

# Electronic Supplementary Information (ESI)

## Stable *N*-Heterocyclic Borylenes with Promising Ligand Properties: A

### Contribution from Theory

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**Table S1** Calculated (M06-D3/Def2-TZVP (Toluene)) Mulliken spin densities at the central boron atom and  $\alpha$ -nitrogen and carbon atoms (w.r.t. the central boron atom) of the triplet states for **1-9**.

<b>Molecules</b>	<b>B</b>	<b>N<math>\alpha</math></b>	<b>C<math>\alpha</math>/N<math>\alpha</math></b>
<b>1</b>	0.586	0.058	0.259
<b>2</b>	1.056	-0.050	0.002
<b>3</b>	1.061	-0.068	0.049
<b>4</b>	1.675	0.015	0.123
<b>5</b>	1.675	-0.018	0.086
<b>6</b>	1.613	-0.057	-0.015
<b>7</b>	1.270	-0.024	-0.087
<b>8</b>	1.003	-0.007	-0.042
<b>9</b>	1.036	-0.056	-0.035

**Table S2** Calculated singlet-triplet energy separation values ( $\Delta E_{S-T}$ , in kcal mol<sup>-1</sup>) for **1-9** with different functionals.

<b>Molecules</b>	<b><math>\Delta E_{S-T}</math></b>			
	<b>M06</b>	<b>PBE0</b>	<b><math>\omega</math>B97XD</b>	<b>B3PW91</b>
<b>1</b>	15.7	13.0	16.1	13.3
<b>2</b>	8.5	4.0	8.5	4.4
<b>3</b>	14.3	11.0	14.7	11.8
<b>4</b>	36.1	30.7	40.2	30.3
<b>5</b>	31.5	25.8	31.8	26.4
<b>6</b>	42.3	37.8	43.6	38.1
<b>7</b>	25.5	21.9	25.4	21.7
<b>8</b>	19.2	15.2	17.9	15.1
<b>9</b>	31.6	28.1	31.2	27.9

**Table S3** Calculated (M06-D3/Def2-TZVP (Toluene)) hydrogenation energy values (in kcal mol<sup>-1</sup>) for **1-9** in their singlet and triplet states. The difference in the calculated hydrogenation energy values for the singlet and triplet states ( $\Delta E_{\text{Hydro}}$ ) of **1-9** are given in kcal mol<sup>-1</sup>.

Molecule	Hydrogenation Energy		$\Delta E_{\text{Hydro}}$
	Singlet	Triplet	
<b>1</b>	53.9	38.2	15.7
<b>2</b>	29.8	21.3	8.5
<b>3</b>	48.3	33.9	14.4
<b>4</b>	51.8	15.6	36.2
<b>5</b>	38.8	7.3	31.5
<b>6</b>	46.9	4.5	42.4
<b>7</b>	39.8	14.3	25.5
<b>8</b>	46.6	27.4	19.2
<b>9</b>	44.6	13.0	31.6

**Table S4** Calculated (M06-D3/Def2-TZVP (Toluene)) important geometrical parameters, natural charges at the pseudo hydridic hydrogen ( $H^{\delta-}$ ) and positively polarized hydrogen atom ( $H^{\delta+}$ ) and occupancies of the formally vacant  $p_{\pi}$  orbital centered at the central E atom (E = B, Al, Ga and C) for the transition state involved in the activation of  $H_2$  by **4-7**, **9**, **II**, **IIIa** and **IIIb**. The bond lengths and bond angles are given in Å and in degree ( $^{\circ}$ ) respectively. The Wiberg Bond Index values (WBI) are given within parenthesis (X = C and N).

Molecules	$H^{\delta+}-H^{\delta-}$	$E-H^{\delta-}$	$E-H^{\delta+}$	E-X	$\angle N-E-X$	$q_{H^{\delta-}}$	$q_{H^{\delta+}}$	Occ $p_{\pi}$
<b>II-TS<sup>H-H</sup></b>	1.076 (0.315)	1.950 (0.465)	1.213 (0.621)	1.325/1.502 (1.298)/(0.997)	108.0	-0.196	0.185	0.756
<b>IIIa-TS<sup>H-H</sup></b>	1.266 (0.228)	1.973 (0.689)	1.591 (0.721)	1.890/1.890 (0.356)/(0.356)	96.9	-0.250	-0.159	0.511
<b>IIIb-TS<sup>H-H</sup></b>	1.398 (0.167)	1.994 (0.727)	1.556 (0.773)	1.948/1.948 (0.404)/(0.404)	96.0	-0.269	-0.097	0.552
<b>4TS<sup>H-H</sup></b>	1.035 (0.457)	2.482 (0.324)	1.525 (0.523)	1.488/1.537 (0.769)/(1.082)	98.3	-0.380	-0.030	0.404
<b>5TS<sup>H-H</sup></b>	0.894 (0.480)	1.865 (0.468)	1.420 (0.499)	1.495/1.632 (0.751)/(0.800)	99.0	-0.046	0.021	0.452
<b>6TS<sup>H-H</sup></b>	1.073 (0.349)	2.180 (0.467)	1.361 (0.628)	1.477/1.480 (0.769)/(0.830)	99.7	-0.269	-0.019	0.425
<b>7TS<sup>H-H</sup></b>	0.922 (0.422)	1.787 (0.518)	1.367 (0.561)	1.564/1.496 (0.650)/(0.774)	99.0	-0.034	0.034	0.497
<b>9TS<sup>H-H</sup></b>	1.035 (0.365)	2.108 (0.505)	1.368 (0.615)	1.440/1.574 (0.839)/(0.620)	98.1	-0.217	-0.023	0.462



**Table S5** Calculated (M06-D3/Def2-TZVP (Toluene)) important geometrical parameters, natural charges at the nitrogen atom of the pseudo amide fragment ( $\text{NH}_2^{\delta-}$ ), positively polarized hydrogen atom ( $\text{H}^{\delta+}$ ) and occupancies of the formally vacant  $p_\pi$  orbital centered at the central E (E = B and C) atom for the transition state involved in the activation of  $\text{NH}_3$  by **4-7**, **9** and **II**. The bond lengths and bond angles are given in Å and in degree ( $^\circ$ ) respectively. The Wiberg Bond Index values (WBI) are given within parenthesis (X = C and N).

Molecules	$\text{H}^{\delta+}-\text{H}_2\text{N}^{\delta-}$	$\text{E}-\text{NH}_2^{\delta-}$	$\text{E}-\text{H}^{\delta+}$	E-X	$\angle\text{N-E-X}$	$q_{\text{NH}_2^{\delta-}}$	$q_{\text{H}^{\delta+}}$	Occ $p_\pi$
<b>II-TS<sup>N-H</sup></b>	1.542 (0.177)	2.428 (0.401)	1.156 (0.695)	1.314/1.496 (1.378)/(0.995)	109.5	-1.165	0.324	0.792
<b>4TS<sup>N-H</sup></b>	1.397 (0.286)	2.833 (0.190)	1.495 (0.660)	1.492/1.528 (0.738)/(1.107)	98.4	-1.277	0.166	0.586
<b>5TS<sup>N-H</sup></b>	1.416 (0.277)	2.731 (0.301)	1.406 (0.678)	1.454/1.626 (0.823)/(0.768)	100.1	-1.224	0.155	0.275
<b>6TS<sup>N-H</sup></b>	1.490 (0.242)	2.745 (0.290)	1.490 (0.712)	1.467/1.467 (0.809)/(0.878)	99.7	-1.241	0.148	0.445
<b>7TS<sup>N-H</sup></b>	1.446 (0.256)	2.700 (0.320)	1.364 (0.709)	1.451/1.541 (0.883)/(0.662)	99.3	-1.222	0.153	0.608
<b>9TS<sup>N-H</sup></b>	1.453 (0.253)	2.743 (0.290)	1.376 (0.707)	1.421/1.558 (0.918)/(0.639)	98.5	-1.236	0.147	0.312

**Table S6** Calculated (M06-D3/Def2-TZVP (Toluene)) important geometrical parameters, natural charges at the carbon atom of the  $\text{CH}_3^{\delta-}$  fragment, positively polarized hydrogen atom ( $\text{H}^{\delta+}$ ) and occupancies of the formally vacant  $p_\pi$  orbital centered at the central E (E = B and C) atom for the transition state involved in the activation of  $\text{CH}_4$  by **4-7**, **9**, and **II** via  $\sigma_{\text{CH}_2}$  approach. The bond lengths and bond angles are given in Å and in degree ( $^\circ$ ) respectively. The Wiberg Bond Index values (WBI) are given within parenthesis (X = C and N).

Molecules	$\text{H}^{\delta+}-\text{H}_3\text{C}^{\delta-}$	$\text{E}-\text{CH}_3^{\delta-}$	$\text{E}-\text{H}^{\delta+}$	$\text{E}-\text{X}$	$\angle\text{N-E-X}$	$q_{\text{CH}_3^{\delta-}}$	$q_{\text{H}^{\delta+}}$	$\text{Occ}_{p_\pi}$
<b>II-TS<sup>C-H</sup></b>	1.557 (0.224)	2.343 (0.518)	1.167 (0.674)	1.338/1.502 (1.247)/(0.995)	108.0	-0.827	0.277	0.832
<b>4TS<sup>C-H</sup></b>	1.540 (0.339)	2.959 (0.271)	1.484 (0.626)	1.497/1.537 (0.773)/(1.090)	98.1	-1.062	0.100	0.542
<b>5TS<sup>C-H</sup></b>	1.436 (0.336)	2.402 (0.510)	1.342 (0.633)	1.495/1.633 (0.762)/(0.799)	99.2	-0.862	0.112	0.374
<b>6TS<sup>C-H</sup></b>	1.624 (0.239)	2.633 (0.460)	1.302 (0.729)	1.481/1.485 (0.830)/(0.776)	99.7	-0.948	0.081	0.448
<b>7TS<sup>C-H</sup></b>	1.439 (0.325)	2.339 (0.538)	1.319 (0.650)	1.560/1.494 (0.652)/(0.781)	99.1	-0.834	0.116	0.439
<b>9TS<sup>C-H</sup></b>	1.509 (0.288)	2.482 (0.496)	1.318 (0.685)	1.574/1.449 (0.838)/(0.629)	98.2	-0.894	0.092	0.438

**Table S7** Calculated (M06-D3/Def2-TZVP (Toluene)) important geometrical parameters, natural charges at the carbon atom of the  $\text{CH}_3^{\delta-}$  fragment, positively polarized hydrogen atom ( $\text{H}^{\delta+}$ ) and occupancies of the formally vacant  $p_\pi$  orbital centered at the central E (E = B and C) atom for the transition state involved in the activation of  $\text{CH}_4$  by **4-7**, **9** and **II** via inverted  $\pi_{\text{CH}_2}$  approach. The bond lengths and bond angles are given in Å and in degree ( $^\circ$ ) respectively. The Wiberg Bond Index values (WBI) are given within parenthesis (X = C and N).

Molecules	$\text{H}^{\delta+}-\text{H}_3\text{C}^{\delta-}$	$\text{E}-\text{CH}_3^{\delta-}$	$\text{E}-\text{H}^{\delta+}$	$\text{E}-\text{X}$	$\angle\text{N-E-X}$	$q_{\text{CH}_3^{\delta-}}$	$q_{\text{H}^{\delta+}}$	$\text{Occ}_{p_\pi}$
<b>II-TS<sup>C-H</sup></b>	1.238 (0.468)	1.833 (0.551)	1.322 (0.401)	1.399/1.521 (1.066)/(0.983)	105.8	-0.649	0.298	0.740
<b>4TS<sup>C-H</sup></b>	1.268 (0.474)	1.862 (0.584)	1.357 (0.404)	1.573/1.589 (0.967)/(0.711)	98.3	-0.783	0.257	0.606
<b>5TS<sup>C-H</sup></b>	1.254 (0.582)	1.865 (0.582)	1.369 (0.403)	1.549/1.642 (0.725)/(0.860)	99.4	-0.781	0.237	0.637
<b>6TS<sup>C-H</sup></b>	1.267 (0.483)	1.844 (0.601)	1.385 (0.430)	1.545/1.528 (0.725)/(0.799)	97.9	-0.779	0.212	0.579
<b>7TS<sup>C-H</sup></b>	1.251 (0.501)	1.834 (0.604)	1.384 (0.397)	1.534/1.573 (0.748)/(0.684)	99.6	-0.796	0.240	0.488
<b>9TS<sup>C-H</sup></b>	1.276 (0.474)	1.831 (0.623)	1.382 (0.425)	1.512/1.594 (0.772)/(0.664)	98.8	-0.799	0.233	0.635

**Table S8** Calculated (M06-D3/Def2-TZVP (Toluene)) important geometrical parameters, natural charges at the fluoride atom ( $F^{\delta-}$ ) and carbon atom of the  $C_6H_5$  fragment and occupancies of the formally vacant  $p_\pi$  orbital centered at the central E atom ( $E = B$  and Al) for the transition state involved in the activation of the C – F bond of  $C_6H_5F$  by **4-7**, **9** and **IIIa**. The bond lengths and bond angles are given in Å and in degree ( $^\circ$ ) respectively. The Wiberg Bond Index values (WBI) are given within parenthesis ( $X = C$  and N).

Molecules	$F^{\delta-}-H_5C_6^{\delta+}$	$E-C_6H_5^{\delta+}$	$E-F^{\delta-}$	E-X	$\angle N-E-X$	$q_{C_6H_5^{\delta+}}$	$q_{F^{\delta-}}$	Occ $_{p_\pi}$
<b>IIIa-TS<sup>C-F</sup></b>	1.529 (0.608)	2.340 (0.458)	2.058 (0.188)	1.932/1.932 (0.261)/(0.261)	92.9	0.159	-0.466	0.280
<b>4TS<sup>C-F</sup></b>	1.370 (0.821)	2.487 (0.334)	2.692 (0.047)	1.494/1.532 (0.729)/(1.046)	98.1	0.408	-0.379	0.367
<b>5TS<sup>C-F</sup></b>	1.370 (0.818)	2.428 (0.373)	2.780 (0.053)	1.444/1.625 (0.705)/(0.644)	99.4	0.397	-0.384	0.250
<b>6TS<sup>C-F</sup></b>	1.374 (0.812)	2.403 (0.371)	2.653 (0.054)	1.454/1.473 (0.867)/(0.763)	98.9	0.399	-0.383	0.262
<b>7TS<sup>C-F</sup></b>	1.403 (0.778)	2.172 (0.443)	2.406 (0.070)	1.451/1.554 (0.831)/(0.608)	98.4	0.316	-0.396	0.374
<b>9TS<sup>C-F</sup></b>	1.375 (0.807)	2.393 (0.394)	2.723 (0.056)	1.421/1.570 (0.830)/(0.542)	97.1	0.392	-0.390	0.379

**Table S9** Calculated (M06-D3/Def2-TZVP (Toluene)) important geometrical parameters, natural charges at the hydrogen atom ( $H^{\delta+}$ ) and carbon atom of the  $C_6H_5$  fragment and occupancies of the formally vacant  $p_\pi$  orbital centered at the central E atom ( $E = B$ ) for the transition state involved in the activation of the *para* C–H bond of  $C_6H_5F$  by **4-7** and **9**. The bond lengths and bond angles are given in Å and in degree ( $^\circ$ ) respectively. The Wiberg Bond Index values (WBI) are given within parenthesis ( $X = C$  and N).

