1.120871
H	1.626349	0.251487	-1.468418
H	0.001870	0.447654	-2.129947

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1 + 2,5b-*c*-$C_5H_4(CH_3)_2$ TS = **1** + 3,5b-*c*-$C_5H_4(CH_3)_2$ TS

C	0.010130	0.015250	-0.004440
C	0.450851	1.146955	0.889307
C	0.336728	0.711829	2.208483
C	0.309171	-0.695741	2.195718
C	0.417926	-1.140211	0.879989
H	0.304051	-2.176584	0.578509
H	0.347669	-1.322899	3.078337
C	0.372322	1.580799	3.431471
H	0.799759	2.558804	3.203082
H	-0.636515	1.743048	3.821429
H	0.963585	1.127636	4.231310
H	0.392042	2.190677	0.594048
C	-1.510855	0.035461	-0.251124
H	-1.792165	0.926130	-0.817558
H	-1.815216	-0.840649	-0.828453
H	-2.054993	0.036145	0.694410
H	0.498130	0.013173	-0.975937
C	2.612593	0.627362	0.497883
C	2.557095	-0.779518	0.475953
C	2.680440	-1.520286	-0.841891
H	3.725029	-1.508967	-1.179670
H	2.390047	-2.567415	-0.726667
H	2.081489	-1.094915	-1.646463
C	3.162866	-1.562112	1.623228
H	4.258972	-1.542092	1.561638
H	2.879362	-1.165721	2.596976
H	2.849012	-2.608643	1.584747
C	3.251554	1.324909	1.678840
H	2.916252	0.925571	2.635589
H	4.343401	1.212247	1.641467
H	3.029221	2.395004	1.664792
C	2.786491	1.402549	-0.792410
H	2.146894	1.056461	-1.603819
H	2.586077	2.465231	-0.637472
H	3.823453	1.314409	-1.142924

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1 + 2,5b-*c*-$C_5H_4(CH_3)_2$ = **1** + 3,5b-*c*-$C_5H_4(CH_3)_2$

C	0.003007	0.000713	0.001431
C	1.330561	0.786543	-0.314160
C	2.497609	-0.091766	0.118220
C	2.492227	-0.103296	1.453253
C	1.335530	0.766144	1.918779
C	0.000521	-0.002334	1.602435

C	-1.188752	0.746759	2.222808
H	-1.258316	1.789041	1.911279
H	-2.135438	0.259963	1.973666
H	-1.092315	0.733672	3.312096
C	0.003068	-1.400742	2.230318
H	0.838252	-2.012703	1.891841
H	0.075115	-1.310165	3.318545
H	-0.924778	-1.934664	2.006300
H	1.388540	1.119657	2.950971
C	1.335369	1.845370	0.810095
C	2.494670	2.831785	0.812043
H	2.454387	3.467064	1.700691
H	3.459294	2.322751	0.802101
H	2.441962	3.484309	-0.063493
H	0.405223	2.416638	0.816556
H	3.139492	-0.688248	2.095851
C	3.391566	-0.816876	-0.832362
H	3.932968	-0.106159	-1.465196
H	4.120953	-1.430705	-0.300793
H	2.815284	-1.462095	-1.502318
H	1.375607	1.152548	-1.343898
C	-1.189189	0.742206	-0.621611
H	-1.100046	0.714896	-1.711311
H	-2.135079	0.261208	-0.359061
H	-1.252369	1.788795	-0.322660
C	0.016166	-1.398883	-0.624432
H	0.117863	-1.314139	-1.711115
H	0.833860	-2.018796	-0.257641
H	-0.921533	-1.924632	-0.423637

35

1 + 5a,5b-*c*-$C_5H_4(CH_3)_2$ TS

C	0.049268	-0.063592	-0.008739
C	-0.710575	-0.836999	-1.079126
C	-0.900682	-2.122820	-0.558062
C	-0.836268	-2.047542	0.838483
C	-0.589009	-0.722534	1.199462
H	-0.394976	-0.393589	2.216280
H	-1.068561	-2.853651	1.521761
H	-1.190924	-2.995022	-1.128442
H	-0.578332	-0.633199	-2.138450
C	1.542867	-0.515951	-0.087484
H	2.095202	-0.113089	0.764724
H	1.638084	-1.599435	-0.090333
H	1.998535	-0.117146	-0.997893
C	0.108539	1.460260	-0.059699
H	-0.823136	1.946253	0.186109
H	0.857553	1.814918	0.653737
H	0.424639	1.790145	-1.053695
C	-2.710232	-0.046800	-0.664446
C	-2.699807	0.074013	0.744871
C	-2.740561	1.432267	1.431057
H	-3.718864	1.541540	1.913246
H	-1.989135	1.529481	2.219990
H	-2.635961	2.277014	0.752819
C	-3.462537	-0.939322	1.578733
H	-4.540370	-0.740088	1.506237
H	-3.296654	-1.969059	1.272626
H	-3.182860	-0.852237	2.632469
C	-3.545602	-1.153433	-1.286962
H	-3.457620	-2.104271	-0.767533
H	-4.604303	-0.863124	-1.271894
H	-3.262395	-1.312618	-2.330911
C	-2.733324	1.170480	-1.576066
H	-2.065810	1.977180	-1.291391
H	-2.477255	0.880111	-2.597996
H	-3.752019	1.577878	-1.607102

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1 + 5a,5b-*c*-$C_5H_4(CH_3)_2$

C	-0.004627	-0.007587	-0.000016
C	1.500669	-0.064871	-0.470764
C	1.441380	-0.424438	-1.949653
C	1.095686	-1.708539	-2.029999
C	0.911653	-2.215556	-0.604540
C	-0.434692	-1.543804	-0.106688
C	-0.984984	-2.155554	1.195763
H	-0.404935	-1.969100	2.092661

H	-1.992100	-1.772728	1.385486
H	-1.070722	-3.239431	1.076229
C	-1.556012	-1.809641	-1.130140
H	-1.320117	-1.465600	-2.134684
H	-1.747864	-2.886169	-1.181738
H	-2.485832	-1.327191	-0.817784
H	0.925899	-3.300738	-0.476180
C	2.054093	-1.413624	0.095628
C	3.462279	-1.751928	-0.435104
H	3.699861	-2.795313	-0.207508
H	3.578716	-1.603989	-1.504435
H	4.203374	-1.132802	0.078954
C	2.204180	-1.565606	1.615212
H	1.294056	-1.528319	2.192928
H	2.678978	-2.527772	1.828135
H	2.872728	-0.785980	1.993517
H	0.897948	-2.278454	-2.928739
H	1.583642	0.268167	-2.769329
H	2.064020	0.837333	-0.218366
C	-0.144440	0.612640	1.401024
H	0.104118	1.676073	1.342399
H	-1.178289	0.541094	1.750641
H	0.497991	0.177707	2.160404
C	-0.817147	0.923811	-0.916355
H	-0.378639	1.926243	-0.895609
H	-0.843642	0.593843	-1.952927
H	-1.848095	1.010681	-0.561271

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1 + 1,2,3-*c*-$C_5H_3(CH_3)_3$ TS = **1** + 2,3,4-*c*-$C_5H_3(CH_3)_3$ TS

C	0.015159	0.005796	-0.007547
C	-0.398041	-0.281892	-1.423988
C	-1.039166	0.872568	-1.889596
C	-0.694333	1.955659	-1.060774
C	0.196676	1.494568	-0.083389
H	0.513479	2.098160	0.761502
C	-1.091440	3.384023	-1.291289
H	-0.856144	3.718592	-2.306952
H	-2.168561	3.516998	-1.152985
H	-0.579098	4.047895	-0.593118
C	-1.868970	0.963773	-3.135774
H	-2.933920	0.848486	-2.908448
H	-1.746453	1.929216	-3.633856
H	-1.600790	0.180921	-3.848194
C	-0.677210	-1.668485	-1.923554
H	-0.517824	-1.743473	-3.003705
H	-0.030611	-2.401317	-1.437800
H	-1.715411	-1.958731	-1.729241
H	-0.843580	-0.205855	0.647052
H	0.862219	-0.569294	0.359655
C	1.749697	0.254750	-2.088666
C	2.039784	1.306193	-1.196132
C	3.000695	1.058076	-0.048326
H	4.029379	1.005424	-0.428417
H	2.963953	1.877672	0.673701
H	2.811848	0.129737	0.489731
C	2.167155	2.720405	-1.726617
H	3.125348	2.842522	-2.248768
H	1.377185	2.983999	-2.427490
H	2.143544	3.445778	-0.908504
C	1.478105	0.566278	-3.543091
H	0.810279	1.417808	-3.672838
H	2.413919	0.799567	-4.069448
H	1.028190	-0.292755	-4.049316
C	2.406599	-1.095987	-1.895349
H	2.317473	-1.487114	-0.880592
H	1.984088	-1.837139	-2.577185
H	3.480179	-1.029015	-2.118040

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1 + 1,2,3-*c*-$C_5H_3(CH_3)_3$ = **1** + 2,3,4-*c*-$C_5H_3(CH_3)_3$

C	0.007469	-0.002863	0.006902
C	0.330493	1.156435	-1.027152
C	-0.128167	2.468502	-0.379276
C	-1.466949	2.469300	-0.373341
C	-1.914863	1.154700	-0.998042
C	-1.593136	-0.003560	0.010967
C	-2.217473	-1.308324	-0.507326

H	-1.892898	-1.571330	-1.514360
H	-1.986953	-2.150374	0.150373
H	-3.305603	-1.200118	-0.528418
C	-2.217847	0.258156	1.385897
H	-1.866232	1.184082	1.840250
H	-3.306163	0.323801	1.287475
H	-2.000784	-0.561134	2.077265
H	-2.950520	1.136237	-1.346529
C	-0.808938	0.965164	-2.045430
H	-0.810912	1.748256	-2.805891
H	-0.804877	-0.012977	-2.531169
C	-2.427459	3.470271	0.182961
H	-3.085861	3.848091	-0.605722
H	-3.072121	3.015280	0.941415
H	-1.917836	4.322495	0.634878
C	0.827146	3.472279	0.183574
H	1.469021	3.885744	-0.600387
H	0.306227	4.301610	0.663978
H	1.490092	3.012296	0.923481
C	1.742018	1.172935	-1.586706
H	2.493236	1.249975	-0.794362
H	1.951059	0.269622	-2.163469
H	1.873210	2.029871	-2.252925
C	0.610329	-1.333308	-0.469775
H	1.700825	-1.288411	-0.411640
H	0.287374	-2.156761	0.171941
H	0.343517	-1.585196	-1.497493
C	0.630235	0.279931	1.380003
H	1.718070	0.356516	1.286495
H	0.265774	1.203232	1.828980
H	0.423255	-0.538021	2.075878

38

1 + 1,2,4-*c*-$C_5H_3(CH_3)_3$ TS = **1** + 1,3,4-*c*-$C_5H_3(CH_3)_3$ TS

C	-0.010062	-0.010531	0.001361
C	0.812222	-1.183308	0.457130
C	0.990465	-1.022513	1.839628
C	0.030781	-0.119301	2.310806
C	-0.779553	0.313229	1.254461
C	-1.729344	1.473184	1.338065
H	-1.180026	2.416246	1.421904
H	-2.362046	1.541303	0.451572
H	-2.375102	1.392246	2.216443
H	-0.135772	0.117683	3.356295
C	1.996040	-1.764516	2.669056
H	3.001338	-1.358469	2.517438
H	1.763490	-1.691797	3.733297
H	2.034245	-2.823041	2.399982
C	1.791836	-1.889005	-0.433655
H	1.974936	-2.912866	-0.093026
H	1.435131	-1.934070	-1.464034
H	2.759267	-1.374579	-0.439090
H	0.675111	0.828564	-0.195338
H	-0.605517	-0.167156	-0.897008
C	-1.070191	-2.459604	0.532102
C	-2.025115	-1.535040	1.000436
C	-3.078480	-1.027892	0.034691
H	-3.734827	-1.853734	-0.270481
H	-3.711168	-0.273772	0.506344
H	-2.666447	-0.596625	-0.879439
C	-2.561266	-1.675667	2.409674
H	-3.256218	-2.524180	2.470109
H	-1.774456	-1.841539	3.143800
H	-3.115169	-0.781213	2.707221
C	-0.595021	-3.563857	1.449732
H	-0.364770	-3.209290	2.453708
H	-1.371133	-4.335565	1.544442
H	0.297285	-4.052347	1.048182
C	-1.122822	-2.899419	-0.916087
H	-1.163591	-2.070501	-1.624530
H	-0.261081	-3.519521	-1.170502
H	-2.020604	-3.508757	-1.087036

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1 + 1,2,4-*c*-$C_5H_3(CH_3)_3$ = **1** + 1,3,4-*c*-$C_5H_3(CH_3)_3$

C	0.012006	-0.007399	-0.021042
C	0.764791	-1.056348	0.901898
C	1.150483	-2.227026	-0.006331

C	0.022518	-2.867345	-0.318161
C	-1.140555	-2.163540	0.367376
C	-1.341389	-0.785293	-0.385014
C	-2.605144	-0.076515	0.127675
H	-2.624315	0.047020	1.211659
H	-2.707750	0.912921	-0.324206
H	-3.490176	-0.650918	-0.156478
C	-1.554579	-0.998215	-1.889091
H	-0.731804	-1.534157	-2.360987
H	-2.468762	-1.575842	-2.054721
H	-1.679177	-0.042241	-2.405407
C	-2.384566	-3.013617	0.555581
H	-3.115505	-2.520455	1.200087
H	-2.868628	-3.234338	-0.400691
H	-2.116630	-3.966051	1.020066
C	-0.422171	-1.692441	1.643865
H	-0.112393	-2.530025	2.273532
H	-1.000280	-0.983334	2.242148
H	-0.083038	-3.697243	-1.009406
C	2.542838	-2.488059	-0.481826
H	3.209440	-2.706150	0.357975
H	2.568236	-3.335769	-1.168633
H	2.955586	-1.613420	-0.994318
C	1.890400	-0.505890	1.759882
H	2.659185	-0.013582	1.155989
H	1.518520	0.217270	2.488404
H	2.371782	-1.316527	2.313551
C	-0.227213	1.298923	0.751472
H	0.727733	1.793999	0.944596
H	-0.834541	1.992081	0.164930
H	-0.723269	1.148281	1.711875
C	0.855488	0.370967	-1.245338
H	1.807293	0.804582	-0.922566
H	1.074121	-0.479781	-1.889816
H	0.345078	1.127065	-1.848423

38

1 + 1,2,5a-*c*-$C_5H_3(CH_3)_3$ TS = **1** + 3,4,5a-*c*-$C_5H_3(CH_3)_3$ TS

C	-0.059107	0.018306	0.015575
C	0.344785	0.401439	1.416015
C	1.004623	1.632655	1.303175
C	0.644753	2.220644	0.085809
C	-0.292195	1.397934	-0.562908
H	-0.599220	1.547086	-1.594145
H	0.931072	3.216921	-0.228268
C	1.892585	2.231762	2.352851
H	2.861014	1.722507	2.380944
H	2.076161	3.290634	2.159656
H	1.451449	2.138547	3.348502
C	0.579447	-0.588982	2.512983
H	0.428266	-0.127421	3.494276
H	-0.098943	-1.441129	2.434427
H	1.604311	-0.977575	2.494650
H	0.896157	-0.262654	-0.461880
C	-0.992202	-1.161613	-0.210640
H	-1.851107	-1.164609	0.452341
H	-1.346745	-1.180563	-1.244023
H	-0.446927	-2.092664	-0.036445
C	-1.832839	1.397094	1.780535
C	-2.067236	1.898559	0.482812
C	-3.125774	1.270343	-0.411276
H	-4.120625	1.598665	-0.084798
H	-3.000772	1.609243	-1.443057
H	-3.124983	0.184687	-0.421927
C	-2.054155	3.405070	0.272451
H	-2.991630	3.836404	0.646595
H	-1.232774	3.902015	0.783081
H	-1.982476	3.647126	-0.791761
C	-1.414769	2.347214	2.880697
H	-0.650423	3.058192	2.572768
H	-2.283627	2.927006	3.222640
H	-1.038246	1.793529	3.746593
C	-2.645051	0.255227	2.356238
H	-3.181428	-0.334891	1.617267
H	-2.038480	-0.419276	2.967847
H	-3.403932	0.679064	3.027368

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1 + 1,2,5a-*c*-$C_5H_3(CH_3)_3$ = **1** + 3,4,5a-*c*-$C_5H_3(CH_3)_3$

C	-0.003106	0.000801	0.000873
C	-0.866078	-0.846433	1.038078
C	-2.291019	-0.291258	0.916809
C	-2.284358	0.928672	1.460650
C	-0.872244	1.209875	1.953096
C	0.014327	1.446211	0.679598
C	1.413216	1.952942	1.067946
H	1.969962	1.285994	1.719990
H	2.021050	2.133581	0.177037
H	1.311963	2.909148	1.589243
C	-0.584733	2.558662	-0.194356
H	-1.605662	2.349819	-0.510064
H	-0.596181	3.495854	0.370708
H	0.022704	2.723701	-1.088873
H	-0.777270	2.008108	2.692719
C	-0.512333	-0.223423	2.418538
H	-1.289695	-0.538523	3.120452
C	0.807515	-0.550571	3.113376
H	1.705880	-0.432346	2.518363
H	0.914848	0.078241	4.001996
H	0.780718	-1.589443	3.454914
H	-3.110053	1.630242	1.482665
C	-3.414624	-1.015635	0.249778
H	-3.637983	-1.952408	0.769741
H	-4.319545	-0.405368	0.240068
H	-3.162361	-1.278817	-0.782065
C	-0.736584	-2.353900	0.927115
H	-1.012871	-2.713151	-0.068991
H	0.286836	-2.678885	1.128488
H	-1.391550	-2.846319	1.651739
C	1.395051	-0.598774	-0.226160
H	1.303052	-1.561025	-0.736888
H	1.981636	0.054479	-0.877577
H	1.971188	-0.766297	0.680249
C	-0.659125	-0.012367	-1.390649
H	-0.743043	-1.042140	-1.752213
H	-1.653313	0.430787	-1.402979
H	-0.040343	0.531117	-2.110015

38

1 + 1,2,5b-*c*-$C_5H_3(CH_3)_3$ TS = **1** + 3,4,5b-*c*-$C_5H_3(CH_3)_3$ TS

C	-0.003782	0.008855	-0.000505
C	-0.414944	-0.279205	-1.424382
C	-1.034642	0.874891	-1.910728
C	-0.676710	1.954376	-1.086349
C	0.197019	1.501564	-0.096345
H	0.514648	2.102802	0.749436
H	-0.928979	2.989803	-1.281323
C	-1.873233	0.945717	-3.152084
H	-2.847304	0.472075	-2.993550
H	-2.048495	1.980305	-3.453020
H	-1.395218	0.425414	-3.986248
C	-0.715577	-1.664283	-1.909266
H	-0.618556	-1.734541	-2.997115
H	-0.045349	-2.400091	-1.460267
H	-1.742764	-1.954832	-1.657631
C	-1.132503	-0.357533	0.982261
H	-1.321434	-1.434304	0.957252
H	-0.856298	-0.088761	2.004263
H	-2.053823	0.165663	0.720722
H	0.886900	-0.537512	0.305305
C	1.763267	0.257866	-2.090414
C	2.053289	1.303353	-1.193489
C	3.004787	1.048078	-0.039469
H	4.036665	1.005754	-0.411906
H	2.957709	1.859888	0.690588
H	2.818142	0.112745	0.487195
C	2.184269	2.718557	-1.721907
H	3.130052	2.833030	-2.267571
H	1.376522	2.991481	-2.398710
H	2.188446	3.438637	-0.899044
C	1.496649	0.577491	-3.542489
H	0.831482	1.431705	-3.668438
H	2.435818	0.815447	-4.060626
H	1.050802	-0.279240	-4.055763
C	2.394421	-1.103746	-1.896055
H	2.293689	-1.496304	-0.883001

H	1.963762	-1.835166	-2.583204
H	3.470165	-1.052306	-2.111722

38

1 + 1,2,5b-*c*-$C_5H_3(CH_3)_3$ = **1** + 3,4,5b-*c*-$C_5H_3(CH_3)_3$

C	-0.003049	0.002834	-0.000306
C	-1.414914	-0.433271	0.585634
C	-2.442233	0.520439	-0.031143
C	-2.256962	1.716985	0.529250
C	-1.107792	1.592959	1.513697
C	0.214836	1.434535	0.683077
C	1.424941	1.497733	1.628331
H	1.398870	0.751240	2.422197
H	2.362714	1.370596	1.081230
H	1.456558	2.482886	2.102163
C	0.388619	2.588980	-0.310731
H	-0.445911	2.677153	-1.005338
H	0.466171	3.532273	0.238778
H	1.307004	2.472539	-0.893162
H	-1.041144	2.375698	2.272623
C	-1.324944	0.150906	2.017357
C	-2.527001	-0.086922	2.920701
H	-2.412483	0.461956	3.858971
H	-3.457452	0.235071	2.450183
H	-2.617366	-1.147692	3.169979
H	-0.437533	-0.228426	2.530409
H	-2.768368	2.636379	0.269389
C	-3.402927	0.126629	-1.105392
H	-4.096298	-0.640758	-0.746896
H	-3.986569	0.985357	-1.441661
H	-2.880877	-0.297957	-1.968632
C	-1.751666	-1.909617	0.475291
H	-1.701972	-2.260043	-0.560279
H	-1.067526	-2.518369	1.071012
H	-2.765549	-2.098089	0.838399
C	1.076986	-1.021755	0.380214
H	0.900675	-1.960466	-0.151313
H	2.067153	-0.665736	0.085474
H	1.106715	-1.246570	1.447500
C	-0.022055	0.048102	-1.533798
H	-0.275767	-0.939126	-1.932666
H	-0.739857	0.765974	-1.928955
H	0.965026	0.309732	-1.925073

38

1 + 1,3,5a-*c*-$C_5H_3(CH_3)_3$ TS = **1** + 2,4,5a-*c*-$C_5H_3(CH_3)_3$ TS

C	0.010809	-0.010605	0.001843
C	0.651649	-0.511932	1.273917
C	1.738834	0.339816	1.494645
C	1.561874	1.532921	0.786352
C	0.314073	1.464735	0.137960
H	-0.004054	2.196105	-0.601098
C	2.484923	2.716464	0.811072
H	2.903934	2.882859	1.807308
H	3.323744	2.564900	0.125658
H	1.968158	3.626545	0.502533
H	2.543821	0.148777	2.196338
C	0.572940	-1.939866	1.718097
H	0.867814	-2.038556	2.766192
H	-0.436907	-2.340608	1.607195
H	1.241846	-2.574469	1.126866
H	0.726381	-0.320933	-0.779367
C	-1.337977	-0.560121	-0.438195
H	-2.067101	-0.607548	0.363425
H	-1.751386	0.038816	-1.253392
H	-1.207271	-1.577624	-0.815258
C	-0.869288	0.731353	2.603588
C	-0.994091	1.880580	1.792377
C	-2.290629	2.172903	1.053247
H	-3.039796	2.545217	1.763732
H	-2.134585	2.959977	0.311136
H	-2.721123	1.319289	0.538504
C	-0.382252	3.182448	2.280864
H	-1.016746	3.608591	3.069055
H	0.616731	3.062399	2.694222
H	-0.327687	3.916614	1.472527
C	-0.013113	0.793829	3.852333
H	0.949901	1.273752	3.692189

H	-0.537057	1.353353	4.639920
H	0.171869	-0.212356	4.240812
C	-2.043587	-0.200710	2.829212
H	-2.828996	-0.130091	2.080767
H	-1.736136	-1.246734	2.913992
H	-2.506556	0.060305	3.790404

38

1 + 1,3,5a-*c*-$C_5H_3(CH_3)_3$ = **1** + 2,4,5a-*c*-$C_5H_3(CH_3)_3$

C	0.007152	-0.002239	0.002644
C	-0.870402	-0.835754	1.030117
C	-2.279147	-0.254810	0.925635
C	-2.281018	0.954921	1.490760
C	-0.853622	1.210149	1.966281
C	0.014770	1.446665	0.676022
C	1.410296	1.975050	1.045804
H	1.972687	1.329570	1.714668
H	2.014399	2.135144	0.148574
H	1.303529	2.944435	1.541147
C	-0.605650	2.542230	-0.204896
H	-1.609188	2.297547	-0.549714
H	-0.662156	3.478063	0.360452
H	0.016396	2.729849	-1.084618
H	-0.744018	2.007329	2.707068
C	-0.502445	-0.229059	2.416685
H	-1.278886	-0.549705	3.117320
C	0.816532	-0.564922	3.108497
H	1.721398	-0.364457	2.546759
H	0.881633	-0.004648	4.045696
H	0.822697	-1.627706	3.368117
C	-3.396521	1.938759	1.622999
H	-3.593904	2.154281	2.677874
H	-3.144006	2.890647	1.146662
H	-4.314492	1.557046	1.172185
H	-3.107320	-0.736834	0.416442
C	-0.778727	-2.345147	0.908673
H	-1.061097	-2.684366	-0.092381
H	0.233568	-2.703026	1.111414
H	-1.454507	-2.821386	1.624448
C	1.408699	-0.603293	-0.198541
H	1.322468	-1.574569	-0.692533
H	2.002354	0.037651	-0.855924
H	1.975014	-0.754493	0.716766
C	-0.631877	-0.030545	-1.396199
H	-0.668180	-1.060477	-1.763424
H	-1.646267	0.363860	-1.412843
H	-0.031291	0.543536	-2.107326

38

1 + 1,3,5b-*c*-$C_5H_3(CH_3)_3$ TS = **1** + 2,4,5b-*c*-$C_5H_3(CH_3)_3$ TS

C	-0.009420	-0.002889	0.000059
C	-0.389498	-0.273266	-1.439725
C	-1.014960	0.886025	-1.899403
C	-0.692498	1.966404	-1.063161
C	0.170690	1.491719	-0.070315
H	0.481190	2.087279	0.783657
C	-1.092364	3.396943	-1.277897
H	-1.068442	3.669019	-2.336532
H	-2.110302	3.573022	-0.918493
H	-0.429223	4.074175	-0.736828
H	-1.568368	0.964616	-2.829225
C	-0.686566	-1.655683	-1.937160
H	-0.712196	-1.684669	-3.029617
H	0.054876	-2.378008	-1.589986
H	-1.664948	-1.992773	-1.576955
C	-1.149615	-0.404317	0.954735
H	-1.312375	-1.485059	0.918902
H	-0.901388	-0.136747	1.984115
H	-2.077980	0.097777	0.677072
H	0.884595	-0.539632	0.313195
C	1.752913	0.244826	-2.081488
C	2.035501	1.305460	-1.197216
C	2.989424	1.071575	-0.041999
H	4.020001	1.023165	-0.417875
H	2.944110	1.894749	0.675055
H	2.804872	0.143652	0.498562
C	2.148900	2.715321	-1.739909
H	3.092067	2.830956	-2.290136

H	1.339762	2.974231	-2.421078
H	2.150530	3.445745	-0.926328
C	1.502587	0.543771	-3.543082
H	0.837851	1.394327	-3.687658
H	2.446886	0.769811	-4.057125
H	1.056576	-0.319299	-4.045013
C	2.421322	-1.098316	-1.869646
H	2.290575	-1.504482	-0.864975
H	2.043678	-1.836730	-2.579793
H	3.502882	-1.012010	-2.039395

38

1 + 1,3,5b-*c*-$C_5H_3(CH_3)_3$ = **1** + 2,4,5b-*c*-$C_5H_3(CH_3)_3$

C	0.003667	-0.002106	0.003278
C	-1.413329	-0.425007	0.576258
C	-2.426228	0.545488	-0.019393
C	-2.258586	1.738273	0.553565
C	-1.099291	1.586906	1.529598
C	0.215518	1.433706	0.681825
C	1.431909	1.510390	1.617178
H	1.402562	0.781121	2.427099
H	2.365237	1.363357	1.067627
H	1.473655	2.505347	2.069396
C	0.372680	2.581809	-0.322218
H	-0.448193	2.634284	-1.036913
H	0.414506	3.535001	0.214628
H	1.304508	2.482928	-0.885993
H	-1.024641	2.365850	2.293863
C	-1.319606	0.141889	2.017506
C	-2.520392	-0.097653	2.921848
H	-2.394516	0.432226	3.869652
H	-3.449254	0.241655	2.460433
H	-2.622834	-1.161631	3.151886
H	-0.432644	-0.245093	2.525495
C	-2.972584	3.024203	0.298709
H	-3.468230	3.372947	1.210508
H	-2.273693	3.810522	-0.002185
H	-3.726560	2.911372	-0.482384
H	-3.115520	0.301177	-0.820934
C	-1.773534	-1.893879	0.445524
H	-1.709073	-2.230347	-0.593531
H	-1.113789	-2.523867	1.047442
H	-2.799206	-2.062210	0.783951
C	1.079423	-1.025356	0.400452
H	0.894261	-1.972870	-0.111838
H	2.070752	-0.682565	0.093644
H	1.114145	-1.230340	1.471402
C	-0.003991	0.029672	-1.530412
H	-0.211507	-0.971366	-1.920045
H	-0.754190	0.707288	-1.936012
H	0.972837	0.330817	-1.919075

38

1 + 1,4,5a-*c*-$C_5H_3(CH_3)_3$ TS

C	-0.029371	0.045300	-0.022240
C	1.038816	1.017418	-0.486256
C	1.668499	0.357978	-1.557443
C	0.815075	-0.617634	-2.067453
C	-0.377952	-0.623597	-1.330344
C	-1.446057	-1.669497	-1.441155
H	-1.111089	-2.619249	-1.010699
H	-2.354737	-1.376070	-0.911385
H	-1.704585	-1.856836	-2.486633
H	0.991235	-1.202434	-2.962301
H	2.616580	0.654833	-1.989640
C	1.753401	1.931077	0.467286
H	2.402187	2.627035	-0.070540
H	1.057895	2.513859	1.074082
H	2.385821	1.357285	1.152457
H	0.579653	-0.719323	0.492126
C	-1.123742	0.424710	0.963441
H	-1.944656	0.970184	0.512151
H	-1.542515	-0.481738	1.407866
H	-0.715233	1.024632	1.781159
C	-0.308386	2.273785	-1.733368
C	-1.208235	1.323454	-2.265939
C	-2.673177	1.357848	-1.873050
H	-3.211030	1.951920	-2.624467

H	-3.129571	0.364982	-1.884107
H	-2.875722	1.822295	-0.911644
C	-1.084401	0.916319	-3.721881
H	-1.447893	1.728770	-4.365988
H	-0.065410	0.687954	-4.024141
H	-1.704312	0.039092	-3.929697
C	0.718504	2.899648	-2.659310
H	1.174953	2.184205	-3.339209
H	0.236631	3.676671	-3.268152
H	1.517484	3.382973	-2.090687
C	-0.795402	3.296131	-0.718974
H	-1.258944	2.868158	0.167700
H	0.033116	3.924265	-0.386016
H	-1.530765	3.961461	-1.189357

38

1 + 1,4,5a-*c*-$C_5H_3(CH_3)_3$

C	-0.001310	0.003362	0.005037
C	0.754395	-1.049207	0.922188
C	1.119110	-2.197749	-0.014280
C	-0.002741	-2.846921	-0.321883
C	-1.157049	-2.155288	0.398086
C	-1.348090	-0.775967	-0.364237
C	-2.631934	-0.049270	0.071432
H	-2.715307	0.121446	1.141856
H	-2.706596	0.919807	-0.428526
H	-3.503489	-0.633321	-0.235102
C	-1.528825	-1.014615	-1.873021
H	-0.685639	-1.528651	-2.331175
H	-2.423890	-1.619471	-2.046120
H	-1.674548	-0.066929	-2.398867
C	-2.406853	-2.996151	0.579645
H	-3.147273	-2.486788	1.200784
H	-2.876816	-3.229532	-0.380283
H	-2.154248	-3.942724	1.065475
C	-0.390489	-1.763666	1.690688
H	0.030120	-2.686300	2.103841
C	-1.100248	-1.093010	2.863860
H	-1.589609	-0.148436	2.655213
H	-1.858343	-1.774397	3.261170
H	-0.378315	-0.917986	3.666998
H	-0.120236	-3.669934	-1.017642
H	2.114374	-2.376850	-0.404928
C	1.896875	-0.505743	1.759691
H	2.658396	-0.026510	1.137426
H	1.547028	0.229630	2.487922
H	2.379165	-1.319406	2.308500
C	-0.230031	1.340620	0.730006
H	0.733229	1.818312	0.926546
H	-0.799759	2.023222	0.094312
H	-0.751558	1.257789	1.680296
C	0.856979	0.365951	-1.218857
H	1.795261	0.821974	-0.889270
H	1.104267	-0.492905	-1.840398
H	0.344625	1.101483	-1.845231

38

1 + 1,4,5b-*c*-$C_5H_3(CH_3)_3$ TS

C	0.002342	0.005382	0.001298
C	0.801143	-1.189114	0.470064
C	0.958834	-1.029974	1.851108
C	0.009613	-0.119792	2.323557
C	-0.777826	0.324651	1.255948
C	-1.720062	1.490295	1.325998
H	-1.164010	2.430695	1.405929
H	-2.346703	1.557317	0.434461
H	-2.371796	1.421349	2.200903
H	-0.170243	0.118808	3.365219
H	1.634450	-1.611869	2.466966
C	1.791316	-1.878265	-0.422114
H	2.079975	-2.851509	-0.016582
H	1.392583	-2.028988	-1.427220
H	2.704207	-1.280617	-0.518884
C	0.928803	1.172821	-0.386647
H	1.541367	0.904770	-1.251345
H	0.341875	2.055477	-0.653477
H	1.589011	1.429379	0.444056
H	-0.632656	-0.210398	-0.858365

C	-1.060863	-2.458767	0.525764
C	-2.018605	-1.540013	1.003499
C	-3.075819	-1.026815	0.046834
H	-3.740390	-1.849686	-0.248390
H	-3.698502	-0.266645	0.522080
H	-2.669168	-0.603384	-0.873328
C	-2.547377	-1.685129	2.414423
H	-3.250328	-2.527270	2.470121
H	-1.759015	-1.866318	3.142864
H	-3.090582	-0.787193	2.721206
C	-0.580699	-3.570610	1.433851
H	-0.347311	-3.222064	2.438318
H	-1.352989	-4.346554	1.523136
H	0.314279	-4.047935	1.025652
C	-1.128782	-2.893927	-0.924135
H	-1.143594	-2.064259	-1.633194
H	-0.287208	-3.540720	-1.178862
H	-2.045079	-3.474550	-1.095059

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1 + 1,4,5b-*c*-$C_5H_3(CH_3)_3$

C	-0.000853	-0.000592	-0.004667
C	1.120964	1.107651	-0.173062
C	1.418990	1.617347	1.231135
C	0.374915	2.336143	1.636272
C	-0.659025	2.333184	0.517614
C	-1.258688	0.865415	0.483137
C	-2.455571	0.798702	-0.478935
H	-2.231748	1.166165	-1.481525
H	-2.820730	-0.226788	-0.572481
H	-3.280067	1.396944	-0.083121
C	-1.800367	0.453597	1.858435
H	-1.040603	0.477859	2.638613
H	-2.608285	1.128833	2.155655
H	-2.219945	-0.555638	1.824893
C	-1.667445	3.467117	0.567803
H	-2.256653	3.521221	-0.350908
H	-2.358548	3.351528	1.407988
H	-1.153223	4.423561	0.692666
C	0.277078	2.286630	-0.713468
C	1.030426	3.566992	-1.045292
H	0.333839	4.354149	-1.345768
H	1.610105	3.929598	-0.194645
H	1.715293	3.402246	-1.881330
H	-0.278043	1.983691	-1.606084
H	0.222666	2.786007	2.610832
H	2.301075	1.355176	1.804277
C	2.338977	0.708385	-0.986943
H	2.802025	-0.201841	-0.594537
H	2.081928	0.533409	-2.034531
H	3.090642	1.501299	-0.954389
C	-0.239991	-0.727110	-1.337742
H	0.646737	-1.307241	-1.605084
H	-1.069588	-1.432773	-1.251100
H	-0.458670	-0.055114	-2.168940
C	0.432681	-1.082866	0.992999
H	1.334168	-1.583552	0.627443
H	0.649820	-0.684679	1.983348
H	-0.341186	-1.848359	1.097307

38

1 + 1,5a,5b-*c*-$C_5H_3(CH_3)_3$ TS

C	0.012343	0.000475	0.009797
C	0.676090	-0.846965	1.094141
C	0.780611	-2.131756	0.544387
C	0.723836	-2.044948	-0.847501
C	0.608063	-0.693504	-1.200752
H	0.420940	-0.349625	-2.214387
H	0.885617	-2.864116	-1.535271
H	0.993269	-3.029351	1.112579
C	0.482752	-0.563283	2.551682
H	1.100901	-1.224996	3.163787
H	0.734034	0.469872	2.801928
H	-0.561699	-0.726286	2.842570
C	-1.514721	-0.322416	0.051264
H	-2.017895	0.152203	-0.794541
H	-1.702311	-1.393471	0.017402
H	-1.950671	0.087176	0.967542

C	0.083097	1.521085	0.098919
H	1.077133	1.926894	-0.003535
H	-0.533028	1.958636	-0.691997
H	-0.331516	1.858199	1.053744
C	2.825965	-0.260064	0.532225
C	2.697426	-0.088628	-0.867215
C	2.801493	1.297547	-1.493896
H	3.738675	1.349176	-2.059289
H	1.993419	1.502172	-2.202176
H	2.832302	2.110354	-0.770721
C	3.341670	-1.104536	-1.798485
H	4.430098	-0.960245	-1.803924
H	3.144963	-2.136943	-1.522187
H	2.986898	-0.957876	-2.822919
C	3.559706	-1.484237	1.045410
H	3.318758	-2.392333	0.498240
H	4.643443	-1.324868	0.960382
H	3.337442	-1.657877	2.101878
C	3.069291	0.913044	1.466131
H	2.374209	1.742889	1.366133
H	3.026323	0.578968	2.505017
H	4.080817	1.307271	1.302912

38

1 + 1,5a,5b-*c*-$C_5H_3(CH_3)_3$

C	-0.002285	0.009467	0.006084
C	-1.506630	0.471782	-0.235340
C	-1.983354	-0.409519	-1.387777
C	-1.389963	0.012115	-2.501957
C	-0.483439	1.173485	-2.112464
C	0.718230	0.504645	-1.332649
C	1.911931	1.455168	-1.118567
H	1.747229	2.281525	-0.436137
H	2.768589	0.893013	-0.735348
H	2.210823	1.877308	-2.082377
C	1.315907	-0.635048	-2.181164
H	0.591736	-1.397400	-2.459672
H	1.730945	-0.215921	-3.103401
H	2.134931	-1.125368	-1.648598
H	-0.157980	1.822468	-2.929442
C	-1.372591	1.829929	-1.015232
C	-2.723417	2.347461	-1.552063
H	-2.544772	3.129448	-2.296085
H	-3.339814	1.579497	-2.010767
H	-3.294006	2.804019	-0.738067
C	-0.802949	3.043505	-0.268820
H	0.208472	2.952081	0.094457
H	-0.828699	3.910668	-0.935408
H	-1.443928	3.280365	0.586171
H	-1.460091	-0.425993	-3.489292
H	-2.641687	-1.263113	-1.273493
C	-2.396401	0.478346	0.993395
H	-2.424501	-0.506080	1.469408
H	-2.048443	1.199279	1.737310
H	-3.421664	0.741883	0.720204
C	0.592235	0.586024	1.304103
H	0.121244	0.100776	2.163198
H	1.661784	0.365930	1.358886
H	0.462366	1.656905	1.433638
C	0.067401	-1.515890	0.202780
H	-0.537650	-1.805830	1.066775
H	-0.287177	-2.080195	-0.657325
H	1.094979	-1.827032	0.411424

38

1 + 2,3,5a-*c*-$C_5H_3(CH_3)_3$ TS

C	-0.039219	-0.027508	0.009499
C	-0.374972	-1.273721	-0.766245
C	-1.340372	-0.897604	-1.707864
C	-1.237078	0.489134	-1.914118
C	-0.193032	0.975454	-1.111301
H	0.007490	2.036408	-0.982782
C	-2.028183	1.274139	-2.918177
H	-1.634352	2.286195	-3.023534
H	-2.021420	0.804213	-3.906788
H	-3.075267	1.352812	-2.609665
C	-2.253067	-1.817519	-2.463932
H	-3.288378	-1.697933	-2.129994

H	-2.239314	-1.616605	-3.539744
H	-1.971442	-2.860565	-2.310757
H	-0.303958	-2.274828	-0.349222
H	-0.947241	0.154464	0.609564
C	1.107098	0.001819	1.008414
H	2.043233	-0.380039	0.622081
H	1.269485	1.022231	1.365980
H	0.841192	-0.609554	1.874633
C	1.484478	-1.115470	-2.071630
C	1.529819	0.280083	-2.278711
C	2.625132	1.141975	-1.671614
H	3.555986	1.007753	-2.237834
H	2.357197	2.198900	-1.746128
H	2.842054	0.936207	-0.627659
C	1.142010	0.824756	-3.641347
H	1.967113	0.668755	-4.348998
H	0.258602	0.347541	-4.059690
H	0.950166	1.900025	-3.592476
C	1.000955	-2.018949	-3.190692
H	0.095808	-1.663443	-3.677509
H	1.778694	-2.107229	-3.961574
H	0.802593	-3.025386	-2.810537
C	2.553287	-1.831009	-1.259092
H	3.225155	-1.163306	-0.723881
H	2.132214	-2.541723	-0.541639
H	3.177516	-2.412224	-1.948436

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1 + 2,3,5a-*c*-$C_5H_3(CH_3)_3$

C	0.004002	0.007940	-0.004570
C	-0.875434	-0.809921	1.011942
C	-2.298964	-0.263549	0.911632
C	-2.291081	0.950211	1.478840
C	-0.862357	1.208575	1.955337
C	0.013636	1.454481	0.671761
C	1.411370	1.978874	1.038368
H	1.969855	1.339043	1.715456
H	2.017079	2.123272	0.139251
H	1.310622	2.955000	1.521566
C	-0.605654	2.553757	-0.205645
H	-1.613051	2.315522	-0.543356
H	-0.653592	3.489193	0.360995
H	0.012280	2.738858	-1.088868
H	-0.760840	2.002162	2.701506
C	-0.508840	-0.233770	2.405374
H	-1.287642	-0.554224	3.102042
C	0.806962	-0.568729	3.104207
H	1.716184	-0.326260	2.567335
H	0.844568	-0.043414	4.063010
H	0.832247	-1.640765	3.320445
C	-3.394288	1.946261	1.635566
H	-3.575393	2.152729	2.695442
H	-3.133279	2.900454	1.167820
H	-4.328774	1.595116	1.195172
C	-3.413460	-1.010894	0.253495
H	-3.602105	-1.954432	0.775906
H	-4.341914	-0.437817	0.244938
H	-3.160243	-1.266889	-0.779822
H	-0.785912	-1.892382	0.881136
C	1.394058	-0.624718	-0.179578
H	1.280245	-1.619479	-0.619970
H	2.003089	-0.032913	-0.868769
H	1.955672	-0.741869	0.742708
C	-0.623106	-0.016744	-1.407393
H	-0.684957	-1.050800	-1.761378
H	-1.625790	0.406897	-1.435970
H	-0.002391	0.534999	-2.119068

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1 + 2,3,5b-*c*-$C_5H_3(CH_3)_3$ TS

C	-0.035290	-0.007194	-0.002396
C	-0.396888	-1.246617	-0.783724
C	-1.359822	-0.877890	-1.723098
C	-1.277916	0.518268	-1.913646
C	-0.264651	1.011485	-1.091719
H	-0.068416	2.071730	-0.957502
C	-2.053066	1.291808	-2.938000
H	-1.689945	2.318128	-3.011071

H	-1.985317	0.836793	-3.931486
H	-3.115099	1.328527	-2.676249
C	-2.234849	-1.802663	-2.515308
H	-3.289991	-1.643362	-2.272303
H	-2.128616	-1.643106	-3.593240
H	-1.995568	-2.845869	-2.303137
H	-0.321997	-2.247657	-0.367851
C	-0.974740	0.211489	1.198595
H	-0.747141	1.158751	1.693077
H	-2.016851	0.228350	0.875936
H	-0.849175	-0.589009	1.931435
H	0.983283	-0.014904	0.377503
C	1.467188	-1.078517	-1.982002
C	1.548241	0.315104	-2.174266
C	2.590864	1.124310	-1.427863
H	3.581790	0.955978	-1.870077
H	2.380007	2.193743	-1.505333
H	2.668598	0.875845	-0.369857
C	1.257808	0.894654	-3.542627
H	2.098538	0.705125	-4.223409
H	0.365659	0.469718	-4.000299
H	1.118686	1.977508	-3.483640
C	1.092503	-1.969400	-3.147649
H	0.246549	-1.586514	-3.716581
H	1.938530	-2.066128	-3.841248
H	0.833884	-2.973517	-2.800790
C	2.422685	-1.768934	-1.028373
H	2.546850	-1.252974	-0.076805
H	2.089346	-2.787571	-0.815219
H	3.418514	-1.842271	-1.485277

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1 + 2,3,5b-*c*-$C_5H_3(CH_3)_3$

C	0.007675	0.011847	-0.002960
C	-1.398475	-0.398857	0.566426
C	-2.440560	0.539331	-0.032555
C	-2.261549	1.736146	0.538869
C	-1.100648	1.592029	1.516840
C	0.221892	1.444003	0.680679
C	1.436902	1.509911	1.618325
H	1.396866	0.785491	2.432056
H	2.368833	1.346424	1.070565
H	1.491727	2.506321	2.065918
C	0.385460	2.595755	-0.317983
H	-0.438839	2.659909	-1.027736
H	0.437370	3.545478	0.223928
H	1.314079	2.492278	-0.886439
H	-1.037356	2.372707	2.280765
C	-1.318942	0.144788	2.009741
C	-2.531514	-0.097748	2.897247
H	-2.411509	0.411716	3.857033
H	-3.450645	0.262810	2.432609
H	-2.648520	-1.165209	3.102155
H	-0.436863	-0.235168	2.529060
C	-2.970430	3.030174	0.304495
H	-3.460205	3.368832	1.223623
H	-2.267118	3.816681	0.013632
H	-3.730446	2.947247	-0.473971
C	-3.406681	0.111977	-1.088918
H	-4.063103	-0.677882	-0.708675
H	-4.032688	0.937374	-1.431472
H	-2.883101	-0.303050	-1.955795
H	-1.611542	-1.465507	0.448555
C	1.056119	-1.034648	0.403664
H	0.819717	-1.986674	-0.080038
H	2.056589	-0.741128	0.074794
H	1.097239	-1.213006	1.478377
C	0.003947	0.044718	-1.535743
H	-0.237460	-0.950444	-1.922666
H	-0.723413	0.747280	-1.941523
H	0.989712	0.316413	-1.923864

38

1 + 2,5a,5b-*c*-$C_5H_3(CH_3)_3$ TS

C	-0.028862	-0.014453	0.011762
C	0.678908	-0.875532	1.047081
C	0.750780	-2.165418	0.504965
C	0.668511	-2.044750	-0.890464

C	0.540187	-0.693935	-1.222050
H	0.347023	-0.333023	-2.228551
H	0.817859	-2.856614	-1.591814
C	0.971940	-3.437521	1.269140
H	1.436354	-3.241008	2.236894
H	0.019586	-3.942205	1.457549
H	1.608901	-4.134787	0.718755
H	0.594508	-0.685092	2.114919
C	-1.553555	-0.344649	0.093676
H	-2.079764	0.125209	-0.740871
H	-1.737431	-1.416656	0.066345
H	-1.967523	0.063389	1.019719
C	0.036241	1.506310	0.112947
H	1.006148	1.924036	-0.106139
H	-0.674387	1.946572	-0.592277
H	-0.261633	1.824843	1.116364
C	2.758272	-0.230847	0.537764
C	2.672254	-0.062921	-0.863967
C	2.776405	1.313220	-1.509935
H	3.719952	1.360774	-2.065182
H	1.976658	1.503802	-2.231838
H	2.796694	2.137827	-0.799577
C	3.323290	-1.095137	-1.769432
H	4.413696	-0.964005	-1.758396
H	3.109682	-2.121779	-1.482480
H	2.987899	-0.959749	-2.801857
C	3.525633	-1.426886	1.070556
H	3.295613	-2.355486	0.552793
H	4.603199	-1.247431	0.958118
H	3.327132	-1.574991	2.135099
C	2.928253	0.941488	1.490111
H	2.330754	1.818172	1.262360
H	2.683909	0.636696	2.510654
H	3.981648	1.251008	1.494429

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1 + 2,5a,5b-*c*-$C_5H_3(CH_3)_3$

C	0.000121	0.004239	-0.001731
C	-1.486634	0.464140	-0.257316
C	-1.998314	-0.418084	-1.393935
C	-1.390930	0.002866	-2.504341
C	-0.478232	1.161661	-2.119761
C	0.727280	0.501238	-1.336773
C	1.919910	1.451094	-1.110033
H	1.765656	2.248811	-0.392027
H	2.785089	0.878996	-0.761899
H	2.200973	1.910596	-2.062108
C	1.330798	-0.635540	-2.184268
H	0.603903	-1.386965	-2.484578
H	1.766931	-0.210679	-3.094099
H	2.135428	-1.138551	-1.641656
H	-0.156666	1.808635	-2.940065
C	-1.370299	1.822773	-1.020130
C	-2.731054	2.325436	-1.544273
H	-2.572128	3.120151	-2.279264
H	-3.337942	1.553690	-2.009996
H	-3.301963	2.759475	-0.718098
C	-0.805095	3.040744	-0.277164
H	0.223287	2.971293	0.041191
H	-0.879868	3.916803	-0.928126
H	-1.416889	3.243797	0.607417
H	-1.478780	-0.430690	-3.493451
C	-2.985020	-1.523278	-1.215639
H	-3.943538	-1.122317	-0.868067
H	-3.154966	-2.056912	-2.152809
H	-2.649919	-2.240903	-0.461201
H	-2.099998	0.462407	0.649567
C	0.560913	0.594075	1.303889
H	0.050294	0.126605	2.150668
H	1.626214	0.366597	1.402236
H	0.434341	1.667464	1.409338
C	0.071815	-1.519263	0.199217
H	-0.558651	-1.807349	1.046358
H	-0.255716	-2.085138	-0.671264
H	1.094555	-1.826542	0.435613

