SUPPORTING INFORMATION

HIGH-YIELD THERMOLYTIC CONVERSION OF IMIDAZOLIUM SALTS INTO ARDUENGO CARBENE ADDUCTS WITH BF3 AND PF5

Chong Tian,[†] Wanli Nie,[†] Maxim V. Borzov,*[,†] and Pengfei Su,[‡]

[†] Key Laboratory of Synthetic and Natural Chemistry of the Ministry of Education, College of Chemistry and Material Science, the North-West University, Taibai Bei avenue 229, Xi'an 710069, P. R. of China

[‡] Xi'an Modern Chemistry Research Institute, East Zhangba road 168, Xi'an 710065, P. R. of China

Table of Contents:

- Views of the NMR Spectra for **2**, **4**, and **12**. p. S2-S7
- IR Spectral Data for **2**, **4**, and **12** and Comparison with Computationally Predicted Ones (for **2** and **4**). p. S8-S11
- Optimized Geometries. p. S12-S20
- Energies and Thermochemistry Computation Results. p. S21-S26
- Computed Vibrational Frequencies. p. S27-S32
- Computed NMR Spectral Parameters for the Stationary Conformations of **2** and **4**. p. S33-S35
- Modeling of **1** → **8a** + C_2H_4 + HF + BF_3 Conversion. p. S36
- Calculation of the Thermodynamic and Kinetic Functions. p. S37
- Additional Thermochemical Plots. p. S38-40
- Intrinsic Reaction Coordinate Path Following for **1** → **2** + HF Conversion. p. S41
- References. p. S42

Views of the NMR Spectra

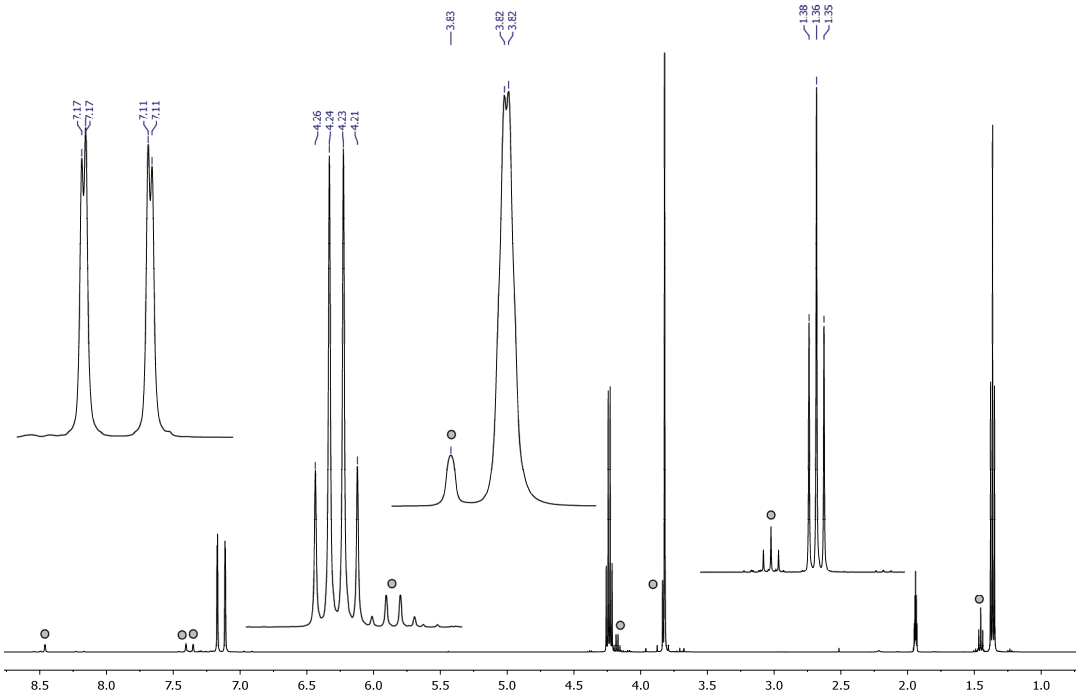


Figure 1. ^{1}H NMR spectrum of **2** [the crude product is chosen to demonstrate the residual signals of **1** (o-labeled)]. Far ^{5}J(H6–F) or through space SSCC (0.7 Hz) is also visible.

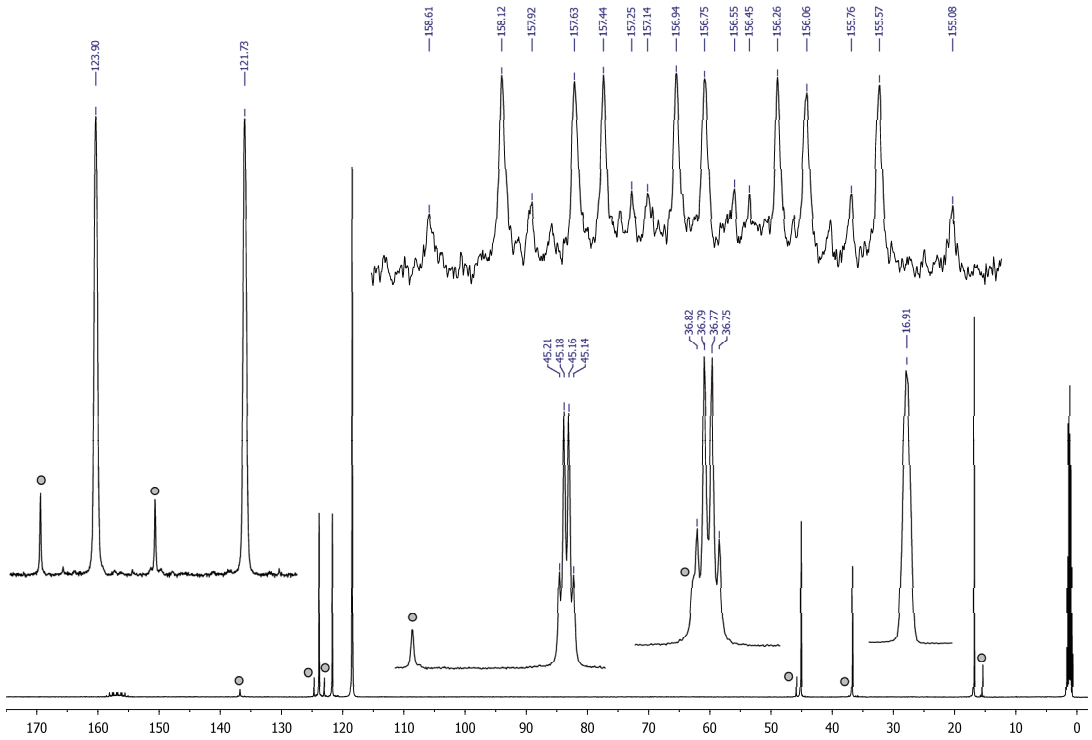


Figure 2. ^{13}C{^{1}H} NMR spectrum of **2** [the crude product is chosen to demonstrate the residual signals of **1** (o-labeled)]. Far ^{4}J(C4–F) and ^{4}J(C6–F) SSCC-s (both 2.8 Hz) are also visible.

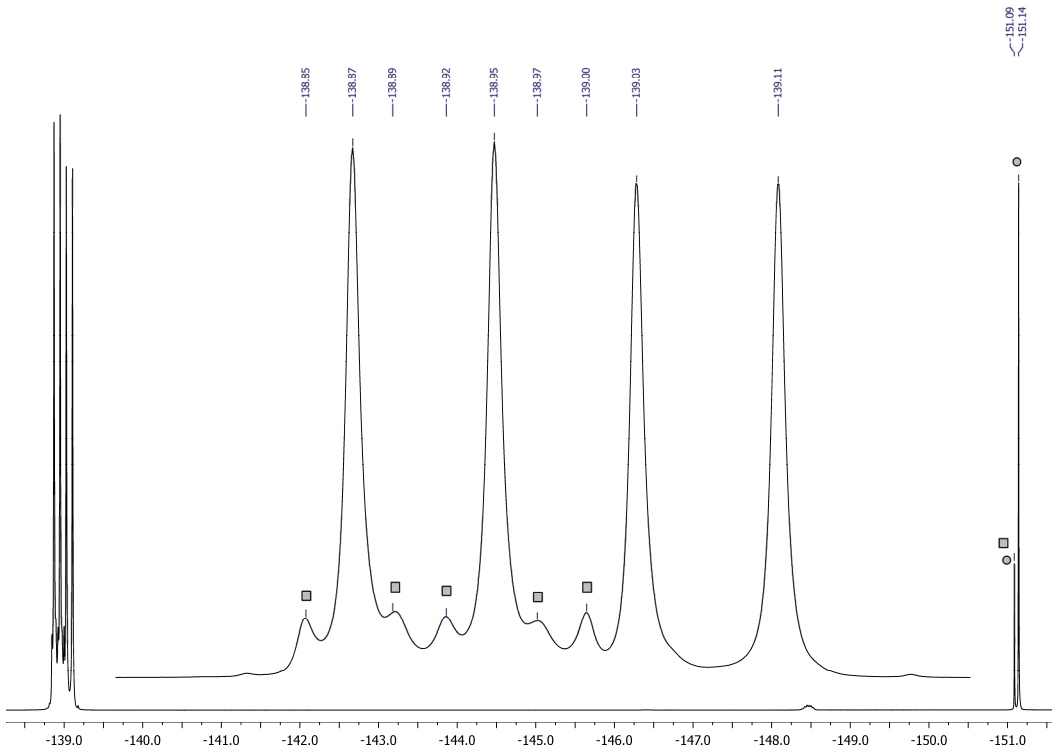


Figure 3. ^{19}F NMR spectrum of **2** [the crude product is chosen to demonstrate the residual signals of **1** (o-labeled)]. □-Labeled signals relate to ^{10}B-containing molecules. The 2nd and the 5th components of the $^{10}BF_3$ 1:1:1:1:1:1:1 septet overlap with the 1st and 2nd components of the $^{11}BF_3$ quartet what results in the increase of the intensity of the latter.

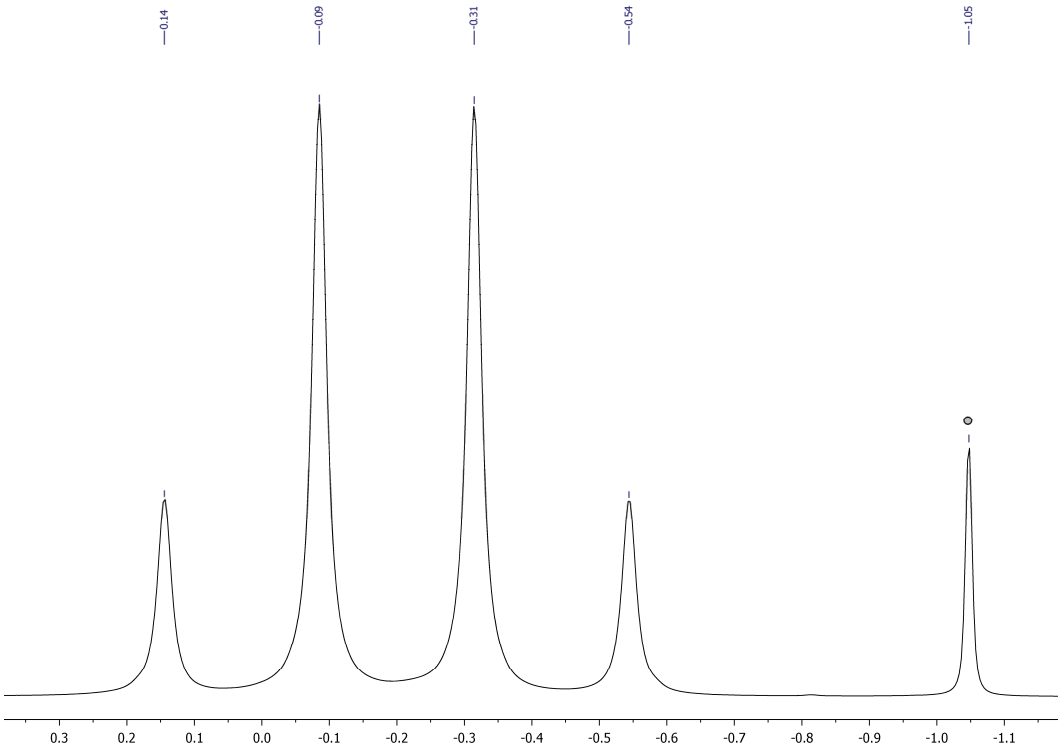


Figure 4. ^{11}B NMR spectrum of **2** [the crude product is chosen to demonstrate the residual signals of **1** (BF_4^-, o-labeled)].

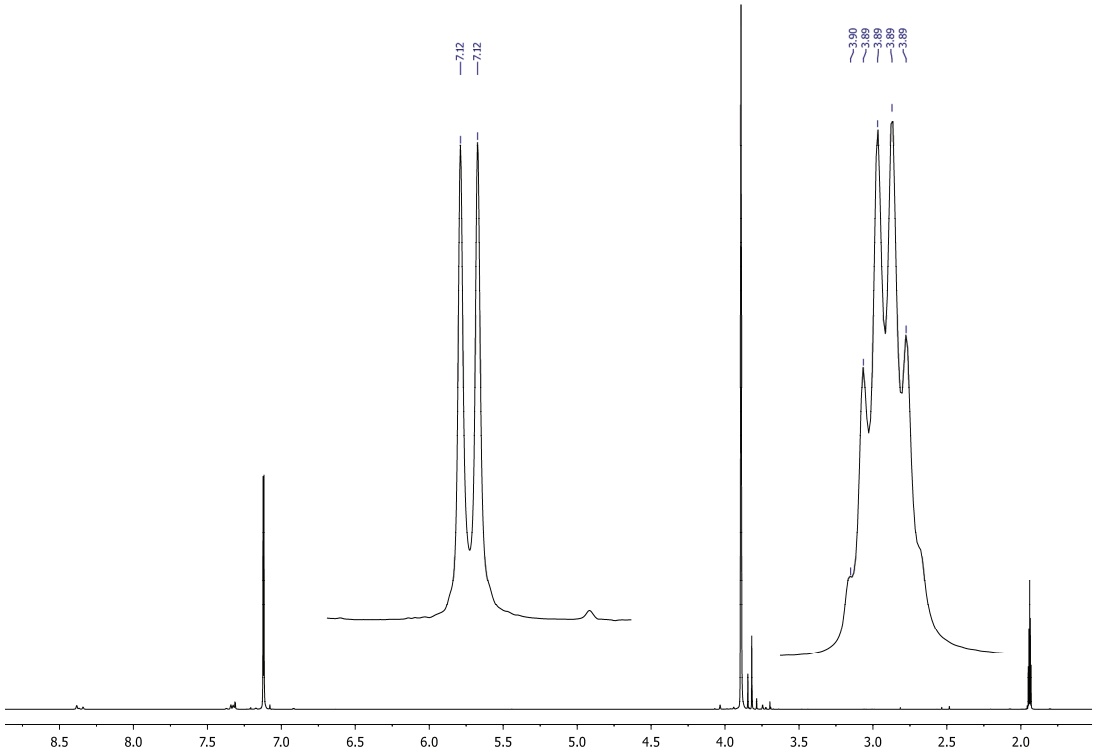


Figure 5. ^{1}H NMR (CD_3CN, 25 °C) spectrum of **4**. Far ^{4}J(P–H) and $^{5}J(F_{cis}–H)$ SSCC-s for the methyl group protons (both equal 1.0 Hz) are also observed.

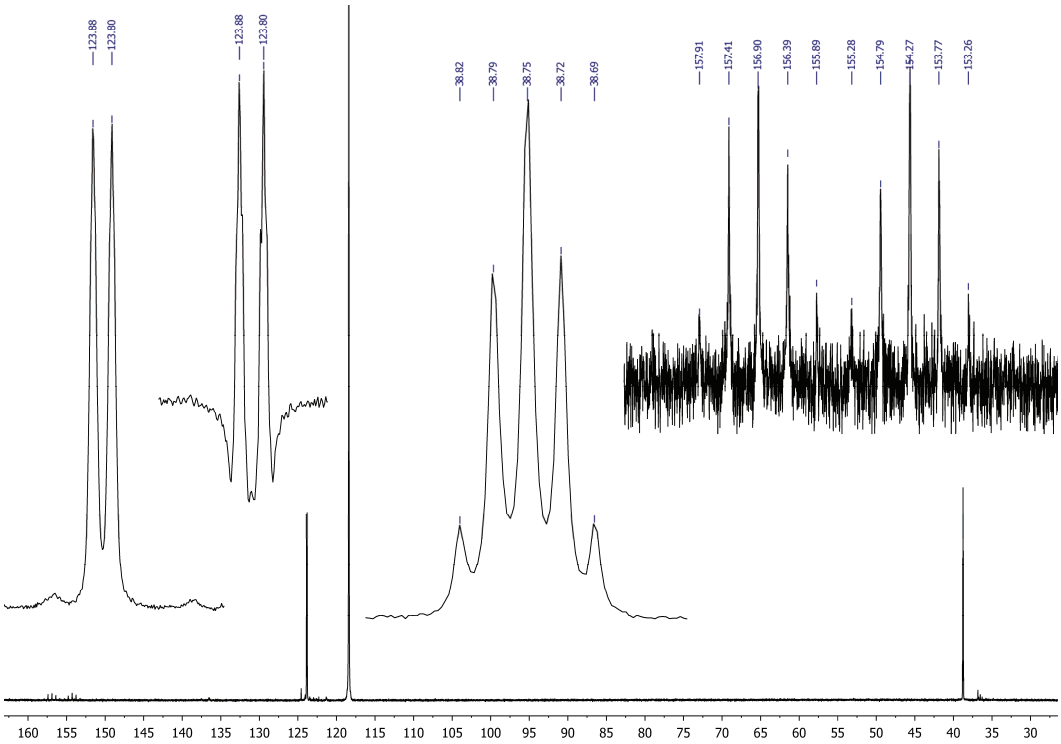


Figure 6. $^{13}C\{^{1}H\}$ NMR spectrum of **4**. Far ^{4}J(C4–F) and $^{4}J(F_{cis}–C2)$ SSCC-s (4.3 and 1.3 Hz; the latter develops in the sine-apodized spectrum) are visible.

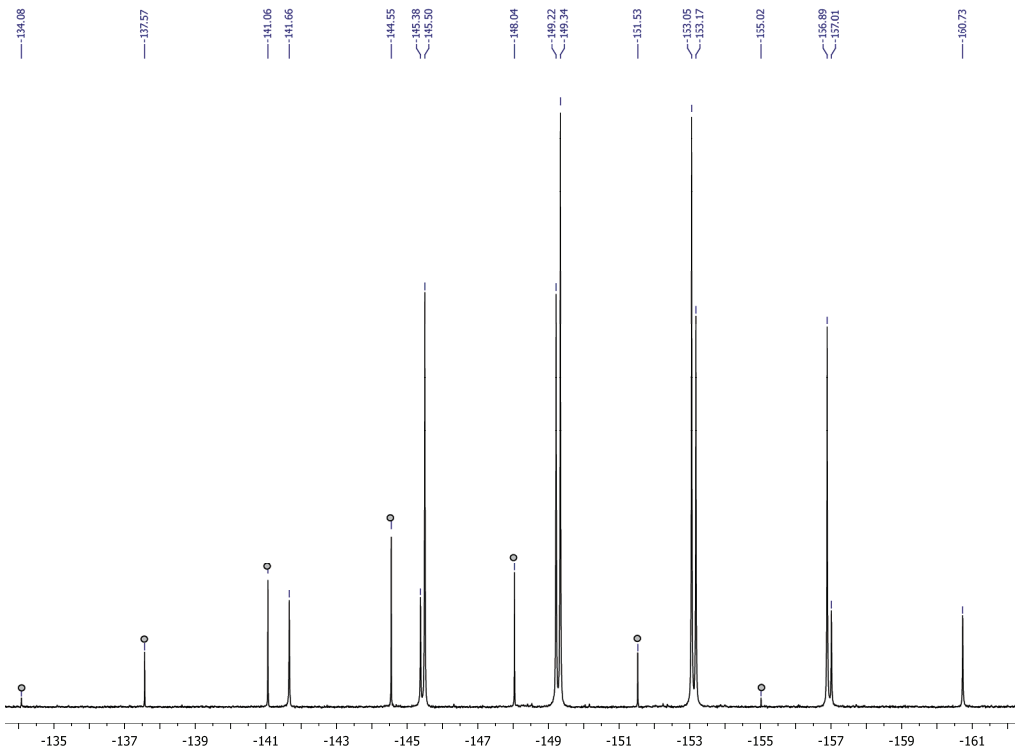


Figure 7. ^{31}P NMR spectrum of **4** [a doublet of quintets; the crude product is chosen to demonstrate the residual signals of **3** (PF_6^-, o-labeled septet)].

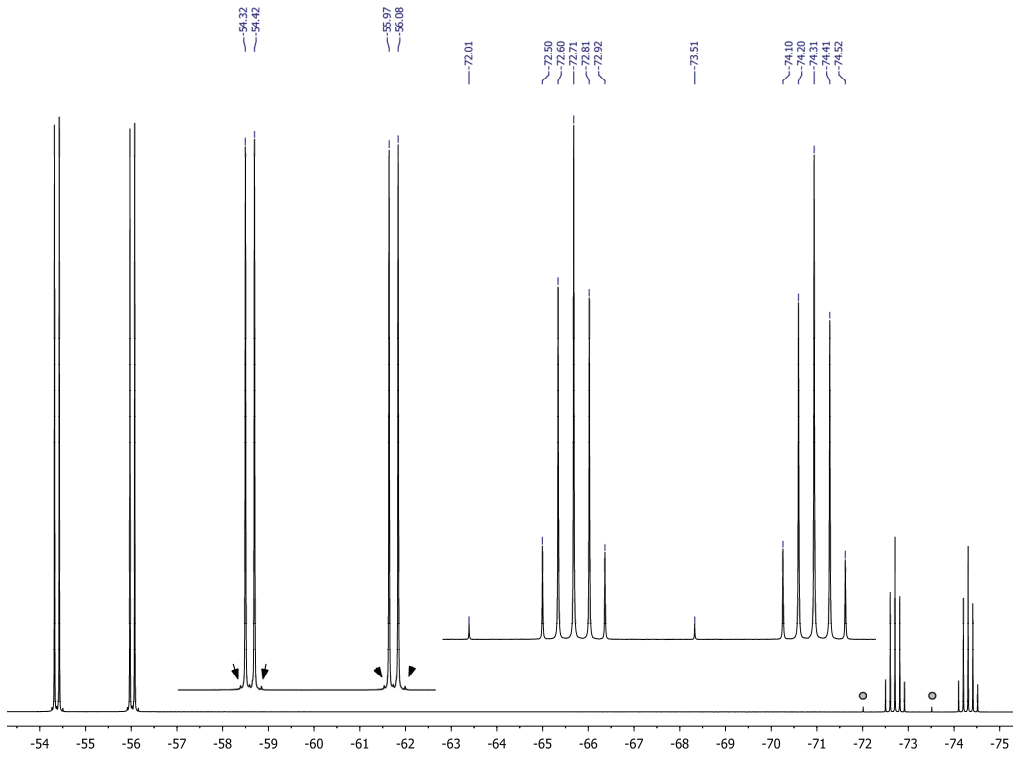


Figure 8. ^{19}F NMR spectrum of **4** [the crude product is chosen to demonstrate the residual signals of **3** (PF_6^-, o-labeled doublet)]. ^{13}C satellites in the lower-field subspectrum are arrow-pointed.

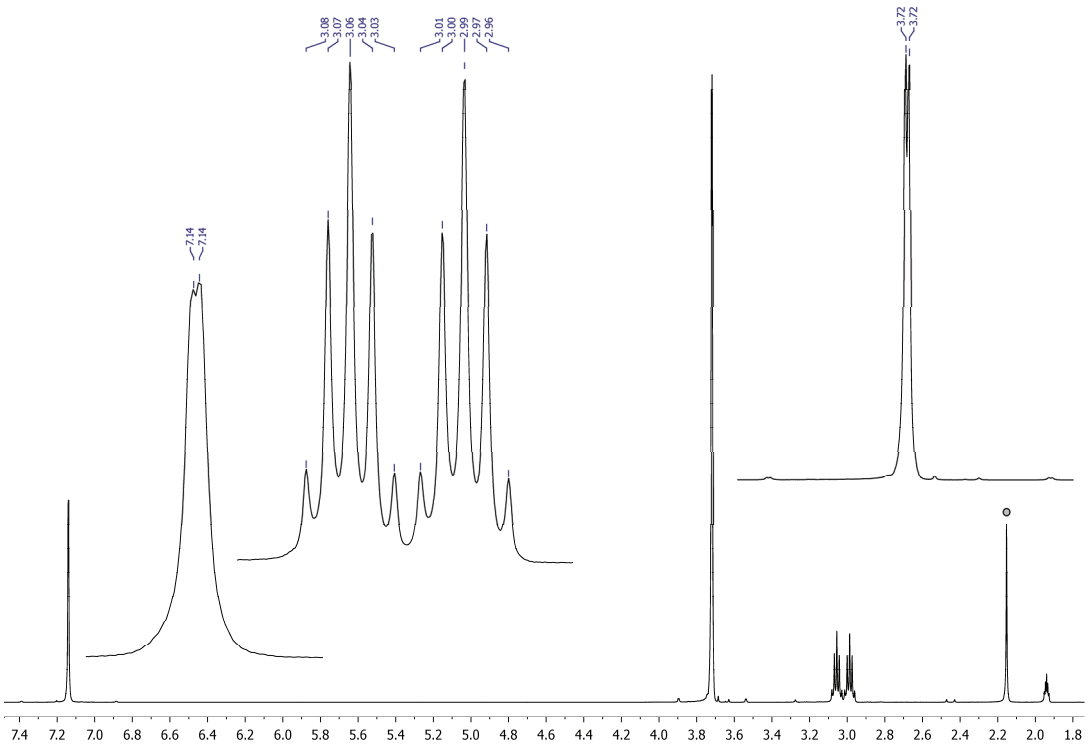


Figure 9. ^{1}H NMR (CD_3CN, 25 °C) spectrum of **12**. Far ^{5}J(P–H) SSCC-s for aromatic and methyl group protons (0.7 and 1.7 Hz) are also observed. o-Labeled signal belongs to water in CD_3CN.