Molecule	$H^{\delta+}-C_6H_4F^{\delta-}$	$E-C_6H_4F^{\delta-}$	$E-H^{\delta+}$	E-X	$\angle N-E-X$	$q_{C_6H_4F^{\delta-}}$	$q_{H^{\delta+}}$	Occ $_{p_\pi}$
<b>4TS<sup>p(C-H)</sup></b>	1.401 (0.424)	2.960 (0.164)	1.608 (0.517)	1.484/1.525 (1.108)/(0.780)	98.2	-0.341	0.148	0.470
<b>5TS<sup>p(C-H)</sup></b>	1.456 (0.343)	2.841 (0.300)	1.442 (0.612)	1.624/1.455 (0.758)/(0.810)	100.2	-0.273	0.091	0.583
<b>6TS<sup>p(C-H)</sup></b>	1.509 (0.334)	2.816 (0.232)	1.442 (0.612)	1.459/1.470 (0.883)/(0.803)	99.3	-0.308	0.120	0.431
<b>7TS<sup>p(C-H)</sup></b>	1.481 (0.309)	2.557 (0.400)	1.345 (0.655)	1.467/1.554 (0.828)/(0.648)	99.2	-0.223	0.100	0.385
<b>9TS<sup>p(C-H)</sup></b>	1.499 (0.317)	2.690 (0.329)	1.383 (0.643)	1.568/1.429 (0.624)/(0.890)	98.5	-0.270	0.095	0.425

**Table S10** Calculated (M06-D3/Def2-TZVP (Toluene)) important geometrical parameters, natural charges at the hydrogen atom ( $H^{\delta+}$ ) and carbon atom of the  $C_6H_5$  fragment and occupancies of the formally vacant  $p_\pi$  orbital centered at the central E atom ( $E = B$ ) for the transition state involved in the activation of the *meta* C–H bond of  $C_6H_5F$  by **4-7** and **9**. The bond lengths and bond angles are given in Å and in degree ( $^\circ$ ) respectively. The Wiberg Bond Index values (WBI) are given within parenthesis ( $X = C$  and  $N$ ).

Molecule	$H^{\delta+}-C_6H_4F^{\delta-}$	$E-C_6H_4F^{\delta-}$	$E-H^{\delta+}$	E-X	$\angle N-E-X$	$q_{C_6H_4F^{\delta-}}$	$q_{H^{\delta+}}$	Occ $p_\pi$
<b>4TS<sup>m(C-H)</sup></b>	1.386 (0.436)	2.947 (0.172)	1.612 (0.504)	1.525/1.485 (1.110)/(0.781)	98.3	-0.298	0.148	0.435
<b>5TS<sup>m(C-H)</sup></b>	1.450 (0.352)	2.840 (0.290)	1.453 (0.603)	1.454/1.624 (0.815)/(0.758)	100.2	-0.231	0.095	0.524
<b>6TS<sup>m(C-H)</sup></b>	1.487 (0.351)	2.810 (0.228)	1.456 (0.596)	1.469/1.458 (0.803)/(0.884)	99.4	-0.268	0.123	0.650
<b>7TS<sup>m(C-H)</sup></b>	1.483 (0.318)	2.601 (0.376)	1.364 (0.646)	1.463/1.553 (0.839)/(0.649)	99.1	-0.195	0.101	0.392
<b>9TS<sup>m(C-H)</sup></b>	1.488 (0.330)	2.717 (0.310)	1.400 (0.629)	1.566/1.427 (0.623)/(0.896)	98.5	-0.236	0.097	0.453

**Table S11** Calculated (M06-D3/Def2-TZVP (Toluene)) important geometrical parameters, natural charges at the hydrogen atom ( $H^{\delta+}$ ) and carbon atom of the  $C_6H_5$  fragment and occupancies of the formally vacant  $p_\pi$  orbital centered at the central E atom ( $E = B$ ) for the transition state involved in the activation of the *ortho* C–H bond of  $C_6H_5F$  by **4-7** and **9**. The bond lengths and bond angles are given in Å and in degree ( $^\circ$ ) respectively. The Wiberg Bond Index values (WBI) are given within parenthesis ( $X = C$  and  $N$ ).

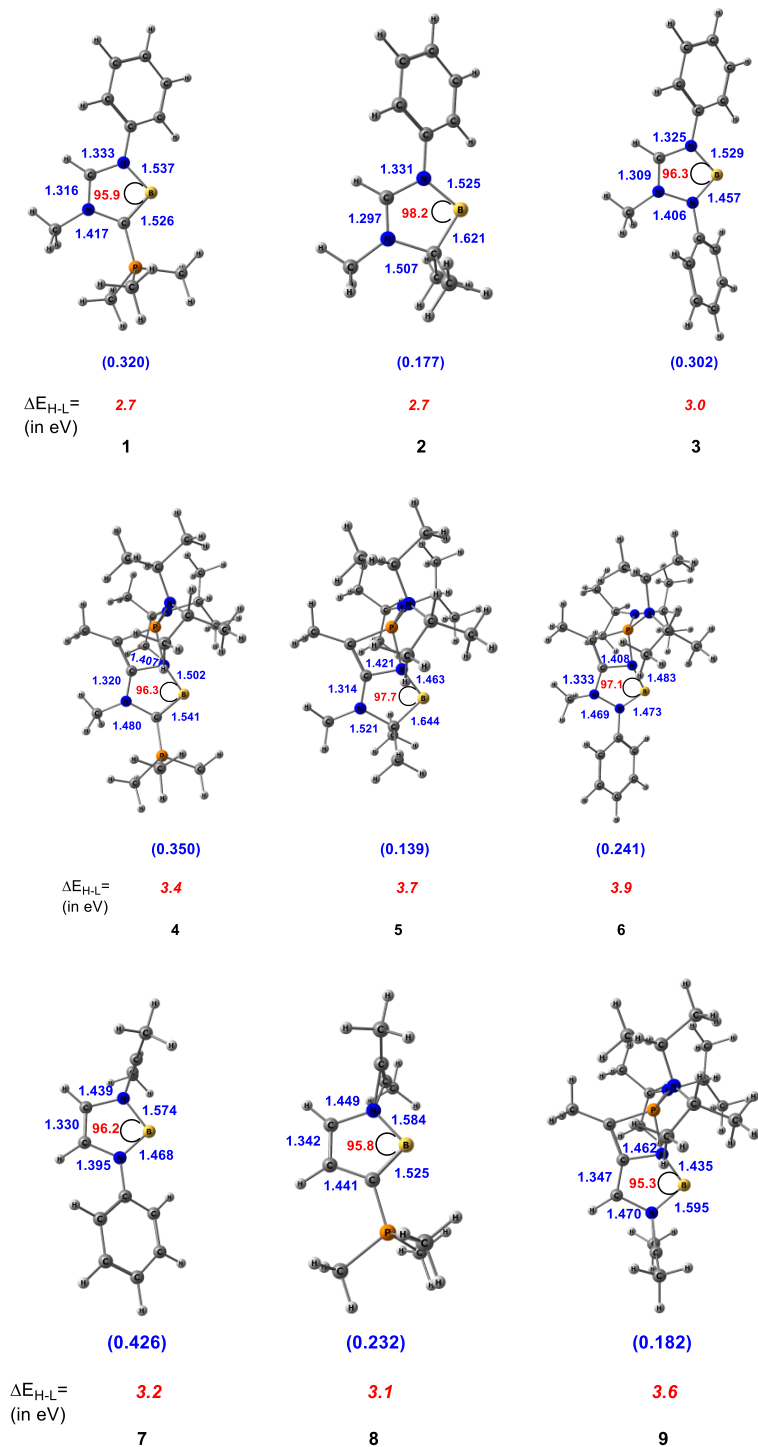
Molecule	$H^{\delta+}-C_6H_4F^{\delta-}$	$E-C_6H_4F^{\delta-}$	$E-H^{\delta+}$	E-X	$\angle N-E-X$	$q_{C_6H_4F^{\delta-}}$	$q_{H^{\delta+}}$	Occ $p_\pi$
<b>4TS<sup>o(C-H)</sup></b>	1.355 (0.460)	2.967 (0.149)	1.668 (0.473)	1.526/1.485 (1.101)/(0.775)	98.1	-0.386	0.168	0.377
<b>5TS<sup>o(C-H)</sup></b>	1.405 (0.405)	2.946 (0.161)	1.608 (0.537)	1.447/1.627 (0.814)/(0.730)	99.9	-0.391	0.138	0.262
<b>6TS<sup>o(C-H)</sup></b>	1.473 (0.362)	2.770 (0.241)	1.467 (0.582)	1.465/1.471 (0.864)/(0.796)	99.0	-0.340	0.130	0.432
<b>7TS<sup>o(C-H)</sup></b>	1.453 (0.356)	2.669 (0.310)	1.423 (0.601)	1.457/1.550 (0.855)/(0.646)	98.9	-0.320	0.119	0.395
<b>9TS<sup>o(C-H)</sup></b>	1.451 (0.367)	2.765 (0.256)	1.462 (0.586)	1.565/1.423 (0.619)/(0.904)	98.2	-0.347	0.118	0.456

**Table S12** Calculated (M06-D3/Def2-TZVP(toluen)) activation energy barriers and reaction free energies (in kcal mol<sup>-1</sup>) for the activation of the C–H (*para*, *meta* and *ortho*) bond of C<sub>6</sub>H<sub>5</sub>F by **4-7** and **9**.

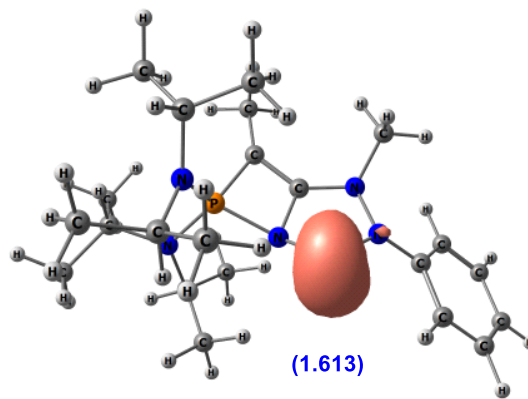
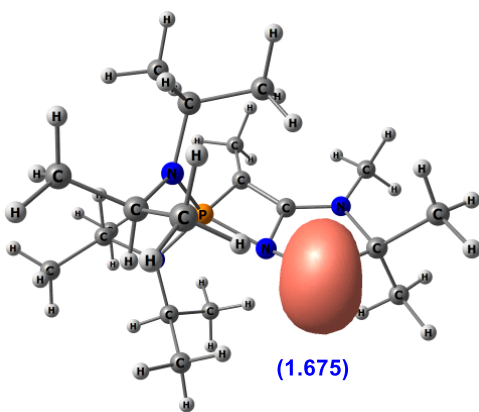
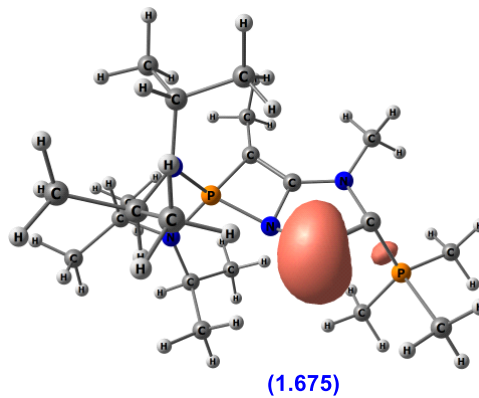
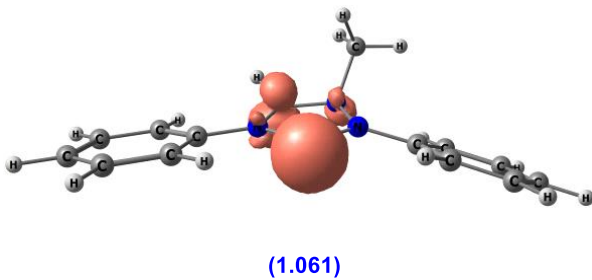
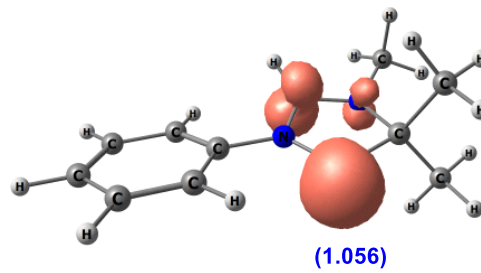
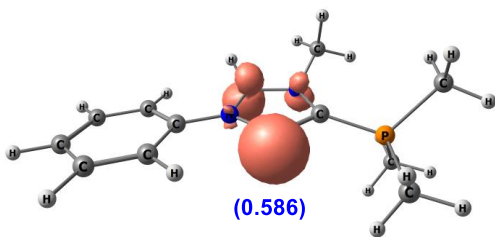
Molecules	<i>para</i>		<i>meta</i>		<i>ortho</i>	
	$\Delta G^{\circ}_{TS}^{\ddagger}$	$\Delta G^{\circ}_{Total}$	$\Delta G^{\circ}_{TS}^{\ddagger}$	$\Delta G^{\circ}_{Total}$	$\Delta G^{\circ}_{TS}^{\ddagger}$	$\Delta G^{\circ}_{Total}$
<b>4</b>	18.3	-48.0	16.6	-48.4	14.7	-48.8
<b>5</b>	22.7	-57.7	20.0	-58.6	17.4	-58.0
<b>6</b>	25.0	-50.8	22.8	-51.3	20.8	-49.5
<b>7</b>	25.1	-60.1	23.8	-60.7	21.6	-61.0
<b>9</b>	24.8	-54.2	23.5	-55.8	20.6	-54.8

**Table S13** Calculated activation energy barriers and reaction free energies (in kcal mol<sup>-1</sup>) for the formation of the E–H (E = H, N and C) splitting products obtained for **4-9** with different functionals.