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1 + 1,2,3,4-*c*-$C_5H_2(CH_3)_4$ TS

C	0.012109	-0.000027	-0.007968
C	-0.096832	-1.160591	-0.956381
C	-0.863322	-0.702053	-2.039802
C	-0.863330	0.701968	-2.039809
C	-0.096846	1.160526	-0.956392
C	-0.069597	2.585361	-0.480972
H	-1.066180	2.916317	-0.170093
H	0.599728	2.702354	0.373122
H	0.267499	3.268262	-1.266303
C	-1.490786	1.566451	-3.093295
H	-1.321653	1.171429	-4.099444
H	-2.574640	1.632032	-2.952617
H	-1.092957	2.582324	-3.062000
C	-1.490774	-1.566553	-3.093274
H	-2.574622	-1.632174	-2.952566
H	-1.321683	-1.171521	-4.099426
H	-1.092909	-2.582413	-3.061993
C	-0.069566	-2.585420	-0.480947
H	0.267523	-3.268326	-1.266275
H	0.599773	-2.702400	0.373140
H	-1.066142	-2.916381	-0.170048
H	-0.882196	-0.000029	0.634194
H	0.885523	-0.000017	0.642934
C	1.948081	-0.705420	-1.766681
C	1.948071	0.705371	-1.766688
C	2.806373	1.435925	-0.753335
H	3.869415	1.272092	-0.976042
H	2.632690	2.513033	-0.795580
H	2.644295	1.109652	0.275273
C	1.869844	1.446774	-3.083923
H	2.836141	1.400254	-3.604468
H	1.117370	1.037256	-3.756384
H	1.639517	2.504401	-2.927075
C	1.869863	-1.446840	-3.083908
H	1.117381	-1.037345	-3.756374
H	2.836159	-1.400312	-3.604455
H	1.639553	-2.504468	-2.927045
C	2.806393	-1.435953	-0.753321
H	2.644307	-1.109676	0.275285
H	2.632729	-2.513064	-0.795560
H	3.869432	-1.272101	-0.976028

41

1 + 1,2,3,4-*c*-$C_5H_2(CH_3)_4$

C	0.007461	0.004804	-0.038227
C	1.254688	0.309604	0.889898
C	2.495897	-0.155042	0.122242
C	2.482201	-1.493069	0.104666
C	1.231534	-1.952216	0.860184
C	-0.008937	-1.597672	-0.059287
C	-1.295832	-2.199639	0.526603
H	-1.462920	-1.931169	1.571095
H	-2.170425	-1.881821	-0.045775
H	-1.253198	-3.289978	0.466708
C	0.139593	-2.200985	-1.461989
H	1.024636	-1.843047	-1.986658
H	0.206367	-3.291247	-1.392594
H	-0.734070	-1.970203	-2.078102
C	1.284758	-3.374730	1.390192
H	0.439425	-3.585649	2.048304
H	1.276772	-4.112265	0.581496
H	2.200409	-3.526152	1.968192
C	1.143572	-0.833877	1.909403
H	1.989204	-0.851622	2.601272
H	0.209546	-0.831786	2.477930
C	3.418106	-2.447324	-0.566824
H	3.903854	-3.099614	0.165411
H	2.881837	-3.100294	-1.262832
H	4.199076	-1.926728	-1.122569
C	3.451317	0.797162	-0.524208
H	3.950178	1.419867	0.224776
H	4.221570	0.275466	-1.093709
H	2.928699	1.479071	-1.202625
C	1.336881	1.716316	1.457076
H	1.344253	2.474847	0.668035
H	0.495845	1.927151	2.120700
H	2.255266	1.833713	2.038640
C	-1.267001	0.617370	0.563639

H	-1.202088	1.707806	0.532340
H	-2.147773	0.332598	-0.016604
H	-1.439775	0.325075	1.600784
C	0.168673	0.641602	-1.424632
H	0.257743	1.728068	-1.326630
H	1.046335	0.279527	-1.958774
H	-0.709374	0.445034	-2.046353

41

1 + 1,2,3,5a-*c*-$C_5H_2(CH_3)_4$ TS = **1** + 2,3,4,5a-*c*-$C_5H_2(CH_3)_4$ TS

C	0.063291	-0.034959	0.062379
C	-0.583404	0.338200	1.372313
C	-1.526446	-0.666788	1.629790
C	-1.195233	-1.806415	0.881042
C	-0.002401	-1.541356	0.181084
H	0.374253	-2.201416	-0.596926
C	-1.923020	-3.118306	0.926445
H	-2.065991	-3.478738	1.950380
H	-2.917330	-3.027052	0.478747
H	-1.377966	-3.886096	0.375216
C	-2.660048	-0.560408	2.606405
H	-3.560209	-0.169517	2.120415
H	-2.917822	-1.531294	3.037009
H	-2.413160	0.117371	3.426483
C	-0.687118	1.748486	1.865688
H	-0.747081	1.779285	2.958400
H	0.179212	2.340322	1.563075
H	-1.583050	2.247395	1.479260
H	-0.724729	0.169464	-0.683027
C	1.290533	0.721815	-0.424286
H	2.032245	0.884800	0.350457
H	1.762849	0.195251	-1.257157
H	0.986600	1.705222	-0.791700
C	1.189647	-0.706227	2.586569
C	1.451624	-1.788621	1.718242
C	2.737551	-1.840937	0.907346
H	3.565985	-2.148148	1.558346
H	2.657546	-2.592155	0.117018
H	3.018631	-0.902966	0.438922
C	1.090878	-3.192686	2.174877
H	1.845856	-3.549911	2.887372
H	0.122874	-3.252547	2.666251
H	1.082578	-3.888131	1.330800
C	0.410912	-0.948316	3.862177
H	-0.463587	-1.581351	3.723584
H	1.054351	-1.433797	4.609424
H	0.076798	-0.000279	4.295818
C	2.197426	0.406208	2.797366
H	2.957011	0.480539	2.022887
H	1.720692	1.384380	2.911410
H	2.730524	0.213584	3.738069

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1 + 1,2,3,5a-*c*-$C_5H_2(CH_3)_4$ = **1** + 2,3,4,5a-*c*-$C_5H_2(CH_3)_4$

C	-0.014358	0.012241	-0.040969
C	1.225103	0.311751	0.908020
C	2.463143	-0.148476	0.122356
C	2.444098	-1.487166	0.093016
C	1.194546	-1.931276	0.848547
C	-0.039501	-1.584942	-0.057472
C	-1.325939	-2.211708	0.505132
H	-1.563585	-1.912927	1.522213
H	-2.185352	-1.967622	-0.125392
H	-1.220898	-3.300506	0.501400
C	0.121940	-2.195168	-1.458093
H	1.012576	-1.844968	-1.977636
H	0.187273	-3.284895	-1.376403
H	-0.746000	-1.966576	-2.083217
H	1.201778	-2.973992	1.179713
C	1.192537	-0.843347	1.948210
H	2.175179	-0.867414	2.428564
C	0.188894	-0.844079	3.099541
H	-0.852483	-0.709254	2.830566
H	0.268355	-1.787659	3.647298
H	0.448846	-0.043189	3.797937
C	3.387016	-2.450621	-0.552712
H	3.843273	-3.100956	0.200786
H	2.862300	-3.103325	-1.256942

H	4.189082	-1.942972	-1.090671
C	3.435288	0.804845	-0.496171
H	3.927690	1.412370	0.269736
H	4.209802	0.282992	-1.060029
H	2.931021	1.500564	-1.174295
C	1.295573	1.717902	1.473924
H	1.325931	2.474035	0.683371
H	0.432678	1.931949	2.108927
H	2.196000	1.837845	2.083343
C	-1.318285	0.650514	0.467709
H	-1.239627	1.739546	0.412501
H	-2.154249	0.357787	-0.173253
H	-1.580972	0.395440	1.491091
C	0.203400	0.636622	-1.430037
H	0.310993	1.721751	-1.335397
H	1.086240	0.255508	-1.940090
H	-0.662410	0.454699	-2.072826

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1 + 1,2,3,5b-*c*-$C_5H_2(CH_3)_4$ TS = **1** + 2,3,4,5b-*c*-$C_5H_2(CH_3)_4$ TS

C	0.012978	0.002426	-0.006023
C	-0.126345	-1.172342	-0.945170
C	-0.880420	-0.726954	-2.035678
C	-0.849897	0.680537	-2.067510
C	-0.048874	1.124226	-1.010333
H	0.031240	2.170144	-0.726814
C	-1.453728	1.534180	-3.143049
H	-1.138963	1.219965	-4.143641
H	-2.546277	1.476410	-3.120194
H	-1.170274	2.580129	-3.015463
C	-1.531658	-1.599838	-3.066863
H	-2.598509	-1.728593	-2.855504
H	-1.450812	-1.171071	-4.069642
H	-1.080322	-2.593634	-3.088566
C	-0.099713	-2.587047	-0.448663
H	0.194728	-3.285220	-1.237952
H	0.602280	-2.701765	0.379798
H	-1.088166	-2.898706	-0.091705
C	-1.157448	0.052431	0.993778
H	-1.138820	-0.826111	1.644764
H	-1.086631	0.940145	1.626317
H	-2.112716	0.075439	0.466306
H	0.936248	-0.023466	0.570683
C	1.967446	-0.699992	-1.785651
C	1.946131	0.709080	-1.752204
C	2.765403	1.438663	-0.704273
H	3.829548	1.399869	-0.971919
H	2.482483	2.493115	-0.654137
H	2.674018	1.019403	0.297185
C	1.899799	1.484346	-3.053571
H	2.884598	1.465576	-3.538938
H	1.178516	1.081662	-3.762298
H	1.641651	2.531525	-2.872702
C	1.854714	-1.415885	-3.112737
H	1.081322	-0.993782	-3.754043
H	2.804077	-1.361050	-3.663097
H	1.626157	-2.475479	-2.965679
C	2.812556	-1.461837	-0.786231
H	2.649491	-1.160296	0.249758
H	2.624980	-2.535640	-0.854729
H	3.879050	-1.307114	-0.998772

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1 + 1,2,3,5b-*c*-$C_5H_2(CH_3)_4$ = **1** + 2,3,4,5b-*c*-$C_5H_2(CH_3)_4$

C	0.036186	0.008828	-0.036012
C	1.314094	0.336431	0.845581
C	2.531518	-0.119090	0.032291
C	2.536097	-1.456675	0.028802
C	1.315647	-1.906242	0.820785
C	0.041470	-1.592902	-0.039793
C	-1.191761	-2.224270	0.625036
H	-1.342036	-1.902886	1.655847
H	-2.104089	-1.997281	0.067340
H	-1.076500	-3.311893	0.631366
C	0.140076	-2.216228	-1.437119
H	1.003816	-1.861444	-1.998576
H	0.220871	-3.304284	-1.347434
H	-0.756798	-2.002409	-2.025414

H	1.346520	-2.941105	1.174489
C	1.243586	-0.802691	1.892458
C	2.333490	-0.813068	2.955179
H	2.261218	-1.716361	3.566587
H	3.330371	-0.780393	2.511423
H	2.228867	0.045232	3.624435
H	0.275618	-0.800258	2.400522
C	3.471127	-2.415524	-0.633542
H	3.965758	-3.043528	0.114999
H	2.931284	-3.090894	-1.304540
H	4.243613	-1.905601	-1.211193
C	3.462585	0.837821	-0.640906
H	3.987530	1.455821	0.094704
H	4.212088	0.319877	-1.240942
H	2.916693	1.524258	-1.296152
C	1.394164	1.750608	1.393109
H	1.344443	2.497879	0.595170
H	0.580365	1.950572	2.094171
H	2.336386	1.901091	1.926820
C	-1.229684	0.609171	0.595574
H	-1.193252	1.699805	0.532877
H	-2.122023	0.285472	0.054091
H	-1.361166	0.342612	1.645397
C	0.145777	0.630486	-1.434439
H	0.226845	1.718913	-1.352313
H	1.009018	0.270436	-1.992898
H	-0.750279	0.418051	-2.024351

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1 + 1,2,4,5a-*c*-$C_5H_2(CH_3)_4$ TS = **1** + 1,3,4,5a-*c*-$C_5H_2(CH_3)_4$ TS

C	0.012973	-0.009316	-0.001342
C	0.324690	1.237556	-0.804963
C	1.564439	0.968898	-1.421298
C	1.747028	-0.413900	-1.467741
C	0.653411	-1.061516	-0.875690
C	0.611919	-2.521981	-0.537801
H	1.293919	-2.752479	0.287519
H	-0.387178	-2.837761	-0.230813
H	0.915753	-3.131119	-1.393037
H	2.562649	-0.913581	-1.979252
C	2.497821	2.003620	-1.976651
H	3.060452	2.489070	-1.172451
H	3.219076	1.556754	-2.664306
H	1.960583	2.790139	-2.510993
C	-0.089272	2.609774	-0.359695
H	-0.005690	3.330578	-1.178303
H	-1.121038	2.626583	-0.003763
H	0.550014	2.970924	0.453839
H	0.727427	0.080767	0.836266
C	-1.339131	-0.266621	0.646061
H	-2.087085	-0.640092	-0.043565
H	-1.225856	-1.013056	1.436403
H	-1.722518	0.642777	1.116498
C	-0.966481	0.679185	-2.559671
C	-0.814226	-0.723381	-2.616540
C	-1.999326	-1.630489	-2.338802
H	-2.462207	-1.887041	-3.301350
H	-1.702605	-2.577344	-1.880629
H	-2.782293	-1.182856	-1.732091
C	0.039017	-1.330265	-3.714742
H	-0.488655	-1.264826	-4.676234
H	1.003635	-0.842738	-3.834066
H	0.218732	-2.391616	-3.519063
C	-0.310139	1.520229	-3.636717
H	0.705304	1.205322	-3.869427
H	-0.897336	1.449794	-4.562532
H	-0.284017	2.575979	-3.353618
C	-2.291806	1.294569	-2.143945
H	-2.678492	0.935324	-1.192746
H	-2.201054	2.380401	-2.072211
H	-3.050831	1.088171	-2.909853

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1 + 1,2,4,5a-*c*-$C_5H_2(CH_3)_4$ = **1** + 1,3,4,5a-*c*-$C_5H_2(CH_3)_4$

C	-0.008721	0.003309	-0.031967
C	1.224090	0.313804	0.921424
C	2.460119	-0.144144	0.136709
C	2.432034	-1.477971	0.110986

C	1.201572	-1.952633	0.878243
C	-0.034153	-1.595767	-0.045992
C	-1.345280	-2.205267	0.479755
H	-1.585033	-1.946176	1.507980
H	-2.185795	-1.897634	-0.147674
H	-1.288728	-3.295288	0.422614
C	0.144229	-2.205340	-1.446677
H	1.056153	-1.878932	-1.943728
H	0.176759	-3.296284	-1.372170
H	-0.703549	-1.952394	-2.089628
C	1.266914	-3.382679	1.381773
H	0.415329	-3.623998	2.022194
H	1.278966	-4.098545	0.554645
H	2.179957	-3.532672	1.964626
C	1.192301	-0.838476	1.960317
H	2.173791	-0.860789	2.445420
C	0.184489	-0.841657	3.107115
H	-0.861323	-0.775588	2.829038
H	0.311449	-1.754276	3.697044
H	0.398884	-0.000483	3.772948
H	3.117855	-2.132858	-0.416744
C	3.438812	0.788758	-0.499233
H	3.936504	1.405673	0.255406
H	4.203443	0.235758	-1.047762
H	2.942513	1.475353	-1.191956
C	1.290950	1.722911	1.480769
H	1.322835	2.474814	0.686264
H	0.427443	1.940562	2.113336
H	2.190457	1.845926	2.090966
C	-1.309672	0.646146	0.478667
H	-1.223694	1.734736	0.427952
H	-2.148133	0.363073	-0.162722
H	-1.571796	0.387751	1.501762
C	0.208862	0.623339	-1.422796
H	0.325387	1.707892	-1.331869
H	1.085799	0.232530	-1.935860
H	-0.660738	0.446403	-2.061727

41

1 + 1,2,4,5b-*c*-$C_5H_2(CH_3)_4$ TS = **1** + 1,3,4,5b-*c*-$C_5H_2(CH_3)_4$ TS

C	-0.007158	0.005814	-0.002301
C	-0.115591	-1.159271	-0.954606
C	-0.856309	-0.707460	-2.055853
C	-0.835182	0.692830	-2.059964
C	-0.087584	1.160979	-0.974287
C	-0.080379	2.587117	-0.506864
H	-1.046476	2.851217	-0.063061
H	0.684904	2.759788	0.252405
H	0.096158	3.275693	-1.337197
H	-1.242410	1.316262	-2.848927
C	-1.496626	-1.589703	-3.085972
H	-2.411848	-2.045014	-2.693718
H	-1.762105	-1.025197	-3.982041
H	-0.834004	-2.406799	-3.381854
C	-0.112101	-2.581433	-0.478164
H	0.179376	-3.270845	-1.276419
H	0.575476	-2.721607	0.358375
H	-1.110415	-2.883960	-0.140340
C	-1.191810	0.027306	0.981701
H	-1.172377	-0.857107	1.623916
H	-1.140856	0.909518	1.625251
H	-2.139156	0.045115	0.439194
H	0.909789	-0.001719	0.587601
C	1.959851	-0.701353	-1.767098
C	1.966021	0.708045	-1.756902
C	2.821250	1.424539	-0.730342
H	3.883643	1.226671	-0.925592
H	2.680788	2.505456	-0.790099
H	2.626120	1.116937	0.298564
C	1.903912	1.457811	-3.071018
H	2.870087	1.397946	-3.590140
H	1.143549	1.064512	-3.743802
H	1.689673	2.517023	-2.904804
C	1.880064	-1.432772	-3.088240
H	1.128430	-1.015342	-3.757228
H	2.846767	-1.380872	-3.607403
H	1.651050	-2.491554	-2.937571
C	2.793653	-1.448104	-0.747162

H	2.626903	-1.121021	0.280472
H	2.604004	-2.522288	-0.794853
H	3.861054	-1.299008	-0.959078

41

1 + 1,2,4,5b-*c*-$C_5H_2(CH_3)_4$ = **1** + 1,3,4,5b-*c*-$C_5H_2(CH_3)_4$

C	0.033641	0.003561	-0.028927
C	1.300769	0.309898	0.876117
C	2.517132	-0.146390	0.066043
C	2.490674	-1.478800	0.039518
C	1.279529	-1.955103	0.829019
C	0.010177	-1.599310	-0.047860
C	-1.261588	-2.198574	0.574130
H	-1.411635	-1.920731	1.618343
H	-2.149016	-1.891071	0.015741
H	-1.215449	-3.289303	0.525129
C	0.116390	-2.207294	-1.452590
H	1.008330	-1.884273	-1.987843
H	0.145590	-3.298617	-1.381741
H	-0.756829	-1.947061	-2.057315
C	1.362859	-3.384591	1.334671
H	0.565168	-3.605803	2.048203
H	1.293164	-4.104122	0.513486
H	2.318727	-3.550714	1.838169
C	1.206101	-0.842537	1.901825
C	2.273590	-0.872046	2.986626
H	2.166175	-1.766441	3.606058
H	3.280491	-0.868553	2.564651
H	2.174366	-0.005829	3.646265
H	0.228364	-0.842250	2.393312
H	3.164586	-2.130422	-0.507161
C	3.474859	0.788470	-0.597837
H	4.002717	1.397606	0.142682
H	4.216280	0.239413	-1.180870
H	2.953502	1.482890	-1.264154
C	1.389255	1.716839	1.441149
H	1.349751	2.473840	0.651864
H	0.574337	1.915750	2.141005
H	2.330310	1.852941	1.980659
C	-1.228343	0.624437	0.590435
H	-1.161552	1.714558	0.549653
H	-2.118237	0.336859	0.025702
H	-1.387199	0.340877	1.632054
C	0.172954	0.635025	-1.420694
H	0.281753	1.720216	-1.327965
H	1.030421	0.256547	-1.975872
H	-0.723022	0.451732	-2.020200

41

1 + 1,2,5a,5b-*c*-$C_5H_2(CH_3)_4$ TS = **1** + 3,4,5a,5b-*c*-$C_5H_2(CH_3)_4$ TS

C	0.002476	0.003651	-0.003280
C	1.188014	0.902044	0.298291
C	0.748315	2.215794	0.097749
C	-0.649095	2.230446	0.173285
C	-1.103110	0.935522	0.477904
H	-2.150433	0.649580	0.416706
H	-1.261153	3.123481	0.145354
C	1.639033	3.404921	-0.106394
H	2.051822	3.411309	-1.120294
H	1.092751	4.339257	0.038933
H	2.485121	3.394507	0.585132
C	2.602898	0.445207	0.144707
H	3.288652	1.089846	0.702856
H	2.734373	-0.578981	0.501826
H	2.918742	0.469219	-0.906061
C	-0.134915	-0.113051	-1.553289
H	-0.238065	0.862385	-2.024610
H	0.746033	-0.616168	-1.962414
H	-1.008873	-0.720914	-1.803581
C	0.072543	-1.437666	0.494404
H	0.458122	-1.526756	1.501447
H	-0.915095	-1.904548	0.448859
H	0.733430	-2.015540	-0.157445
C	0.639997	0.929888	2.668742
C	-0.770077	0.888238	2.559362
C	-1.552639	-0.343649	2.993132
H	-1.666684	-0.328642	4.084249
H	-2.560087	-0.322486	2.568657

H	-1.105162	-1.294663	2.724356
C	-1.559763	2.129552	2.952686
H	-1.602807	2.203803	4.046802
H	-1.128509	3.052627	2.574147
H	-2.588585	2.064736	2.586710
C	1.317130	2.243825	2.991109
H	0.924327	3.087098	2.426803
H	1.187272	2.475946	4.057649
H	2.393720	2.177781	2.804827
C	1.441627	-0.217750	3.250607
H	0.894414	-1.153284	3.341051
H	2.364351	-0.407049	2.693257
H	1.749165	0.061010	4.266709

41

1 + 1,2,5a,5b-*c*-$C_5H_2(CH_3)_4$ = **1** + 3,4,5a,5b-*c*-$C_5H_2(CH_3)_4$

C	0.000884	0.011586	-0.001024
C	1.255828	0.317591	0.937476
C	2.460833	-0.138520	0.102836
C	2.432757	-1.470868	0.070114
C	1.224776	-1.928583	0.876901
C	-0.027799	-1.586746	-0.013211
C	-1.326886	-2.221657	0.516071
H	-1.639761	-1.899556	1.503159
H	-2.152768	-2.019534	-0.172001
H	-1.199732	-3.307459	0.553714
C	0.139232	-2.204742	-1.413740
H	1.042768	-1.879849	-1.925270
H	0.182167	-3.294611	-1.322965
H	-0.717403	-1.964019	-2.049322
H	1.241792	-2.969059	1.212381
C	1.244970	-0.842118	1.994772
C	2.524738	-0.892766	2.854621
H	2.521004	-1.805569	3.457917
H	3.445009	-0.874953	2.276715
H	2.540321	-0.049671	3.551373
C	0.119594	-0.851375	3.038392
H	-0.885472	-0.741674	2.662632
H	0.160192	-1.789976	3.599856
H	0.286606	-0.042141	3.755564
H	3.107804	-2.118226	-0.477121
C	3.435293	0.795371	-0.535615
H	3.978815	1.364982	0.225941
H	4.163341	0.248042	-1.137366
H	2.932436	1.525382	-1.177120
C	1.325819	1.730753	1.485026
H	1.313275	2.474952	0.682952
H	0.481126	1.939182	2.146353
H	2.245260	1.879875	2.057635
C	-1.301762	0.672090	0.487846
H	-1.221151	1.757026	0.378008
H	-2.138488	0.349723	-0.137720
H	-1.567785	0.476424	1.522228
C	0.214942	0.621852	-1.399831
H	0.346688	1.705146	-1.316211
H	1.078393	0.217592	-1.923872
H	-0.665968	0.454106	-2.025511

41

1 + 1,3,5a,5b-*c*-$C_5H_2(CH_3)_4$ TS = **1** + 2,4,5a,5b-*c*-$C_5H_2(CH_3)_4$ TS

C	-0.010946	0.022741	0.000941
C	1.062161	1.017561	-0.444867
C	1.702053	0.395642	-1.527105
C	0.859049	-0.569878	-2.085666
C	-0.342303	-0.552793	-1.360746
H	-1.135316	-1.282970	-1.507169
C	1.152468	-1.403969	-3.298607
H	1.742338	-0.853238	-4.036344
H	1.723386	-2.295634	-3.022996
H	0.231439	-1.739597	-3.778334
H	2.655902	0.703846	-1.941448
C	1.752362	1.923070	0.529329
H	2.414253	2.622263	0.011936
H	1.041019	2.500123	1.123984
H	2.368403	1.342485	1.225757
C	0.712274	-1.079876	0.836177
H	1.574404	-1.485190	0.310059
H	1.044726	-0.659306	1.790297

H	0.017742	-1.893521	1.058554
C	-1.150736	0.493592	0.898090
H	-1.825500	1.192354	0.429427
H	-1.741810	-0.371196	1.213399
H	-0.747830	0.955346	1.804645
C	-0.311044	2.293448	-1.716994
C	-1.210479	1.318496	-2.211958
C	-2.667656	1.300538	-1.765922
H	-3.289905	1.612097	-2.612606
H	-3.007144	0.302300	-1.474677
H	-2.890605	1.986376	-0.950777
C	-1.134689	0.918818	-3.675763
H	-1.553615	1.722445	-4.296191
H	-0.124886	0.726185	-4.028302
H	-1.732689	0.021051	-3.858088
C	0.714701	2.877225	-2.671563
H	1.169447	2.134021	-3.322161
H	0.236665	3.631263	-3.311757
H	1.517075	3.377889	-2.122536
C	-0.757539	3.361660	-0.731928
H	-1.250008	2.993548	0.164795
H	0.101357	3.953663	-0.408452
H	-1.449006	4.054755	-1.228567

41

1 + 1,3,5a,5b-*c*-$C_5H_2(CH_3)_4$ = **1** + 2,4,5a,5b-*c*-$C_5H_2(CH_3)_4$

C	-0.007247	0.009748	-0.002134
C	1.254096	0.314799	0.925458
C	2.446762	-0.158129	0.095678
C	2.441533	-1.490655	0.074041
C	1.222956	-1.930703	0.883292
C	-0.025511	-1.589045	-0.013074
C	-1.313778	-2.231850	0.530303
H	-1.549296	-1.990277	1.561789
H	-2.171958	-1.948248	-0.085224
H	-1.218312	-3.319776	0.468025
C	0.137855	-2.194787	-1.418282
H	1.006570	-1.816476	-1.953930
H	0.238751	-3.281819	-1.337537
H	-0.747404	-1.994758	-2.028478
H	1.237388	-2.971919	1.221666
C	1.244220	-0.838587	1.993330
C	2.524315	-0.900686	2.851889
H	2.473725	-1.770976	3.513155
H	3.441959	-0.965342	2.273044
H	2.588757	-0.016775	3.493076
C	0.120145	-0.831928	3.038746
H	-0.877195	-0.652670	2.668346
H	0.111398	-1.790970	3.566029
H	0.329649	-0.058976	3.784069
C	3.393364	-2.432694	-0.584377
H	3.905232	-3.040769	0.169672
H	2.873074	-3.126932	-1.250556
H	4.147499	-1.894324	-1.161762
H	3.140348	0.498923	-0.418643
C	1.342560	1.731158	1.461094
H	1.306886	2.466631	0.652053
H	0.520116	1.948406	2.147870
H	2.282217	1.879598	1.999503
C	-1.319910	0.659492	0.475815
H	-1.211887	1.747375	0.466544
H	-2.123869	0.415519	-0.224383
H	-1.660276	0.377257	1.466804
C	0.207140	0.631837	-1.396857
H	0.277038	1.719904	-1.306112
H	1.107679	0.282105	-1.896224
H	-0.645698	0.418520	-2.046782

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1 + 1,4,5a,5b-*c*-$C_5H_2(CH_3)_4$ TS

C	-0.001146	0.000090	-0.001392
C	1.038533	1.009528	-0.489020
C	1.665043	0.377793	-1.580730
C	0.819889	-0.601930	-2.091852
C	-0.359764	-0.636805	-1.333591
C	-1.409865	-1.698631	-1.446727
H	-1.066193	-2.636902	-0.995899
H	-2.332082	-1.414637	-0.934687

H	-1.647508	-1.906775	-2.492918
H	0.990166	-1.171592	-2.997451
H	2.601876	0.696725	-2.021387
C	1.760778	1.910926	0.469500
H	2.380948	2.635455	-0.064336
H	1.071015	2.461260	1.112836
H	2.424454	1.329840	1.119276
C	0.768505	-1.058615	0.846687
H	1.649800	-1.430431	0.327427
H	1.076458	-0.614312	1.798012
H	0.108756	-1.900027	1.075842
C	-1.148999	0.457769	0.893476
H	-1.910073	1.019084	0.370403
H	-1.635022	-0.416351	1.335837
H	-0.769445	1.063962	1.721278
C	-0.305792	2.262945	-1.707408
C	-1.217320	1.317304	-2.240734
C	-2.685886	1.362129	-1.854456
H	-3.234161	1.853818	-2.668407
H	-3.124050	0.365942	-1.749321
H	-2.901115	1.931012	-0.952970
C	-1.102044	0.917149	-3.700310
H	-1.461207	1.736842	-4.337620
H	-0.087986	0.680237	-4.010979
H	-1.732766	0.047558	-3.908554
C	0.708154	2.890970	-2.648533
H	1.146860	2.181756	-3.345780
H	0.217208	3.676498	-3.238588
H	1.520803	3.364721	-2.091183
C	-0.775563	3.303409	-0.701956
H	-1.262568	2.900299	0.182794
H	0.068595	3.908178	-0.364528
H	-1.482335	3.988317	-1.187540

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1 + 1,4,5a,5b-*c*-$C_5H_2(CH_3)_4$

C	0.000496	-0.000261	0.003211
C	1.255752	0.310605	0.937128
C	2.447216	-0.154854	0.102438
C	2.430496	-1.484263	0.075769
C	1.234103	-1.956339	0.899355
C	-0.022086	-1.599281	-0.005817
C	-1.327486	-2.226661	0.517878
H	-1.549281	-2.030059	1.562758
H	-2.176588	-1.880308	-0.077040
H	-1.278205	-3.312270	0.398888
C	0.142579	-2.201444	-1.413793
H	1.026011	-1.842921	-1.938149
H	0.213388	-3.290720	-1.344271
H	-0.731814	-1.975930	-2.030701
C	1.305150	-3.392341	1.385259
H	0.476192	-3.631002	2.056093
H	1.271994	-4.097027	0.549381
H	2.239164	-3.566820	1.925659
C	1.247670	-0.839903	1.999907
C	2.521510	-0.882044	2.869426
H	2.463390	-1.726166	3.562838
H	3.442463	-0.972410	2.299841
H	2.584302	0.023555	3.479554
C	0.116511	-0.831985	3.037613
H	-0.881113	-0.675151	2.657782
H	0.118415	-1.779034	3.586134
H	0.310667	-0.043030	3.770195
H	3.092932	-2.142783	-0.474430
H	3.125044	0.508273	-0.422784
C	1.337709	1.728882	1.469922
H	1.289177	2.462289	0.659820
H	0.520101	1.941795	2.163543
H	2.280759	1.886465	1.999331
C	-1.310355	0.657090	0.476030
H	-1.191637	1.743792	0.479451
H	-2.109986	0.429498	-0.234284
H	-1.662850	0.366502	1.460380
C	0.220723	0.619442	-1.392290
H	0.300996	1.706900	-1.302473
H	1.116262	0.260467	-1.894081
H	-0.634499	0.414214	-2.041379

41

1 + 2,3,5a,5b-*c*-$C_5H_2(CH_3)_4$ TS

C	-0.007615	0.006528	-0.001839
C	1.037733	0.989776	-0.512843
C	1.712249	0.330105	-1.551428
C	0.855592	-0.659490	-2.068064
C	-0.337154	-0.624393	-1.340600
H	-1.135651	-1.352164	-1.466702
C	1.150756	-1.525092	-3.257022
H	1.863768	-2.312996	-2.993725
H	0.243435	-2.006732	-3.625186
H	1.592445	-0.956899	-4.081392
C	3.065120	0.674427	-2.099115
H	3.788476	-0.113256	-1.864084
H	3.055216	0.782893	-3.188299
H	3.436894	1.606440	-1.670734
H	1.531778	1.699627	0.148061
C	0.737899	-1.046782	0.877142
H	1.612104	-1.451625	0.370869
H	1.056064	-0.583636	1.815380
H	0.061224	-1.868119	1.125299
C	-1.155889	0.491841	0.878317
H	-1.903309	1.064737	0.351730
H	-1.661174	-0.372278	1.318697
H	-0.767078	1.096122	1.703345
C	-0.294964	2.251572	-1.693943
C	-1.198043	1.307249	-2.237431
C	-2.669105	1.286770	-1.845959
H	-3.257909	1.624152	-2.706979
H	-3.025340	0.282935	-1.595872
H	-2.920709	1.952982	-1.022839
C	-1.057863	0.907110	-3.694142
H	-1.432395	1.714233	-4.338712
H	-0.033619	0.699444	-3.993668
H	-1.656187	0.015945	-3.905014
C	0.730012	2.884919	-2.619536
H	1.199663	2.176262	-3.297214
H	0.242346	3.653713	-3.233297
H	1.521280	3.376110	-2.046601
C	-0.730604	3.281696	-0.662904
H	-1.394454	2.913191	0.112081
H	0.143443	3.711408	-0.166548
H	-1.243537	4.107109	-1.173322

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1 + 2,3,5a,5b-*c*-$C_5H_2(CH_3)_4$

C	0.010773	0.024967	0.007239
C	-1.407897	-0.625967	-0.240254
C	-2.277547	0.491551	-0.817602
C	-2.535205	1.338065	0.184664
C	-1.847050	0.776170	1.428443
C	-0.306199	1.020673	1.218596
C	0.502279	0.762460	2.502140
H	0.319522	-0.198124	2.973724
H	1.574676	0.841945	2.302198
H	0.252790	1.532741	3.237518
C	-0.034295	2.497714	0.884729
H	-0.523718	2.830572	-0.028785
H	-0.389828	3.128510	1.705570
H	1.039462	2.676925	0.778448
H	-2.219348	1.167846	2.380958
C	-2.061543	-0.750105	1.171256
C	-3.552846	-1.140651	1.122776
H	-3.957033	-1.170639	2.139030
H	-4.166903	-0.464256	0.533062
H	-3.657472	-2.146515	0.704939
C	-1.462308	-1.759783	2.159515
H	-0.386456	-1.771989	2.237905
H	-1.867451	-1.573588	3.159181
H	-1.773396	-2.767360	1.868169
C	-3.343843	2.593642	0.198425
H	-4.221298	2.471414	0.843679
H	-2.768937	3.431826	0.603338
H	-3.692638	2.868743	-0.798341
C	-2.718242	0.527698	-2.244103
H	-1.866368	0.444814	-2.925607
H	-3.377210	-0.321636	-2.456977
H	-3.260143	1.444141	-2.483803

H	-1.365938	-1.538868	-0.843119
C	1.122316	-1.004002	0.286420
H	1.155176	-1.727704	-0.533215
H	2.094250	-0.502389	0.311362
H	1.031222	-1.562199	1.211632
C	0.491648	0.738039	-1.271239
H	0.618471	0.001040	-2.070993
H	-0.195228	1.503077	-1.627242
H	1.464224	1.209146	-1.106492

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1 + 1,2,3,4,5a-*c*-$C_5H(CH_3)_5$ TS

C	-0.037381	-0.000912	-0.044573
C	0.257439	1.240130	-0.864766
C	1.512490	0.984230	-1.458805
C	1.730556	-0.398600	-1.487428
C	0.631062	-1.047993	-0.899316
C	0.594925	-2.508826	-0.560629
H	1.386190	-2.775568	0.148869
H	-0.359967	-2.788663	-0.111366
H	0.738218	-3.128665	-1.450883
C	2.911972	-1.085244	-2.107523
H	3.271391	-0.560023	-2.996653
H	3.748658	-1.137116	-1.402844
H	2.666699	-2.108346	-2.399125
C	2.431608	2.017674	-2.041745
H	3.285480	2.198675	-1.380481
H	2.836124	1.707412	-3.009654
H	1.920986	2.971103	-2.185478
C	-0.185465	2.604969	-0.417863
H	-0.144063	3.327443	-1.237375
H	-1.210638	2.590554	-0.043688
H	0.456692	2.986879	0.383122
H	0.661477	0.120101	0.801990
C	-1.393377	-0.279450	0.586796
H	-2.116667	-0.695850	-0.104892
H	-1.272602	-0.998312	1.401134
H	-1.812812	0.630227	1.024203
C	-1.012910	0.676740	-2.593601
C	-0.832107	-0.722919	-2.662206
C	-1.992180	-1.663897	-2.393242
H	-2.425762	-1.956440	-3.359071
H	-1.674110	-2.590112	-1.906596
H	-2.801835	-1.228954	-1.812564
C	0.046102	-1.303030	-3.753441
H	-0.480187	-1.259087	-4.717081
H	0.993360	-0.782556	-3.875037
H	0.262574	-2.357694	-3.556940
C	-0.374647	1.541767	-3.664455
H	0.639377	1.239014	-3.916178
H	-0.972657	1.487446	-4.584355
H	-0.347237	2.592175	-3.361854
C	-2.359034	1.257436	-2.190853
H	-2.750855	0.882335	-1.248022
H	-2.294709	2.344569	-2.109651
H	-3.102535	1.040531	-2.968887

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1 + 1,2,3,4,5a-*c*-$C_5H(CH_3)_5$

C	-0.009120	-0.020394	0.004514
C	1.281116	0.305831	0.866282
C	2.472686	0.046774	-0.066212
C	2.574055	-1.277576	-0.231057
C	1.452400	-1.931696	0.587783
C	0.111970	-1.602493	-0.192376
C	-1.087377	-2.395749	0.355068
H	-1.256092	-2.282991	1.423208
H	-2.004497	-2.101389	-0.161527
H	-0.939936	-3.460913	0.158609
C	0.217976	-2.031365	-1.665799
H	1.022163	-1.531776	-2.203027
H	0.391736	-3.110279	-1.726240
H	-0.717875	-1.826996	-2.193517
C	1.671780	-3.392347	0.938497
H	0.893602	-3.760851	1.610606
H	1.674820	-4.029256	0.048687
H	2.634560	-3.520495	1.441739
C	1.448027	-0.937435	1.777290

H	2.469136	-0.908470	2.172429
C	0.558487	-1.157540	2.998755
H	-0.508010	-1.215699	2.812957
H	0.855539	-2.085116	3.497125
H	0.722915	-0.346027	3.713890
C	3.532760	-2.064098	-1.067511
H	4.141980	-2.726266	-0.444162
H	3.003736	-2.702959	-1.781648
H	4.208113	-1.415907	-1.627601
C	3.286941	1.147968	-0.667671
H	3.801503	1.721831	0.109558
H	4.041303	0.764588	-1.356084
H	2.654974	1.854888	-1.214370
C	1.285559	1.652809	1.566471
H	1.176404	2.480428	0.858973
H	0.473661	1.725398	2.293553
H	2.227505	1.797294	2.103578
C	-1.303441	0.426540	0.706226
H	-1.320955	1.517151	0.778172
H	-2.175505	0.133035	0.116318
H	-1.433551	0.032783	1.711277
C	0.003947	0.765520	-1.317726
H	0.012903	1.840105	-1.110152
H	0.863762	0.538258	-1.945414
H	-0.900380	0.558054	-1.896707

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1 + 1,2,3,4,5b-*c*-$C_5H(CH_3)_5$ TS

C	-0.091947	-0.020030	0.097628
C	-0.173058	-1.154317	1.089010
C	0.508691	-0.722302	2.236344
C	0.610275	0.678634	2.206330
C	-0.005555	1.155224	1.039500
C	0.126439	2.559711	0.524644
H	1.170862	2.796824	0.292266
H	-0.454875	2.700372	-0.388952
H	-0.217341	3.295806	1.256950
C	1.195208	1.524702	3.298242
H	0.885410	1.182163	4.290165
H	2.289592	1.492625	3.275691
H	0.894613	2.568910	3.196381
C	0.969306	-1.596778	3.364749
H	2.056031	-1.729667	3.339585
H	0.721876	-1.167986	4.340494
H	0.515501	-2.587862	3.310433
C	-0.246131	-2.583681	0.634536
H	-0.690379	-3.230958	1.396084
H	-0.844071	-2.677608	-0.274323
H	0.752653	-2.978364	0.416067
C	1.173316	-0.130432	-0.772850
H	1.133449	-1.027141	-1.397005
H	1.260677	0.734829	-1.435387
H	2.065993	-0.181205	-0.146062
H	-0.950090	0.027692	-0.573716
C	-2.252348	-0.537140	1.674722
C	-2.150347	0.869612	1.644825
C	-2.849133	1.630985	0.536280
H	-3.937905	1.551293	0.657502
H	-2.599589	2.693435	0.572502
H	-2.614544	1.264750	-0.464554
C	-2.146842	1.641790	2.946487
H	-3.160697	1.682452	3.367534
H	-1.498328	1.198352	3.700637
H	-1.821363	2.674077	2.789271
C	-2.356584	-1.246020	3.007845
H	-1.648958	-0.868811	3.744660
H	-3.364622	-1.122571	3.426680
H	-2.183289	-2.320100	2.895505
C	-3.056599	-1.236151	0.597005
H	-2.773951	-0.950712	-0.417628
H	-2.962907	-2.320970	0.679281
H	-4.122177	-0.995143	0.710615

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1 + 1,2,3,4,5b-*c*-$C_5H(CH_3)_5$

C	0.033979	-0.020722	0.000041
C	1.348949	0.309108	0.819318
C	2.523034	0.050036	-0.129131

C	2.623596	-1.272964	-0.294068
C	1.518873	-1.927467	0.540455
C	0.154468	-1.606861	-0.197644
C	-1.002577	-2.390761	0.442406
H	-1.081441	-2.248618	1.521293
H	-1.958213	-2.105189	-0.003557
H	-0.870169	-3.459741	0.257412
C	0.194406	-2.045627	-1.667631
H	0.981650	-1.553209	-2.237119
H	0.358728	-3.125983	-1.728948
H	-0.759292	-1.836941	-2.160483
C	1.753916	-3.386004	0.894259
H	1.025629	-3.737948	1.628748
H	1.687053	-4.033334	0.014482
H	2.749857	-3.518696	1.325145
C	1.445943	-0.938460	1.724303
C	2.608357	-0.972373	2.706780
H	2.633394	-1.926348	3.240226
H	3.567618	-0.837184	2.202465
H	2.501423	-0.183715	3.456347
H	0.521063	-1.079518	2.292600
C	3.562901	-2.057105	-1.153878
H	4.202270	-2.704099	-0.544649
H	3.016384	-2.711687	-1.840371
H	4.209738	-1.408225	-1.745929
C	3.319022	1.151135	-0.753951
H	3.869116	1.715388	0.006047
H	4.041587	0.770424	-1.477088
H	2.668022	1.866465	-1.266666
C	1.370992	1.655457	1.522662
H	1.190151	2.480362	0.826730
H	0.613614	1.704468	2.308627
H	2.344662	1.826607	1.989391
C	-1.214620	0.402464	0.790520
H	-1.245676	1.491719	0.874503
H	-2.125443	0.095887	0.270779
H	-1.251586	-0.008636	1.800505
C	-0.018982	0.764456	-1.317416
H	-0.017681	1.839172	-1.110248
H	0.821663	0.548197	-1.975515
H	-0.940331	0.543302	-1.863483

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1 + 1,2,3,5a,5b-*c*-$C_5H(CH_3)_5$ TS = **1** + 2,3,4,5a,5b-*c*-$C_5H(CH_3)_5$ TS

C	1.157773	-0.000605	-0.019264
C	0.622245	0.020480	2.314301
C	-1.130912	0.026606	0.118133
C	-0.789583	-0.016128	2.215137
C	0.713605	1.308040	-0.247387
C	-0.688890	1.326138	-0.194969
C	-0.018804	-0.905291	-0.341248
C	1.305955	1.332815	2.636573
C	1.416311	-1.126818	2.909692
C	-1.576258	-1.243556	2.653004
C	-1.573482	1.225026	2.613837
H	0.913003	2.179014	2.076782
H	1.189244	1.563455	3.704926
H	2.380539	1.265171	2.438709
H	0.863710	-2.058765	3.006182
H	2.339984	-1.327177	2.357606
H	1.721858	-0.842098	3.924852
H	-1.684576	-1.227483	3.744887
H	-2.585780	-1.216869	2.233598
H	-1.135682	-2.197179	2.382801
H	-1.616200	1.290721	3.708734
H	-1.138230	2.151159	2.247804
H	-2.603206	1.169628	2.249263
C	2.575846	-0.456320	-0.160091
H	-2.178779	-0.259807	0.046082
C	1.596109	2.502791	-0.454491
C	-1.549283	2.545958	-0.346428
C	-0.126021	-1.027988	-1.892672
C	0.043528	-2.345888	0.160888
H	3.251421	0.155241	0.445767
H	2.692560	-1.496135	0.153972
H	2.918379	-0.385025	-1.199818
H	1.816817	2.644493	-1.518059
H	1.128247	3.422270	-0.093654
H	2.550953	2.385426	0.062236

H	-1.522279	2.913305	-1.377436
H	-2.588552	2.324467	-0.099136
H	-1.220219	3.370745	0.294001
H	-0.226375	-0.054982	-2.370468
H	0.765567	-1.526043	-2.284923
H	-0.991199	-1.642501	-2.157151
H	0.426940	-2.434582	1.168517
H	-0.946311	-2.808098	0.114737
H	0.702342	-2.929461	-0.487944

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1 + 1,2,3,5a,5b-*c*-$C_5H(CH_3)_5$ = **1** + 2,3,4,5a,5b-*c*-$C_5H(CH_3)_5$

C	-0.000446	-0.000564	0.000121
C	-1.268901	0.903479	-0.340219
C	-2.448753	-0.081760	-0.331096
C	-2.339629	-0.844540	-1.422926
C	-1.089176	-0.380306	-2.167383
C	0.131919	-0.892433	-1.320208
C	1.466193	-0.750438	-2.074191
H	1.718654	0.257921	-2.384666
H	2.291204	-1.126880	-1.462869
H	1.428313	-1.366892	-2.977096
C	0.008052	-2.404199	-1.059056
H	-0.900759	-2.678675	-0.526938
H	0.012804	-2.939868	-2.013732
H	0.861467	-2.766235	-0.478887
H	-1.039030	-0.680398	-3.219430
C	-1.176407	1.148088	-1.887311
C	-2.448456	1.782996	-2.485997
H	-2.353473	1.826492	-3.575259
H	-3.363550	1.246106	-2.246649
H	-2.555550	2.813369	-2.134520
C	-0.051630	2.056361	-2.403850
H	0.932940	1.875525	-2.001125
H	0.014157	1.965341	-3.492595
H	-0.302240	3.098407	-2.184045
C	-3.220608	-1.942618	-1.922177
H	-3.693192	-1.647332	-2.865991
H	-2.645723	-2.850324	-2.128319
H	-4.011109	-2.192217	-1.212457
C	-3.486309	-0.100857	0.744144
H	-4.066999	0.828197	0.737379
H	-4.182008	-0.932410	0.621396
H	-3.031333	-0.180614	1.736320
C	-1.431565	2.139374	0.525162
H	-1.467248	1.886614	1.589179
H	-0.601768	2.834925	0.375593
H	-2.358553	2.665305	0.281278
C	1.264329	0.802722	0.357473
H	1.097988	1.345469	1.291981
H	2.098149	0.117312	0.532732
H	1.589001	1.529020	-0.381019
C	-0.266552	-0.831678	1.271086
H	-0.448816	-0.163139	2.118258
H	-1.119467	-1.501099	1.183210
H	0.610172	-1.434606	1.522590

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1 + 1,2,4,5a,5b-*c*-$C_5H(CH_3)_5$ TS = **1** + 1,3,4,5a,5b-*c*-$C_5H(CH_3)_5$ TS

C	0.006533	-0.006210	-0.002118
C	-0.091035	1.185473	-0.952352
C	0.682930	0.823830	-2.075971
C	0.772853	-0.566927	-2.120074
C	0.088810	-1.122855	-1.030037
C	0.169235	-2.563727	-0.628147
H	1.147131	-2.791549	-0.188286
H	-0.586804	-2.821309	0.116873
H	0.038731	-3.220694	-1.491633
H	1.219122	-1.133819	-2.929951
C	1.278163	1.779936	-3.065983
H	2.193597	2.228205	-2.664393
H	1.537598	1.273917	-3.998534
H	0.597703	2.600673	-3.301611
C	-0.173229	2.593394	-0.440689
H	-0.456913	3.287976	-1.236443
H	-0.904022	2.690690	0.364918
H	0.796847	2.927003	-0.052663
C	1.393926	0.104683	0.702406

H	1.378522	0.934534	1.415660
H	1.599474	-0.809508	1.266378
H	2.199320	0.266825	-0.012205
C	-0.996145	-0.166401	1.136571
H	-1.975036	-0.488541	0.811849
H	-0.625520	-0.914335	1.843184
H	-1.099060	0.770788	1.691303
C	-2.067470	0.661298	-1.843760
C	-2.026523	-0.753710	-1.879428
C	-2.990244	-1.572711	-1.036572
H	-3.800324	-1.920141	-1.690630
H	-2.528849	-2.471563	-0.618449
H	-3.465663	-1.021797	-0.228098
C	-1.817701	-1.451315	-3.211483
H	-2.732301	-1.379851	-3.816128
H	-1.002165	-1.036673	-3.798450
H	-1.616901	-2.515948	-3.057718
C	-1.968290	1.411112	-3.159320
H	-1.201353	1.020161	-3.824680
H	-2.928613	1.341884	-3.687984
H	-1.769171	2.473537	-2.994800
C	-3.024301	1.390911	-0.914680
H	-2.972936	1.088374	0.128190
H	-2.840849	2.466837	-0.952831
H	-4.055711	1.233044	-1.255802

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1 + 1,2,4,5a,5b-*c*-$C_5H(CH_3)_5$ = **1** + 1,3,4,5a,5b-*c*-$C_5H(CH_3)_5$