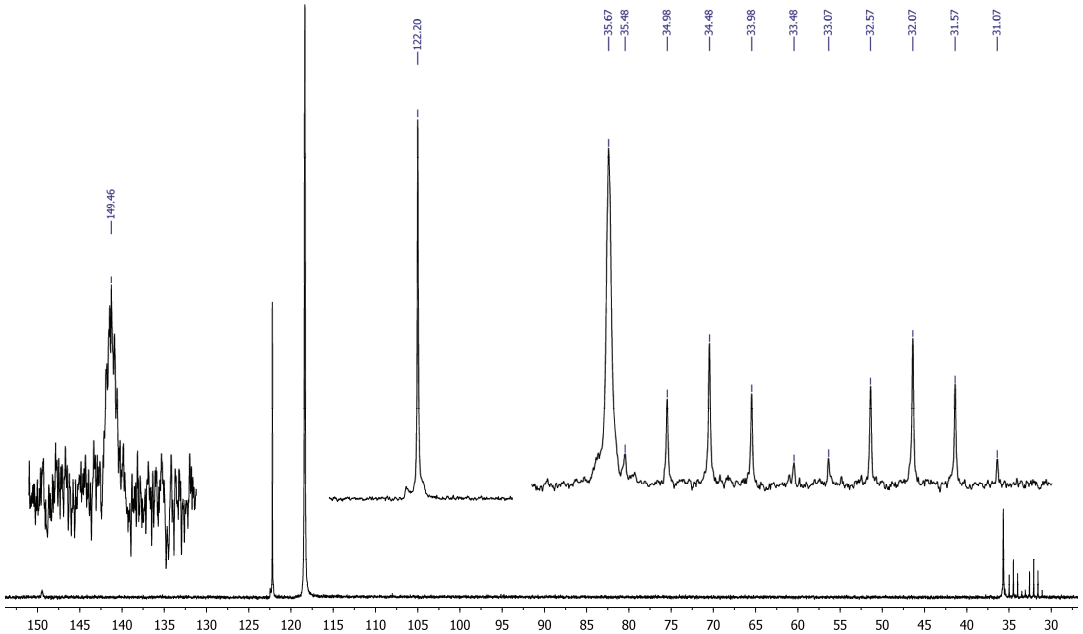


Figure 10. $^{13}C\{^{1}H\}$ NMR spectrum of **12**. The signals of quaternary and Me-group carbons are evidently broadened ($\Delta\nu_{1/2}$ = 21 and 7 Hz *vs* 2 Hz for CH aromatic carbon signals).

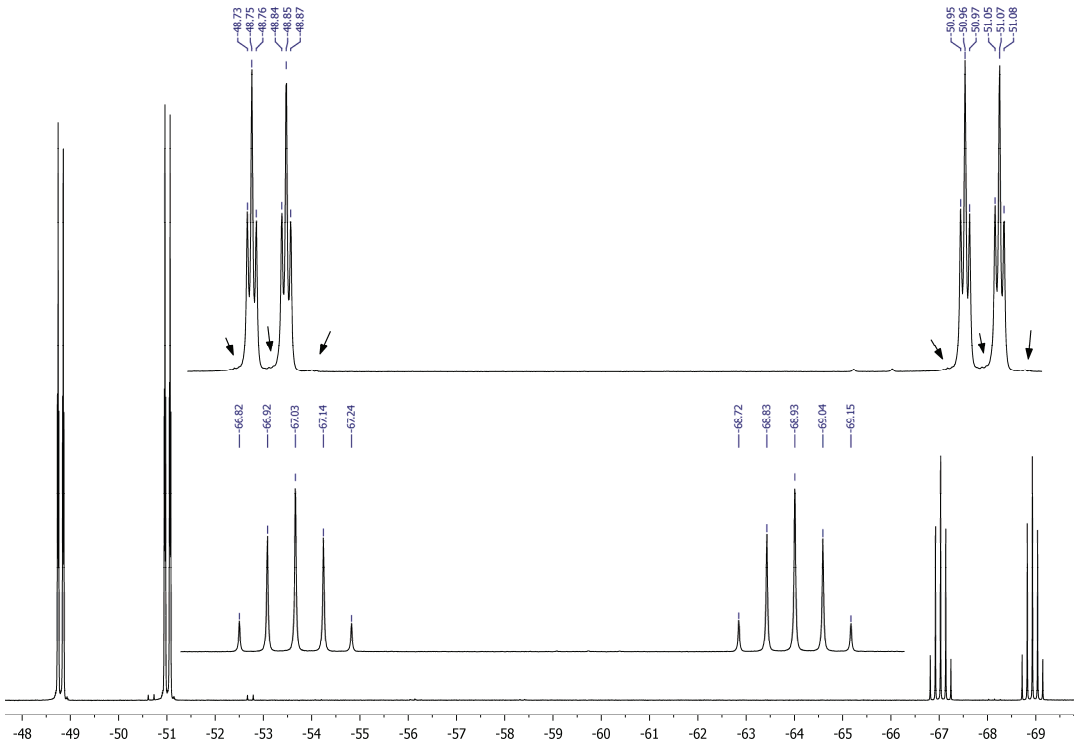


Figure 11. ^{19}F NMR spectrum of **12**. ^{13}C satellites in the lower-field subspectrum are arrow-pointed.

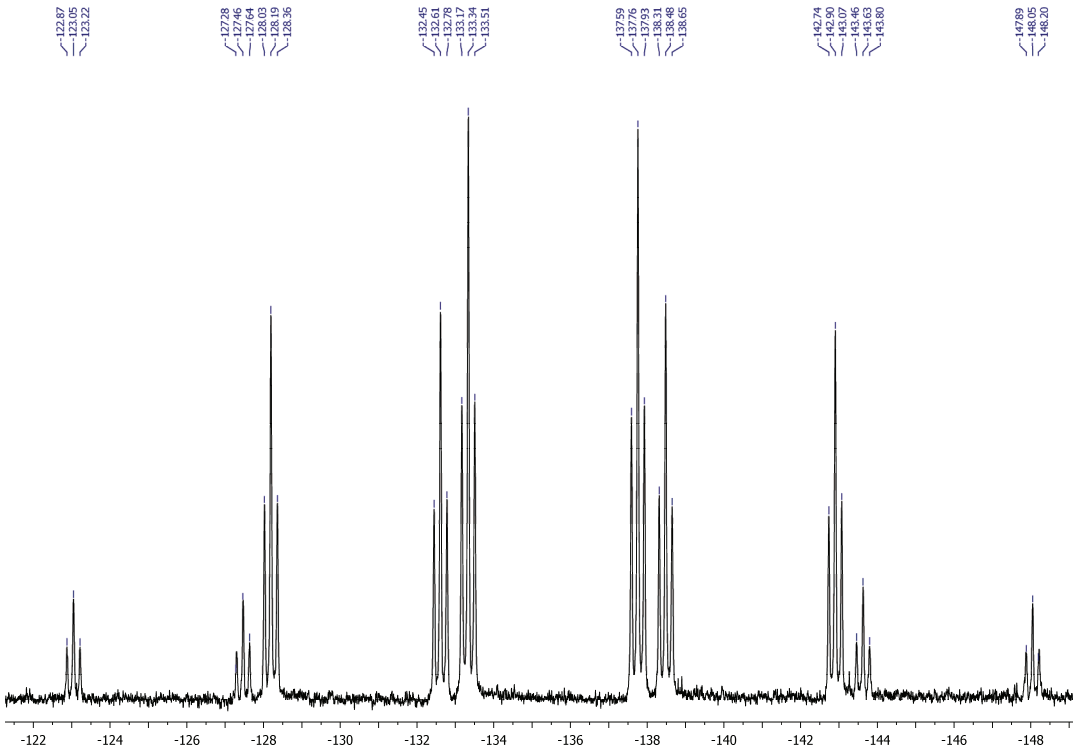


Figure 12. ^{31}P NMR spectrum of **12** [a doublet of quintets of triplets].

IR Spectral Data for 2, 4, and 12 and Comparison with Computationally Predicted Ones (for 2 and 4).

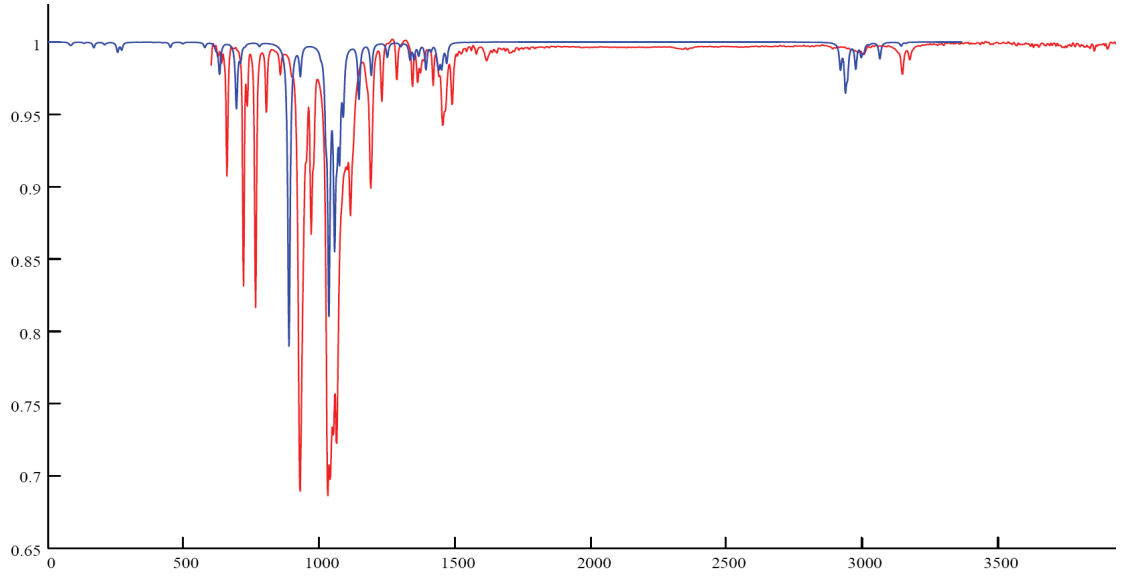


Figure 13. Experimental (red) and computed (blue) IR-spectra of **2** (transmittance *vs* wavenumber [cm^{-1}] plot). IR (neat, solid): 3172 (w), 3147 (w), 3000-2927 (v. w; a set of broad bands), 1489 (m), 1454 (m), 1421 (w), 1361 (w), 1342 (w), 1284 (w), 1230 (w), 1188 (m), 927 (v. s), 854 (w), 802 (m), 764 (s), 732 (w), 719 (s), 658 (m). The computed spectrum is scaled by an empirical factor 0.9613 (recommended by Foresman and Frisch[1]). Area of the stretching vibrations of the aliphatic protons is instrumentally suppressed.

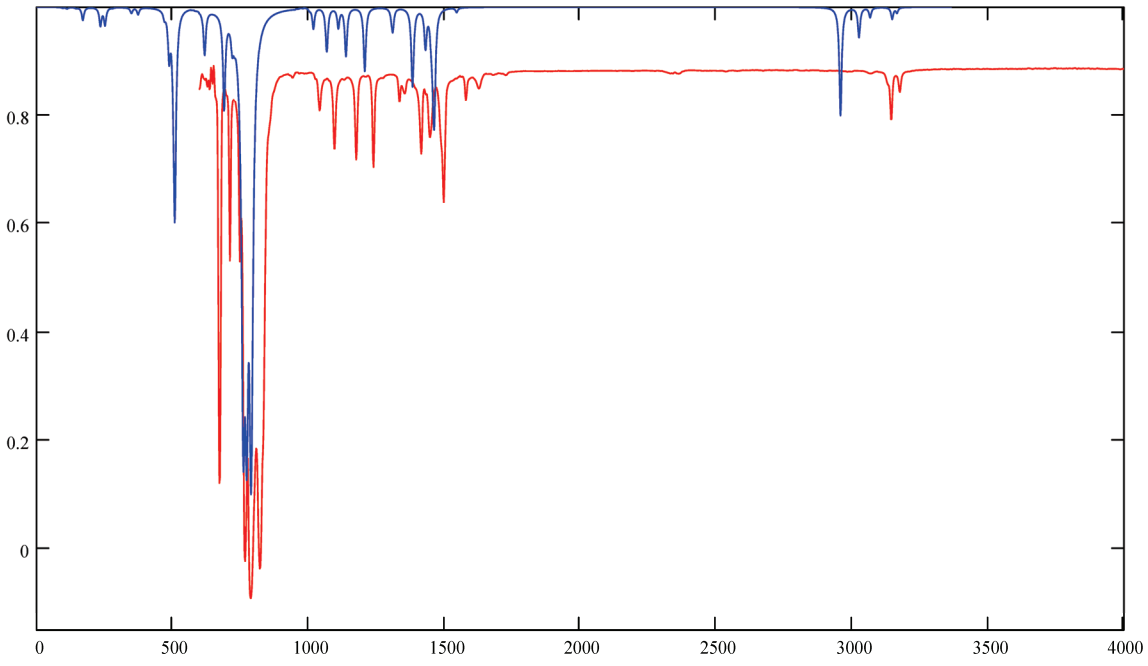


Figure 14. Experimental (red) and computed (blue) IR-spectra of 4 (transmittance vs wavenumber [cm–1] plot). IR (neat, solid): 3176 (w), 3145 (w), 3000-2927 (v. w; a set of broad bands), 1628 (w), 1581 (w), 1489 (m), 1448 (m-w), 1416 (m-w), 1354 (w), 1335 (w), 1240 (m), 1176 (m), 1097 (m-w), 1041 (w), 821 (v. s), 788 (v. s.), 768 (v. s.), 748 (s), 712 (s), 673 (s). The computed spectrum is scaled by an empirical factor 0.9613 (recommended by Foresman and Frisch[1]). Experimental spectrum is offsetted by 0.1 units down the transmittance axis for clarity. Area of the stretching vibrations of the aliphatic protons is instrumentally suppressed.

Table 1. Computed frequencies (ν / cm^{-1}; non-scaled), reduced masses *m*, force constants *f*, and IR spectrum intensities *I* (all in atomic units) for two stationary conformations of 2 with assignment.[a]

Freq. No.	2a				2b				Assignment
	ν	*m*	*f*	*I*	ν	*m*	*f*	*I*	
1	32.2	9.127	0.006	0.032	32.9	8.122	0.005	0.069	ρ(C–BF_3)
2	66.0	1.067	0.003	0.045	62.9	1.437	0.003	0.792	ρ(N–CH_3)
3	82.7	2.604	0.011	1.766	63.9	1.642	0.004	0.922	ρ(N–C_2H_5)
4	87.9	3.389	0.015	1.936	90.8	3.677	0.018	1.605	δ_{as}(non-H)
5	136.0	5.320	0.058	0.978	133.2	5.357	0.056	1.383	δ_{s}(non-H)
6	174.0	3.894	0.070	4.913	175.0	5.307	0.096	4.112	τ_{as}(non-H)
7	215.7	3.764	0.103	2.163	213.5	1.376	0.037	2.079	δ_{as}(non-H)
8	226.0	1.298	0.039	0.334	220.1	2.777	0.079	1.916	ρ(CH_2–CH_3)
9	265.3	5.667	0.235	8.459	272.7	6.982	0.306	7.230	τ_{as}(non-H)
10	280.9	4.728	0.220	6.208	274.5	3.138	0.139	6.163	τ_{as}(non-H)+ρ(CH_2–CH_3)
11	318.4	6.065	0.362	0.202	313.5	6.656	0.386	0.012	δ_{as}(non-H)+ω(BF_3)
12	353.8	2.928	0.216	0.154	352.6	3.034	0.222	0.069	τ_{s}(non-H)+β_{s}(CBF)
13	402.8	4.217	0.403	0.336	408.7	4.484	0.441	0.127	δ_{as}(non-H)+β_{as}+β_{as}
14	437.3	5.716	0.644	0.575	436.5	5.271	0.592	0.165	τ_{as}(non-H)+β_{as}(CBF)
15	467.8	10.123	1.305	4.584	468.5	9.438	1.221	4.371	δ_{as}(non-H)+σ_{s}(CBF)
16	515.5	4.186	0.656	1.460	515.6	4.191	0.656	0.872	τ_{as}(non-H)+σ_{s}(CBF)
17	599.4	4.011	0.849	4.425	599.8	4.052	0.859	3.996	π_{s}+β_{s}(CBF)
18	642.3	3.660	0.890	4.670	642.8	3.623	0.882	3.125	π_{as}+β_{s}(CBF)
19	656.0	8.466	2.147	27.338	656.0	8.873	2.250	25.924	π_{as}+β_{s}(CBF)+ν(CB)
20	720.8	1.408	0.431	57.886	718.8	1.359	0.414	61.220	δ_{s}(H)
21	736.6	4.103	1.312	12.525	738.5	3.783	1.216	11.448	ϕ_{as}+β_{s}(NCC)+2ν(CN)
22	753.5	4.573	1.530	1.745	753.6	5.223	1.748	0.889	π_{s}+ δ_{s}(H)
23	809.2	1.163	0.448	3.117	805.9	1.182	0.452	2.879	ω(CH_3)+γ(CH_2)
24	834.0	1.382	0.566	0.098	830.1	1.391	0.565	0.013	δ_{as}(H)
25	922.1	10.031	5.025	294.528	923.4	9.575	4.810	294.787	ν(CB)+β_{s}(CBF)+ν_{s}(BF)
26	965.7	2.498	1.373	25.606	968.2	2.514	1.388	24.615	ν(CB)+ω(CH_3) in C_2H_5
27	1043.8	2.755	1.769	3.806	1045.1	2.955	1.901	6.768	ϕ_{as}+ω(NCH_3)
28	1063.3	2.794	1.861	50.709	1067.0	2.367	1.588	20.142	τ_{s}(H)+ϕ_{s}+ω(CH_3)
29	1075.1	8.649	5.890	243.535	1073.3	9.915	6.730	257.240	τ_{s}(H)+ϕ_{s}+δ(B)+ν_{as}(BF)
30	1096.9	2.569	1.821	164.063	1099.3	3.126	2.225	176.057	τ_{s}(H)+ϕ_{as}+ν_{as}(BF)+ω(NCH_3)
31	1106.3	2.295	1.655	54.027	1107.8	2.156	1.559	53.769	τ_{as}(H)+ϕ_{as}+ν_{as}(BF)+ω(CCH_3)+ν(CC)
32	1116.2	1.628	1.195	80.473	1114.3	1.426	1.043	34.196	τ_{s}(H)+ϕ_{s}+ω(NCH_3)+ν_{as}(BF)+ω(CH_3)
33	1130.5	1.960	1.476	49.413	1129.8	2.233	1.679	89.191	complicated skeletal
34	1162.4	1.313	1.045	0.322	1157.2	1.328	1.048	8.276	ω(NCH_3)+δ(NCH_3)+π(NCH_3)
35	1190.3	2.431	2.029	48.595	1192.1	2.491	2.086	48.919	complicated skeletal
36	1237.4	1.723	1.555	27.971	1240.2	1.718	1.557	18.453	τ_{as}(H)+ϕ_{as}+ω(NCH_3)
37	1299.1	1.554	1.545	12.828	1303.8	1.589	1.591	11.359	τ_{as}(H)+ϕ_{as}+ω(CH_3)+α(CH_2)
38	1349.9	7.829	8.406	3.375	1356.8	7.295	7.912	8.025	ϕ_{as}+2ν(CN)
39	1385.8	1.736	1.964	13.996	1386.3	2.269	2.569	5.472	τ_{as}(H)+ϕ_{as}+ω(CH_2)
40	1401.2	1.654	1.913	13.089	1397.2	1.340	1.542	21.372	τ_{as}(H)+ϕ_{as}+ω(CH_2)
41	1419.4	1.263	1.499	10.107	1419.3	1.250	1.484	9.606	ν(CC)+β_{s}(CCH) in Et
42	1447.2	1.549	1.912	22.921	1449.2	1.592	1.970	23.184	ν(CN)+β_{s}(CCH) in Me
43	1466.5	3.028	3.837	5.817	1470.3	2.705	3.445	6.109	ϕ_{as}+ν(CB)+γ(CH_2)+β_{as}(HCH) in Me
44	1490.4	1.099	1.438	9.171	1486.9	1.140	1.485	7.229	β_{as}(HCH)+σ(CH_2) in Et +β_{s}(CCH) in Me
45	1496.4	1.381	1.822	16.458	1494.3	1.119	1.472	14.421	β_{as}(HCH)+σ(CH_2) in Et +β_{s}(CCH) in Me
46	1506.1	1.112	1.486	7.943	1497.3	1.082	1.429	7.903	β_{as}(HCH)+σ(CH_2) in Et +β_{s}(CCH) in Me
47	1508.0	1.042	1.396	11.488	1504.3	1.143	1.524	7.152	β_{as}(NCH_3)
48	1512.8	1.225	1.652	1.574	1512.2	1.258	1.695	5.993	β_{as}(NCH_3)+ β_{as}(HCH)+σ(CH_2) in Et
49	1526.6	1.332	1.829	16.557	1518.8	1.500	2.039	25.637	σ(CH_2)+)+β_{as}(HCH) in NCH_3
50	1608.4	4.261	6.494	0.212	1603.3	4.264	6.457	0.226	ϕ_{s} +τ_{s}(H)
51	3035.6	1.037	5.631	21.410	3036.2	1.036	5.629	17.605	ν_{s}(CH) CH_3 in Et
52	3054.5	1.036	5.696	36.924	3062.1	1.034	5.713	26.695	ν_{s}(CH) CH_3 in Me
53	3062.7	1.069	5.910	22.313	3069.2	1.069	5.935	21.756	ν_{s}(CH) CH_2 in Et
54	3094.4	1.101	6.210	21.877	3096.6	1.102	6.223	20.018	ν_{as}(CH) CH_3 in Et
55	3115.3	1.106	6.322	10.412	3121.6	1.100	6.314	11.384	ν_{as}(CH) CH_3 in Me
56	3125.1	1.099	6.326	7.218	3129.9	1.106	6.382	8.505	ν_{as}(CH) CH_3 in Et
57	3146.6	1.099	6.413	1.312	3152.9	1.099	6.436	0.602	ν_{as}(CH) CH_2 in Et
58	3186.8	1.101	6.586	14.401	3170.8	1.104	6.537	1.817	ν_{as}(CH) CH_3 in Me
59	3268.1	1.091	6.868	3.380	3268.9	1.092	6.872	3.396	ν_{as}(CH), ring
60	3286.7	1.109	7.056	0.900	3287.3	1.109	7.058	0.839	ν_{s}(CH), ring

[a] ν - stretching, β – bending, α – twisting, γ – rocking, σ – scissoring, ω – wagging, τ – in-plane deformation, δ – out of plane deformation, ϕ – in-plane ring deformation, π – out of plane ring deformation, ρ – rotation; *s* and *as* indices denote symmetric and asymmetric vibrations.

Table 2. Computed frequencies (ν / cm^{-1}; non-scaled), reduced masses *m*, force constants *f*, and IR spectrum intensities *I* (all in atomic units) for 4 with assignment.[a]

Freq. No.	ν	*m*	*f*	*I*	Assignment
1	86.8	6.725	0.030	0.000	ρ(C–PF_5)
2	100.7	4.671	0.028	0.282	δ_s(non-H)
3	116.7	1.039	0.008	0.195	ρ(N–CH_3)
4	116.8	1.049	0.008	0.308	ρ(N–CH_3)
5	152.0	9.169	0.125	0.342	ω(PF_5)
6	177.4	3.656	0.068	4.765	δ_{as}(non-H)
7	244.6	6.887	0.243	6.662	ν(CP)
8	262.2	4.940	0.200	6.431	τ(CP)
9	269.9	3.896	0.167	0.029	δ_{as}(N–Me)
10	289.9	12.969	0.642	0.004	δ_{as}(N–Me)+α_{as}(P–F_{cis})
11	291.8	8.786	0.441	0.211	δ_s(non-H)+β(CPF)+σ_s(FPF)
12	360.6	12.807	0.981	0.284	τ_{as}(N–Me)+σ_s(FPF)+ω(PF_{cis})
13	363.6	3.080	0.240	1.792	τ_s(N–Me)+ν(CP)
14	388.8	10.900	0.971	2.470	δ_s(non-H)+σ_s(FPF)
15	443.1	16.201	1.874	0.000	σ_s(F_{cis}–P–F_{cis})+τ_s(N–Me)
16	489.5	6.132	0.866	2.511	τ_{as}(N–Me)+β(CPF)
17	507.6	18.044	2.739	17.047	β(CPF)+σ_s(FPF)
18	523.3	4.770	0.770	8.540	τ_{as}(non-H)+σ_s(FPF+β(PF_{trans})
19	529.2	19.414	3.204	96.824	ν(CP)+ν(PF_{trans})+ω(PF_{cis})
20	537.5	18.689	3.181	0.718	ν_{as}(PF_{cis})+ν(CP)
21	607.2	4.622	1.004	0.081	ϕ_s
22	633.6	3.309	0.783	0.156	π_{as}
23	643.6	16.635	4.060	17.323	ν_s(PF_{cis})+ν(CP)+ϕ_s+ω(PF_{cis})
24	718.1	1.538	0.467	38.478	δ_s(H)+π(C)
25	749.1	3.677	1.216	8.457	δ_s(H,N–Me)+π(C=C,C)
26	757.3	4.812	1.626	3.788	τ_{as}(all)+ϕ_{as}
27	791.9	22.580	8.343	331.844	ν_{as}(PF_{cis})+β(F_{cis}–P–F_{cis})+β(CPF_{trans})
28	804.2	21.783	8.301	332.335	ν_{as}(PF_{cis})+β(F_{cis}–P–F_{cis})+β(CPF_{trans})
29	821.1	21.691	8.617	422.308	ν(PF_{trans})+ν(CP)+ω(PF_{cis})
30	833.8	1.385	0.567	0.063	δ_{as}(H)+π_{as}(C=C)
31	1044.6	3.309	2.127	0.750	ϕ_{as}+τ(P)+ω_{as}(CH_3)+ν_{as}(N–Me)
32	1059.8	2.387	1.579	7.864	ϕ_s+τ_s(H)+ω_s(CH_3)
33	1110.0	1.922	1.395	10.064	ϕ_{as}+τ(all)+ω_{as}(CH_3)+ν_{as}(N–Me)
34	1112.1	1.181	0.860	7.659	τ_s(H)+ϕ_s+ω_s(CH_3)+ν_s(N–Me)
35	1151.8	1.316	1.029	0.004	ω_{as}(CH_3)+π_{as}(N)
36	1155.1	1.322	1.039	7.225	ω_s(CH_3)+π_s(N)
37	1184.3	2.339	1.933	18.844	ϕ_s+τ_s(H)+ω_s(CH_3)+ν(CP)
38	1256.3	1.589	1.478	25.147	ϕ_{as}+τ_{as}(H)+ω_{as}(CH_3)+τ(P)
39	1358.7	7.908	8.601	2.366	ϕ_s+τ_s(H)+β_s(CH_3)+ν_s(N–Me)
40	1363.5	3.919	4.293	7.949	ϕ_{as}+τ_{as}(all)+ω_{as}(CH_3)+τ(P)
41	1438.3	1.581	1.927	23.886	ϕ_{as}+τ_{as}(H)+β_{as}(CH_3)+ν_{as}(N–Me)
42	1441.1	3.121	3.819	9.157	ϕ_s+σ_s(CH_3)+ν(CP)
43	1472.1	1.203	1.537	0.063	β_s(CH_3)+ϕ_s
44	1488.5	1.050	1.371	14.225	β_{as}(CH_3)
45	1490.3	1.113	1.456	0.449	β_{as}(CH_3)+ϕ_{as}
46	1510.4	1.275	1.714	7.913	β_{as}(CH_3)+ϕ_{as}+τ_{as}(all)
47	1518.2	1.193	1.620	21.441	β_{as}(CH_3)
48	1522.6	1.622	2.216	36.557	β_{as}(CH_3)+ϕ_{as}+τ_{as}(P,H)
49	1607.8	4.199	6.395	1.667	ν(C=C)+τ_s(H)+ϕ_s+β_s(CH_3)+ν(CP)
50	3076.9	1.034	5.769	36.167	ν_s(CH_3)–ν_s(CH_3)
51	3077.0	1.034	5.770	8.452	ν_s(CH_3)+ν_s(CH_3)
52	3147.5	1.106	6.457	5.751	ν_{as}(CH_3)–ν_{as}(CH_3)
53	3147.7	1.106	6.459	5.390	ν_{as}(CH_3)+ν_{as}(CH_3)
54	3190.1	1.103	6.611	2.353	ν_{as}(CH_3)–ν_{as}(CH_3)
55	3190.3	1.103	6.612	1.254	ν_{as}(CH_3)+ν_{as}(CH_3)
56	3274.6	1.092	6.897	4.261	ν_{as}(=CH)
57	3292.8	1.109	7.085	1.940	ν_s(=CH)

[a] ν - stretching, β – bending, α – twisting, γ – rocking, σ – scissoring, ω – wagging, τ – in-plane deformation, δ – out of plane deformation, ϕ – in-plane ring deformation, π – out of plane ring deformation, ρ – rotation; *s* and *as* indices denote symmetric and asymmetric vibrations.