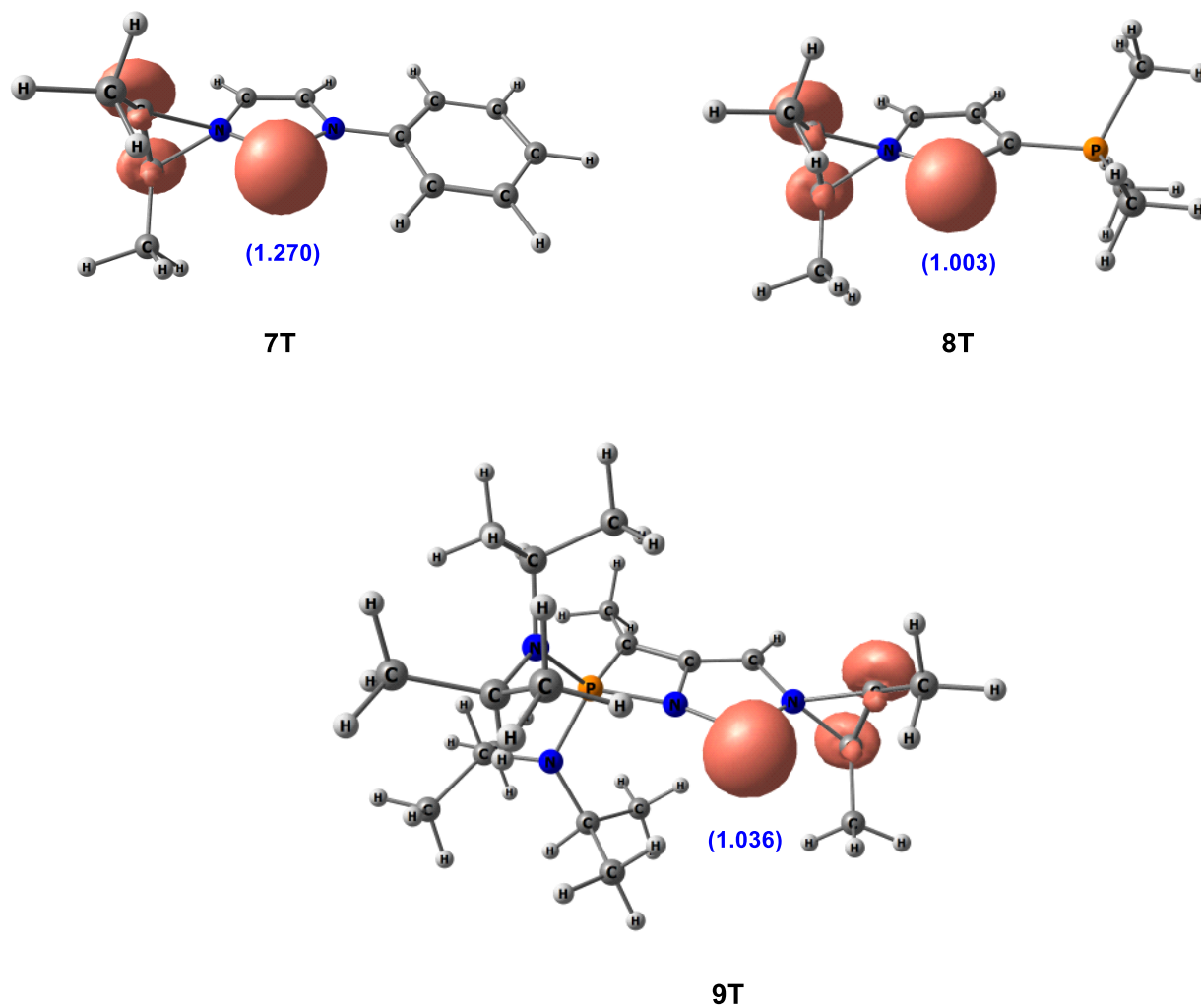
Molecules	M06		PBE0		$\omega$ B97XD	
	$\Delta G^{\circ}_{TS}^{\ddagger}$	$\Delta G^{\circ}_{Total}$	$\Delta G^{\circ}_{TS}^{\ddagger}$	$\Delta G^{\circ}_{Total}$	$\Delta G^{\circ}_{TS}^{\ddagger}$	$\Delta G^{\circ}_{Total}$
<b>4 + H<sub>2</sub></b>	14.4	-48.8	11.6	-47.0	14.7	-46.9
<b>7 + H<sub>2</sub></b>	18.1	-61.4	14.5	-62.8	18.8	-60.7
<b>5 + NH<sub>3</sub></b>	16.4	-63.4	14.0	-63.6	15.9	-62.7
<b>7 + NH<sub>3</sub></b>	19.4	-67.4	17.1	-68.1	20.2	-65.8
<b>6 + CH<sub>4</sub></b>	31.7	-45.0	31.8	-44.6	35.6	-44.0
<b>9 + CH<sub>4</sub></b>	29.9	-49.2	29.4	-49.2	33.3	-48.4



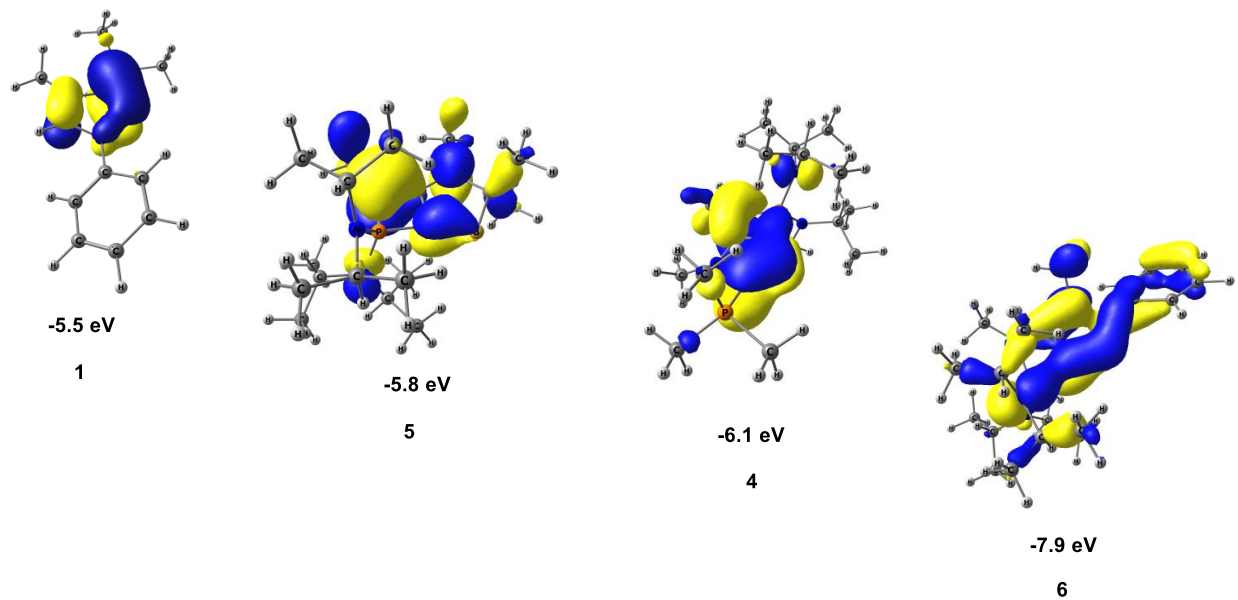
**Fig. S1** Pictorial representation of the singlet state optimized geometries of **1-9** calculated at M06-D3/Def2-TZVP (Toluene) level of theory. The occupancy of the formally vacant  $p_{\pi}$  orbital centered at the boron atom for **1-9** are given within parenthesis. Bond lengths and bond angles are given in Å and degree ( $^{\circ}$ ) respectively. The HOMO-LUMO ( $\Delta E_{H-L}$ , in eV) gap values for **1-9** are given in *italics*.







**Fig. S2** Mulliken spin density plots for the triplet states of **1-9** calculated at M06-D3/Def2-TZVP (Toluene) level of theory. The spin density values at the central boron atom are given within parenthesis.

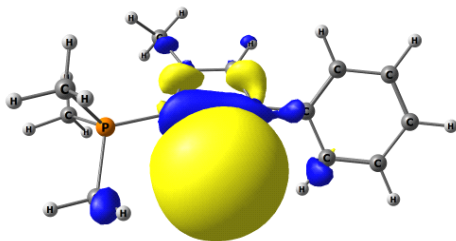


**Fig. S3** Pictorial representation of the occupied  $\pi$ -symmetric molecular orbitals (along with their energies in eV) for **1**, **4-6** calculated at the M06-D3/Def2-TZVP (Toluene) level of theory.