C	0.000517	-0.000101	0.000182
C	-1.126780	1.129266	-0.024908
C	-1.541642	1.199626	-1.501151
C	-0.530105	1.761055	-2.160980
C	0.570133	2.107640	-1.161133
C	1.207529	0.709113	-0.772378
C	2.502248	0.850599	0.050116
H	2.422974	1.472685	0.936683
H	2.860586	-0.133991	0.361814
H	3.282264	1.286604	-0.579619
C	1.651477	-0.049028	-2.037073
H	0.841383	-0.228184	-2.741065
H	2.425723	0.521932	-2.557437
H	2.090473	-1.014693	-1.770794
C	1.551591	3.169958	-1.621865
H	2.238456	3.457075	-0.821777
H	2.150849	2.817644	-2.466345
H	1.018144	4.066360	-1.948661
C	-0.335732	2.476117	0.065638
C	-1.212099	3.718039	-0.199511
H	-0.593844	4.619491	-0.153885
H	-1.719022	3.703096	-1.161304
H	-1.967725	3.814512	0.585535
C	0.343298	2.805138	1.402884
H	0.897135	2.003728	1.867459
H	1.027161	3.649008	1.268543
H	-0.418157	3.127296	2.119345
H	-0.459134	1.917580	-3.232464
C	-2.845707	0.698385	-2.028329
H	-3.677083	1.276727	-1.611215
H	-2.884293	0.780730	-3.116186
H	-3.017507	-0.346271	-1.751916
C	-2.254727	0.938855	0.972390
H	-2.731002	-0.039919	0.860993
H	-1.888967	1.016645	1.999358
H	-3.029317	1.697632	0.833673
C	0.351200	-0.498899	1.415062
H	-0.529529	-0.964100	1.865716
H	1.119444	-1.274143	1.350108
H	0.710179	0.254206	2.109462
C	-0.510593	-1.273206	-0.705327
H	-1.395666	-1.653143	-0.185458
H	-0.774912	-1.118963	-1.749108
H	0.246125	-2.060942	-0.664542

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1 + 1,2,3,4,5a,5b-*c*-$C_5(CH_3)_6$ TS

C	-0.000103	0.000016	0.000093
C	-0.120136	1.192836	-0.946492
C	0.673243	0.850819	-2.063742

C	0.803615	-0.541393	-2.118288
C	0.112011	-1.105514	-1.032471
C	0.201009	-2.548606	-0.636886
H	1.226418	-2.825408	-0.363838
H	-0.438135	-2.766520	0.221549
H	-0.103479	-3.207644	-1.455292
C	1.521330	-1.314630	-3.184892
H	1.445873	-0.833162	-4.163519
H	2.587540	-1.404385	-2.949656
H	1.122331	-2.326593	-3.277477
C	1.241441	1.816655	-3.061287
H	2.304144	1.997700	-2.865149
H	1.163428	1.443213	-4.086303
H	0.733705	2.781421	-3.019259
C	-0.227671	2.592672	-0.413115
H	-0.549196	3.294447	-1.187211
H	-0.944659	2.655640	0.408028
H	0.740158	2.945914	-0.038114
C	1.379564	0.134502	0.714838
H	1.341387	0.953053	1.440433
H	1.604423	-0.783367	1.265515
H	2.184826	0.327869	0.007355
C	-1.007008	-0.188025	1.131676
H	-1.968503	-0.553775	0.800700
H	-0.614062	-0.911526	1.851378
H	-1.153810	0.749610	1.675213
C	-2.077427	0.662817	-1.825168
C	-2.009080	-0.749987	-1.898292
C	-2.949133	-1.618180	-1.079060
H	-3.746367	-1.977913	-1.742234
H	-2.457365	-2.509686	-0.678705
H	-3.443399	-1.100326	-0.260022
C	-1.774533	-1.407080	-3.244973
H	-2.691813	-1.354815	-3.847749
H	-0.977554	-0.948363	-3.825213
H	-1.535447	-2.467940	-3.120368
C	-1.992971	1.451665	-3.119945
H	-1.230062	1.084970	-3.802755
H	-2.956963	1.396812	-3.643623
H	-1.793224	2.509244	-2.926725
C	-3.058343	1.345414	-0.884473
H	-3.013939	1.011578	0.148902
H	-2.894729	2.425343	-0.886858
H	-4.082866	1.180405	-1.242643

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1 + 1,2,3,4,5a,5b-*c*-$C_5(CH_3)_6$ TS

C	-0.031428	-0.035308	-0.001263
C	-1.116833	0.067372	-1.161713
C	-1.966662	1.286255	-0.774667
C	-2.706768	0.938814	0.281508
C	-2.377696	-0.523670	0.617102
C	-0.924558	-0.472126	1.250648
C	-0.509759	-1.805284	1.901308
H	-0.605723	-2.680509	1.265228
H	0.526855	-1.750738	2.243688
H	-1.127070	-1.981808	2.786235
C	-0.875530	0.537966	2.412368
H	-1.121052	1.555057	2.113663
H	-1.578551	0.238040	3.195404
H	0.120048	0.550505	2.864790
C	-3.421616	-1.252033	1.445366
H	-3.174774	-2.310998	1.552279
H	-3.507787	-0.827995	2.450120
H	-4.406064	-1.183065	0.974836
C	-2.151999	-1.058793	-0.836611
C	-3.430070	-0.977324	-1.697325
H	-4.128422	-1.763298	-1.394873
H	-3.945388	-0.021231	-1.631521
H	-3.184841	-1.161198	-2.747386
C	-1.698252	-2.514464	-1.016696
H	-0.740805	-2.772768	-0.590919
H	-2.446167	-3.186519	-0.584435
H	-1.648699	-2.743439	-2.085468
C	-3.702818	1.744330	1.052053
H	-4.711596	1.335500	0.926127
H	-3.487717	1.725045	2.124928
H	-3.720711	2.785990	0.728121

C	-1.907472	2.585571	-1.511302
H	-2.286801	2.467685	-2.532376
H	-2.500830	3.358687	-1.020812
H	-0.878869	2.949013	-1.598074
C	-0.554139	0.076107	-2.571696
H	0.188372	0.868456	-2.705708
H	-0.071481	-0.875567	-2.808118
H	-1.346327	0.242305	-3.306337
C	1.137230	-0.988345	-0.318460
H	1.683143	-0.616702	-1.189715
H	1.843224	-0.994852	0.516494
H	0.868030	-2.019965	-0.521931
C	0.667598	1.325890	0.192134
H	1.190149	1.606491	-0.727678
H	-0.013441	2.133899	0.449773
H	1.422415	1.258364	0.980001

Table S13. Cartesian coordinates for Diels-Alder transition states and product norbornenes formed from **1** + *c*-$C_5H_x(CF_3)_{6-x}$

32
1 + 1-*c*-$C_5H_5(CF_3)$ TS = **1** + 4-*c*-$C_5H_5(CF_3)$ TS

C	-0.001856	0.007157	0.016161
C	-0.009369	1.168382	-0.933032
C	0.779666	0.818952	-2.024997
C	0.917940	-0.572535	-2.047183
C	0.195256	-1.107480	-0.972959
H	0.239022	-2.149401	-0.677211
H	1.382729	-1.143609	-2.839097
H	1.131302	1.506054	-2.784033
C	-0.153385	2.570534	-0.462768
F	-0.660332	3.378197	-1.413638
F	-0.960238	2.662921	0.609038
F	1.021586	3.123386	-0.092527
H	0.899181	0.071479	0.644332
H	-0.864246	-0.071510	0.671705
C	-2.078237	0.364165	-1.772188
C	-1.831381	-1.019956	-1.686949
C	-2.512956	-1.824296	-0.595074
H	-3.576088	-1.943709	-0.837974
H	-2.083279	-2.826128	-0.522864
H	-2.462190	-1.362676	0.390136
C	-1.679703	-1.824260	-2.964567
H	-2.662760	-1.975351	-3.427769
H	-1.039937	-1.337083	-3.697857
H	-1.260959	-2.811675	-2.753251
C	-2.052029	1.028205	-3.127751
H	-1.160596	0.768788	-3.699838
H	-2.919066	0.703527	-3.718162
H	-2.093497	2.113664	-3.033251
C	-3.008679	1.029074	-0.781976
H	-2.791989	0.785629	0.257951
H	-2.978851	2.114521	-0.883143
H	-4.039403	0.706334	-0.981140

32
1 + 1-*c*-$C_5H_5(CF_3)$ = **1** + 4-*c*-$C_5H_5(CF_3)$

C	-0.003704	-0.001222	0.014328
C	-0.175805	0.342542	-1.527370
C	-1.640523	0.126102	-1.882073
C	-1.849112	-1.189169	-1.883317
C	-0.534940	-1.861528	-1.527575
C	-0.252526	-1.586915	-0.006891
C	0.967204	-2.411524	0.431052
H	1.855890	-2.226528	-0.172395
H	1.224377	-2.216600	1.474771
H	0.726016	-3.474663	0.348355
C	-1.427251	-2.050564	0.861553
H	-2.358457	-1.537989	0.622692
H	-1.586063	-3.122576	0.710826
H	-1.217082	-1.897305	1.923233
H	-0.450072	-2.916124	-1.790669
C	0.449544	-0.892290	-2.201178
H	0.344462	-0.864005	-3.285836
H	1.493968	-1.047107	-1.932023
H	-2.797430	-1.694541	-2.010493
H	-2.367343	0.918584	-2.004313
C	0.373077	1.659190	-2.007998
F	-0.065508	2.702726	-1.278934
F	1.715924	1.703380	-1.982331
F	0.010237	1.902054	-3.279764
C	1.394415	0.382609	0.523943
H	1.504292	1.469069	0.529359
H	1.522191	0.037673	1.552451
H	2.206527	-0.027759	-0.075630
C	-1.009260	0.763111	0.886543
H	-0.800974	1.833588	0.849311
H	-2.042138	0.608901	0.576244
H	-0.919193	0.445082	1.928173

32
1 + 2-*c*-$C_5H_5(CF_3)$ TS = **1** + 3-*c*-$C_5H_5(CF_3)$ TS

C	0.006435	-0.002433	-0.017124
C	-0.221275	-1.028074	1.057863
C	0.508517	-0.583063	2.160800
C	0.763541	0.789733	2.033043
C	0.206863	1.220059	0.833604

H	0.327522	2.217840	0.429540
H	1.187515	1.419242	2.804052
C	0.835651	-1.391161	3.364798
F	2.148255	-1.673695	3.445207
F	0.523943	-0.753331	4.512812
F	0.183996	-2.564545	3.378510
H	-0.443429	-2.070809	0.864818
H	0.961468	-0.238437	-0.510124
H	-0.757710	0.064099	-0.785325
C	-2.216118	-0.208022	1.496942
C	-1.972546	1.176781	1.417175
C	-2.492457	1.970330	0.235333
H	-3.582837	2.073103	0.308969
H	-2.071170	2.977700	0.228320
H	-2.280898	1.511552	-0.730244
C	-1.916657	1.990594	2.691905
H	-2.928775	2.125406	3.095077
H	-1.316870	1.516345	3.467756
H	-1.500385	2.982677	2.501515
C	-2.469256	-0.845427	2.848330
H	-1.777139	-0.510190	3.618601
H	-3.482490	-0.597335	3.189429
H	-2.398714	-1.933410	2.785206
C	-2.996072	-0.898617	0.394404
H	-2.704996	-0.599261	-0.611470
H	-2.894829	-1.983781	0.467602
H	-4.063018	-0.665325	0.501337

32

1 + 2-*c*-$C_5H_5(CF_3)$ = **1** + 3-*c*-$C_5H_5(CF_3)$

C	-0.000582	0.000736	0.010627
C	0.298027	-0.139522	-1.529595
C	1.414213	0.827665	-1.881888
C	0.932848	2.067324	-1.801521
C	-0.527435	1.944045	-1.407273
C	-0.584386	1.486011	0.097167
C	-2.038691	1.552747	0.584939
H	-2.729452	0.981700	-0.035894
H	-2.126299	1.184173	1.610018
H	-2.373406	2.593583	0.582128
C	0.223359	2.433031	0.992313
H	1.274226	2.492440	0.709666
H	-0.197558	3.441037	0.929474
H	0.173073	2.121001	2.038755
H	-1.142469	2.821476	-1.608337
C	-0.885087	0.636521	-2.143228
H	-0.804738	0.729275	-3.226508
H	-1.863419	0.234220	-1.882695
H	1.490235	2.986317	-1.927716
C	2.797668	0.435274	-2.249232
F	2.814687	-0.266236	-3.398961
F	3.598451	1.495666	-2.423323
F	3.376653	-0.352325	-1.324532
H	0.449536	-1.171072	-1.849809
C	-1.006649	-1.087564	0.414835
H	-0.537311	-2.068509	0.302378
H	-1.298746	-0.983581	1.462548
H	-1.915173	-1.085173	-0.187873
C	1.253064	-0.226177	0.860814
H	1.647943	-1.228977	0.676894
H	2.050663	0.483113	0.644944
H	1.013458	-0.153040	1.925168

32

1 + 5a-*c*-$C_5H_5(CF_3)$ TS

C	-0.127607	-0.003345	-0.011611
C	-0.233753	1.162209	-0.967156
C	0.593982	0.787353	-2.037759
C	0.699687	-0.607581	-2.057559
C	-0.034177	-1.138008	-0.995756
H	-0.051299	-2.182728	-0.709927
H	1.155950	-1.189603	-2.846718
H	0.955316	1.456947	-2.805913
H	-0.360469	2.182490	-0.623245
H	0.894801	0.103525	0.383893
C	-0.930838	-0.110166	1.265266
F	-2.041459	-0.852126	1.201211
F	-0.174966	-0.683144	2.223935

F	-1.281713	1.101013	1.728457
C	-2.181086	0.713106	-1.795844
C	-2.134825	-0.685978	-1.980954
C	-3.071716	-1.627820	-1.246508
H	-3.863469	-1.918639	-1.948139
H	-2.571499	-2.548499	-0.936629
H	-3.553635	-1.193593	-0.378134
C	-1.828499	-1.227821	-3.361877
H	-2.709279	-1.096553	-4.004403
H	-0.993713	-0.731381	-3.851505
H	-1.611693	-2.298272	-3.314820
C	-2.091723	1.619957	-3.013447
H	-1.332688	1.311569	-3.728272
H	-3.057840	1.622807	-3.533526
H	-1.878545	2.650039	-2.715323
C	-3.107171	1.327281	-0.759593
H	-3.184813	0.769482	0.167447
H	-2.792309	2.344206	-0.513560
H	-4.115758	1.396957	-1.185476

32

1 + 5a-*c*-$C_5H_5(CF_3)$

C	0.047069	0.002327	0.040640
C	0.199563	-0.243473	-1.517052
C	1.342714	0.673041	-1.951082
C	0.894171	1.927559	-1.890465
C	-0.562334	1.872374	-1.443907
C	-0.563968	1.474512	0.076206
C	-1.991218	1.541318	0.639975
H	-2.707017	0.905609	0.125739
H	-1.998241	1.257364	1.695520
H	-2.356363	2.569633	0.571789
C	0.263129	2.477513	0.890420
H	1.297239	2.548000	0.554830
H	-0.185232	3.472302	0.810862
H	0.268171	2.204679	1.949186
H	-1.165517	2.752979	-1.664482
C	-0.937893	0.569776	-2.194112
H	-0.679001	0.709610	-3.243933
C	-2.375218	0.089439	-2.307744
F	-2.821116	-0.770441	-1.380985
F	-3.230659	1.127907	-2.317473
F	-2.535283	-0.549286	-3.484335
H	1.460531	2.836252	-2.045512
H	2.352456	0.344502	-2.158530
H	0.295923	-1.293950	-1.791920
C	-0.815273	-1.060573	0.740495
H	-0.376354	-2.047878	0.570782
H	-0.807527	-0.885616	1.820069
H	-1.848641	-1.095353	0.419920
C	1.424986	-0.122529	0.718804
H	1.819297	-1.129841	0.551886
H	2.161732	0.589385	0.353483
H	1.330723	0.014443	1.798711

32

1 + 5b-*c*-$C_5H_5(CF_3)$ TS

C	0.002238	0.001367	0.005879
C	-0.201151	-1.062701	1.055323
C	0.509509	-0.651965	2.178681
C	0.759631	0.726501	2.080901
C	0.210086	1.202104	0.894562
H	0.356186	2.200625	0.500971
H	1.188337	1.342200	2.860085
H	0.715335	-1.266095	3.044910
H	-0.423095	-2.093093	0.805623
C	1.214903	-0.280860	-0.868316
F	1.014541	-1.395132	-1.598829
F	1.402364	0.724532	-1.745386
F	2.364406	-0.445972	-0.213341
H	-0.810366	0.098217	-0.709602
C	-2.219740	-0.208014	1.495266
C	-1.969542	1.175310	1.395899
C	-2.484612	1.954960	0.202232
H	-3.568494	2.099355	0.296676
H	-2.028141	2.946050	0.158805
H	-2.314904	1.466908	-0.757285
C	-1.930010	2.010976	2.657425

H	-2.944756	2.142067	3.054640
H	-1.327003	1.557104	3.442599
H	-1.523540	3.004095	2.451631
C	-2.442208	-0.821180	2.861240
H	-1.699269	-0.501044	3.590407
H	-3.428685	-0.533827	3.247159
H	-2.412385	-1.912004	2.805965
C	-3.004157	-0.916672	0.408676
H	-2.697517	-0.657675	-0.604560
H	-2.924351	-2.000501	0.515640
H	-4.067413	-0.658258	0.493707

32

1 + 5b-*c*-$C_5H_5(CF_3)$

C	-0.000192	0.002818	-0.006363
C	0.315351	-0.129138	-1.546743
C	1.450749	0.831632	-1.861924
C	0.962734	2.067893	-1.788577
C	-0.508935	1.958932	-1.422874
C	-0.587547	1.490446	0.081968
C	-2.043746	1.556382	0.565490
H	-2.739688	0.991849	-0.055790
H	-2.134350	1.183474	1.588644
H	-2.375445	2.597993	0.566489
C	0.215086	2.430825	0.987316
H	1.267554	2.486884	0.712487
H	-0.202250	3.440337	0.926510
H	0.152714	2.112290	2.031211
H	-1.131032	2.828527	-1.636136
C	-0.882760	0.642970	-2.129517
C	-1.041140	0.668990	-3.630250
F	-2.087512	1.448515	-3.969717
F	0.005110	1.107399	-4.334794
F	-1.318354	-0.569943	-4.084785
H	-1.837781	0.245952	-1.783790
H	1.509638	2.996448	-1.881102
H	2.479223	0.540349	-2.027029
H	0.444284	-1.161489	-1.872893
C	-1.000249	-1.086606	0.407892
H	-0.532404	-2.067488	0.289602
H	-1.280602	-0.982726	1.458947
H	-1.917721	-1.088529	-0.181449
C	1.263614	-0.224918	0.829682
H	1.643931	-1.234710	0.648938
H	2.059742	0.479660	0.593058
H	1.043447	-0.143174	1.897358

35

1 + 1,2-*c*-$C_5H_4(CF_3)_2$ TS = **1** + 3,4-*c*-$C_5H_4(CF_3)_2$ TS

C	-0.003469	0.013838	0.019290
C	-0.012629	1.181973	-0.922117
C	0.794017	0.825084	-2.003289
C	0.938838	-0.566709	-2.029908
C	0.212342	-1.100993	-0.961613
H	0.264547	-2.141428	-0.664562
H	1.430492	-1.121628	-2.815938
C	1.396912	1.742439	-3.024876
F	2.210429	1.062897	-3.848612
F	0.488629	2.355654	-3.798492
F	2.127008	2.707663	-2.451896
C	-0.173054	2.571968	-0.407562
F	-0.575958	3.423338	-1.362168
F	-1.077912	2.623674	0.586378
F	0.967018	3.068999	0.106182
H	0.894400	0.091979	0.652028
H	-0.867910	-0.069089	0.671120
C	-2.099890	0.316065	-1.769984
C	-1.812975	-1.059783	-1.692953
C	-2.467509	-1.885590	-0.600607
H	-3.531293	-2.016617	-0.833321
H	-2.023442	-2.881738	-0.544134
H	-2.412687	-1.432544	0.388450
C	-1.632821	-1.855096	-2.972597
H	-2.609017	-2.020541	-3.444429
H	-0.995998	-1.354969	-3.699396
H	-1.199725	-2.835825	-2.760520
C	-2.101514	0.993184	-3.116291
H	-1.254972	0.703772	-3.736250

H	-3.011636	0.709312	-3.661800
H	-2.090880	2.078759	-3.015319
C	-3.041187	0.947614	-0.769558
H	-2.810622	0.711540	0.268821
H	-3.052622	2.032920	-0.871587
H	-4.059559	0.585340	-0.963815

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1 + 1,2-*c*-$C_5H_4(CF_3)_2$ = **1** + 3,4-*c*-$C_5H_4(CF_3)_2$

C	-0.004174	-0.013411	0.006100
C	-0.294388	0.307736	1.536023
C	0.195712	1.732164	1.800999
C	1.526796	1.706675	1.764234
C	1.948234	0.279384	1.495906
C	1.599751	-0.037793	-0.002833
C	2.199332	-1.403397	-0.369427
H	1.878173	-2.210138	0.289411
H	1.943647	-1.684829	-1.393350
H	3.289127	-1.341141	-0.311300
C	2.239780	0.988916	-0.944614
H	1.905127	2.008877	-0.756603
H	3.326474	0.964446	-0.821133
H	2.023679	0.750264	-1.988888
H	2.977201	0.033103	1.756138
C	0.834921	-0.471962	2.240690
H	0.843576	-0.296703	3.316935
H	0.800172	-1.541343	2.039168
H	2.179659	2.568396	1.812820
C	-0.622355	2.971256	1.965324
F	-0.973617	3.185407	3.240804
F	0.059861	4.059514	1.568372
F	-1.754737	2.926823	1.249608
C	-1.674015	-0.035908	2.056082
F	-2.669628	0.340417	1.241245
F	-1.809257	-1.361344	2.240617
F	-1.898141	0.543364	3.245049
C	-0.626850	-1.359396	-0.399708
H	-1.715821	-1.285927	-0.388895
H	-0.328317	-1.610553	-1.419531
H	-0.343514	-2.187127	0.249700
C	-0.604916	1.046958	-0.925760
H	-1.691758	1.056119	-0.834178
H	-0.245050	2.054445	-0.718957
H	-0.357699	0.811128	-1.963702

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1 + 1,3-*c*-$C_5H_4(CF_3)_2$ TS = **1** + 2,4-*c*-$C_5H_4(CF_3)_2$ TS

C	0.004552	0.005109	0.009611
C	-0.004644	1.189717	-0.911155
C	0.770236	0.871535	-2.016795
C	0.905873	-0.519797	-2.061546
C	0.177986	-1.090446	-1.006959
H	0.245491	-2.139017	-0.741802
C	1.591396	-1.260315	-3.153528
F	1.185360	-0.863925	-4.378341
F	2.921650	-1.075652	-3.128750
F	1.375536	-2.581848	-3.075478
H	1.119247	1.567180	-2.769499
C	-0.168504	2.583557	-0.419151
F	-0.684879	3.394140	-1.360582
F	-0.978594	2.644412	0.650944
F	0.998178	3.142003	-0.039776
H	0.914459	0.042079	0.627502
H	-0.850747	-0.082721	0.672527
C	-2.080148	0.354952	-1.784361
C	-1.829918	-1.028561	-1.678904
C	-2.502206	-1.814752	-0.567017
H	-3.562908	-1.948760	-0.810496
H	-2.063791	-2.811143	-0.476583
H	-2.458581	-1.334117	0.408970
C	-1.711492	-1.857316	-2.945662
H	-2.711806	-2.024012	-3.363158
H	-1.110786	-1.383037	-3.718650
H	-1.276575	-2.836129	-2.732572
C	-2.032193	1.005715	-3.144018
H	-1.150460	0.714980	-3.716297
H	-2.908295	0.696043	-3.729023
H	-2.047607	2.092645	-3.059248

C	-3.003847	1.036582	-0.801693
H	-2.789024	0.802749	0.240652
H	-2.971878	2.120281	-0.917059
H	-4.034492	0.712416	-0.998654

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1 + 1,3-*c*-$C_5H_4(CF_3)_2$ = **1** + 2,4-*c*-$C_5H_4(CF_3)_2$

C	0.000406	-0.011975	0.007237
C	-0.252247	0.282494	1.546236
C	0.211422	1.704617	1.824427
C	1.540370	1.679098	1.784034
C	1.983846	0.263663	1.462008
C	1.605142	-0.038631	-0.032614
C	2.195255	-1.404758	-0.415437
H	1.890588	-2.214406	0.247569
H	1.916642	-1.682956	-1.434042
H	3.285958	-1.341065	-0.382562
C	2.219647	0.984707	-0.992356
H	1.876856	2.002503	-0.812601
H	3.307413	0.980416	-0.884067
H	1.989054	0.727126	-2.029179
H	3.020348	0.027731	1.703605
C	0.888272	-0.508457	2.218393
H	0.921711	-0.347964	3.296178
H	0.856217	-1.575094	2.001243
C	2.452888	2.829923	2.013079
F	3.209484	2.630743	3.107016
F	3.308014	3.019001	0.993399
F	1.785940	3.976141	2.192658
H	-0.430126	2.564746	1.965203
C	-1.624069	-0.011344	2.096967
F	-2.605520	0.556410	1.374240
F	-1.884701	-1.326216	2.151986
F	-1.749036	0.457106	3.350605
C	-0.634975	-1.344969	-0.417086
H	-1.723674	-1.268676	-0.382312
H	-0.357503	-1.572946	-1.448490
H	-0.342077	-2.188227	0.207814
C	-0.617967	1.071627	-0.887551
H	-1.705611	1.049777	-0.805321
H	-0.280277	2.076808	-0.636399
H	-0.361681	0.884686	-1.932844

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1 + 1,4-*c*-$C_5H_4(CF_3)_2$ TS

C	-0.011652	0.004583	0.014873
C	-0.225656	-1.029155	1.079574
C	0.454067	-0.606086	2.224022
C	0.698857	0.763281	2.110050
C	0.173403	1.205107	0.893717
C	0.542272	2.525853	0.304294
F	1.870205	2.634555	0.104107
F	-0.034423	2.721360	-0.892070
F	0.194298	3.557154	1.092315
H	1.130078	1.398702	2.872063
H	0.662147	-1.220385	3.089880
C	-0.348615	-2.472681	0.720500
F	-1.007718	-3.181441	1.652677
F	-0.989540	-2.647929	-0.445786
F	0.855419	-3.060819	0.580170
H	0.939699	-0.207853	-0.496475
H	-0.791190	0.081242	-0.738267
C	-2.301906	-0.178277	1.546605
C	-2.053534	1.206712	1.433705
C	-2.620787	1.958717	0.247524
H	-3.715102	1.979720	0.331318
H	-2.273304	2.991896	0.231673
H	-2.383207	1.507996	-0.715897
C	-2.006021	2.033806	2.700184
H	-3.011176	2.085781	3.137753
H	-1.349029	1.606100	3.457024
H	-1.677225	3.051982	2.494790
C	-2.509164	-0.761222	2.927788
H	-1.722780	-0.476883	3.626430
H	-3.456416	-0.390641	3.339955
H	-2.561972	-1.848905	2.893323
C	-3.125590	-0.865025	0.476950
H	-2.775519	-0.678662	-0.538197

H	-3.153753	-1.943772	0.631669
H	-4.158044	-0.496375	0.533226

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1 + 1,4-*c*-$C_5H_4(CF_3)_2$

C	0.002184	-0.014606	0.001034
C	-0.263486	0.271801	1.536907
C	0.209715	1.689281	1.824875
C	1.538586	1.673487	1.792353
C	1.963222	0.245494	1.481954
C	1.615113	-0.033021	-0.038998
C	2.191425	-1.379622	-0.504491
H	1.909784	-2.220721	0.128266
H	1.862258	-1.594071	-1.522991
H	3.281890	-1.328290	-0.521365
C	2.212822	1.037290	-0.962627
H	1.900855	2.047644	-0.700827
H	3.302104	0.997461	-0.921549
H	1.916288	0.849772	-1.997017
C	3.356333	-0.085568	1.952894
F	3.592135	-1.406624	1.980534
F	4.309016	0.469105	1.182483
F	3.560356	0.365113	3.201988
C	0.857811	-0.534698	2.209493
H	0.886202	-0.391787	3.289979
H	0.839164	-1.596422	1.966780
H	2.214252	2.515060	1.868524
H	-0.441160	2.546625	1.933858
C	-1.638885	-0.026190	2.077110
F	-2.615584	0.548615	1.353004
F	-1.903073	-1.341464	2.120403
F	-1.770565	0.431423	3.333346
C	-0.627549	-1.347719	-0.433206
H	-1.716016	-1.271674	-0.393785
H	-0.356274	-1.569276	-1.467155
H	-0.332886	-2.195312	0.184784
C	-0.615997	1.068739	-0.893434
H	-1.702522	1.054253	-0.797944
H	-0.267897	2.071676	-0.649394
H	-0.375859	0.873656	-1.940987

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1 + 1,5a-*c*-$C_5H_4(CF_3)_2$ TS = **1** + 4,5a-*c*-$C_5H_4(CF_3)_2$ TS

C	-0.001069	0.011110	0.009709
C	-0.094433	1.185109	-0.927892
C	0.669304	0.816765	-2.035459
C	0.781837	-0.572393	-2.075484
C	0.040780	-1.110269	-1.005277
H	0.089922	-2.148404	-0.696813
H	1.222143	-1.145557	-2.878511
H	1.021790	1.506809	-2.790692
C	-0.198738	2.600148	-0.486280
F	-0.453359	3.409123	-1.530140
F	-1.173457	2.791424	0.414781
F	0.934948	3.055314	0.086018
H	1.033327	0.026599	0.390698
C	-0.787846	-0.083060	1.300941
F	-2.053034	0.334899	1.268448
F	-0.798594	-1.354482	1.741572
F	-0.178506	0.652337	2.245744
C	-2.199174	0.317612	-1.936773
C	-1.927205	-1.059490	-1.774808
C	-2.698538	-1.878995	-0.751723
H	-3.682692	-2.122739	-1.168937
H	-2.190433	-2.826383	-0.556383
H	-2.862377	-1.384495	0.199102
C	-1.677896	-1.899225	-3.020933
H	-2.638569	-2.113987	-3.503836
H	-1.041083	-1.410724	-3.753931
H	-1.223737	-2.858575	-2.758746
C	-1.987941	0.950924	-3.290991
H	-1.048058	0.669875	-3.762278
H	-2.792388	0.623415	-3.963203
H	-2.031219	2.039187	-3.220096
C	-3.298398	1.021505	-1.173071
H	-3.595098	0.531141	-0.253979
H	-3.042452	2.058015	-0.948819
H	-4.176967	1.047484	-1.831391

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1 + 1,5a-*c*-$C_5H_4(CF_3)_2$ = **1** + 4,5a-*c*-$C_5H_4(CF_3)_2$

C	0.009200	-0.006710	-0.002367
C	-0.050531	0.317769	-1.564341
C	-1.516736	0.118227	-1.954936
C	-1.754299	-1.191344	-1.928046
C	-0.456214	-1.888293	-1.541482
C	-0.214301	-1.592012	-0.020145
C	0.985384	-2.400378	0.496599
H	1.920690	-2.197946	-0.016255
H	1.144820	-2.208558	1.560362
H	0.769432	-3.466187	0.384933
C	-1.421787	-2.062158	0.802697
H	-2.353222	-1.576549	0.514533
H	-1.549650	-3.140636	0.671760
H	-1.259402	-1.880447	1.868011
H	-0.383114	-2.944609	-1.797512
C	0.506273	-0.938201	-2.293238
H	0.183682	-0.890357	-3.334255
C	1.985356	-1.263118	-2.465011
F	2.837700	-0.912724	-1.496569
F	2.131752	-2.588974	-2.646976
F	2.436723	-0.664250	-3.579750
H	-2.706307	-1.684557	-2.069644
H	-2.216763	0.927736	-2.113595
C	0.523937	1.631998	-2.025695
F	-0.009371	2.675644	-1.366938
F	1.851641	1.697116	-1.861595
F	0.281874	1.833164	-3.331439
C	1.311804	0.434019	0.686057
H	1.390175	1.523219	0.660821
H	1.270074	0.138691	1.737423
H	2.217428	0.024828	0.255569
C	-1.100026	0.754069	0.751333
H	-0.925837	1.829047	0.684574
H	-2.102800	0.549961	0.382630
H	-1.070934	0.483212	1.809000

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1 + 1,5b-*c*-$C_5H_4(CF_3)_2$ TS = **1** + 4,5b-*c*-$C_5H_4(CF_3)_2$ TS

C	0.000992	-0.004090	0.004841
C	0.030849	1.182319	-0.920165
C	0.802005	0.832756	-2.020119
C	0.913983	-0.561933	-2.072424
C	0.181938	-1.108302	-1.012158
H	0.235983	-2.148377	-0.712515
H	1.372638	-1.125233	-2.872638
H	1.162108	1.527466	-2.767936
C	-0.138331	2.586735	-0.458312
F	-0.640213	3.367890	-1.435570
F	-0.972368	2.675959	0.589289
F	1.018153	3.160660	-0.079928
C	1.138647	-0.006307	1.022393
F	0.972160	0.977358	1.918448
F	1.133255	-1.164887	1.708922
F	2.355426	0.136587	0.498106
H	-0.898507	-0.078600	0.611757
C	-2.085042	0.355116	-1.761435
C	-1.828491	-1.029093	-1.672913
C	-2.502246	-1.833266	-0.575129
H	-3.565886	-1.951470	-0.813713
H	-2.071669	-2.834526	-0.505819
H	-2.449307	-1.374700	0.411694
C	-1.692006	-1.834555	-2.952408
H	-2.681314	-1.983075	-3.401541
H	-1.061245	-1.347951	-3.693742
H	-1.273160	-2.822482	-2.745232
C	-2.036246	1.017113	-3.114060
H	-1.125091	0.770410	-3.661800
H	-2.878429	0.670941	-3.727554
H	-2.101742	2.101359	-3.024572
C	-3.008860	1.023757	-0.770427
H	-2.793844	0.782913	0.270889
H	-2.978313	2.108428	-0.875021
H	-4.039819	0.699934	-0.966477

35
1 + 1,5b-*c*-$C_5H_4(CF_3)_2$ = **1** + 4,5b-*c*-$C_5H_4(CF_3)_2$

C	0.013221	-0.004480	-0.001776
C	-0.174539	0.345193	-1.548968
C	-1.644831	0.123812	-1.878734
C	-1.856013	-1.188356	-1.871037
C	-0.539821	-1.867629	-1.531869
C	-0.240285	-1.590769	-0.015353
C	0.976124	-2.420899	0.422300
H	1.869643	-2.246226	-0.177440
H	1.232394	-2.223340	1.465435
H	0.728714	-3.482534	0.343057
C	-1.414698	-2.048925	0.856558
H	-2.343464	-1.529023	0.625745
H	-1.580761	-3.119212	0.703043
H	-1.195982	-1.901020	1.916824
H	-0.449741	-2.918772	-1.804415
C	0.463569	-0.905482	-2.192671
C	0.582562	-1.002931	-3.701162
F	0.947881	-2.259375	-4.028528
F	-0.520055	-0.728421	-4.398293
F	1.549816	-0.190072	-4.154041
H	1.484285	-1.060041	-1.841169
H	-2.802674	-1.696286	-1.993448
H	-2.366407	0.919410	-2.006013
C	0.364866	1.678531	-2.009709
F	-0.078133	2.691068	-1.241745
F	1.704466	1.728329	-1.989677
F	-0.019831	1.952616	-3.263973
C	1.414138	0.378108	0.501022
H	1.524224	1.464093	0.508782
H	1.543708	0.030462	1.528128
H	2.227768	-0.030018	-0.098513
C	-0.986978	0.759788	0.876405
H	-0.769401	1.828048	0.855905
H	-2.021005	0.617648	0.564983
H	-0.898633	0.424924	1.912532

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1 + 2,3-*c*-$C_5H_4(CF_3)_2$ TS

C	0.000478	0.000428	0.000329
C	-0.224413	-1.007263	1.091416
C	0.524598	-0.567654	2.184132
C	0.787322	0.804104	2.021251
C	0.207706	1.232219	0.831320
H	0.344561	2.226688	0.425377
C	1.485844	1.707895	2.983331
F	1.149517	1.469111	4.259743
F	2.818533	1.584039	2.904399
F	1.198443	2.995907	2.731451
C	0.887882	-1.407860	3.365150
F	2.183815	-1.267182	3.676325
F	0.194910	-1.112800	4.478950
F	0.668792	-2.708456	3.115325
H	-0.451162	-2.051293	0.913706
H	0.955001	-0.240744	-0.491830
H	-0.765270	0.060316	-0.765629
C	-2.214997	-0.163286	1.516404
C	-1.954804	1.219584	1.429271
C	-2.467053	2.010461	0.241748
H	-3.555711	2.124211	0.319496
H	-2.035874	3.013187	0.228320
H	-2.264257	1.542545	-0.721284
C	-1.888978	2.040626	2.698775
H	-2.899089	2.173522	3.106414
H	-1.287587	1.573223	3.478159
H	-1.474925	3.031062	2.501548
C	-2.491473	-0.791436	2.866360
H	-1.854735	-0.409313	3.658997
H	-3.531623	-0.589576	3.152006
H	-2.368137	-1.876707	2.826880
C	-2.992143	-0.853920	0.411812
H	-2.693235	-0.568635	-0.595417
H	-2.908645	-1.939470	0.497723
H	-4.055464	-0.602757	0.511728

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1 + 2,3-*c*-$C_5H_4(CF_3)_2$

C	0.000976	0.002740	0.010082
C	0.270442	-0.154865	-1.534523

C	1.387954	0.803703	-1.902900
C	0.892531	2.040842	-1.842612
C	-0.563517	1.924288	-1.422813
C	-0.599497	1.480273	0.087053
C	-2.053955	1.537882	0.576763
H	-2.745539	0.967529	-0.043642
H	-2.136238	1.165164	1.600343
H	-2.390926	2.577778	0.579522
C	0.200757	2.440858	0.972510
H	1.260283	2.474122	0.724706
H	-0.196672	3.454851	0.866270
H	0.110588	2.160949	2.025331
H	-1.172836	2.802649	-1.631836
C	-0.920226	0.609492	-2.143092
H	-0.854553	0.693200	-3.228063
H	-1.892153	0.204770	-1.865484
C	1.611293	3.331342	-2.092802
F	0.739596	4.300297	-2.415005
F	2.295307	3.767705	-1.024218
F	2.481296	3.225985	-3.102566
C	2.790810	0.376888	-2.203833
F	3.009034	0.288555	-3.522829
F	3.705349	1.213989	-1.700113
F	3.037684	-0.837550	-1.686110
H	0.429254	-1.187880	-1.842516
C	-0.982342	-1.091374	0.449534
H	-0.510529	-2.069836	0.328422
H	-1.241914	-0.981754	1.505134
H	-1.909470	-1.096619	-0.124044
C	1.281580	-0.200304	0.827762
H	1.663613	-1.211822	0.668551
H	2.077034	0.498256	0.564807
H	1.078857	-0.084684	1.895564

35

1 + 2,5a-*c*-$C_5H_4(CF_3)_2$ TS = **1** + 3,5a-*c*-$C_5H_4(CF_3)_2$ TS

C	0.012263	-0.024432	0.000304
C	-0.102753	1.120903	-0.980615
C	0.732527	0.705060	-2.033043
C	0.823265	-0.691873	-2.033711
C	0.095247	-1.183338	-0.955980
H	0.055404	-2.221329	-0.651493
H	1.273211	-1.285993	-2.817652
C	1.325632	1.583699	-3.074194
F	2.666410	1.629419	-2.986388
F	1.054189	1.156743	-4.326689
F	0.884108	2.846372	-2.983353
H	-0.198010	2.154016	-0.666035
H	1.038114	0.097320	0.384111
C	-0.780445	-0.112375	1.286635
F	-1.886411	-0.862591	1.238170
F	-0.012253	-0.669167	2.242554
F	-1.131364	1.103026	1.732660
C	-2.048853	0.713113	-1.761125
C	-2.014450	-0.683339	-1.974797
C	-2.940867	-1.636927	-1.247095
H	-3.767557	-1.871057	-1.929750
H	-2.451374	-2.584324	-1.010780
H	-3.374637	-1.237785	-0.338072
C	-1.704054	-1.196969	-3.364051
H	-2.586212	-1.049236	-4.000916
H	-0.872672	-0.687561	-3.846949
H	-1.489888	-2.268229	-3.340545
C	-1.994907	1.639860	-2.966728
H	-1.271041	1.342695	-3.721005
H	-2.981251	1.649967	-3.446069
H	-1.768624	2.664185	-2.663109
C	-2.958588	1.310110	-0.699804
H	-3.047999	0.725413	0.208768
H	-2.625335	2.313420	-0.424570
H	-3.964544	1.411616	-1.123977

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1 + 2,5a-*c*-$C_5H_4(CF_3)_2$ = **1** + 3,5a-*c*-$C_5H_4(CF_3)_2$

C	-0.011669	-0.016700	0.005905
C	0.170686	-0.245343	-1.552494
C	1.301903	0.693486	-1.963884
C	0.854526	1.945560	-1.884955

C	-0.607102	1.868162	-1.464614
C	-0.634708	1.450350	0.047916
C	-2.073490	1.498947	0.582357
H	-2.771821	0.858153	0.050962
H	-2.095483	1.206762	1.635180
H	-2.448818	2.523482	0.515283
C	0.168069	2.453859	0.886227
H	1.209172	2.536325	0.574711
H	-0.287488	3.444992	0.804506
H	0.153778	2.173593	1.942440
H	-1.207126	2.750120	-1.685870
C	-0.958450	0.573042	-2.244268
H	-0.677904	0.725416	-3.287046
C	-2.394793	0.093290	-2.393763
F	-2.849894	-0.790196	-1.496116
F	-3.246542	1.133768	-2.386423
F	-2.534273	-0.510817	-3.588433
H	1.423813	2.850690	-2.049205
C	2.653070	0.257296	-2.403121
F	2.591000	-0.356768	-3.599276
F	3.497654	1.288487	-2.529897
F	3.216238	-0.622614	-1.559169
H	0.290377	-1.288757	-1.844873
C	-0.882662	-1.098538	0.664577
H	-0.424246	-2.077156	0.498493
H	-0.910816	-0.935206	1.745183
H	-1.904579	-1.142937	0.310721
C	1.344666	-0.132499	0.724559
H	1.756918	-1.132952	0.571162
H	2.089971	0.585364	0.388374
H	1.208590	0.006897	1.799369

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1 + 2,5b-*c*-$C_5H_4(CF_3)_2$ TS = **1** + 3,5b-*c*-$C_5H_4(CF_3)_2$ TS

C	0.019279	0.023063	-0.009025
C	-0.199536	-1.005298	1.073375
C	0.532394	-0.557349	2.169741
C	0.797957	0.814760	2.035218
C	0.247185	1.248814	0.838791
H	0.379449	2.237465	0.418188
H	1.232929	1.442970	2.800766
C	0.858028	-1.364478	3.376913
F	2.168284	-1.638546	3.461898
F	0.534008	-0.723062	4.519014
F	0.207420	-2.537355	3.385288
H	-0.415513	-2.046743	0.868944
C	1.228635	-0.311452	-0.873400
F	1.006847	-1.446325	-1.561159
F	1.430493	0.660607	-1.781381
F	2.371173	-0.471939	-0.207087
H	-0.793732	0.107317	-0.725137
C	-2.197918	-0.187355	1.478844
C	-1.956251	1.199628	1.401841
C	-2.468567	1.997488	0.220489
H	-3.558647	2.101341	0.293030
H	-2.045179	3.003523	0.218007
H	-2.259816	1.543623	-0.748389
C	-1.892543	2.005049	2.679989
H	-2.900548	2.119649	3.098607
H	-1.276158	1.532426	3.444089
H	-1.494404	3.004365	2.491187
C	-2.452432	-0.825078	2.829528
H	-1.760047	-0.491816	3.600381
H	-3.464579	-0.572276	3.169079
H	-2.386464	-1.913038	2.765343
C	-2.971817	-0.880041	0.373432
H	-2.690229	-0.575366	-0.633842
H	-2.862445	-1.964364	0.442097
H	-4.039473	-0.654319	0.485225

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1 + 2,5b-*c*-$C_5H_4(CF_3)_2$ = **1** + 3,5b-*c*-$C_5H_4(CF_3)_2$

C	-0.014030	-0.015484	-0.000531
C	0.299891	-0.150944	-1.541240
C	1.420861	0.820811	-1.869504
C	0.941451	2.058187	-1.789447
C	-0.526300	1.940559	-1.416899
C	-0.598612	1.473582	0.087065

C	-2.053747	1.542021	0.572149
H	-2.750313	0.972434	-0.043713
H	-2.139329	1.173771	1.597187
H	-2.386748	2.583041	0.569632
C	0.207852	2.417887	0.985691
H	1.259765	2.476514	0.708129
H	-0.212449	3.425984	0.924902
H	0.151977	2.101380	2.030101
H	-1.145497	2.811511	-1.630290
C	-0.897282	0.623114	-2.127431
C	-1.046129	0.654610	-3.630427
F	-2.097987	1.425030	-3.968704
F	0.003044	1.115037	-4.316690
F	-1.301829	-0.582461	-4.093012
H	-1.852366	0.225467	-1.784327
H	1.495607	2.978514	-1.914100
C	2.803563	0.422313	-2.236600
F	2.818739	-0.257953	-3.394691
F	3.611096	1.479932	-2.382201
F	3.365827	-0.386158	-1.318672
H	0.441933	-1.179801	-1.873214
C	-1.018699	-1.105601	0.402172
H	-0.547039	-2.085175	0.290797
H	-1.308918	-0.999976	1.449925
H	-1.930413	-1.110348	-0.195924
C	1.238404	-0.242206	0.851002
H	1.633677	-1.244686	0.667912
H	2.035890	0.467937	0.639259
H	0.993419	-0.169945	1.913803

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1 + 5a,5b-*c*-$C_5H_4(CF_3)_2$ TS

C	0.002167	0.001895	-0.000747
C	-0.201664	1.151235	-0.988649
C	0.570167	0.770715	-2.101335
C	0.697639	-0.618923	-2.103893
C	0.024569	-1.144210	-0.999197
H	0.049540	-2.182338	-0.691585
H	1.129134	-1.208076	-2.901105
H	0.896230	1.437442	-2.886506
H	-0.300189	2.174132	-0.641720
C	1.439588	0.152923	0.630761
F	1.412352	1.088567	1.594881
F	1.845060	-0.997320	1.183194
F	2.402889	0.517013	-0.209682
C	-0.937580	-0.085166	1.220914
F	-2.013670	-0.838753	0.998629
F	-0.351090	-0.631212	2.294423
F	-1.355311	1.133330	1.589217
C	-2.152090	0.711101	-1.732836
C	-2.119330	-0.697023	-1.935572
C	-3.088682	-1.643561	-1.246622
H	-3.812611	-1.976367	-1.999210
H	-2.591746	-2.539242	-0.867583
H	-3.651754	-1.196855	-0.434613
C	-1.818808	-1.211793	-3.327745
H	-2.700223	-1.048485	-3.961795
H	-0.982379	-0.717082	-3.814813
H	-1.622891	-2.286925	-3.305877
C	-2.085960	1.616553	-2.957128
H	-1.338215	1.316244	-3.685879
H	-3.060782	1.606286	-3.459245
H	-1.881782	2.649611	-2.662932
C	-3.113916	1.330321	-0.728930
H	-3.285409	0.750384	0.169679
H	-2.772629	2.323671	-0.428735
H	-4.082830	1.460192	-1.225630

35

1 + 5a,5b-*c*-$C_5H_4(CF_3)_2$

C	-0.011850	0.000796	-0.005669
C	0.205985	-0.193913	-1.578319
C	1.367552	0.736754	-1.913329
C	0.911816	1.980872	-1.817560
C	-0.574843	1.911440	-1.463345
C	-0.613333	1.484546	0.048995
C	-2.029686	1.619723	0.631937
H	-2.808115	1.101350	0.081479

H	-2.051576	1.259531	1.663573
H	-2.295791	2.679860	0.652384
C	0.243399	2.460615	0.874731
H	1.295404	2.457393	0.596477
H	-0.136043	3.478763	0.748442
H	0.174481	2.215922	1.937764
H	-1.162167	2.802367	-1.687064
C	-0.920419	0.628663	-2.292413
C	-0.653449	0.876132	-3.833058
F	-1.788930	0.949272	-4.543750
F	-0.026748	2.023774	-4.118629
F	0.074284	-0.119371	-4.354127
C	-2.322486	-0.013456	-2.267732
F	-2.640772	-0.640178	-1.136310
F	-3.287106	0.888742	-2.487909
F	-2.407130	-0.969217	-3.209027
H	1.466298	2.901722	-1.931726
H	2.381712	0.415401	-2.103873
H	0.311338	-1.232164	-1.891611
C	-0.859617	-1.090584	0.697289
H	-0.782124	-2.036967	0.156053
H	-0.466411	-1.262596	1.701233
H	-1.910951	-0.858872	0.808273
C	1.365230	-0.138921	0.683248
H	1.712270	-1.170954	0.569870
H	2.136862	0.520774	0.296022
H	1.266194	0.053305	1.753408

38

1 + 1,2,3-*c*-$C_5H_3(CF_3)_3$ TS = **1** + 2,3,4-*c*-$C_5H_3(CF_3)_3$ TS

C	0.001566	0.007091	0.010802
C	0.001553	1.190205	-0.913035
C	0.798120	0.849229	-2.005662
C	0.918737	-0.550818	-2.043623
C	0.172491	-1.096225	-0.990147
H	0.235528	-2.142009	-0.715039
C	1.617926	-1.369912	-3.080800
F	1.333614	-0.970440	-4.331666
F	2.948895	-1.333544	-2.949498
F	1.257060	-2.661257	-2.987398
C	1.392964	1.782571	-3.027437
F	2.583616	1.328199	-3.433089
F	0.630399	1.915727	-4.122596
F	1.578788	3.007845	-2.532621
C	-0.207090	2.566318	-0.364088
F	-0.772845	3.395684	-1.252255
F	-1.018501	2.522268	0.708981
F	0.928929	3.142242	0.057933
H	0.910886	0.050773	0.630582
H	-0.854930	-0.066251	0.672672
C	-2.105107	0.336331	-1.750500
C	-1.828969	-1.045144	-1.671801
C	-2.478415	-1.857979	-0.565133
H	-3.546637	-1.972582	-0.783717
H	-2.048784	-2.860589	-0.516692
H	-2.402919	-1.406362	0.422934
C	-1.713335	-1.845103	-2.956898
H	-2.711148	-1.967859	-3.394528
H	-1.084906	-1.371452	-3.708588
H	-1.312863	-2.840973	-2.760291
C	-2.114316	1.006931	-3.098428
H	-1.289407	0.693440	-3.734429
H	-3.042002	0.737712	-3.621561
H	-2.085336	2.092722	-3.002896
C	-3.023574	0.982051	-0.740012
H	-2.799575	0.727846	0.295105
H	-3.013124	2.067922	-0.833626
H	-4.048945	0.642545	-0.939027