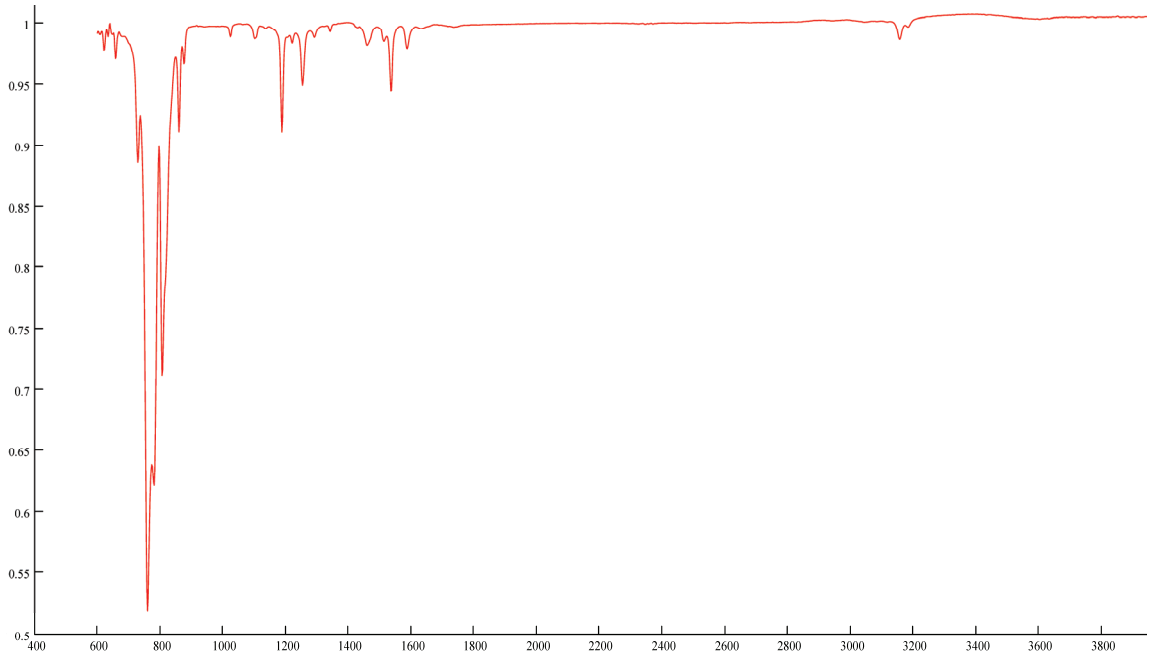


Figure 15. IR-spectrum of **12** (transmittance vs wavenumber [cm–1] plot). IR (neat, solid): 3182 (w), 3157 (w), 3000-2927 (v. w; a set of broad bands), 1587 (w), 1535 (w), 1512 (w), 1458 (w), 1429 (wq, sh), 1340 (w), 1292 (-w), 1254 (m), 1221 (w), 1188 (m), 1101 (w), 1024 (w), 876 (w), 860 (m), 806 (s), 781 (s.), 760 (v. s.), 729 (m), 658 (w), 621 (w). Area of the stretching vibrations of the aliphatic protons is instrumentally suppressed.

Optimized Geometries

Table 3. Cartesian coordinates for the optimized geometry of the salt 1 [Å]. Atom numbering is brought into accordance with that in the structure of 2.

B1	2.24199700	–0.47343900	–0.13691500
C1	–0.70366900	0.33946400	0.44665500
C2	–2.44061700	0.67644400	–0.86362900
C3	–1.90242100	1.88599300	–0.56286800
C4	–1.83325400	–1.74249700	–0.30422000
C5	–2.71248700	–2.29633300	0.80980700
C6	0.14075400	2.64562300	0.74850700
F1	1.76835200	0.51288700	–1.03071900
F2	3.54551000	–0.81207700	–0.38775700
F3	1.38039700	–1.60210000	–0.22902900
F4	2.09093100	0.05222700	1.18818900
H1	0.09090900	–0.13487200	1.00130400
H2	–3.28147300	0.41698900	–1.48195600
H3	–2.18391000	2.87644300	–0.87340100
H4A	–2.25592700	–1.95498000	–1.28635100
H4B	–0.82605400	–2.15751500	–0.27695400
H5A	–3.71688700	–1.86854900	0.78317200
H5B	–2.80001300	–3.37810800	0.69520500
H5C	–2.27601600	–2.09752700	1.79009100
H6A	–0.33137300	3.27486800	1.50264400
H6B	0.99442600	2.11383000	1.16186100
H6C	0.47885600	3.24941300	–0.09126900
N1	–1.67506300	–0.27832400	–0.22404600
N2	–0.81908900	1.65212600	0.25955300

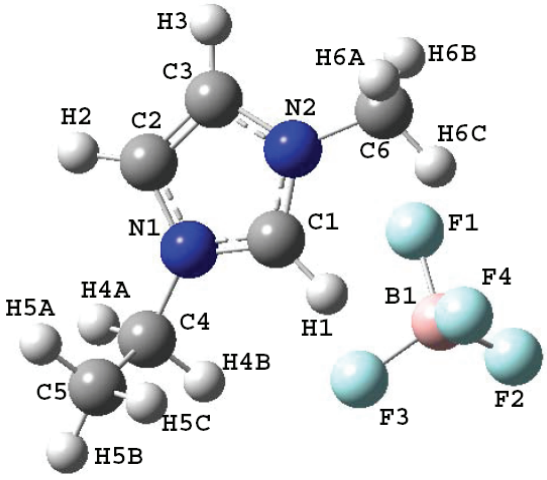


Table 4. Cartesian coordinates for the optimized geometry of 2 [Å]. The first conformation 2a. Atom numbering is brought into accordance with that in the X-ray diffraction analysis.

B1	–0.54659100	–1.45244600	0.05512800
C1	–0.30895500	0.20348600	0.08898800
C2	0.78065000	2.15194600	0.27109800
C3	–0.52045400	2.43302100	0.03033200
C4	2.16078000	0.05468900	0.50859000
C5	2.96132200	–0.08378500	–0.78089500
C6	–2.61592000	1.11102000	–0.33121800
F1	–1.88737200	–1.73818500	–0.19171000
F2	0.27271500	–1.95266800	–0.96071200
F3	–0.14558500	–1.94220500	1.30086600
H2	1.62282300	2.80377000	0.42394600
H3	–1.03220500	3.37455500	–0.06440600
H4A	2.71983100	0.60855200	1.26514000
H4B	1.90936800	–0.91832800	0.92247500
H5A	3.20952300	0.89079100	–1.20782100
H5B	3.89565100	–0.60847500	–0.57110700
H5C	2.39931800	–0.66307100	–1.51277700
H6A	–2.85774400	1.61856900	–1.26519200
H6B	–2.87870900	0.06166300	–0.40109300
H6C	–3.16333900	1.57662500	0.48868300
N1	0.89266900	0.77750300	0.30709800
N2	–1.17751500	1.22147400	–0.08007500

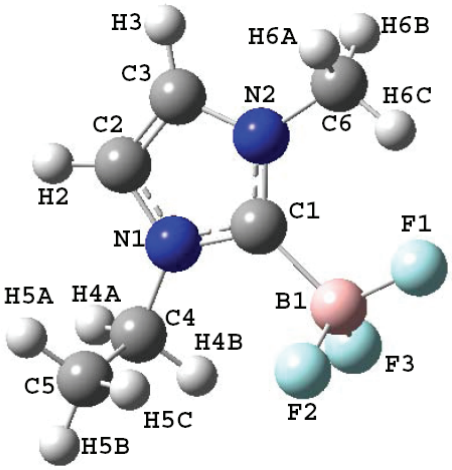


Table 5. Cartesian coordinates for the optimized geometry of 2 [Å]. The second conformation 2b. Atom numbering is brought into accordance with that in the X-ray diffraction analysis.

B1	0.83459700	–1.29664400	–0.07375100
C1	0.17075400	0.23469200	–0.09500100
C2	–1.18286900	2.01030400	–0.24195000
C3	0.06542600	2.46907100	0.01058200
C4	–2.26228800	–0.24818500	–0.52332500
C5	–2.87717800	–0.72735300	0.78572300
C6	2.32986400	1.40872800	0.32066000
F1	1.80823000	–1.32515700	–1.07354100
F2	1.41463400	–1.46917900	1.18799500
F3	–0.16548800	–2.23856400	–0.30317500
H2	–2.11041700	2.53741900	–0.37961300
H3	0.43580900	3.47191600	0.13043600
H4A	–2.97887900	0.32891500	–1.10964400
H4B	–1.92581900	–1.09173200	–1.11883600
H5A	–3.19990700	0.11049700	1.40787700
H5B	–3.74917800	–1.34843900	0.57096500
H5C	–2.16075400	–1.33018700	1.34340800
H6A	2.55697400	2.25410700	0.96838600
H6B	2.64294400	0.48501300	0.79763400
H6C	2.84922800	1.51945300	–0.63077600
N1	–1.09937400	0.63228500	–0.30855100
N2	0.88342800	1.36183000	0.10101900

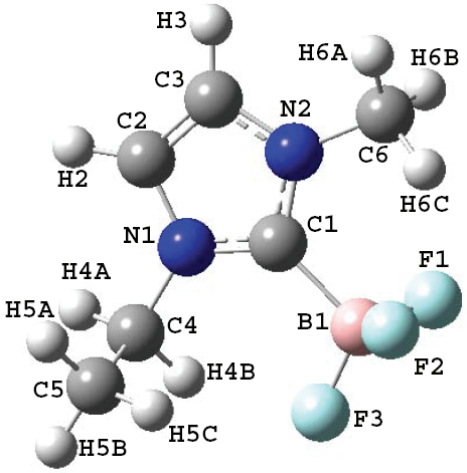


Table 6. Cartesian coordinates for the optimized geometry of 2…HF [Å].

B1	0.96317800	–1.04002600	–0.62229700
C1	0.23812900	0.41607400	–0.29436800
C2	–1.17284900	2.13417200	–0.07248600
C3	0.03347500	2.53553600	0.39161200
C4	–2.15218000	0.01320500	–0.99946400
C5	–3.02434000	–0.52380000	0.12991200
C6	2.30720300	1.48489300	0.61553100
F1	2.12929600	–0.78904600	–1.32661400
F2	1.30249300	–1.61795500	0.64908800
F3	0.10346600	–1.88182300	–1.30269400
F4	–0.57634500	–1.70045500	2.38488900
H1	0.14660900	–1.76896000	1.77857700
H2	–2.11002200	2.65825500	–0.13545600
H3	0.35112100	3.47658700	0.80473100
H4A	–2.72316200	0.65566300	–1.67229100
H4B	–1.72209500	–0.79615300	–1.58028000
H5A	–3.47997200	0.28551200	0.70488900
H5B	–3.82696600	–1.13031900	–0.29430600
H5C	–2.44166400	–1.14441400	0.81141500
H6A	2.43144800	2.13176600	1.48232500
H6B	2.90397000	1.85755100	–0.21618300
H6C	2.62780400	0.47797300	0.86254700
N1	–1.02936100	0.82725000	–0.49362000
N2	0.88939300	1.46413600	0.25063000

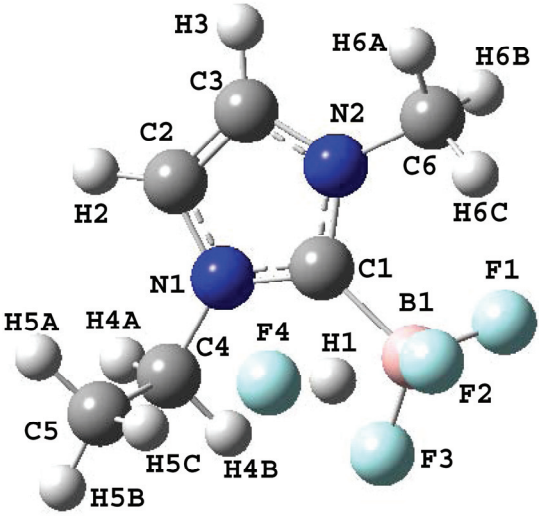


Table 7. Cartesian coordinates for the optimized geometry of the TS [Å]. Atom numbering is brought into accordance with that in the structures of 1 and 2.

B1	2.31690500	–0.58357900	–0.68016800
C1	–0.50766200	0.32658000	0.49625500
C2	–2.05335700	0.87179400	–1.06572800
C3	–1.44763900	2.01902900	–0.67913200
C4	–1.84967800	–1.55789400	–0.40677500
C5	–3.12185800	–1.85927700	0.37877500
C6	0.37268200	2.59681400	0.96071300
F1	1.66022700	–0.25460300	–1.77712600
F2	2.94196400	0.35159200	0.00007600
F3	2.41026100	–1.84497100	–0.33597200
F4	0.71594700	–0.92354000	2.46345700
H1	0.26378100	–0.46238100	1.70156100
H2	–2.83222900	0.70218300	–1.78915900
H3	–1.59644900	3.03436800	–1.00434000
H4A	–1.96711300	–1.82367700	–1.45970900
H4B	–1.01120700	–2.12856900	–0.01061300
H5A	–3.97178700	–1.28702300	0.00050700
H5B	–3.36497500	–2.92062300	0.29601800
H5C	–2.98584400	–1.62022600	1.43455800
H6A	–0.21329800	3.34999300	1.48934700
H6B	0.96926600	2.03749600	1.67658100
H6C	1.03452000	3.08829900	0.24633200
N1	–1.46339900	–0.14696900	–0.33811000
N2	–0.51084500	1.66260900	0.27542400

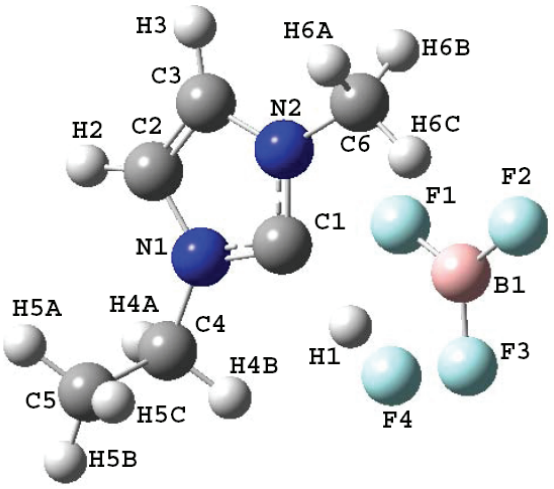


Table 8. Cartesian coordinates for the optimized geometry of 7 [Å]. Atom numbering is brought into accordance with that in the structures of 1 and 2.

C1	–0.39121900	0.38991800	–0.12365100
C2	0.31251600	–1.76111500	–0.24164500
C3	–1.01883500	–1.78501500	–0.00054300
C4	2.03613500	0.06670900	–0.52165500
C5	2.87882500	0.01643900	0.74873700
C6	–2.79373600	–0.02477000	0.30659100
F1	–0.45357500	3.01151400	–0.11146700
H1	–0.42630000	2.00679500	–0.11851900
H2	–1.69505400	–2.61442300	0.11694100
H3	1.01391400	–2.56765700	–0.37012200
H4A	2.49292500	–0.52704900	–1.31690900
H4B	1.94345200	1.09068400	–0.88031500
H5A	2.97284000	–1.00373300	1.12747600
H5B	3.88231700	0.39518700	0.54346500
H5C	2.43190200	0.63485400	1.52862900
H6A	–3.14810400	–0.39232700	1.27101700
H6C	–2.80474800	1.06225800	0.30977100
H6B	–3.45319900	–0.39002600	–0.48238300
N1	0.67283000	–0.42515200	–0.31619400
N2	–1.42567200	–0.46216000	0.06864400

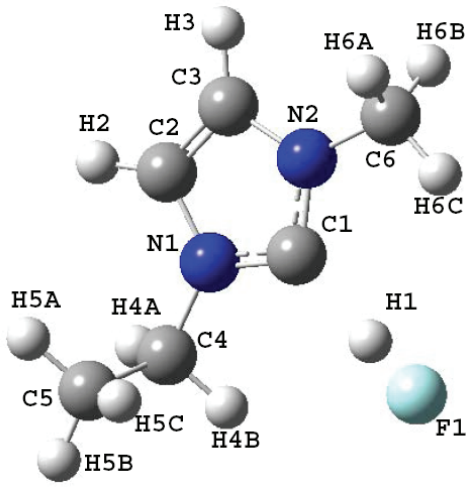


Table 9. Cartesian coordinates for the optimized geometry of 9 [Å]. Atom numbering is brought into accordance with that in the structures of 1 and 2.

C1	0.39542200	–0.91841800	–0.24863200
C2	–0.13461400	1.30430300	–0.10742000
C3	1.19412100	1.19594200	0.11830200
C4	–1.99183500	–0.33086700	–0.57521600
C5	–2.84144900	–0.31235900	0.69261400
C6	2.82135100	–0.71256700	0.20161800
H2	–0.76851300	2.17477500	–0.13412000
H3	1.93307600	1.95296800	0.32111400
H4A	–2.39461700	0.36219800	–1.31914300
H4B	–1.98357000	–1.32663300	–1.01577800
H5A	–2.85200000	0.67810100	1.15318200
H5B	–3.87277000	–0.58650100	0.45801000
H5C	–2.45188600	–1.02462300	1.42195400
H6A	3.20789400	–0.48864800	1.19839100
H6B	3.50942700	–0.31025900	–0.54534600
H6C	2.74774000	–1.79002000	0.07832000
N1	–0.59573100	0.01428700	–0.32994200
N2	1.49105000	–0.15679700	0.02934500

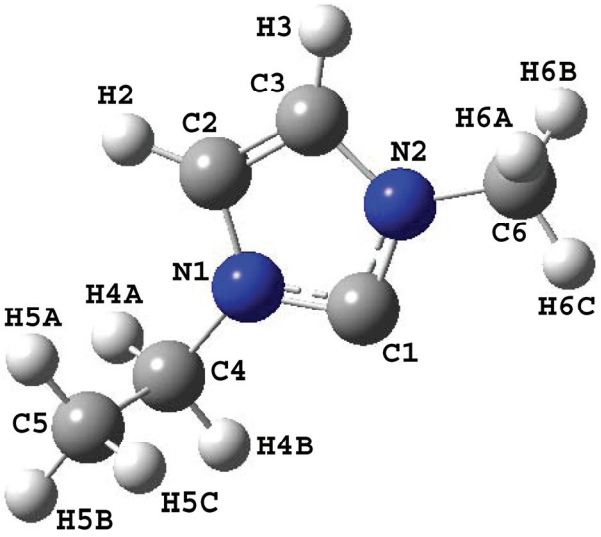


Table 10. Cartesian coordinates for the optimized geometry of 5a [Å].

B1	1.74468200	0.15537400	–0.00002700
C1	–0.82553100	0.72665900	0.00007700
C2	–1.79435800	–1.24942900	0.00037200
C3	–0.44318800	–1.41497400	–0.00030100
C4	–3.32331100	0.76847500	–0.00039700
F1	1.81582600	1.53769600	–0.00437400
F2	2.25051000	–0.42144100	–1.14389800
F3	2.24851700	–0.41380400	1.14853400
H1	–0.67190600	1.79195800	0.00023200
H3	0.14750100	–2.31403500	–0.00066300
H4	–2.59916900	–1.96345400	0.00054400
H4A	–3.17637200	1.84625200	0.00733400
H4B	–3.88873900	0.48099200	0.88592900
H4C	–3.88212600	0.49262400	–0.89464000
N1	–2.02213000	0.11348500	0.00059200
N2	0.14099300	–0.17314800	–0.00051600

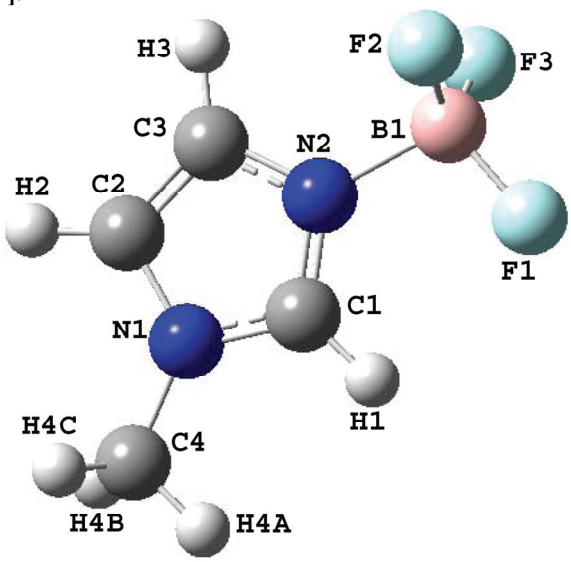


Table 11. Cartesian coordinates for the optimized geometry of 8a (Å).

C1	–0.19667100	–1.08400100	–0.00022300
C2	–0.22789800	1.11064000	–0.00019000
C3	–1.50075600	0.60545900	0.00009700
C4	2.05936100	0.03295000	0.00013900
H1	0.20691700	–2.08540300	–0.00029500
H2	0.15105000	2.11894200	–0.00028000
H3	–2.43081800	1.15118700	0.00022100
H4A	2.44041800	0.53765800	0.88968500
H4B	2.44047800	0.53919900	–0.88849400
H4C	2.42386300	–0.99314500	–0.00075800
N1	0.60848500	0.01640600	–0.00002000
N2	–1.47078800	–0.76765300	0.00016100

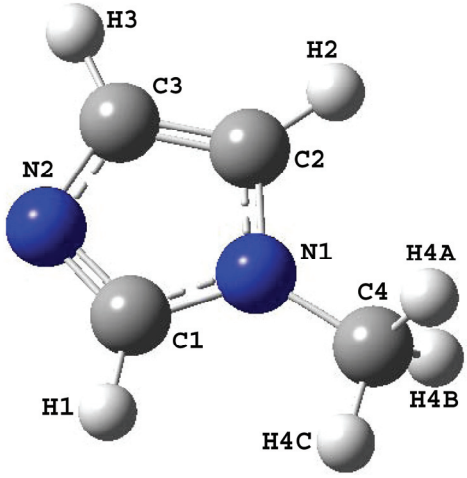


Table 12. Cartesian coordinates for the optimized geometry of 5b [Å].

B1	–2.12231600	–0.23492700	0.06896300
C1	0.45853600	–0.58255500	–0.31411400
C2	1.29076300	1.44093900	–0.08792900
C3	–0.05818300	1.49226600	0.08671700
C4	2.94616400	–0.43184000	–0.55528000
C5	3.74270300	–0.56207000	0.73877400
F1	–2.11890600	–1.58343300	–0.24493000
F2	–2.81736700	0.53663800	–0.83629300
F3	–2.49046300	0.01704900	1.37266800
H1	0.37330500	–1.64251600	–0.48112300
H2	2.04010300	2.21243000	–0.06110100
H3	–0.70209100	2.32895300	0.29299700
H4A	2.81907600	–1.40368900	–1.03270500
H4B	3.46045400	0.21383900	–1.26906100
H5A	3.88802100	0.40840500	1.21603800
H5B	4.72630000	–0.98350600	0.52304300
H5C	3.23500500	–1.21914700	1.44662400
N1	1.60482400	0.11936500	–0.34424300
N2	–0.55737600	0.22165500	–0.05740600

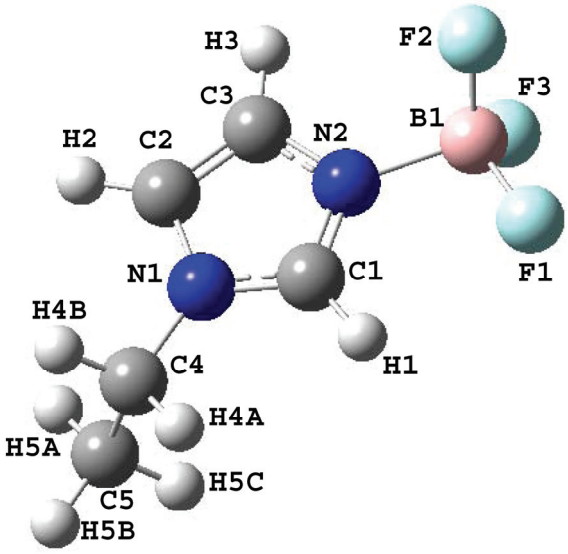


Table 13. Cartesian coordinates for the optimized geometry of 8b [Å].

C1	0.74194000	–1.09647900	0.01262800
C2	0.60169100	1.08268800	–0.20162100
C3	1.87300000	0.70859100	0.14300100
C4	–1.54613000	–0.21373100	–0.57910300
C5	–2.43959000	0.17924600	0.59535900
H1	0.43130400	–2.13059000	0.01646700
H2	0.16020600	2.04563700	–0.39650600
H3	2.73220400	1.34194000	0.29647000
H4A	–1.77278700	0.39777700	–1.45563600
H4B	–1.72359500	–1.25283800	–0.86138600
H5A	–2.28538100	1.22226200	0.87694400
H5B	–2.23102800	–0.44235500	1.46791300
H5C	–3.49033500	0.05237600	0.32484700
N1	–0.12332100	–0.08593600	–0.28773900
N2	1.95102900	–0.65636400	0.27478200

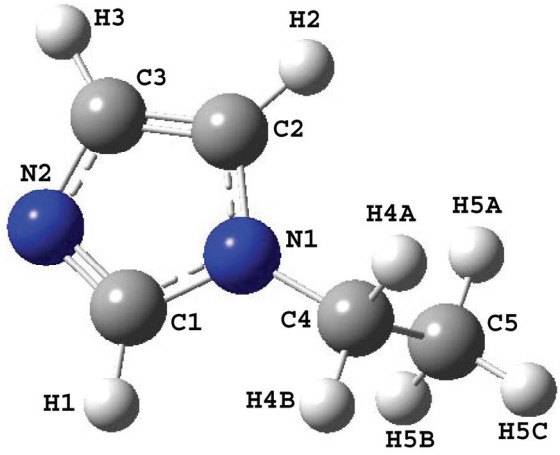


Table 14. Cartesian coordinates for the optimized geometry of TS-a [Å].