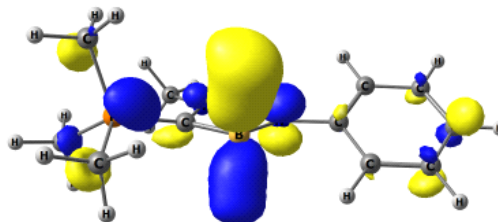
$\sigma$ -symmetric donor orbital

$\pi$ -symmetric acceptor orbital

1

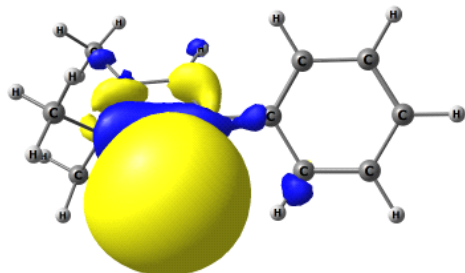


-3.2 eV

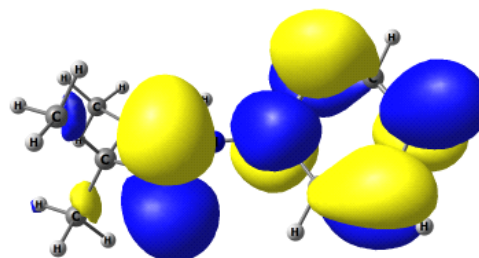


1.4 eV

2

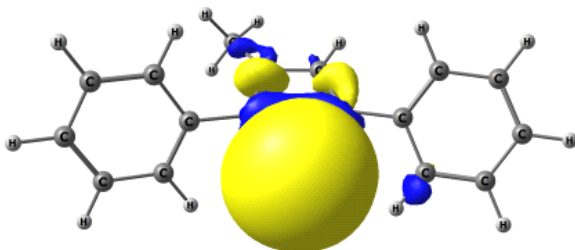


-3.9 eV

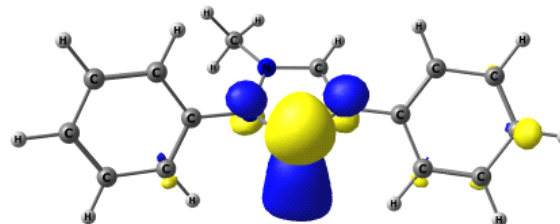


-0.3 eV

3

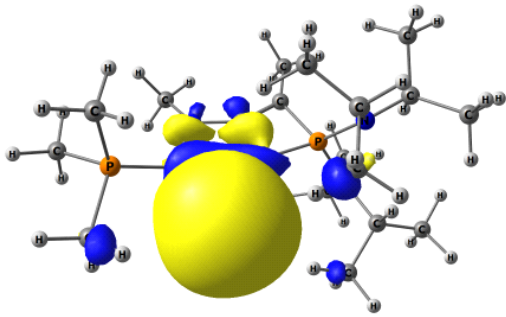


-4.1 eV

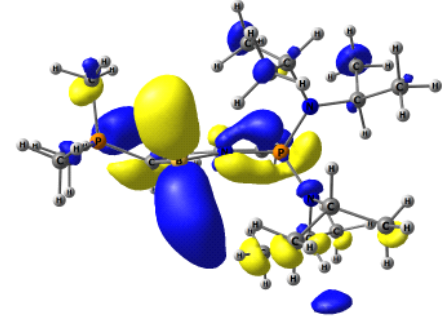


1.1 eV

4

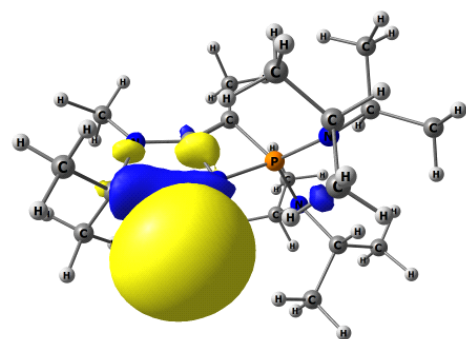


-3.0 eV

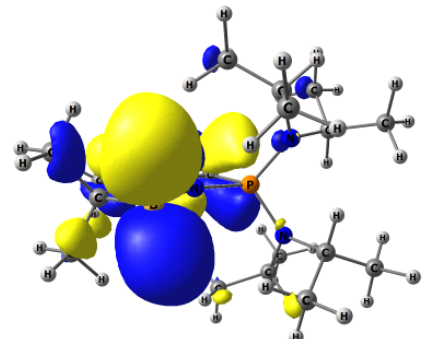


1.0 eV

5

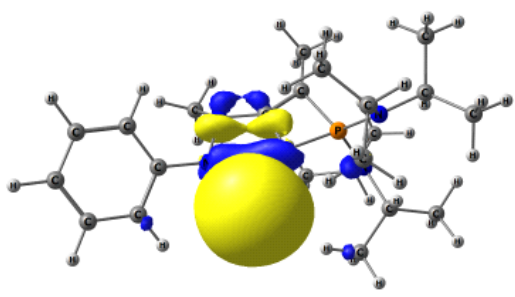


-3.4 eV

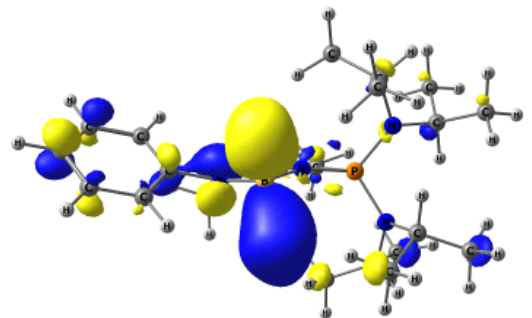


0.4 eV

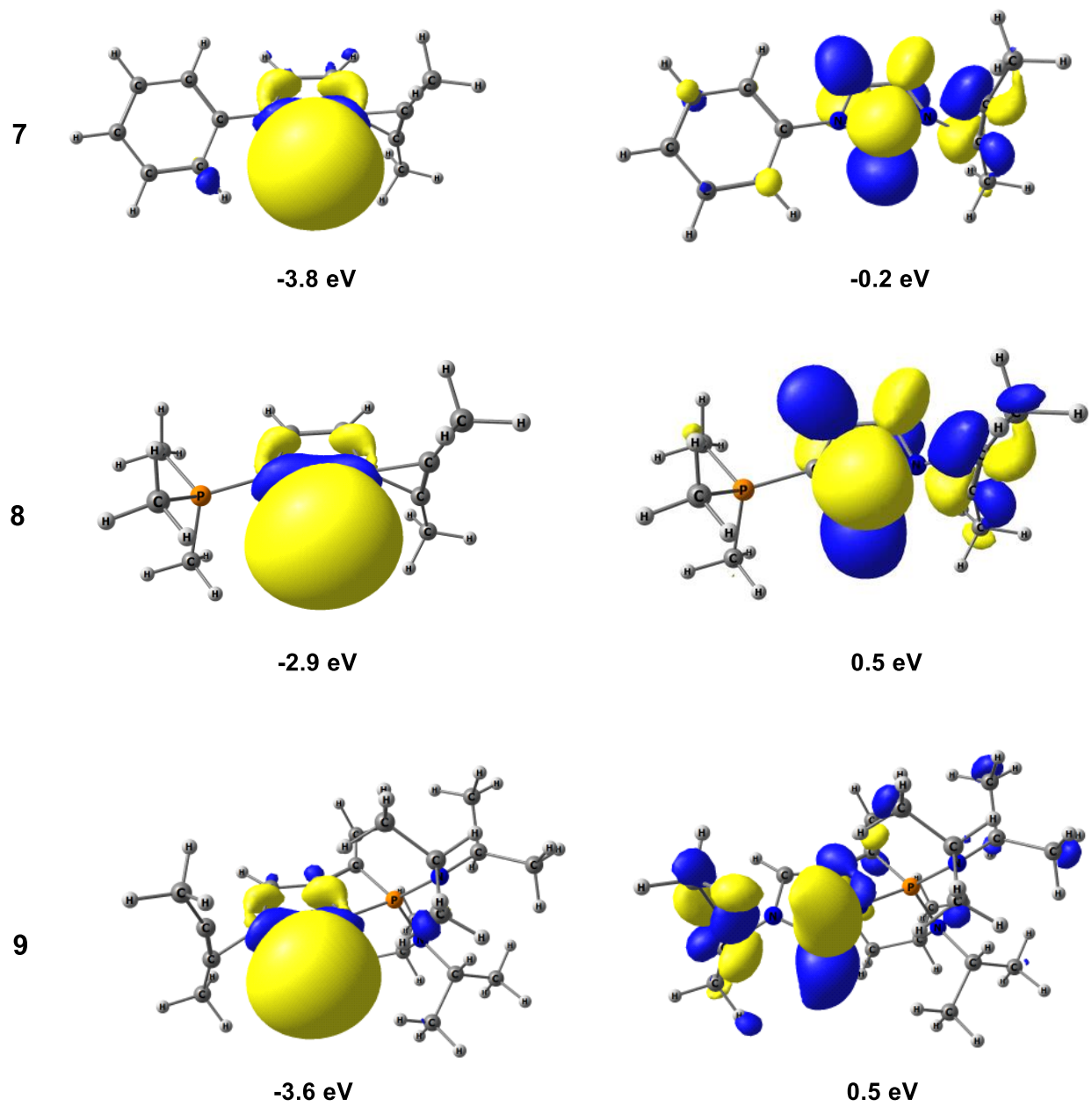
6



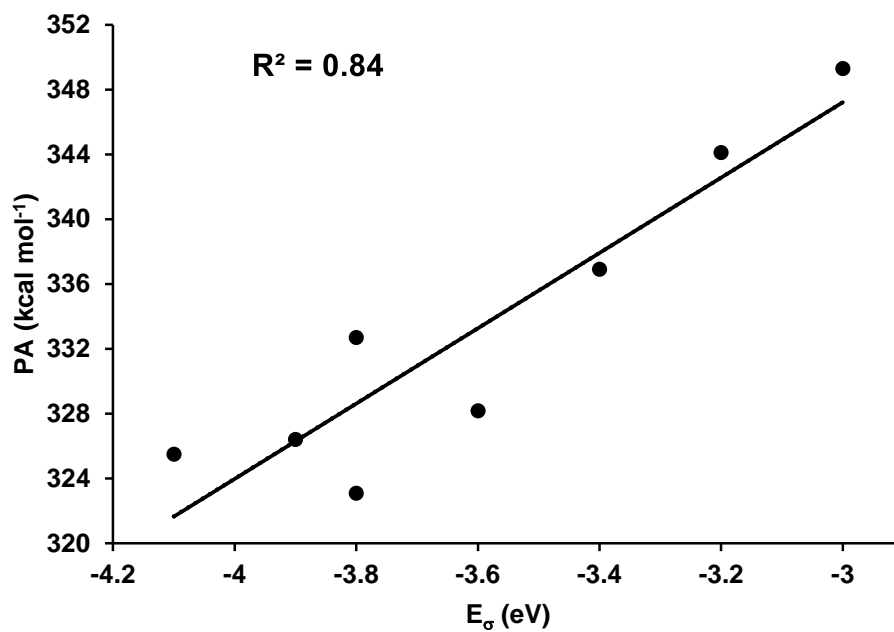
-3.8 eV



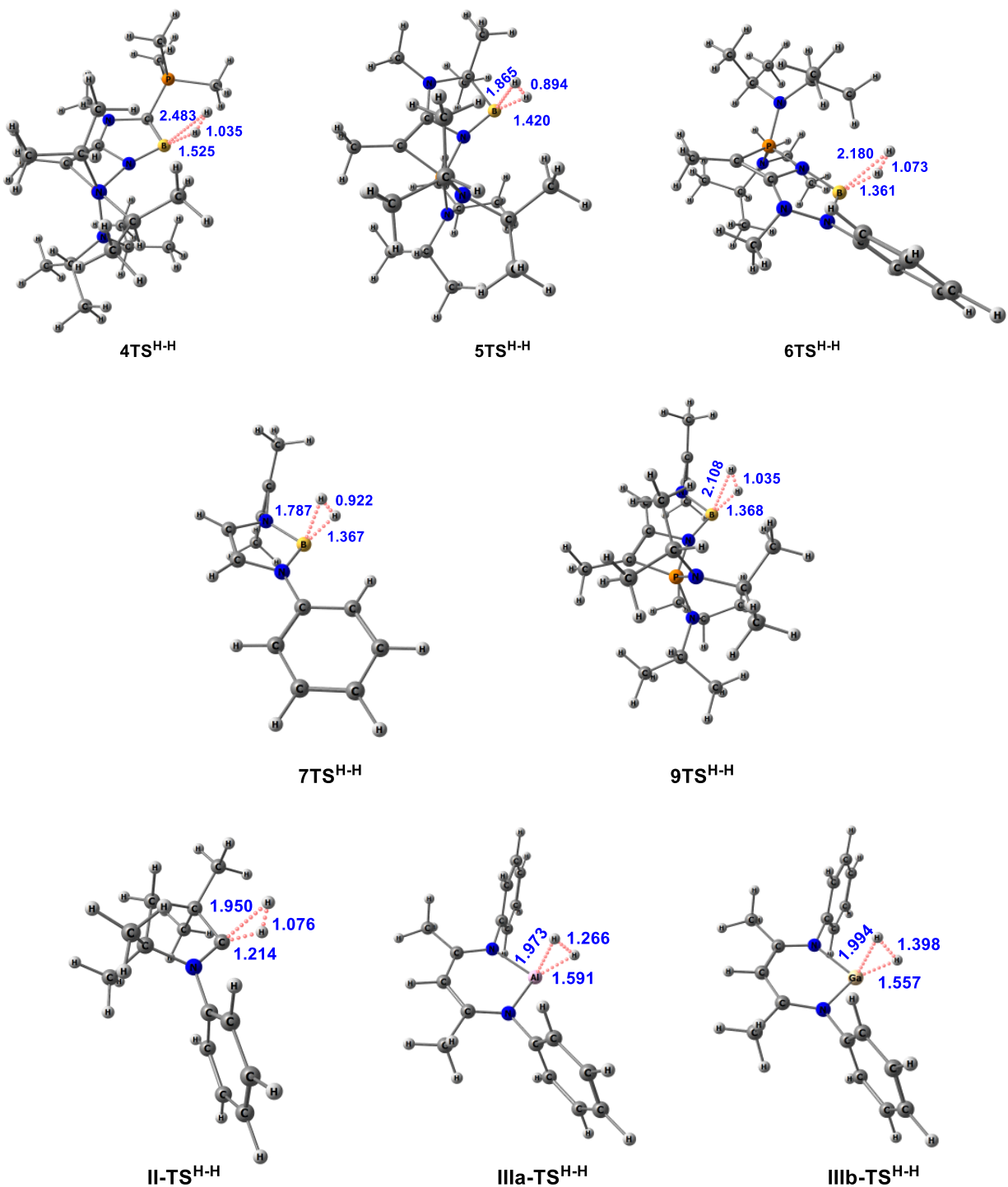
1.1 eV



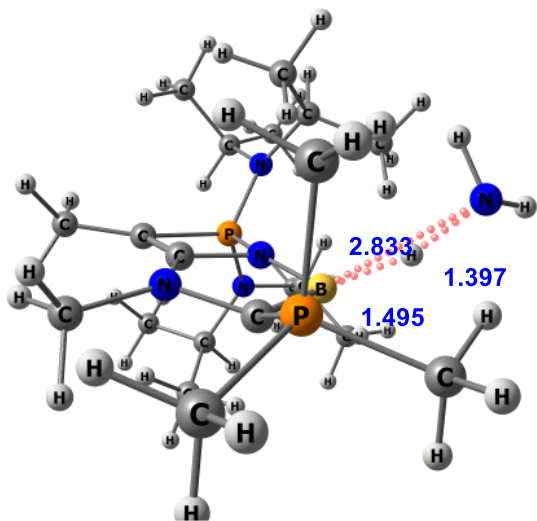
**Fig. S4** Pictorial representation of the  $\sigma$ -symmetric donor and  $\pi$ -symmetric acceptor orbitals (along with their energies in eV) concentrated at the boron atom for **1-9**. (M06-D3/Def2-TZVP (Toluene))



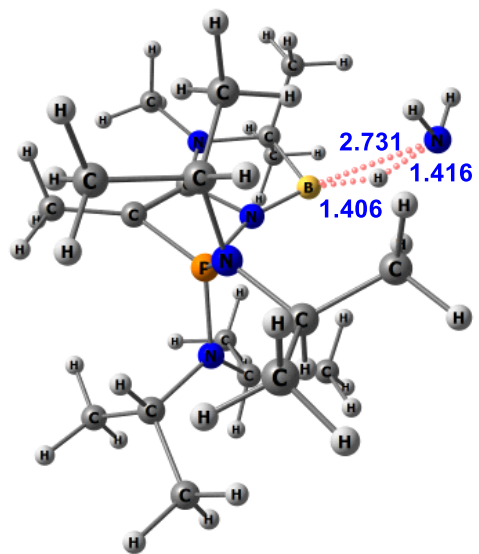
**Fig. S5** Correlation plot between proton affinity (PA, in  $\text{kcal mol}^{-1}$ ) and  $E_\sigma$  (in eV) values for **1-9** (omitting the point corresponding to **8**).



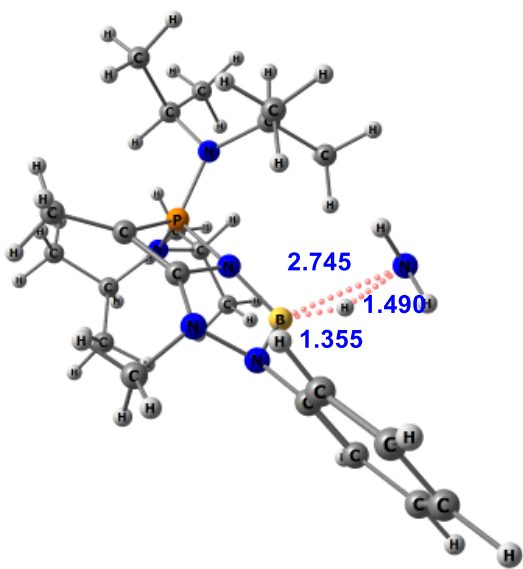
**Fig. S6** Optimized geometries of the transition states (TS) involved in the activation of dihydrogen by **4-7**, **9**, **II**, **IIIa** and **IIIb** (bond lengths are given in Å) at M06-D3/Def2-TZVP (Toluene) level of theory.