38

1 + 1,2,3-*c*-$C_5H_3(CF_3)_3$ = **1** + 2,3,4-*c*-$C_5H_3(CF_3)_3$

C	-0.013275	-0.009537	0.001722
C	-0.303784	0.302973	1.531474
C	0.188121	1.726603	1.809436
C	1.521310	1.682335	1.793884
C	1.938090	0.256255	1.496926
C	1.589233	-0.047978	-0.004115
C	2.182009	-1.418203	-0.365853

H	1.863350	-2.221792	0.298020
H	1.919655	-1.702412	-1.386911
H	3.272058	-1.357109	-0.314983
C	2.236490	0.972082	-0.946197
H	1.878493	1.988833	-0.794979
H	3.319609	0.974802	-0.791575
H	2.054626	0.703143	-1.989652
H	2.965185	0.012515	1.763065
C	0.818196	-0.487573	2.236632
H	0.827382	-0.319311	3.314030
H	0.776187	-1.554583	2.027914
C	2.484220	2.819605	1.984346
F	3.682155	2.349195	2.365424
F	2.685155	3.529123	0.865925
F	2.070031	3.667485	2.928476
C	-0.661581	2.958922	1.956207
F	-0.839904	3.294910	3.235492
F	-0.107115	4.011169	1.337854
F	-1.870964	2.777135	1.413741
C	-1.686265	-0.043749	2.054325
F	-2.686841	0.273779	1.224337
F	-1.787786	-1.364265	2.285714
F	-1.923332	0.573970	3.221514
C	-0.644501	-1.348782	-0.412053
H	-1.732808	-1.272232	-0.400220
H	-0.347057	-1.592618	-1.433854
H	-0.361832	-2.182372	0.230198
C	-0.609958	1.066273	-0.915480
H	-1.697476	1.069809	-0.830028
H	-0.253594	2.072123	-0.690730
H	-0.355427	0.851501	-1.955929

38

1 + 1,2,4-*c*-$C_5H_3(CF_3)_3$ TS = **1** + 1,3,4-*c*-$C_5H_3(CF_3)_3$ TS

C	-0.034230	0.006972	0.009107
C	-0.244033	-1.013241	1.092910
C	0.468353	-0.554948	2.208902
C	0.713253	0.812902	2.066711
C	0.175772	1.224370	0.852351
C	0.517376	2.541613	0.237470
F	1.838878	2.661841	0.014627
F	-0.083803	2.709309	-0.949747
F	0.167702	3.575649	1.019346
H	1.153804	1.452933	2.819770
C	0.860708	-1.322385	3.430054
F	2.151885	-1.678161	3.395165
F	0.696772	-0.580825	4.541651
F	0.143511	-2.438819	3.585187
C	-0.387453	-2.458803	0.697869
F	-1.263593	-3.151690	1.434015
F	-0.797654	-2.548815	-0.578957
F	0.784985	-3.108465	0.776901
H	0.907171	-0.231694	-0.510607
H	-0.821198	0.071269	-0.736635
C	-2.306551	-0.172814	1.561509
C	-2.064005	1.213877	1.460458
C	-2.636947	1.977123	0.285953
H	-3.730162	2.000422	0.382765
H	-2.286910	3.009235	0.274483
H	-2.412858	1.531006	-0.682768
C	-1.979085	2.029008	2.731121
H	-2.975514	2.087868	3.187344
H	-1.314942	1.587554	3.473936
H	-1.643294	3.045058	2.526287
C	-2.515665	-0.766834	2.938636
H	-1.756584	-0.458545	3.656745
H	-3.481440	-0.423711	3.330763
H	-2.535308	-1.854796	2.905544
C	-3.129060	-0.847073	0.481199
H	-2.773026	-0.655785	-0.531122
H	-3.170364	-1.925454	0.629591
H	-4.157521	-0.468077	0.532670

38

1 + 1,2,4-*c*-$C_5H_3(CF_3)_3$ = **1** + 1,3,4-*c*-$C_5H_3(CF_3)_3$

C	-0.016644	-0.024753	0.014461
C	-0.290632	0.260491	1.550514
C	0.211543	1.674113	1.845755

C	1.539887	1.645391	1.799192
C	1.945866	0.216855	1.495833
C	1.594961	-0.052077	-0.026166
C	2.166482	-1.400191	-0.492193
H	1.879020	-2.241238	0.137941
H	1.837673	-1.609813	-1.511629
H	3.257077	-1.353744	-0.507407
C	2.199413	1.019240	-0.945090
H	1.899731	2.032596	-0.678865
H	3.288336	0.967890	-0.910397
H	1.894543	0.840982	-1.978436
C	3.337621	-0.123037	1.968690
F	3.556915	-1.444929	2.003082
F	4.292241	0.419763	1.194995
F	3.541518	0.334939	3.214594
C	0.832228	-0.548247	2.224926
H	0.859573	-0.405596	3.305853
H	0.802558	-1.609264	1.983723
H	2.211616	2.491619	1.863443
C	-0.597171	2.916606	2.047198
F	-0.925292	3.103154	3.330785
F	0.087508	4.004560	1.659391
F	-1.738636	2.888717	1.347069
C	-1.666811	-0.088205	2.082053
F	-2.669376	0.308722	1.288199
F	-1.801833	-1.415446	2.242328
F	-1.867830	0.470466	3.283865
C	-0.650738	-1.359197	-0.411696
H	-1.738556	-1.281000	-0.373527
H	-0.379668	-1.584577	-1.444477
H	-0.355860	-2.204970	0.208499
C	-0.629876	1.058484	-0.882305
H	-1.713046	1.076633	-0.757752
H	-0.252698	2.058374	-0.669611
H	-0.418348	0.837728	-1.930874

38

1 + 1,2,5a-*c*-$C_5H_3(CF_3)_3$ TS = **1** + 3,4,5a-*c*-$C_5H_3(CF_3)_3$ TS

C	-0.112950	-0.004099	-0.022425
C	-0.203773	1.175698	-0.963303
C	0.601448	0.796847	-2.043762
C	0.728970	-0.590343	-2.082578
C	-0.026424	-1.126741	-1.028595
H	0.020069	-2.163567	-0.718225
H	1.199779	-1.147510	-2.879051
C	1.233212	1.694078	-3.063732
F	1.386207	1.054270	-4.236855
F	0.516476	2.795840	-3.302002
F	2.453689	2.087642	-2.677124
C	-0.378129	2.590035	-0.500431
F	-1.197253	3.295327	-1.295354
F	-0.903707	2.628640	0.730933
F	0.783816	3.264655	-0.453423
H	0.913404	0.036795	0.380738
C	-0.930706	-0.163244	1.249519
F	-2.182141	0.291795	1.210354
F	-0.987726	-1.465999	1.585967
F	-0.326002	0.464478	2.267253
C	-2.278438	0.279201	-2.002855
C	-1.987732	-1.096012	-1.865008
C	-2.763063	-1.947528	-0.872381
H	-3.735809	-2.193854	-1.313903
H	-2.246610	-2.891978	-0.687215
H	-2.950427	-1.474549	0.085101
C	-1.685877	-1.904393	-3.119254
H	-2.629210	-2.126377	-3.631754
H	-1.039908	-1.389519	-3.825933
H	-1.221868	-2.860553	-2.863654
C	-2.064883	0.944587	-3.341006
H	-1.128459	0.674781	-3.826085
H	-2.868796	0.625554	-4.017809
H	-2.113351	2.029935	-3.249082
C	-3.394549	0.945668	-1.227562
H	-3.734574	0.389309	-0.362479
H	-3.137441	1.958781	-0.916779
H	-4.244775	1.037163	-1.915454

38

1 + 1,2,5a-*c*-$C_5H_3(CF_3)_3$ = **1** + 3,4,5a-*c*-$C_5H_3(CF_3)_3$

C	0.020876	0.004382	-0.005581
C	-0.041215	0.339473	-1.568628
C	-1.511975	0.113457	-1.964775
C	-1.733020	-1.199299	-1.922450
C	-0.430830	-1.878834	-1.543929
C	-0.194739	-1.581446	-0.022642
C	1.006319	-2.387140	0.494533
H	1.944803	-2.170113	-0.005818
H	1.152014	-2.206373	1.561975
H	0.799658	-3.453073	0.368773
C	-1.402780	-2.059240	0.796319
H	-2.340713	-1.590515	0.500540
H	-1.514777	-3.140548	0.676277
H	-1.249235	-1.863495	1.860088
H	-0.355744	-2.933892	-1.802452
C	0.517991	-0.920363	-2.299653
H	0.193671	-0.872061	-3.340636
C	1.997350	-1.249926	-2.479572
F	2.854525	-0.927177	-1.507692
F	2.123261	-2.574873	-2.681265
F	2.448518	-0.640142	-3.585909
H	-2.686352	-1.689663	-2.065171
C	-2.561432	1.132728	-2.281376
F	-2.372297	1.689436	-3.484331
F	-3.776742	0.563507	-2.299123
F	-2.604689	2.133454	-1.392852
C	0.582231	1.640813	-2.023776
F	0.099474	2.701223	-1.363797
F	1.910488	1.633882	-1.846357
F	0.366009	1.847713	-3.329330
C	1.328009	0.447244	0.673768
H	1.389568	1.537569	0.674851
H	1.303480	0.125105	1.717249
H	2.233098	0.062005	0.220741
C	-1.084338	0.755591	0.759571
H	-0.946698	1.832480	0.654911
H	-2.093665	0.515686	0.433646
H	-1.012542	0.512690	1.821835

38

1 + 1,2,5b-*c*-$C_5H_3(CF_3)_3$ TS = **1** + 3,4,5b-*c*-$C_5H_3(CF_3)_3$ TS

C	-0.012807	0.002909	0.018321
C	0.020630	1.201553	-0.892667
C	0.802897	0.846154	-1.986685
C	0.916159	-0.548872	-2.051278
C	0.181163	-1.097271	-0.997274
H	0.244695	-2.136947	-0.699950
H	1.399420	-1.094176	-2.848575
C	1.408882	1.774406	-3.000722
F	2.245014	1.104740	-3.807168
F	0.497512	2.363148	-3.789422
F	2.107320	2.751969	-2.417444
C	-0.174113	2.592802	-0.386553
F	-0.624649	3.406416	-1.355608
F	-1.071025	2.622078	0.612770
F	0.949691	3.143725	0.092814
C	1.120288	0.000108	1.045324
F	0.926453	0.957345	1.961328
F	1.131573	-1.174897	1.700874
F	2.334381	0.179687	0.527835
H	-0.916009	-0.075065	0.618728
C	-2.122510	0.309933	-1.748220
C	-1.830413	-1.066119	-1.663324
C	-2.475889	-1.886125	-0.560466
H	-3.540517	-2.017140	-0.786632
H	-2.030902	-2.881485	-0.502945
H	-2.417244	-1.431803	0.428039
C	-1.671377	-1.868676	-2.942239
H	-2.655974	-2.032894	-3.395430
H	-1.045659	-1.373365	-3.681687
H	-1.238464	-2.849497	-2.731562
C	-2.091839	0.981929	-3.092923
H	-1.221256	0.699773	-3.683595
H	-2.976601	0.677779	-3.668418
H	-2.102287	2.067556	-2.997155
C	-3.050799	0.955678	-0.748133
H	-2.826082	0.717565	0.291533

H	-3.048413	2.040490	-0.852512
H	-4.073674	0.605217	-0.940754

38

1 + 1,2,5b-*c*-$C_5H_3(CF_3)_3$ = **1** + 3,4,5b-*c*-$C_5H_3(CF_3)_3$

C	0.012798	0.002216	-0.006385
C	-0.165358	0.359322	-1.554575
C	-1.636640	0.108479	-1.895341
C	-1.834138	-1.205816	-1.871857
C	-0.514155	-1.865864	-1.537083
C	-0.226477	-1.585033	-0.019593
C	0.995026	-2.406803	0.418908
H	1.888304	-2.224152	-0.178699
H	1.246706	-2.207600	1.462591
H	0.755751	-3.470030	0.338324
C	-1.401379	-2.053105	0.847150
H	-2.337774	-1.550209	0.607996
H	-1.550062	-3.127176	0.703882
H	-1.191839	-1.890390	1.906844
H	-0.418880	-2.915664	-1.810829
C	0.475008	-0.892417	-2.201235
C	0.575260	-0.988149	-3.713403
F	0.923892	-2.247019	-4.044996
F	-0.540169	-0.703846	-4.386818
F	1.537343	-0.182123	-4.180665
H	1.499047	-1.035689	-1.855974
H	-2.784219	-1.709935	-1.985142
C	-2.709592	1.120236	-2.137289
F	-2.750322	1.522710	-3.411592
F	-3.919366	0.611448	-1.850784
F	-2.548045	2.216279	-1.382208
C	0.430602	1.681738	-2.003735
F	0.133430	2.697549	-1.182233
F	1.769519	1.613795	-2.064509
F	-0.006945	2.017151	-3.222302
C	1.411126	0.392602	0.499372
H	1.516298	1.478589	0.508982
H	1.536437	0.044794	1.526558
H	2.228580	-0.013592	-0.095936
C	-0.995516	0.760111	0.866943
H	-0.816655	1.833792	0.807458
H	-2.032085	0.577946	0.586361
H	-0.874691	0.457736	1.909711

38

1 + 1,3,5a-*c*-$C_5H_3(CF_3)_3$ TS = **1** + 2,4,5a-*c*-$C_5H_3(CF_3)_3$ TS

C	-0.004294	-0.021457	0.025917
C	-0.099070	1.182198	-0.875219
C	0.654361	0.854411	-1.994871
C	0.775369	-0.534786	-2.063194
C	0.024314	-1.116668	-1.020456
H	0.100846	-2.163183	-0.747613
C	1.490864	-1.258791	-3.146662
F	1.099611	-0.866922	-4.378372
F	2.815046	-1.041148	-3.096886
F	1.304914	-2.583850	-3.074289
H	1.007310	1.558779	-2.737203
C	-0.232025	2.586394	-0.403277
F	-0.481881	3.410219	-1.435299
F	-1.224141	2.740181	0.483806
F	0.885303	3.040378	0.196065
H	1.035266	-0.025063	0.394781
C	-0.772567	-0.145303	1.327956
F	-2.035612	0.280245	1.328295
F	-0.779496	-1.425838	1.734797
F	-0.141824	0.567103	2.274737
C	-2.202070	0.288536	-1.941026
C	-1.941659	-1.087000	-1.747396
C	-2.712381	-1.874788	-0.699270
H	-3.675899	-2.167656	-1.131573
H	-2.184645	-2.797006	-0.444865
H	-2.919202	-1.338951	0.219415
C	-1.729888	-1.959553	-2.978553
H	-2.706854	-2.158820	-3.433663
H	-1.102841	-1.507071	-3.741613
H	-1.295278	-2.923129	-2.704733
C	-1.962488	0.891823	-3.302191
H	-1.037175	0.563311	-3.772230

H	-2.779688	0.580604	-3.966813
H	-1.967450	1.981846	-3.251293
C	-3.275632	1.031281	-1.183838
H	-3.504598	0.628937	-0.205163
H	-3.038438	2.091008	-1.082141
H	-4.189963	0.968542	-1.789723

38

1 + 1,3,5a-*c*-$C_5H_3(CF_3)_3$ = **1** + 2,4,5a-*c*-$C_5H_3(CF_3)_3$

C	0.006870	-0.001299	-0.005820
C	-0.034484	0.298692	-1.571353
C	-1.491779	0.083561	-1.980096
C	-1.705794	-1.228132	-1.943008
C	-0.415793	-1.915800	-1.518472
C	-0.193053	-1.589782	0.000269
C	1.017972	-2.375046	0.527140
H	1.949664	-2.176383	0.006752
H	1.178928	-2.157805	1.585301
H	0.809879	-3.444520	0.440634
C	-1.390237	-2.056581	0.837584
H	-2.327374	-1.575597	0.563204
H	-1.524150	-3.134464	0.715756
H	-1.208423	-1.864376	1.897797
H	-0.340351	-2.974956	-1.763133
C	0.543374	-0.964117	-2.278115
H	0.231277	-0.938780	-3.323440
C	2.030195	-1.271064	-2.429127
F	2.864215	-0.877507	-1.462467
F	2.196951	-2.597425	-2.572304
F	2.477731	-0.693630	-3.555086
C	-2.968323	-1.928315	-2.301361
F	-2.804584	-2.660312	-3.416589
F	-3.373905	-2.779025	-1.345637
F	-3.968677	-1.069796	-2.527518
H	-2.203480	0.869879	-2.194907
C	0.527556	1.614218	-2.049807
F	-0.025008	2.659056	-1.412466
F	1.851204	1.693816	-1.876439
F	0.290345	1.786723	-3.360087
C	1.293945	0.468460	0.691043
H	1.362541	1.557446	0.644650
H	1.237116	0.194247	1.747295
H	2.209441	0.057455	0.283661
C	-1.124483	0.759193	0.715696
H	-0.956748	1.834408	0.639676
H	-2.119748	0.544016	0.331459
H	-1.116036	0.500651	1.776335

38

1 + 1,3,5b-*c*-$C_5H_3(CF_3)_3$ TS = **1** + 2,4,5b-*c*-$C_5H_3(CF_3)_3$ TS

C	-0.013477	-0.037912	0.028032
C	0.026896	1.171350	-0.866532
C	0.785433	0.849746	-1.977320
C	0.887421	-0.545080	-2.053773
C	0.143742	-1.123101	-1.015197
H	0.220179	-2.169787	-0.744360
C	1.563380	-1.277232	-3.157671
F	1.127756	-0.883334	-4.373995
F	2.888229	-1.075152	-3.155783
F	1.359613	-2.599592	-3.075521
H	1.150085	1.551727	-2.716709
C	-0.161707	2.565950	-0.380777
F	-0.675372	3.352962	-1.345769
F	-0.997535	2.620177	0.666868
F	0.985894	3.146485	0.006980
C	1.134413	-0.076873	1.035992
F	0.986131	0.893583	1.947675
F	1.117825	-1.247532	1.697629
F	2.345435	0.060498	0.498921
H	-0.909513	-0.116028	0.639045
C	-2.102734	0.306071	-1.756018
C	-1.842669	-1.076625	-1.639306
C	-2.510644	-1.857545	-0.520159
H	-3.570142	-1.995691	-0.763982
H	-2.068168	-2.851279	-0.424021
H	-2.471522	-1.373661	0.454700
C	-1.734791	-1.913151	-2.903198
H	-2.739716	-2.083862	-3.306268

H	-1.144293	-1.441686	-3.685545
H	-1.295495	-2.889349	-2.688094
C	-2.017737	0.951100	-3.112488
H	-1.114649	0.663924	-3.654008
H	-2.867782	0.623690	-3.725674
H	-2.049844	2.037803	-3.035022
C	-3.018551	0.999914	-0.778405
H	-2.812097	0.768068	0.266435
H	-2.977014	2.082369	-0.898816
H	-4.051102	0.682315	-0.976680

38

1 + 1,3,5b-*c*-$C_5H_3(CF_3)_3$ = **1** + 2,4,5b-*c*-$C_5H_3(CF_3)_3$

C	0.009902	0.001612	-0.007699
C	-0.157453	0.324656	-1.561169
C	-1.621454	0.098792	-1.910153
C	-1.817979	-1.213841	-1.888676
C	-0.513502	-1.893669	-1.510170
C	-0.230845	-1.586890	0.004164
C	0.991486	-2.402498	0.454265
H	1.884545	-2.235832	-0.148304
H	1.245989	-2.183454	1.493100
H	0.747711	-3.466115	0.396171
C	-1.398499	-2.032979	0.889450
H	-2.331177	-1.519033	0.663380
H	-1.570694	-3.103692	0.754031
H	-1.165129	-1.865774	1.943595
H	-0.429808	-2.948879	-1.769764
C	0.490564	-0.936611	-2.180887
C	0.614313	-1.057731	-3.688742
F	0.982323	-2.315784	-3.994312
F	-0.491751	-0.794391	-4.385318
F	1.577353	-0.246398	-4.149324
H	1.509022	-1.080683	-1.819850
C	-3.085108	-1.925833	-2.203672
F	-2.947275	-2.678773	-3.305345
F	-3.459809	-2.760181	-1.217836
F	-4.096615	-1.077569	-2.416102
H	-2.350789	0.876594	-2.092639
C	0.381164	1.653501	-2.041282
F	-0.068252	2.675531	-1.292766
F	1.718874	1.700808	-2.015108
F	-0.000617	1.902318	-3.301156
C	1.401697	0.403686	0.503828
H	1.506038	1.490088	0.491588
H	1.517682	0.077157	1.539295
H	2.225179	-0.013311	-0.075736
C	-1.008209	0.776750	0.840701
H	-0.795092	1.845288	0.803874
H	-2.038105	0.624412	0.519348
H	-0.934325	0.461373	1.883600

38

1 + 1,4,5a-*c*-$C_5H_3(CF_3)_3$ TS

C	-0.097941	0.016496	-0.050999
C	-0.211716	1.164186	-1.037955
C	0.552367	0.743754	-2.140658
C	0.630681	-0.644453	-2.137292
C	-0.075019	-1.130035	-1.033664
C	0.026892	-2.558232	-0.611122
F	1.226744	-2.841483	-0.071892
F	-0.890313	-2.895475	0.302714
F	-0.130037	-3.378272	-1.663633
H	1.056170	-1.261979	-2.916037
H	0.919164	1.401607	-2.915140
C	-0.136400	2.605431	-0.620164
F	0.099610	3.391253	-1.684706
F	-1.247301	3.070967	-0.040571
F	0.868236	2.807841	0.250243
H	0.943499	0.098803	0.299463
C	-0.836845	-0.064063	1.275541
F	-2.056784	-0.600564	1.257141
F	-0.112404	-0.815332	2.120482
F	-0.945491	1.153493	1.820667
C	-2.291501	0.683425	-1.839142
C	-2.191763	-0.717568	-2.016442
C	-3.124292	-1.649469	-1.273487
H	-4.083631	-1.639843	-1.809248

H	-2.759705	-2.676893	-1.292926
H	-3.321352	-1.368102	-0.246503
C	-1.888886	-1.246779	-3.401056
H	-2.785950	-1.119682	-4.020946
H	-1.081273	-0.721309	-3.905796
H	-1.651618	-2.311108	-3.371729
C	-2.203318	1.581685	-3.060689
H	-1.389681	1.325377	-3.735422
H	-3.140146	1.495592	-3.625972
H	-2.092493	2.627941	-2.771436
C	-3.300198	1.221718	-0.838085
H	-3.154788	0.890060	0.184660
H	-3.306749	2.309361	-0.842735
H	-4.297331	0.883372	-1.147516

38

1 + 1,4,5a-*c*-$C_5H_3(CF_3)_3$

C	-0.006789	-0.002902	-0.001446
C	0.288745	-0.936855	-1.256951
C	0.685662	0.021984	-2.377219
C	-0.415380	0.659841	-2.755609
C	-1.576574	0.126585	-1.911514
C	-1.372789	0.719063	-0.455206
C	-2.556999	0.418451	0.478898
H	-2.858781	-0.624805	0.500919
H	-2.300880	0.717552	1.496639
H	-3.422571	1.008721	0.177368
C	-1.258100	2.251778	-0.497767
H	-0.466087	2.608708	-1.154528
H	-2.199186	2.687142	-0.836137
H	-1.064137	2.634966	0.506445
C	-2.900013	0.376645	-2.604821
F	-3.972661	-0.008305	-1.910996
F	-3.056836	1.688736	-2.865772
F	-2.939591	-0.259155	-3.786246
C	-1.093831	-1.351059	-1.837272
H	-0.937836	-1.690287	-2.862889
C	-1.914911	-2.514650	-1.290140
F	-2.103221	-2.598703	0.029696
F	-3.128400	-2.511706	-1.857310
F	-1.315336	-3.657855	-1.657808
H	-0.508925	1.470707	-3.464867
H	1.703396	0.192146	-2.701197
C	1.271427	-2.067758	-1.070126
F	2.469062	-1.617830	-0.656750
F	0.860486	-2.973172	-0.175964
F	1.477984	-2.716319	-2.226066
C	-0.118879	-0.762051	1.331390
H	0.839908	-1.226780	1.568510
H	-0.330534	-0.046291	2.128561
H	-0.881015	-1.532114	1.355436
C	1.155910	0.986269	0.216723
H	2.064648	0.438521	0.469141
H	1.367797	1.615809	-0.644754
H	0.925794	1.639522	1.060431

38

1 + 1,4,5b-*c*-$C_5H_3(CF_3)_3$ TS

C	-0.007402	0.015385	-0.001960
C	-0.218964	-1.023887	1.074483
C	0.465816	-0.592814	2.211130
C	0.711563	0.776206	2.094680
C	0.184099	1.224619	0.883534
C	0.532302	2.573980	0.333588
F	1.852157	2.713341	0.131763
F	-0.070378	2.820350	-0.836271
F	0.177000	3.555587	1.182489
H	1.143646	1.412191	2.855359
H	0.674499	-1.205610	3.077562
C	-0.366028	-2.481961	0.763650
F	-1.001830	-3.131946	1.755269
F	-1.055948	-2.697976	-0.362963
F	0.821677	-3.090730	0.618192
C	1.230048	-0.279653	-0.859157
F	1.043880	-1.399796	-1.570270
F	1.431737	0.710786	-1.738424
F	2.351735	-0.429707	-0.156691
H	-0.823851	0.101579	-0.717343

C	-2.298638	-0.168447	1.521807
C	-2.048982	1.219433	1.411165
C	-2.623890	1.972634	0.230239
H	-3.718254	1.974420	0.314055
H	-2.292737	3.010630	0.224451
H	-2.380903	1.535171	-0.738484
C	-2.004295	2.035460	2.683899
H	-3.003373	2.050188	3.137153
H	-1.324423	1.617588	3.426542
H	-1.710982	3.064945	2.486057
C	-2.509760	-0.743751	2.904936
H	-1.706805	-0.484053	3.594920
H	-3.437982	-0.337748	3.326006
H	-2.602298	-1.827958	2.874109
C	-3.129117	-0.847575	0.453250
H	-2.776302	-0.673823	-0.563720
H	-3.177508	-1.924014	0.614424
H	-4.154013	-0.458319	0.505537

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1 + 1,4,5b-*c*-$C_5H_3(CF_3)_3$

C	0.002091	-0.014263	0.002444
C	-0.277072	0.296963	1.537353
C	0.200992	1.717860	1.799617
C	1.527200	1.705031	1.770683
C	1.965629	0.275249	1.488411
C	1.613614	-0.029830	-0.032815
C	2.196882	-1.379047	-0.483380
H	1.923137	-2.219199	0.154638
H	1.866092	-1.604176	-1.498784
H	3.286464	-1.321839	-0.504159
C	2.203143	1.030535	-0.974470
H	1.901890	2.045004	-0.716630
H	3.291398	0.983861	-0.960087
H	1.882509	0.834214	-1.999346
C	3.389837	-0.012002	1.918335
F	3.660252	-1.321436	1.974320
F	4.281466	0.538171	1.073774
F	3.646962	0.505053	3.126323
C	0.851437	-0.529833	2.201662
C	0.883278	-0.625786	3.722434
F	1.959644	-1.325304	4.112380
F	0.906843	0.538043	4.369189
F	-0.187251	-1.307236	4.157920
H	0.834322	-1.570143	1.874259
H	2.203088	2.545869	1.845010
H	-0.454579	2.571528	1.903163
C	-1.686521	0.038058	2.029607
F	-2.603151	0.607721	1.225762
F	-1.981126	-1.265602	2.096456
F	-1.879240	0.558200	3.248246
C	-0.626520	-1.351712	-0.421517
H	-1.714657	-1.273203	-0.394893
H	-0.344835	-1.582991	-1.450281
H	-0.341826	-2.197410	0.204305
C	-0.607615	1.057700	-0.912791
H	-1.694811	1.033441	-0.848821
H	-0.274142	2.065726	-0.669913
H	-0.337935	0.854620	-1.950949

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1 + 1,5a,5b-*c*-$C_5H_3(CF_3)_3$ TS

C	0.003214	-0.014526	0.001859
C	-0.149802	1.174540	-0.933528
C	0.584837	0.833344	-2.071403
C	0.699411	-0.549383	-2.149234
C	-0.006900	-1.116375	-1.065629
H	0.089889	-2.155400	-0.768657
H	1.139101	-1.103646	-2.964759
H	0.919623	1.544213	-2.815503
C	-0.310340	2.592645	-0.502308
F	-1.003053	3.292130	-1.424064
F	-0.971860	2.694390	0.656797
F	0.855037	3.245942	-0.349141
C	1.441090	0.019230	0.653621
F	1.631490	1.160167	1.319407
F	1.568786	-0.996887	1.520453
F	2.451858	-0.086749	-0.203101

C	-0.952643	-0.199927	1.205399
F	-2.169060	0.292029	0.994611
F	-1.084607	-1.506489	1.484799
F	-0.509460	0.387146	2.318811
C	-2.262962	0.283368	-1.948749
C	-1.951341	-1.098145	-1.790277
C	-2.762153	-1.962100	-0.832050
H	-3.674533	-2.273783	-1.352767
H	-2.213500	-2.870818	-0.574543
H	-3.061523	-1.479645	0.089688
C	-1.690437	-1.911016	-3.056587
H	-2.648562	-2.115320	-3.547351
H	-1.051477	-1.409254	-3.777520
H	-1.239280	-2.875638	-2.808894
C	-2.039693	0.918169	-3.298139
H	-1.081157	0.672355	-3.750554
H	-2.812137	0.544880	-3.984173
H	-2.138263	2.002572	-3.236936
C	-3.406769	0.962630	-1.223970
H	-3.853782	0.367299	-0.435869
H	-3.117409	1.930266	-0.809588
H	-4.185352	1.160527	-1.969797

38

1 + 1,5a,5b-*c*-$C_5H_3(CF_3)_3$

C	0.013473	-0.008856	-0.000601
C	-0.085199	0.341601	-1.583252
C	-1.568349	0.135859	-1.888003
C	-1.799277	-1.169454	-1.852699
C	-0.477947	-1.871368	-1.562172
C	-0.200709	-1.594148	-0.035919
C	0.972571	-2.414596	0.527203
H	1.939638	-2.230666	0.076973
H	1.068394	-2.218081	1.598045
H	0.749445	-3.477946	0.407016
C	-1.422683	-2.075320	0.769105
H	-2.343287	-1.551509	0.519497
H	-1.577877	-3.141978	0.582804
H	-1.245633	-1.955431	1.840111
H	-0.416370	-2.924224	-1.836565
C	0.470468	-0.918710	-2.362942
C	0.169493	-1.001621	-3.909735
F	0.743456	-2.121879	-4.386156
F	-1.106897	-1.088502	-4.280319
F	0.679924	0.037923	-4.569011
C	1.997780	-1.251648	-2.305807
F	2.641742	-0.702397	-1.279079
F	2.171509	-2.579658	-2.219468
F	2.663252	-0.840521	-3.387617
H	-2.748185	-1.672129	-1.973715
H	-2.273256	0.943609	-2.026509
C	0.438183	1.702385	-2.000788
F	0.105996	2.654937	-1.111739
F	1.770880	1.715703	-2.116295
F	-0.071580	2.097597	-3.173884
C	1.280190	0.453626	0.754949
H	1.497833	1.497853	0.523886
H	1.065504	0.406060	1.825343
H	2.175258	-0.125255	0.586080
C	-1.115717	0.729834	0.759774
H	-0.897491	1.796992	0.802505
H	-2.108766	0.599210	0.338814
H	-1.143627	0.363591	1.787214

38

1 + 2,3,5a-*c*-$C_5H_3(CF_3)_3$ TS

C	-0.126896	-0.001306	-0.026090
C	-0.258124	1.104238	-1.049252
C	0.601789	0.678738	-2.084017
C	0.709523	-0.719776	-2.019229
C	-0.021000	-1.189994	-0.936257
H	-0.041780	-2.221744	-0.610528
C	1.451936	-1.623250	-2.954026
F	1.418105	-1.206273	-4.224484
F	2.742516	-1.721212	-2.607405
F	0.942258	-2.864760	-2.924537
C	1.206630	1.574189	-3.113959
F	2.527209	1.368069	-3.214728

F	0.704754	1.410271	-4.352327
F	1.018340	2.863968	-2.795142
H	-0.354225	2.146152	-0.766300
H	0.897537	0.151198	0.352739
C	-0.916412	-0.070403	1.264566
F	-2.009392	-0.839962	1.232318
F	-0.136408	-0.594444	2.227031
F	-1.283082	1.149061	1.681949
C	-2.185048	0.704613	-1.792317
C	-2.149997	-0.690444	-2.021237
C	-3.060102	-1.658683	-1.297612
H	-3.919916	-1.845149	-1.954045
H	-2.576160	-2.623792	-1.134870
H	-3.445237	-1.297925	-0.351770
C	-1.812160	-1.188578	-3.406202
H	-2.685638	-1.035358	-4.053646
H	-0.982636	-0.663274	-3.876953
H	-1.591158	-2.257415	-3.394409
C	-2.153051	1.646689	-2.988137
H	-1.473582	1.339280	-3.775977
H	-3.159286	1.693208	-3.420358
H	-1.885730	2.660793	-2.680876
C	-3.095381	1.284488	-0.721250
H	-3.193118	0.684698	0.175912
H	-2.762721	2.282933	-0.428517
H	-4.097641	1.393975	-1.150875

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1 + 2,3,5a-*c*-$C_5H_3(CF_3)_3$

C	0.047548	0.005770	0.050321
C	0.205567	-0.234263	-1.510453
C	1.337271	0.696645	-1.933846
C	0.878316	1.947132	-1.864639
C	-0.580756	1.874517	-1.425378
C	-0.590997	1.464617	0.089918
C	-2.029272	1.502512	0.627271
H	-2.727141	0.859443	0.098677
H	-2.043975	1.208351	1.679337
H	-2.408852	2.525574	0.564411
C	0.203336	2.478384	0.922306
H	1.254759	2.537720	0.646837
H	-0.231722	3.474787	0.800487
H	0.149622	2.225273	1.984087
H	-1.173775	2.759048	-1.651872
C	-0.930210	0.575218	-2.196993
H	-0.662523	0.726114	-3.243532
C	-2.362178	0.076283	-2.326232
F	-2.785100	-0.811296	-1.417762
F	-3.227525	1.103020	-2.310362
F	-2.505086	-0.534637	-3.515806
C	1.624076	3.217421	-2.148943
F	0.768109	4.229069	-2.352792
F	2.429835	3.585308	-1.142718
F	2.383287	3.106048	-3.243611
C	2.705680	0.222858	-2.316374
F	2.811122	0.075648	-3.643642
F	3.668876	1.061141	-1.923608
F	2.966156	-0.973746	-1.769062
H	0.331890	-1.278025	-1.795499
C	-0.800382	-1.079222	0.732039
H	-0.344591	-2.056907	0.554882
H	-0.798433	-0.913034	1.812556
H	-1.831919	-1.124844	0.406885
C	1.421883	-0.092177	0.740072
H	1.827237	-1.097977	0.605953
H	2.162614	0.617784	0.372737
H	1.311626	0.078384	1.813045

38

1 + 2,3,5b-*c*-$C_5H_3(CF_3)_3$ TS

C	-0.055423	0.004994	0.042457
C	-0.266607	-1.006167	1.140512
C	0.479708	-0.560048	2.227833
C	0.747966	0.811899	2.058585
C	0.174456	1.240735	0.870434
H	0.319439	2.226745	0.448067
C	1.451331	1.718120	3.017869
F	1.109138	1.482254	4.292689

F	2.779787	1.587840	2.937962
F	1.163369	3.003854	2.759092
C	0.843607	-1.398486	3.411935
F	2.136934	-1.255480	3.721162
F	0.146578	-1.095077	4.520675
F	0.620537	-2.697045	3.163848
H	-0.485279	-2.049765	0.952309
C	1.156654	-0.335863	-0.820132
F	0.936924	-1.481533	-1.487019
F	1.349091	0.624599	-1.739852
F	2.298353	-0.478929	-0.149862
H	-0.869588	0.079927	-0.672363
C	-2.270651	-0.161492	1.531821
C	-2.009679	1.222630	1.447829
C	-2.512193	2.019117	0.260610
H	-3.601295	2.130119	0.331925
H	-2.081994	3.021925	0.256515
H	-2.305027	1.559522	-0.705941
C	-1.934274	2.035085	2.720815
H	-2.941031	2.157912	3.139143
H	-1.324377	1.563580	3.491390
H	-1.527574	3.028906	2.526885
C	-2.544701	-0.792008	2.880676
H	-1.899607	-0.419146	3.671030
H	-3.580553	-0.578894	3.172499
H	-2.433870	-1.878098	2.835578
C	-3.040270	-0.854197	0.423854
H	-2.757726	-0.554634	-0.584272
H	-2.939855	-1.938858	0.498139
H	-4.106057	-0.619808	0.534562

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1 + 2,3,5b-*c*-$C_5H_3(CF_3)_3$

C	0.074290	0.012744	-0.039781
C	0.360530	-0.139737	-1.584712
C	1.481204	0.825258	-1.930273
C	0.986192	2.059251	-1.869553
C	-0.477500	1.945770	-1.471847
C	-0.526634	1.494412	0.037935
C	-1.980733	1.554624	0.528081
H	-2.679432	0.986650	-0.086815
H	-2.059565	1.181739	1.551591
H	-2.315229	2.594976	0.532230
C	0.275128	2.453969	0.922928
H	1.334824	2.486052	0.676545
H	-0.121827	3.468015	0.817589
H	0.182846	2.172224	1.974697
H	-1.091504	2.817738	-1.692880
C	-0.844678	0.621483	-2.167207
C	-1.001632	0.644227	-3.670580
F	-2.071734	1.385720	-4.005855
F	0.037100	1.131199	-4.355551
F	-1.223121	-0.600552	-4.127253
H	-1.792988	0.219947	-1.811261
C	1.699558	3.352343	-2.126233
F	0.820347	4.315865	-2.438564
F	2.389646	3.787069	-1.060755
F	2.559882	3.246177	-3.140789
C	2.883159	0.396011	-2.232424
F	3.098709	0.302045	-3.547729
F	3.793933	1.236610	-1.729292
F	3.126263	-0.816144	-1.706202
H	0.511145	-1.170132	-1.904754
C	-0.909576	-1.082669	0.395384
H	-0.436348	-2.060122	0.274394
H	-1.168811	-0.972765	1.450739
H	-1.838787	-1.092767	-0.175137
C	1.351933	-0.190808	0.781764
H	1.734866	-1.201826	0.623306
H	2.147795	0.509010	0.524954
H	1.141510	-0.076845	1.847922

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1 + 2,5a,5b-*c*-$C_5H_3(CF_3)_3$ TS = **1** + 3,5a,5b-*c*-$C_5H_3(CF_3)_3$ TS

C	0.005594	-0.003180	0.002534
C	-0.212154	1.121385	-1.014663
C	0.581391	0.706048	-2.103561
C	0.708802	-0.684550	-2.080416

C	0.044667	-1.175374	-0.962111
H	0.055868	-2.206109	-0.632500
H	1.148466	-1.283201	-2.866610
C	1.160512	1.583797	-3.153611
F	2.498978	1.630788	-3.076860
F	0.876183	1.148503	-4.400904
F	0.715223	2.844519	-3.062311
H	-0.286596	2.157281	-0.700630
C	1.442482	0.189222	0.632731
F	1.391911	1.135058	1.583242
F	1.871100	-0.945162	1.196025
F	2.392132	0.564230	-0.217428
C	-0.933248	-0.088371	1.224702
F	-2.002211	-0.852641	1.001434
F	-0.339233	-0.628206	2.295389
F	-1.358058	1.127288	1.587974
C	-2.146821	0.714287	-1.724073
C	-2.126722	-0.691726	-1.949406
C	-3.086559	-1.646902	-1.265346
H	-3.820891	-1.959077	-2.016883
H	-2.587881	-2.553411	-0.916579
H	-3.635607	-1.215482	-0.436161
C	-1.805619	-1.188432	-3.341042
H	-2.681931	-1.013861	-3.979392
H	-0.968512	-0.683240	-3.816852
H	-1.612439	-2.263708	-3.332365
C	-2.110587	1.630328	-2.942743
H	-1.392944	1.335956	-3.702771
H	-3.101394	1.620908	-3.411283
H	-1.897099	2.660346	-2.649741
C	-3.101810	1.321009	-0.704390
H	-3.279524	0.726689	0.183043
H	-2.752990	2.306466	-0.388264
H	-4.068055	1.467356	-1.200227

38

1 + 2,5a,5b-*c*-$C_5H_3(CF_3)_3$ = **1** + 3,5a,5b-*c*-$C_5H_3(CF_3)_3$

C	-0.008690	-0.015065	-0.000111
C	0.214191	-0.220112	-1.575899
C	1.367209	0.720993	-1.903367
C	0.918576	1.966468	-1.801329
C	-0.569795	1.889089	-1.469861
C	-0.626081	1.461356	0.042957
C	-2.051340	1.572076	0.607519
H	-2.807831	1.000418	0.080845
H	-2.061877	1.253639	1.652891
H	-2.357155	2.621225	0.582329
C	0.204698	2.454894	0.874671
H	1.258636	2.477794	0.602531
H	-0.198758	3.463672	0.748910
H	0.138314	2.206989	1.936554
H	-1.153125	2.780457	-1.700806
C	-0.906863	0.604420	-2.299988
C	-0.661675	0.839753	-3.840617
F	-1.806074	1.171797	-4.458094
F	0.175367	1.833370	-4.156093
F	-0.186783	-0.269786	-4.411689
C	-2.329501	-0.006319	-2.264693
F	-2.584867	-0.743226	-1.185036
F	-3.270483	0.943808	-2.324138
F	-2.518709	-0.847280	-3.291631
H	1.486464	2.878512	-1.921283
C	2.738135	0.299686	-2.296103
F	2.771651	-0.107685	-3.574348
F	3.619896	1.301038	-2.173708
F	3.190116	-0.729135	-1.559432
H	0.334420	-1.257269	-1.887849
C	-0.848590	-1.113867	0.700249
H	-0.740202	-2.064910	0.173417
H	-0.469937	-1.264110	1.712716
H	-1.906110	-0.902066	0.788461
C	1.358752	-0.125849	0.711083
H	1.733757	-1.147655	0.610060
H	2.127516	0.548949	0.343569
H	1.229255	0.072992	1.776394

41

1 + 1,2,3,4-*c*-$C_5H_2(CF_3)_4$ TS

C	-0.050946	0.009682	0.014142
C	-0.245728	-1.027429	1.076298
C	0.479003	-0.600771	2.195684
C	0.721855	0.777348	2.065168
C	0.153381	1.223445	0.867072
C	0.490037	2.524815	0.181548
F	1.812348	2.747184	0.174375
F	0.095224	2.473413	-1.102329
F	-0.086458	3.604775	0.717541
C	1.424614	1.636651	3.079577
F	1.076084	1.314226	4.332806
F	2.751173	1.518098	2.988886
F	1.125764	2.928623	2.907701
C	0.908418	-1.429043	3.379965
F	2.161493	-1.118862	3.728729
F	0.140333	-1.243078	4.462675
F	0.877264	-2.733730	3.104393
C	-0.439187	-2.453685	0.635867
F	-1.184670	-3.176050	1.478718
F	-1.052937	-2.484849	-0.560160
F	0.726636	-3.093209	0.472204
H	0.891630	-0.207714	-0.514544
H	-0.840265	0.078668	-0.727469
C	-2.324029	-0.134610	1.571601
C	-2.054320	1.246549	1.438547
C	-2.625554	1.976161	0.238556
H	-3.720193	1.964321	0.311694
H	-2.309525	3.017594	0.217838
H	-2.369812	1.522254	-0.719036
C	-1.976507	2.096445	2.688626
H	-2.982167	2.190375	3.117247
H	-1.343610	1.663958	3.463103
H	-1.611284	3.097679	2.464666
C	-2.531715	-0.707974	2.953590
H	-1.816932	-0.339869	3.684257
H	-3.530315	-0.415411	3.303414
H	-2.490625	-1.797126	2.944505
C	-3.164645	-0.817436	0.513842
H	-2.832178	-0.636748	-0.507560
H	-3.208698	-1.894049	0.675333
H	-4.189312	-0.431356	0.589609

41

1 + 1,2,3,4-*c*-$C_5H_2(CF_3)_4$

C	0.000449	0.014535	-0.028690
C	-0.298904	0.279305	1.507735
C	0.181731	1.700106	1.824282
C	1.517144	1.669474	1.817991
C	1.945487	0.240790	1.489322
C	1.611374	-0.007286	-0.041058
C	2.187810	-1.354303	-0.507821
H	1.881012	-2.199621	0.107184
H	1.876433	-1.551471	-1.534823
H	3.277793	-1.315489	-0.503321
C	2.234631	1.075451	-0.931917
H	1.918132	2.086519	-0.672917
H	3.322234	1.035581	-0.857870
H	1.963219	0.902166	-1.975514
C	3.320202	-0.189326	1.977411
F	3.353144	-1.518104	2.174183
F	4.320337	0.095367	1.137274
F	3.604404	0.385910	3.154487
C	0.817037	-0.525358	2.190224
H	0.827823	-0.398770	3.273696
H	0.794990	-1.582219	1.934040
C	2.449385	2.843896	1.990532
F	2.646486	3.126005	3.278575
F	3.642198	2.583448	1.444141
F	1.981739	3.947979	1.399276
C	-0.653762	2.951945	1.982567
F	-0.194334	3.696238	2.991654
F	-0.639062	3.715615	0.880965
F	-1.931842	2.671524	2.234447
C	-1.665802	-0.125440	2.031575
F	-2.683742	0.327142	1.291630
F	-1.779080	-1.464700	2.067292
F	-1.843909	0.298425	3.289299
C	-0.622368	-1.313300	-0.490783

H	-1.710946	-1.237460	-0.471254
H	-0.331161	-1.511964	-1.523345
H	-0.337187	-2.172200	0.114720
C	-0.606096	1.107116	-0.918025
H	-1.687993	1.143622	-0.775051
H	-0.206116	2.099307	-0.722824
H	-0.420693	0.875418	-1.969212

41

1 + 1,2,3,5a-*c*-$C_5H_2(CF_3)_4$ TS = **1** + 2,3,4,5a-*c*-$C_5H_2(CF_3)_4$ TS

C	-0.118308	-0.020696	-0.034266
C	-0.193371	1.204977	-0.906805
C	0.574201	0.884783	-2.025838
C	0.669214	-0.513444	-2.131001
C	-0.098253	-1.093533	-1.096255
H	-0.016631	-2.143036	-0.838922
C	1.370872	-1.320741	-3.177938
F	1.005367	-0.994833	-4.430740
F	2.700475	-1.198942	-3.111601
F	1.095535	-2.627016	-3.021141
C	1.206281	1.895047	-2.954775
F	2.142329	1.325700	-3.716146
F	0.325430	2.475923	-3.776996
F	1.799367	2.869437	-2.257780
C	-0.393362	2.585085	-0.371476
F	-0.705242	3.441168	-1.353722
F	-1.394984	2.618870	0.519672
F	0.689177	3.064704	0.258964
H	0.926160	-0.038903	0.324807
C	-0.860426	-0.180715	1.282323
F	-2.136711	0.197063	1.324584
F	-0.812861	-1.469116	1.660752
F	-0.228228	0.534026	2.224200
C	-2.335158	0.272834	-2.007186
C	-2.065573	-1.097253	-1.798805
C	-2.820235	-1.876955	-0.733807
H	-3.756856	-2.230726	-1.178805
H	-2.260304	-2.763859	-0.428216
H	-3.077363	-1.312162	0.153700
C	-1.864939	-1.982555	-3.023170
H	-2.843924	-2.155750	-3.484031
H	-1.218468	-1.555689	-3.784490
H	-1.461882	-2.955527	-2.736592
C	-2.102943	0.849031	-3.375487
H	-1.177379	0.514039	-3.841394
H	-2.917517	0.508915	-4.029746
H	-2.114991	1.938525	-3.356259
C	-3.376068	1.038181	-1.231427
H	-3.515572	0.715118	-0.207740
H	-3.167087	2.108468	-1.237746
H	-4.330284	0.897769	-1.758054

41

1 + 1,2,3,5a-*c*-$C_5H_2(CF_3)_4$ = **1** + 2,3,4,5a-*c*-$C_5H_2(CF_3)_4$

C	-0.039229	0.009754	0.060530
C	-0.088488	0.351248	-1.497486
C	-1.553486	0.114525	-1.913440
C	-1.753786	-1.203761	-1.889394
C	-0.449772	-1.871484	-1.487661
C	-0.234136	-1.576796	0.036895
C	0.972700	-2.374053	0.554421
H	1.908526	-2.162892	0.046905
H	1.123168	-2.181379	1.618749
H	0.765117	-3.441073	0.441442
C	-1.440522	-2.069728	0.847159
H	-2.373207	-1.569714	0.593591
H	-1.578461	-3.141670	0.678073
H	-1.264800	-1.927873	1.916076
H	-0.369590	-2.923216	-1.754888
C	0.493115	-0.898267	-2.233275
H	0.177466	-0.850346	-3.277303
C	1.976156	-1.230700	-2.402202
F	2.828651	-0.893762	-1.432079
F	2.096432	-2.559107	-2.579085
F	2.429998	-0.644266	-3.518200
C	-3.023222	-1.953211	-2.192208
F	-2.751366	-3.247841	-2.409929
F	-3.911213	-1.903947	-1.192341