B1	3.32445100	–0.24324000	0.16763500
C1	–2.66210500	0.69972500	–0.01199600
C2	–3.43849000	–1.35436800	–0.02277600
C3	–2.08324600	–1.36576900	–0.19460000
C4	–5.14478300	0.48630200	0.29342800
C5	0.56842700	0.37581300	–0.48251300
C6	0.52795300	1.81719300	–0.11105000
F1	2.70985100	–1.36567000	0.69501500
F2	3.34329700	0.80289500	1.06883100
F3	4.52224200	–0.49163300	–0.42679500
F4	2.38781100	0.22296400	–0.95950200
H1	–2.65221100	1.77671100	0.04377900
H2	–4.16143100	–2.15035400	0.03044700
H3	–1.42666000	–2.21177400	–0.31697800
H4A	–5.10331000	1.57263000	0.34278400
H4B	–5.56127600	0.10683400	1.22683400
H4C	–5.79004000	0.19547500	–0.53589400
H5A	0.70746700	–0.37789700	0.27297900
H5B	0.34678500	0.04594400	–1.48014400
H6A	1.54347300	2.13499100	0.12683800
H6B	0.13810700	2.43700600	–0.91760700
H6C	–0.06546400	1.95862100	0.79221500
N1	–3.79859500	–0.02984000	0.09286900
N2	–1.61183700	–0.07621400	–0.18491600

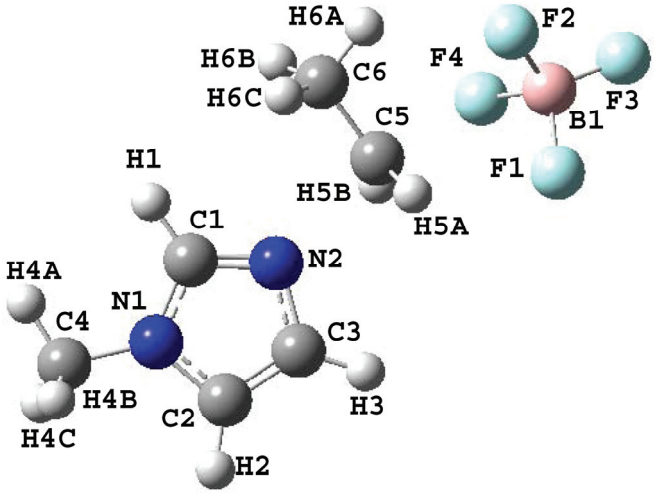


Table 15. Cartesian coordinates for the optimized geometry of TS-b [Å].

B1	–3.54076400	–0.43363500	–0.01714100
C1	1.69345300	–0.20920900	0.35121900
C11	4.70068200	–1.52695400	–0.71885000
C2	1.97393700	1.85430200	–0.20188800
C3	3.22025200	1.31986600	–0.03389300
C4	–1.12223500	0.95660600	–0.06015900
C5	4.07257900	–0.99626000	0.56611900
F1	–3.08601100	–0.90042200	1.19693100
F2	–4.87983300	–0.23158900	–0.08363800
F3	–3.00737400	–1.13136600	–1.07768900
F4	–2.90846700	0.99257500	–0.13944300
H1	1.25233900	–1.16140600	0.60181500
H2	1.70477700	2.86163500	–0.47372600
H3	4.20175900	1.75203700	–0.12730000
H4A	–1.11900100	0.50804000	0.91568400
H4B	–1.04922700	2.02497100	–0.15260800
H4C	–1.03667100	0.33801200	–0.93380700
H5A	3.61251700	–1.80522800	1.13457400
H5B	4.82650200	–0.53946500	1.20967400
H6A	5.17350100	–0.72602200	–1.28958900
H6B	5.46562800	–2.26708900	–0.47632500
H6C	3.95159300	–2.00338700	–1.35331600
N1	1.03074700	0.88764700	0.04240500
N2	3.02971900	0.00280900	0.32186500

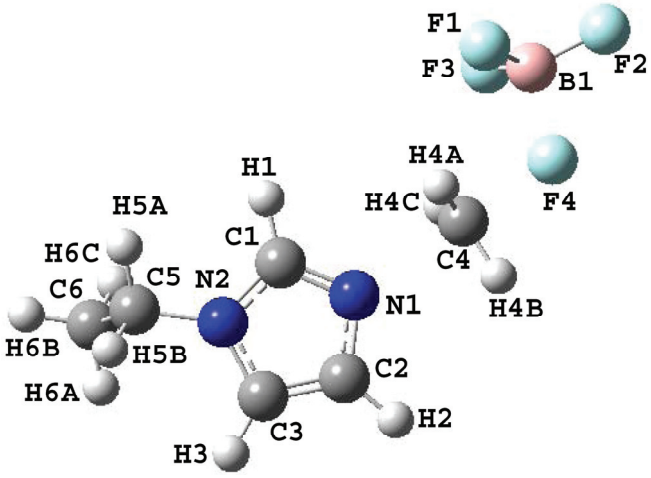


Table 16. Cartesian coordinates for the optimized geometry of 3 [Å]. Atom numbering is brought into accordance with that in the X-ray diffraction analysis for 4.

C1	–1.66077700	–0.02654100	–0.57127500
C2	–3.48104400	–0.49752100	0.57778900
C3	–3.33859200	0.85177500	0.55298100
C4	–2.12166200	–2.44934500	–0.32600700
C5	–1.58378400	2.44151200	–0.37467400
F1	0.93600500	–1.38472900	–0.29896800
F2	2.48333000	–0.81798200	1.33273300
F3	2.65612000	1.30766300	0.41607000
F4	1.10800200	0.73090700	–1.20862900
F5	3.00739000	–0.55742800	–0.90723300
F6	0.58953100	0.47356600	1.02334600
H1	–0.73174300	–0.12483800	–1.10882300
H2	–4.22920800	–1.11633900	1.04044000
H3	–3.93766000	1.62866100	0.99388700
H4A	–1.06890100	–2.54378600	–0.58104800
H4B	–2.74878500	–2.85856300	–1.11765600
H4C	–2.30851600	–2.97879800	0.60625200
H5A	–0.61692700	2.29845100	–0.84995500
H5B	–1.43038100	2.91211300	0.59464700
H5C	–2.23329200	3.05678300	–0.99636200
N1	–2.42030900	–1.02843800	–0.13064400
N2	–2.19578500	1.12490700	–0.17201400
P1	1.84732100	–0.04241500	0.07789800

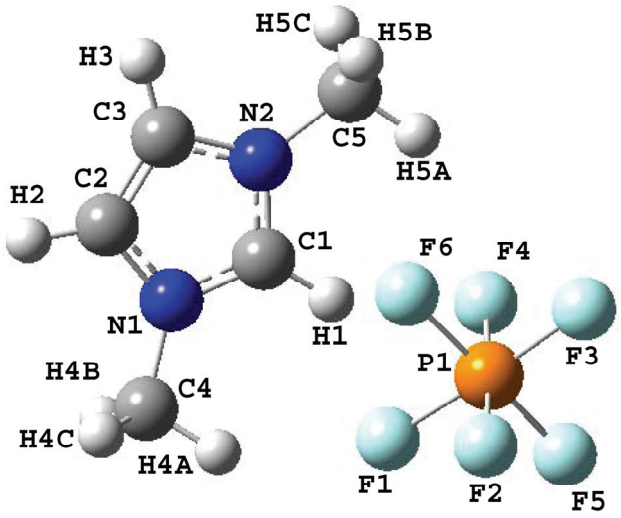


Table 17. Cartesian coordinates for the optimized geometry of 4 [Å]. Atom numbering is brought into accordance with that in the X-ray diffraction analysis.

C1	0.69708500	0.00000800	0.00001500
C2	2.82329400	–0.67596700	0.00716000
C3	2.82331300	0.67593000	–0.00720300
C4	1.10994000	–2.49373300	–0.00695800
C5	1.10999300	2.49373700	0.00698700
F1	–1.17441100	–1.05229300	1.25735800
F2	–1.17351700	–1.25087400	–1.05459600
F3	–1.17441900	1.05231900	–1.25732900
F4	–1.17363700	1.25088800	1.05458000
F5	–2.81446700	–0.00006000	–0.00005500
H2	3.63603700	–1.38005200	0.01183600
H3	3.63606800	1.38000000	–0.01179300
H4A	0.24820500	–2.63945200	0.63403000
H4B	1.95284800	–3.07636300	0.35921800
H4C	0.85864800	–2.79315000	–1.02201700
H5A	0.85926700	2.79328900	1.02215300
H5B	1.95269500	3.07632300	–0.35972300
H5C	0.24789700	2.63938200	–0.63352200
N1	1.50505000	–1.07951200	0.01318900
N2	1.50507400	1.07950900	–0.01318000
P1	–1.21668100	0.00002500	0.00000800

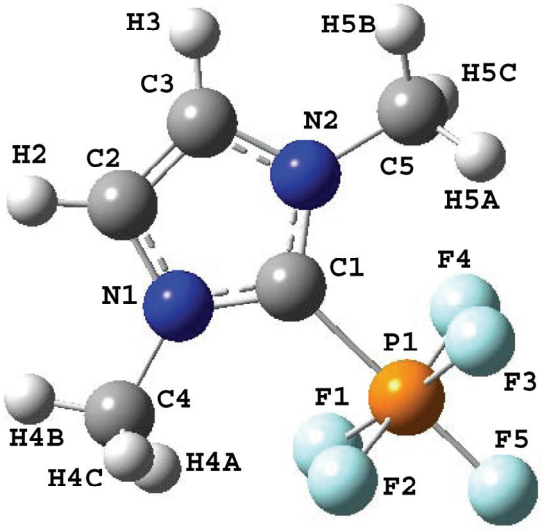


Table 18. Cartesian coordinates for the optimized geometry of 6 [Å].

C1	1.43341500	–0.70676800	–0.00134000
C2	2.47381400	1.23256300	–0.00021200
C3	1.13227900	1.45380700	0.00070400
C4	3.92315100	–0.84553000	0.00161100
F1	–1.12673900	–1.07315300	1.25969800
F2	–1.08103900	–1.31902500	–1.00965300
F3	–1.45744700	0.93036100	–1.26063300
F4	–1.49810200	1.17675900	1.01210600
F5	–2.94552000	–0.34550800	–0.00167700
H1	1.24369300	–1.76549500	–0.00458900
H2	3.30534600	1.91502300	–0.00086900
H3	0.57552300	2.37287300	0.00293500
H4A	3.73426100	–1.91625200	–0.02913100
H4B	4.50798700	–0.56259500	–0.87327500
H4C	4.48127800	–0.60788800	0.90704800
N1	2.64823900	–0.13928600	–0.00110600
N2	0.50211000	0.23294900	0.00002800
P1	–1.37979100	–0.08137600	0.00015300

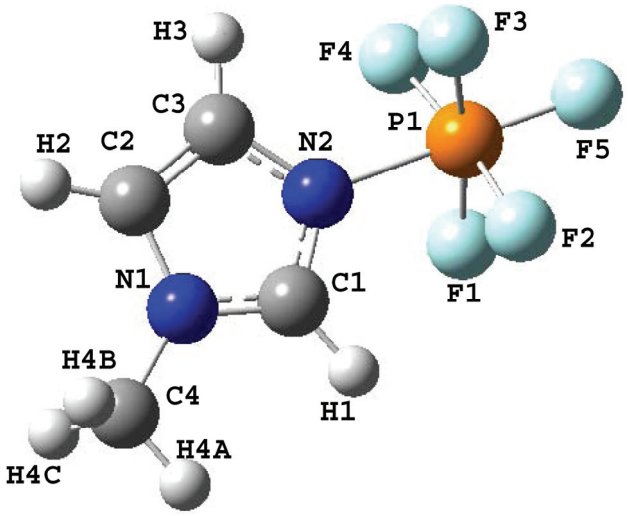


Table 19. Cartesian coordinates for the optimized geometry of 10 [Å].

C1	–0.00004800	–0.97721900	0.00004100
C2	–0.67596500	1.21081000	–0.00016900
C3	0.67604600	1.21084000	0.00012700
C4	–2.44261900	–0.57102200	0.00021900
C5	2.44241800	–0.57100800	–0.00015100
H2	–1.37491100	2.03041200	–0.00003000
H3	1.37511900	2.03032600	0.00028800
H4A	–2.96858600	–0.20703700	–0.88520000
H4B	–2.43643500	–1.65794500	–0.00703000
H4C	–2.96395200	–0.21907700	0.89325200
H5A	2.96618500	–0.21412900	0.88955400
H5B	2.96667900	–0.21239900	–0.88855200
H5C	2.43622600	–1.65801400	–0.00159300
N1	–1.06182700	–0.12183200	–0.00060100
N2	1.06192300	–0.12196000	0.00044600

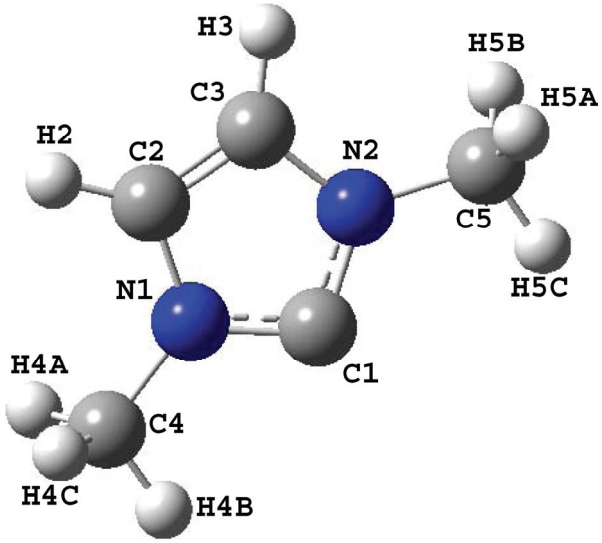


Table 20. Cartesian coordinates for the optimized geometry of EtF [Å].

C1	–0.10276900	0.54920400	–0.00000300
C2	1.19420500	–0.22394900	–0.00000400
F1	–1.19031100	–0.34001000	–0.00000100
H1A	–0.20683200	1.17460500	0.88968600
H1B	–0.20686000	1.17465900	–0.88965300
H2A	2.03848600	0.47098100	–0.00026800
H2B	1.26958900	–0.85605600	–0.88656100
H2C	1.26980400	–0.85562800	0.88684400

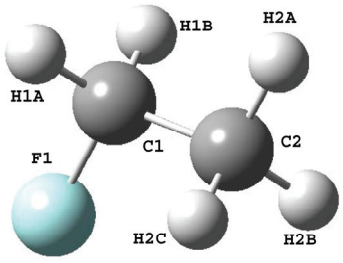


Table 21. Cartesian coordinates for the optimized geometry of $F_3B{\leftarrow}OEt_2$ [Å].

B1	1.11635500	–0.60009900	–0.01077200
C1	–0.49633800	1.46644800	–0.68103900
C2	–0.03809400	2.46095000	0.36724100
C3	–1.47486000	–0.41411600	0.61441100
C4	–2.59273900	–1.00447700	–0.21836300
F1	0.87059100	–1.93159900	–0.15063500
F2	1.47796800	–0.23119000	1.25410800
F3	1.85764000	–0.03039500	–0.99990100
H1A	0.12042800	1.51329600	–1.57455900
H1B	–1.53770400	1.61878100	–0.96622100
H2A	1.00614100	2.29945100	0.63055700
H2B	–0.14203900	3.46931900	–0.04140100
H2C	–0.63827300	2.40694100	1.27716200
H3A	–1.81100600	0.41515200	1.23766500
H3B	–1.01632900	–1.16174800	1.25620800
H4A	–3.04448400	–0.26342600	–0.88083200
H4B	–3.37571100	–1.38019800	0.44504400
H4C	–2.22277500	–1.83447600	–0.82058400
O1	–0.39545300	0.07540300	–0.24185400

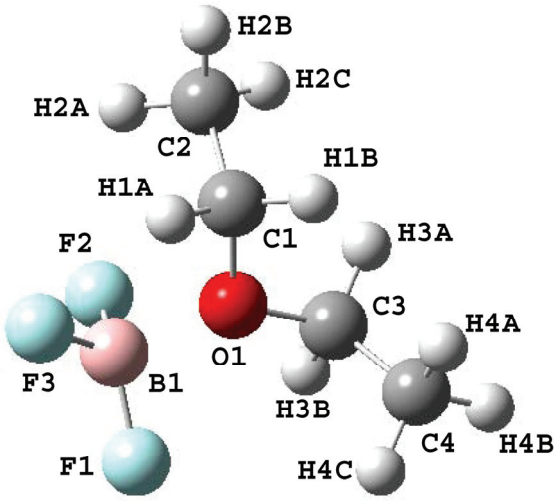
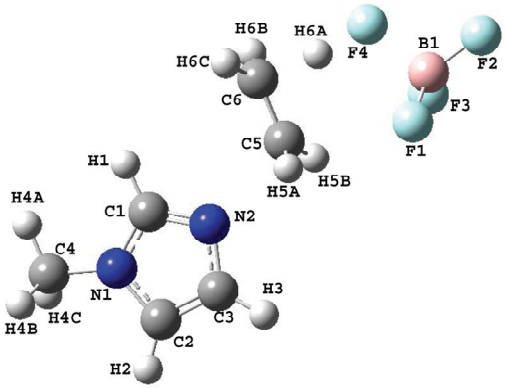


Table 22. Cartesian coordinates for the optimized geometry of TS-C_2H_4 [Å].

B1	–3.63734400	–0.27746300	0.07102800
C1	2.86821200	0.63997300	0.00337300
C2	3.91761700	–1.28852600	–0.01316100
C3	2.56728700	–1.48515200	–0.09701500
C4	5.37292500	0.77339600	0.15249000
C5	–0.38055200	0.24788500	–0.16561400
C6	–0.64661500	1.59185500	–0.13325300
F1	–3.06873200	–0.95672800	–0.98195500
F2	–4.98928500	–0.26271300	0.08251800
F3	–3.04521300	–0.59124500	1.27247800
F4	–3.20889400	1.22416000	–0.17796900
H1	2.71403100	1.70742900	0.03712200
H2	4.74453800	–1.97791800	0.00707200
H3	2.02789900	–2.41591000	–0.16327700
H4A	5.18641600	1.84515100	0.18657500
H4B	5.99908200	0.55271800	–0.71262900
H4C	5.89728100	0.47892800	1.06218000
H5A	–0.38284200	–0.29291200	–1.10037300
H5B	–0.45962100	–0.34898000	0.73092800
H6A	–1.99501000	1.30459100	–0.16948300
H6B	–0.58586000	2.12616500	0.80992200
H6C	–0.52146900	2.18567700	–1.03341900
N1	4.10080000	0.07524800	0.05074900
N2	1.92464800	–0.27174400	–0.08593800



Geometry for HF: H–F 0.92419 Å.
Geometry for CH_3F: C–F 1.39403 Å, C–H 1.09109 Å, F–C–H 108.574° (point group C_{3v}).
Geometry for BF_3: B–F 1.31373 Å (point group D_{3h}).
Geometry for PF_5: P–F 1.549445 (apical) and 1.55571 Å (equatorial) (point group D_{3h}).
Geometry for PH_3: P–H 1.41897 Å, C–Cl 1.78960 Å, H–P–H 93.385° (point group C_{3v}).
Geometry for C_2H_4: C=C 1.32535 Å, C–H 1.08430 Å, C=C–H 121.703º (point group D_{2h})

Energies and Thermochemistry Computation Results

Table 23. SCF- (E_{SCF}), zero-point corrected (ZPE) energies [Hartrees], thermal corrections to E_{SCF} [$\Delta E(T)$ / kcal·mol^{-1}], and entropies [$S(T)$ / cal·mol^{-1}·K^{-1}] for geometry-optimized 1, 2 (2a is used), HF, and TS. For 1, 2, and TS, both internal hindered rotation corrected and non-corrected values of $\Delta E(T)$ and $S(T)$ are provided. The computed vibrational frequencies were scaled by an empirical factor of 0.9613 (recommended by Foresman and Frisch[1]). Thermochemistry was modeled for the case of 0.001 atm pressure and the ^{1}H, ^{11}B, ^{12}C, ^{14}N, and ^{19}F set of isotopes.

T, °C	**1** (E_{SCF}; ZPE) −769.472384; −769.295707				**2** (E_{SCF}; ZPE) −668.953710; −668.790078				HF (E_{SCF}; ZPE) −100.483154; −100.474198		**TS** (E_{SCF}; ZPE) −769.411990; −769.239332			
	$\Delta E(T)$ corr./non-corr.		$S(T)$ corr./non-corr.		$\Delta E(T)$ corr./non-corr.		$S(T)$ corr./non-corr.		$\Delta E(T)$	$S(T)$	$\Delta E(T)$ corr./non-corr.		$S(T)$ corr./non-corr.	
25	120.234	120.317	141.036	144.358	110.653	110.604	126.186	126.340	7.101	55.221	118.262	117.680	152.720	148.117
50	121.574	121.647	145.511	148.799	111.840	111.788	130.166	130.312	7.225	55.781	119.588	118.904	157.150	152.218
70	122.705	122.768	149.026	152.283	112.844	112.791	133.299	133.443	7.324	56.199	120.704	119.936	160.620	155.437
90	123.888	123.937	152.488	155.709	113.896	113.842	136.390	136.533	7.424	56.593	121.869	121.016	164.030	158.606
110	125.121	125.155	155.898	159.079	114.994	114.940	139.440	139.581	7.523	56.966	123.081	122.141	167.386	161.729
130	126.402	126.420	159.259	162.396	116.138	116.083	142.450	142.588	7.622	57.320	124.340	123.312	170.688	164.808
150	127.731	127.729	162.571	165.661	117.325	117.268	145.421	145.554	7.722	57.657	125.643	124.527	173.941	167.845
170	129.104	129.081	165.834	168.876	118.555	118.494	148.352	148.476	7.821	57.978	126.991	125.785	177.144	170.841
190	130.522	130.476	169.050	172.040	119.825	119.759	151.244	151.356	7.921	58.285	128.381	127.084	180.299	173.797
210	131.981	131.910	172.218	175.156	121.135	121.062	154.096	154.194	8.020	58.579	129.812	128.424	183.407	176.712
230	133.481	133.382	175.340	178.222	122.483	122.400	156.909	156.988	8.119	58.861	131.282	129.802	186.469	179.587
250	135.019	134.891	178.415	181.241	123.866	123.772	159.683	159.740	8.219	59.132	132.790	131.217	189.486	183.801
270	136.594	136.435	181.443	184.212	125.284	125.178	162.417	162.450	8.318	59.394	134.334	132.669	192.457	186.598
290	138.204	138.013	184.427	187.136	126.735	126.614	165.113	165.119	8.418	59.645	135.914	134.155	195.384	189.356
310	139.848	139.624	187.365	190.015	128.219	128.081	167.770	167.748	8.517	59.888	137.526	135.674	198.267	192.881
330	141.525	141.265	190.259	192.849	129.732	129.577	170.389	170.337	8.617	60.123	139.172	137.225	201.108	195.563
350	143.233	142.935	193.110	195.639	131.275	131.101	172.970	172.888	8.717	60.351	140.848	138.806	203.907	198.208
370	144.971	144.634	195.918	198.385	132.846	132.652	175.514	175.400	8.816	60.571	142.554	140.417	206.664	200.815
390	146.738	146.361	198.684	201.09	134.444	134.229	178.021	177.875	8.916	60.785	144.288	142.057	209.381	203.386
410	148.532	148.114	201.409	203.752	136.068	135.831	180.493	180.315	9.016	60.993	146.050	143.724	212.057	205.922
430	150.353	149.892	204.093	206.375	137.716	137.457	182.929	182.718	9.116	61.194	147.839	145.417	214.695	208.422
450	152.200	151.694	206.738	208.958	139.389	139.107	185.330	185.087	9.217	61.391	149.653	147.135	217.295	210.887

Table 24. SCF- (E_{SCF}), zero-point corrected (*ZPE*) energies [Hartrees], thermal corrections to E_{SCF} [$\Delta E(T)$ / kcal·mol^{-1}], and entropies [$S(T)$ / cal·mol^{-1}·K^{-1}] for geometry-optimized 3, 4, MeF, and 6. For 3, 4, and 6, both internal hindered rotation corrected and non-corrected values of $\Delta E(T)$ and $S(T)$ are provided. The computed vibrational frequencies were scaled by an empirical factor of 0.9613 (recommended by Foresman and Frisch[1]). Thermochemistry was modeled for the case of 0.001 atm pressure and the ^{1}H, ^{31}P, ^{12}C, ^{14}N, and ^{19}F set of isotopes.

T, °C	**3** (E_{SCF}; *ZPE*) –1246.373980; –1246.214399				**4** (E_{SCF}; *ZPE*) –1145.861175; –1145.714702				MeF (E_{SCF}; *ZPE*) –139.794296; –139.755275		**6** (E_{SCF}; *ZPE*) –1106.552535; –1106.434702			
	$\Delta E(T)$ corr./non-corr.		$S(T)$ corr./non-corr.		$\Delta E(T)$ corr./non-corr.		$S(T)$ corr./non-corr.		$\Delta E(T)$	$S(T)$	$\Delta E(T)$ corr./non-corr.		$S(T)$ corr./non-corr.	
25	106.104	106.138	144.227	143.481	96.723	96.692	126.292	125.557	25.378	67.003	78.352	78.560	123.690	124.007
50	107.521	107.592	148.947	148.321	97.995	97.989	130.549	129.892	25.561	67.751	79.451	79.702	127.390	127.843
70	108.710	108.814	152.637	152.108	99.066	99.081	133.882	133.290	25.714	68.330	80.379	80.664	130.295	130.851
90	109.947	110.085	156.254	155.821	100.181	100.219	137.153	136.626	25.874	68.896	81.348	81.668	133.151	133.807
110	111.231	111.404	159.800	159.463	101.339	101.402	140.364	139.903	26.041	69.449	82.356	82.711	135.959	136.710
130	112.558	112.769	163.278	163.036	102.539	102.628	143.517	143.121	26.215	69.992	83.401	83.792	138.718	139.560
150	113.928	114.178	166.689	166.542	103.778	103.894	146.613	146.282	26.395	70.525	84.481	84.909	141.430	142.360
170	115.338	115.628	170.037	169.982	105.055	105.199	149.653	149.386	26.583	71.050	85.595	86.059	144.093	145.108
190	116.787	117.118	173.321	173.358	106.369	106.540	152.639	152.435	26.778	71.568	86.741	87.242	146.710	147.805
210	118.272	118.646	176.545	176.671	107.717	107.918	155.572	155.430	26.979	72.078	87.917	88.455	149.280	150.453
230	119.792	120.210	179.709	179.924	109.097	109.328	158.453	158.371	27.187	72.581	89.122	89.697	151.804	153.053
250	121.346	121.808	182.814	183.116	110.510	110.771	161.282	161.261	27.402	73.077	90.354	90.967	154.282	155.604
270	122.932	123.439	185.864	186.250	111.952	112.244	164.062	164.099	27.624	73.567	91.612	92.262	156.716	158.108
290	124.548	125.102	188.857	189.327	113.423	113.747	166.793	166.887	27.852	74.050	92.894	93.582	159.106	160.566
310	126.194	126.794	191.798	192.349	114.921	115.277	169.477	169.626	28.086	74.528	94.200	94.925	161.454	162.980
330	127.867	128.515	194.686	195.318	116.445	116.833	172.114	172.317	28.326	75.000	95.527	96.291	163.760	165.349
350	129.567	130.262	197.523	198.233	117.995	118.415	174.705	174.962	28.571	75.465	96.876	97.678	166.024	167.676
370	131.292	132.036	200.310	201.098	119.568	120.021	177.253	177.562	28.823	75.926	98.245	99.085	168.249	169.961
390	133.041	133.835	203.050	203.913	121.164	121.651	179.758	180.117	29.080	76.380	99.633	100.511	170.435	172.206
410	134.814	135.658	205.743	206.680	122.782	123.302	182.220	182.629	29.343	76.829	101.040	101.956	172.584	174.411
430	136.610	137.504	208.391	209.400	124.421	124.975	184.642	185.100	29.611	77.273	102.463	103.418	174.695	176.578
450	138.427	139.371	210.994	212.075	126.080	126.668	187.025	187.530	29.883	77.712	103.904	104.897	176.771	178.707

Table 25. SCF- (E_{SCF}), zero-point corrected (*ZPE*) energies [Hartrees], thermal corrections to E_{SCF} [$\Delta E(T)$ / kcal·mol^{-1}], and entropies [$S(T)$ / cal·mol^{-1}·K^{-1}] for geometry-optimized 7, 8a, 8b, and 9. Both internal hindered rotation corrected and non-corrected values of $\Delta E(T)$ and $S(T)$ are provided. The computed vibrational frequencies were scaled by an empirical factor of 0.9613 (recommended by Foresman and Frisch[1]). Thermochemistry was modeled for the case of 0.001 atm pressure and the ^{1}H, ^{11}B, ^{12}C, ^{14}N, and ^{19}F set of isotopes.