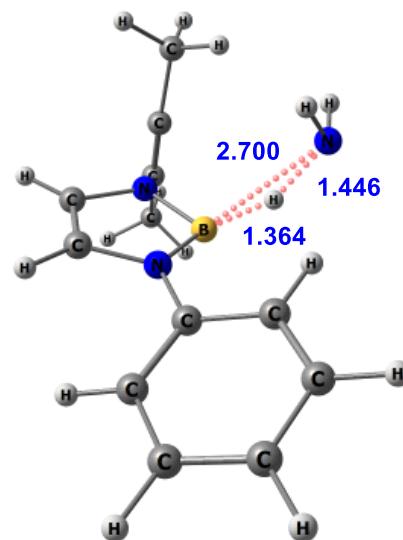
4TS<sup>N-H</sup>



5TS<sup>N-H</sup>

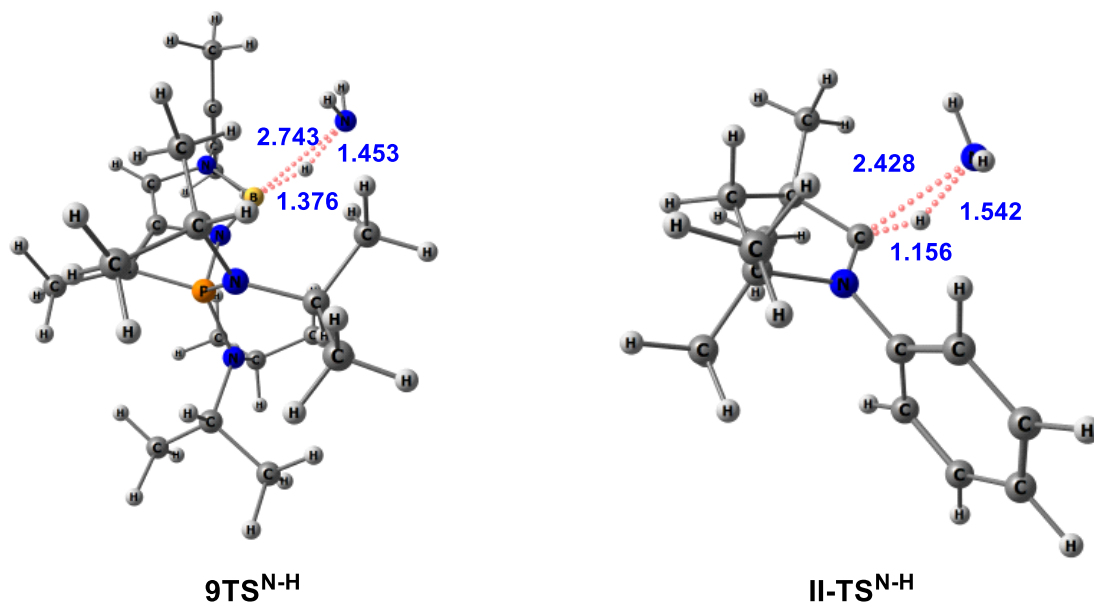


6TS<sup>N-H</sup>

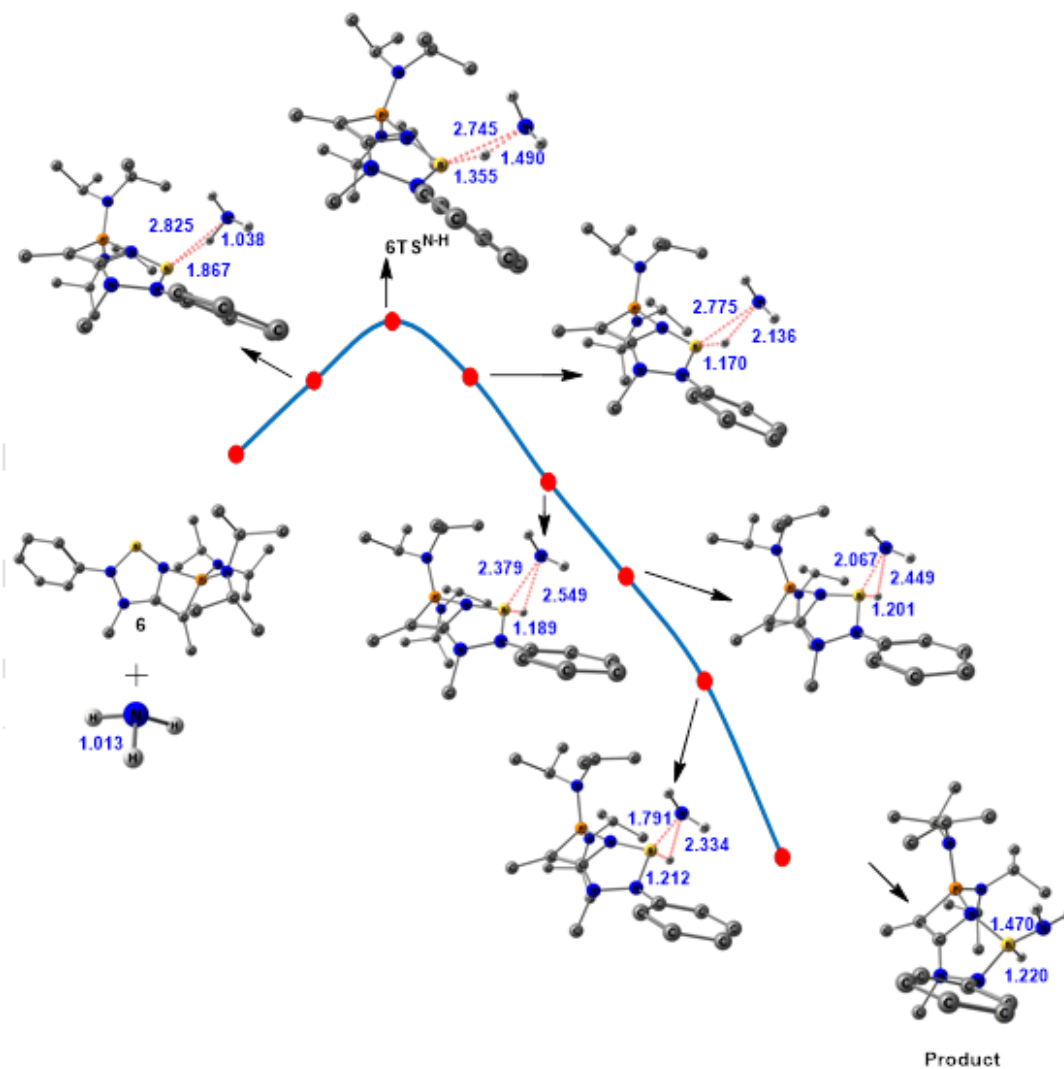


7TS<sup>N-H</sup>

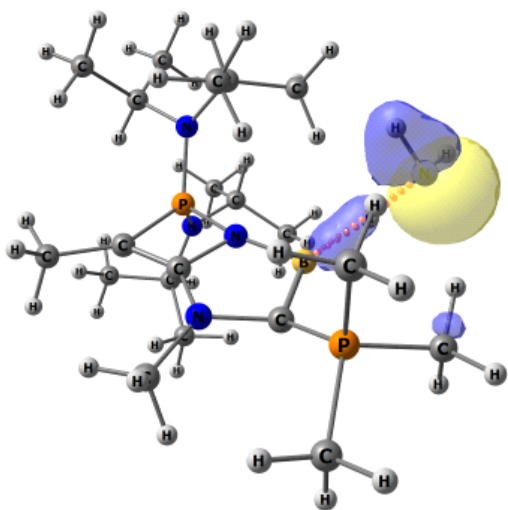




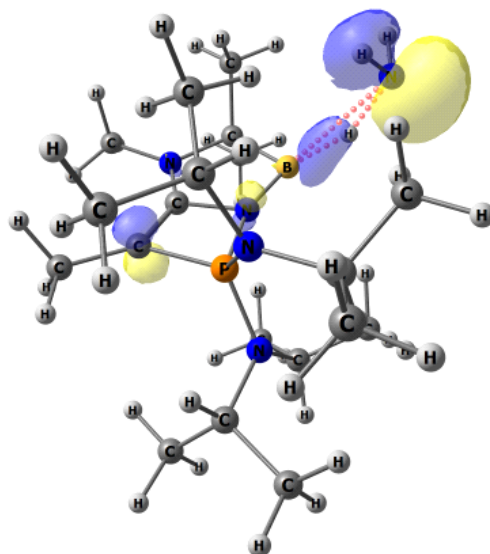
**Fig. S7** Optimized geometries of the TSs involved in the activation of  $\text{NH}_3$  by **4-7**, **9** and **II** (bond lengths are given in Å) at M06-D3/Def2-TZVP (Toluene) level of theory.



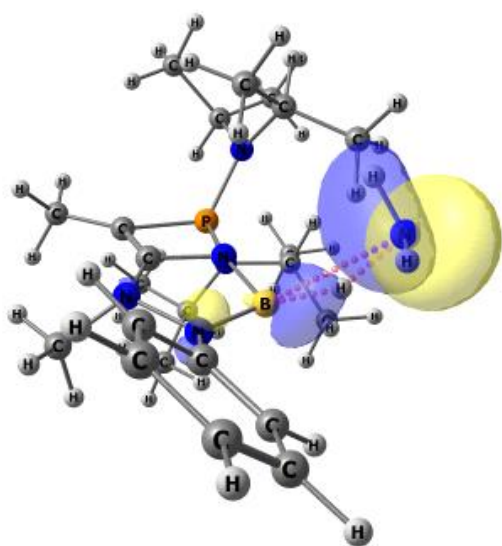
**Fig. S8** Some structures along the reaction pathway obtained from the IRC calculation (M06-D3/Def2-TZVP (Toluene)) for the activation of N–H bond of ammonia by **6** (bond lengths are given in Å). The hydrogen atoms of the methyl groups are omitted for clarity.