F	-3.622360	-1.479376	-3.287106
C	-2.588328	1.160536	-2.232120
F	-2.680729	1.370424	-3.547255
F	-3.798422	0.789724	-1.796712
F	-2.299747	2.329575	-1.654592
C	0.532960	1.668231	-1.931072
F	0.223386	2.697264	-1.137237
F	1.869356	1.575263	-1.937669
F	0.150549	1.986136	-3.176063
C	1.261160	0.462144	0.744969
H	1.328763	1.551293	0.732295
H	1.227029	0.153831	1.792347
H	2.167103	0.062911	0.305082
C	-1.163675	0.755256	0.804712
H	-1.008805	1.832404	0.731441
H	-2.165833	0.533685	0.438846
H	-1.136495	0.486893	1.862732

41

1 + 1,2,3,5b-*c*-$C_5H_2(CF_3)_4$ TS = **1** + 2,3,4,5b-*c*-$C_5H_2(CF_3)_4$ TS

C	-0.130722	-0.018284	-0.158644
C	-0.070528	1.197732	-1.042908
C	0.695875	0.859690	-2.150234
C	0.773630	-0.543230	-2.237639
C	0.011079	-1.102140	-1.199936
H	0.090928	-2.147340	-0.925011
C	1.446581	-1.352445	-3.299531
F	1.113691	-0.947356	-4.538400
F	2.778241	-1.311177	-3.214619
F	1.091555	-2.644866	-3.199982
C	1.296554	1.822762	-3.145407
F	2.409770	1.313831	-3.676973
F	0.463026	2.100391	-4.157836
F	1.617257	2.982621	-2.571782
C	-0.311070	2.573368	-0.506380
F	-0.838427	3.380312	-1.441203
F	-1.181265	2.528942	0.517188
F	0.791563	3.169008	-0.039857
C	1.018627	-0.077532	0.850740
F	0.874760	0.877716	1.776427
F	0.993929	-1.259244	1.490144
F	2.228406	0.062435	0.312042
H	-1.027921	-0.079944	0.451567
C	-2.250804	0.288610	-1.923156
C	-1.961714	-1.089182	-1.807879
C	-2.603866	-1.877603	-0.678313
H	-3.669222	-2.009477	-0.897814
H	-2.162245	-2.873089	-0.602255
H	-2.538940	-1.402284	0.299450
C	-1.868759	-1.921241	-3.076423
H	-2.876918	-2.061521	-3.482437
H	-1.263387	-1.462252	-3.855124
H	-1.456318	-2.908629	-2.863725
C	-2.191679	0.933310	-3.276513
H	-1.322892	0.619415	-3.853957
H	-3.076136	0.629153	-3.853096
H	-2.189328	2.020685	-3.202916
C	-3.162404	0.967823	-0.934533
H	-2.953937	0.728239	0.107728
H	-3.134556	2.051029	-1.048877
H	-4.190977	0.638358	-1.135791

41

1 + 1,2,3,5b-*c*-$C_5H_2(CF_3)_4$ = **1** + 2,3,4,5b-*c*-$C_5H_2(CF_3)_4$

C	-0.058006	0.014041	-0.014012
C	-0.227385	0.372167	-1.561464
C	-1.698058	0.121223	-1.913478
C	-1.878272	-1.197776	-1.906570
C	-0.558889	-1.854517	-1.548748
C	-0.282392	-1.573765	-0.030536
C	0.945573	-2.389807	0.401496
H	1.834466	-2.208593	-0.203081
H	1.203180	-2.185331	1.442345
H	0.706799	-3.453477	0.327653
C	-1.452497	-2.052769	0.834987
H	-2.384815	-1.529044	0.632172
H	-1.623281	-3.118579	0.657310
H	-1.221270	-1.930023	1.895600

H	-0.468577	-2.902400	-1.829178
C	0.421262	-0.874170	-2.212480
C	0.513407	-0.977640	-3.726413
F	0.898588	-2.226414	-4.046985
F	-0.621578	-0.737466	-4.386575
F	1.439936	-0.143871	-4.211090
H	1.446249	-1.009886	-1.868199
C	-3.144102	-1.959936	-2.183160
F	-2.853750	-3.231092	-2.496397
F	-3.968810	-1.998034	-1.127989
F	-3.820487	-1.437258	-3.205771
C	-2.757606	1.162379	-2.148884
F	-2.939048	1.402462	-3.446689
F	-3.934540	0.776622	-1.638681
F	-2.433820	2.320360	-1.561963
C	0.374748	1.697370	-2.006874
F	0.129813	2.707718	-1.164959
F	1.708933	1.598490	-2.105956
F	-0.092424	2.053281	-3.208847
C	1.333865	0.413567	0.501250
H	1.437053	1.499358	0.507803
H	1.449570	0.069757	1.530839
H	2.157171	0.004819	-0.084154
C	-1.082437	0.769217	0.843667
H	-0.898424	1.842640	0.793309
H	-2.115273	0.590943	0.543497
H	-0.985317	0.460908	1.886928

41

1 + 1,2,4,5a-*c*-$C_5H_2(CF_3)_4$ TS = **1** + 1,3,4,5a-*c*-$C_5H_2(CF_3)_4$ TS

C	0.001122	0.000155	-0.000330
C	-0.092100	1.120540	-1.026256
C	0.729608	0.661550	-2.079718
C	0.807888	-0.730231	-2.025995
C	0.075897	-1.180305	-0.932989
C	0.171980	-2.595656	-0.463963
F	1.346384	-2.846287	0.138670
F	-0.786027	-2.915479	0.412237
F	0.073707	-3.442861	-1.500751
H	1.286220	-1.358892	-2.763352
C	1.481421	1.451464	-3.115795
F	2.172099	0.613074	-3.906381
F	0.714618	2.191355	-3.924747
F	2.369482	2.276786	-2.548279
C	-0.091827	2.565351	-0.598672
F	0.056920	3.379154	-1.649224
F	-1.218327	2.932595	0.018096
F	0.918190	2.811332	0.250666
H	1.033140	0.117061	0.372370
C	-0.754459	-0.076964	1.318973
F	-1.987864	-0.579290	1.280517
F	-0.053340	-0.867558	2.146918
F	-0.829157	1.128432	1.889604
C	-2.173047	0.574686	-1.880151
C	-2.032639	-0.824991	-2.019610
C	-2.951759	-1.760131	-1.266821
H	-3.906535	-1.772869	-1.810821
H	-2.572312	-2.781887	-1.267429
H	-3.161730	-1.463000	-0.246462
C	-1.660193	-1.387576	-3.372987
H	-2.532298	-1.295821	-4.033256
H	-0.842478	-0.861675	-3.861854
H	-1.404726	-2.445368	-3.300720
C	-2.092144	1.439588	-3.122560
H	-1.330680	1.129460	-3.830358
H	-3.061461	1.378299	-3.634262
H	-1.922652	2.487930	-2.874257
C	-3.207298	1.118031	-0.909549
H	-3.064835	0.833679	0.127206
H	-3.247086	2.204025	-0.961197
H	-4.188923	0.736588	-1.217899

41

1 + 1,2,4,5a-*c*-$C_5H_2(CF_3)_4$ = **1** + 1,3,4,5a-*c*-$C_5H_2(CF_3)_4$

C	0.019780	0.039109	0.043003
C	0.328253	-0.895187	-1.215007
C	0.706897	0.074685	-2.346055
C	-0.403550	0.708100	-2.706880

C	-1.552849	0.163614	-1.864102
C	-1.346940	0.759325	-0.410217
C	-2.531548	0.462483	0.524111
H	-2.816751	-0.584186	0.571823
H	-2.282996	0.791516	1.534321
H	-3.404009	1.033322	0.206161
C	-1.235575	2.293211	-0.457986
H	-0.464209	2.655967	-1.136138
H	-2.186950	2.726234	-0.768770
H	-1.012456	2.676244	0.539831
C	-2.877891	0.412298	-2.558745
F	-3.945592	0.009822	-1.870753
F	-3.040837	1.725497	-2.803459
F	-2.905671	-0.210085	-3.747015
C	-1.058364	-1.309889	-1.798701
H	-0.900625	-1.647694	-2.824983
C	-1.884282	-2.476239	-1.258530
F	-2.102510	-2.548216	0.056373
F	-3.083760	-2.474298	-1.854038
F	-1.277238	-3.619084	-1.606255
H	-0.493726	1.511439	-3.425587
C	2.056359	0.346293	-2.942648
F	2.543779	-0.729301	-3.568959
F	1.970275	1.331837	-3.846847
F	2.969370	0.718821	-2.037893
C	1.283890	-2.054328	-1.009538
F	2.496444	-1.633586	-0.624721
F	0.843902	-2.908061	-0.078325
F	1.440301	-2.752955	-2.139417
C	-0.098156	-0.728139	1.371318
H	0.871471	-1.155794	1.631691
H	-0.355055	-0.020243	2.161293
H	-0.831042	-1.526217	1.376933
C	1.171000	1.034392	0.277917
H	2.100077	0.493465	0.461324
H	1.342151	1.721031	-0.546874
H	0.955324	1.629772	1.167001

41

1 + 1,2,4,5b-*c*-$C_5H_2(CF_3)_4$ TS = **1** + 1,3,4,5b-*c*-$C_5H_2(CF_3)_4$ TS

C	0.000509	-0.000337	0.000582
C	-0.220709	-1.032625	1.088143
C	0.482487	-0.572323	2.206816
C	0.720308	0.799203	2.072692
C	0.191591	1.224228	0.861594
C	0.520029	2.574272	0.297622
F	1.836474	2.731664	0.098206
F	-0.086570	2.796067	-0.874053
F	0.145983	3.554915	1.138001
H	1.153381	1.435261	2.833106
C	0.896912	-1.331885	3.428897
F	2.180892	-1.699622	3.357527
F	0.771693	-0.567928	4.529668
F	0.173287	-2.435510	3.623974
C	-0.425650	-2.482785	0.722716
F	-1.243460	-3.133773	1.558840
F	-0.967584	-2.589296	-0.498582
F	0.732810	-3.154682	0.711155
C	1.267130	-0.288016	-0.828688
F	1.140357	-1.421641	-1.524248
F	1.456584	0.696893	-1.716163
F	2.372938	-0.389904	-0.093004
H	-0.806456	0.068057	-0.727254
C	-2.302585	-0.175466	1.541147
C	-2.060247	1.211699	1.429758
C	-2.628831	1.963375	0.246482
H	-3.723208	1.966684	0.330363
H	-2.296465	3.000737	0.238484
H	-2.386869	1.521009	-0.720148
C	-1.992625	2.029282	2.699500
H	-2.986021	2.044622	3.165126
H	-1.305583	1.611646	3.435794
H	-1.701758	3.058055	2.495639
C	-2.502713	-0.750715	2.926236
H	-1.721677	-0.455996	3.627071
H	-3.448919	-0.371942	3.332514
H	-2.557545	-1.836913	2.906675
C	-3.131273	-0.855100	0.470916

H	-2.781584	-0.673536	-0.545671
H	-3.177668	-1.931799	0.627634
H	-4.156676	-0.468592	0.527507

41

1 + 1,2,4,5b-*c*-$C_5H_2(CF_3)_4$ = **1** + 1,3,4,5b-*c*-$C_5H_2(CF_3)_4$

C	-0.017132	-0.021554	0.004673
C	-0.308128	0.278171	1.541988
C	0.194714	1.697552	1.815881
C	1.520647	1.673384	1.770069
C	1.944781	0.244499	1.492739
C	1.592118	-0.050197	-0.029037
C	2.169051	-1.402993	-0.476651
H	1.884666	-2.241511	0.158761
H	1.843066	-1.623895	-1.494274
H	3.258919	-1.353213	-0.490788
C	2.190909	1.008410	-0.967728
H	1.914268	2.027705	-0.699555
H	3.277914	0.939941	-0.969819
H	1.850492	0.828068	-1.988983
C	3.370371	-0.047262	1.921941
F	3.628317	-1.357120	1.987139
F	4.259921	0.490948	1.069746
F	3.632019	0.479955	3.123880
C	0.823335	-0.545918	2.212203
C	0.867863	-0.613436	3.737368
F	1.933936	-1.328951	4.123872
F	0.931831	0.567072	4.352273
F	-0.210095	-1.252972	4.206329
H	0.795498	-1.589372	1.896330
H	2.190627	2.520225	1.836286
C	-0.612940	2.940691	2.023052
F	-0.957673	3.109536	3.301966
F	0.086557	4.026379	1.658075
F	-1.742416	2.929367	1.303346
C	-1.718828	-0.048095	2.015751
F	-2.663157	0.376773	1.165636
F	-1.893070	-1.369792	2.150430
F	-1.973335	0.521792	3.197059
C	-0.649504	-1.354547	-0.429386
H	-1.737027	-1.273414	-0.411491
H	-0.360057	-1.578293	-1.457274
H	-0.369478	-2.204751	0.192188
C	-0.619661	1.062067	-0.901165
H	-1.703397	1.083685	-0.794535
H	-0.241668	2.061425	-0.689252
H	-0.394433	0.834489	-1.944830

41

1 + 1,2,5a,5b-*c*-$C_5H_2(CF_3)_4$ TS = **1** + 3,4,5a,5b-*c*-$C_5H_2(CF_3)_4$ TS

C	-0.025943	0.009228	0.046073
C	-0.163007	1.200121	-0.894428
C	0.576874	0.822394	-2.021942
C	0.671069	-0.562047	-2.091754
C	-0.043214	-1.103878	-1.005407
H	0.038075	-2.140945	-0.699225
H	1.111495	-1.116802	-2.906156
C	1.184238	1.732810	-3.047149
F	1.308270	1.105906	-4.230004
F	0.455381	2.833537	-3.253465
F	2.408921	2.122748	-2.682021
C	-0.334391	2.614462	-0.427126
F	-1.236067	3.280359	-1.168501
F	-0.768453	2.648866	0.838652
F	0.800753	3.326517	-0.481381
C	1.415740	0.039512	0.697409
F	1.610568	1.182786	1.354854
F	1.536154	-0.973728	1.566425
F	2.422062	-0.075572	-0.162916
C	-0.984385	-0.165580	1.250727
F	-2.192823	0.344332	1.034174
F	-1.133708	-1.472668	1.518640
F	-0.535454	0.403140	2.368599
C	-2.301528	0.287344	-1.920376
C	-1.985475	-1.091231	-1.757568
C	-2.795074	-1.950122	-0.795278
H	-3.715352	-2.249261	-1.309314
H	-2.254105	-2.865470	-0.546155

H	-3.080142	-1.466207	0.130392
C	-1.707947	-1.906380	-3.018289
H	-2.662742	-2.123421	-3.509607
H	-1.074177	-1.400170	-3.740913
H	-1.247127	-2.864829	-2.765311
C	-2.063124	0.934008	-3.259801
H	-1.120313	0.662481	-3.729879
H	-2.851174	0.591666	-3.944414
H	-2.128930	2.019895	-3.185603
C	-3.451693	0.954061	-1.196744
H	-3.890416	0.355707	-0.406573
H	-3.176609	1.928039	-0.790741
H	-4.231363	1.136585	-1.945453

41

1 + 1,2,5a,5b-*c*-$C_5H_2(CF_3)_4$ = **1** + 3,4,5a,5b-*c*-$C_5H_2(CF_3)_4$

C	0.009702	0.003109	-0.004209
C	-0.072554	0.357105	-1.586815
C	-1.559189	0.131434	-1.899190
C	-1.783451	-1.174938	-1.849234
C	-0.462877	-1.865940	-1.562231
C	-0.191166	-1.582860	-0.035870
C	0.989811	-2.393782	0.525851
H	1.963804	-2.156399	0.118341
H	1.044877	-2.243916	1.606627
H	0.805387	-3.456857	0.351619
C	-1.408487	-2.072110	0.771476
H	-2.345181	-1.592945	0.491911
H	-1.524003	-3.150353	0.629579
H	-1.250115	-1.899846	1.838014
H	-0.403966	-2.918848	-1.834811
C	0.480814	-0.912338	-2.364488
C	0.172068	-0.978665	-3.911667
F	0.725434	-2.100452	-4.403222
F	-1.109439	-1.043520	-4.270760
F	0.691184	0.064602	-4.554825
C	2.005866	-1.272179	-2.316925
F	2.674816	-0.740010	-1.297950
F	2.141947	-2.604162	-2.226098
F	2.669579	-0.882481	-3.405422
H	-2.738767	-1.668076	-1.962276
C	-2.611208	1.159072	-2.170873
F	-2.708637	1.448545	-3.472264
F	-3.816683	0.711757	-1.780513
F	-2.381032	2.308456	-1.523664
C	0.503155	1.705596	-2.004312
F	0.313199	2.654954	-1.079815
F	1.822836	1.616486	-2.210163
F	-0.054566	2.152174	-3.133724
C	1.266159	0.467817	0.762563
H	1.348793	1.553996	0.715465
H	1.123084	0.207117	1.814042
H	2.207519	0.042445	0.451774
C	-1.130235	0.736450	0.743189
H	-0.983027	1.814528	0.683475
H	-2.132081	0.512138	0.386357
H	-1.093062	0.457356	1.797416

41

1 + 1,3,5a,5b-*c*-$C_5H_2(CF_3)_4$ TS = **1** + 2,4,5a,5b-*c*-$C_5H_2(CF_3)_4$ TS

C	-0.017359	-0.039413	0.026625
C	-0.141254	1.167282	-0.890089
C	0.557244	0.824727	-2.042306
C	0.640084	-0.561431	-2.127300
C	-0.081885	-1.132992	-1.051707
H	0.022765	-2.176367	-0.771327
C	1.358580	-1.290944	-3.205132
F	0.975523	-0.895498	-4.438782
F	2.680610	-1.077925	-3.144634
F	1.165220	-2.614514	-3.132979
H	0.909172	1.527017	-2.787732
C	-0.279061	2.587319	-0.455171
F	-0.968250	3.293374	-1.374015
F	-0.931195	2.696007	0.707201
F	0.896383	3.220386	-0.310688
C	1.434131	-0.062464	0.655562
F	1.676230	1.073397	1.310761
F	1.535241	-1.079258	1.522038

F	2.421327	-0.210152	-0.221546
C	-0.960287	-0.194681	1.244195
F	-2.165866	0.328451	1.043023
F	-1.120450	-1.494360	1.533354
F	-0.484907	0.390673	2.343583
C	-2.310616	0.273538	-1.914438
C	-2.019269	-1.109206	-1.722969
C	-2.833559	-1.931552	-0.730218
H	-3.755286	-2.240181	-1.234908
H	-2.297881	-2.843235	-0.457572
H	-3.115876	-1.421725	0.181686
C	-1.819834	-1.955751	-2.978955
H	-2.801672	-2.136542	-3.429490
H	-1.197369	-1.491610	-3.737785
H	-1.391513	-2.927934	-2.727397
C	-2.063024	0.881510	-3.269076
H	-1.124024	0.581469	-3.729870
H	-2.858594	0.532646	-3.941858
H	-2.114790	1.969886	-3.221955
C	-3.415806	1.001060	-1.183217
H	-3.864960	0.436268	-0.374527
H	-3.090193	1.969517	-0.799031
H	-4.199732	1.206066	-1.921629

41

1 + 1,3,5a,5b-*c*-$C_5H_2(CF_3)_4$ = **1** + 2,4,5a,5b-*c*-$C_5H_2(CF_3)_4$

C	0.008456	-0.000411	-0.006557
C	-0.082747	0.321758	-1.588680
C	-1.562288	0.103177	-1.902335
C	-1.778273	-1.204064	-1.859246
C	-0.460697	-1.897876	-1.539301
C	-0.186161	-1.588054	-0.014559
C	0.998578	-2.385407	0.560478
H	1.968091	-2.187652	0.123419
H	1.077513	-2.180498	1.630647
H	0.793610	-3.452747	0.445327
C	-1.392532	-2.058444	0.816530
H	-2.319376	-1.542037	0.581115
H	-1.554855	-3.126877	0.652957
H	-1.189750	-1.916596	1.880091
H	-0.399107	-2.954195	-1.800265
C	0.485183	-0.945746	-2.353968
C	0.198504	-1.014765	-3.904508
F	0.696725	-2.174002	-4.363577
F	-1.074700	-0.995585	-4.291962
F	0.792845	-0.013941	-4.554058
C	2.011057	-1.301815	-2.282998
F	2.660675	-0.719568	-1.278430
F	2.150449	-2.628490	-2.142068
F	2.691387	-0.958589	-3.376438
C	-3.058918	-1.893669	-2.188220
F	-2.891427	-2.752618	-3.202792
F	-3.547362	-2.612426	-1.163195
F	-4.004439	-1.017589	-2.543483
H	-2.276438	0.890229	-2.102488
C	0.430515	1.679014	-2.033803
F	0.094775	2.647675	-1.166726
F	1.761291	1.690339	-2.151881
F	-0.086455	2.040320	-3.214701
C	1.266988	0.489673	0.741636
H	1.441961	1.546445	0.532987
H	1.066157	0.408739	1.812724
H	2.179949	-0.051767	0.547186
C	-1.133065	0.743718	0.730865
H	-0.930043	1.814451	0.742702
H	-2.125197	0.588708	0.314245
H	-1.159895	0.406772	1.767879

41

1 + 1,4,5a,5b-*c*-$C_5H_2(CF_3)_4$ TS

C	-0.000928	-0.001142	0.000273
C	-0.193633	1.157694	-1.005613
C	0.552272	0.751966	-2.134955
C	0.658594	-0.626865	-2.142193
C	-0.017035	-1.138892	-1.027621
C	0.093282	-2.597526	-0.684835
F	1.359585	-3.037587	-0.645373
F	-0.469397	-2.882352	0.492665

F	-0.518574	-3.351261	-1.618384
H	1.088434	-1.230535	-2.929622
H	0.895442	1.422109	-2.908781
C	-0.130199	2.626590	-0.649080
F	-0.003245	3.355130	-1.774063
F	-1.206382	3.096383	-0.014380
F	0.928332	2.915616	0.118230
C	1.451389	0.085969	0.638050
F	1.456984	0.917234	1.682184
F	1.833277	-1.115648	1.076798
F	2.390767	0.505988	-0.201612
C	-0.941374	-0.099495	1.230916
F	-2.070697	-0.752125	0.979136
F	-0.371946	-0.743735	2.251195
F	-1.263923	1.122952	1.663074
C	-2.238222	0.693891	-1.760838
C	-2.163404	-0.723564	-1.939575
C	-3.144060	-1.647570	-1.236954
H	-3.888231	-1.943990	-1.985421
H	-2.677650	-2.566169	-0.880642
H	-3.676749	-1.187839	-0.413067
C	-1.881074	-1.232780	-3.336690
H	-2.756559	-1.005535	-3.958397
H	-1.029049	-0.761890	-3.821189
H	-1.743226	-2.313469	-3.339012
C	-2.171387	1.561230	-3.009085
H	-1.355449	1.306756	-3.681152
H	-3.107463	1.430806	-3.565877
H	-2.091109	2.617089	-2.750948
C	-3.275409	1.265000	-0.803316
H	-3.224859	0.905534	0.217488
H	-3.222906	2.350596	-0.783452
H	-4.263347	0.994127	-1.196039

41

1 + 1,4,5a,5b-*c*-$C_5H_2(CF_3)_4$

C	-0.009931	-0.005859	0.003732
C	0.330323	-0.940337	-1.273943
C	0.726624	0.068089	-2.346111
C	-0.372378	0.701085	-2.723061
C	-1.552943	0.113571	-1.946513
C	-1.385463	0.679256	-0.462262
C	-2.577897	0.381230	0.467433
H	-2.914600	-0.649533	0.484788
H	-2.306006	0.665298	1.485821
H	-3.428433	0.997062	0.176752
C	-1.292949	2.218098	-0.482736
H	-0.496812	2.599826	-1.119672
H	-2.234717	2.650990	-0.816754
H	-1.116032	2.578238	0.532456
C	-2.871679	0.455884	-2.637193
F	-3.965216	0.118142	-1.955823
F	-2.938583	1.787035	-2.838732
F	-2.962838	-0.110504	-3.843905
C	-1.058487	-1.395624	-1.900074
C	-0.962886	-2.063859	-3.338185
F	-2.152030	-2.580246	-3.671172
F	-0.615427	-1.268362	-4.344824
F	-0.080496	-3.064479	-3.324749
C	-1.905715	-2.449416	-1.106241
F	-1.683273	-2.446774	0.204587
F	-3.210749	-2.229947	-1.287076
F	-1.654035	-3.699098	-1.499071
H	-0.467581	1.516812	-3.425420
H	1.744758	0.251404	-2.658554
C	1.386006	-2.017271	-1.040820
F	2.339782	-1.600508	-0.190010
F	0.857821	-3.130697	-0.525216
F	2.030824	-2.347932	-2.164553
C	-0.076501	-0.686488	1.392919
H	0.756656	-1.377947	1.520541
H	0.042543	0.091076	2.150938
H	-0.991341	-1.210708	1.622153
C	1.135526	1.022720	0.191608
H	2.032879	0.514219	0.541453
H	1.387645	1.593216	-0.697879
H	0.850515	1.733676	0.966855

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1 + 2,3,5a,5b-*c*-$C_5H_2(CF_3)_4$ TS

C	0.001243	-0.000909	-0.000110
C	-0.242421	1.083620	-1.055383
C	0.573290	0.664477	-2.134598
C	0.728692	-0.724741	-2.048003
C	0.075448	-1.199805	-0.920252
H	0.110650	-2.224239	-0.573995
C	1.463581	-1.626109	-2.993738
F	1.411571	-1.204971	-4.261368
F	2.754181	-1.719285	-2.657705
F	0.953890	-2.867270	-2.959737
C	1.167737	1.570180	-3.161851
F	2.490368	1.384985	-3.252090
F	0.676749	1.397048	-4.403882
F	0.954162	2.855415	-2.842987
H	-0.313320	2.127497	-0.767872
C	1.434539	0.246830	0.626369
F	1.353631	1.210375	1.554747
F	1.894202	-0.861936	1.210647
F	2.369343	0.630462	-0.236509
C	-0.936725	-0.088674	1.221638
F	-1.995832	-0.866830	0.997219
F	-0.333672	-0.618554	2.290462
F	-1.374162	1.122775	1.580030
C	-2.149405	0.708143	-1.726291
C	-2.150853	-0.695969	-1.970792
C	-3.101940	-1.654907	-1.287315
H	-3.850336	-1.947546	-2.033135
H	-2.600854	-2.571253	-0.970142
H	-3.632307	-1.236461	-0.439883
C	-1.799925	-1.184019	-3.352911
H	-2.660962	-0.992661	-4.007551
H	-0.956064	-0.673218	-3.812690
H	-1.613759	-2.259404	-3.353306
C	-2.123509	1.639466	-2.935926
H	-1.450288	1.325922	-3.725792
H	-3.131910	1.677762	-3.361838
H	-1.857583	2.656701	-2.638536
C	-3.099418	1.306977	-0.695725
H	-3.278084	0.704980	0.185869
H	-2.747993	2.288885	-0.372083
H	-4.065051	1.459110	-1.189749

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1 + 2,3,5a,5b-*c*-$C_5H_2(CF_3)_4$

C	-0.002943	0.021388	0.029559
C	0.199134	-0.189657	-1.546753
C	1.354605	0.742404	-1.889819
C	0.899683	1.987813	-1.794819
C	-0.587409	1.916554	-1.438514
C	-0.630402	1.491900	0.074169
C	-2.058006	1.597202	0.634698
H	-2.817167	1.044919	0.091368
H	-2.074849	1.254854	1.671995
H	-2.354023	2.649306	0.633671
C	0.194645	2.486901	0.907095
H	1.256841	2.481428	0.674816
H	-0.179729	3.502204	0.746396
H	0.085826	2.263077	1.970924
H	-1.159997	2.813735	-1.671235
C	-0.925868	0.631059	-2.266778
C	-0.680638	0.870773	-3.810256
F	-1.828628	1.120296	-4.451456
F	0.094829	1.918533	-4.111401
F	-0.119789	-0.208523	-4.361891
C	-2.336034	-0.004448	-2.229827
F	-2.591775	-0.716743	-1.134589
F	-3.293991	0.922504	-2.330387
F	-2.482246	-0.878496	-3.235824
C	1.651888	3.263065	-2.051375
F	0.799400	4.272510	-2.272060
F	2.426323	3.622896	-1.017491
F	2.443471	3.156141	-3.119295
C	2.730984	0.277143	-2.253930
F	2.891321	0.219390	-3.578809
F	3.681761	1.079335	-1.763090
F	2.956901	-0.955541	-1.774602

H	0.324059	-1.226210	-1.856674
C	-0.825503	-1.076236	0.747877
H	-0.681240	-2.039634	0.252832
H	-0.457837	-1.183424	1.770024
H	-1.889021	-0.889829	0.813727
C	1.380188	-0.084183	0.713915
H	1.748334	-1.108909	0.617310
H	2.145932	0.585828	0.327458
H	1.275350	0.128538	1.779002

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1 + 1,2,3,4,5a-*c*-$C_5H(CF_3)_5$ TS

C	-0.000136	-0.000382	-0.000246
C	-0.075092	1.177273	-0.950159
C	0.732249	0.783846	-2.027854
C	0.781747	-0.623938	-2.072636
C	0.016529	-1.139058	-1.009802
C	0.008014	-2.572872	-0.522831
F	1.235841	-2.969636	-0.159952
F	-0.783714	-2.689574	0.550108
F	-0.452755	-3.450922	-1.414311
C	1.507974	-1.424837	-3.128353
F	1.264222	-0.963066	-4.364042
F	2.828271	-1.395321	-2.932147
F	1.142352	-2.706730	-3.119396
C	1.499361	1.733614	-2.928054
F	2.490184	1.107058	-3.562140
F	0.738700	2.320388	-3.857237
F	2.068413	2.702575	-2.202407
C	-0.196352	2.609332	-0.491591
F	-0.291953	3.432767	-1.543283
F	-1.287505	2.818454	0.250607
F	0.855496	2.991947	0.241834
H	1.053840	0.040053	0.330329
C	-0.674076	-0.033770	1.371496
F	-1.972019	-0.326995	1.406673
F	-0.041575	-0.920557	2.149457
F	-0.514507	1.155897	1.961248
C	-2.210088	0.585021	-1.923368
C	-2.097067	-0.820339	-1.971149
C	-3.014861	-1.663621	-1.111245
H	-4.013890	-1.608994	-1.564484
H	-2.720341	-2.711870	-1.117568
H	-3.105569	-1.329331	-0.084361
C	-1.825340	-1.473370	-3.310051
H	-2.738941	-1.390867	-3.912777
H	-1.033822	-0.999056	-3.883912
H	-1.596464	-2.531985	-3.201603
C	-2.042414	1.367669	-3.204402
H	-1.219030	1.025401	-3.825018
H	-2.961496	1.245239	-3.793234
H	-1.912263	2.432109	-3.013404
C	-3.225731	1.211408	-0.992646
H	-3.126759	0.922228	0.048839
H	-3.197052	2.297369	-1.055247
H	-4.220261	0.887447	-1.327351

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1 + 1,2,3,4,5a-*c*-$C_5H(CF_3)_5$

C	-0.004161	0.038241	0.085194
C	0.324047	0.186429	-1.460250
C	-0.240493	1.566343	-1.855815
C	-1.572818	1.461390	-1.886124
C	-1.931425	0.010959	-1.487578
C	-1.600461	-0.115909	0.067693
C	-2.071193	-1.452824	0.667387
H	-1.775414	-2.331060	0.099541
H	-1.666588	-1.547625	1.675525
H	-3.157013	-1.458507	0.755524
C	-2.316244	0.974078	0.880561
H	-2.036588	1.987643	0.602593
H	-3.396861	0.882050	0.764838
H	-2.085802	0.841289	1.939763
C	-3.325905	-0.430586	-1.929265
F	-3.651359	-1.655183	-1.513561
F	-4.261724	0.396314	-1.439051
F	-3.428321	-0.429331	-3.261850
C	-0.739229	-0.664334	-2.231968

H	-0.763788	-0.314076	-3.266118
C	-0.633908	-2.176535	-2.469478
F	-0.294883	-2.950992	-1.437962
F	-1.803164	-2.631665	-2.932977
F	0.264961	-2.393243	-3.438014
C	-2.561109	2.557088	-2.236372
F	-3.407865	2.148654	-3.183276
F	-3.285332	2.939930	-1.180552
F	-1.948446	3.637981	-2.714737
C	0.575207	2.831443	-2.054851
F	0.572886	3.219568	-3.329078
F	0.117141	3.840870	-1.304157
F	1.846415	2.645249	-1.697821
C	1.762067	-0.128476	-1.864369
F	2.686882	0.412695	-1.067832
F	1.974499	-1.449631	-1.824219
F	2.000018	0.282678	-3.116310
C	0.727661	-1.142221	0.748940
H	1.805344	-0.983682	0.697200
H	0.462785	-1.166033	1.807335
H	0.506188	-2.112745	0.320736
C	0.483394	1.282980	0.853057
H	1.567929	1.365406	0.775688
H	0.047890	2.220760	0.513369
H	0.236820	1.175461	1.910717

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1 + 1,2,3,4,5b-*c*-$C_5H(CF_3)_5$ TS

C	-0.007039	-0.009913	0.023725
C	-0.226284	-1.048236	1.100159
C	0.489163	-0.611217	2.219041
C	0.734373	0.769542	2.086679
C	0.175524	1.218128	0.886017
C	0.448043	2.556195	0.230844
F	1.759598	2.800848	0.140161
F	-0.056556	2.571478	-1.011265
F	-0.102165	3.593889	0.870359
C	1.443761	1.617051	3.110655
F	1.079609	1.291009	4.358524
F	2.766239	1.474488	3.023327
F	1.168097	2.913087	2.948298
C	0.919772	-1.436862	3.408859
F	2.164283	-1.110429	3.765696
F	0.136880	-1.257562	4.482002
F	0.908058	-2.740185	3.134272
C	-0.465679	-2.488210	0.709083
F	-1.209263	-3.143482	1.609530
F	-1.123761	-2.548149	-0.458507
F	0.668840	-3.173491	0.549070
C	1.267458	-0.331526	-0.793221
F	1.075991	-1.435287	-1.522178
F	1.550849	0.655964	-1.645502
F	2.344389	-0.527423	-0.033026
H	-0.808388	0.063833	-0.709107
C	-2.325783	-0.147628	1.564484
C	-2.054043	1.234258	1.436248
C	-2.631650	1.967597	0.243478
H	-3.724873	1.965632	0.338125
H	-2.306687	3.005715	0.214482
H	-2.398657	1.507839	-0.717091
C	-1.981330	2.068319	2.696388
H	-2.980638	2.110826	3.147206
H	-1.317474	1.647397	3.451585
H	-1.664308	3.087265	2.484390
C	-2.539008	-0.711164	2.948695
H	-1.802360	-0.368504	3.670380
H	-3.519640	-0.372718	3.307941
H	-2.545756	-1.799725	2.944708
C	-3.166488	-0.824013	0.504194
H	-2.820022	-0.661845	-0.516042
H	-3.235878	-1.896945	0.676699
H	-4.182290	-0.412783	0.565042

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1 + 1,2,3,4,5b-*c*-$C_5H(CF_3)_5$

C	0.000497	0.058299	0.013586
C	0.318393	0.290902	-1.529190
C	-0.244072	1.674067	-1.886635

C	-1.573600	1.569143	-1.907525
C	-1.936297	0.128045	-1.544846
C	-1.603104	-0.046758	0.003406
C	-2.115311	-1.398733	0.528656
H	-1.764110	-2.258434	-0.041382
H	-1.798491	-1.528653	1.564313
H	-3.205028	-1.416360	0.521552
C	-2.287388	1.041364	0.843994
H	-2.024728	2.055165	0.540774
H	-3.370410	0.941417	0.781279
H	-2.003263	0.927512	1.891878
C	-3.318146	-0.372018	-1.967293
F	-3.324796	-1.708594	-2.064171
F	-4.285336	-0.055457	-1.098465
F	-3.671724	0.130801	-3.152960
C	-0.746818	-0.621880	-2.192054
C	-0.717984	-0.753242	-3.718143
F	-1.779975	-1.440514	-4.150233
F	-0.699905	0.409226	-4.372807
F	0.361911	-1.447832	-4.094319
H	-0.675832	-1.645822	-1.824193
C	-2.565658	2.675488	-2.177354
F	-2.776310	2.822415	-3.484030
F	-3.741792	2.409174	-1.599241
F	-2.152762	3.850231	-1.695255
C	0.524340	2.966148	-2.076989
F	0.094632	3.606825	-3.164776
F	0.380120	3.794326	-1.032600
F	1.832091	2.757886	-2.215496
C	1.751080	-0.024284	-1.955919
F	2.664480	0.517798	-1.141500
F	1.961971	-1.348989	-1.940447
F	2.006322	0.400822	-3.193820
C	0.684399	-1.214726	0.541116
H	1.766491	-1.079421	0.546687
H	0.376498	-1.388005	1.572987
H	0.464627	-2.113661	-0.033380
C	0.527900	1.215320	0.873880
H	1.611165	1.292576	0.777582
H	0.094586	2.180137	0.620922
H	0.306367	1.018857	1.924825

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1 + 1,2,3,5a,5b-*c*-$C_5H(CF_3)_5$ TS = **1** + 2,3,4,5a,5b-*c*-$C_5H(CF_3)_5$ TS

C	0.002341	-0.007880	-0.004662
C	-0.069675	1.232919	-0.880386
C	0.608879	0.887781	-2.049706
C	0.637625	-0.505685	-2.180045
C	-0.109860	-1.071536	-1.107205
H	0.016661	-2.116590	-0.840864
C	1.344745	-1.327021	-3.210653
F	0.991019	-1.012641	-4.471225
F	2.672372	-1.208600	-3.133619
F	1.064788	-2.631278	-3.042588
C	1.222600	1.879078	-3.017483
F	2.166321	1.298294	-3.758249
F	0.324787	2.404353	-3.860307
F	1.792786	2.891271	-2.363539
C	-0.279955	2.633124	-0.395256
F	-0.737386	3.397712	-1.402071
F	-1.197925	2.672380	0.582424
F	0.811246	3.232118	0.090802
C	1.460366	-0.110176	0.615545
F	1.754948	0.987886	1.306420
F	1.526501	-1.159306	1.444293
F	2.431237	-0.266937	-0.279462
C	-0.936809	-0.160516	1.215147
F	-2.156254	0.325113	1.009522
F	-1.067844	-1.457705	1.527400
F	-0.465913	0.458532	2.296897
C	-2.355970	0.249615	-1.941446
C	-2.006896	-1.117846	-1.726992
C	-2.790217	-1.949489	-0.714794
H	-3.702981	-2.294044	-1.211289
H	-2.224556	-2.839448	-0.432071
H	-3.084338	-1.435041	0.190382
C	-1.829221	-1.972387	-2.984584
H	-2.818804	-2.139750	-3.421787

H	-1.207052	-1.522126	-3.751782
H	-1.412808	-2.947920	-2.729535
C	-2.098898	0.849352	-3.287443
H	-1.156462	0.544689	-3.736893
H	-2.883845	0.481500	-3.964092
H	-2.157642	1.937484	-3.257918
C	-3.446915	0.973835	-1.196068
H	-3.885499	0.407893	-0.382337
H	-3.112463	1.940545	-0.814801
H	-4.236978	1.183796	-1.926400

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1 + 1,2,3,5a,5b-*c*-$C_5H(CF_3)_5$ = **1** + 2,3,4,5a,5b-*c*-$C_5H(CF_3)_5$

C	0.019870	0.003627	0.056184
C	0.380631	0.184771	-1.515743
C	-0.173845	1.586135	-1.826333
C	-1.499335	1.489204	-1.820465
C	-1.869965	0.038691	-1.544016
C	-1.566406	-0.175638	-0.013514
C	-2.091945	-1.523224	0.511834
H	-1.646784	-2.409718	0.080369
H	-1.932124	-1.571256	1.591187
H	-3.169706	-1.572560	0.337954
C	-2.345053	0.877757	0.794527
H	-2.056112	1.904169	0.583399
H	-3.414005	0.778520	0.584530
H	-2.206086	0.708033	1.864203
H	-2.874791	-0.250288	-1.847477
C	-0.704452	-0.642192	-2.330210
C	-0.812384	-0.340809	-3.878228
F	-1.755485	-1.140705	-4.397852
F	-1.178589	0.894284	-4.222206
F	0.338582	-0.580558	-4.499780
C	-0.690575	-2.210380	-2.300900
F	-0.041389	-2.744470	-1.270704
F	-1.953162	-2.659168	-2.250562
F	-0.123794	-2.744177	-3.381985
C	-2.508846	2.569549	-2.110300
F	-3.699363	2.018312	-2.384411
F	-2.691728	3.404288	-1.079664
F	-2.151043	3.304021	-3.162710
C	0.624189	2.840967	-2.061531
F	0.846394	3.047572	-3.358554
F	-0.023602	3.911036	-1.584462
F	1.810646	2.790560	-1.446488
C	1.835387	-0.062264	-1.910897
F	2.702145	0.310728	-0.963592
F	2.041441	-1.364047	-2.140849
F	2.162393	0.602153	-3.023137
C	0.747098	-1.118689	0.826096
H	1.826015	-0.972502	0.773813
H	0.466036	-1.024735	1.877793
H	0.524329	-2.130309	0.525000
C	0.453020	1.277541	0.821695
H	1.538431	1.374544	0.797007
H	0.021486	2.206912	0.456714
H	0.153848	1.177123	1.865999

44

1 + 1,2,4,5a,5b-*c*-$C_5H(CF_3)_5$ TS = **1** + 1,3,4,5a,5b-*c*-$C_5H(CF_3)_5$ TS

C	-0.020539	0.002324	0.021525
C	-0.180899	1.161332	-1.004557
C	0.581203	0.716644	-2.116913
C	0.672906	-0.663496	-2.099943
C	0.003090	-1.151080	-0.980329
C	0.137429	-2.607288	-0.628424
F	1.417247	-3.006835	-0.589089
F	-0.412057	-2.911143	0.547151
F	-0.456407	-3.370780	-1.564283
H	1.112492	-1.272500	-2.878413
C	1.229562	1.513958	-3.209459
F	2.532622	1.690647	-2.972952
F	1.135348	0.852599	-4.381093
F	0.685457	2.717236	-3.392564
C	-0.061358	2.632967	-0.600107
F	-0.800815	3.430952	-1.379740
F	-0.432712	2.879358	0.650701
F	1.211009	3.045878	-0.715338

C	1.417129	0.140897	0.678519
F	1.369902	1.055363	1.651393
F	1.816517	-1.016118	1.203982
F	2.366045	0.520325	-0.169283
C	-0.999279	-0.163050	1.235691
F	-2.048815	-0.921978	0.930308
F	-0.396875	-0.765137	2.262742
F	-1.473372	0.991050	1.690479
C	-2.210311	0.692316	-1.782816
C	-2.162310	-0.726092	-1.960783
C	-3.151726	-1.651807	-1.275735
H	-3.858116	-1.974770	-2.048339
H	-2.684355	-2.555523	-0.883415
H	-3.724700	-1.183605	-0.483585
C	-1.835852	-1.249760	-3.342044
H	-2.706066	-1.061560	-3.983547
H	-0.990211	-0.764656	-3.823998
H	-1.669977	-2.326426	-3.318766
C	-2.184628	1.515977	-3.062687
H	-1.344835	1.296475	-3.717638
H	-3.093716	1.274634	-3.626393
H	-2.198325	2.582482	-2.857208
C	-3.160084	1.313500	-0.774100
H	-3.277614	0.759744	0.149398
H	-2.859192	2.333240	-0.530636
H	-4.147042	1.377520	-1.248081

44

1 + 1,2,4,5a,5b-*c*-$C_5H(CF_3)_5$ = **1** + 1,3,4,5a,5b-*c*-$C_5H(CF_3)_5$

C	0.007715	-0.015807	0.035728
C	0.361595	0.148041	-1.537535
C	-0.191119	1.539101	-1.864688
C	-1.512137	1.463689	-1.836430
C	-1.905561	0.018084	-1.553981
C	-1.586947	-0.184091	-0.002580
C	-2.087916	-1.523490	0.572828
H	-1.828836	-2.406985	0.000483
H	-1.683664	-1.643208	1.579327
H	-3.173184	-1.498800	0.662159
C	-2.307822	0.889004	0.838078
H	-2.088465	1.911027	0.532447
H	-3.386347	0.744973	0.792846
H	-2.010901	0.779663	1.882746
C	-3.358822	-0.223652	-1.966175
F	-3.856742	-1.398906	-1.591226
F	-4.139725	0.723461	-1.410958
F	-3.522206	-0.121062	-3.287333
C	-0.727121	-0.692699	-2.347325
C	-0.764036	-0.399575	-3.910664
F	-1.555536	-1.288663	-4.518746
F	-1.212602	0.798384	-4.275222
F	0.457685	-0.523999	-4.426611
C	-0.637736	-2.258857	-2.311337
F	-0.063597	-2.751900	-1.218711
F	-1.863692	-2.784242	-2.384613
F	0.068667	-2.746634	-3.330244
H	-2.217206	2.274379	-1.957764
C	0.568464	2.804075	-2.125498
F	0.852841	2.956496	-3.420927
F	-0.159259	3.869313	-1.754665
F	1.723263	2.850856	-1.451489
C	1.832658	-0.080888	-1.903158
F	2.664501	0.310859	-0.929265
F	2.072842	-1.377018	-2.123543
F	2.192552	0.598733	-2.993134
C	0.735186	-1.134721	0.816512
H	1.811814	-1.064743	0.666746
H	0.556189	-0.961437	1.880018
H	0.423620	-2.145411	0.604708
C	0.456542	1.264846	0.784727
H	1.541130	1.355358	0.748407
H	0.026024	2.190751	0.412457
H	0.173227	1.178484	1.833559

47

1 + 1,2,3,4,5a,5b-*c*-$C_5(CF_3)_6$ TS

C	0.012808	0.032809	0.026948

C	-0.164570	1.199196	-0.970460
C	0.640272	0.806955	-2.070511
C	0.711366	-0.589838	-2.101954
C	0.013407	-1.114899	-0.999475
C	0.111062	-2.570747	-0.571186
F	1.363923	-3.033908	-0.622871
F	-0.321173	-2.719407	0.683924
F	-0.635655	-3.383578	-1.328488
C	1.379884	-1.415520	-3.183049
F	1.169217	-0.902319	-4.403725
F	2.693145	-1.502800	-2.987805
F	0.896270	-2.660382	-3.211095
C	1.439385	1.726454	-2.979987
F	2.450910	1.062380	-3.541612
F	0.716452	2.266738	-3.966437
F	1.992873	2.722906	-2.286863
C	-0.236527	2.667491	-0.575503
F	-0.329809	3.420874	-1.681650
F	-1.294163	2.984962	0.169318
F	0.845106	3.058761	0.103685
C	1.476041	0.136531	0.662661
F	1.464189	0.983256	1.691060
F	1.868677	-1.055465	1.108359
F	2.410192	0.559155	-0.182232
C	-0.917886	-0.072755	1.277178
F	-2.057055	-0.704656	1.019050
F	-0.339391	-0.730317	2.280651
F	-1.226013	1.136974	1.739951
C	-2.227752	0.651237	-1.829274
C	-2.158889	-0.772280	-1.913166
C	-3.137780	-1.635829	-1.135178
H	-3.857297	-2.017469	-1.868054
H	-2.672904	-2.506728	-0.676206
H	-3.693931	-1.099501	-0.375541
C	-1.882940	-1.387361	-3.267466
H	-2.781539	-1.238012	-3.879836
H	-1.065681	-0.932300	-3.817919
H	-1.712206	-2.459478	-3.187367
C	-2.113903	1.419609	-3.130507
H	-1.295316	1.095329	-3.766542
H	-3.042119	1.253347	-3.692180
H	-2.019369	2.490358	-2.961776
C	-3.246141	1.294298	-0.903843
H	-3.155145	1.028829	0.144722
H	-3.206946	2.377806	-0.986527
H	-4.240754	0.977533	-1.240164

47

1 + 1,2,3,4,5a,5b-*c*-$C_5(CF_3)_6$ TS

C	-0.027761	-0.005231	-0.016872
C	1.219413	0.316430	0.955317
C	2.427038	-0.148931	0.125571
C	2.439894	-1.481299	0.129482
C	1.210303	-1.960714	0.941360
C	-0.052497	-1.605999	0.014857
C	-1.388835	-2.179851	0.527772
H	-1.589966	-2.025958	1.583232
H	-2.198180	-1.723513	-0.043414
H	-1.425541	-3.251131	0.336876
C	0.116776	-2.219734	-1.388024
H	1.002935	-1.880547	-1.918721
H	0.155017	-3.306357	-1.327984
H	-0.755025	-1.959030	-1.991136
C	1.272347	-3.436745	1.375330
F	0.142826	-3.885863	1.919608
F	1.500926	-4.209746	0.301662
F	2.241625	-3.659842	2.260116
C	1.267197	-0.837497	2.062388
C	2.610754	-0.900129	2.921226
F	2.451078	-1.717190	3.963413
F	3.691063	-1.340488	2.277157
F	2.909086	0.306863	3.394248
C	0.169474	-0.826257	3.188224
F	-0.988178	-0.290930	2.818371
F	-0.086246	-2.069150	3.596763
F	0.564358	-0.130402	4.253635
C	3.516036	-2.355260	-0.494601
F	3.876008	-3.345674	0.318238

F	3.115757	-2.898123	-1.649428
F	4.619662	-1.650261	-0.737487
C	3.359009	0.769911	-0.644862
F	4.524964	0.925725	-0.025963
F	3.591354	0.307860	-1.880033
F	2.816527	1.981596	-0.800143
C	1.281012	1.762669	1.482763
F	0.789328	2.652740	0.613777
F	0.553846	1.878347	2.597912
F	2.525678	2.149633	1.763634
C	-1.385051	0.656921	0.325682
H	-1.255757	1.721214	0.514878
H	-2.020902	0.572583	-0.558064
H	-1.932063	0.226258	1.149097
C	0.272359	0.561311	-1.427619
H	0.293364	1.649592	-1.393700
H	1.196291	0.215060	-1.882645
H	-0.535432	0.271993	-2.099361

Table S14. Cartesian coordinates for Diels-Alder transition states and product norbornenes formed from **1** + *c*-$C_5H_xF_{6-x}$