T, °C	**7** (E_{SCF}; *ZPE*) –444.729124; –444.562340				**8a** (E_{SCF}; *ZPE*) –265.608028; –265.509447				**8b** (E_{SCF}; *ZPE*) –304.935866; –304.808813				**9** (E_{SCF}; *ZPE*) –344.214732; –344.060272			
	$\Delta E(T)$ corr./non-corr.		$S(T)$ corr./non-corr.		$\Delta E(T)$ corr./non-corr.		$S(T)$ corr./non-corr.		$\Delta E(T)$ corr./non-corr.		$S(T)$ corr./non-corr.		$\Delta E(T)$ corr./non-corr.		$S(T)$ corr./non-corr.	
25	107.385	107.360	122.089	118.544	62.873	62.938	88.523	88.476	80.941	80.885	96.229	95.608	98.595	98.511	104.873	103.887
50	108.327	108.320	125.284	121.794	63.364	63.449	90.266	90.281	81.582	81.528	98.453	97.837	99.391	99.316	107.594	106.637
70	109.127	109.135	127.804	124.359	63.788	63.889	91.656	91.719	82.132	82.080	100.224	99.615	100.069	100.003	109.750	108.820
90	109.967	109.991	130.295	126.897	64.237	64.355	93.042	93.152	82.715	82.666	101.987	101.388	100.785	100.730	111.888	110.989
110	110.847	110.889	132.759	129.409	64.713	64.847	94.423	94.578	83.330	83.286	103.740	103.155	101.536	101.494	114.009	113.144
130	111.765	111.827	135.197	131.896	65.214	65.365	95.798	95.996	83.975	83.938	105.484	104.914	102.323	102.296	116.111	115.285
150	112.722	112.804	137.608	134.358	65.740	65.908	97.167	97.407	84.651	84.621	107.216	106.664	103.144	103.134	118.196	117.410
170	113.715	113.820	139.993	136.795	66.289	66.475	98.528	98.808	85.356	85.335	108.935	108.405	103.999	104.008	120.262	119.519
190	114.744	114.873	142.351	139.206	66.862	67.066	99.881	100.199	86.089	86.079	110.640	110.133	104.887	104.916	122.308	121.611
210	115.807	115.962	144.683	141.592	67.458	67.679	101.223	101.579	86.849	86.851	112.331	111.849	105.806	105.858	124.334	123.685
230	116.904	117.085	146.987	143.951	68.075	68.314	102.554	102.947	87.636	87.650	114.006	113.551	106.755	106.831	126.340	125.740
250	118.033	118.243	149.265	146.284	68.712	68.969	103.874	104.302	88.447	88.476	115.665	115.237	107.734	107.835	128.324	127.774
270	119.193	119.432	151.515	148.589	69.370	69.645	105.182	105.643	89.282	89.327	117.307	116.908	108.741	108.870	130.288	129.789
290	120.382	120.653	153.737	150.868	70.046	70.340	106.477	106.971	90.141	90.202	118.931	118.562	109.775	109.932	132.229	131.782
310	121.601	121.903	155.933	153.120	70.741	71.053	107.758	108.284	91.022	91.101	120.537	120.199	110.835	111.023	134.148	133.754
330	122.847	123.183	158.101	155.344	71.453	71.783	109.026	109.583	91.924	92.022	122.126	121.819	111.920	112.140	136.045	135.704
350	124.120	124.490	160.242	157.541	72.182	72.531	110.280	110.867	92.847	92.964	123.696	123.421	113.030	113.282	137.920	137.632
370	125.419	125.825	162.356	159.711	72.927	73.294	111.519	112.136	93.790	93.927	125.247	125.005	114.163	114.449	139.773	139.538
390	126.742	127.185	164.444	161.855	73.688	74.074	112.745	113.390	94.752	94.910	126.781	126.571	115.319	115.640	141.603	141.423
410	128.090	128.570	166.505	163.971	74.463	74.868	113.956	114.629	95.732	95.913	128.296	128.119	116.497	116.854	143.412	143.285
430	129.461	129.979	168.540	166.061	75.253	75.677	115.154	115.854	96.730	96.933	129.792	129.649	117.696	118.090	145.199	145.125
450	130.854	131.411	170.549	168.126	76.057	76.499	116.337	117.063	97.744	97.971	131.271	131.160	118.915	119.347	146.964	146.943

Table 26. SCF- (E_{SCF}), zero-point corrected (*ZPE*) energies [Hartrees], thermal corrections to E_{SCF} [$\Delta E(T)$ / kcal·mol^{-1}], and entropies [$S(T)$ / cal·mol^{-1}·K^{-1}] for geometry-optimized 5a, TS-a, 5b, and TS-b. Both internal hindered rotation corrected and non-corrected values of $\Delta E(T)$ and $S(T)$ are provided. The computed vibrational frequencies were scaled by an empirical factor of 0.9613 (recommended by Foresman and Frisch[1]). Thermochemistry was modeled for the case of 0.001 atm pressure and the ^{1}H, ^{11}B, ^{12}C, ^{14}N, and ^{19}F set of isotopes.

T, °C	**5a** (E_{SCF}; *ZPE*) –590.325023; –590.211450				**TS-a** (E_{SCF}; *ZPE*) –769.400296; –769.220329				**5b** (E_{SCF}; *ZPE*) –629.653501; –629.511477				**TS-b** (E_{SCF}; *ZPE*) –769.400859; –769.219918			
	$\Delta E(T)$ corr./non-corr.		$S(T)$ corr./non-corr.		$\Delta E(T)$ corr./non-corr.		$S(T)$ corr./non-corr.		$\Delta E(T)$ corr./non-corr.		$S(T)$ corr./non-corr.		$\Delta E(T)$ corr./non-corr.		$S(T)$ corr./non-corr.	
25	74.476	74.685	113.830	114.147	118.170	118.223	151.129	148.106	92.541	92.627	121.465	121.141	118.648	118.540	148.618	145.498
50	75.334	75.585	116.751	117.205	119.471	119.570	155.480	152.601	93.546	93.659	124.860	124.622	119.994	119.876	153.113	149.961
70	76.061	76.346	119.053	119.610	120.568	120.705	158.891	156.128	94.399	94.533	127.538	127.366	121.128	121.004	156.637	153.465
90	76.823	77.144	121.324	121.981	121.712	121.890	162.246	159.597	95.293	95.451	130.182	130.077	122.311	122.182	160.100	156.915
110	77.620	77.976	123.566	124.318	122.904	123.124	165.547	163.012	96.227	96.410	132.793	132.754	123.542	123.410	163.504	160.312
130	78.450	78.842	125.778	126.621	124.142	124.406	168.796	166.374	97.201	97.410	135.370	135.398	124.818	124.686	166.852	163.658
150	79.312	79.740	127.960	128.891	125.424	125.734	171.995	169.684	98.211	98.448	137.914	138.008	126.138	126.008	170.144	166.955
170	80.204	80.669	130.113	131.128	126.749	127.106	175.146	172.943	99.259	99.524	140.423	140.583	127.501	127.375	173.381	170.202
190	81.127	81.628	132.236	133.332	128.114	128.520	178.247	176.152	100.340	100.636	142.897	143.124	128.903	128.784	176.564	173.400
210	82.077	82.615	134.328	135.503	129.519	129.975	181.301	179.311	101.455	101.782	145.337	145.631	130.345	130.235	179.694	176.549
230	83.054	83.629	136.391	137.640	130.962	131.469	184.307	182.422	102.601	102.961	147.742	148.102	131.823	131.724	182.773	179.651
250	84.057	84.670	138.423	139.745	132.441	133.001	187.266	185.484	103.777	104.171	150.112	150.538	133.337	133.252	185.800	182.705
270	85.084	85.735	140.425	141.817	133.954	134.568	190.179	188.498	104.983	105.412	152.448	152.940	134.884	134.815	188.778	185.713
290	86.135	86.823	142.396	143.857	135.501	136.170	193.047	191.466	106.215	106.681	154.749	155.306	136.464	136.413	191.706	188.673
310	87.209	87.934	144.338	145.865	137.079	137.804	195.870	194.387	107.475	107.977	157.015	157.638	138.075	138.044	194.586	191.588
330	88.303	89.067	146.251	147.841	138.687	139.470	198.649	197.262	108.759	109.300	159.248	159.935	139.716	139.707	197.420	194.459
350	89.418	90.219	148.134	149.786	140.325	141.166	201.385	200.093	110.068	110.648	161.447	162.198	141.385	141.400	200.207	197.284
370	90.553	91.392	149.989	151.701	141.991	142.890	204.079	202.880	111.400	112.020	163.614	164.427	143.082	143.122	202.950	200.067
390	91.706	92.583	151.815	153.586	143.683	144.643	206.731	205.624	112.754	113.415	165.747	166.624	144.805	144.871	205.649	202.806
410	92.877	93.792	153.614	155.441	145.402	146.422	209.343	208.326	114.129	114.831	167.850	168.788	146.554	146.648	208.306	205.505
430	94.065	95.019	155.385	157.268	147.145	148.227	211.915	210.987	115.525	116.270	169.920	170.920	148.326	148.450	210.920	208.162
450	95.269	96.261	157.130	159.066	148.912	150.056	214.449	213.608	116.940	117.728	171.961	173.021	150.122	150.277	213.495	210.779

Table 27. SCF- (E_{SCF}), zero-point corrected (*ZPE*) energies [Hartrees], thermal corrections to E_{SCF} [$\Delta E(T)$ / kcal·mol^{-1}], and entropies [$S(T)$ / cal·mol^{-1}·K^{-1}] for geometry-optimized EtF, BF_3, and 2…HF. For EtF and 2…HF, both internal hindered rotation corrected and non-corrected values of $\Delta E(T)$ and $S(T)$ are provided. The computed vibrational frequencies were scaled by an empirical factor of 0.9613 (recommended by Foresman and Frisch[1]). Thermochemistry was modeled for the case of 0.001 atm pressure and the ^{1}H, ^{11}B, ^{12}C, ^{14}N, and ^{19}F set of isotopes.

T, °C	EtF (E_{SCF}; *ZPE*) –179.127044; –179.059472				BF_3 (E_{SCF}; *ZPE*) –324.679084; –324.666840		**2…HF** (E_{SCF}; *ZPE*) –769.454034; –769.271245				PF_5 (E_{SCF}; *ZPE*) –840.906298; –840.890078		**10** (E_{SCF}; *ZPE*) –304.886891; –304.760850			
	$\Delta E(T)$ corr./non-corr.		$S(T)$ corr./non-corr.		$\Delta E(T)$	$S(T)$	$\Delta E(T)$ corr./non-corr		$S(T)$ corr./non-corr.		$\Delta E(T)$	$S(T)$	$\Delta E(T)$ corr./non-corr		$S(T)$ corr./non-corr.	
25	43.277	43.233	77.347	77.085	9.626	74.785	119.575	119.756	140.840	140.157	13.345	90.508	80.531	80.569	97.107	96.616
50	43.601	43.547	78.551	78.255	9.892	75.800	120.925	121.129	145.344	144.739	13.841	92.265	81.172	81.242	99.329	98.942
70	43.876	43.813	79.497	79.174	10.112	76.582	122.061	122.287	148.876	148.333	14.254	93.625	81.719	81.816	101.090	100.785
90	44.165	44.093	80.428	80.080	10.340	77.338	123.247	123.495	152.346	151.869	14.680	94.946	82.296	82.422	102.837	102.613
110	44.468	44.388	81.345	80.976	10.574	78.071	124.480	124.754	155.758	155.348	15.119	96.228	82.904	83.059	104.572	104.427
130	44.784	44.696	82.251	81.862	10.814	78.783	125.759	126.060	159.112	158.772	15.568	97.472	83.541	83.727	106.295	106.227
150	45.113	45.018	83.143	82.737	11.059	79.474	127.083	127.413	162.411	162.143	16.028	98.681	84.208	84.425	108.005	108.013
170	45.455	45.354	84.024	83.604	11.311	80.146	128.448	128.810	165.656	165.461	16.497	99.855	84.903	85.152	109.701	109.783
190	45.809	45.703	84.894	84.462	11.567	80.800	129.854	130.251	168.847	168.728	16.974	100.995	85.626	85.907	111.384	111.537
210	46.175	46.065	85.752	85.310	11.829	81.436	131.300	131.732	171.986	171.943	17.459	102.104	86.375	86.689	113.052	113.275
230	46.553	46.439	86.599	86.150	12.095	82.056	132.782	133.253	175.073	175.107	17.950	103.182	87.150	87.498	114.705	114.995
250	46.942	46.826	87.434	86.981	12.365	82.661	134.300	134.811	178.109	178.222	18.448	104.230	87.951	88.332	116.342	116.698
270	47.342	47.224	88.259	87.803	12.639	83.250	135.852	136.406	181.095	181.287	18.952	105.250	88.775	89.191	117.963	118.384
290	47.753	47.634	89.074	88.616	12.918	83.825	137.437	138.035	184.032	184.305	19.462	106.243	89.623	90.073	119.567	120.050
310	48.174	48.055	89.878	89.420	13.200	84.387	139.053	139.697	186.920	187.274	19.976	107.210	90.493	90.978	121.155	121.698
330	48.605	48.487	90.671	90.215	13.485	84.935	140.699	141.391	189.762	190.197	20.495	108.152	91.384	91.904	122.725	123.327
350	49.046	48.929	91.455	91.001	13.774	85.471	142.373	143.116	192.558	193.075	21.019	109.070	92.296	92.852	124.277	124.937
370	49.496	49.381	92.229	91.778	14.066	85.994	144.075	144.869	195.309	195.907	21.546	109.966	93.229	93.819	125.812	126.529
390	49.955	49.844	92.993	92.547	14.360	86.506	145.803	146.651	198.016	198.696	22.076	110.839	94.180	94.807	127.330	128.101
410	50.423	50.315	93.747	93.306	14.658	87.007	147.557	148.460	200.680	201.442	22.611	111.692	95.150	95.812	128.830	129.654
430	50.900	50.796	94.492	94.057	14.958	87.497	149.335	150.294	203.302	204.146	23.148	112.524	96.138	96.836	130.312	204.146
450	51.385	51.286	95.228	94.800	15.260	87.977	151.136	152.153	205.884	206.809	23.688	113.337	97.143	97.878	131.778	206.809

Table 28. SCF- (E_{SCF}), zero-point corrected (ZPE) energies [Hartrees], thermal corrections to E_{SCF} [$\Delta E(T)$ / kcal·mol^{-1}], and entropies [$S(T)$ / cal·mol^{-1}·K^{-1}] for geometry-optimized TS-C_2H_4 and C_2H_4. For TS-C_2H_4, both internal hindered rotation corrected and non-corrected values of $\Delta E(T)$ and $S(T)$ are provided. The computed vibrational frequencies were scaled by an empirical factor of 0.9613 (recommended by Foresman and Frisch[1]). Thermochemistry was modeled for the case of 0.001 atm pressure and the ^{1}H and ^{12}C set of isotopes.

T, °C	**TS-C_2H_4** (E_{SCF}; ZPE) −769.383353; −769.209495				C_2H_4 (E_{SCF}; ZPE) −78.617639; −78.566807	
	$\Delta E(T)$ corr./non-corr.		$S(T)$ corr./non-corr.		$\Delta E(T)$	$S(T)$
25	114.449	114.784	155.111	151.205	32.592	67.494
50	115.755	116.161	159.473	155.798	32.808	68.350
70	116.856	117.322	162.899	159.403	32.992	69.021
90	118.008	118.535	166.273	162.950	33.186	69.681
110	119.208	119.798	169.596	166.440	33.389	70.332
130	120.455	121.109	172.870	169.877	33.602	70.975
150	121.748	122.467	176.097	173.260	33.824	71.609
170	123.085	123.870	179.275	176.591	34.056	72.236
190	124.465	125.316	182.407	179.870	34.297	72.856
210	125.884	126.803	185.491	183.097	34.546	73.467
230	127.343	128.330	188.529	186.274	34.805	74.072
250	128.838	129.894	191.521	189.401	35.072	74.669
270	130.369	131.495	194.467	192.478	35.346	75.260
290	131.934	133.130	197.368	195.506	35.629	75.843
310	133.531	134.798	200.225	198.485	35.920	76.419
330	135.160	136.498	203.037	201.418	36.217	76.988
350	136.818	138.228	205.806	204.304	36.522	77.550
370	138.504	139.986	208.532	207.144	36.834	78.105
390	140.218	141.773	211.217	209.940	37.153	78.654
410	141.958	143.585	213.861	212.692	37.478	79.197
430	143.723	145.423	216.465	215.402	37.810	79.732
450	145.512	147.286	219.029	218.069	38.148	80.262

Computed Vibrational Frequencies

Table 29. Computed frequencies (ν / cm^{-1}; non-scaled), reduced masses *m*, force constants *f*, and IR spectrum intensities *I* (all in atomic units) for 1, TS, and 7.

Freq.	1				TS				7			
No.	ν	*m*	*f*	*I*	ν	*m*	*f*	*I*	ν	*m*	*f*	*I*
1	23.7	9.088	0.003	0.118	*i*31.1	10.487	0.006	0.255	30.2	7.046	0.004	4.769
2	36.0	2.770	0.002	1.779	9.1	10.911	0.001	0.469	46.3	2.481	0.003	0.625
3	45.0	5.203	0.006	4.178	23.4	7.052	0.002	1.776	64.7	4.049	0.010	1.041
4	68.0	10.906	0.030	2.539	31.4	4.022	0.002	2.211	102.6	1.087	0.007	0.104
5	77.3	3.619	0.013	5.274	42.3	5.958	0.006	3.413	134.6	3.304	0.035	3.064
6	91.8	5.863	0.029	3.743	48.2	4.496	0.006	1.848	197.1	2.534	0.058	1.476
7	106.3	2.249	0.015	6.419	53.0	4.631	0.008	0.112	230.2	2.703	0.084	3.187
8	128.8	1.484	0.015	5.016	66.9	12.097	0.032	0.228	233.0	1.633	0.052	5.683
9	172.9	4.933	0.087	19.877	76.5	6.774	0.023	0.805	319.9	2.374	0.143	12.705
10	213.8	1.173	0.032	0.143	101.6	1.108	0.007	0.118	390.3	3.238	0.291	1.565
11	246.5	3.430	0.123	2.029	138.5	3.342	0.038	6.173	444.0	2.667	0.310	3.301
12	302.6	2.030	0.110	1.176	191.7	2.385	0.052	0.418	609.4	3.734	0.817	3.367
13	345.9	18.833	1.327	0.138	223.2	1.540	0.045	2.987	630.1	3.981	0.931	2.253
14	348.1	18.632	1.331	0.099	237.8	3.253	0.108	7.222	660.0	4.038	1.036	6.624
15	390.9	3.425	0.308	0.514	318.8	2.415	0.145	9.778	718.6	1.255	0.382	53.570
16	425.4	2.500	0.267	1.399	390.5	3.250	0.292	3.256	726.5	3.859	1.200	13.953
17	504.0	18.191	2.723	1.727	444.8	2.688	0.313	3.154	806.3	1.162	0.445	0.700
18	507.6	18.040	2.738	1.492	467.4	17.728	2.282	10.178	819.4	1.384	0.548	0.064
19	515.6	17.501	2.741	18.845	472.3	17.768	2.335	9.532	959.6	2.481	1.346	9.490
20	598.6	3.666	0.774	2.273	607.5	3.763	0.818	2.351	1020.4	2.674	1.641	6.589
21	637.7	3.336	0.799	6.625	630.1	4.227	0.989	4.894	1036.8	3.420	2.166	3.135
22	674.5	3.597	0.964	37.209	647.3	7.982	1.971	135.204	1069.6	1.080	0.728	49.526
23	707.2	3.621	1.067	10.603	664.1	4.507	1.171	54.342	1080.1	1.705	1.172	7.295
24	731.0	1.257	0.396	34.053	723.0	1.279	0.394	51.402	1100.8	1.539	1.099	2.496
25	746.1	18.665	6.122	9.981	725.9	3.704	1.150	13.204	1110.6	1.442	1.048	5.492
26	808.5	1.134	0.437	1.911	805.2	1.161	0.444	0.729	1136.5	1.881	1.432	9.116
27	840.0	1.387	0.577	0.057	823.7	1.386	0.554	0.131	1157.3	1.318	1.040	0.021
28	939.5	1.431	0.744	139.570	876.6	18.932	8.571	1.606	1177.2	1.320	1.077	96.049
29	961.8	6.075	3.311	234.086	959.7	2.478	1.345	8.472	1235.3	1.649	1.483	16.905
30	964.2	2.416	1.323	5.120	1020.9	2.681	1.646	6.282	1284.9	1.693	1.646	6.834
31	1009.7	7.788	4.678	248.763	1036.4	3.127	1.979	4.779	1353.9	4.028	4.351	0.926
32	1043.8	3.820	2.452	17.503	1071.0	1.146	0.774	40.897	1373.5	4.158	4.622	5.935
33	1048.4	3.143	2.035	25.601	1079.5	1.452	0.997	15.242	1392.3	1.411	1.611	23.831
34	1106.8	1.752	1.265	7.687	1100.6	1.599	1.141	2.123	1412.0	2.487	2.922	2.698
35	1112.2	1.341	0.978	8.306	1109.3	1.364	0.989	6.912	1417.0	1.264	1.495	11.940
36	1121.6	1.471	1.090	1.675	1136.1	1.822	1.385	11.573	1438.6	1.732	2.112	22.788
37	1138.4	1.676	1.280	17.373	1152.8	1.443	1.130	61.350	1478.6	1.426	1.837	12.986
38	1161.0	1.455	1.156	55.144	1158.0	1.316	1.040	0.462	1493.0	1.054	1.384	6.309
39	1168.5	5.755	4.630	483.768	1233.4	1.724	1.545	27.498	1495.2	1.040	1.370	9.900
40	1183.0	1.850	1.526	129.265	1284.4	1.701	1.654	9.903	1498.1	1.130	1.494	6.768
41	1272.2	1.391	1.326	7.175	1355.0	4.464	4.829	1.492	1509.0	1.086	1.458	5.474
42	1318.3	1.442	1.477	0.205	1373.5	4.148	4.611	5.288	1512.4	1.134	1.528	12.986
43	1353.3	4.876	5.262	8.217	1391.4	1.425	1.626	11.539	1598.4	4.350	6.549	1.712
44	1395.8	1.552	1.781	12.804	1409.0	6.991	8.178	257.201	2473.5	1.077	3.882	3015.460
45	1411.1	1.925	2.259	6.429	1411.4	2.710	3.181	65.190	3033.7	1.035	5.612	17.157
46	1423.2	1.279	1.526	6.812	1417.6	1.273	1.508	14.216	3042.4	1.035	5.644	44.406
47	1450.8	2.854	3.539	3.481	1439.8	1.879	2.295	4.927	3050.5	1.067	5.852	24.354
48	1467.6	1.242	1.576	8.333	1445.9	8.822	10.867	390.995	3092.3	1.101	6.205	16.270
49	1493.4	1.043	1.371	8.927	1480.5	1.368	1.766	7.421	3100.0	1.105	6.258	15.508
50	1496.4	1.056	1.393	13.317	1491.8	1.052	1.379	6.743	3106.7	1.100	6.253	20.440
51	1498.5	1.050	1.389	5.033	1496.0	1.050	1.384	12.221	3122.6	1.102	6.331	9.200
52	1509.9	1.169	1.571	10.252	1497.8	1.141	1.509	6.925	3151.4	1.102	6.447	0.331
53	1516.2	1.107	1.499	8.319	1509.4	1.090	1.463	6.771	3256.5	1.091	6.814	1.375
54	1595.3	3.489	5.232	37.906	1512.7	1.130	1.524	10.441	3276.0	1.108	7.008	0.058
55	1605.3	3.714	5.639	25.646	1597.4	4.300	6.465	0.684				
56	3036.7	1.035	5.626	13.202	2573.9	1.076	4.199	2631.250				
57	3059.6	1.033	5.696	25.602	3034.4	1.035	5.615	16.643				
58	3074.3	1.062	5.915	10.405	3046.3	1.035	5.658	38.433				
59	3097.6	1.103	6.237	19.263	3053.4	1.067	5.861	20.373				
60	3109.7	1.100	6.269	16.432	3093.1	1.101	6.208	14.840				
61	3130.2	1.107	6.392	6.120	3105.3	1.105	6.281	13.719				
62	3138.4	1.105	6.413	3.805	3107.5	1.100	6.257	18.909				
63	3160.2	1.107	6.514	6.644	3123.2	1.103	6.336	9.947				
64	3240.5	1.106	6.843	180.131	3155.0	1.102	6.463	0.394				
65	3274.9	1.092	6.903	6.579	3257.8	1.091	6.821	1.551				
66	3292.2	1.109	7.080	1.943	3277.2	1.108	7.014	0.009				

Table 30. Computed frequencies (ν /cm^{-1}; non-scaled), reduced masses *m*, force constants *f*, and IR spectrum intensities *I* (all in atomic units) for 5a, 5b, TS-a, and TS-b.