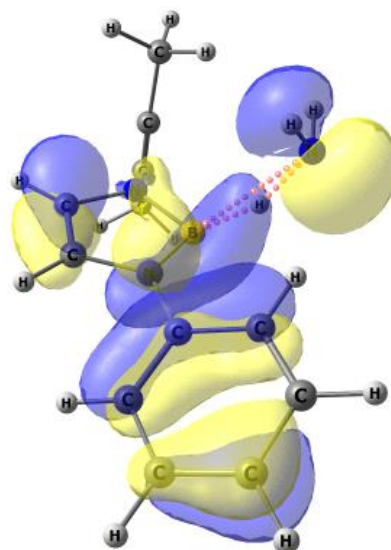
4TS<sup>N-H</sup>



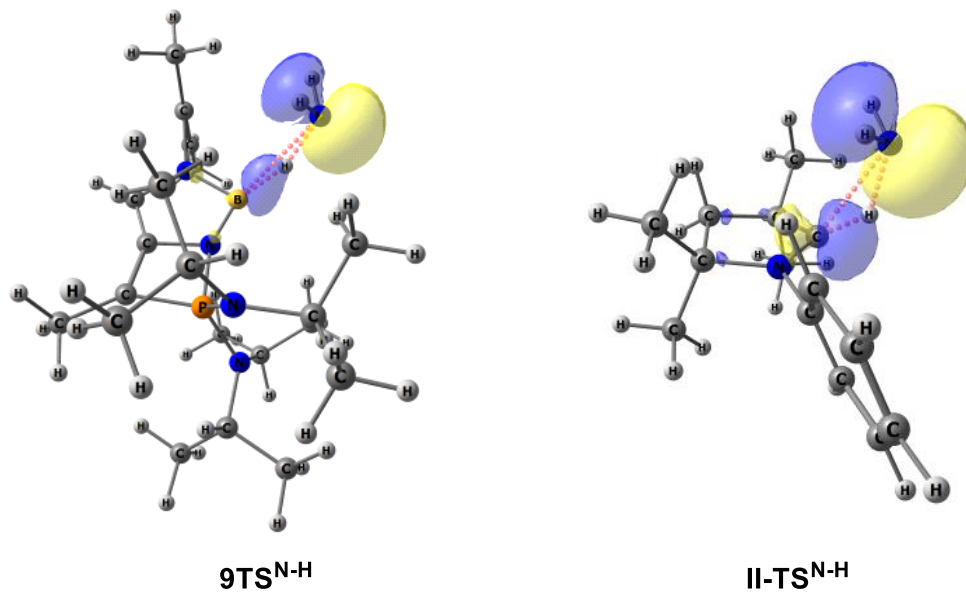
5TS<sup>N-H</sup>



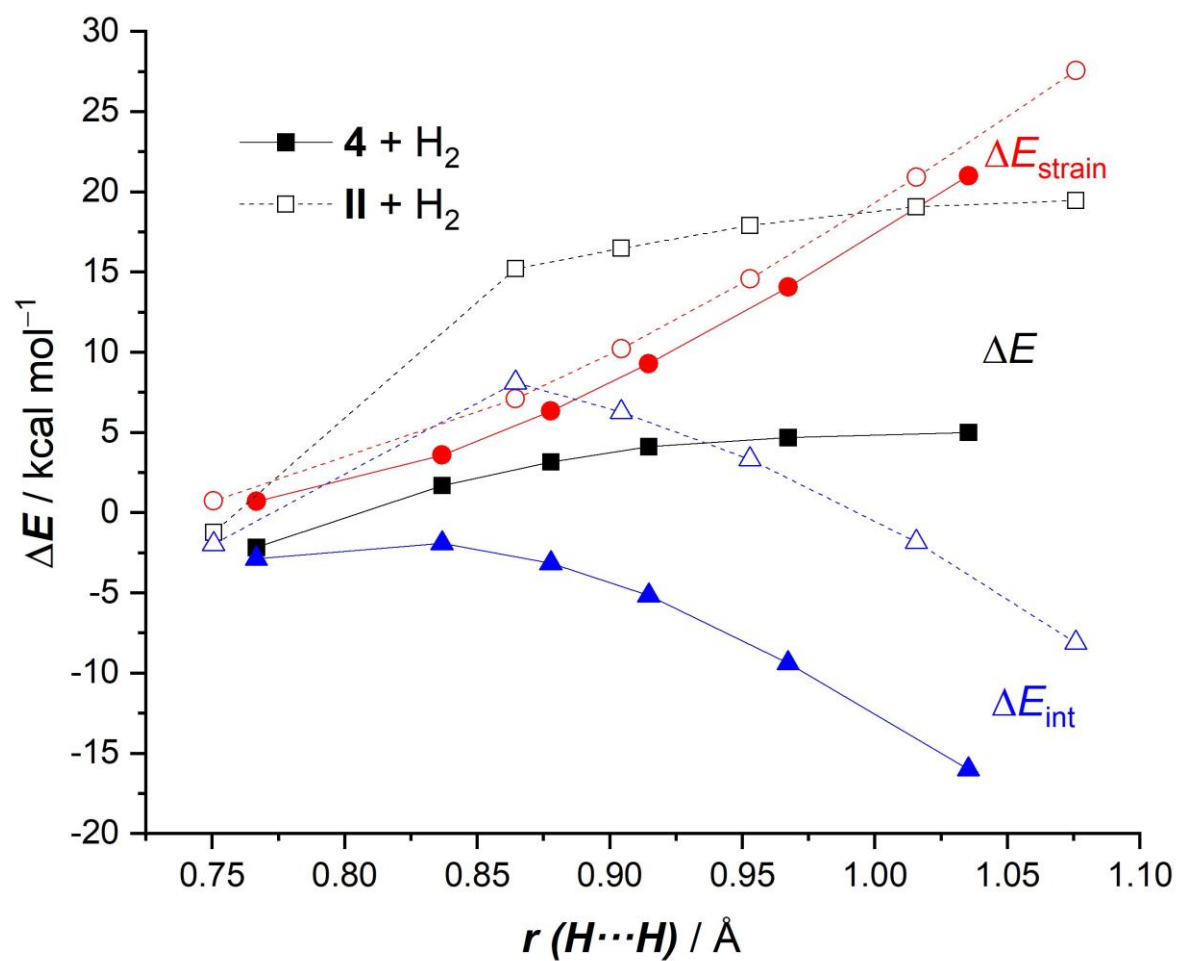
6TS<sup>N-H</sup>



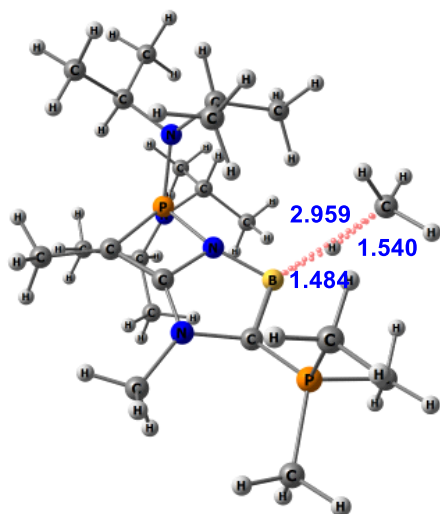
7TS<sup>N-H</sup>



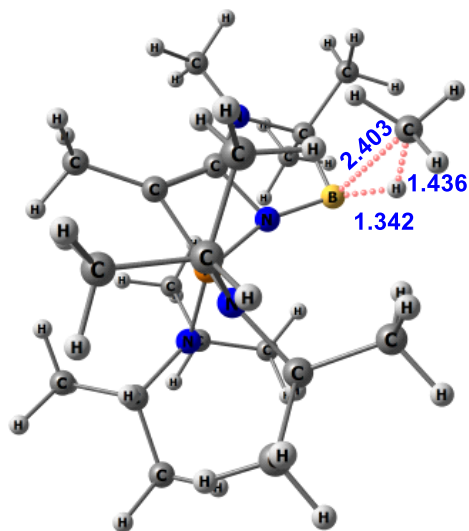
**Fig. S9** Pictorial representation of the molecular orbital showing the orientation of the amino lone pair for the transition states (TS) involved in the activation of NH<sub>3</sub> by **4-7**, **9** and **II** at M06-D3/Def2-TZVP (Toluene) level of theory.



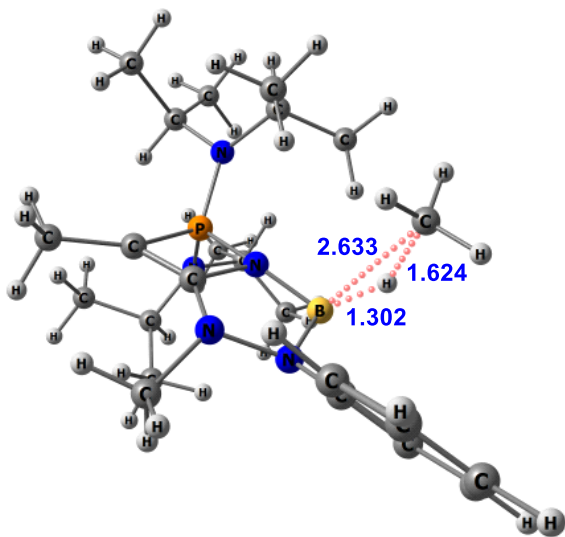
**Fig. S10** Comparative activation strain diagrams for the  $\text{H}_2$ -activation reactions mediated by **4** (solid lines) and **II** (dotted lines) along the reaction coordinate projected onto the breaking  $\text{H}\cdots\text{H}$  bond distance. All data have been computed at the PCM(toluene)-M06-D3/def2-TZVP level.



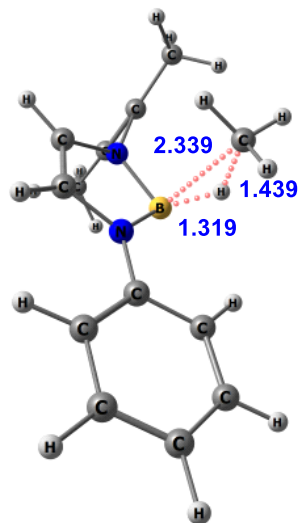
4TS<sub>σ</sub><sup>C-H</sup>



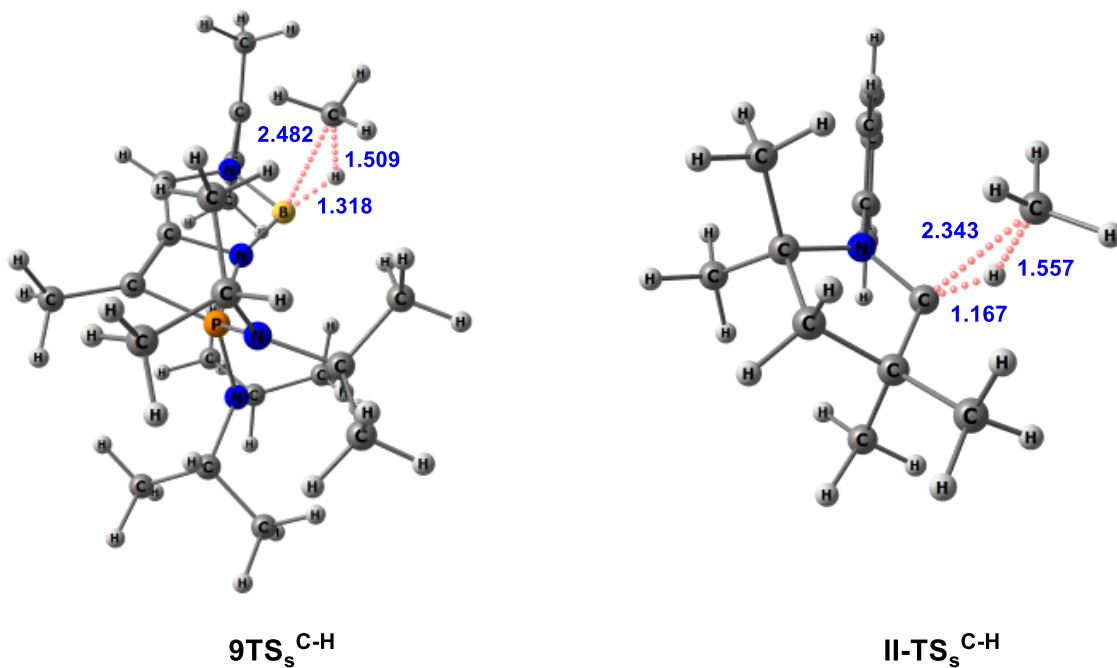
5TS<sub>σ</sub><sup>C-H</sup>



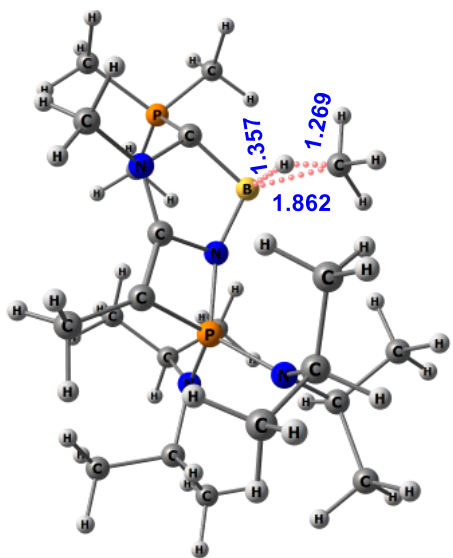
6TS<sub>σ</sub><sup>C-H</sup>



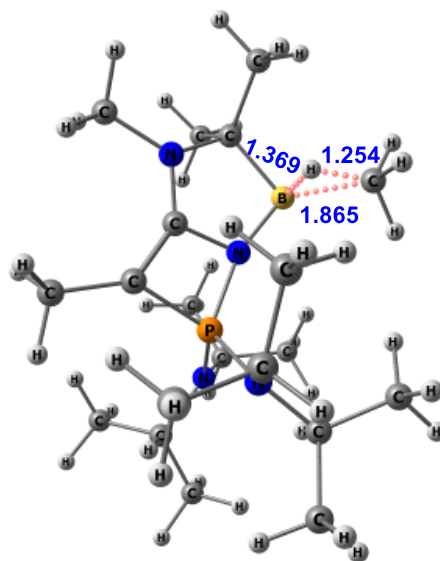
7TS<sub>σ</sub><sup>C-H</sup>



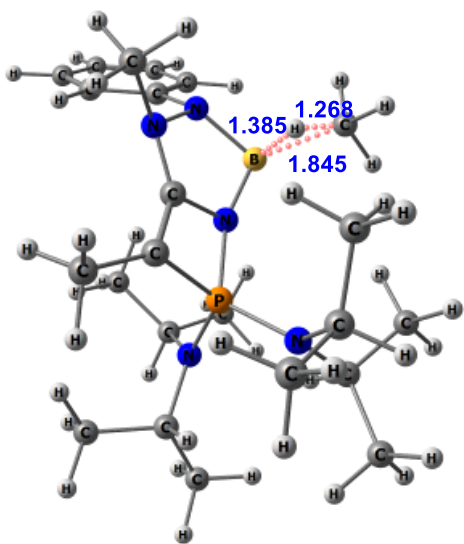
**Fig. S11** Optimized geometries of the transition states (TS) involved in the activation of C-H bond of CH<sub>4</sub> by **4-7**, **9** and **II** (bond lengths are given in Å) via  $\sigma_{\text{CH}_2}$  approach at M06-D3/Def2-TZVP (Toluene) level of theory.



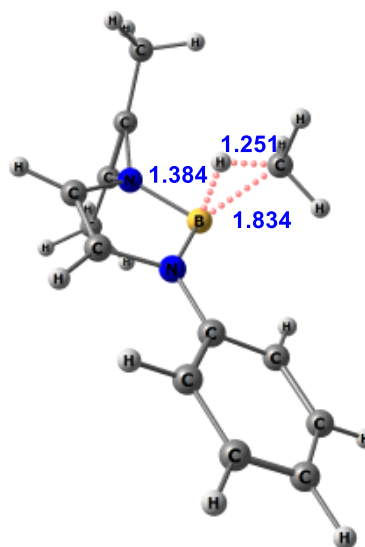
4TS $\pi^{C-H}$  (inverted)



5TS $\pi^{C-H}$  (inverted)

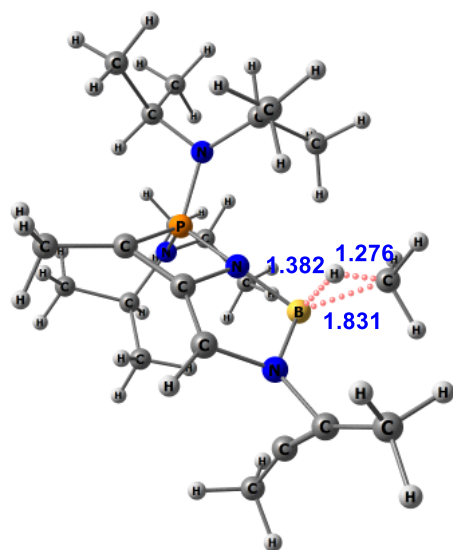


6TS $\pi^{C-H}$  (inverted)

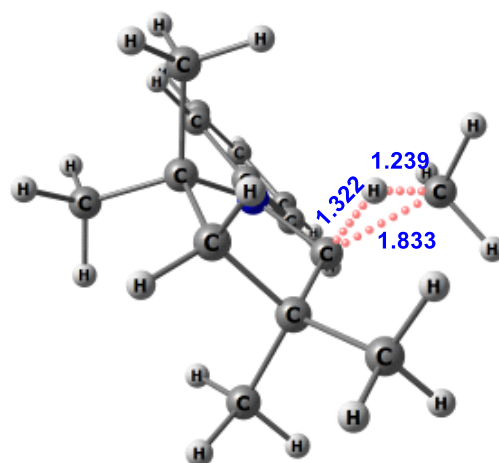


7TS $\pi^{C-H}$  (inverted)