29
1 + 1-*c*-C_5H_5F TS = **1** + 4-*c*-C_5H_5F TS

C	-0.001862	0.000381	0.012992
H	-0.653839	-0.324100	0.822817
H	-0.564529	-0.125523	-0.920825
H	0.852034	-0.678487	-0.026438
C	0.456846	1.440416	0.127236
C	1.504229	1.776858	-0.914152
H	1.990696	2.733660	-0.733596
H	2.276702	1.003597	-0.940640
H	1.044929	1.818809	-1.910122
C	-0.426903	2.430362	0.587819
C	-1.848412	2.066798	0.968909
H	-1.921925	1.193312	1.616222
H	-2.432324	1.846381	0.065999
H	-2.337345	2.900995	1.476885
C	-0.314772	3.838464	0.045075
H	-0.717563	3.881860	-0.975308
H	-0.888495	4.537766	0.658424
H	0.714096	4.192916	0.006146
C	0.353968	2.766863	2.677248
C	1.560864	3.387267	2.365521
C	2.467934	2.428541	1.888109
C	1.802135	1.210480	1.888556
C	0.641794	1.296840	2.829350
H	1.020469	1.113596	3.844289
H	-0.179264	0.613570	2.636842
F	2.423424	0.038085	1.660473
H	3.446722	2.605860	1.465884
H	1.726445	4.456308	2.350561
H	-0.487049	3.256930	3.150871

29
1 + 1-*c*-C_5H_5F = **1** + 4-*c*-C_5H_5F

C	0.004567	-0.004173	-0.002862
C	-1.418246	-0.224369	0.488564
C	-1.671195	0.715333	1.399095
H	-2.537726	0.832482	2.036175
C	-0.415977	1.552919	1.504590
C	0.067013	1.536455	0.054618
H	-0.642439	2.016900	-0.618023
H	1.062785	1.955268	-0.084140
C	0.688213	0.727786	2.250121
C	0.170338	0.207737	3.595437
H	0.949829	-0.348663	4.122372
H	-0.699110	-0.440817	3.493633
H	-0.113231	1.056243	4.224346
C	1.882968	1.641178	2.559391
H	2.687871	1.070903	3.029140
H	1.570280	2.418074	3.259419
H	2.291278	2.137764	1.679452
C	0.989693	-0.402353	1.163871
C	2.430278	-0.380993	0.634635
H	2.705498	0.565833	0.169649
H	3.147565	-0.582832	1.434115
H	2.547893	-1.165660	-0.117766
C	0.719031	-1.828719	1.651770
H	-0.297430	-1.963137	2.020272
H	0.870915	-2.530435	0.825908
H	1.410413	-2.106813	2.451944
F	-0.615835	2.795078	2.071401
H	-2.052623	-1.057052	0.214144
H	0.260923	-0.477653	-0.950728

29
1 + 2-*c*-C_5H_5F TS = **1** + 3-*c*-C_5H_5F TS

C	0.007996	-0.000533	0.003984
H	-0.526422	-0.376278	0.876539
H	-0.670433	-0.099713	-0.853464
H	0.859896	-0.659107	-0.177665
C	0.458626	1.439257	0.139435
C	1.517715	1.827731	-0.868109
H	2.054900	2.734414	-0.588507
H	2.254038	1.029962	-0.988019
H	1.058966	2.011081	-1.848554
C	-0.434819	2.418493	0.612573
C	-1.853924	2.028139	0.980529

H	-1.924211	1.108124	1.559642
H	-2.447122	1.878627	0.069329
H	-2.339220	2.822611	1.552930
C	-0.367135	3.821811	0.042646
H	-0.800030	3.842280	-0.965797
H	-0.940692	4.518116	0.660433
H	0.651473	4.199517	-0.028966
C	0.365922	2.810051	2.613858
C	1.603094	3.392325	2.328790
C	2.447153	2.357083	1.927249
C	1.803235	1.132965	1.951979
C	0.618925	1.342654	2.850820
H	0.937648	1.218182	3.895421
H	-0.225434	0.682377	2.677164
H	2.288466	0.183150	1.768973
F	3.664695	2.554122	1.400342
H	1.831923	4.446529	2.266418
H	-0.456765	3.345621	3.073855

29

1 + 2-*c*-C_5H_5F = **1** + 3-*c*-C_5H_5F

C	-0.005598	-0.003199	0.005166
C	-1.430521	-0.233476	0.496789
C	-1.639498	0.730807	1.383797
C	-0.417992	1.602071	1.513926
C	0.061189	1.536957	0.052702
H	-0.638002	2.007102	-0.638606
H	1.059858	1.945025	-0.101082
C	0.677071	0.741547	2.250141
C	0.143608	0.209292	3.584639
H	0.898612	-0.394056	4.095601
H	-0.753657	-0.399578	3.470123
H	-0.108041	1.048442	4.239710
C	1.881897	1.635125	2.574363
H	2.687157	1.057872	3.035764
H	1.579191	2.404353	3.289988
H	2.291372	2.139987	1.698899
C	0.985660	-0.392354	1.164223
C	2.425183	-0.363311	0.629398
H	2.695821	0.584267	0.162936
H	3.147753	-0.563068	1.424699
H	2.544229	-1.147185	-0.123638
C	0.731610	-1.820654	1.657440
H	-0.279475	-1.963148	2.037099
H	0.881033	-2.522926	0.831629
H	1.433846	-2.092987	2.450212
H	-0.587070	2.580425	1.964691
F	-2.693004	0.884004	2.193941
H	-2.068092	-1.076479	0.274410
H	0.242489	-0.479905	-0.943877

29

1 + 5a-*c*-C_5H_5F TS

C	0.004918	-0.005335	0.007041
H	-0.648549	-0.350733	0.802184
H	-0.534031	-0.106981	-0.944092
H	0.865524	-0.677056	-0.041356
C	0.453620	1.434339	0.163562
C	1.509683	1.807318	-0.857040
H	2.029416	2.732642	-0.614543
H	2.256519	1.014586	-0.947857
H	1.043725	1.937433	-1.842525
C	-0.433969	2.420619	0.621775
C	-1.867851	2.075439	0.973687
H	-1.977384	1.127571	1.491737
H	-2.457957	2.027755	0.049070
H	-2.313145	2.855914	1.595610
C	-0.312544	3.831655	0.082810
H	-0.701360	3.871502	-0.943120
H	-0.901465	4.527708	0.685372
H	0.714244	4.192653	0.059254
C	0.370981	2.827264	2.703606
C	1.588973	3.421076	2.397807
C	2.481018	2.429907	1.938201
C	1.835641	1.199942	1.948809
C	0.704995	1.379406	2.920508
H	1.119920	1.282830	3.934558
F	-0.333096	0.476714	2.851888

H	2.306506	0.242539	1.760994
H	3.465573	2.617765	1.531545
H	1.785153	4.484806	2.397160
H	-0.463169	3.320005	3.188404

29

1 + 5a-*c*-C_5H_5F

C	0.004513	-0.000446	0.006516
C	-1.413429	-0.209804	0.500309
C	-1.670135	0.739633	1.405751
C	-0.428152	1.599649	1.532349
C	-0.011801	1.535991	0.054006
H	-0.749491	1.976074	-0.616656
F	1.202370	2.139165	-0.234107
C	0.686914	0.753607	2.251737
C	0.166073	0.218257	3.591481
H	0.936976	-0.364672	4.102590
H	-0.718885	-0.408508	3.485472
H	-0.094051	1.058457	4.242392
C	1.894670	1.644174	2.583068
H	2.682768	1.058711	3.064128
H	1.584675	2.416917	3.292344
H	2.316667	2.139713	1.712122
C	0.993737	-0.381001	1.169875
C	2.441440	-0.378171	0.654250
H	2.739653	0.569579	0.212468
H	3.137282	-0.617608	1.462795
H	2.550146	-1.153989	-0.109025
C	0.713538	-1.807292	1.659923
H	-0.303934	-1.940301	2.026322
H	0.868263	-2.511469	0.836832
H	1.403195	-2.084956	2.461562
H	-0.568617	2.592275	1.960903
H	-2.572772	0.856782	1.990994
H	-2.065333	-1.020040	0.201083
H	0.256770	-0.459831	-0.949527

29

1 + 5b-*c*-C_5H_5F TS

C	0.003214	-0.001349	0.003914
H	-0.599463	-0.351952	0.840499
H	-0.604564	-0.124114	-0.901697
H	0.863747	-0.666635	-0.092582
C	0.448024	1.443117	0.117397
C	1.487041	1.810137	-0.919871
H	2.015902	2.730097	-0.675421
H	2.227338	1.013795	-1.025012
H	1.007365	1.952588	-1.896948
C	-0.440668	2.430587	0.576053
C	-1.860308	2.068988	0.964746
H	-1.947219	1.146652	1.537242
H	-2.463863	1.940043	0.057166
H	-2.320064	2.870454	1.546723
C	-0.334307	3.834235	0.020380
H	-0.709039	3.858499	-1.011182
H	-0.935455	4.530375	0.609636
H	0.690264	4.202931	0.007333
C	0.380184	2.859999	2.643408
C	1.597449	3.445880	2.360526
C	2.494335	2.450024	1.897934
C	1.847331	1.230903	1.886372
C	0.633749	1.373736	2.780122
H	-0.204294	0.726731	2.548411
F	0.977010	1.067840	4.103716
H	2.317101	0.274673	1.693232
H	3.485673	2.639177	1.507969
H	1.802435	4.508118	2.376098
H	-0.455629	3.353287	3.123464

29

1 + 5b-*c*-C_5H_5F

C	-0.016370	-0.006011	0.006796
C	-1.435099	-0.219967	0.505931
C	-1.691286	0.727116	1.407865
C	-0.448842	1.592727	1.529306
C	0.057784	1.522277	0.085194
H	1.053886	1.935759	-0.066277
F	-0.769594	2.160253	-0.819675
C	0.667912	0.752403	2.252199

C	0.164972	0.218232	3.597129
H	0.942032	-0.362178	4.101739
H	-0.718471	-0.411087	3.496615
H	-0.093836	1.058212	4.248641
C	1.871994	1.655141	2.561809
H	2.683900	1.084131	3.019189
H	1.569244	2.424003	3.277584
H	2.275405	2.163493	1.685670
C	0.976452	-0.387781	1.166331
C	2.418614	-0.365648	0.636781
H	2.701809	0.581325	0.176469
H	3.134043	-0.575135	1.435972
H	2.534988	-1.146407	-0.119534
C	0.714638	-1.813691	1.661875
H	-0.300812	-1.951441	2.031294
H	0.871223	-2.518992	0.840260
H	1.408740	-2.082373	2.462737
H	-0.586573	2.588638	1.950944
H	-2.583346	0.832713	2.010581
H	-2.075521	-1.044568	0.222935
H	0.238014	-0.459269	-0.951548

29

1 + 1,2-*c*-$C_5H_4F_2$ TS = **1** + 3,4-*c*-$C_5H_4F_2$ TS

C	0.002135	-0.002232	0.001680
H	-0.555077	-0.355771	0.868627
H	-0.654195	-0.121010	-0.869767
H	0.854504	-0.670316	-0.143023
C	0.462388	1.438550	0.108307
C	1.507365	1.782790	-0.932343
H	2.005654	2.730197	-0.734175
H	2.273349	1.004657	-0.985661
H	1.041526	1.856468	-1.923459
C	-0.421022	2.432082	0.556765
C	-1.842407	2.080671	0.943467
H	-1.933963	1.139120	1.484017
H	-2.450963	1.988445	0.034935
H	-2.286970	2.867041	1.555831
C	-0.298704	3.850188	0.041481
H	-0.708023	3.917884	-0.974515
H	-0.864565	4.539321	0.672962
H	0.731163	4.204193	0.001480
C	0.341917	2.804154	2.656791
C	1.548868	3.413784	2.358911
C	2.449509	2.461005	1.879946
C	1.799389	1.229785	1.895688
C	0.623845	1.348457	2.834396
H	0.976688	1.184436	3.861338
H	-0.213339	0.685097	2.642338
H	2.281544	0.284868	1.681172
H	3.406528	2.685519	1.431138
F	1.740430	4.734536	2.349392
F	-0.661423	3.429836	3.286787

29

1 + 1,2-*c*-$C_5H_4F_2$ = **1** + 3,4-*c*-$C_5H_4F_2$

C	-0.015665	0.006584	0.008018
C	-1.442421	-0.230200	0.493771
C	-1.656270	0.724867	1.387445
C	-0.414576	1.579089	1.506633
C	0.054752	1.548863	0.054990
H	1.052764	1.959588	-0.088930
H	-0.654812	2.028957	-0.617372
C	0.676608	0.742049	2.256020
C	0.133205	0.222771	3.591584
H	0.894372	-0.355918	4.120574
H	-0.750082	-0.406056	3.477189
H	-0.141320	1.070517	4.224787
C	1.872533	1.648227	2.577247
H	2.668446	1.071925	3.054535
H	1.558572	2.427038	3.274523
H	2.292397	2.140372	1.700019
C	0.979369	-0.387133	1.166762
C	2.417045	-0.357457	0.629829
H	2.686072	0.589103	0.160740
H	3.139771	-0.553538	1.425607
H	2.535108	-1.143545	-0.120947
C	0.721166	-1.814214	1.658005

H	-0.290276	-1.955193	2.037174
H	0.869304	-2.515353	0.831078
H	1.422491	-2.087627	2.450961
F	-0.638194	2.807825	2.073837
F	-2.686946	0.892716	2.210014
H	-2.074826	-1.074794	0.263372
H	0.233190	-0.463468	-0.943212

29

1 + 1,3-*c*-$C_5H_4F_2$ TS = **1** + 2,4-*c*-$C_5H_4F_2$ TS

C	0.015513	-0.002463	-0.002252
H	-0.493648	-0.387403	0.881442
H	-0.681559	-0.107878	-0.843511
H	0.872019	-0.648603	-0.204474
C	0.450727	1.442221	0.126457
C	1.525094	1.835889	-0.860588
H	2.049664	2.747729	-0.573991
H	2.269068	1.043608	-0.967144
H	1.080378	2.015407	-1.847937
C	-0.445006	2.415862	0.598380
C	-1.860559	2.024244	0.977709
H	-1.937084	1.061897	1.481958
H	-2.472728	1.958750	0.069683
H	-2.313379	2.780727	1.621454
C	-0.391537	3.829390	0.051959
H	-0.895757	3.874355	-0.921365
H	-0.913646	4.516816	0.723194
H	0.624221	4.195470	-0.084826
C	0.376747	2.818159	2.585615
C	1.608209	3.407008	2.312404
C	2.433615	2.347997	1.928532
C	1.782582	1.131613	1.980617
C	0.590066	1.359893	2.869298
H	0.888965	1.267086	3.921360
H	-0.266339	0.717196	2.690906
H	2.243569	0.172287	1.792730
F	3.644851	2.524038	1.386317
H	1.828730	4.461803	2.255196
F	-0.618253	3.490091	3.191194

29

1 + 1,3-*c*-$C_5H_4F_2$ = **1** + 2,4-*c*-$C_5H_4F_2$

C	-0.000504	0.000383	-0.002926
C	-1.405166	-0.203294	0.501729
C	-1.702055	0.707755	1.418545
C	-0.438969	1.545756	1.514593
C	0.047434	1.540178	0.064450
H	1.042364	1.961847	-0.068980
H	-0.662328	2.020210	-0.607561
C	0.673202	0.728868	2.256992
C	0.166719	0.209903	3.606543
H	0.954861	-0.334680	4.132736
H	-0.695725	-0.448862	3.513048
H	-0.122689	1.058710	4.232256
C	1.866875	1.647071	2.556451
H	2.677746	1.080529	3.020013
H	1.555999	2.421943	3.259474
H	2.267378	2.146764	1.674735
C	0.973528	-0.405133	1.171928
C	2.415886	-0.395055	0.650263
H	2.701738	0.552454	0.192839
H	3.125107	-0.606823	1.454098
H	2.531403	-1.177296	-0.104714
C	0.676970	-1.828542	1.653022
H	-0.349993	-1.955225	1.996870
H	0.839892	-2.533424	0.832676
H	1.344682	-2.110850	2.471097
F	-0.643985	2.786631	2.076951
H	-2.559819	0.774806	2.070499
F	-2.124560	-1.267904	0.141754
H	0.230526	-0.481430	-0.952779

29

1 + 1,4-*c*-$C_5H_4F_2$ TS

C	0.007029	-0.001094	0.008072
H	-0.601678	-0.345274	0.843185
H	-0.596995	-0.123776	-0.899734
H	0.867250	-0.666921	-0.077462
C	0.452211	1.443134	0.118304

C	1.512406	1.785893	-0.906333
H	1.987537	2.747405	-0.721043
H	2.291259	1.019028	-0.921873
H	1.065648	1.823821	-1.908033
C	-0.434438	2.428914	0.576578
C	-1.852600	2.065783	0.967959
H	-1.936008	1.137441	1.531558
H	-2.456943	1.943925	0.060245
H	-2.307448	2.860892	1.560825
C	-0.339992	3.845485	0.051140
H	-0.808844	3.908876	-0.939100
H	-0.871897	4.534645	0.712263
H	0.686116	4.194904	-0.047321
C	0.365003	2.781635	2.649165
C	1.563182	3.405303	2.349753
C	2.453068	2.415852	1.890501
C	1.781726	1.206431	1.918084
C	0.611000	1.315642	2.849267
H	0.967327	1.159773	3.875523
H	-0.225863	0.653809	2.653581
F	2.380117	0.020936	1.704884
H	3.427891	2.579535	1.454128
H	1.724154	4.473623	2.333163
F	-0.656102	3.397081	3.271784

29

1 + 1,4-*c*-$C_5H_4F_2$

C	0.003666	-0.001436	0.001529
C	-1.416459	-0.234426	0.468321
C	-1.673376	0.712039	1.369883
C	-0.416934	1.547925	1.477370
C	0.071274	1.529206	0.025089
H	1.070752	1.935433	-0.116748
H	-0.638773	1.988980	-0.659915
C	0.686547	0.722735	2.227284
C	0.164988	0.201692	3.569989
H	0.942786	-0.358147	4.095356
H	-0.705832	-0.444644	3.465750
H	-0.116855	1.049399	4.200352
C	1.881879	1.634804	2.535681
H	2.688014	1.061298	2.998702
H	1.571784	2.407725	3.240940
H	2.286757	2.135254	1.656534
C	0.994816	-0.412223	1.146047
C	2.431571	-0.389575	0.606406
H	2.712196	0.561134	0.153907
H	3.142048	-0.604936	1.407645
H	2.541249	-1.162174	-0.156497
C	0.719993	-1.841542	1.623597
H	-0.290051	-1.973674	2.009954
H	0.855041	-2.532864	0.787394
H	1.424339	-2.128652	2.408378
F	-0.616318	2.789770	2.037324
H	-2.541558	0.830436	2.004216
H	-2.021898	-1.083656	0.181288
F	0.305749	-0.606350	-1.197754

29

1 + 1,5a-*c*-$C_5H_4F_2$ TS = **1** + 4,5a-*c*-$C_5H_4F_2$ TS

C	0.020695	-0.007937	0.005339
H	-0.573272	-0.378945	0.835443
H	-0.573344	-0.116056	-0.911325
H	0.895534	-0.653419	-0.101893
C	0.442352	1.440207	0.153504
C	1.513506	1.830034	-0.841707
H	2.013980	2.762202	-0.584597
H	2.272692	1.048452	-0.922506
H	1.063939	1.961513	-1.834545
C	-0.451557	2.417712	0.612223
C	-1.880601	2.066972	0.976809
H	-2.010151	1.050220	1.333292
H	-2.501889	2.196188	0.081677
H	-2.269889	2.748226	1.736551
C	-0.356386	3.838296	0.089071
H	-0.801182	3.892139	-0.912542
H	-0.919043	4.518253	0.734214
H	0.665482	4.205401	0.017719
C	0.385822	2.856419	2.657769

C	1.608281	3.436185	2.368241
C	2.470763	2.403231	1.944527
C	1.807887	1.187516	1.995750
C	0.661086	1.404891	2.942902
H	1.039772	1.343110	3.972594
F	-0.400050	0.541542	2.866102
H	2.248990	0.215189	1.820614
H	3.455978	2.559170	1.526640
H	1.811698	4.497206	2.365001
F	-0.615282	3.501355	3.273832

29

1 + 1,5a-*c*-$C_5H_4F_2$ = **1** + 4,5a-*c*-$C_5H_4F_2$

C	0.003229	0.000892	0.004390
C	-1.417179	-0.210766	0.493818
C	-1.670428	0.728042	1.408107
C	-0.420604	1.566852	1.526098
C	-0.006015	1.539723	0.049062
H	-0.751071	1.994939	-0.602550
F	1.204539	2.139404	-0.226673
C	0.694751	0.747733	2.256242
C	0.167426	0.222481	3.597473
H	0.944791	-0.338591	4.121940
H	-0.704630	-0.422232	3.492740
H	-0.111847	1.069430	4.230149
C	1.892819	1.652522	2.583511
H	2.673472	1.068066	3.076546
H	1.572294	2.431617	3.277807
H	2.322499	2.138605	1.711724
C	0.995166	-0.382672	1.170068
C	2.442015	-0.380137	0.654797
H	2.741959	0.567461	0.214280
H	3.136069	-0.620184	1.464415
H	2.549552	-1.155881	-0.108591
C	0.709633	-1.807595	1.657739
H	-0.308780	-1.938569	2.022126
H	0.863800	-2.510413	0.833478
H	1.397147	-2.087132	2.460314
F	-0.624139	2.809683	2.074828
H	-2.556114	0.871411	2.012328
H	-2.069887	-1.016512	0.185749
H	0.258543	-0.456102	-0.951325

29

1 + 1,5b-*c*-$C_5H_4F_2$ TS = **1** + 4,5b-*c*-$C_5H_4F_2$ TS

C	0.016591	-0.002002	-0.004545
H	-0.519446	-0.380557	0.865068
H	-0.648383	-0.123206	-0.868859
H	0.883500	-0.644945	-0.167925
C	0.441383	1.448300	0.109792
C	1.499918	1.834456	-0.897553
H	2.016444	2.754538	-0.627096
H	2.246963	1.044512	-1.000329
H	1.038824	1.993369	-1.880824
C	-0.454688	2.427908	0.565118
C	-1.867562	2.057441	0.967908
H	-1.965355	1.066051	1.406934
H	-2.503289	2.075391	0.074086
H	-2.277405	2.784945	1.671025
C	-0.382412	3.841282	0.025716
H	-0.850514	3.884976	-0.965785
H	-0.930279	4.525098	0.679063
H	0.637266	4.208593	-0.071393
C	0.395077	2.882505	2.593974
C	1.616148	3.456862	2.324054
C	2.480833	2.416237	1.904704
C	1.810536	1.209947	1.928840
C	0.590234	1.398395	2.803175
H	-0.269556	0.776862	2.580853
F	0.896525	1.159454	4.142750
H	2.252718	0.238811	1.752362
H	3.474218	2.570467	1.505196
H	1.828282	4.516031	2.333245
F	-0.615334	3.521502	3.200467

29

1 + 1,5b-*c*-$C_5H_4F_2$ = **1** + 4,5b-*c*-$C_5H_4F_2$

C	0.001609	-0.001106	-0.002359
C	-1.421761	-0.213394	0.492039

C	-1.675651	0.725793	1.401105
C	-0.422454	1.564286	1.514952
C	0.075718	1.529439	0.069941
F	-0.765193	2.169138	-0.811042
H	1.067591	1.954603	-0.073104
C	0.692513	0.746383	2.248006
C	0.181117	0.223469	3.594115
H	0.964501	-0.332267	4.115360
H	-0.688003	-0.425508	3.494337
H	-0.100048	1.070719	4.225493
C	1.886031	1.663768	2.553749
H	2.689192	1.095200	3.027981
H	1.570835	2.442993	3.249760
H	2.299171	2.158580	1.674989
C	0.995679	-0.386381	1.158089
C	2.436501	-0.363300	0.627569
H	2.716915	0.582424	0.163334
H	3.151789	-0.566736	1.428145
H	2.553572	-1.147399	-0.125035
C	0.727987	-1.811378	1.650291
H	-0.288898	-1.947255	2.016496
H	0.884939	-2.515110	0.827533
H	1.418879	-2.081886	2.453062
F	-0.614447	2.811378	2.057650
H	-2.552323	0.856304	2.020369
H	-2.064116	-1.033524	0.201655
H	0.256585	-0.454058	-0.960084

29

1 + 2,3-*c*-$C_5H_4F_2$ TS

C	0.000061	-0.001084	0.003855
H	-0.564533	-0.361664	0.863607
H	-0.654002	-0.100012	-0.871923
H	0.846878	-0.674215	-0.148368
C	0.469337	1.434289	0.136673
C	1.515252	1.799199	-0.896886
H	2.045144	2.721797	-0.661116
H	2.260140	1.005756	-0.994152
H	1.044645	1.935172	-1.879069
C	-0.421095	2.424216	0.596678
C	-1.845548	2.050472	0.956447
H	-1.924642	1.150635	1.566329
H	-2.425533	1.868689	0.042589
H	-2.337043	2.864783	1.493746
C	-0.313773	3.832295	0.047756
H	-0.696230	3.867155	-0.980457
H	-0.906840	4.529162	0.644816
H	0.709868	4.205426	0.025443
C	0.346315	2.806679	2.649136
C	1.568718	3.387359	2.355074
C	2.450468	2.407420	1.900261
C	1.810605	1.179215	1.893421
C	0.646021	1.342350	2.834450
H	-0.190606	0.676620	2.647142
H	0.993270	1.177233	3.862912
H	2.310739	0.240210	1.693153
F	3.637135	2.676779	1.350377
F	1.818743	4.697352	2.287985
H	-0.470362	3.331342	3.128466

29

1 + 2,3-*c*-$C_5H_4F_2$

C	0.002747	0.002556	-0.005458
C	-1.403670	-0.211915	0.498583
C	-1.658418	0.730026	1.396776
C	-0.428285	1.596609	1.514862
C	0.053877	1.541152	0.052838
H	-0.643471	2.012357	-0.638868
H	1.052899	1.950036	-0.092859
C	0.675552	0.744331	2.246850
C	0.151953	0.211982	3.584947
H	0.913904	-0.383493	4.094638
H	-0.741078	-0.404274	3.477632
H	-0.102832	1.051441	4.238265
C	1.879065	1.642636	2.562783
H	2.689327	1.069173	3.019767
H	1.577481	2.410355	3.280394
H	2.282459	2.149906	1.685864

C	0.983426	-0.393067	1.161741
C	2.425174	-0.375841	0.635993
H	2.707040	0.572577	0.177541
H	3.138952	-0.585941	1.436356
H	2.542689	-1.157067	-0.119773
C	0.701760	-1.818848	1.647548
H	-0.320723	-1.953463	2.001346
H	0.862450	-2.523578	0.826602
H	1.379309	-2.097273	2.458955
H	-0.598928	2.577075	1.960646
F	-2.699914	0.822371	2.225232
F	-2.127514	-1.294036	0.207507
H	0.228111	-0.481280	-0.956376

29

1 + 2,5a-*c*-$C_5H_4F_2$ TS = **1** + 3,5a-*c*-$C_5H_4F_2$ TS

C	-0.006334	-0.004949	0.006323
H	-0.718079	-0.319025	0.763008
H	-0.480996	-0.121073	-0.976256
H	0.841344	-0.695002	0.031649
C	0.459721	1.431459	0.154610
C	1.504289	1.777944	-0.890635
H	2.019575	2.715302	-0.689986
H	2.256138	0.987208	-0.960866
H	1.027814	1.865103	-1.875213
C	-0.424502	2.429386	0.595055
C	-1.861296	2.107001	0.949066
H	-1.975883	1.186557	1.514430
H	-2.443067	2.009863	0.022993
H	-2.309211	2.919776	1.524997
C	-0.251703	3.843028	0.085240
H	-0.575750	3.901368	-0.962077
H	-0.859587	4.543642	0.661495
H	0.781465	4.189083	0.120546
C	0.352305	2.824969	2.755819
C	1.547570	3.424444	2.422494
C	2.468321	2.505966	1.900676
C	1.835012	1.265416	1.878981
C	0.735466	1.380834	2.902777
H	1.189429	1.235166	3.892860
F	-0.288526	0.466722	2.818378
H	2.331242	0.326840	1.661181
H	3.429267	2.757677	1.476271
F	1.760161	4.745291	2.441150
H	-0.468576	3.301524	3.274221

29

1 + 2,5a-*c*-$C_5H_4F_2$ = **1** + 3,5a-*c*-$C_5H_4F_2$

C	-0.002967	-0.000919	-0.004800
C	-1.427882	-0.224574	0.484098
C	-1.638388	0.735080	1.378470
C	-0.422055	1.608049	1.515937
C	-0.014523	1.535942	0.034361
H	-0.752411	1.975596	-0.636016
F	1.199711	2.133864	-0.251704
C	0.686144	0.754360	2.238059
C	0.144481	0.219036	3.569468
H	0.899197	-0.384693	4.079757
H	-0.752886	-0.389596	3.453893
H	-0.105609	1.057367	4.225927
C	1.894112	1.639647	2.578244
H	2.674851	1.048763	3.064198
H	1.583562	2.413589	3.285671
H	2.325004	2.131768	1.709600
C	0.993173	-0.379300	1.152356
C	2.439658	-0.371408	0.632926
H	2.736395	0.576331	0.190600
H	3.137785	-0.610184	1.439475
H	2.548188	-1.146987	-0.130512
C	0.721078	-1.806170	1.644251
H	-0.292405	-1.943734	2.019265
H	0.871835	-2.509170	0.819538
H	1.418780	-2.081665	2.439468
H	-0.593344	2.593543	1.948579
F	-2.714495	0.910994	2.148282
H	-2.085169	-1.039411	0.219156
H	0.243148	-0.458937	-0.962994

29

1 + 2,5b-*c*-$C_5H_4F_2$ TS = **1** + 3,5b-*c*-$C_5H_4F_2$ TS

C	-0.009422	0.000257	0.002370
H	-0.644005	-0.322555	0.826235
H	-0.589189	-0.133472	-0.919211
H	0.842553	-0.681417	-0.053598
C	0.457079	1.440942	0.097449
C	1.467650	1.774281	-0.982999
H	1.985580	2.714331	-0.802104
H	2.219576	0.985441	-1.064402
H	0.963747	1.852328	-1.954549
C	-0.424796	2.440948	0.545450
C	-1.848134	2.106253	0.936413
H	-1.941920	1.208785	1.547130
H	-2.446056	1.939634	0.031069
H	-2.306104	2.934054	1.480626
C	-0.255411	3.849656	0.028992
H	-0.552836	3.901336	-1.026426
H	-0.876503	4.550339	0.589954
H	0.777409	4.196185	0.086777
C	0.370175	2.850327	2.700013
C	1.564827	3.444931	2.385656
C	2.483121	2.531275	1.831614
C	1.847835	1.302602	1.783237
C	0.676131	1.375261	2.750731
F	1.101076	0.999223	4.029149
H	-0.157667	0.721989	2.521678
H	2.342111	0.365621	1.557695
H	3.444750	2.791983	1.413937
F	1.788404	4.762393	2.429111
H	-0.451365	3.323530	3.218955

29

1 + 2,5b-*c*-$C_5H_4F_2$ = **1** + 3,5b-*c*-$C_5H_4F_2$

C	0.005758	-0.002283	-0.002059
C	-1.417288	-0.227017	0.493129
C	-1.627888	0.737629	1.377264
C	-0.407521	1.611474	1.511121
C	0.086402	1.529282	0.064391
F	-0.744887	2.166911	-0.833398
H	1.083629	1.937361	-0.091986
C	0.698407	0.761063	2.238839
C	0.169773	0.226810	3.573865
H	0.928640	-0.374908	4.080334
H	-0.726341	-0.383639	3.460916
H	-0.080627	1.065256	4.229879
C	1.903128	1.656749	2.560437
H	2.705884	1.079058	3.025108
H	1.599137	2.427526	3.273364
H	2.318093	2.160449	1.686852
C	1.008741	-0.377791	1.149442
C	2.447824	-0.345508	0.611648
H	2.723300	0.601275	0.146292
H	3.169394	-0.547471	1.406972
H	2.565507	-1.128099	-0.142459
C	0.760468	-1.804473	1.648205
H	-0.250304	-1.949225	2.027257
H	0.914338	-2.509003	0.825549
H	1.464034	-2.068079	2.442335
H	-0.572919	2.601757	1.934980
F	-2.687573	0.907994	2.170652
H	-2.065840	-1.054074	0.247016
H	0.252715	-0.455736	-0.962053

29

1 + 5a,5b-*c*-$C_5H_4F_2$ TS

C	-0.001593	-0.010373	0.000986
H	-0.674108	-0.354810	0.780100
H	-0.519011	-0.114485	-0.961435
H	0.860749	-0.680525	-0.026979
C	0.439911	1.430566	0.156626
C	1.496684	1.809555	-0.859530
H	2.024451	2.726792	-0.604038
H	2.235152	1.011446	-0.965313
H	1.027333	1.960963	-1.840092
C	-0.448647	2.418009	0.615224
C	-1.881888	2.078940	0.971138
H	-2.001002	1.121220	1.467773
H	-2.474566	2.056105	0.047566

H	-2.316906	2.851334	1.609648
C	-0.319917	3.827714	0.077345
H	-0.689279	3.862761	-0.955676
H	-0.920988	4.523150	0.667729
H	0.706787	4.189573	0.070369
C	0.383009	2.860223	2.701160
C	1.592425	3.443488	2.387767
C	2.491667	2.444394	1.924505
C	1.860574	1.218667	1.939714
C	0.709078	1.396153	2.906301
F	1.153579	1.198879	4.194725
F	-0.319778	0.521258	2.795277
H	2.324698	0.255812	1.768995
H	3.474394	2.637507	1.516893
H	1.792463	4.506104	2.383193
H	-0.450342	3.338987	3.199123

29

1 + 5a,5b-*c*-$C_5H_4F_2$

C	-0.001726	-0.001799	-0.002156
C	-1.413884	-0.218259	0.511373
C	-1.669989	0.729735	1.415055
C	-0.436330	1.606892	1.531153
C	0.002052	1.528957	0.065098
F	-0.860226	2.122463	-0.802051
F	1.202118	2.111809	-0.206286
C	0.687655	0.766238	2.245127
C	0.168619	0.227130	3.584089
H	0.942283	-0.355046	4.091100
H	-0.714933	-0.400908	3.478603
H	-0.090770	1.065719	4.237036
C	1.897677	1.652065	2.580726
H	2.679469	1.060896	3.064472
H	1.588213	2.424365	3.290353
H	2.330475	2.147616	1.715415
C	0.995763	-0.374523	1.158042
C	2.445391	-0.375889	0.648098
H	2.755813	0.569565	0.210563
H	3.134191	-0.620743	1.460680
H	2.554143	-1.151321	-0.115218
C	0.715609	-1.799267	1.652733
H	-0.300924	-1.932281	2.020391
H	0.871450	-2.505578	0.831942
H	1.406614	-2.071931	2.454432
H	-0.576402	2.608496	1.936963
H	-2.568879	0.845816	2.004857
H	-2.061635	-1.031844	0.214967
H	0.247223	-0.439770	-0.968448

29

1 + 1,2,3-*c*-$C_5H_3F_3$ TS = **1** + 2,3,4-*c*-$C_5H_3F_3$ TS

C	0.006992	-0.002661	-0.001354
H	-0.528387	-0.373739	0.872678
H	-0.669023	-0.112030	-0.858910
H	0.861188	-0.660417	-0.176029
C	0.455506	1.439197	0.121033
C	1.523316	1.811634	-0.884210
H	2.042501	2.736562	-0.633965
H	2.273949	1.022444	-0.968166
H	1.073487	1.950833	-1.875570
C	-0.433945	2.422063	0.583871
C	-1.853623	2.048315	0.961786
H	-1.937621	1.098171	1.488329
H	-2.459165	1.963415	0.050935
H	-2.307878	2.821723	1.583699
C	-0.345117	3.841200	0.058134
H	-0.803191	3.900900	-0.936928
H	-0.888839	4.527779	0.711865
H	0.677759	4.205033	-0.031202
C	0.354683	2.816363	2.616054
C	1.579478	3.406099	2.337935
C	2.444355	2.395665	1.911879
C	1.800329	1.175432	1.942863
C	0.616781	1.361899	2.858638
H	0.933637	1.235407	3.901157
H	-0.227150	0.708055	2.663334
H	2.275040	0.225210	1.742458
F	3.628822	2.639530	1.350922

F	1.821544	4.711231	2.263057
F	-0.635614	3.472244	3.234067

29

1 + 1,2,3-*c*-$C_5H_3F_3$ = **1** + 2,3,4-*c*-$C_5H_3F_3$

C	0.001932	0.001748	-0.005459
C	-1.405198	-0.219233	0.492199
C	-1.664046	0.713601	1.397719
C	-0.414357	1.563914	1.504875
C	0.057427	1.542759	0.053457
H	-0.650344	2.024477	-0.618902
H	1.056059	1.953757	-0.083227
C	0.684593	0.733752	2.250687
C	0.150663	0.214801	3.589972
H	0.919030	-0.354915	4.118127
H	-0.727709	-0.422015	3.483124
H	-0.127867	1.062855	4.220891
C	1.880336	1.642960	2.563846
H	2.681012	1.069207	3.035921
H	1.568312	2.420023	3.263892
H	2.294073	2.137923	1.685308
C	0.985933	-0.399229	1.162277
C	2.425961	-0.382336	0.634541
H	2.707078	0.565041	0.173882
H	3.139763	-0.589832	1.435265
H	2.541722	-1.165563	-0.119316
C	0.699122	-1.823467	1.646169
H	-0.323821	-1.955856	1.999480
H	0.858063	-2.527517	0.824416
H	1.375523	-2.102926	2.457951
F	-0.639888	2.793352	2.067202
F	-2.679479	0.815161	2.245113
F	-2.119045	-1.302925	0.194980
H	0.229105	-0.474191	-0.959369

29

1 + 1,2,4-*c*-$C_5H_3F_3$ TS = **1** + 1,3,4-*c*-$C_5H_3F_3$ TS

C	-0.003040	-0.002401	0.012225
H	-0.642900	-0.323930	0.832830
H	-0.578488	-0.137232	-0.911950
H	0.851997	-0.679263	-0.034372
C	0.456509	1.439183	0.107266
C	1.513485	1.754958	-0.931222
H	1.976367	2.729306	-0.787883
H	2.301638	0.997267	-0.916298
H	1.066606	1.744269	-1.933128
C	-0.420134	2.436588	0.554740
C	-1.841256	2.098460	0.952587
H	-1.932011	1.184454	1.538930
H	-2.446003	1.959005	0.047781
H	-2.289477	2.911232	1.525722
C	-0.276439	3.857340	0.056806
H	-0.682164	3.939686	-0.959389
H	-0.832854	4.548975	0.693477
H	0.758868	4.195617	0.019897
C	0.348370	2.773017	2.689083
C	1.533584	3.406553	2.375532
C	2.456152	2.481748	1.869007
C	1.804406	1.259366	1.874521
C	0.650425	1.313460	2.835754
H	1.033933	1.121446	3.845366
H	-0.174021	0.639907	2.626302
F	2.435246	0.096838	1.642020
H	3.409696	2.708988	1.417158
F	1.700099	4.728457	2.359922
F	-0.673260	3.360677	3.323436

29

1 + 1,2,4-*c*-$C_5H_3F_3$ = **1** + 1,3,4-*c*-$C_5H_3F_3$

C	0.006359	-0.000423	0.005056
C	-1.416719	-0.248781	0.470471
C	-1.636813	0.714637	1.354196
C	-0.393205	1.565547	1.473733
C	0.081475	1.530538	0.019806
H	-0.628062	1.990190	-0.665484
H	1.083296	1.928822	-0.126418
C	0.696502	0.726264	2.227292
C	0.149010	0.205128	3.559648
H	0.908262	-0.377758	4.086381

H	-0.735860	-0.420979	3.442294
H	-0.123477	1.051395	4.195293
C	1.893789	1.629840	2.548752
H	2.690133	1.049285	3.019480
H	1.582744	2.404543	3.251548
H	2.311181	2.125908	1.672755
C	1.006829	-0.407613	1.142209
C	2.441423	-0.376542	0.596967
H	2.715642	0.573295	0.138851
H	3.156652	-0.584312	1.395778
H	2.552864	-1.151842	-0.162910
C	0.744252	-1.837792	1.622848
H	-0.259877	-1.976239	2.021660
H	0.873659	-2.528279	0.785133
H	1.459756	-2.121013	2.398773
F	-0.611086	2.796254	2.032107
F	-2.665050	0.879679	2.175549
H	-2.016188	-1.116095	0.237912
F	0.300820	-0.600598	-1.196757

29

1 + 1,2,5a-*c*-$C_5H_3F_3$ TS = **1** + 3,4,5a-*c*-$C_5H_3F_3$ TS

C	0.012751	-0.008346	0.003346
H	-0.622534	-0.360133	0.810348
H	-0.537254	-0.127915	-0.938618
H	0.884345	-0.665448	-0.052327
C	0.443877	1.438582	0.143067
C	1.511638	1.805718	-0.867168
H	2.002977	2.752039	-0.648580
H	2.279494	1.029658	-0.920149
H	1.061240	1.891869	-1.864230
C	-0.443697	2.424965	0.589861
C	-1.874286	2.097643	0.962825
H	-2.012791	1.089309	1.339912
H	-2.495801	2.214572	0.066128
H	-2.255882	2.798552	1.708455
C	-0.307020	3.850422	0.094401
H	-0.699963	3.923934	-0.927450
H	-0.888465	4.531384	0.720558
H	0.721472	4.208841	0.073133
C	0.364849	2.859516	2.702572
C	1.576981	3.441808	2.392482
C	2.471106	2.468683	1.923788
C	1.819306	1.244751	1.954799
C	0.686971	1.410884	2.935180
H	1.090990	1.309689	3.951566
F	-0.359375	0.533890	2.841857
H	2.279768	0.285732	1.757020
H	3.438080	2.679550	1.490428
F	1.803167	4.754639	2.389703
F	-0.625126	3.487129	3.341062

29

1 + 1,2,5a-*c*-$C_5H_3F_3$ = **1** + 3,4,5a-*c*-$C_5H_3F_3$

C	-0.007472	-0.005981	-0.002235
C	-1.433733	-0.237292	0.480462
C	-1.647976	0.710264	1.383822
C	-0.412931	1.569854	1.514031
C	-0.010480	1.532803	0.035116
H	-0.755610	1.988022	-0.616311
F	1.201198	2.125744	-0.241039
C	0.692471	0.740444	2.246062
C	0.143417	0.216781	3.579316
H	0.904531	-0.364129	4.105316
H	-0.741018	-0.410509	3.464503
H	-0.127308	1.063236	4.215708
C	1.891836	1.638862	2.582445
H	2.663885	1.049575	3.082862
H	1.570681	2.420951	3.273058
H	2.332012	2.119351	1.712622
C	0.992174	-0.389256	1.156262
C	2.437432	-0.382889	0.636239
H	2.736199	0.564311	0.194557
H	3.134265	-0.622587	1.443390
H	2.543515	-1.158697	-0.127237
C	0.714484	-1.814582	1.646381
H	-0.299762	-1.950008	2.019918
H	0.864433	-2.516746	0.820879

H	1.410296	-2.091504	2.442529
F	-0.643323	2.797862	2.065746
F	-2.700367	0.900868	2.168686
H	-2.085284	-1.053894	0.207398
H	0.240723	-0.458983	-0.961612

29

1 + 1,2,5b-*c*-$C_5H_3F_3$ TS = **1** + 3,4,5b-*c*-$C_5H_3F_3$ TS

C	0.004482	-0.002112	-0.003684
H	-0.572357	-0.354624	0.850338
H	-0.624368	-0.138191	-0.892062
H	0.869074	-0.659678	-0.117033
C	0.443002	1.446544	0.090035
C	1.487922	1.797807	-0.947705
H	1.992930	2.738877	-0.736927
H	2.247104	1.015025	-1.014977
H	1.016472	1.889945	-1.934289
C	-0.443760	2.437882	0.534034
C	-1.861614	2.097524	0.938597
H	-1.971423	1.120457	1.406848
H	-2.492598	2.094918	0.041115
H	-2.267319	2.849546	1.617587
C	-0.312173	3.856471	0.026354
H	-0.697225	3.923030	-0.999032
H	-0.894782	4.542232	0.645594
H	0.718205	4.211108	0.009557
C	0.361344	2.877733	2.644616
C	1.566898	3.467895	2.359208
C	2.469452	2.502312	1.869585
C	1.822179	1.283056	1.863712
C	0.618663	1.402092	2.783833
H	-0.227070	0.765644	2.550239
F	0.975939	1.100919	4.096094
H	2.293054	0.330315	1.662762
H	3.439675	2.728371	1.451057
F	1.792209	4.779789	2.375998
F	-0.648049	3.483529	3.274512

29

1 + 1,2,5b-*c*-$C_5H_3F_3$ = **1** + 3,4,5b-*c*-$C_5H_3F_3$

C	0.001058	-0.002076	-0.004461
C	-1.425246	-0.229610	0.484957
C	-1.640878	0.726195	1.375799
C	-0.399151	1.580092	1.503022
C	0.083450	1.531025	0.055896
F	-0.761453	2.172040	-0.817210
H	1.077541	1.947754	-0.095031
C	0.701714	0.749618	2.240187
C	0.163035	0.228011	3.576325
H	0.927458	-0.349128	4.101699
H	-0.719330	-0.401994	3.462850
H	-0.110575	1.075023	4.210705
C	1.896794	1.658929	2.558715
H	2.690716	1.083645	3.040030
H	1.580831	2.439802	3.252508
H	2.321345	2.149523	1.682808
C	1.006165	-0.382143	1.147189
C	2.443630	-0.349729	0.607757
H	2.717244	0.596128	0.139779
H	3.165211	-0.547692	1.403820
H	2.560681	-1.134665	-0.143910
C	0.752194	-1.807818	1.643278
H	-0.259999	-1.950995	2.019098
H	0.906945	-2.511286	0.819985
H	1.452527	-2.072445	2.439687
F	-0.613695	2.814664	2.045674
F	-2.679749	0.910757	2.180020
H	-2.069509	-1.058168	0.232827
H	0.247440	-0.453359	-0.965031

29

1 + 1,3,5a-*c*-$C_5H_3F_3$ TS = **1** + 2,4,5a-*c*-$C_5H_3F_3$ TS

C	0.025971	-0.008751	0.007856
H	-0.554960	-0.391289	0.842371
H	-0.580822	-0.112974	-0.901016
H	0.905122	-0.644163	-0.117648
C	0.432672	1.440504	0.164445
C	1.527703	1.856250	-0.789435
H	2.043815	2.765603	-0.480379

H	2.273381	1.066632	-0.900641
H	1.096871	2.053951	-1.779548
C	-0.462109	2.408019	0.642836
C	-1.888626	2.039002	1.005599
H	-2.007773	1.019199	1.356910
H	-2.512132	2.166472	0.112317
H	-2.283994	2.712176	1.769358
C	-0.392049	3.829064	0.111461
H	-0.869520	3.875618	-0.874721
H	-0.939307	4.507773	0.771112
H	0.624306	4.202611	0.005081
C	0.404288	2.854643	2.618146
C	1.643021	3.420059	2.342127
C	2.468681	2.346633	1.977577
C	1.826330	1.134733	2.059579
C	0.665964	1.410132	2.974570
H	1.003365	1.393509	4.019102
F	-0.394399	0.548994	2.892200
H	2.268535	0.161598	1.903469
F	3.687370	2.517098	1.457938
H	1.882746	4.471179	2.297760
F	-0.579625	3.533224	3.223385

29

1 + 1,3,5a-*c*-$C_5H_3F_3$ = **1** + 2,4,5a-*c*-$C_5H_3F_3$

C	-0.002801	0.001107	-0.004865
C	-1.404107	-0.196013	0.502263
C	-1.699252	0.719312	1.416898
C	-0.439127	1.558952	1.523320
C	-0.022581	1.540824	0.046964
H	-0.767759	1.996617	-0.603878
F	1.187873	2.136782	-0.225561
C	0.681931	0.746348	2.252182
C	0.162893	0.221628	3.596470
H	0.947586	-0.328694	4.121183
H	-0.702746	-0.432280	3.498200
H	-0.122329	1.068856	4.226006
C	1.879768	1.653846	2.573431
H	2.663619	1.071401	3.063444
H	1.559943	2.431420	3.269710
H	2.305756	2.142142	1.701270
C	0.981861	-0.387655	1.166933
C	2.429620	-0.393652	0.656964
H	2.737985	0.554661	0.223639
H	3.116868	-0.642334	1.469518
H	2.535480	-1.166586	-0.109231
C	0.674931	-1.810216	1.648213
H	-0.352767	-1.935725	1.990451
H	0.840202	-2.515885	0.829199
H	1.341019	-2.092525	2.467215
F	-0.648517	2.799598	2.069824
H	-2.579101	0.823132	2.033647
F	-2.148268	-1.228046	0.109151
H	0.224616	-0.465312	-0.962831

29

1 + 1,3,5b-*c*-$C_5H_3F_3$ TS = **1** + 2,4,5b-*c*-$C_5H_3F_3$ TS

C	0.020783	-0.003416	-0.000523
H	-0.516310	-0.390783	0.864852
H	-0.644389	-0.117775	-0.865887
H	0.890461	-0.640270	-0.170276
C	0.434330	1.446432	0.128367
C	1.520991	1.858932	-0.833252
H	2.051472	2.755208	-0.508322
H	2.254572	1.061690	-0.964780
H	1.083541	2.085222	-1.814050
C	-0.461131	2.417931	0.603804
C	-1.870715	2.027773	1.006620
H	-1.953020	1.044590	1.467084
H	-2.503691	2.015438	0.111308
H	-2.295557	2.761855	1.693642
C	-0.418905	3.829558	0.050611
H	-0.933082	3.863402	-0.917548
H	-0.940331	4.516090	0.722656
H	0.593164	4.200687	-0.096789
C	0.415392	2.871051	2.553292
C	1.651535	3.433960	2.300273
C	2.480506	2.351937	1.947413

C	1.829934	1.145878	1.995889
C	0.604831	1.391912	2.837575
H	-0.252840	0.765380	2.619923
F	0.867889	1.226135	4.194636
H	2.275052	0.176291	1.829410
F	3.705853	2.522682	1.446761
H	1.901209	4.482934	2.266333
F	-0.577261	3.534437	3.159064