Freq.	5a				5b				TS-a				TS-b			
No.	ν	*m*	*f*	*I*	ν	*m*	*f*	*I*	ν	*m*	*f*	*I*	ν	*m*	*f*	*I*
1	19.2	4.991	0.001	0.016	17.3	5.664	0.001	0.124	*i*360.6	8.876	0.680	886.238	*i*422.9	11.359	1.197	1237.209
2	68.3	1.157	0.003	0.000	35.7	2.832	0.002	0.935	12.1	5.938	0.001	1.131	7.5	4.841	0.000	0.473
3	101.4	4.638	0.028	0.062	94.6	4.874	0.026	0.098	14.9	4.022	0.001	0.245	26.6	4.720	0.002	2.559
4	130.1	6.186	0.062	0.857	125.6	4.481	0.042	0.882	34.9	5.910	0.004	0.289	32.8	6.343	0.004	0.973
5	213.8	3.375	0.091	1.333	145.1	4.223	0.052	0.224	52.6	2.895	0.005	0.971	50.3	3.258	0.005	1.620
6	269.7	7.726	0.331	1.396	220.1	1.252	0.036	0.062	74.0	1.248	0.004	1.427	66.8	5.129	0.014	0.283
7	311.4	7.295	0.417	1.238	264.2	6.474	0.266	1.180	82.7	1.793	0.007	6.182	104.4	6.160	0.040	9.374
8	323.7	9.383	0.579	2.029	313.3	4.925	0.285	1.047	85.8	2.163	0.009	4.414	120.3	1.058	0.009	0.287
9	386.0	3.698	0.325	1.804	320.9	8.727	0.529	1.543	101.5	3.644	0.022	8.314	141.2	3.816	0.045	1.893
10	476.5	12.313	1.647	1.006	371.8	3.132	0.255	1.569	147.3	9.473	0.121	16.461	178.8	10.078	0.190	25.173
11	503.1	9.948	1.483	0.212	414.5	3.641	0.369	0.993	211.0	3.251	0.085	5.697	220.1	1.154	0.033	0.833
12	631.3	3.302	0.775	6.893	477.8	11.728	1.577	0.876	223.8	4.075	0.120	8.953	278.3	4.926	0.225	8.782
13	646.3	11.768	2.896	90.918	504.7	9.063	1.360	0.246	275.7	3.455	0.155	14.283	301.5	3.753	0.201	23.503
14	680.6	3.039	0.829	17.281	636.4	4.832	1.153	28.544	291.8	3.620	0.182	14.101	347.0	10.225	0.726	2.114
15	689.2	4.655	1.303	30.744	655.0	5.605	1.417	65.544	342.9	8.671	0.601	9.651	354.9	4.498	0.334	11.825
16	737.3	1.239	0.397	31.999	672.8	3.612	0.963	34.244	365.0	3.229	0.254	0.804	365.5	3.512	0.277	3.898
17	859.5	1.433	0.624	21.484	681.0	2.942	0.804	20.171	381.5	5.596	0.480	3.278	402.8	3.365	0.322	0.190
18	868.4	1.433	0.637	7.820	738.0	1.244	0.399	29.931	471.0	11.595	1.516	21.856	460.5	11.016	1.376	37.075
19	872.7	13.313	5.975	407.294	800.9	1.142	0.431	1.282	497.0	17.079	2.486	7.151	492.9	17.227	2.466	6.859
20	1011.4	5.182	3.124	95.932	859.5	1.467	0.638	21.637	514.6	15.594	2.433	16.765	517.0	14.337	2.258	23.642
21	1040.4	3.219	2.053	25.124	868.1	1.429	0.635	6.844	629.0	3.100	0.723	6.554	636.9	3.488	0.833	5.964
22	1091.2	1.518	1.065	22.756	874.0	13.137	5.912	421.713	668.7	3.441	0.907	6.842	661.3	3.301	0.851	9.564
23	1120.7	1.342	0.993	57.278	961.5	2.439	1.329	2.025	673.6	4.888	1.307	62.974	667.8	10.856	2.853	144.883
24	1136.5	1.937	1.474	81.692	1012.7	4.759	2.876	108.118	680.8	8.334	2.276	130.654	672.9	3.042	0.811	19.360
25	1152.1	1.328	1.038	3.020	1044.9	3.212	2.066	31.242	737.9	1.254	0.402	33.092	735.4	1.251	0.399	35.262
26	1162.0	11.091	8.824	335.535	1100.6	1.905	1.360	3.361	824.1	1.412	0.565	27.970	801.3	1.144	0.433	1.197
27	1162.8	6.139	4.891	230.094	1117.9	1.457	1.072	90.448	831.4	1.077	0.439	0.171	834.0	1.436	0.589	25.897
28	1273.2	1.473	1.407	5.784	1126.5	1.471	1.100	5.764	858.7	9.755	4.237	239.266	856.4	1.400	0.605	0.639
29	1323.2	4.192	4.325	21.851	1138.4	2.002	1.529	80.463	866.1	1.387	0.613	7.742	858.3	13.917	6.041	167.795
30	1396.0	4.083	4.688	3.887	1159.2	8.999	7.125	307.947	937.8	5.555	2.879	8.682	943.4	5.691	2.984	14.557
31	1407.0	5.637	6.575	0.109	1162.5	6.972	5.551	247.425	995.1	1.476	0.861	66.818	962.8	2.417	1.320	11.645
32	1460.2	1.234	1.550	9.707	1260.2	1.383	1.295	1.817	1042.8	2.384	1.527	7.615	1048.4	3.364	2.179	11.671
33	1488.0	1.038	1.354	11.983	1287.6	2.095	2.047	12.437	1044.3	2.854	1.834	7.065	1095.8	1.230	0.871	5.236
34	1514.3	1.126	1.521	9.895	1325.7	2.429	2.515	22.375	1057.4	1.141	0.751	34.080	1101.1	1.607	1.148	3.351
35	1576.2	3.307	4.841	44.859	1387.9	1.457	1.653	12.875	1085.2	1.557	1.080	9.010	1106.9	1.328	0.959	40.498
36	1583.1	4.259	6.289	37.035	1397.9	3.754	4.322	6.377	1106.1	1.390	1.002	28.838	1110.4	1.164	0.846	44.346
37	3054.6	1.033	5.679	24.025	1422.5	1.265	1.508	6.032	1131.9	1.937	1.462	12.280	1123.9	1.616	1.203	1.107
38	3119.5	1.106	6.343	6.335	1431.8	2.583	3.120	4.501	1138.1	7.090	5.411	352.319	1134.5	1.813	1.375	47.460
39	3146.5	1.104	6.439	3.320	1492.1	1.074	1.408	7.805	1150.1	1.313	1.023	0.060	1162.8	5.093	4.057	319.306
40	3271.5	1.093	6.890	5.216	1493.5	1.041	1.368	12.257	1202.3	1.995	1.699	132.965	1233.5	6.554	5.876	414.295
41	3283.5	1.099	6.979	17.153	1509.8	1.111	1.492	7.927	1216.5	1.609	1.403	46.946	1258.2	1.581	1.475	11.444
42	3290.3	1.109	7.070	2.228	1565.4	3.411	4.925	44.921	1228.1	2.089	1.856	314.443	1269.2	1.404	1.332	15.156
43					1582.1	4.346	6.409	40.076	1268.2	1.798	1.704	16.346	1286.9	1.572	1.533	46.035
44					3040.1	1.035	5.635	9.780	1312.7	2.037	2.067	15.000	1319.6	1.858	1.906	27.002
45					3062.0	1.061	5.863	15.002	1384.5	5.552	6.270	0.027	1381.0	4.969	5.584	0.769
46					3095.1	1.104	6.231	0.452	1388.5	4.066	4.619	2.144	1389.2	1.334	1.517	20.926
47					3109.0	1.101	6.272	20.170	1407.3	1.194	1.393	15.502	1401.3	1.105	1.279	2.854
48					3119.2	1.106	6.337	17.630	1456.9	1.265	1.582	21.314	1420.4	1.481	1.761	3.423
49					3271.4	1.093	6.889	4.620	1476.9	1.103	1.417	7.373	1422.4	1.113	1.327	5.627
50					3281.8	1.099	6.971	16.497	1479.0	1.041	1.342	8.139	1424.0	1.818	2.172	7.675
51					3290.3	1.108	7.069	2.411	1487.7	1.038	1.354	10.587	1490.3	1.103	1.443	13.798
52									1502.2	1.134	1.508	3.174	1493.8	1.039	1.366	12.190
53									1513.2	1.170	1.579	7.416	1508.1	1.131	1.516	9.554
54									1548.4	2.997	4.234	76.271	1546.0	2.949	4.153	37.392
55									1554.8	2.892	4.119	15.467	1547.9	3.271	4.617	46.792
56									3050.6	1.033	5.664	32.647	3039.4	1.035	5.632	10.952
57									3054.3	1.035	5.687	12.831	3059.6	1.061	5.853	17.176
58									3114.0	1.106	6.320	7.601	3092.8	1.104	6.222	0.212
59									3118.6	1.099	6.298	4.839	3107.8	1.101	6.268	22.047
60									3130.8	1.105	6.381	9.803	3117.6	1.105	6.330	18.752
61									3139.5	1.104	6.408	4.677	3157.8	1.009	5.925	15.647
62									3215.7	1.054	6.423	17.572	3246.5	1.097	6.813	4.170
63									3248.3	1.094	6.804	0.254	3249.9	1.093	6.800	5.523
64									3249.8	1.095	6.814	6.239	3272.3	1.105	6.974	0.059
65									3272.3	1.106	6.974	0.050	3347.1	1.125	7.424	1.442
66									3335.9	1.126	7.382	5.293	3357.4	1.126	7.476	4.664

Table 31. Computed frequencies (ν / cm^{-1}; non-scaled), reduced masses *m*, force constants *f*, and IR spectrum intensities *I* (all in atomic units) for 3, 6, and 2...HF.

Freq.	3				6				2…HF			
No.	ν	*m*	*f*	*I*	ν	*m*	*f*	*I*	ν	*m*	*f*	*I*
1	22.9	6.466	0.002	0.171	12.8	4.180	0.000	0.153	19.6	8.926	0.002	2.962
2	37.2	5.383	0.004	3.322	69.6	1.238	0.004	0.061	43.1	5.439	0.006	1.016
3	57.4	6.751	0.013	0.163	94.1	3.686	0.019	0.321	56.4	8.052	0.015	1.739
4	75.3	4.487	0.015	4.771	124.4	6.528	0.060	0.234	74.5	3.296	0.011	1.848
5	79.6	8.383	0.031	3.074	208.0	3.538	0.090	0.705	83.7	1.161	0.005	0.356
6	100.2	1.147	0.007	1.047	222.4	8.257	0.241	1.894	94.7	3.295	0.017	2.698
7	107.3	1.150	0.008	1.550	268.3	6.828	0.290	3.302	141.9	5.233	0.062	1.902
8	134.5	2.900	0.031	27.417	279.5	18.633	0.858	0.111	175.2	5.387	0.098	3.097
9	206.7	3.442	0.087	3.394	286.8	8.337	0.404	1.914	200.4	4.029	0.095	9.163
10	268.7	3.514	0.150	0.706	367.7	5.084	0.405	1.511	217.4	1.549	0.043	1.621
11	284.5	17.173	0.819	0.036	402.3	11.348	1.082	0.162	221.5	2.621	0.076	1.679
12	290.2	2.858	0.142	1.896	424.4	5.289	0.561	2.043	278.0	6.703	0.305	5.928
13	293.9	14.788	0.752	0.068	460.6	18.995	2.374	0.795	288.9	3.741	0.184	9.341
14	297.4	18.632	0.971	0.084	511.6	17.031	2.626	15.175	316.0	6.537	0.385	2.203
15	425.1	2.676	0.285	1.973	513.7	20.175	3.137	175.445	355.8	3.217	0.240	0.196
16	441.3	18.956	2.176	0.164	524.5	15.207	2.465	13.051	402.8	4.293	0.410	0.125
17	445.1	18.003	2.101	0.328	559.2	18.500	3.409	0.268	439.8	5.523	0.629	5.269
18	449.4	18.774	2.234	3.325	629.3	3.201	0.747	6.718	470.3	9.663	1.259	3.712
19	505.8	18.358	2.767	8.395	668.4	10.823	2.849	4.450	520.6	4.115	0.657	2.260
20	518.6	18.940	3.001	2.875	674.9	3.015	0.809	14.018	598.7	4.097	0.865	4.570
21	529.6	20.202	3.338	32.163	688.2	5.323	1.485	10.970	644.5	4.286	1.049	6.645
22	529.8	19.668	3.253	31.645	733.5	1.238	0.392	29.233	655.0	5.456	1.379	13.122
23	530.4	19.446	3.223	38.554	823.7	22.216	8.881	478.254	707.7	1.083	0.320	126.429
24	607.0	4.489	0.975	1.022	840.4	19.625	8.167	313.037	721.9	1.480	0.454	47.063
25	632.2	3.257	0.767	0.226	844.9	22.152	9.316	310.893	737.2	4.108	1.316	9.952
26	653.7	3.566	0.898	62.257	857.7	1.499	0.650	46.929	752.6	3.559	1.187	7.296
27	676.0	18.995	5.114	67.851	878.6	1.432	0.652	21.891	773.5	1.067	0.376	196.056
28	720.3	4.273	1.306	10.770	992.1	5.692	3.301	59.022	814.4	1.163	0.455	3.138
29	733.6	1.238	0.393	33.771	1039.4	3.207	2.041	8.104	837.0	1.396	0.576	0.030
30	814.6	19.787	7.737	454.413	1097.2	1.521	1.079	5.167	901.9	10.212	4.894	310.826
31	817.5	23.192	9.133	343.778	1122.3	1.260	0.935	13.494	964.3	2.464	1.350	10.055
32	830.1	24.570	9.976	419.749	1132.6	1.842	1.392	83.379	1028.7	9.709	6.053	258.356
33	844.2	1.379	0.579	0.057	1152.6	1.317	1.030	0.026	1047.2	3.029	1.958	6.155
34	938.0	1.272	0.659	10.677	1278.7	1.475	1.421	3.500	1071.6	2.219	1.501	32.032
35	1038.9	3.997	2.542	2.318	1316.5	3.771	3.851	14.109	1104.1	1.826	1.311	2.284
36	1043.8	2.964	1.902	4.248	1391.2	4.747	5.413	2.599	1112.6	1.391	1.015	10.911
37	1106.8	1.544	1.114	5.126	1411.1	4.618	5.417	0.173	1127.5	1.994	1.493	39.311
38	1111.2	1.216	0.885	13.583	1460.7	1.232	1.548	11.757	1146.0	3.918	3.032	244.955
39	1127.6	1.515	1.135	0.505	1488.1	1.038	1.354	12.142	1155.6	1.473	1.159	63.720
40	1156.9	1.323	1.043	3.915	1514.0	1.128	1.523	9.668	1200.1	2.560	2.172	63.946
41	1163.7	1.319	1.053	1.458	1577.3	3.901	5.718	76.069	1241.7	1.762	1.601	19.432
42	1191.4	1.829	1.530	96.257	1583.6	3.581	5.292	13.460	1305.6	1.545	1.551	11.367
43	1310.3	1.282	1.296	1.749	3056.4	1.033	5.685	22.026	1354.2	6.125	6.619	7.773
44	1353.1	7.217	7.786	4.085	3122.6	1.106	6.356	5.317	1386.5	2.043	2.313	5.322
45	1394.1	3.019	3.458	0.973	3148.3	1.104	6.448	2.824	1404.6	1.538	1.788	20.179
46	1432.3	3.532	4.269	0.879	3276.2	1.095	6.923	6.262	1428.1	1.232	1.480	7.606
47	1457.9	1.244	1.558	9.941	3291.2	1.099	7.016	20.068	1452.3	1.593	1.980	20.523
48	1476.2	1.197	1.536	0.831	3301.3	1.106	7.104	6.877	1473.0	2.823	3.609	12.861
49	1494.0	1.043	1.372	12.889					1492.8	1.096	1.438	9.147
50	1499.8	1.043	1.382	17.569					1495.3	1.106	1.457	17.496
51	1509.3	1.211	1.626	20.836					1498.4	1.111	1.470	10.602
52	1510.8	1.107	1.488	1.484					1508.7	1.214	1.628	3.129
53	1605.9	3.498	5.316	37.962					1511.0	1.258	1.692	4.003
54	1608.4	3.695	5.633	25.558					1523.6	1.397	1.910	23.173
55	3061.7	1.033	5.706	21.035					1606.9	4.316	6.566	0.296
56	3062.7	1.033	5.707	20.368					3035.5	1.036	5.624	18.584
57	3136.9	1.105	6.407	3.325					3063.8	1.072	5.928	26.279
58	3138.9	1.106	6.420	3.587					3065.6	1.035	5.729	21.826
59	3162.9	1.106	6.521	4.865					3096.2	1.101	6.220	20.571
60	3166.1	1.106	6.533	5.979					3120.1	1.102	6.319	4.658
61	3259.2	1.105	6.917	196.313					3133.7	1.106	6.398	6.722
62	3275.9	1.093	6.909	7.723					3164.6	1.096	6.467	2.849
63	3293.2	1.109	7.087	1.649					3175.1	1.103	6.553	0.306
64									3270.5	1.092	6.880	3.831
65									3288.8	1.109	7.065	1.492
66									3635.5	1.061	8.261	754.887

Table 32. Computed frequencies (ν /cm^{-1}; non-scaled), reduced masses *m*, force constants *f*, and IR spectrum intensities *I* (all in atomic units) for 8a, 8b, 9, and 10.

Freq.	8a				8b				9				10			
No.	ν	*m*	*f*	*I*	ν	*m*	*f*	*I*	ν	*m*	*f*	*I*	ν	*m*	*f*	*I*
1	83.1	1.131	0.005	0.132	51.0	2.475	0.004	1.306	52.9	2.438	0.004	0.383	105.0	1.149	0.008	0.321
2	205.7	2.862	0.071	0.861	134.0	3.599	0.038	0.168	105.5	1.179	0.008	0.993	107.3	1.068	0.007	0.069
3	349.3	2.682	0.193	0.560	215.1	1.140	0.031	0.191	135.1	2.706	0.029	7.662	190.4	2.517	0.054	17.744
4	625.6	3.117	0.719	6.290	347.6	2.148	0.153	0.475	213.1	1.200	0.032	1.229	262.3	3.239	0.131	0.000
5	675.5	4.354	1.170	3.985	396.8	3.238	0.300	0.791	230.4	2.939	0.092	6.231	291.4	2.620	0.131	4.186
6	675.6	3.368	0.906	14.387	635.2	3.415	0.812	6.181	303.5	1.984	0.108	2.740	437.7	2.698	0.305	8.871
7	721.3	1.254	0.385	36.217	662.5	3.027	0.783	2.855	387.5	3.211	0.284	3.511	616.0	7.784	1.740	0.163
8	815.3	1.400	0.548	32.533	677.5	3.301	0.893	17.685	443.5	2.679	0.311	9.571	617.5	4.358	0.979	2.471
9	860.4	1.379	0.602	2.089	721.3	1.265	0.388	33.748	606.7	4.110	0.892	1.848	625.0	3.289	0.757	0.000
10	919.3	6.320	3.147	8.587	798.1	1.147	0.430	1.205	620.7	4.518	1.025	0.112	709.3	1.225	0.363	63.832
11	1043.2	3.453	2.214	10.013	816.1	1.415	0.555	30.515	651.5	3.879	0.970	0.615	748.7	4.616	1.524	26.249
12	1073.7	1.594	1.083	12.729	861.0	1.381	0.603	2.331	709.3	1.237	0.367	61.330	806.7	1.379	0.529	0.000
13	1096.3	1.354	0.959	11.105	920.1	6.229	3.107	8.959	730.9	3.827	1.205	22.169	1005.5	2.604	1.551	3.365
14	1135.6	2.072	1.574	18.190	959.3	2.379	1.290	6.262	803.6	1.178	0.448	1.244	1006.4	4.953	2.955	0.745
15	1147.0	1.309	1.015	0.156	1046.6	3.392	2.189	14.710	807.9	1.378	0.530	0.027	1060.0	2.466	1.632	0.375
16	1264.2	1.753	1.651	23.287	1093.9	1.435	1.012	19.475	953.6	2.581	1.383	10.277	1074.7	1.603	1.091	0.343
17	1308.1	1.926	1.941	21.416	1097.0	1.823	1.293	5.288	1005.6	3.421	2.038	2.244	1099.8	1.244	0.886	6.951
18	1374.6	4.611	5.134	3.350	1116.9	1.623	1.193	1.716	1017.8	3.144	1.919	0.811	1153.4	1.326	1.039	0.002
19	1381.8	5.495	6.181	1.016	1136.6	2.109	1.605	16.884	1066.8	2.162	1.450	0.205	1155.7	1.309	1.030	0.440
20	1452.6	1.293	1.607	16.987	1256.2	1.619	1.505	28.488	1092.5	1.697	1.193	1.603	1231.5	1.881	1.681	54.073
21	1487.2	1.040	1.355	9.469	1274.9	1.887	1.807	8.993	1099.9	1.308	0.932	7.814	1316.5	3.347	3.418	2.330
22	1511.6	1.316	1.772	6.554	1310.1	1.811	1.831	24.993	1113.8	1.898	1.387	3.754	1339.7	4.318	4.566	3.446
23	1534.2	2.788	3.866	56.928	1376.9	4.679	5.227	1.405	1155.1	1.317	1.036	0.277	1376.5	10.471	11.690	0.339
24	1539.1	2.319	3.236	7.055	1388.2	1.415	1.607	22.105	1226.5	1.897	1.682	52.437	1419.4	1.999	2.373	38.987
25	3038.3	1.034	5.622	46.436	1411.8	1.963	2.306	4.951	1263.8	2.041	1.921	13.521	1451.1	1.171	1.453	1.659
26	3094.5	1.106	6.237	15.707	1417.9	1.334	1.580	10.560	1328.3	3.289	3.419	1.846	1471.8	1.566	1.999	14.550
27	3127.4	1.102	6.349	8.178	1486.7	1.171	1.525	15.526	1366.9	5.720	6.297	0.584	1494.3	1.041	1.369	0.001
28	3232.3	1.095	6.742	2.659	1492.1	1.041	1.365	10.791	1381.7	1.915	2.154	10.969	1495.6	1.041	1.371	16.029
29	3237.1	1.092	6.742	3.042	1505.8	1.151	1.537	6.237	1389.6	1.413	1.607	30.568	1507.0	1.087	1.454	25.337
30	3261.9	1.104	6.922	1.766	1529.1	2.357	3.247	31.986	1412.5	1.284	1.509	15.448	1509.4	1.071	1.438	0.775
31					1533.2	3.356	4.649	26.619	1425.7	1.876	2.247	22.361	1599.6	4.338	6.540	0.965
32					3034.8	1.035	5.615	17.209	1462.2	1.417	1.785	10.248	3031.5	1.036	5.610	113.843
33					3045.5	1.062	5.805	26.583	1490.8	1.066	1.395	3.529	3032.4	1.036	5.614	9.293
34					3081.5	1.102	6.167	1.756	1492.7	1.068	1.402	8.498	3083.6	1.105	6.189	18.888
35					3100.1	1.101	6.235	30.644	1494.3	1.042	1.371	8.852	3084.1	1.105	6.191	27.622
36					3110.9	1.104	6.297	24.798	1506.4	1.073	1.435	4.557	3147.2	1.099	6.415	3.188
37					3229.4	1.095	6.731	2.312	1508.9	1.081	1.450	13.365	3147.7	1.099	6.417	1.617
38					3236.6	1.092	6.738	3.584	1596.1	4.481	6.726	1.643	3246.7	1.090	6.769	0.320
39					3261.3	1.104	6.919	1.755	3029.8	1.035	5.597	29.412	3267.1	1.108	6.971	1.912
40									3031.2	1.036	5.609	59.107				
41									3037.5	1.069	5.811	32.944				
42									3083.1	1.105	6.187	23.065				
43									3087.0	1.101	6.182	16.800				
44									3101.2	1.099	6.228	25.983				
45									3117.7	1.100	6.298	15.433				
46									3147.2	1.099	6.415	2.429				
47									3245.6	1.090	6.764	0.234				
48									3266.0	1.108	6.965	1.895				

Table 33. Computed frequencies (ν / cm^{-1}; non-scaled), reduced masses *m*, force constants *f*, and IR spectrum intensities *I* (all in atomic units) for $F_3B{\cdot}OEt_2$, EtF, MeF, BF_3, PF_5, PH_3, HF, and C_2H_4.

Freq. No.	$F_3B{\cdot}OEt_2$ ν	*m*	*f*	*I*
1	24.0	2.708	0.001	0.846
2	41.9	5.722	0.006	0.212
3	85.7	2.688	0.012	0.686
4	117.7	3.887	0.032	1.654
5	187.3	1.974	0.041	0.290
6	207.7	1.191	0.030	0.159
7	256.2	1.483	0.057	1.818
8	261.6	3.448	0.139	7.307
9	274.3	6.336	0.281	1.949
10	324.7	2.342	0.145	1.545
11	328.9	6.187	0.394	6.064
12	444.3	5.207	0.606	0.173
13	487.8	5.745	0.806	5.387
14	495.4	4.482	0.648	8.185
15	528.3	4.279	0.704	17.901
16	609.6	11.077	2.426	360.089
17	752.5	2.965	0.989	100.099
18	797.6	1.129	0.423	5.818
19	815.8	1.454	0.570	38.968
20	872.5	3.466	1.555	53.039
21	912.6	2.402	1.179	12.168
22	1003.2	2.561	1.519	6.851
23	1032.9	4.096	2.575	115.195
24	1108.8	1.935	1.402	1.456
25	1110.9	2.001	1.455	11.378
26	1170.8	1.711	1.382	3.654
27	1206.4	8.015	6.873	312.623
28	1223.2	1.911	1.685	26.607
29	1247.9	9.356	8.585	377.221
30	1317.7	1.103	1.128	9.384
31	1361.3	1.140	1.245	4.966
32	1392.3	1.205	1.376	10.835
33	1413.7	1.212	1.428	2.719
34	1424.0	1.271	1.519	9.176
35	1426.2	1.266	1.518	21.864
36	1487.3	1.039	1.354	0.926
37	1489.1	1.040	1.359	7.882
38	1490.8	1.072	1.403	0.909
39	1501.3	1.053	1.398	0.708
40	1508.4	1.070	1.434	14.796
41	1511.8	1.081	1.455	7.900
42	3036.7	1.036	5.629	9.114
43	3040.6	1.038	5.654	8.515
44	3069.3	1.067	5.922	16.966
45	3076.1	1.067	5.949	15.688
46	3094.0	1.102	6.212	8.114
47	3097.0	1.100	6.218	29.782
48	3116.6	1.099	6.291	10.428
49	3127.9	1.098	6.329	4.814
50	3146.4	1.103	6.431	7.354
51	3149.3	1.105	6.455	7.980

Freq. No.	EtF ν	*m*	*f*	*I*
1	248.1	1.130	0.041	0.470
2	408.2	2.933	0.288	6.428
3	814.3	1.082	0.423	0.889
4	877.4	2.378	1.079	25.488
5	1042.9	4.008	2.569	91.871
6	1118.0	2.066	1.521	19.539
7	1183.0	1.518	1.251	4.530
8	1295.6	1.107	1.095	0.123
9	1399.2	1.208	1.393	1.876
10	1419.6	1.297	1.540	23.340
11	1481.4	1.039	1.343	6.242
12	1498.9	1.057	1.399	1.679
13	1517.4	1.089	1.478	2.039
14	3032.4	1.036	5.612	13.616
15	3039.2	1.056	5.748	31.602
16	3077.2	1.109	6.187	11.759
17	3095.5	1.099	6.207	26.479
18	3112.6	1.106	6.312	38.171

Freq. No.	BF_3 ν	*m*	*f*	*I*
1	470.9	17.868	2.335	13.466
2	470.9	17.868	2.335	13.472
3	680.7	11.814	3.225	99.710
4	881.1	18.998	8.690	0.000
5	1435.4	12.298	14.928	450.610
6	1435.5	12.297	14.929	450.476

Freq. No.	PH_3 ν	*m*	*f*	*I*
1	1024.3	1.075	0.665	23.773
2	1145.2	1.025	0.792	12.674
3	1145.2	1.025	0.792	12.670
4	2386.4	1.032	3.463	39.166
5	2391.7	1.041	3.508	63.563
6	2391.7	1.041	3.508	63.550

Freq. No.	MeF ν	*m*	*f*	*I*
1	1031.1	8.881	5.563	113.416
2	1188.9	1.247	1.038	0.969
3	1188.9	1.247	1.038	0.969
4	1479.9	1.129	1.457	0.955
5	1492.6	1.052	1.381	5.658
6	1492.6	1.052	1.381	5.657
7	3029.7	1.026	5.547	30.647
8	3112.1	1.109	6.326	28.495
9	3112.2	1.109	6.326	28.497

Freq. No.	PF_5 ν	*m*	*f*	*I*
1	163.4	19.034	0.299	0.075
2	163.4	19.034	0.299	0.075
3	489.1	18.998	2.677	0.000
4	489.1	18.998	2.677	0.000
5	505.7	20.658	3.112	38.374
6	505.7	20.658	3.113	38.372
7	553.8	20.454	3.696	52.057
8	618.1	18.998	4.277	0.000
9	771.0	18.998	6.654	0.000
10	907.0	24.370	11.812	415.336
11	976.9	24.029	13.511	278.175
12	976.9	24.030	13.512	278.250

Freq. No.	HF ν	*m*	*f*	*I*
1	4089.2	1.058	10.427	122.402

Freq. No.	C_2H_4 ν	*m*	*f*	*I*
1	838.9	1.043	0.432	0.256
2	973.7	1.161	0.648	104.358
3	976.5	1.519	0.854	0.000
4	1057.9	1.008	0.665	0.000
5	1247.6	1.526	1.400	0.000
6	1379.9	1.235	1.385	0.000
7	1478.6	1.112	1.432	9.526
8	1686.9	3.081	5.166	0.000
9	3123.2	1.048	6.021	16.843
10	3135.7	1.072	6.208	0.000
11	3192.9	1.115	6.696	0.000
12	3221.0	1.118	6.833	20.656

Table 34. Computed frequencies (ν / cm^{-1}; non-scaled), reduced masses *m*, force constants *f*, and IR spectrum intensities *I* (all in atomic units) for TS-C_2H_4.