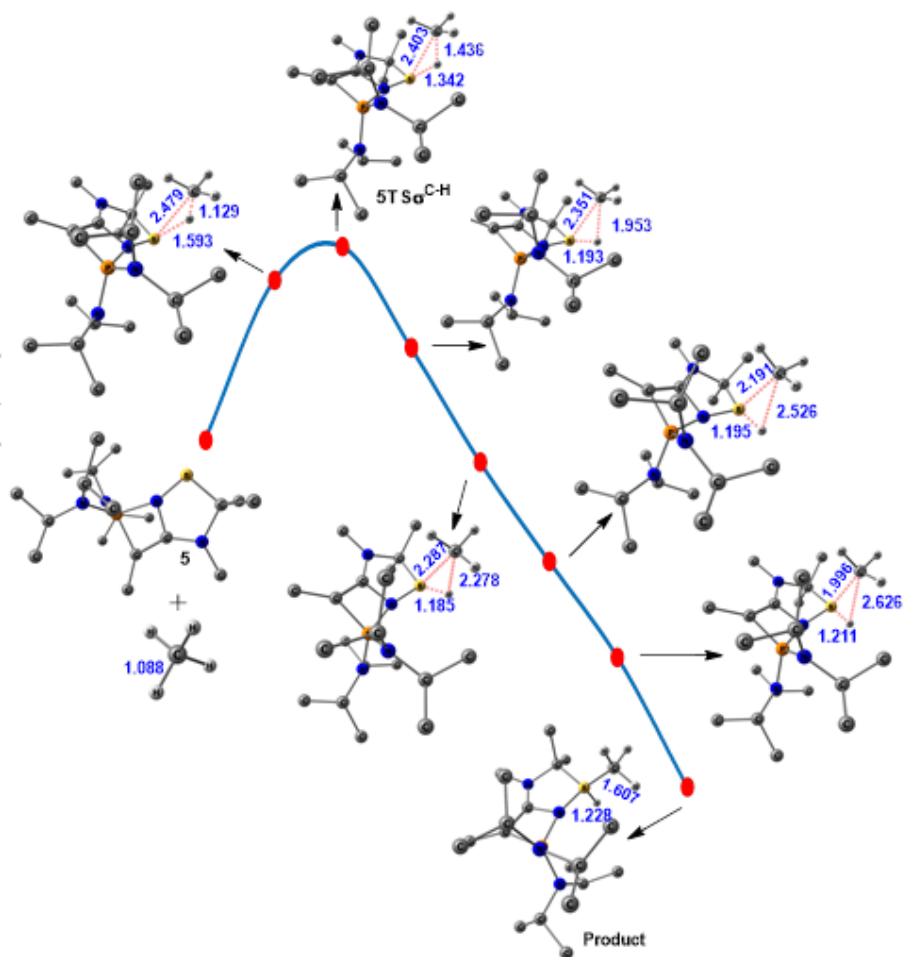


**9TSp<sup>C-H</sup> (inverted)**

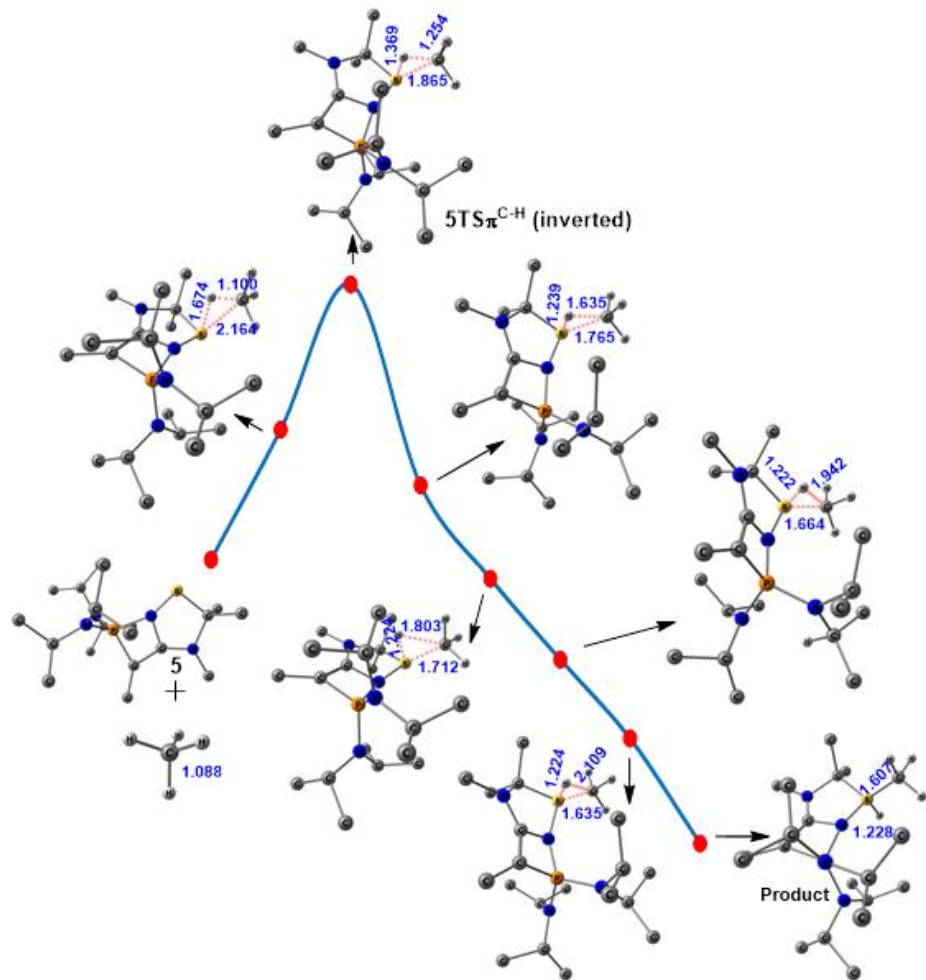


**II-TSp<sup>C-H</sup> (inverted)**

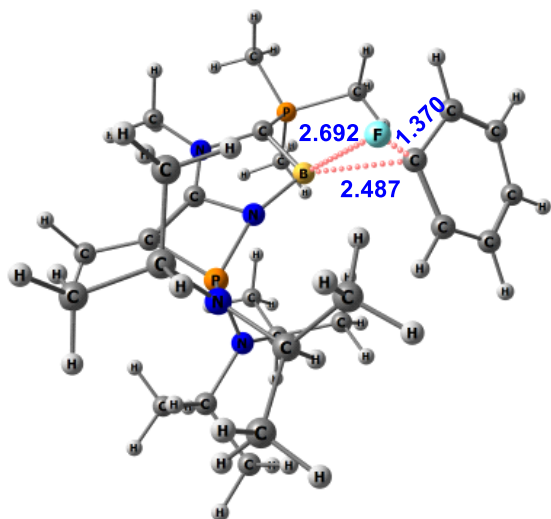
**Fig. S12** Optimized geometries of the transition states (TS) involved in the activation of C–H bond of CH<sub>4</sub> by **4-7**, **9** and **II** (bond lengths are given in Å) via inverted  $\pi_{\text{CH}_2}$  approach at M06-D3/Def2-TZVP (Toluene) level of theory.



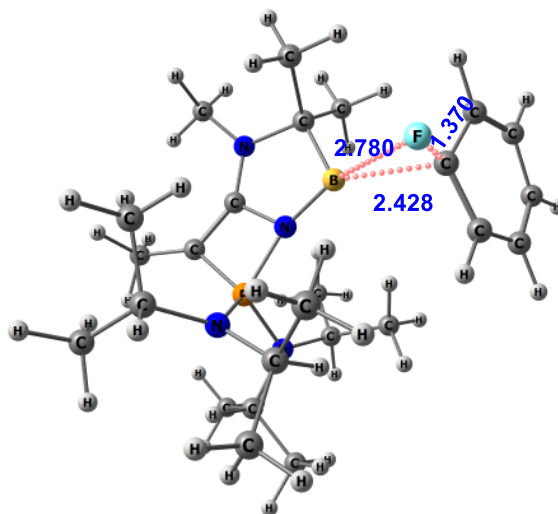
**Fig. S13** Some structures along the reaction pathway obtained from the IRC calculation (M06-D3/Def2-TZVP (Toluene)) for the activation of methane by **5** (bond lengths are given in Å) via  $\sigma_{\text{CH}_2}$  approach. The hydrogen atoms of the methyl groups are omitted for clarity.



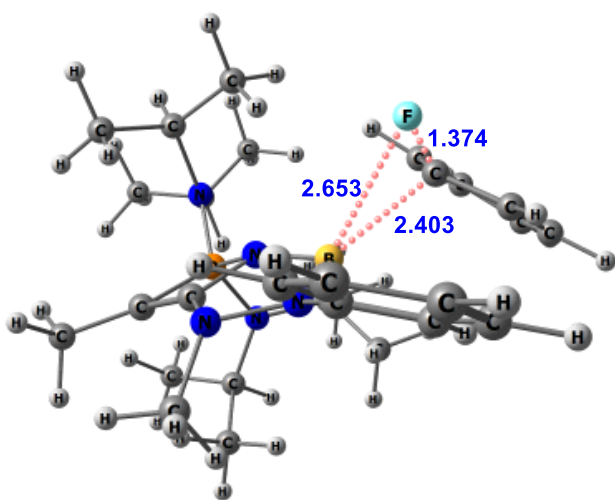
**Fig. S14** Some structures along the reaction pathway obtained from the IRC calculation (M06-D3/Def2-TZVP (Toluene)) for the activation of methane by **5** (bond lengths are given in Å) via inverted  $\pi_{\text{CH}_2}$  approach. The hydrogen atoms of the methyl groups are omitted for clarity.



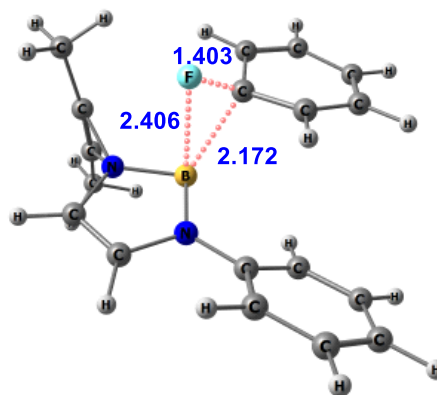
4TS<sup>C-F</sup>



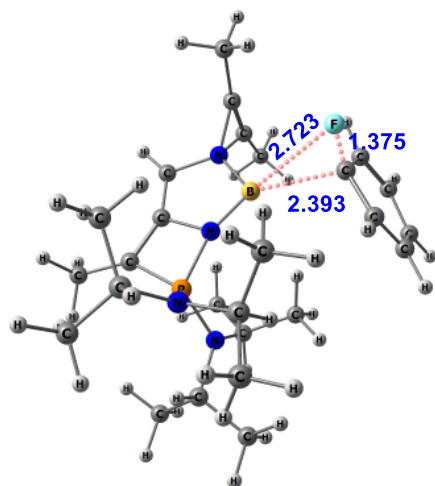
5TS<sup>C-F</sup>



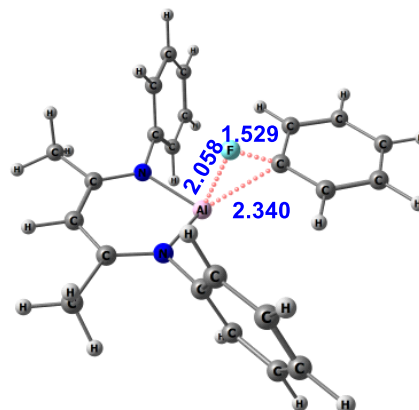
6TS<sup>C-F</sup>



7TS<sup>C-F</sup>

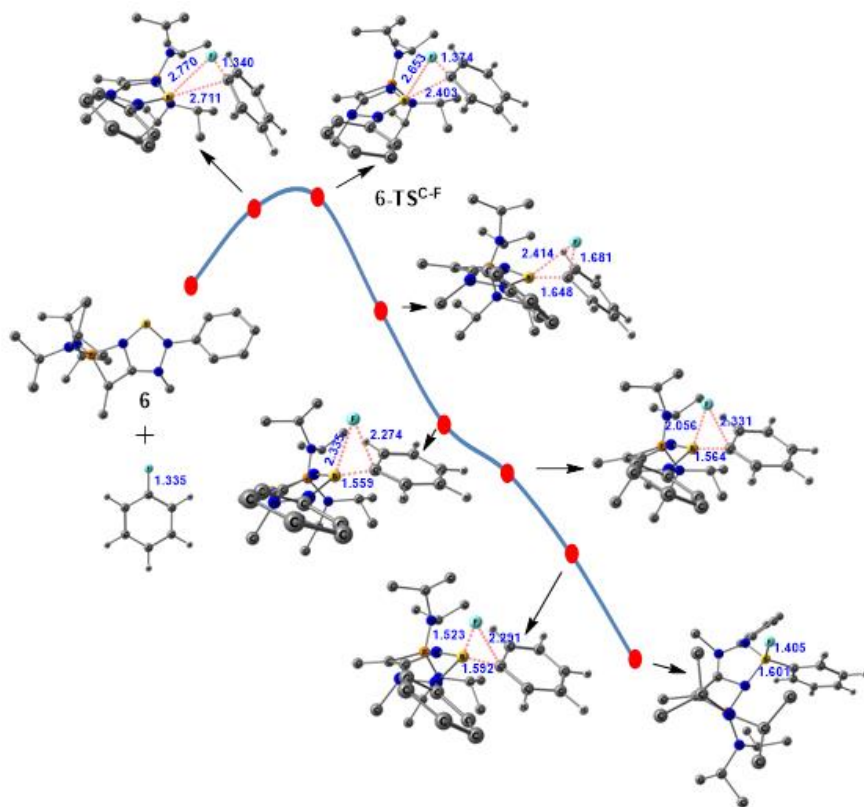


**9TS<sup>C-F</sup>**

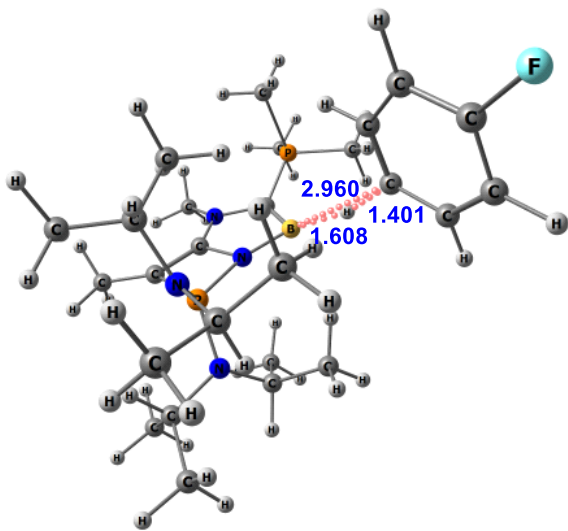


**IIIa-TS<sup>C-F</sup>**

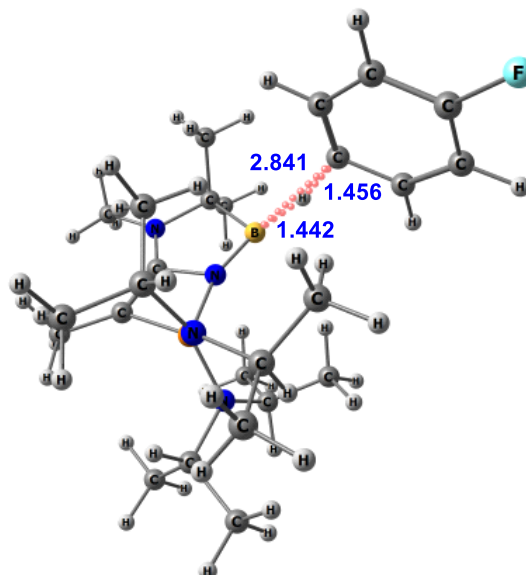
**Fig. S15** Optimized geometries of the transition states (TS) involved in the activation of C–F bond of C<sub>6</sub>H<sub>5</sub>F by **4-7**, **9** and **IIIa** (bond lengths are given in Å) at M06-D3/Def2-TZVP (Toluene) level of theory.