29

1 + 1,3,5b-*c*-$C_5H_3F_3$ = **1** + 2,4,5b-*c*-$C_5H_3F_3$

C	0.003274	0.002015	-0.004570
C	-1.403830	-0.194469	0.501231
C	-1.700007	0.714978	1.418354
C	-0.440078	1.553818	1.523525
C	0.061239	1.531823	0.077281
F	-0.781731	2.163791	-0.803776
H	1.051336	1.962242	-0.060818
C	0.683810	0.745532	2.252910
C	0.185238	0.223694	3.603695
H	0.977438	-0.321112	4.122974
H	-0.677624	-0.434615	3.512828
H	-0.100347	1.071204	4.232602
C	1.875865	1.668688	2.547410
H	2.685936	1.104693	3.014906
H	1.562379	2.445881	3.246416
H	2.280084	2.166761	1.666380
C	0.985412	-0.391252	1.164233
C	2.428124	-0.379916	0.641687
H	2.719147	0.566575	0.185325
H	3.135115	-0.593581	1.446720
H	2.543119	-1.161477	-0.113631
C	0.691080	-1.813505	1.649136
H	-0.335794	-1.940786	1.992404
H	0.857061	-2.519802	0.830988
H	1.359325	-2.089828	2.468416
F	-0.639375	2.798937	2.063178
H	-2.572231	0.801462	2.047623
F	-2.129222	-1.244763	0.122840
H	0.233419	-0.458145	-0.964944

29

1 + 1,4,5a-*c*-$C_5H_3F_3$ TS

C	0.009612	-0.007749	0.011940
H	-0.720169	-0.330622	0.747194
H	-0.428617	-0.143198	-0.984809
H	0.874239	-0.671481	0.074247
C	0.430916	1.440732	0.150504
C	1.508455	1.799673	-0.852062
H	1.994494	2.750304	-0.641978
H	2.275839	1.021998	-0.882760
H	1.067392	1.867417	-1.854536
C	-0.453981	2.425054	0.608259
C	-1.883034	2.097485	0.990111
H	-2.013378	1.110408	1.421786
H	-2.501772	2.158139	0.086055
H	-2.273938	2.832917	1.696003
C	-0.331524	3.846776	0.099315
H	-0.774195	3.916005	-0.902340
H	-0.879761	4.533753	0.749000
H	0.697752	4.192747	0.028235
C	0.385414	2.824708	2.700242
C	1.579625	3.437957	2.390769
C	2.474918	2.444725	1.928729
C	1.820427	1.232949	1.960150
C	0.684602	1.367643	2.940959
F	-0.348908	0.484808	2.834788
H	1.093576	1.265145	3.954961
F	2.412823	0.047905	1.761899
H	3.457011	2.613743	1.511658
H	1.752646	4.504295	2.390932
F	-0.631642	3.425237	3.332488

29

1 + 1,4,5a-*c*-$C_5H_3F_3$

C	-0.000521	-0.001641	0.000983
C	-1.418638	-0.222416	0.469007
C	-1.675875	0.724917	1.371662
C	-0.425069	1.561654	1.490404

C	-0.001795	1.536029	0.012372
F	1.208091	2.123441	-0.259236
H	-0.744021	1.970951	-0.655695
C	0.690008	0.740711	2.224834
C	0.158052	0.214318	3.563060
H	0.933162	-0.350461	4.086486
H	-0.715549	-0.427778	3.455394
H	-0.119529	1.060533	4.197097
C	1.889301	1.642705	2.553099
H	2.668249	1.054545	3.043901
H	1.570142	2.420132	3.249594
H	2.320308	2.129599	1.682630
C	0.998343	-0.394724	1.143213
C	2.441326	-0.390220	0.616317
H	2.745594	0.559880	0.185746
H	3.129446	-0.640990	1.426983
H	2.541319	-1.156195	-0.154813
C	0.710938	-1.822529	1.622667
H	-0.301378	-1.951997	2.004089
H	0.850173	-2.516111	0.789182
H	1.410994	-2.108809	2.411163
F	-0.626297	2.804004	2.034743
H	-2.563301	0.871126	1.972315
H	-2.043114	-1.044572	0.146857
F	0.295870	-0.591838	-1.200689

29

1 + 1,4,5b-*c*-$C_5H_3F_3$ TS

C	0.008572	-0.002509	0.008155
H	-0.642935	-0.339428	0.812782
H	-0.541514	-0.145005	-0.930092
H	0.878311	-0.660567	-0.019968
C	0.433833	1.447940	0.108245
C	1.497512	1.796391	-0.909568
H	1.979361	2.751662	-0.710495
H	2.269152	1.023190	-0.936264
H	1.048409	1.852499	-1.909153
C	-0.452436	2.432934	0.565965
C	-1.867766	2.082505	0.976313
H	-1.966698	1.126030	1.486948
H	-2.493192	2.031138	0.076636
H	-2.287410	2.855520	1.621802
C	-0.349579	3.849564	0.044777
H	-0.799065	3.909503	-0.954405
H	-0.895769	4.536839	0.695419
H	0.677881	4.199624	-0.034282
C	0.389501	2.842684	2.636003
C	1.587075	3.450558	2.351353
C	2.484081	2.452363	1.888316
C	1.819774	1.250948	1.897383
C	0.615915	1.357639	2.805762
H	-0.223121	0.713127	2.570583
F	0.977072	1.073888	4.116206
F	2.401266	0.061209	1.691934
H	3.472035	2.619584	1.484691
H	1.768202	4.515436	2.364025
F	-0.635297	3.440526	3.259174

29

1 + 1,4,5b-*c*-$C_5H_3F_3$

C	0.004755	-0.001493	0.002015
C	-1.417420	-0.223111	0.468541
C	-1.674614	0.723220	1.368843
C	-0.419713	1.560096	1.487613
C	0.080445	1.527989	0.040158
H	1.074562	1.943236	-0.112508
F	-0.763795	2.142006	-0.846536
C	0.693367	0.741851	2.225106
C	0.176555	0.218676	3.568431
H	0.956995	-0.342089	4.088299
H	-0.695048	-0.426564	3.465783
H	-0.101760	1.065558	4.201147
C	1.887495	1.657783	2.530369
H	2.692166	1.085847	2.997395
H	1.575074	2.432831	3.231990
H	2.296721	2.156587	1.652213
C	1.002743	-0.396116	1.142509
C	2.439000	-0.371274	0.599559

H	2.723410	0.578962	0.148262
H	3.149086	-0.589102	1.400208
H	2.547034	-1.142449	-0.164772
C	0.731801	-1.824163	1.624997
H	-0.278199	-1.957553	2.010539
H	0.870278	-2.517659	0.791394
H	1.437025	-2.104568	2.411035
F	-0.614049	2.805701	2.026752
H	-2.553431	0.854674	1.984753
H	-2.033527	-1.058145	0.165101
F	0.308067	-0.586376	-1.200415

29

1 + 1,5a,5b-*c*-$C_5H_3F_3$ TS

C	0.024822	-0.007695	0.005705
H	-0.570899	-0.386326	0.830969
H	-0.567729	-0.112824	-0.912087
H	0.903053	-0.647401	-0.103509
C	0.437176	1.440928	0.158875
C	1.515148	1.847707	-0.818693
H	2.027772	2.763235	-0.526257
H	2.261328	1.057983	-0.928482
H	1.067248	2.027066	-1.804591
C	-0.458419	2.417546	0.622073
C	-1.884970	2.064140	0.992620
H	-2.020721	1.036685	1.313703
H	-2.512579	2.228586	0.108362
H	-2.262058	2.723312	1.777603
C	-0.371176	3.836980	0.094252
H	-0.823978	3.883760	-0.903758
H	-0.932938	4.515891	0.741023
H	0.648337	4.207766	0.013813
C	0.406846	2.888288	2.641473
C	1.630475	3.447819	2.352618
C	2.494901	2.394802	1.953064
C	1.840092	1.184896	2.018116
C	0.668174	1.419342	2.940623
F	1.047836	1.300861	4.253384
F	-0.382738	0.581260	2.829976
H	2.270487	0.204425	1.868688
H	3.483095	2.544079	1.540290
H	1.847501	4.505477	2.336916
F	-0.592225	3.524745	3.258665

29

1 + 1,5a,5b-*c*-$C_5H_3F_3$

C	-0.002478	-0.002711	-0.002925
C	-1.418575	-0.217639	0.506047
C	-1.672509	0.720534	1.418154
C	-0.429686	1.573379	1.530605
C	0.006837	1.529132	0.056265
F	-0.863116	2.130674	-0.788523
F	1.201841	2.113033	-0.205437
C	0.693735	0.756712	2.251630
C	0.169789	0.227092	3.592562
H	0.950471	-0.332079	4.113479
H	-0.700263	-0.419755	3.488561
H	-0.109818	1.072222	4.227394
C	1.892166	1.660039	2.581825
H	2.668993	1.072994	3.077243
H	1.570728	2.438475	3.276295
H	2.329834	2.146991	1.714710
C	0.996208	-0.377467	1.160311
C	2.444973	-0.378309	0.650833
H	2.755897	0.567521	0.214693
H	3.132256	-0.623056	1.464485
H	2.553437	-1.153346	-0.112793
C	0.709949	-1.801093	1.651893
H	-0.308364	-1.932263	2.015280
H	0.867049	-2.505967	0.830232
H	1.396945	-2.075491	2.456191
F	-0.626780	2.819522	2.057478
H	-2.556804	0.861058	2.024024
H	-2.067473	-1.027159	0.202171
H	0.248192	-0.443554	-0.967069

29

1 + 2,3,5a-*c*-$C_5H_3F_3$ TS

C	0.002925	-0.005421	0.006740

H	-0.659947	-0.351616	0.793866
H	-0.527824	-0.100188	-0.949294
H	0.860829	-0.680871	-0.038080
C	0.456230	1.431373	0.173681
C	1.522942	1.807580	-0.835689
H	2.051821	2.727295	-0.587991
H	2.265193	1.011642	-0.931948
H	1.063923	1.952284	-1.821928
C	-0.432075	2.419026	0.632787
C	-1.868595	2.075450	0.974391
H	-1.983392	1.126189	1.488997
H	-2.452626	2.030732	0.046204
H	-2.316983	2.855588	1.594518
C	-0.299999	3.834390	0.105972
H	-0.676462	3.881845	-0.923790
H	-0.892766	4.529556	0.705152
H	0.726419	4.199319	0.091194
C	0.371414	2.837682	2.704689
C	1.587839	3.414607	2.395505
C	2.473854	2.431050	1.938315
C	1.846119	1.200605	1.943445
C	0.728462	1.392853	2.934010
F	-0.308770	0.497223	2.849747
H	1.137278	1.290134	3.947599
H	2.340817	0.254943	1.763392
F	3.667370	2.701961	1.411655
F	1.848823	4.720354	2.349684
H	-0.444421	3.347043	3.201077

29

1 + 2,3,5a-*c*-$C_5H_3F_3$

C	-0.001814	0.002174	-0.006718
C	-1.407826	-0.207825	0.498548
C	-1.662820	0.734813	1.397953
C	-0.434811	1.602737	1.520299
C	-0.025774	1.539216	0.039231
F	1.188852	2.134272	-0.239961
H	-0.762636	1.979636	-0.631329
C	0.680302	0.757269	2.240748
C	0.145626	0.221760	3.574777
H	0.905926	-0.374924	4.084835
H	-0.747897	-0.393377	3.464895
H	-0.107634	1.060506	4.229370
C	1.887518	1.645443	2.576329
H	2.669859	1.056910	3.062305
H	1.576565	2.419331	3.283559
H	2.317220	2.138002	1.707550
C	0.987956	-0.379769	1.156042
C	2.435621	-0.380546	0.643010
H	2.740544	0.567700	0.207108
H	3.126569	-0.626797	1.453283
H	2.543403	-1.154015	-0.122424
C	0.693718	-1.804579	1.641599
H	-0.329746	-1.936790	1.993566
H	0.856259	-2.510163	0.821937
H	1.369111	-2.083813	2.454091
H	-0.608999	2.589962	1.948656
F	-2.731246	0.867570	2.180394
F	-2.157787	-1.252872	0.156761
H	0.217726	-0.465634	-0.966598

29

1 + 2,3,5b-*c*-$C_5H_3F_3$ TS

C	0.001158	-0.001776	0.002736
H	-0.590265	-0.357516	0.845823
H	-0.622540	-0.112123	-0.893187
H	0.855790	-0.671184	-0.115508
C	0.456887	1.438465	0.125803
C	1.497915	1.809298	-0.909370
H	2.037624	2.723513	-0.663072
H	2.232963	1.010030	-1.025848
H	1.018142	1.966803	-1.883625
C	-0.428833	2.428071	0.593933
C	-1.848945	2.065181	0.979574
H	-1.934582	1.144974	1.556627
H	-2.450487	1.929295	0.072079
H	-2.312542	2.868531	1.555926
C	-0.316253	3.836722	0.049964

H	-0.687067	3.870491	-0.982311
H	-0.916003	4.531529	0.641731
H	0.708031	4.208841	0.037943
C	0.393088	2.857846	2.640270
C	1.612189	3.422339	2.356382
C	2.498348	2.433082	1.888074
C	1.864191	1.215400	1.862272
C	0.675408	1.376983	2.786916
F	1.035350	1.076771	4.101328
H	-0.165023	0.732009	2.559393
H	2.349857	0.268047	1.672233
F	3.691675	2.714363	1.368880
F	1.891676	4.723574	2.320140
H	-0.422951	3.363679	3.137929

29

1 + 2,3,5b-*c*-$C_5H_3F_3$

C	0.003648	0.002406	-0.005448
C	-1.403170	-0.206950	0.500315
C	-1.657994	0.734277	1.396868
C	-0.429761	1.603298	1.519512
C	0.067761	1.532394	0.071060
F	-0.761205	2.165098	-0.828681
H	1.064893	1.943057	-0.076887
C	0.686040	0.762583	2.242738
C	0.168793	0.228412	3.581946
H	0.934963	-0.365628	4.086327
H	-0.723398	-0.389103	3.477016
H	-0.083808	1.067198	4.236544
C	1.888860	1.664343	2.554631
H	2.697777	1.091516	3.014243
H	1.585706	2.433443	3.269630
H	2.296407	2.170878	1.679164
C	0.995552	-0.379957	1.154281
C	2.436948	-0.359673	0.625776
H	2.723366	0.588027	0.168595
H	3.149642	-0.571991	1.426213
H	2.553251	-1.139580	-0.131097
C	0.719441	-1.804443	1.645341
H	-0.302239	-1.940902	2.000123
H	0.883181	-2.510926	0.826852
H	1.399284	-2.075312	2.456988
H	-0.598665	2.594694	1.939873
F	-2.711687	0.852512	2.201901
F	-2.137060	-1.270368	0.179522
H	0.227802	-0.457708	-0.967799

29

1 + 2,5a,5b-*c*-$C_5H_3F_3$ TS

C	-0.008969	0.000182	-0.002259
H	-0.749289	-0.300750	0.731571
H	-0.449592	-0.126378	-0.998662
H	0.833967	-0.692952	0.061239
C	0.457628	1.437757	0.135706
C	1.491847	1.775166	-0.924100
H	2.009081	2.714208	-0.738577
H	2.241521	0.982764	-0.994665
H	1.002486	1.851545	-1.902715
C	-0.430816	2.440410	0.564698
C	-1.867939	2.132214	0.918905
H	-1.992643	1.215590	1.488230
H	-2.446397	2.031386	-0.008838
H	-2.310482	2.952864	1.486733
C	-0.223558	3.851408	0.071391
H	-0.489929	3.913486	-0.991814
H	-0.852175	4.555981	0.618624
H	0.812111	4.184050	0.155452
C	0.358607	2.866361	2.784112
C	1.535716	3.471316	2.432945
C	2.457274	2.567309	1.861657
C	1.840986	1.327065	1.821330
C	0.742496	1.412091	2.872015
F	-0.274906	0.527085	2.754842
F	1.278052	1.122496	4.105082
H	2.342239	0.390708	1.607823
H	3.407856	2.840544	1.428405
F	1.748556	4.787647	2.471813
H	-0.458742	3.310579	3.333497

29

1 + 2,5a,5b-*c*-$C_5H_3F_3$

C	-0.001758	-0.001356	-0.004132
C	-1.419942	-0.231913	0.504260
C	-1.632674	0.728678	1.394067
C	-0.422662	1.617694	1.522100
C	0.005827	1.530935	0.053028
F	-0.859631	2.124461	-0.807807
F	1.205402	2.108715	-0.220257
C	0.693697	0.769829	2.239824
C	0.153470	0.231263	3.570530
H	0.911162	-0.370651	4.077796
H	-0.741907	-0.379665	3.455512
H	-0.097139	1.068305	4.228131
C	1.903086	1.651575	2.583546
H	2.678715	1.055985	3.071354
H	1.592822	2.424824	3.291499
H	2.343132	2.144048	1.719922
C	1.003569	-0.370190	1.149613
C	2.452032	-0.365772	0.635882
H	2.760855	0.579919	0.198224
H	3.143256	-0.610354	1.446283
H	2.560731	-1.140528	-0.128043
C	0.732610	-1.795536	1.646744
H	-0.279959	-1.933651	2.022737
H	0.885199	-2.500921	0.824654
H	1.431691	-2.065186	2.442268
H	-0.593817	2.612683	1.931372
F	-2.701477	0.904564	2.169721
H	-2.074508	-1.047615	0.237734
H	0.240231	-0.439651	-0.972065

29

1 + 1,2,3,4-*c*-$C_5H_2F_4$ TS

C	0.006638	-0.003481	0.006652
H	-0.606990	-0.346306	0.839242
H	-0.592274	-0.129938	-0.903707
H	0.867930	-0.668577	-0.073770
C	0.448617	1.441390	0.116150
C	1.528845	1.786331	-0.887402
H	2.011931	2.742713	-0.691317
H	2.303432	1.015739	-0.901177
H	1.097667	1.838657	-1.894824
C	-0.436611	2.425714	0.573655
C	-1.854424	2.065435	0.967429
H	-1.938683	1.134147	1.526812
H	-2.462300	1.948973	0.061685
H	-2.306050	2.859465	1.564221
C	-0.327250	3.850247	0.071711
H	-0.783787	3.930242	-0.922629
H	-0.861301	4.535366	0.734584
H	0.700460	4.200972	-0.014161
C	0.365791	2.794578	2.659367
C	1.568130	3.402273	2.357266
C	2.455001	2.416655	1.899403
C	1.798675	1.202149	1.919571
C	0.638093	1.332949	2.861535
H	-0.200233	0.677006	2.649978
H	0.986269	1.169344	3.887965
F	2.405874	0.029591	1.708375
F	3.625778	2.668810	1.326282
F	1.790193	4.708610	2.273912
F	-0.641648	3.416172	3.281436

29

1 + 1,2,3,4-*c*-$C_5H_2F_4$

C	0.005071	0.001624	-0.000145
C	-1.411736	-0.232732	0.478100
C	-1.668195	0.709688	1.375245
C	-0.417927	1.556368	1.480294
C	0.061749	1.530273	0.027784
H	1.063633	1.931861	-0.107898
H	-0.645034	1.991670	-0.658655
C	0.679520	0.726169	2.232544
C	0.141621	0.204687	3.568516
H	0.908801	-0.368419	4.094353
H	-0.737587	-0.430481	3.458693
H	-0.135958	1.050858	4.201976

C	1.875673	1.633717	2.546849
H	2.676765	1.056321	3.013150
H	1.565361	2.406524	3.252034
H	2.287365	2.132875	1.669919
C	0.989476	-0.412029	1.148404
C	2.427608	-0.393765	0.614687
H	2.714454	0.556998	0.165795
H	3.132877	-0.613368	1.419006
H	2.537920	-1.166101	-0.148299
C	0.698421	-1.839559	1.621427
H	-0.317715	-1.969327	1.994394
H	0.838135	-2.532492	0.787968
H	1.389614	-2.129655	2.416182
F	-0.640204	2.788939	2.031531
F	-2.675457	0.806739	2.229253
F	-2.093123	-1.332057	0.194292
F	0.282179	-0.601197	-1.196922

29

1 + 1,2,3,5a-*c*-$C_5H_2F_4$ TS = **1** + 2,3,4,5a-*c*-$C_5H_2F_4$ TS

C	0.018650	-0.008504	0.002967
H	-0.591664	-0.379064	0.821407
H	-0.559019	-0.115029	-0.924068
H	0.893691	-0.655874	-0.090232
C	0.438903	1.438073	0.159272
C	1.529063	1.833919	-0.812544
H	2.038934	2.757841	-0.540520
H	2.282617	1.047934	-0.897716
H	1.095422	1.988143	-1.808855
C	-0.452874	2.413919	0.624422
C	-1.882500	2.063027	0.987060
H	-2.010545	1.049800	1.354359
H	-2.501111	2.180250	0.088877
H	-2.276692	2.752344	1.736972
C	-0.350439	3.840611	0.116222
H	-0.790881	3.904536	-0.886191
H	-0.912047	4.518599	0.763718
H	0.671433	4.210633	0.047150
C	0.383070	2.861856	2.654828
C	1.614597	3.426374	2.366140
C	2.476377	2.398670	1.957456
C	1.833755	1.184438	2.015205
C	0.686908	1.418105	2.964332
H	1.048151	1.362472	3.998814
F	-0.362109	0.547326	2.867266
H	2.287621	0.219462	1.840105
F	3.672026	2.627330	1.421170
F	1.884141	4.724627	2.306829
F	-0.591211	3.527809	3.277442

29

1 + 1,2,3,5a-*c*-$C_5H_2F_4$ = **1** + 2,3,4,5a-*c*-$C_5H_2F_4$

C	-0.002732	0.000972	-0.006769
C	-1.408781	-0.218400	0.491293
C	-1.666549	0.711795	1.400565
C	-0.421032	1.569179	1.515905
C	-0.016858	1.540394	0.038258
H	-0.760577	1.997206	-0.613259
F	1.196101	2.128083	-0.233169
C	0.690746	0.746963	2.246743
C	0.148698	0.223711	3.582902
H	0.916066	-0.348384	4.109287
H	-0.730779	-0.411372	3.474229
H	-0.126661	1.070613	4.216596
C	1.889929	1.647577	2.578085
H	2.664228	1.060238	3.077096
H	1.568897	2.428880	3.269617
H	2.327856	2.129397	1.708070
C	0.990220	-0.386538	1.158260
C	2.436830	-0.389805	0.645046
H	2.744950	0.557965	0.210817
H	3.125999	-0.638635	1.455812
H	2.541469	-1.162837	-0.121186
C	0.689339	-1.809465	1.642008
H	-0.335248	-1.939093	1.991627
H	0.851432	-2.514699	0.822064
H	1.361958	-2.089853	2.456195
F	-0.657099	2.796262	2.065134

F	-2.707384	0.854134	2.205690
F	-2.147117	-1.266496	0.142856
H	0.220716	-0.459610	-0.968898

29

1 + 1,2,3,5b-*c*-$C_5H_2F_4$ TS = **1** + 2,3,4,5b-*c*-$C_5H_2F_4$ TS

C	0.011418	-0.002760	-0.004347
H	-0.536791	-0.378016	0.859542
H	-0.647199	-0.118963	-0.874087
H	0.874722	-0.651924	-0.162441
C	0.443183	1.443954	0.115860
C	1.512045	1.832503	-0.879886
H	2.042071	2.743689	-0.601746
H	2.251219	1.036932	-0.992444
H	1.058383	2.012169	-1.862746
C	-0.443711	2.424286	0.587926
C	-1.856129	2.054189	0.994280
H	-1.946105	1.077555	1.467829
H	-2.488114	2.034223	0.098239
H	-2.276354	2.801012	1.670154
C	-0.362512	3.844272	0.063942
H	-0.827980	3.900992	-0.927599
H	-0.905712	4.526874	0.721851
H	0.658373	4.211503	-0.032238
C	0.406527	2.869941	2.594396
C	1.634441	3.433191	2.329243
C	2.497571	2.401734	1.908930
C	1.850971	1.193689	1.928165
C	0.645122	1.394655	2.819410
F	0.955997	1.171181	4.155562
H	-0.205906	0.761635	2.595117
H	2.306980	0.232683	1.740995
F	3.692716	2.644037	1.380305
F	1.916504	4.728133	2.276945
F	-0.579797	3.513213	3.221175

29

1 + 1,2,3,5b-*c*-$C_5H_2F_4$ = **1** + 2,3,4,5b-*c*-$C_5H_2F_4$

C	0.002783	0.001352	-0.006142
C	-1.406288	-0.211718	0.492685
C	-1.665807	0.720317	1.396966
C	-0.417209	1.571038	1.513345
C	0.068558	1.533262	0.065715
H	1.062592	1.952592	-0.077369
F	-0.774107	2.169717	-0.809381
C	0.693048	0.749563	2.246786
C	0.165969	0.228329	3.587432
H	0.938414	-0.339823	4.110751
H	-0.711598	-0.409691	3.482688
H	-0.110724	1.075529	4.220091
C	1.887160	1.663655	2.555377
H	2.686618	1.092595	3.032248
H	1.572326	2.443570	3.250723
H	2.305017	2.156180	1.677358
C	0.996032	-0.386287	1.154856
C	2.436042	-0.366817	0.625101
H	2.720921	0.579385	0.164235
H	3.148624	-0.574521	1.426589
H	2.551516	-1.149945	-0.128466
C	0.713147	-1.809411	1.643273
H	-0.309979	-1.943476	1.994869
H	0.877096	-2.515273	0.824429
H	1.389534	-2.081367	2.457233
F	-0.637102	2.805360	2.052294
F	-2.695172	0.846057	2.220282
F	-2.130512	-1.277304	0.168089
H	0.228008	-0.454960	-0.969798

29

1 + 1,2,4,5a-*c*-$C_5H_2F_4$ TS = **1** + 1,3,4,5a-*c*-$C_5H_2F_4$ TS

C	-0.003008	-0.008101	0.013533
H	-0.771940	-0.303966	0.719365
H	-0.394840	-0.159790	-0.999576
H	0.846731	-0.684103	0.130484
C	0.435855	1.437622	0.138807
C	1.509960	1.767901	-0.880033
H	1.988520	2.730256	-0.711477
H	2.283441	0.995276	-0.881515
H	1.067026	1.789086	-1.883231

C	-0.439474	2.434799	0.582703
C	-1.870147	2.135129	0.973882
H	-2.007878	1.163253	1.437625
H	-2.489248	2.170662	0.068687
H	-2.254201	2.896737	1.655058
C	-0.265157	3.859036	0.103143
H	-0.645697	3.948919	-0.922084
H	-0.833036	4.550987	0.729057
H	0.773168	4.189234	0.089913
C	0.367590	2.821252	2.752429
C	1.543714	3.449139	2.420530
C	2.469546	2.523895	1.904797
C	1.835725	1.296829	1.908107
C	0.722722	1.368813	2.927704
F	-0.298647	0.475690	2.806885
H	1.165382	1.221456	3.921236
F	2.467896	0.139286	1.683143
H	3.432071	2.756312	1.475236
F	1.725987	4.766680	2.425468
F	-0.649478	3.386711	3.403637

29

1 + 1,2,4,5a-*c*-$C_5H_2F_4$ = **1** + 1,3,4,5a-*c*-$C_5H_2F_4$

C	-0.000305	-0.001621	-0.000522
C	-1.423507	-0.240865	0.466085
C	-1.644893	0.717088	1.356005
C	-0.408402	1.573271	1.484209
C	0.004313	1.535132	0.004368
H	-0.736899	1.970029	-0.664859
F	1.215148	2.118013	-0.264747
C	0.696244	0.740779	2.220943
C	0.142142	0.215291	3.550653
H	0.900521	-0.370600	4.074693
H	-0.744443	-0.408375	3.432529
H	-0.125975	1.060423	4.189519
C	1.897045	1.635801	2.559508
H	2.666284	1.042426	3.058905
H	1.576879	2.416623	3.251681
H	2.339952	2.116506	1.691424
C	1.005739	-0.393913	1.135446
C	2.447687	-0.384723	0.605376
H	2.749693	0.564416	0.171613
H	3.138430	-0.632335	1.414620
H	2.547753	-1.152435	-0.164005
C	0.726969	-1.822275	1.617477
H	-0.280141	-1.956359	2.010187
H	0.860251	-2.514999	0.782365
H	1.436936	-2.106188	2.397793
F	-0.631117	2.803584	2.028121
F	-2.695355	0.907764	2.138906
H	-2.042064	-1.081062	0.188477
F	0.288199	-0.588828	-1.203952

29

1 + 1,2,4,5b-*c*-$C_5H_2F_4$ TS = **1** + 1,3,4,5b-*c*-$C_5H_2F_4$ TS

C	-0.005661	-0.003237	0.012613
H	-0.684504	-0.312424	0.805639
H	-0.531594	-0.160597	-0.936587
H	0.854848	-0.674468	0.021728
C	0.440288	1.443750	0.090079
C	1.492811	1.754719	-0.954500
H	1.957743	2.728767	-0.817982
H	2.278581	0.995048	-0.941427
H	1.037257	1.739571	-1.952133
C	-0.434989	2.443185	0.534443
C	-1.855578	2.125066	0.945753
H	-1.966138	1.186143	1.486673
H	-2.476683	2.050487	0.044609
H	-2.270361	2.922295	1.563872
C	-0.265836	3.863131	0.048226
H	-0.630593	3.948175	-0.983036
H	-0.841365	4.556174	0.665359
H	0.773492	4.192329	0.048672
C	0.360486	2.830436	2.689366
C	1.539131	3.460818	2.388033
C	2.470932	2.543054	1.854258
C	1.832771	1.324563	1.828699
C	0.655031	1.358069	2.785812

H	-0.171283	0.698983	2.544182
F	1.078624	1.014444	4.061061
F	2.458570	0.164347	1.600960
H	3.436336	2.785587	1.437402
F	1.721364	4.777045	2.409065
F	-0.670760	3.387970	3.327611

29

1 + 1,2,4,5b-*c*-$C_5H_2F_4$ = **1** + 1,3,4,5b-*c*-$C_5H_2F_4$

C	0.004585	-0.001555	0.000534
C	-1.419716	-0.237529	0.466027
C	-1.641488	0.727151	1.346778
C	-0.397367	1.578036	1.477562
C	0.087589	1.529081	0.028057
H	1.083848	1.936318	-0.131847
F	-0.760095	2.144732	-0.851602
C	0.701016	0.745283	2.219283
C	0.157007	0.222456	3.552187
H	0.918698	-0.360010	4.075288
H	-0.727685	-0.403779	3.435656
H	-0.113677	1.068303	4.188936
C	1.897202	1.652388	2.538293
H	2.691996	1.073104	3.012770
H	1.583961	2.429006	3.237751
H	2.318686	2.147033	1.663379
C	1.012907	-0.391576	1.132870
C	2.446610	-0.357120	0.583323
H	2.723971	0.592752	0.126980
H	3.162215	-0.567669	1.380801
H	2.556071	-1.130317	-0.178739
C	0.755486	-1.820483	1.618915
H	-0.248978	-1.960882	2.015788
H	0.889892	-2.513447	0.784283
H	1.471323	-2.095812	2.397021
F	-0.609193	2.813389	2.014226
F	-2.679151	0.908668	2.148406
H	-2.033411	-1.087957	0.211215
F	0.299077	-0.583444	-1.203994

29

1 + 1,2,5a,5b-*c*-$C_5H_2F_4$ TS = **1** + 3,4,5a,5b-*c*-$C_5H_2F_4$ TS

C	0.012824	-0.006513	0.001082
H	-0.632869	-0.359196	0.799155
H	-0.526786	-0.125755	-0.946605
H	0.885302	-0.662632	-0.045205
C	0.440329	1.440835	0.140508
C	1.507301	1.812889	-0.867722
H	2.008751	2.750791	-0.636091
H	2.265977	1.029711	-0.937279
H	1.051702	1.921602	-1.859951
C	-0.448705	2.429057	0.586625
C	-1.878128	2.106446	0.963544
H	-2.025956	1.091052	1.316981
H	-2.502502	2.249288	0.072966
H	-2.249244	2.795294	1.725593
C	-0.304776	3.853092	0.092622
H	-0.682240	3.923867	-0.935100
H	-0.895411	4.534521	0.709256
H	0.724232	4.210591	0.083950
C	0.374505	2.894806	2.704245
C	1.581371	3.468235	2.393007
C	2.478883	2.487431	1.917274
C	1.840862	1.265246	1.945137
C	0.692354	1.429802	2.922387
F	1.128917	1.240300	4.207388
F	-0.344874	0.579125	2.800021
H	2.299327	0.302681	1.763530
H	3.443419	2.705393	1.482371
F	1.818500	4.776235	2.383213
F	-0.620379	3.497277	3.350146

29

1 + 1,2,5a,5b-*c*-$C_5H_2F_4$ = **1** + 3,4,5a,5b-*c*-$C_5H_2F_4$

C	-0.002643	-0.002555	-0.004745
C	-1.423880	-0.236385	0.497295
C	-1.640985	0.712546	1.396191
C	-0.411101	1.584802	1.522150
C	0.012082	1.530032	0.045723
F	-0.861311	2.133260	-0.791767

F	1.207701	2.107059	-0.220473
C	0.701500	0.757921	2.245703
C	0.155324	0.230181	3.578608
H	0.919811	-0.348100	4.101972
H	-0.726659	-0.400038	3.464317
H	-0.116759	1.074998	4.216502
C	1.900805	1.655507	2.584406
H	2.669965	1.064127	3.086244
H	1.578866	2.436693	3.275514
H	2.347588	2.137178	1.718721
C	1.004414	-0.375666	1.151131
C	2.451688	-0.372197	0.637025
H	2.761459	0.573411	0.200094
H	3.141806	-0.617050	1.448071
H	2.558739	-1.146902	-0.127100
C	0.726741	-1.799730	1.645562
H	-0.287631	-1.935862	2.017324
H	0.880710	-2.504152	0.823012
H	1.421679	-2.070745	2.444018
F	-0.635086	2.816943	2.051583
F	-2.689210	0.902585	2.183540
H	-2.073242	-1.054142	0.224532
H	0.240263	-0.441054	-0.971980

29

1 + 1,3,5a,5b-*c*-$C_5H_2F_4$ TS = **1** + 2,4,5a,5b-*c*-$C_5H_2F_4$ TS

C	0.029730	-0.009643	0.013656
H	-0.551666	-0.400137	0.844037
H	-0.578782	-0.108115	-0.894767
H	0.911059	-0.639952	-0.117564
C	0.428386	1.438356	0.176642
C	1.534502	1.872822	-0.750048
H	2.059870	2.762280	-0.398621
H	2.266853	1.076781	-0.893301
H	1.110964	2.126727	-1.730418
C	-0.463362	2.405675	0.668152
C	-1.886838	2.030984	1.038404
H	-2.005264	1.007233	1.377773
H	-2.514574	2.168052	0.150164
H	-2.277306	2.696694	1.810889
C	-0.406891	3.823939	0.125376
H	-0.899063	3.858491	-0.853531
H	-0.949364	4.503598	0.787613
H	0.605744	4.201476	0.002152
C	0.430724	2.867987	2.592886
C	1.672913	3.416754	2.325278
C	2.506069	2.325501	2.003733
C	1.874932	1.115786	2.107237
C	0.686745	1.410243	2.980367
F	1.005747	1.374444	4.311678
F	-0.354744	0.562204	2.868741
H	2.308462	0.135626	1.979557
F	3.727243	2.489943	1.497995
H	1.924591	4.463962	2.268541
F	-0.547818	3.538826	3.204988

29

1 + 1,3,5a,5b-*c*-$C_5H_2F_4$ = **1** + 2,4,5a,5b-*c*-$C_5H_2F_4$

C	-0.001380	0.000504	-0.004545
C	-1.400665	-0.199326	0.519227
C	-1.694270	0.713661	1.434492
C	-0.442228	1.567088	1.536077
C	-0.003998	1.532842	0.061197
F	-0.875208	2.127698	-0.783954
F	1.189353	2.116792	-0.197785
C	0.687608	0.758094	2.255663
C	0.172278	0.229254	3.599887
H	0.960406	-0.318888	4.121092
H	-0.691309	-0.426849	3.502545
H	-0.113343	1.074755	4.231445
C	1.885758	1.664364	2.579408
H	2.665456	1.080001	3.073191
H	1.564542	2.442243	3.274580
H	2.320357	2.152430	1.711575
C	0.988813	-0.379931	1.165277
C	2.438193	-0.388794	0.660601
H	2.755813	0.557608	0.230134
H	3.119424	-0.640036	1.477113

H	2.545490	-1.161926	-0.104854
C	0.680897	-1.801141	1.650439
H	-0.346627	-1.926704	1.992028
H	0.848555	-2.508780	0.833880
H	1.346611	-2.078654	2.470920
F	-0.647326	2.810595	2.061426
H	-2.574321	0.818025	2.050096
F	-2.136942	-1.235669	0.130738
H	0.222017	-0.449606	-0.971012

29

1 + 1,4,5a,5b-*c*-$C_5H_2F_4$ TS

C	0.010520	-0.007764	0.012577
H	-0.741022	-0.327665	0.726585
H	-0.398848	-0.148967	-0.995226
H	0.873771	-0.670210	0.102078
C	0.425787	1.441728	0.149379
C	1.503292	1.804873	-0.850535
H	1.996099	2.749651	-0.630442
H	2.264150	1.021664	-0.893313
H	1.058552	1.889136	-1.849910
C	-0.459914	2.427584	0.607788
C	-1.888000	2.105385	0.994330
H	-2.027681	1.111261	1.405922
H	-2.509995	2.189517	0.094775
H	-2.268289	2.831787	1.715190
C	-0.331534	3.847883	0.098832
H	-0.759335	3.912877	-0.909341
H	-0.889994	4.535233	0.738967
H	0.698393	4.194080	0.040528
C	0.394059	2.854791	2.699187
C	1.584966	3.457592	2.387249
C	2.485922	2.459460	1.921785
C	1.843937	1.248777	1.950725
C	0.688190	1.382069	2.927281
F	1.133526	1.189115	4.204757
F	-0.333447	0.521756	2.793059
F	2.423755	0.060710	1.764403
H	3.466654	2.635958	1.505489
H	1.763427	4.522686	2.385150
F	-0.623705	3.436538	3.338168

29

1 + 1,4,5a,5b-*c*-$C_5H_2F_4$

C	0.001040	-0.001949	0.002347
C	-1.414482	-0.222119	0.485696
C	-1.671860	0.724765	1.386755
C	-0.427921	1.576025	1.503771
C	0.014796	1.537874	0.029190
F	-0.853357	2.115365	-0.825904
F	1.208223	2.111770	-0.232997
C	0.694295	0.757300	2.228934
C	0.164169	0.227564	3.566785
H	0.941465	-0.336520	4.087066
H	-0.708369	-0.415408	3.459534
H	-0.112951	1.072498	4.202577
C	1.893913	1.657953	2.559661
H	2.669037	1.067650	3.053436
H	1.573957	2.435671	3.255328
H	2.332852	2.144575	1.693123
C	1.004069	-0.382500	1.144639
C	2.447949	-0.380566	0.620323
H	2.760996	0.568005	0.193006
H	3.132077	-0.635615	1.432727
H	2.547425	-1.145776	-0.151508
C	0.717384	-1.808953	1.629187
H	-0.294287	-1.938484	2.011237
H	0.857904	-2.504915	0.798014
H	1.418411	-2.090619	2.418048
F	-0.626506	2.820101	2.030164
H	-2.558072	0.867099	1.989268
H	-2.038001	-1.046273	0.168433
F	0.296489	-0.575596	-1.200910

29

1 + 2,3,5a,5b-*c*-$C_5H_2F_4$ TS

C	0.002975	-0.005082	0.007815
H	-0.671814	-0.351242	0.784588
H	-0.516051	-0.098881	-0.954478

H	0.860995	-0.680530	-0.026704
C	0.453414	1.431597	0.175322
C	1.520485	1.812321	-0.830591
H	2.055289	2.725995	-0.573385
H	2.256231	1.012318	-0.938425
H	1.058932	1.973545	-1.812879
C	-0.436092	2.421037	0.635065
C	-1.872246	2.080920	0.977488
H	-1.993307	1.127523	1.482583
H	-2.455242	2.045710	0.048504
H	-2.316958	2.858565	1.602837
C	-0.297492	3.835133	0.109317
H	-0.657752	3.879138	-0.926188
H	-0.899741	4.530089	0.698553
H	0.729010	4.200173	0.107661
C	0.384171	2.866108	2.708959
C	1.596210	3.433670	2.399971
C	2.489331	2.443208	1.938747
C	1.871806	1.216310	1.940434
C	0.737199	1.408716	2.925807
F	1.186419	1.216465	4.208790
F	-0.288183	0.536282	2.812622
H	2.359706	0.264623	1.779250
F	3.676670	2.725980	1.412829
F	1.865586	4.734025	2.347636
H	-0.431022	3.359486	3.220599

29

1 + 2,3,5a,5b-*c*-$C_5H_2F_4$

C	-0.000801	0.001627	-0.006097
C	-1.402562	-0.214709	0.516294
C	-1.657552	0.726978	1.413751
C	-0.436496	1.610646	1.527137
C	-0.006602	1.533420	0.057604
F	-0.871004	2.121425	-0.805121
F	1.192106	2.111824	-0.208823
C	0.687338	0.771592	2.242849
C	0.154365	0.233071	3.576367
H	0.917535	-0.362031	4.083252
H	-0.737449	-0.383989	3.467255
H	-0.098959	1.070625	4.232168
C	1.896061	1.656321	2.581530
H	2.673248	1.063433	3.069919
H	1.585305	2.430020	3.288710
H	2.334967	2.148705	1.717479
C	0.996934	-0.371846	1.153465
C	2.446225	-0.375563	0.645553
H	2.761534	0.570741	0.213377
H	3.131028	-0.626054	1.459407
H	2.554540	-1.148657	-0.119864
C	0.703290	-1.795214	1.643732
H	-0.319271	-1.927844	1.996983
H	0.867109	-2.502865	0.826338
H	1.380093	-2.069359	2.456325
H	-0.612065	2.606572	1.933355
F	-2.720877	0.864215	2.198755
F	-2.145431	-1.261463	0.172497
H	0.214694	-0.446385	-0.975908

29

1 + 1,2,3,4,5a-*c*-C_5HF_5 TS

C	0.009704	-0.009452	0.010540
H	-0.731056	-0.330596	0.735728
H	-0.413091	-0.149575	-0.991899
H	0.873951	-0.672485	0.086891
C	0.426954	1.439651	0.150390
C	1.524450	1.800331	-0.830591
H	2.016103	2.747297	-0.612375
H	2.289074	1.020250	-0.857315
H	1.100502	1.879361	-1.839190
C	-0.456920	2.422681	0.607483
C	-1.886164	2.098900	0.990059
H	-2.020722	1.106858	1.409165
H	-2.508106	2.174716	0.089683
H	-2.271562	2.828003	1.705700
C	-0.320439	3.852224	0.122982
H	-0.754504	3.939919	-0.880579
H	-0.867946	4.535093	0.777063

H	0.710077	4.198863	0.059884
C	0.389274	2.840010	2.712545
C	1.587342	3.438822	2.394738
C	2.477900	2.450141	1.934899
C	1.838147	1.231689	1.964683
C	0.710965	1.385631	2.956564
F	-0.323761	0.510282	2.833737
H	1.111148	1.274279	3.971774
F	2.444326	0.061082	1.770309
F	3.659169	2.704892	1.390373
F	1.824385	4.741644	2.337706
F	-0.610280	3.451608	3.346991

29

1 + 1,2,3,4,5a-*c*-C_5HF_5

C	0.000517	0.001279	-0.000963
C	-1.415938	-0.227503	0.483733
C	-1.672265	0.714313	1.380830
C	-0.425699	1.567362	1.490638
C	-0.009037	1.536664	0.013157
F	1.203345	2.116263	-0.248884
H	-0.747858	1.973855	-0.656975
C	0.684797	0.743639	2.228358
C	0.137387	0.217512	3.560520
H	0.902457	-0.359260	4.084789
H	-0.743727	-0.414662	3.448215
H	-0.136242	1.062530	4.197094
C	1.884903	1.640970	2.563365
H	2.656360	1.049378	3.061290
H	1.564075	2.420214	3.257009
H	2.325761	2.124126	1.695824
C	0.994785	-0.395206	1.143739
C	2.439304	-0.395909	0.622971
H	2.752081	0.554522	0.199434
H	3.121097	-0.655522	1.435871
H	2.538370	-1.159218	-0.150874
C	0.692261	-1.821553	1.618420
H	-0.325721	-1.949394	1.987187
H	0.836633	-2.516507	0.787545
H	1.379550	-2.110657	2.416493
F	-0.655593	2.798268	2.029308
F	-2.704183	0.854310	2.194467
F	-2.119358	-1.294554	0.147497
F	0.266955	-0.591371	-1.199240

29

1 + 1,2,3,4,5b-*c*-C_5HF_5 TS

C	0.007365	-0.004356	0.006208
H	-0.642025	-0.340549	0.813476
H	-0.546964	-0.146721	-0.929329
H	0.875959	-0.663792	-0.026638
C	0.433828	1.445370	0.107246
C	1.516765	1.794958	-0.890693
H	2.005609	2.745947	-0.682712
H	2.284747	1.018444	-0.914545
H	1.084223	1.863903	-1.896346
C	-0.451262	2.429522	0.564631
C	-1.866868	2.079156	0.973295
H	-1.963071	1.127711	1.494764
H	-2.490074	2.013893	0.073221
H	-2.292588	2.857856	1.607879
C	-0.334458	3.853986	0.066389
H	-0.775078	3.932402	-0.935052
H	-0.879583	4.537761	0.721104
H	0.694664	4.204092	-0.004521
C	0.386348	2.849704	2.643595
C	1.590093	3.442174	2.360544
C	2.484503	2.448231	1.898504
C	1.833514	1.241411	1.895769
C	0.645728	1.371876	2.820302
F	1.009625	1.091799	4.126786
H	-0.193570	0.727438	2.582139
F	2.423847	0.063448	1.693456
F	3.666687	2.712457	1.363173
F	1.840694	4.741481	2.306505
F	-0.625499	3.452022	3.268492

29

1 + 1,2,3,4,5b-*c*-C_5HF_5

C	0.006113	0.001907	0.000078
C	-1.413676	-0.221191	0.477368
C	-1.670324	0.720927	1.373265
C	-0.420547	1.568236	1.489712
C	0.069344	1.530062	0.040839
F	-0.774628	2.140699	-0.842974
H	1.065230	1.942570	-0.107891
C	0.686832	0.745957	2.229340
C	0.153626	0.222792	3.566251
H	0.923122	-0.350979	4.087426
H	-0.726296	-0.411418	3.457704
H	-0.120601	1.068532	4.201507
C	1.881597	1.657890	2.539745
H	2.681936	1.082630	3.009528
H	1.569005	2.432803	3.241372
H	2.296523	2.155456	1.663354
C	0.997889	-0.395308	1.143783
C	2.435280	-0.374186	0.606109
H	2.724885	0.576319	0.158288
H	3.140835	-0.595856	1.409358
H	2.543885	-1.144976	-0.158469
C	0.710912	-1.821868	1.621406
H	-0.305403	-1.952714	1.993198
H	0.854450	-2.516617	0.790292
H	1.402602	-2.105826	2.417594
F	-0.638959	2.804486	2.020645
F	-2.691224	0.840189	2.204415
F	-2.107364	-1.302729	0.166961
F	0.283534	-0.581710	-1.200036

29

1 + 1,2,3,5a,5b-*c*-C_5HF_5 TS = **1** + 2,3,4,5a,5b-*c*-C_5HF_5 TS

C	0.022193	-0.008455	0.004578
H	-0.587084	-0.386272	0.820510
H	-0.558845	-0.109370	-0.920912
H	0.898525	-0.652282	-0.095550
C	0.437246	1.437202	0.166778
C	1.534468	1.847614	-0.787477
H	2.053024	2.757703	-0.485137
H	2.277649	1.055445	-0.896676
H	1.104379	2.043112	-1.778009
C	-0.454572	2.412856	0.638934
C	-1.881693	2.057693	1.006582
H	-2.010598	1.039825	1.360162
H	-2.503280	2.186619	0.112540
H	-2.271884	2.738846	1.765846
C	-0.360666	3.838075	0.124501
H	-0.808765	3.894404	-0.874624
H	-0.921473	4.515573	0.772973
H	0.658923	4.211945	0.046449
C	0.402369	2.882897	2.638393
C	1.636533	3.431115	2.358962
C	2.503331	2.386476	1.973713
C	1.869371	1.174885	2.040465
C	0.700695	1.424856	2.963420
F	1.067275	1.328675	4.277785
F	-0.333753	0.572486	2.843946
H	2.314488	0.202803	1.888240
F	3.698328	2.613990	1.444680
F	1.922360	4.722573	2.279220
F	-0.571498	3.535447	3.266375

29

1 + 1,2,3,5a,5b-*c*-C_5HF_5 = **1** + 2,3,4,5a,5b-*c*-C_5HF_5

C	-0.001634	0.000396	-0.006695
C	-1.405318	-0.221021	0.507865
C	-1.663539	0.708314	1.415737
C	-0.423852	1.578182	1.527521
C	0.000849	1.532939	0.051424
F	-0.871333	2.131470	-0.787666
F	1.196398	2.108436	-0.209966
C	0.695561	0.759297	2.249622
C	0.156633	0.232229	3.585631
H	0.927171	-0.337700	4.109109
H	-0.720838	-0.405192	3.477706
H	-0.119397	1.077604	4.220978
C	1.894801	1.659120	2.582768
H	2.666106	1.070128	3.083924

H	1.572876	2.440166	3.274036
H	2.339453	2.141396	1.716524
C	0.997208	-0.378211	1.156166
C	2.445522	-0.384001	0.648395
H	2.762964	0.562177	0.217755
H	3.128701	-0.636217	1.462873
H	2.551516	-1.156574	-0.117786
C	0.695565	-1.799867	1.643736
H	-0.329018	-1.929783	1.992167
H	0.860609	-2.507049	0.826323
H	1.367497	-2.075329	2.459713
F	-0.655351	2.808674	2.055429
F	-2.701546	0.853090	2.221425
F	-2.137039	-1.271325	0.159851
H	0.216852	-0.445491	-0.976753