Freq.	**3**				Freq.	**6**			
No.	ν	*m*	*f*	*I*	No.	ν	*m*	*f*	*I*
1	*i*712.9	1.730	0.518	5756.840	34	1043.2	3.394	2.176	7.772
2	11.1	4.527	0.000	0.033	35	1082.2	1.558	1.075	8.777
3	22.6	4.891	0.002	0.350	36	1105.4	1.346	0.969	11.467
4	30.4	5.883	0.003	0.151	37	1134.3	1.973	1.495	10.789
5	46.3	3.640	0.005	0.329	38	1143.6	1.379	1.062	445.305
6	52.7	3.046	0.005	0.643	39	1148.9	1.312	1.021	0.069
7	62.9	6.103	0.014	14.412	40	1160.6	7.742	6.144	322.683
8	72.7	1.242	0.004	0.523	41	1208.2	1.530	1.316	213.203
9	96.2	7.046	0.038	3.170	42	1242.1	1.356	1.232	204.550
10	108.8	3.848	0.027	7.134	43	1256.6	1.492	1.388	7.643
11	170.7	5.129	0.088	105.648	44	1264.0	1.771	1.667	29.627
12	216.1	3.059	0.084	0.772	45	1279.6	1.962	1.893	409.999
13	275.6	9.072	0.406	9.348	46	1310.1	2.069	2.092	19.561
14	323.6	14.822	0.914	0.200	47	1360.3	1.353	1.475	24.755
15	336.8	3.193	0.213	13.903	48	1382.8	5.602	6.311	0.484
16	364.6	2.988	0.234	4.859	49	1386.1	4.287	4.853	1.251
17	419.9	5.708	0.593	26.833	50	1455.8	1.268	1.584	12.955
18	485.4	3.917	0.544	8.788	51	1481.5	1.117	1.444	8.926
19	492.4	10.281	1.469	92.791	52	1488.0	1.039	1.355	10.483
20	500.8	1.466	0.217	11.978	53	1512.5	1.199	1.616	7.560
21	543.3	6.381	1.110	15.414	54	1543.7	3.035	4.261	37.514
22	628.6	3.108	0.724	6.135	55	1550.0	2.744	3.885	20.388
23	670.6	3.239	0.858	10.877	56	1605.9	1.938	2.944	35.777
24	674.8	4.403	1.181	9.001	57	3048.2	1.033	5.656	34.821
25	729.1	7.365	2.307	277.615	58	3108.8	1.055	6.008	0.471
26	734.5	1.254	0.399	34.420	59	3110.0	1.106	6.303	9.074
27	824.0	1.229	0.492	18.523	60	3137.0	1.103	6.396	5.209
28	825.3	1.167	0.469	12.407	61	3185.3	1.058	6.327	9.345
29	862.1	1.378	0.604	1.933	62	3191.4	1.115	6.692	2.385
30	869.3	1.993	0.888	220.152	63	3241.5	1.096	6.786	2.123
31	935.3	5.628	2.901	16.498	64	3247.3	1.092	6.786	4.206
32	953.5	1.043	0.559	19.370	65	3269.5	1.105	6.962	0.325
33	1008.6	1.657	0.993	521.344	66	3281.8	1.120	7.105	1.072

Computed NMR Spectral Parameters for the Stationary Conformations of 2 and 4

Table 35. Isotropic components of the GIAO magnetic shielding tensors Δ / ppm for 2a,b and 4 and chemical shifts δ / ppm.[a]

Nucleus	Δ (**2a**)	Δ (**2b**)	δ (**2a**)	δ (**2b**)
B1	102.0800	102.223	–2.9444	–3.0874
C1	11.4922	11.0916	170.9734	171.374
C2	58.3607	59.5480	124.1049	123.7573
C3	58.7104	58.7083	123.7552	123.7573
C4	133.9350	133.3910	48.5306	49.0746
C5	164.9130	164.2680	17.5526	18.1976
C6	147.6660	145.6680	34.7996	36.7976
F1	328.4180	323.2550	–173.1019	–167..9389
F2	318.4180	323.8720	–163.1019	–168.5559
F3	324.7970	333.3910	–169.4809	–178.0749
H2	25.0430	25.1953	6.8391	6.6868
H3	25.1475	25.1433	6.7346	6.7388
H4A	28.3460	28.4435	3.5361	3.4386
H4B	26.7303	26.7274	5.1518	5.1547
H5A	30.8784	30.8353	1.0037	1.0468
H5B	30.7388	30.7259	1.1433	1.1562
H5C	29.8750	30.0222	2.0071	1.8599
H6A	28.6365	28.7105	3.2456	3.1716
H6B	28.6181	28.3533	3.2640	3.5288
H6C	26.2220	26.9652	5.6601	4.9169
N1	41.6981	42.3526	216.6858	216.0313
N2	59.4959	56.8809	198.8880	201.5030

Nucleus	Δ (**4**)	δ (**4**)
C1	12.6245	169.8411
C2	58.6380	123.8276
C3	58.6406	123.8250
C4	142.537	39.9286
C5	142.5400	39.9256
F1	226.8110	–71.4949
F2	222.3090	–66.9929
F3	226.8170	–71.5009
F4	222.3250	–67.0089
F5	246.6910	–91.3749
H2	25.2189	6.6632
H3	25.2191	6.6630
H4A	26.9443	4.9378
H4B	28.7761	3.1060
H4C	28.0967	3.7854
H5A	26.9436	4.9385
H5B	28.7760	3.1061
H5C	28.0976	3.7845
N1	57.6881	200.6958
N2	57.6870	200.6969
P1	431.121	–109.879

[a] Chemical shifts referenced to: ^{1}H and ^{13}C (TMS); ^{19}F ($CFCl_3$); ^{11}B ($Et_2O{\cdot}BF_3$); ^{14}N (NH_3); and H_3PO_4 (85% aq.). Correspondent isotropic components of the GIAO magnetic shielding tensors Δ / ppm: 31.8821, 182.4656, 155.3161, 99.1356, 258.3839, and 321.242.

Table 36. Computed spin-spin coupling constants [Hz] for 2a (upper triangle) and 2b (lower triangle). ^{1}H, ^{11}B, ^{13}C, ^{14}N, and ^{19}F set of isotopes.

	B1	C1	C2	C3	C4	C5	C6	F1	F2	F3	H2	H3	H4A	H4B	H5A	H5B	H5C	H6A	H6B	H6C	N1	N2
B1	—	79.0	2.1	2.3	0.3	–0.2	0.1	–89.7	–89.7	–84.3	0.4	0.5	–0.2	–0.1	0.0	–0.1	0.0	–0.3	0.0	–0.3	1.4	1.7
C1	78.6	—	–0.3	–0.2	5.5	0.3	5.5	63.1	59.8	54.6	2.6	2.7	5.1	2.8	–0.1	0.2	0.0	3.1	3.2	2.6	4.9	5.2
C2	2.3	–0.2	—	80.9	1.9	0.2	2.0	0.4	1.0	2.1	184.1	11.4	3.1	6.0	–0.1	–0.2	–0.1	–0.3	0.5	–0.3	7.2	2.1
C3	2.1	–0.2	80.8	—	1.9	–0.2	1.8	1.5	1.4	2.0	11.4	184.5	–0.3	0.3	0.0	0.0	0.0	1.5	7.9	1.3	2.1	7.1
C4	0.1	5.0	2.0	2.0	—	34.5	0.0	0.5	5.1	–0.1	1.7	0.3	128.2	140.1	–5.2	0.1	–5.7	0.1	0.0	0.0	5.7	0.8
C5	–0.1	0.3	0.1	–0.1	34.5	—	–0.1	4.4	–0.2	–0.2	–0.1	–0.1	–2.3	–2.9	119.2	118.7	128.9	0.2	0.0	0.2	–0.2	0.0
C6	0.3	5.9	2.1	2.0	0.0	–0.1	—	0.0	–0.1	18.6	0.3	1.8	0.2	0.0	0.0	0.0	0.0	130.0	139.9	130.4	0.8	6.8
F1	–90.6	62.5	1.4	0.4	–0.1	0.1	1.5	—	30.4	19.5	–0.3	0.1	0.1	2.1	0.4	–0.1	3.0	0.3	–0.1	–0.1	–1.1	1.7
F2	–91.1	60.4	1.4	1.0	–0.1	0.0	4.8	32.9	—	21.7	–0.4	0.1	0.3	0.7	1.3	0.4	0.2	0.0	–0.1	0.3	–1.4	1.5
F3	–85.2	59.4	1.1	2.0	11.1	1.2	–0.1	13.6	20.9	—	0.5	–0.3	–0.3	–0.6	–0.2	–0.2	–0.1	–0.3	–8.3	–0.6	2.6	–2.2
H2	0.5	2.6	184.7	11.5	1.8	–0.2	0.4	0.1	0.1	–0.2	—	1.5	0.0	–0.4	0.2	–0.2	–0.1	–0.3	0.2	–0.3	2.1	3.0
H3	0.4	2.6	11.6	184.5	0.3	–0.1	1.8	–0.3	–0.4	0.6	1.5	—	–0.2	0.2	–0.1	–0.1	–0.1	–0.2	–0.2	–0.2	3.0	2.3
H4A	–0.2	5.4	4.0	–0.2	127.8	–2.4	0.2	0.1	–0.3	2.2	0.1	–0.1	—	–13.4	4.1	2.6	12.8	–0.1	–0.1	0.1	–0.4	0.1
H4B	–0.1	2.0	5.3	0.3	140.5	–3.0	0.0	0.0	0.2	1.8	–0.4	0.1	–12.7	—	13.2	2.8	4.5	–0.1	–0.1	–0.1	–0.8	–0.2
H5A	0.0	–0.1	–0.1	0.0	–5.1	120.2	0.0	–0.2	–0.1	0.1	0.1	–0.1	3.9	12.8	—	–13.0	–11.0	0.0	–0.1	–0.1	1.0	0.0
H5B	–0.1	0.0	–0.1	0.1	0.1	118.7	0.0	–0.1	–0.1	0.3	–0.1	–0.1	2.8	2.6	–12.9	—	–13.8	0.0	–0.1	–0.1	5.1	0.2
H5C	0.0	–0.1	–0.1	0.0	–5.6	127.8	0.0	–0.3	0.1	1.7	–0.1	–0.2	12.9	4.7	–11.1	–13.9	—	0.0	0.0	–0.1	0.8	0.0
H6A	–0.2	5.8	–0.2	3.4	0.2	0.0	127.3	1.4	0.4	–0.2	–0.2	0.0	–0.2	–0.1	0.0	–0.1	–0.1	—	–13.2	–11.3	0.0	–0.6
H6B	–0.1	2.7	0.3	6.5	0.0	0.0	139.5	3.4	0.6	–0.5	0.1	–0.3	–0.1	–0.1	–0.1	–0.1	0.0	–13.1	—	–13.3	–0.2	–1.0
H6C	–0.4	1.0	–0.4	0.4	–0.1	0.2	135.3	0.4	–0.3	–0.5	–0.3	–0.4	0.0	0.0	–0.1	–0.1	–0.1	–11.2	–13.7	—	0.0	–0.7
N1	1.6	4.8	7.0	2.0	5.7	–0.2	0.9	1.5	1.6	–2.0	2.2	2.9	–0.3	–0.8	1.0	5.1	0.8	0.1	–0.1	–0.1	—	0.5
N2	1.3	5.2	2.2	7.4	0.8	0.0	6.9	–1.2	–1.5	2.8	3.1	2.2	0.1	–0.2	0.0	0.1	0.0	–0.6	–1.0	–0.9	0.5	—

Table 37. Computed spin-spin coupling constants for 4 (isotope independent *K* / Hz, upper triangle and isotope dependent *J* / Hz, lower triangle). ^{1}H, ^{31}P, ^{13}C, ^{14}N, and ^{19}F set of isotopes.

	C1	C2	C3	C4	C5	F1	F2	F3	F4	F5	H2	H3	H4A	H4B	H4C	H5A	H5B	H5C	N1	N2	P1
C1	0.0	0.3	0.3	2.1	2.1	7.0	7.2	7.0	7.2	0.2	0.4	0.4	0.8	0.2	0.1	0.8	0.2	0.1	13.5	13.5	92.7
C2	0.6	0.0	40.0	1.0	1.1	0.2	0.2	0.2	0.1	0.0	23.9	1.4	0.6	0.7	0.1	0.0	0.0	–0.1	13.3	3.0	3.1
C3	0.6	78.9	0.0	1.1	1.0	0.2	0.1	0.2	0.2	0.0	1.4	23.9	0.0	0.0	–0.1	0.6	0.7	0.1	3.0	13.3	3.1
C4	4.1	1.9	2.3	0.0	0.0	1.4	0.0	0.0	1.2	0.0	0.3	0.0	16.1	18.1	17.6	0.0	0.0	0.0	11.3	1.1	–0.1
C5	4.1	2.3	1.9	0.0	0.0	0.0	1.2	1.4	0.0	0.0	0.0	0.3	0.0	0.0	0.0	16.1	18.1	17.6	1.1	11.3	–0.1
F1	51.6	1.2	1.3	10.1	–0.3	0.0	–4.6	–0.1	–4.3	–5.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	–0.4	0.8	–84.5
F2	53.3	1.4	0.5	–0.2	9.2	–126.6	0.0	–4.3	–0.1	–5.2	0.0	0.0	0.0	0.0	0.0	0.2	0.2	0.2	0.9	–0.4	–85.7
F3	51.6	1.3	1.2	–0.3	10.1	–3.4	–118.8	0.0	–4.6	–5.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.8	–0.4	–84.5
F4	53.3	0.5	1.4	9.2	–0.2	–118.8	–1.8	–126.6	0.0	–5.2	0.0	0.0	0.2	0.2	0.2	0.0	0.0	0.0	–0.4	0.9	–85.7
F5	1.4	0.0	0.0	0.2	0.2	–141.5	–142.7	–141.5	–142.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	–101.5
H2	3.3	187.2	11.2	2.2	0.4	–0.2	0.3	0.2	–0.1	–0.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.3	0.2
H3	3.3	11.2	187.2	0.4	2.2	0.2	–0.1	–0.2	0.3	–0.3	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.3	1.0	0.2
H4A	6.1	4.7	–0.1	126.5	0.2	1.3	0.1	–0.3	6.9	–0.1	0.1	–0.1	0.0	–0.4	–0.4	0.0	0.0	0.0	–0.1	0.0	–0.1
H4B	1.8	5.4	0.2	141.8	–0.1	–0.7	–0.5	0.3	5.9	–0.2	–0.3	0.1	–12.3	0.0	–0.5	0.0	0.0	0.0	–0.5	–0.1	0.0
H4C	1.1	0.8	–0.4	138.2	–0.2	–0.9	0.0	–0.2	5.2	–0.1	–0.5	–0.2	–11.3	–14.1	0.0	0.0	0.0	0.0	–0.5	0.0	–0.1
H5A	6.1	–0.1	4.7	0.2	126.5	–0.3	6.9	1.3	0.1	–0.1	–0.1	0.1	–0.1	–0.1	–0.1	0.0	–0.4	–0.4	0.0	–0.1	–0.1
H5B	1.8	0.2	5.4	–0.1	141.8	0.3	5.9	–0.7	–0.5	–0.2	0.1	–0.3	–0.1	–0.1	0.1	–12.4	0.0	–0.5	–0.1	–0.5	0.0
H5C	1.1	–0.4	0.8	–0.2	138.2	–0.2	5.2	–0.9	0.0	–0.1	–0.2	–0.5	–0.1	0.1	0.5	–11.3	–14.1	0.0	0.0	–0.5	–0.1
N1	7.7	7.5	1.7	6.4	0.7	–0.8	1.8	1.6	–0.8	0.0	2.3	2.9	–0.3	–1.1	–1.0	0.1	–0.1	0.0	0.0	4.9	7.1
N2	7.7	1.7	7.5	0.7	6.4	1.6	–0.8	–0.8	1.8	0.0	2.9	2.3	0.1	–0.1	0.0	–0.3	–1.1	–1.0	0.8	0.0	7.1
P1	294.7	9.8	9.8	–0.4	–0.4	–1006.0	–1019.4	–1006.1	–1019.2	–1207.7	2.7	2.7	–0.8	–0.6	–1.5	–0.8	–0.6	–1.6	6.5	6.5	0.0

Modeling of 1 → 8a + C_2H_4 + HF + BF_3 conversion

The less chemically evident thermolytic decomposition of **1** into 1-methy-1*H*-limidazole (**8a**), C_2H_4, HF, and BF_3 by a β-elimination mechanism was also modeled (see Figure 16, +-labeled lines). Unexpectedly, from the thermodynamical viewpoint, **8a**, C_2H_4, HF, and BF_3 present the most favored set of products even in respect to **8a**, EtF, and BF_3 within the entire 25 through 450 ºC temperature range. This instantly suggests that EtF is, actually, a metastable compound under the conditions of question (what itself presents a rather strange fact from a "regular" organic chemist's viewpoint). However, examination of the empirical thermodynamical data for EtF, HF, and C_2H_4 demonstrates that at 1 atm pressure ΔG for EtF → C_2H_4 + HF conversion [linear r. m. s. approximation: $\Delta G(T) = -0.0317 \cdot T + 1.813$, where T denotes temperature (ºC) and $\Delta G(T)$ is in kcal·mol^{-1}]* zeroes [$\Delta G(57.11\ ^\circ C) = 0$] and quickly becomes strongly negative at temperatures above *ca*. 60 C. Reduction of the pressure down to 0.001 atm would, evidently, drop down the thermal "metastability limit" and move it to the ambient temperature range.

As for the transition state leading to **8a**, HF, BF_3, and ethene (**TS-C_2H_4**; see Table 22 and the view with numbering attached thereto), it is the highest by $\Delta G^{\neq}$ within the entire temperature range studied (in Figure 16, see the upmost line) and drops down from 46.8 to 42.4 kcal·mol^{-1} with the increase of temperature from 25 to 450 ºC). It exceeds the actual **TS** by 12.7 through 10.5 kcal·mol^{-1}, with the relative rate of **8a**, HF, BF_3, and ethene formation lower than 0.001 even at 450 ºC (see Figure 19, brown curve). Thus, the most thermodynamically favored set of products **8a**, HF, BF_3, and ethene is, at the same time, the most kinetically disfavored, if not negligible, one.

Table 38. Standard enthalpies [$\Delta_f H^\circ$ / kJ·mol^{-1}] and Gibbs free energies of formation [$\Delta_f G^\circ$ / kJ·mol^{-1}] along with standard entropies [S° / J·mol^{-1}·K^{-1}] and heat capacities [at constant pressure (1 atm) and 298.15, 400, 600, and 800 K; C_p / J·mol^{-1}·K^{-1}] for EtF, HF, and C_2H_4 (all in gas phase; *Lange's Handbook of Chemistry*. 15 ed.; McGraw-Hill, Inc.: N.-Y., 1999, Ch. 6).

Compound	$\Delta_f H^\circ$	$\Delta_f G^\circ$	S°	C_p at different T [K]				
				298.15	400	600	800	1000
C_2H_5F	–263.2	–211.0	264.5	58.6	74.1	98.6	116.4	129.7
HF	–273.30(70)	–275.4	173.779(3)	29.14	29.1	29.2	29.5	30.2
C_2H_4	52.5	68.4	219.3	42.9	53.1	70.7	83.8	93.9

* Dependencies of ΔH_f, and S from temperature for all these compounds were elucidated by the known formulas:

$$\Delta H_f(T) = \Delta H^\circ_f + \int_{T_0}^{T} C_p(T)dT \text{ and } S(T) = S^\circ + \int_{T_0}^{T} \frac{C_p(T)}{T} dT$$

where constant pressure heat capacities $C_p(T)$ for all seven compounds were interpolated with the 4th order polynoms and the subsequent integrations were performed analytically. Empirical $\Delta G(T)$ for EtF→C_2H_4+HF reaction was then calculated as

$$\Delta G(T) = \Delta H_f^{C_2H_4}(T) + \Delta H_f^{HF}(T) - \Delta H_f^{EtF}(T) - T\left[S^{C_2H_4}(T) + S^{HF}(T) - S^{EtF}(T)\right].$$

Calculation of the Thermodynamic and Kinetic Functions

Changes in free Gibbs and free Gibbs activation energies, $\Delta G(T)$ and $\Delta G^{\neq}(T)$, either accounting or not accounting for the free intrinsic rotation were made according to Eqs. (1a-m) and Eq. (2a-d), respectively:

$$\Delta G^{[2+HF]}(T) = E_{SCF}^{[2]} + E_{SCF}^{[HF]} - E_{SCF}^{[1]} + \Delta E^{[2]}(T) + \Delta E^{[HF]}(T) - \Delta E^{[1]}(T) - T\left(S^{[2]}(T) + S^{[HF]}(T) - S^{[1]}(T)\right) + RT \qquad \text{Eqs. (1a-m)}$$

$$\Delta G^{[2...HF]}(T) = E_{SCF}^{[2...HF]} - E_{SCF}^{[1]} + \Delta E^{[2...HF]}(T) - \Delta E^{[1]}(T) - T\left(S^{[2...HF]}(T) - S^{[1]}(T)\right)$$

$$\Delta G^{[7+BF_3]}(T) = E_{SCF}^{[7]} + E_{SCF}^{[BF_3]} - E_{SCF}^{[1]} + \Delta E^{[7]}(T) + \Delta E^{[BF_3]}(T) - \Delta E^{[1]}(T) - T\left(S^{[7]}(T) + S^{[BF_3]}(T) - S^{[1]}(T)\right) + RT$$

$$\Delta G^{[9+HF+BF_3]}(T) = E_{SCF}^{[9]} + E_{SCF}^{[HF]} + E_{SCF}^{[BF_3]} - E_{SCF}^{[1]} + \Delta E^{[9]}(T) + \Delta E^{[HF]}(T) + \Delta E^{[BF_3]}(T) - \Delta E^{[1]}(T) - T\left(S^{[9]}(T) + S^{[HF]}(T) + S^{[BF_3]}(T) - S^{[1]}(T)\right) + 2RT$$

$$\Delta G^{[5a+EtF]}(T) = E_{SCF}^{[5a]} + E_{SCF}^{[EtF]} - E_{SCF}^{[1]} + \Delta E^{[5a]}(T) + \Delta E^{[EtF]}(T) - \Delta E^{[1]}(T) - T\left(S^{[5a]}(T) + S^{[EtF]}(T) - S^{[1]}(T)\right) + RT$$

$$\Delta G^{[5b+MeF]}(T) = E_{SCF}^{[5b]} + E_{SCF}^{[MeF]} - E_{SCF}^{[1]} + \Delta E^{[5b]}(T) + \Delta E^{[MeF]}(T) - \Delta E^{[1]}(T) - T\left(S^{[5b]}(T) + S^{[MeF]}(T) - S^{[1]}(T)\right) + RT$$

$$\Delta G^{[8a+EtF+BF_3]}(T) = E_{SCF}^{[8a]} + E_{SCF}^{[EtF]} + E_{SCF}^{[BF_3]} - E_{SCF}^{[1]} + \Delta E^{[8a]}(T) + \Delta E^{[EtF]}(T) + \Delta E^{[BF_3]}(T) - \Delta E^{[1]}(T) - T\left(S^{[8a]}(T) + S^{[EtF]}(T) + S^{[BF_3]}(T) - S^{[1]}(T)\right) + 2RT$$

$$\Delta G^{[8b+MeF+BF_3]}(T) = E_{SCF}^{[8b]} + E_{SCF}^{[MeF]} + E_{SCF}^{[BF_3]} - E_{SCF}^{[1]} + \Delta E^{[8b]}(T) + \Delta E^{[MeF]}(T) + \Delta E^{[BF_3]}(T) - \Delta E^{[1]}(T) - T\left(S^{[8b]}(T) + S^{[MeF]}(T) + S^{[BF_3]}(T) - S^{[1]}(T)\right) + 2RT$$

$$\Delta G^{[4+HF]}(T) = E_{SCF}^{[4]} + E_{SCF}^{[HF]} - E_{SCF}^{[3]} + \Delta E^{[4]}(T) + \Delta E^{[HF]}(T) - \Delta E^{[3]}(T) - T\left(S^{[4]}(T) + S^{[HF]}(T) - S^{[3]}(T)\right) + RT$$

$$\Delta G^{[6+MeF]}(T) = E_{SCF}^{[6]} + E_{SCF}^{[MeF]} - E_{SCF}^{[3]} + \Delta E^{[6]}(T) + \Delta E^{[MeF]}(T) - \Delta E^{[3]}(T) - T\left(S^{[6]}(T) + S^{[MeF]}(T) - S^{[3]}(T)\right) + RT$$

$$\Delta G^{[10+HF+PF_5]}(T) = E_{SCF}^{[10]} + E_{SCF}^{[HF]} + E_{SCF}^{[PF_5]} - E_{SCF}^{[3]} + \Delta E^{[10]}(T) + \Delta E^{[HF]}(T) + \Delta E^{[PF_5]}(T) - \Delta E^{[3]}(T) - T\left(S^{[10]}(T) + S^{[HF]}(T) + S^{[PF_5]}(T) - S^{[3]}(T)\right) + 2RT$$

$$\Delta G^{[8a+MeF+PF_5]}(T) = E_{SCF}^{[8a]} + E_{SCF}^{[MeF]} + E_{SCF}^{[PF_5]} - E_{SCF}^{[3]} + \Delta E^{[8a]}(T) + \Delta E^{[MeF]}(T) + \Delta E^{[PF_5]}(T) - \Delta E^{[3]}(T) - T\left(S^{[8a]}(T) + S^{[MeF]}(T) + S^{[PF_5]}(T) - S^{[3]}(T)\right) + 2RT$$

$$\Delta G^{[8a+HF+C2H4+BF_3]}(T) = E_{SCF}^{[8a]} + E_{SCF}^{[HF]} + E_{SCF}^{[C2H4]} + E_{SCF}^{[BF_3]} - E_{SCF}^{[1]} + \Delta E^{[8a]}(T) + \Delta E^{[HF]}(T) + \Delta E^{[C2H4]}(T) + \Delta E^{[BF_3]}(T) - \Delta E^{[1]}(T) -$$
$$- T\left(S^{[8a]}(T) + S^{[HF]}(T) + S^{[C2H4]}(T) + S^{[BF_3]}(T) - S^{[1]}(T)\right) + 3RT$$

$$\Delta G^{\neq[2+HF]}(T) = E_{SCF}^{[TS]} - E_{SCF}^{[1]} + \Delta E^{[TS]}(T) - \Delta E^{[1]}(T) - T\left(S^{[TS]}(T) - S^{[1]}(T)\right) \qquad \text{Eq. (2a)}$$

$$\Delta G^{\neq[5a+EtF]}(T) = E_{SCF}^{[TS\text{-}a]} - E_{SCF}^{[1]} + \Delta E^{[TS\text{-}a]}(T) - \Delta E^{[1]}(T) - T\left(S^{[TS\text{-}a]}(T) - S^{[1]}(T)\right) \qquad \text{Eq. (2b)}$$

$$\Delta G^{\neq[5b+MeF]}(T) = E_{SCF}^{[TS\text{-}b]} - E_{SCF}^{[1]} + \Delta E^{[TS\text{-}b]}(T) - \Delta E^{[1]}(T) - T\left(S^{[TS\text{-}b]}(T) - S^{[1]}(T)\right) \qquad \text{Eq. (2c)}$$

$$\Delta G^{\neq[8a+HF+C2H4+BF_3]}(T) = E_{SCF}^{[TS\text{-}C2H4]} - E_{SCF}^{[1]} + \Delta E^{[TS\text{-}C2H4]}(T) - \Delta E^{[1]}(T) - T\left(S^{[TS\text{-}C2H4]}(T) - S^{[1]}(T)\right) \qquad \text{Eq. (2d)}$$

where T is the absolute temperature [K], R is the universal gas constant (8.314511212 J·mol^{-1} K^{-1}), and other functions as defined in the caption to Tables 27-31. The square-bracketed superscripts denote the component(s).

Equilibrium constant, rate constant, and half-conversion time [$K(T)$, $k(T)$, and $\tau(T)$] either accounting or not accounting for the free intrinsic rotation were calculated according to Eqs. (3), (4) and (5), respectively:

$$K(T) = e^{-\frac{\Delta G(T)}{RT}} \quad \text{Eq. (3)} \qquad k(T) = A\frac{k_B T}{h}e^{-\frac{\Delta G^{\neq}(T)}{RT}} \quad \text{Eq. (4)} \qquad \tau(T) = \left(k(T)\right)^{-1}\ln 2 \quad \text{Eq. (5)}$$

where k_B and h are the Boltzmann and Plank's constants (1.380658·10^{-23} J·K^{-1} and 6.626075·10^{-34} J·s), with the dimensionless transition coefficient A put to 1 (*i.e.*, tunneling effects were not accounted for due to evident reasons). The following conversion factors were used: 1 cal = 4.184 J (exactly); 1 Hartree = 627.5095 kcal·mol^{-1}; T[K] = T[°C] + 273.15; 1 atm = 760 Torr = 101325 Pa.

Additional Thermochemical Plots

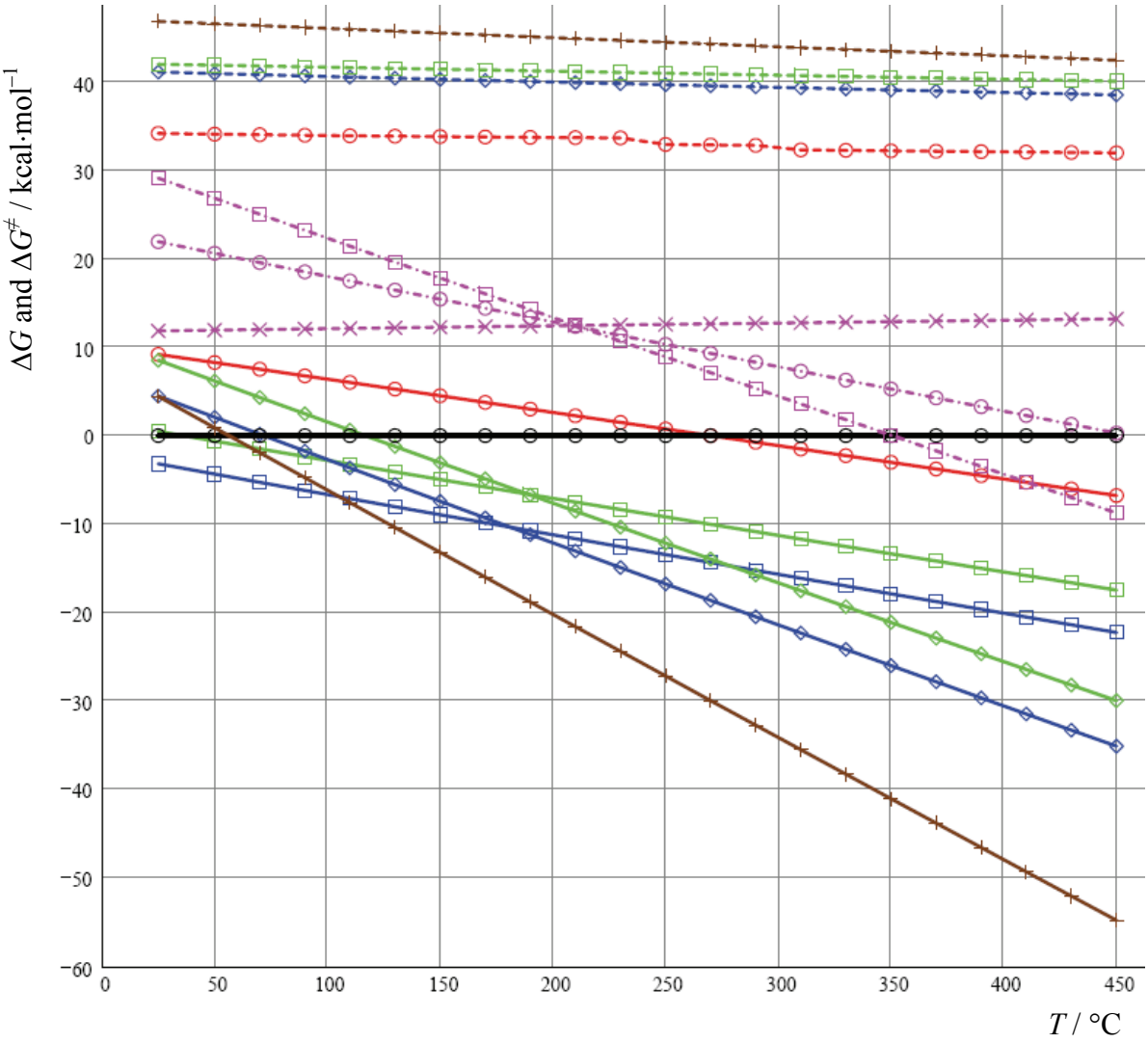


Figure 16. Thermochemistry 2D-plot for **1** → **2** + HF conversion and related reactions. $\Delta G(T)$ / kcal·mol^{-1} for actual and alternative products: initial **1** (black, o-s; reference compound); actual product **2** + HF (red, o-s), **5a** + EtF (blue, boxes), **8a** + EtF + BF_3 (blue, diamonds), **8a** + C_2H_4 + HF + BF_3 (brown, crosses), **5b** + MeF (green, boxes), **8b** + MeF + BF_3 (green, diamonds), **2**···HF (pink, x-ses, dashes), **7** + BF_3 (pink, o-s, da-dot), and **9** + HF +BF_3 (pink, boxes, da-dot). $\Delta G^{\neq}(T)$ / kcal·mol^{-1} for transition states: **TS** (red, o-s, dashes), **TS-a** (blue, boxes, dashes), **TS-b** (green, diamonds, dashes), and **TS_C_2H_4** (brown, crosses, dashes).

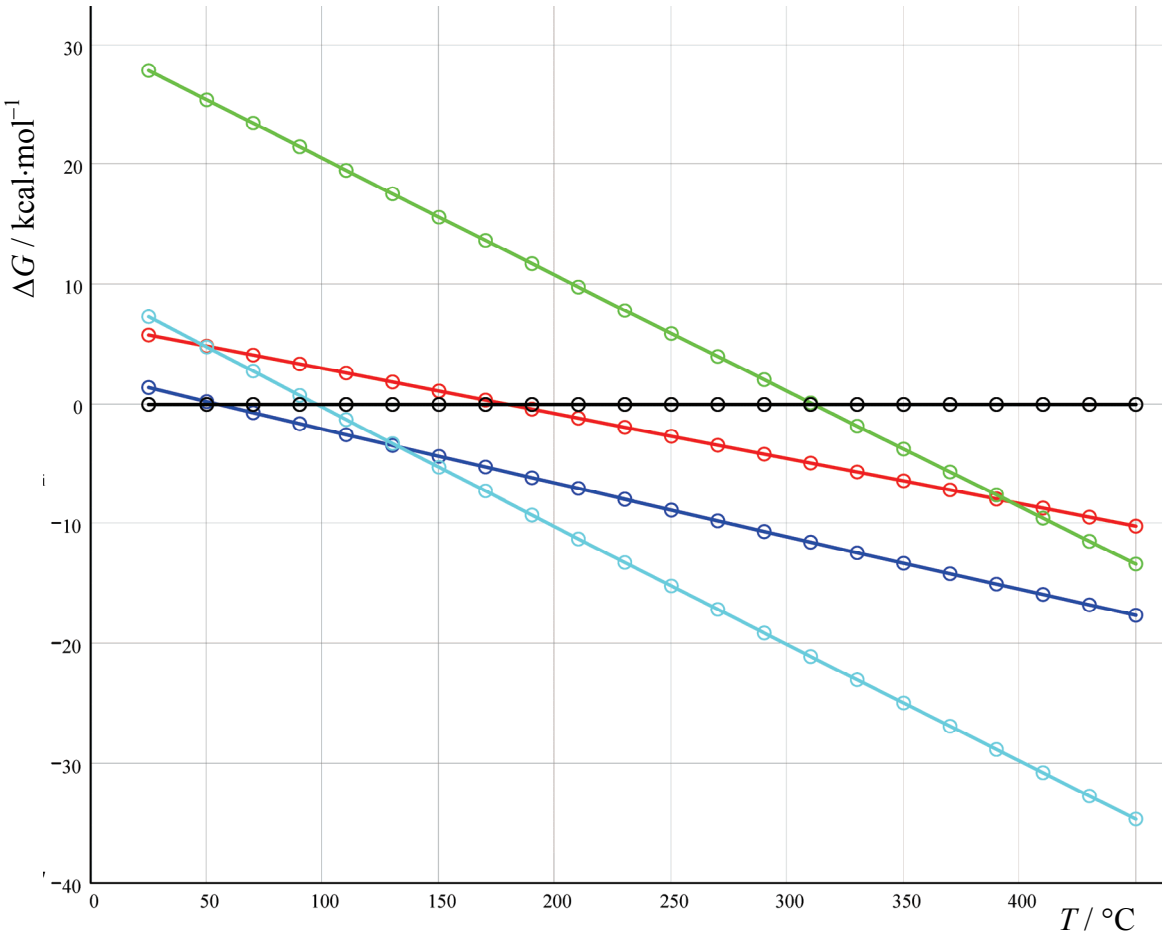


Figure 17. Thermochemistry 2D-plot for **3** → **4** + HF conversion and related reactions. $\Delta G(T)$ / kcal·mol^{-1} for actual and alternative products: initial **3** (black; reference compound); actual product **4** + HF (red), **6** + MeF (blue), **8a** + MeF +PF_5 (cyan), and **10** + HF +PF_5 (green).

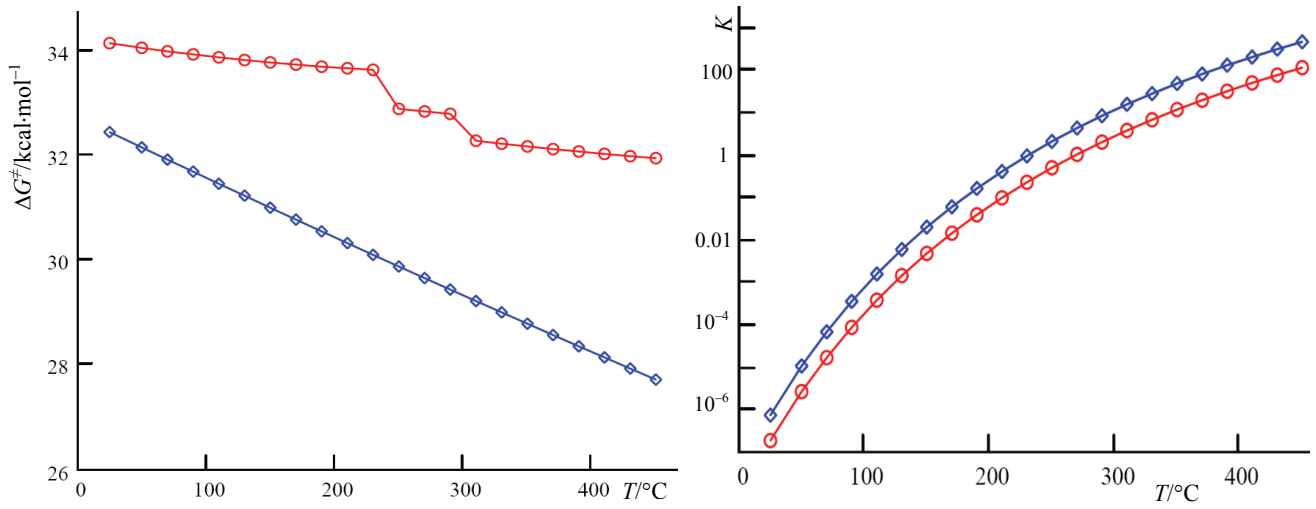


Figure 18. Influence of accounting for the free intrinsic rotation on $\Delta G\neq$(T) / kcal·mol–1 (for **TS**; left) and equilibrium constant $K(T)$ for **1**→**2**+HF interconversion (right; logarithmic plot). The red (circles) and blue (diamonds) curves correspond to models with accounted and non-accounted free intrinsic rotation, respectively.

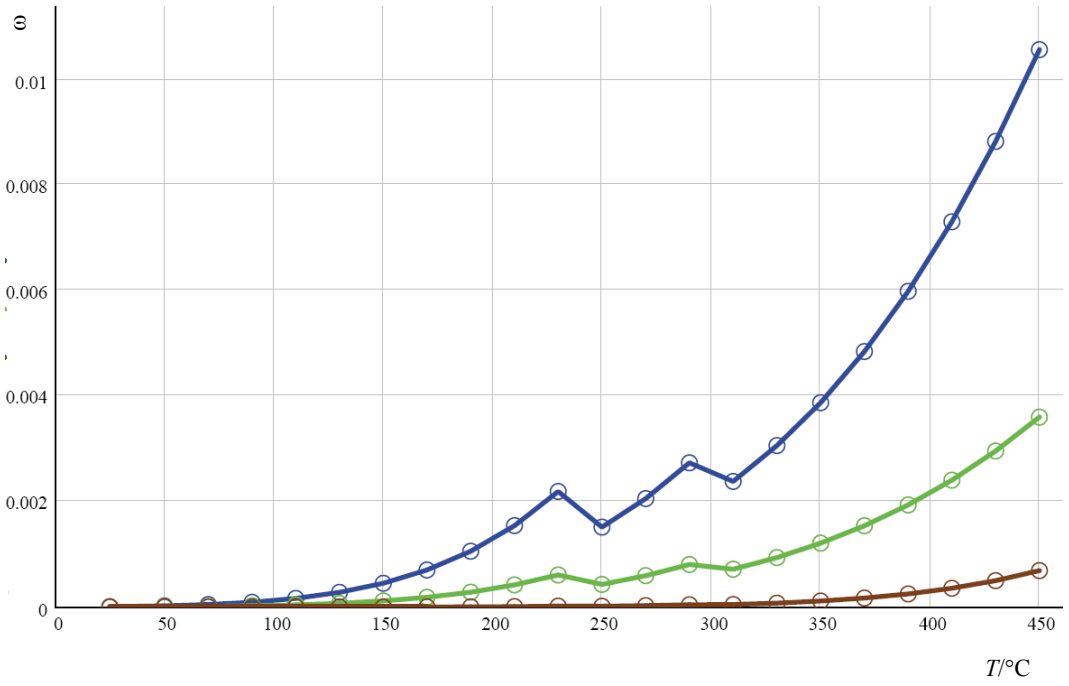


Figure 19. Computed rates of **5a** (blue), **5b** (green), and **8a** + C_2H_4 + HF + BF_3 (brown) formation relatively to that of **2** [ω; defined as rate constant ratios $k(T)^{[\mathbf{1}\rightarrow\mathbf{5a}+\mathrm{EtF}]}/k(T)^{[\mathbf{1}\rightarrow\mathbf{2}+\mathrm{HF}]}$, $k(T)^{[\mathbf{1}\rightarrow\mathbf{5b}+\mathrm{MeF}]}/k(T)^{[\mathbf{1}\rightarrow\mathbf{2}+\mathrm{HF}]}$, and $k(T)^{[\mathbf{1}\rightarrow\mathbf{8a}+\mathrm{C2H4+HF+BF3}]}/k(T)^{[\mathbf{1}\rightarrow\mathbf{2}+\mathrm{HF}]}$, respectively].

Table 39. Intrinsic reaction coordinate path following for 1 → 2 + HF conversion. Point numbers, weighted reaction coordinate (ζ / amu$^{1/2}$·Bohr), SCF-energies (E_{SCF} / Hartrees), and SCF-energies scaled to that of 1 (ΔE_{SCF} / kcal·mol^{-1}). Negative point numbers and ζ stay for the "initial compound" side of the path.

	ζ	E_{SCF}	ΔE_{SCF}		ζ	E_{SCF}	ΔE_{SCF}		ζ	E_{SCF}	ΔE_{SCF}
-98	-32.345	-769.471830000	0.347	-35	-9.422	-769.415664803	35.592	28	5.440	-769.412137494	37.805
-97	-32.036	-769.471773131	0.383	-34	-9.099	-769.415329294	35.802	29	5.695	-769.412144118	37.801
-96	-31.728	-769.471713024	0.421	-33	-8.778	-769.415020465	35.996	30	5.945	-769.412150941	37.797
-95	-31.438	-769.471654819	0.457	-32	-8.477	-769.414758408	36.160	31	6.200	-769.412158166	37.792
-94	-31.102	-769.471581090	0.504	-31	-8.191	-769.414529633	36.304	32	6.402	-769.412163455	37.789
-93	-30.778	-769.471507944	0.550	-30	-7.908	-769.414317550	36.437	33	6.644	-769.412170297	37.784
-92	-30.398	-769.471413353	0.609	-29	-7.637	-769.414129718	36.555	34	6.890	-769.412177360	37.780
-91	-30.015	-769.471313833	0.671	-28	-7.367	-769.413954463	36.665	35	7.098	-769.412183244	37.776
-90	-29.631	-769.471209540	0.737	-27	-7.052	-769.413752600	36.792	36	7.304	-769.412189186	37.773
-89	-29.308	-769.471124189	0.790	-26	-6.701	-769.413535702	36.928	37	7.519	-769.412195717	37.769
-88	-29.050	-769.471059691	0.831	-25	-6.349	-769.413337340	37.052	38	7.724	-769.412202229	37.764
-87	-28.732	-769.470970793	0.887	-24	-6.002	-769.413161296	37.163	39	7.946	-769.412210030	37.760
-86	-28.418	-769.470878137	0.945	-23	-5.680	-769.413016280	37.254	40	8.180	-769.412219345	37.754
-85	-28.092	-769.470777956	1.008	-22	-5.409	-769.412912610	37.319	41	8.425	-769.412230848	37.746
-84	-27.735	-769.470663604	1.079	-21	-5.080	-769.412789258	37.396	42	8.675	-769.412245035	37.738
-83	-27.348	-769.470527733	1.165	-20	-4.703	-769.412656488	37.479	43	8.931	-769.412263228	37.726
-82	-26.953	-769.470385479	1.254	-19	-4.341	-769.412546981	37.548	44	9.186	-769.412286211	37.712
-81	-26.554	-769.470239218	1.346	-18	-3.966	-769.412446261	37.611	45	9.504	-769.412294872	37.706
-80	-26.156	-769.470090885	1.439	-17	-3.589	-769.412358083	37.667	46	9.819	-769.412397691	37.642
-79	-25.759	-769.469937956	1.535	-16	-3.244	-769.412291026	37.709	47	10.157	-769.412507355	37.573
-78	-25.364	-769.469779584	1.634	-15	-2.903	-769.412232697	37.745	48	10.497	-769.412645356	37.486
-77	-24.968	-769.469611575	1.740	-14	-2.681	-769.412203460	37.764	49	10.841	-769.412832501	37.369
-76	-24.571	-769.469433612	1.851	-13	-2.501	-769.412182389	37.777	50	11.182	-769.413080680	37.213
-75	-24.172	-769.469247289	1.968	-12	-2.294	-769.412159277	37.791	51	11.510	-769.413387111	37.021
-74	-23.774	-769.469056403	2.088	-11	-2.061	-769.412134563	37.807	52	11.856	-769.413817152	36.751
-73	-23.399	-769.468879451	2.199	-10	-1.817	-769.412110931	37.822	53	12.218	-769.414403339	36.383
-72	-23.018	-769.468699943	2.312	-9	-1.596	-769.412092099	37.834	54	12.580	-769.415139762	35.921
-71	-22.628	-769.468520354	2.424	-8	-1.422	-769.412079180	37.842	55	12.940	-769.416027314	35.364
-70	-22.327	-769.468403200	2.498	-7	-1.264	-769.412068287	37.849	56	13.303	-769.417084833	34.701
-69	-22.004	-769.468279553	2.575	-6	-1.084	-769.412057078	37.856	57	13.673	-769.418325926	33.922
-68	-21.688	-769.468162557	2.649	-5	-0.923	-769.412047402	37.862	58	14.051	-769.419753870	33.026
-67	-21.387	-769.468055307	2.716	-4	-0.759	-769.412038595	37.867	59	14.434	-769.421316636	32.045
-66	-21.074	-769.467942808	2.787	-3	-0.643	-769.412032840	37.871	60	14.820	-769.422968402	31.009
-65	-20.724	-769.467807157	2.872	-2	-0.542	-769.412028658	37.873	61	15.209	-769.424659727	29.947
-64	-20.343	-769.467634151	2.980	-1	-0.328	-769.412018996	37.879	62	15.600	-769.426357305	28.882
-63	-19.952	-769.467417976	3.116	0	0.000	-769.411990156	37.898	63	15.989	-769.428038452	27.827
-62	-19.558	-769.467150235	3.284	1	0.241	-769.411996625	37.893	64	16.380	-769.429793928	26.725
-61	-19.159	-769.466821741	3.490	2	0.455	-769.412001343	37.891	65	16.771	-769.431662264	25.553
-60	-18.761	-769.466424769	3.739	3	0.635	-769.412006125	37.888	66	17.165	-769.433515647	24.390
-59	-18.367	-769.465946300	4.040	4	0.819	-769.412011325	37.884	67	17.556	-769.435129427	23.377
-58	-17.989	-769.465280249	4.457	5	0.993	-769.412016970	37.881	68	17.948	-769.436444869	22.552
-57	-17.672	-769.464669171	4.841	6	1.167	-769.412022824	37.877	69	18.341	-769.437541571	21.864
-56	-17.276	-769.462420388	6.252	7	1.349	-769.412029310	37.873	70	18.736	-769.438521090	21.249
-55	-16.877	-769.458930757	8.442	8	1.531	-769.412035987	37.869	71	19.128	-769.439423253	20.683
-54	-16.477	-769.454664741	11.119	9	1.692	-769.412041819	37.865	72	19.521	-769.440275917	20.148
-53	-16.077	-769.450092654	13.988	10	1.869	-769.412048383	37.861	73	19.910	-769.441071544	19.649
-52	-15.678	-769.445560691	16.832	11	2.050	-769.412055035	37.857	74	20.301	-769.441833929	19.170
-51	-15.280	-769.441292716	19.510	12	2.234	-769.412061651	37.853	75	20.694	-769.442567299	18.710
-50	-14.882	-769.437399999	21.953	13	2.421	-769.412068075	37.849	76	21.087	-769.443264782	18.272
-49	-14.486	-769.433937764	24.125	14	2.594	-769.412073894	37.845	77	21.481	-769.443936847	17.851
-48	-14.093	-769.430899667	26.032	15	2.763	-769.412079028	37.842	78	21.870	-769.444571595	17.452
-47	-13.700	-769.428230889	27.706	16	2.924	-769.412083857	37.839	79	22.262	-769.445192089	17.063
-46	-13.310	-769.425918807	29.157	17	3.090	-769.412088489	37.836	80	22.652	-769.445795789	16.684
-45	-12.922	-769.423917321	30.413	18	3.256	-769.412092999	37.833	81	23.041	-769.446387415	16.313
-44	-12.541	-769.422198953	31.491	19	3.440	-769.412097562	37.830	82	23.429	-769.446967842	15.949
-43	-12.169	-769.420722111	32.418	20	3.635	-769.412102201	37.827	83	23.804	-769.447516536	15.604
-42	-11.805	-769.419492338	33.190	21	3.837	-769.412106420	37.825	84	24.179	-769.448054686	15.267
-41	-11.443	-769.418612517	33.742	22	4.037	-769.412110257	37.822	85	24.564	-769.448603942	14.922
-40	-11.085	-769.417928109	34.171	23	4.252	-769.412113987	37.820	86	24.950	-769.449132110	14.591
-39	-10.732	-769.417344046	34.538	24	4.474	-769.412117659	37.818	87	25.338	-769.449636352	14.274
-38	-10.387	-769.416833963	34.858	25	4.708	-769.412121805	37.815	88	25.594	-769.449610434	14.290
-37	-10.064	-769.416409825	35.124	26	4.941	-769.412126049	37.812	89	25.945	-769.450172453	13.938
-36	-9.754	-769.416041503	35.355	27	5.189	-769.412131463	37.809	90	26.325	-769.450620050	13.657

References

(1) Foresman, J. B.; Frisch, Æ. Exploring Chemistry with Electronic Structure Methods. Second ed.; Gaussian Inc.: Pittsburg, PA, USA, 1996.

(2) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. J. Montgomery, T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. A.-. Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople *Gaussian 03W*, Revision 6.1; Gaussian, Inc.: Pittsburgh PA, 2003.