29

1 + 1,2,4,5a,5b-*c*-C_5HF_5 TS = **1** + 1,3,4,5a,5b-*c*-C_5HF_5 TS

C	-0.005711	-0.007309	0.015617
H	-0.789885	-0.296899	0.706886
H	-0.378043	-0.165939	-1.003284
H	0.840796	-0.683393	0.153222
C	0.433086	1.438982	0.133561
C	1.500499	1.764784	-0.894062
H	1.980546	2.727535	-0.733632
H	2.272565	0.990995	-0.897855
H	1.048787	1.781189	-1.893080
C	-0.443298	2.440123	0.573212
C	-1.873284	2.151343	0.968073
H	-2.021542	1.175133	1.419121
H	-2.494365	2.203733	0.065212
H	-2.246989	2.909810	1.658434
C	-0.248029	3.861659	0.100566
H	-0.589041	3.950472	-0.938496
H	-0.834389	4.556798	0.704983
H	0.792683	4.185391	0.120961
C	0.366289	2.851527	2.770251
C	1.533787	3.478764	2.432102
C	2.463512	2.560941	1.889064
C	1.844541	1.332481	1.875792
C	0.722933	1.388464	2.909926
F	1.237906	1.123489	4.146181
F	-0.289318	0.519558	2.769916
F	2.474901	0.177206	1.661499
H	3.421425	2.810416	1.459561
F	1.716285	4.793191	2.441198
F	-0.657149	3.388094	3.428389

29

1 + 1,2,4,5a,5b-*c*-C_5HF_5 = **1** + 1,3,4,5a,5b-*c*-C_5HF_5

C	0.000965	-0.001677	0.000465
C	-1.419070	-0.239077	0.481882
C	-1.642771	0.720331	1.368010
C	-0.410817	1.589035	1.496182
C	0.020110	1.538013	0.019663
F	-0.850566	2.117125	-0.829361
F	1.213998	2.107153	-0.244014
C	0.699667	0.758228	2.224107
C	0.146828	0.229565	3.553283
H	0.907277	-0.355225	4.074917
H	-0.738424	-0.395436	3.435242
H	-0.121583	1.073543	4.193423
C	1.900567	1.652283	2.564558
H	2.667378	1.056843	3.064739
H	1.580198	2.432411	3.257262
H	2.349243	2.133987	1.700010
C	1.011559	-0.380797	1.136093
C	2.454417	-0.373643	0.608629
H	2.765235	0.574482	0.179190
H	3.141322	-0.626724	1.419148
H	2.553728	-1.139623	-0.162463
C	0.733895	-1.807845	1.623355
H	-0.272892	-1.942283	2.015774
H	0.869514	-2.503104	0.790843
H	1.444288	-2.086617	2.404706
F	-0.630108	2.821712	2.021949
F	-2.689206	0.908891	2.153678
H	-2.037789	-1.079323	0.206133

F	0.287741	-0.573556	-1.204207

29

1 + 1,2,3,4,5a,5b-*c*-C_5F_6 TS

C	0.010875	-0.008883	0.010766
H	-0.737440	-0.329886	0.728150
H	-0.402950	-0.151120	-0.994856
H	0.875239	-0.670683	0.095324
C	0.424637	1.440647	0.148114
C	1.521088	1.805050	-0.831468
H	2.017390	2.747859	-0.605823
H	2.281114	1.021140	-0.868441
H	1.093741	1.897258	-1.837344
C	-0.460567	2.425000	0.605778
C	-1.888288	2.102844	0.992242
H	-2.027031	1.107415	1.401698
H	-2.511961	2.188357	0.094215
H	-2.269033	2.827973	1.714315
C	-0.320820	3.853030	0.120186
H	-0.742474	3.936346	-0.888861
H	-0.877475	4.536245	0.765843
H	0.709887	4.200806	0.067107
C	0.395409	2.867213	2.707351
C	1.593340	3.454748	2.392240
C	2.489302	2.459647	1.929656
C	1.857915	1.242976	1.952259
C	0.716019	1.400375	2.942710
F	-0.305540	0.544023	2.805812
F	1.162361	1.209995	4.217041
F	2.449746	0.067494	1.771023
F	3.663665	2.727200	1.382752
F	1.839817	4.752596	2.324183
F	-0.605653	3.460475	3.348342

29

1 + 1,2,3,4,5a,5b-*c*-C_5F_6 TS

C	0.001619	0.001110	-0.000025
C	-1.413981	-0.225259	0.497071
C	-1.670538	0.716371	1.392907
C	-0.429006	1.581665	1.503478
C	0.005263	1.538946	0.028619
F	-0.863034	2.113124	-0.823782
F	1.199300	2.108446	-0.228060
C	0.687603	0.760005	2.232033
C	0.141577	0.230752	3.563739
H	0.908340	-0.345842	4.085104
H	-0.738898	-0.401813	3.451594
H	-0.131283	1.074633	4.202017
C	1.887998	1.656251	2.568523
H	2.656599	1.063068	3.068488
H	1.566766	2.435802	3.261497
H	2.335155	2.139213	1.704102
C	0.999058	-0.383270	1.144629
C	2.444249	-0.385608	0.626083
H	2.763927	0.563500	0.204807
H	3.122915	-0.647895	1.440444
H	2.543311	-1.148505	-0.148046
C	0.696819	-1.808314	1.624033
H	-0.320816	-1.935993	1.992916
H	0.842626	-2.505501	0.795379
H	1.384588	-2.093235	2.422784
F	-0.656583	2.814295	2.024902
F	-2.699219	0.856203	2.208160
F	-2.113501	-1.293591	0.162840
F	0.267077	-0.575712	-1.199945

Table S15. Cartesian coordinates for Diels-Alder transition states and product norbornenes formed from **1** + randomly substituted cyclopentadienes *c*-$C_5H_a(CH_3)_b(F)_c(CF_3)_d$ (a+b+c+d=6)

35
1 + 1-CH_3-2-F-4-CF_3-C_5H_3 TS

C	0.019785	-0.017530	0.066194
C	1.498277	0.163833	0.036962
F	1.887241	0.942048	-0.987358
F	1.972808	0.719897	1.165428
F	2.158240	-1.003878	-0.111583
C	-0.751101	-0.150647	-1.219078
C	-2.121400	-0.458484	-0.686413
C	-3.319449	-0.721738	-1.543867
H	-3.351116	-0.043191	-2.396572
H	-3.295216	-1.745205	-1.929928
H	-4.243338	-0.612331	-0.971825
C	-2.308135	1.673284	0.100964
C	-0.997055	1.958265	0.535233
C	-0.732784	2.033777	2.024083
H	-1.098356	1.158346	2.560462
H	0.332439	2.138714	2.229759
H	-1.246185	2.907655	2.445360
C	-0.152514	2.926510	-0.268171
H	-0.574489	3.936090	-0.177353
H	0.869763	2.964102	0.109500
H	-0.106631	2.692541	-1.332014
C	-2.823148	2.341839	-1.156558
H	-3.818967	1.978977	-1.415677
H	-2.906539	3.423104	-0.987799
H	-2.174067	2.208659	-2.023721
C	-3.393157	1.439074	1.129406
H	-3.680335	2.392862	1.590837
H	-4.290041	1.018882	0.668824
H	-3.084379	0.771339	1.933079
C	-1.886200	-1.070856	0.541332
C	-0.600904	-0.838445	1.011778
H	-0.209698	-1.132498	1.975518
F	-2.846226	-1.687100	1.244738
H	-0.691851	0.704598	-1.888093
H	-0.378575	-1.033474	-1.759227

35
1 + 1-CH_3-2-F-4-CF_3-C_5H_3

C	0.000347	0.029061	0.022224
C	0.713833	-1.033690	0.818254
F	1.897363	-1.371869	0.279982
F	0.953838	-0.658161	2.088011
F	-0.011026	-2.162802	0.882217
C	-0.095209	-0.278480	-1.482657
C	-1.005404	0.923521	-1.782633
C	-1.570056	1.040217	-3.185128
H	-0.770574	1.038358	-3.927668
H	-2.231120	0.196776	-3.396386
H	-2.152408	1.956671	-3.305950
C	-0.108045	2.123545	-1.263466
C	0.631432	1.484064	0.014926
C	0.350953	2.237551	1.322027
H	-0.710072	2.291756	1.562142
H	0.861293	1.748097	2.152993
H	0.734267	3.258710	1.255711
C	2.160715	1.431895	-0.133321
H	2.561384	2.443376	-0.226171
H	2.604872	0.989567	0.760748
H	2.500080	0.851973	-0.991270
C	0.863085	2.564675	-2.367452
H	0.302607	3.009093	-3.193071
H	1.548239	3.329640	-1.996330
H	1.461380	1.746774	-2.771878
C	-0.976947	3.343228	-0.931875
H	-0.361274	4.179167	-0.591254
H	-1.504700	3.674650	-1.830191
H	-1.724315	3.140758	-0.164392
C	-2.028482	0.691587	-0.694335
C	-1.474896	0.159855	0.385354
H	-1.916532	-0.016669	1.355070
F	-3.283952	1.121533	-0.836618
H	0.866681	-0.237390	-1.994615
H	-0.583974	-1.233511	-1.680452

35
1 + 1-CH_3-5a-F-3-CF_3-C_5H_3 TS

C	0.059347	-0.006581	-0.069150
H	0.419225	0.679535	-0.826393
C	-0.994239	-1.048991	-0.328691
C	-1.128660	-1.695781	1.023953
C	-2.165789	-2.730420	1.324559
H	-3.130327	-2.451379	0.898411
H	-1.884408	-3.701454	0.905748
H	-2.284681	-2.855669	2.403373
C	-1.925041	0.377082	1.901647
C	-1.211171	1.292706	1.108198
C	-0.122823	2.137426	1.746334
H	0.533955	1.578512	2.409254
H	0.495197	2.616296	0.983583
H	-0.588573	2.933118	2.340918
C	-1.928966	2.069853	0.019260
H	-2.426905	2.931791	0.480951
H	-1.218004	2.466656	-0.709672
H	-2.678381	1.494642	-0.514847
C	-3.406247	0.160367	1.682148
H	-3.766458	-0.685900	2.270128
H	-3.950756	1.047445	2.031916
H	-3.675639	-0.003485	0.641210
C	-1.505719	0.158822	3.337212
H	-1.845621	1.002673	3.952585
H	-1.962092	-0.746984	3.744001
H	-0.426224	0.082328	3.460032
C	0.141998	-1.607777	1.570748
C	0.869816	-0.614962	0.888248
C	2.253368	-0.205739	1.243818
F	3.160605	-1.137185	0.899580
F	2.615774	0.934802	0.638926
F	2.404678	-0.016833	2.571890
H	0.493128	-2.144458	2.443434
F	-2.166638	-0.636131	-0.917500
H	-0.555152	-1.791972	-1.011901

35
1 + 1-CH_3-5a-F-3-CF_3-C_5H_3

C	0.008420	0.080968	0.077191
H	1.097227	0.119768	0.036161
C	-0.728443	-0.326320	-1.209376
C	-2.138907	-0.267079	-0.586286
C	-3.288456	-0.670265	-1.489362
H	-3.286262	-0.078649	-2.406178
H	-3.204627	-1.724193	-1.765664
H	-4.251503	-0.527669	-0.992345
C	-2.185923	1.203621	0.008487
C	-0.671589	1.443022	0.463011
C	-0.509042	1.730172	1.960212
H	-0.956623	0.969111	2.597928
H	0.553785	1.785064	2.210575
H	-0.959075	2.693413	2.214160
C	0.034664	2.592918	-0.273813
H	-0.428922	3.550233	-0.023764
H	1.075119	2.639987	0.059286
H	0.033309	2.481052	-1.355253
C	-2.669262	2.209477	-1.047992
H	-3.712927	2.006430	-1.300470
H	-2.629167	3.223230	-0.642153
H	-2.087244	2.184629	-1.967061
C	-3.199139	1.274294	1.159711
H	-3.241031	2.284854	1.573472
H	-4.199394	1.037020	0.786316
H	-2.974320	0.586963	1.975019
C	-1.849956	-1.203444	0.573041
C	-0.584341	-1.008243	0.946068
C	0.154277	-1.750361	2.000175
F	1.165374	-2.463582	1.471019
F	0.707645	-0.933624	2.912789
F	-0.634690	-2.608162	2.659555
H	-2.557132	-1.894960	1.014932
F	-0.555950	0.528732	-2.281858
H	-0.461916	-1.326633	-1.555041

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1 + 2-CH_3-4-F-C_5H_4 TS

C	0.247012	0.094448	0.147918
C	0.411690	-0.662834	1.428938
F	1.339439	-1.633469	1.544116
C	-0.822605	-0.728855	2.063243
C	-1.611116	0.318254	1.553236
C	-2.964234	0.718360	2.062919
H	-3.211250	1.734719	1.751890
H	-3.735367	0.051536	1.667954
H	-3.016908	0.670994	3.153358
C	-0.871518	0.999361	0.587001
H	-1.266846	1.799610	-0.027773
H	-1.063534	-1.373744	2.897578
H	1.140537	0.573073	-0.240634
H	-0.133200	-0.606768	-0.607152
C	0.559366	2.117071	1.955804
C	1.368361	1.061817	2.410199
C	1.266368	0.585807	3.845619
H	0.238875	0.518234	4.198722
H	1.724780	-0.401311	3.951127
H	1.804607	1.272455	4.511481
C	2.775666	0.895644	1.870574
H	3.449180	1.581722	2.399824
H	3.141446	-0.118262	2.043612
H	2.872757	1.112244	0.807629
C	1.082016	3.092914	0.921165
H	0.275066	3.724900	0.543768
H	1.830968	3.754470	1.375649
H	1.557847	2.614231	0.065674
C	-0.436453	2.749875	2.901376
H	0.085556	3.389499	3.625289
H	-1.147491	3.376839	2.357627
H	-1.003384	2.013516	3.469765

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1 + 2-CH_3-4-F-C_5H_4

C	0.022912	0.054545	-0.118139
F	0.740181	-0.878016	0.605169
C	-0.094161	-0.198515	-1.621457
C	-1.011850	1.027013	-1.802846
H	-1.394723	1.222286	-2.806585
C	-0.095204	2.191897	-1.261553
C	0.667049	1.479060	-0.053350
C	0.443976	2.119742	1.320762
H	-0.610497	2.217311	1.576495
H	0.919946	1.501028	2.086537
H	0.900129	3.112146	1.366432
C	2.186281	1.365174	-0.245424
H	2.646406	2.356251	-0.250646
H	2.612515	0.802673	0.587275
H	2.473006	0.856515	-1.165503
C	0.835316	2.661713	-2.388145
H	0.237388	3.125638	-3.177543
H	1.543948	3.412083	-2.028787
H	1.406586	1.850632	-2.840344
C	-0.927413	3.406755	-0.840231
H	-0.282506	4.219586	-0.495245
H	-1.494515	3.778486	-1.699544
H	-1.635105	3.178259	-0.043673
C	-2.071389	0.726777	-0.747664
C	-1.436711	0.142443	0.270835
H	-1.830193	-0.137440	1.239926
C	-3.504231	1.125307	-0.871260
H	-3.599113	2.204963	-1.020090
H	-3.960238	0.642649	-1.740941
H	-4.071551	0.845019	0.017508
H	0.852850	-0.141564	-2.157025
H	-0.594819	-1.141371	-1.838316

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1 + 2-CH_3-5b-F-1-CF_3-C_5H_3 TS

C	0.070695	-0.027099	0.095476
H	0.893041	-0.354280	-0.529490
C	-1.031380	0.860495	-0.452851
C	-1.899915	0.958614	0.771619
C	-3.145555	1.764956	0.787092
F	-4.251671	1.038647	0.537002
F	-3.364893	2.356395	1.984917
F	-3.111664	2.746959	-0.128319

C	-0.039253	2.294845	1.647078
C	1.039264	1.612872	1.054262
C	1.985235	0.817453	1.936279
H	1.465557	0.195437	2.662128
H	2.623563	0.169510	1.330645
H	2.639520	1.503642	2.487639
C	1.769586	2.244739	-0.116979
H	2.447620	3.020339	0.258684
H	2.382584	1.505875	-0.638098
H	1.117709	2.718894	-0.848696
C	-0.481424	3.646537	1.137529
H	-1.439368	3.934836	1.570434
H	0.258584	4.400009	1.438832
H	-0.572261	3.705422	0.053303
C	-0.343528	2.036242	3.098296
H	0.454491	2.453928	3.726262
H	-1.287905	2.494920	3.391571
H	-0.390221	0.967796	3.321554
C	-1.709187	-0.186482	1.525007
C	-0.502793	-0.794523	1.100318
H	-0.055217	-1.659396	1.572250
C	-2.578947	-0.666346	2.646869
H	-2.027847	-1.332214	3.312398
H	-2.972095	0.168544	3.228867
H	-3.433586	-1.217015	2.244890
H	-0.718344	1.806173	-0.880948
F	-1.704201	0.190295	-1.479483

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1 + 2-CH_3-5b-F-1-CF_3-C_5H_3

C	0.021388	0.021849	-0.023782
H	0.781577	0.092818	0.754125
C	-1.413032	-0.186530	0.458610
C	-2.016881	-0.115395	-0.952390
C	-3.525167	-0.142047	-0.984131
F	-4.052605	1.006885	-0.540929
F	-4.008741	-0.333079	-2.228017
F	-4.034225	-1.119433	-0.215370
C	-1.260115	-1.329141	-1.648812
C	0.186772	-1.231541	-0.949479
C	1.346042	-1.030709	-1.930973
H	1.216525	-0.154726	-2.565205
H	2.274973	-0.902013	-1.367923
H	1.471465	-1.905042	-2.574659
C	0.548039	-2.457345	-0.095033
H	0.648974	-3.352861	-0.712392
H	1.514448	-2.281885	0.384544
H	-0.174130	-2.676260	0.691403
C	-1.963156	-2.671069	-1.386657
H	-2.927228	-2.693942	-1.898670
H	-1.359440	-3.486312	-1.791251
H	-2.145466	-2.875286	-0.332004
C	-1.207166	-1.157596	-3.172779
H	-0.648796	-1.983900	-3.619133
H	-2.216005	-1.178272	-3.588668
H	-0.729696	-0.227823	-3.478722
C	-1.380523	1.182256	-1.459890
C	-0.172108	1.245052	-0.898919
H	0.581737	1.996576	-1.095578
C	-1.998979	2.100671	-2.463305
H	-1.287559	2.874879	-2.753664
H	-2.310132	1.556034	-3.359088
H	-2.889702	2.582068	-2.053409
H	-1.600977	-1.132283	0.965245
F	-1.865057	0.808874	1.295782

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1 + 3-CH_3-5a-F-1-CF_3-C_5H_3 TS

C	0.048950	0.037110	0.045774
H	0.894531	-0.084421	0.713842
C	-1.349479	-0.342909	0.439077
C	-2.068793	-0.066370	-0.853019
C	-3.539462	-0.233305	-1.001456
F	-4.235120	0.762297	-0.408737
F	-3.905692	-0.229952	-2.296124
F	-3.988646	-1.372323	-0.458937
C	-0.889135	-1.841367	-1.912929
C	0.347861	-1.728126	-1.255932

C	1.546719	-1.195688	-2.018450
H	1.324053	-0.315419	-2.618374
H	2.361659	-0.945108	-1.334146
H	1.919190	-1.972606	-2.697934
C	0.766773	-2.772372	-0.238786
H	1.207196	-3.621274	-0.777277
H	1.540103	-2.384401	0.429134
H	-0.050788	-3.147388	0.368087
C	-1.814911	-3.003879	-1.621917
H	-2.784253	-2.856973	-2.099684
H	-1.376784	-3.917789	-2.044767
H	-1.984138	-3.171990	-0.561555
C	-1.007834	-1.318518	-3.326157
H	-0.446734	-1.970983	-4.008105
H	-2.048037	-1.303016	-3.653086
H	-0.601023	-0.313001	-3.438082
C	-1.387914	1.004569	-1.415064
C	-0.090224	1.079628	-0.871585
C	0.978397	2.043306	-1.293648
H	1.966345	1.680677	-1.006744
H	0.970974	2.199926	-2.375146
H	0.829722	3.017117	-0.819637
H	-1.768347	1.629907	-2.213996
F	-1.518862	-1.585225	0.997853
H	-1.703233	0.380894	1.187890

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1 + 3-CH_3-5a-F-1-CF_3-C_5H_3

C	0.064655	0.041256	-0.027756
H	0.205585	-0.800266	0.652473
C	-0.928455	1.119286	0.418985
C	-0.697280	1.994109	-0.830266
C	-1.396963	3.328539	-0.803951
F	-0.932525	4.095122	0.200019
F	-1.202663	4.024797	-1.939569
F	-2.719436	3.226764	-0.626039
C	-1.024273	1.012036	-2.030954
C	-0.471212	-0.375682	-1.443307
C	0.659661	-0.995859	-2.274485
H	1.487789	-0.310329	-2.452751
H	1.052655	-1.873863	-1.752572
H	0.286983	-1.334792	-3.244198
C	-1.545067	-1.466015	-1.299009
H	-1.923022	-1.765341	-2.279625
H	-1.091722	-2.350532	-0.842777
H	-2.387514	-1.164249	-0.681792
C	-2.525264	0.975443	-2.364910
H	-2.834660	1.937065	-2.779942
H	-2.707953	0.218591	-3.131266
H	-3.157204	0.762333	-1.506205
C	-0.309702	1.455958	-3.316044
H	-0.471075	0.717853	-4.105390
H	-0.721399	2.404433	-3.663930
H	0.764432	1.582503	-3.185111
C	0.813245	2.105982	-0.701286
C	1.269462	0.946916	-0.218039
C	2.675589	0.536953	0.064996
H	2.946011	-0.351328	-0.512800
H	3.375404	1.338335	-0.175903
H	2.792168	0.279888	1.121789
H	1.392346	2.971778	-0.997693
F	-2.226332	0.677007	0.578831
H	-0.642247	1.625381	1.340977

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1 + 3-CH_3-5b-F-4-CF_3-C_5H_3 TS

C	0.102943	-0.087645	-0.052104
C	1.330318	0.745646	-0.015981
F	1.288842	1.728884	-0.929776
F	1.518702	1.338915	1.186208
F	2.455622	0.044082	-0.250787
C	-0.745252	-0.200317	-1.289539
C	-1.835757	-1.113348	-0.760195
H	-2.641573	-1.456157	-1.398202
C	-2.853535	0.501933	0.188968
C	-1.798845	1.204958	0.799820
C	-1.510207	0.947638	2.254443
H	-1.442897	-0.120389	2.474411

H	-0.580603	1.425959	2.563136
H	-2.326366	1.345018	2.872178
C	-1.378482	2.567614	0.301091
H	-2.139552	3.303844	0.592392
H	-0.434133	2.875433	0.750153
H	-1.271426	2.631758	-0.781362
C	-3.580144	1.122238	-0.990692
H	-4.169307	0.372321	-1.523387
H	-4.280243	1.881562	-0.622325
H	-2.927984	1.613190	-1.710989
C	-3.794925	-0.316970	1.054332
H	-4.472600	0.352855	1.597505
H	-4.409437	-0.977012	0.437226
H	-3.272657	-0.929582	1.786323
C	-1.260596	-1.871581	0.250678
C	-0.073924	-1.239128	0.694894
C	0.789307	-1.704076	1.827979
H	1.163800	-0.862531	2.412615
H	0.239947	-2.376276	2.488620
H	1.656183	-2.243671	1.437325
H	-1.696318	-2.747431	0.713391
H	-1.072329	0.739842	-1.719331
F	-0.043045	-0.852297	-2.308212

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1 + 3-CH_3-5b-F-4-CF_3-C_5H_3

C	-0.039597	-0.024596	0.022268
C	0.576916	-1.136502	-0.790441
F	1.750815	-0.778580	-1.337367
F	0.811117	-2.241140	-0.053894
F	-0.217130	-1.512323	-1.801866
C	-0.068660	1.336567	-0.689684
C	-0.875650	2.020956	0.412095
H	-1.161151	3.055683	0.222698
C	0.107651	1.852932	1.620445
C	0.698227	0.375497	1.373675
C	0.366770	-0.604592	2.506909
H	-0.701913	-0.682993	2.701492
H	0.745681	-1.599447	2.266360
H	0.852777	-0.280493	3.430248
C	2.227818	0.359708	1.218992
H	2.692710	0.738042	2.131959
H	2.578071	-0.664333	1.074798
H	2.592722	0.953540	0.381533
C	1.170678	2.962506	1.576527
H	0.676910	3.930590	1.693823
H	1.883016	2.858926	2.398222
H	1.738962	2.993856	0.646952
C	-0.636491	2.017056	2.949553
H	0.044759	1.908942	3.797298
H	-1.065262	3.022122	2.999391
H	-1.448700	1.301382	3.069600
C	-2.005478	1.021404	0.568437
C	-1.527618	-0.202513	0.339283
C	-2.223583	-1.519748	0.455262
H	-1.692465	-2.188553	1.138235
H	-3.240204	-1.377504	0.824065
H	-2.271633	-2.021368	-0.513904
H	-3.009589	1.261342	0.893983
H	0.920860	1.754823	-0.869922
F	-0.712314	1.301556	-1.906357

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1 + 3-F-5a-CF_3-C_5H_4 TS

C	-0.045507	-0.117532	0.028814
H	0.169050	-0.477885	1.026747
C	1.009741	0.194175	-1.003374
C	0.139816	0.709972	-2.125564
H	0.541203	1.131451	-3.039651
C	-0.717976	2.507949	-0.975139
C	-0.737426	1.976036	0.332455
C	-2.069249	1.623528	0.970999
H	-2.748950	1.090914	0.309248
H	-1.924601	1.010863	1.863933
H	-2.571842	2.547574	1.283532
C	0.247629	2.451373	1.384575
H	-0.131207	3.383641	1.821979
H	0.327842	1.725937	2.197161

H	1.247334	2.650717	1.013139
C	0.190750	3.666326	-1.354355
H	0.624912	3.542971	-2.349754
H	-0.425254	4.572737	-1.388613
H	0.997522	3.851763	-0.654276
C	-2.027911	2.618633	-1.733609
H	-2.606365	3.461392	-1.334039
H	-1.841831	2.822251	-2.791904
H	-2.655539	1.733535	-1.663228
C	-1.009614	-0.085132	-2.062327
C	-1.099479	-0.568747	-0.761166
F	-2.165793	-1.219720	-0.279014
H	-1.775290	-0.175479	-2.818527
C	2.329974	0.840320	-0.635214
F	2.418330	2.155896	-0.848430
F	2.641530	0.616987	0.651222
F	3.316238	0.291174	-1.371390
H	1.340410	-0.795764	-1.351644

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1 + 3-F-5a-CF_3-C_5H_4

C	-0.018861	-0.027514	0.017153
H	0.311764	-0.451695	-0.930630
C	1.070253	0.352152	1.050645
C	0.028878	0.917185	2.058522
H	0.415680	1.317369	2.995691
C	-1.062699	-0.215384	2.242764
C	-1.043229	-0.917801	0.809568
C	-2.398782	-0.919323	0.091826
H	-2.815797	0.079389	-0.039097
H	-2.289511	-1.365858	-0.900458
H	-3.126141	-1.519269	0.644722
C	-0.563068	-2.375777	0.836541
H	-1.268729	-2.997175	1.393600
H	-0.519479	-2.759478	-0.186153
H	0.418707	-2.515063	1.281601
C	-0.766961	-1.161995	3.417317
H	-0.690959	-0.577551	4.338602
H	-1.600857	-1.857621	3.545568
H	0.137537	-1.748075	3.318729
C	-2.414429	0.427497	2.607554
H	-3.169455	-0.344561	2.772803
H	-2.307394	0.983035	3.544454
H	-2.795685	1.113307	1.854514
C	-0.605224	1.948049	1.116005
C	-0.636089	1.350157	-0.067366
F	-1.212519	1.781878	-1.191201
H	-1.054599	2.887680	1.400217
C	2.185590	-0.613694	1.420404
F	1.993661	-1.410343	2.480109
F	2.489610	-1.412375	0.382225
F	3.298576	0.089800	1.704664
H	1.639524	1.187848	0.643366

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1 + 4-CH_3-1-F-5b-CF_3-C_5H_3 TS

C	-0.066505	0.002547	-0.089831
C	-0.396792	1.412877	0.294459
H	0.281993	2.111364	-0.201322
H	-1.417842	1.670044	-0.003099
H	-0.326306	1.565933	1.372124
C	-0.559852	-1.200795	0.689475
C	0.098450	-2.288153	-0.118542
F	-0.085021	-3.581940	0.197732
C	2.051197	-1.857153	0.730104
C	2.074841	-0.450052	0.732934
C	2.876670	0.285763	-0.314257
H	2.748286	-0.132538	-1.311531
H	2.597678	1.341847	-0.349098
H	3.946641	0.235689	-0.073023
C	1.979347	0.300383	2.044129
H	2.876036	0.107423	2.646770
H	1.928091	1.376998	1.874106
H	1.122558	0.017937	2.658893
C	1.921169	-2.603058	2.044295
H	1.628965	-3.640806	1.877078
H	2.896048	-2.611381	2.547371
H	1.210951	-2.159911	2.741980

C	2.891948	-2.630972	-0.265643
H	3.937266	-2.650540	0.066287
H	2.547478	-3.666394	-0.331201
H	2.870156	-2.201588	-1.265362
C	0.228115	-1.841113	-1.426944
C	0.161612	-0.442062	-1.389156
H	0.375803	0.210956	-2.226042
H	0.479938	-2.462399	-2.274057
H	-0.298848	-1.197910	1.745720
C	-2.078409	-1.307008	0.675040
F	-2.629808	-1.270768	-0.538757
F	-2.483444	-2.441528	1.264475
F	-2.614133	-0.291177	1.381318

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1 + 4-CH_3-1-F-5b-CF_3-C_5H_3

C	0.057069	-0.033148	0.001522
C	0.945477	0.926871	-0.769455
H	1.676298	1.390827	-0.101733
H	1.494080	0.393940	-1.548905
H	0.366238	1.717218	-1.249631
C	-1.136901	-0.666904	-0.756928
C	-1.502031	-1.579595	0.420354
F	-2.526574	-2.470932	0.213617
C	-1.840078	-0.527123	1.531019
C	-0.720511	0.580003	1.249787
C	0.232461	0.804267	2.429251
H	0.725996	-0.109426	2.757623
H	1.006605	1.524191	2.150034
H	-0.306625	1.223341	3.282711
C	-1.305160	1.955038	0.895942
H	-1.935750	2.322984	1.708301
H	-0.496060	2.676379	0.761185
H	-1.903685	1.957191	-0.016395
C	-3.283177	-0.034647	1.345038
H	-3.967652	-0.874926	1.472408
H	-3.528996	0.714099	2.101118
H	-3.480401	0.402624	0.366246
C	-1.774918	-1.173911	2.918893
H	-2.033838	-0.448733	3.694154
H	-2.503081	-1.987867	2.970996
H	-0.793166	-1.583854	3.151924
C	-0.170878	-2.219402	0.745449
C	0.752735	-1.293726	0.510726
H	1.816322	-1.357381	0.703978
H	-0.061407	-3.205477	1.175299
H	-1.924004	0.057168	-0.970740
C	-0.847914	-1.298784	-2.100537
F	0.222814	-2.096957	-2.154975
F	-1.896827	-2.014635	-2.529312
F	-0.642629	-0.325944	-3.015105

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1 + 4-CH_3-3-F-5b-CF_3-C_5H_3 TS

C	-0.190603	0.151545	-0.034302
C	-0.575081	1.020620	1.120457
H	-0.537427	0.468216	2.059958
H	0.095358	1.880660	1.188806
H	-1.593681	1.403006	1.002794
C	-0.601699	-1.288708	-0.213859
C	0.107368	-1.631474	-1.507354
H	0.019419	-2.611504	-1.961130
C	2.005713	-1.784073	-0.542425
C	1.992164	-0.675460	0.329408
C	2.743789	0.576731	-0.051212
H	2.567156	0.877398	-1.084652
H	2.466780	1.412886	0.594786
H	3.824866	0.418057	0.056940
C	1.880346	-0.885722	1.822442
H	2.803529	-1.342363	2.202394
H	1.752052	0.065185	2.342167
H	1.061227	-1.543956	2.118474
C	1.912313	-3.183544	0.038280
H	1.702518	-3.916074	-0.744632
H	2.872565	-3.459011	0.491451
H	1.154397	-3.296197	0.813256
C	2.901056	-1.747392	-1.766675
H	3.948451	-1.879887	-1.468843

H	2.648826	-2.558934	-2.454356
H	2.830318	-0.809089	-2.313908
C	0.201818	-0.443422	-2.236241
C	0.043045	0.597884	-1.323739
F	0.247253	1.887740	-1.618321
H	0.496506	-0.333907	-3.269545
H	-0.339193	-1.928064	0.626878
C	-2.109681	-1.447233	-0.332887
F	-2.703454	-1.135584	0.836295
F	-2.683334	-0.693427	-1.271847
F	-2.431716	-2.726606	-0.597793

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1 + 4-CH_3-3-F-5b-CF_3-C_5H_3

C	-0.017600	0.058108	0.086944
C	0.711617	-0.986431	0.910934
H	1.689404	-1.210366	0.482064
H	0.850514	-0.640917	1.937813
H	0.137546	-1.914529	0.947432
C	-0.204939	-0.195315	-1.423898
C	-1.117935	1.026368	-1.640324
H	-1.522065	1.155752	-2.644194
C	-0.137168	2.178460	-1.209312
C	0.626198	1.512976	0.034593
C	0.404677	2.244270	1.363954
H	-0.648370	2.341853	1.628082
H	0.902759	1.704684	2.173862
H	0.837050	3.247223	1.327561
C	2.144914	1.414315	-0.165146
H	2.577502	2.407548	-0.304975
H	2.608098	0.981923	0.724669
H	2.435442	0.801080	-1.020035
C	0.781228	2.537113	-2.387710
H	0.173264	2.928975	-3.207410
H	1.493087	3.317647	-2.109131
H	1.351995	1.693722	-2.777512
C	-0.913316	3.452862	-0.862110
H	-0.231984	4.257852	-0.574598
H	-1.468322	3.791765	-1.741954
H	-1.626835	3.307193	-0.052343
C	-2.145659	0.839082	-0.531388
C	-1.469050	0.282660	0.460444
F	-1.887578	0.021816	1.700339
H	-3.164922	1.194250	-0.526561
H	0.735450	-0.107833	-1.970041
C	-0.732264	-1.552976	-1.829617
F	0.262595	-2.463029	-1.774510
F	-1.727926	-2.042448	-1.083630
F	-1.167478	-1.533351	-3.102270

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1 + 4-F-2-CF_3-C_5H_4 TS

C	0.005037	-0.135715	-0.122441
F	0.902913	-1.127947	-0.024570
C	-0.098776	0.692112	-1.364571
C	-1.171788	1.642119	-0.902035
H	-1.538634	2.471539	-1.492430
C	0.243961	2.667855	0.472125
C	0.958414	1.570865	0.985695
C	0.710062	1.106110	2.404945
H	-0.346450	1.090940	2.668254
H	1.113758	0.101593	2.554957
H	1.217669	1.775720	3.110774
C	2.381510	1.308596	0.537319
H	3.053943	2.007097	1.051132
H	2.694133	0.297579	0.802451
H	2.542333	1.440752	-0.532025
C	0.895275	3.590369	-0.539844
H	0.152729	4.245113	-1.001070
H	1.623727	4.233519	-0.030341
H	1.430868	3.074200	-1.335370
C	-0.739085	3.404266	1.357403
H	-0.190508	4.046096	2.058462
H	-1.394307	4.045909	0.764626
H	-1.365952	2.741015	1.950165
C	-1.946582	0.930831	0.011530
C	-1.232608	-0.173215	0.499552
H	-1.525490	-0.836486	1.300682

C	-3.281727	1.349647	0.518295
F	-4.263526	0.550538	0.066826
F	-3.356590	1.307552	1.863697
F	-3.591772	2.599376	0.143079
H	0.825588	1.135332	-1.719467
H	-0.513717	0.057126	-2.159908

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1 + 4-F-2-CF_3-C_5H_4

C	-0.024415	0.027870	-0.066166
F	0.370077	-0.597315	1.094509
C	1.064153	0.272387	-1.114831
C	0.043463	0.856182	-2.116985
H	0.414340	1.146148	-3.100134
C	-0.555200	2.061324	-1.292378
C	-0.601263	1.460512	0.186011
C	-1.999026	1.382770	0.810441
H	-2.718192	0.855899	0.183786
H	-1.936496	0.857799	1.767529
H	-2.391768	2.383296	1.006637
C	0.295863	2.193469	1.193145
H	-0.057538	3.216553	1.340086
H	0.251266	1.682037	2.156197
H	1.342379	2.238567	0.892519
C	0.381512	3.268633	-1.440847
H	0.369194	3.604506	-2.481054
H	0.044675	4.103913	-0.822623
H	1.416208	3.051739	-1.175177
C	-1.921900	2.495338	-1.827650
H	-2.302962	3.346648	-1.257353
H	-1.826914	2.807771	-2.870994
H	-2.668112	1.703066	-1.791066
C	-0.969523	-0.276823	-2.106575
C	-1.023158	-0.773753	-0.873688
H	-1.677114	-1.540964	-0.481382
C	-1.755738	-0.727439	-3.284110
F	-0.948344	-1.219140	-4.241275
F	-2.632187	-1.688909	-2.970044
F	-2.447492	0.274446	-3.854711
H	1.833218	0.972896	-0.794371
H	1.517479	-0.655350	-1.461994

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1 + 5a-CH_3-2-F-3-CF_3-C_5H_3 TS

C	0.043498	-0.020646	0.035228
H	0.268145	-1.083097	0.033021
C	-0.827834	0.625622	1.098272
C	-0.774463	2.052931	0.623916
H	-1.359643	2.869639	1.026773
C	-1.779899	1.442571	-1.466472
C	-1.274608	0.132401	-1.611573
C	-0.289540	-0.145246	-2.738046
H	0.457542	0.632539	-2.870122
H	0.231983	-1.091534	-2.576760
H	-0.842399	-0.231638	-3.681363
C	-2.170755	-1.082940	-1.423059
H	-2.728688	-1.259562	-2.350202
H	-1.566538	-1.976337	-1.244245
H	-2.892007	-1.006403	-0.616613
C	-3.239279	1.717531	-1.163999
H	-3.368848	2.560007	-0.480682
H	-3.727590	1.999270	-2.105590
H	-3.787322	0.864404	-0.773380
C	-1.173269	2.560558	-2.284921
H	-1.505354	2.466730	-3.327511
H	-1.504455	3.534268	-1.916721
H	-0.083793	2.555869	-2.297309
C	0.485646	2.191147	0.078620
C	1.023893	0.947110	-0.256410
C	2.336725	0.728066	-0.912325
F	2.498931	-0.554451	-1.275237
F	2.503762	1.475607	-2.022316
F	3.362205	1.039138	-0.101279
F	1.060457	3.353817	-0.234368
C	-2.150396	0.041037	1.567265
H	-2.983339	0.288707	0.919462
H	-2.082963	-1.045331	1.657978
H	-2.380298	0.441137	2.557177

H	-0.158464	0.592848	1.975045

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1 + 5a-CH_3-2-F-3-CF_3-C_5H_3

C	-0.014518	-0.004947	0.019130
H	0.434460	-0.858740	-0.492429
C	-0.142909	1.315321	-0.796510
C	-0.841356	2.045690	0.385226
H	-1.180256	3.071403	0.232740
C	0.127908	1.860306	1.616528
C	0.740374	0.411932	1.335313
C	0.488669	-0.590156	2.470023
H	-0.559951	-0.676649	2.748847
H	0.829276	-1.583390	2.166658
H	1.053572	-0.303476	3.361336
C	2.260321	0.393207	1.105788
H	2.788273	0.767035	1.986651
H	2.581238	-0.640138	0.949469
H	2.592813	0.967849	0.245828
C	1.167780	2.988061	1.694182
H	0.654519	3.949692	1.779335
H	1.781608	2.867741	2.590981
H	1.841118	3.046236	0.844363
C	-0.674936	1.963018	2.924325
H	-0.023946	1.819435	3.789897
H	-1.113958	2.961809	3.003714
H	-1.487304	1.239936	2.995821
C	-1.949884	1.045297	0.594188
C	-1.488519	-0.184369	0.378820
C	-2.209002	-1.475832	0.432766
F	-1.557741	-2.395851	1.168279
F	-3.439691	-1.355893	0.941286
F	-2.337379	-2.012786	-0.797514
F	-3.156279	1.413654	1.004247
C	1.043156	1.946385	-1.518017
H	1.832015	2.339284	-0.888272
H	1.488398	1.210131	-2.192835
H	0.678312	2.772890	-2.133146
H	-0.891894	1.138089	-1.571665

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1 + 5a-CH_3-3-F-2-CF_3-C_5H_3 TS

C	-0.078519	-0.063284	-0.292480
H	0.497337	-0.879923	-0.708708
C	-0.018433	1.368496	-0.752335
C	-0.876440	2.009896	0.324381
H	-1.093135	3.073888	0.339742
C	0.453878	1.829049	1.959287
C	0.947845	0.516761	1.795766
C	0.339506	-0.605453	2.607111
H	-0.749762	-0.592671	2.628680
H	0.660183	-1.577601	2.225711
H	0.680934	-0.525427	3.647830
C	2.402576	0.234215	1.478225
H	2.896734	-0.060459	2.412782
H	2.520034	-0.602311	0.785480
H	2.953581	1.087143	1.091344
C	1.357856	3.039494	1.776748
H	0.759084	3.939594	1.613984
H	1.925639	3.200830	2.700697
H	2.071114	2.966821	0.962857
C	-0.520233	2.101830	3.096396
H	0.040663	2.173975	4.036167
H	-1.035957	3.053606	2.949388
H	-1.272011	1.328155	3.225959
C	-1.861631	1.046341	0.613638
C	-1.335319	-0.198045	0.261245
F	-1.916237	-1.359725	0.566516
C	-3.167586	1.268176	1.282229
F	-3.317296	2.547981	1.659767
F	-4.201727	0.973260	0.476167
F	-3.331514	0.510297	2.385644
C	1.304416	1.948382	-1.226222
H	2.140804	1.688272	-0.587831
H	1.523418	1.556739	-2.221970
H	1.244044	3.036065	-1.305471
H	-0.694666	1.415226	-1.623185

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1 + 5a-CH_3-3-F-2-CF_3-C_5H_3

C	0.023783	-0.028335	0.112912
H	-0.842253	0.556578	0.426073
C	0.027483	-1.555821	0.403210
C	1.393805	-1.748635	-0.318851
H	1.782605	-2.767449	-0.374211
C	2.367054	-0.738219	0.393789
C	1.400188	0.502337	0.672965
C	1.796296	1.790408	-0.068231
H	1.874441	1.666047	-1.148164
H	1.046846	2.564241	0.121845
H	2.756292	2.165309	0.294378
C	1.292870	0.906386	2.150918
H	2.242672	1.327073	2.492113
H	0.534930	1.686831	2.259737
H	1.033921	0.097037	2.826825
C	2.968112	-1.378287	1.655689
H	3.630263	-2.195038	1.356233
H	3.574873	-0.653601	2.204406
H	2.235645	-1.792203	2.343133
C	3.567606	-0.390697	-0.496754
H	4.250106	0.280833	0.031430
H	4.120942	-1.300995	-0.741058
H	3.288499	0.083032	-1.436161
C	1.015786	-1.139787	-1.668323
C	0.208295	-0.121682	-1.380611
F	-0.328965	0.764439	-2.208439
C	1.458996	-1.635811	-2.990165
F	2.790350	-1.824587	-3.046174
F	0.905917	-2.833002	-3.271271
F	1.130686	-0.806117	-3.986044
C	-0.234436	-2.088508	1.807839
H	0.324958	-1.620616	2.608729
H	-1.295484	-1.961569	2.037335
H	-0.022057	-3.160882	1.832651
H	-0.733606	-2.019569	-0.228361

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1 + 5b-CH_3-1-F-5a-CF_3-C_5H_3 TS

C	-0.011139	0.119089	-0.068635
H	0.234433	-0.447906	-0.958761
C	1.033083	0.410507	1.004126
C	0.086984	1.080628	1.982321
F	0.530106	1.457475	3.192368
C	-1.411534	-0.673193	2.298564
C	-1.321409	-1.282063	1.023648
C	-2.511673	-1.191010	0.080781
H	-2.980386	-0.211304	0.055557
H	-2.217710	-1.454873	-0.938785
H	-3.273269	-1.914002	0.398908
C	-0.641087	-2.626531	0.826559
H	-1.382503	-3.413210	1.013521
H	-0.307814	-2.743462	-0.207451
H	0.205060	-2.817801	1.474830
C	-0.916731	-1.339524	3.571728
H	-0.300831	-0.667047	4.174547
H	-1.795295	-1.591860	4.175043
H	-0.363123	-2.257840	3.406759
C	-2.635182	0.165705	2.618744
H	-3.477325	-0.503915	2.835709
H	-2.457383	0.769462	3.513056
H	-2.946635	0.826586	1.814382
C	-0.792374	1.838281	1.214039
C	-0.863249	1.231986	-0.043333
H	-1.571620	1.488322	-0.818327
H	-1.405030	2.645692	1.587579
C	1.942930	-0.725074	1.479703
F	1.485732	-1.432278	2.511435
F	2.183803	-1.581492	0.469769
F	3.144164	-0.272484	1.881600
C	2.019810	1.488956	0.442967
H	1.461183	2.265930	-0.066741
H	2.598414	1.926190	1.256277
H	2.712742	1.024280	-0.260869

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1 + 5b-CH_3-1-F-5a-CF_3-C_5H_3

C	-0.012166	-0.025431	0.059827

H	-0.333752	0.994688	0.271848
C	-0.815961	-1.157192	0.789915
C	0.069591	-2.235232	0.095587
F	-0.246022	-3.539988	0.387288
C	1.595073	-1.879186	0.363775
C	1.515091	-0.282597	0.367308
C	2.379674	0.373820	-0.722072
H	2.207778	-0.032580	-1.716862
H	2.168741	1.446910	-0.756049
H	3.440783	0.255887	-0.487691
C	1.945626	0.399870	1.674841
H	2.992658	0.171567	1.890911
H	1.866559	1.482512	1.543894
H	1.361108	0.135762	2.549572
C	2.197632	-2.536778	1.628221
H	1.676534	-3.470860	1.848148
H	3.242796	-2.786817	1.436558
H	2.176311	-1.921398	2.517947
C	2.440483	-2.468368	-0.786906
H	3.488301	-2.191081	-0.656091
H	2.381677	-3.559978	-0.740728
H	2.133760	-2.153507	-1.781227
C	-0.181727	-1.838552	-1.351561
C	-0.214618	-0.510412	-1.374952
H	-0.295409	0.132450	-2.241083
H	-0.223994	-2.542345	-2.171450
C	-0.898486	-1.137468	2.324982
F	0.160113	-1.579266	3.006047
F	-1.139562	0.119772	2.751723
F	-1.918052	-1.894509	2.768169
C	-2.311349	-1.185499	0.378403
H	-2.453801	-0.885683	-0.651840
H	-2.718033	-2.188749	0.510508
H	-2.883278	-0.507308	1.013516

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1 + 5b-CH_3-3-CF_3-C_5H_3 TS

C	-0.087476	0.038225	-0.022532
H	-0.392837	-0.096733	-1.054339
C	0.840697	1.139307	0.434107
C	0.916923	0.786975	1.900169
H	1.564727	1.304072	2.599038
C	2.090686	-1.087544	1.403740
C	1.482625	-1.486283	0.197483
C	0.630378	-2.739061	0.169899
H	-0.054789	-2.811866	1.012462
H	0.039733	-2.787706	-0.747401
H	1.276702	-3.625687	0.196677
C	2.206620	-1.271786	-1.118057
H	2.994426	-2.027945	-1.226809
H	1.523957	-1.394480	-1.961953
H	2.686520	-0.298468	-1.210098
C	3.464040	-0.447795	1.387809
H	3.709810	-0.031368	2.366810
H	4.222309	-1.207066	1.156295
H	3.573230	0.345395	0.648561
C	1.831458	-1.890632	2.659485
H	2.380033	-2.840613	2.616020
H	2.173619	-1.349238	3.544583
H	0.777283	-2.128830	2.795870
C	-0.290864	0.197873	2.247088
C	-0.906942	-0.249099	1.066620
C	-2.171506	-1.027249	1.019232
F	-3.251167	-0.255326	1.242810
F	-2.358085	-1.619189	-0.171100
F	-2.213438	-1.999833	1.954255
H	-0.639708	-0.009830	3.249901
H	1.804661	1.128249	-0.067068
C	0.213851	2.530266	0.212089
H	-0.764622	2.594682	0.690059
H	0.859116	3.305448	0.630330
H	0.096340	2.727374	-0.855477

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1 + 5b-CH_3-3-CF_3-C_5H_3

C	-0.111972	0.049481	-0.038778
H	0.243664	-0.405722	-0.965198
C	0.950661	0.418399	1.024628

C	-0.103341	1.053486	1.965244
H	0.262320	1.509902	2.886645
C	-1.070478	-0.161856	2.219987
C	-1.075842	-0.880402	0.790066
C	-2.464122	-0.981634	0.149602
H	-2.968309	-0.020135	0.064139
H	-2.375970	-1.395949	-0.858314
H	-3.106330	-1.650353	0.729167
C	-0.502244	-2.305699	0.806107
H	-1.111523	-2.966001	1.428053
H	-0.517576	-2.708872	-0.209981
H	0.524616	-2.360571	1.167830
C	-0.504057	-1.032983	3.350762
H	-0.503845	-0.460194	4.282096
H	-1.125572	-1.917406	3.511721
H	0.516497	-1.371150	3.170789
C	-2.448682	0.318197	2.690957
H	-3.114173	-0.528243	2.879713
H	-2.340795	0.867398	3.631144
H	-2.938291	0.976960	1.974323
C	-0.800246	1.995481	1.001437
C	-0.793653	1.397298	-0.188061
C	-1.327008	1.945230	-1.458954
F	-0.331621	2.188189	-2.334905
F	-2.169121	1.098247	-2.078140
F	-1.984574	3.099821	-1.282620
H	-1.262665	2.943042	1.245038
H	1.379517	-0.478823	1.472429
C	2.092315	1.313630	0.564873
H	1.732446	2.224301	0.084069
H	2.716894	1.600134	1.414594
H	2.726262	0.782610	-0.149148