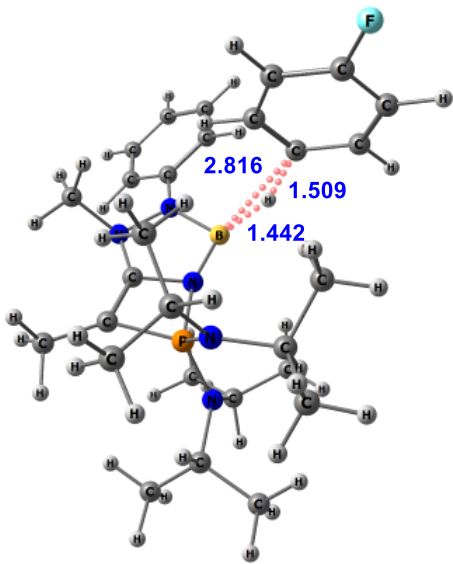
**Fig. S16** Some structures along the reaction pathway obtained from the IRC calculation (M06-D3/Def2-TZVP (Toluene)) for the activation of C-F bond of C<sub>6</sub>H<sub>5</sub>F by **6** (bond lengths are given in Å). The hydrogen atoms of the methyl groups are omitted for clarity.



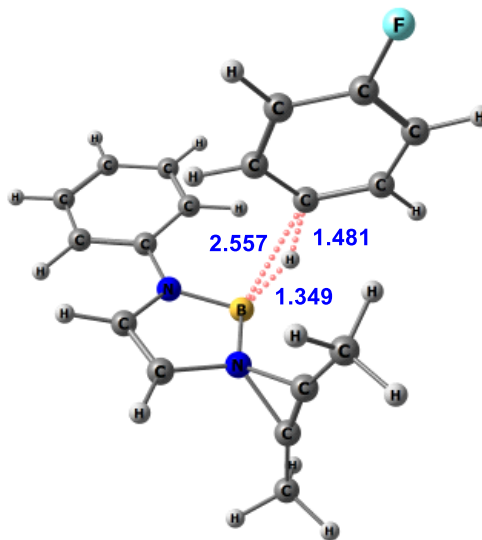
4TS<sup>p</sup>(C-H)



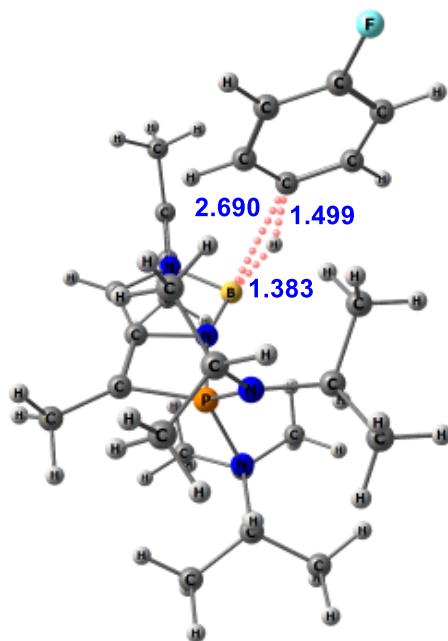
5TS<sup>p</sup>(C-H)



6TS<sup>p</sup>(C-H)



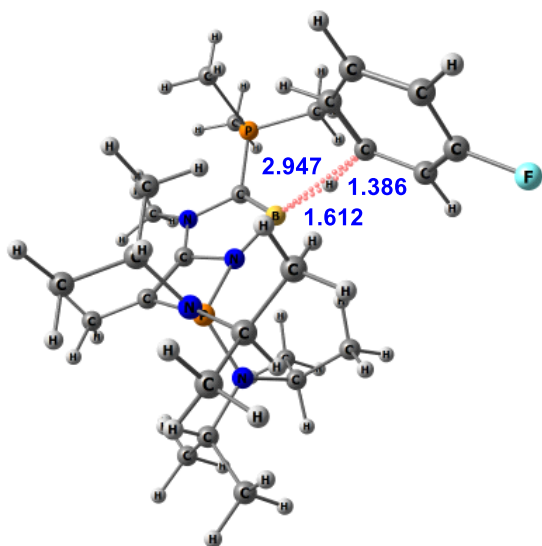
7TS<sup>p</sup>(C-H)



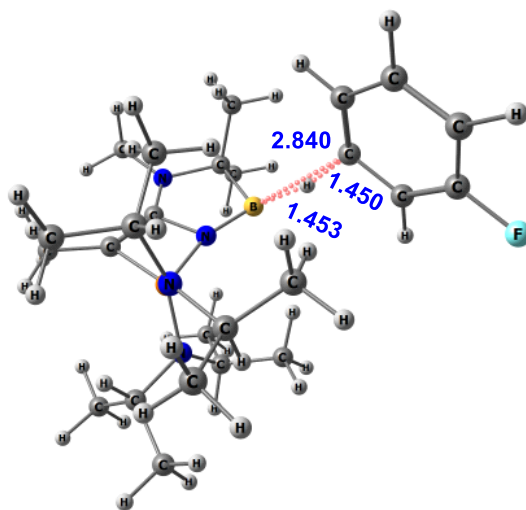
**9TS <sup>$\rho$</sup> (C-H)**

**Fig. S17** Optimized geometries of the transition states (TS) involved in the activation of *para* C–H bond of C<sub>6</sub>H<sub>5</sub>F by **4-7** and **9** (bond lengths are given in Å) at M06-D3/Def2-TZVP (Toluene) level of theory.

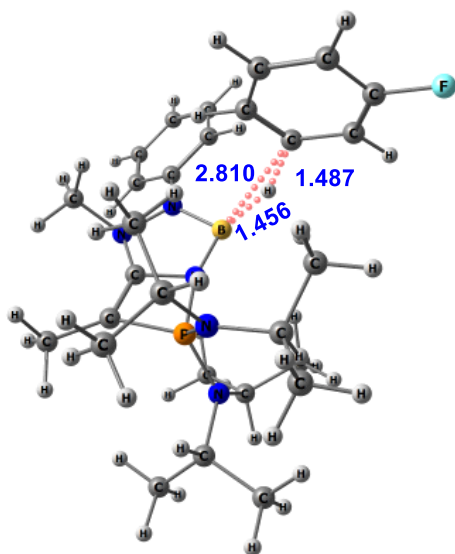




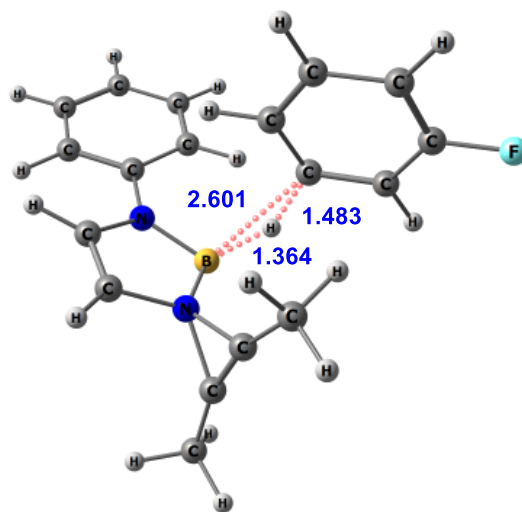
4TS<sup>m</sup>(C-H)



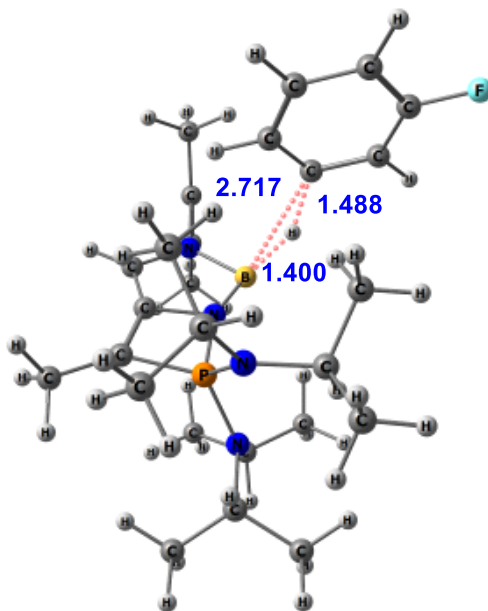
5TS<sup>m</sup>(C-H)



6TS<sup>m</sup>(C-H)

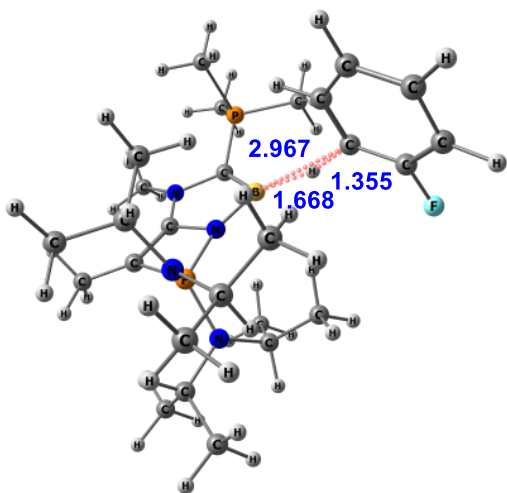


7TS<sup>m</sup>(C-H)

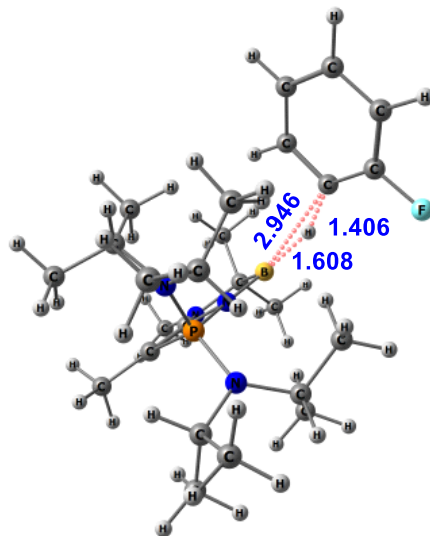


**9TS<sup>m</sup>(C-H)**

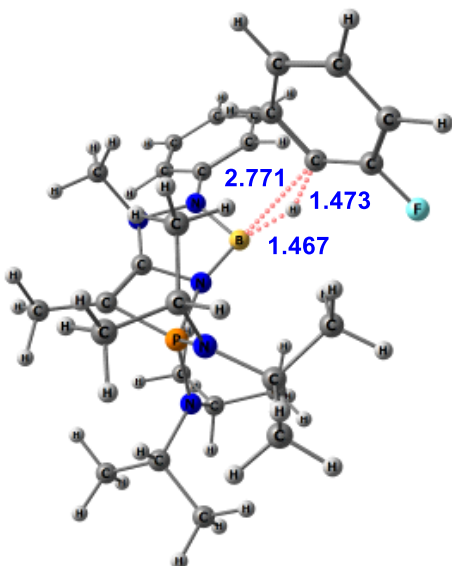
**Fig. S18** Optimized geometries of the transition states (TS) involved in the activation of *meta* C–H bond of C<sub>6</sub>H<sub>5</sub>F by **4-7** and **9** (bond lengths are given in Å) at M06-D3/Def2-TZVP (Toluene) level of theory.



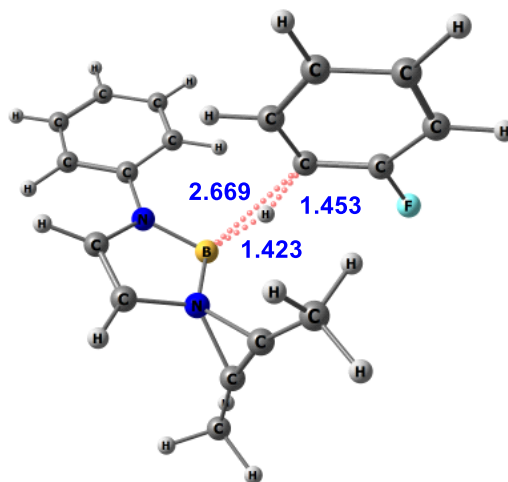
4TS<sup>o</sup>(C-H)



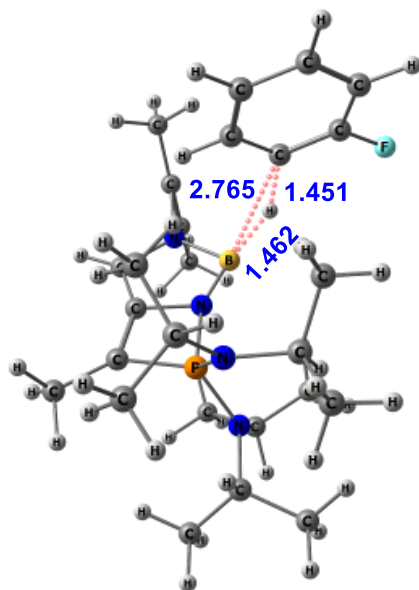
5TS<sup>o</sup>(C-H)



6TS<sup>o</sup>(C-H)

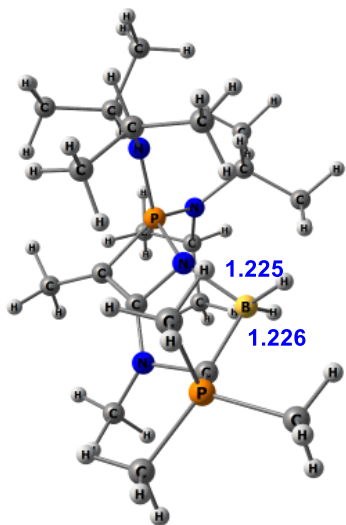


7TS<sup>o</sup>(C-H)

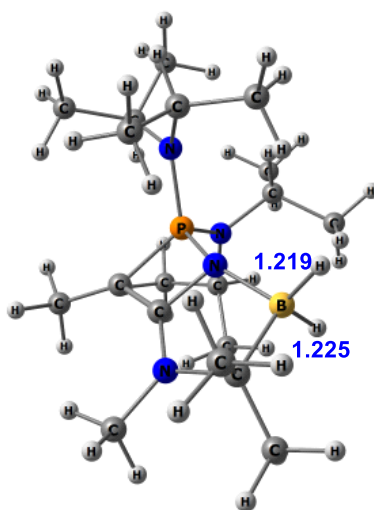


**9TS<sup>o</sup>(C-H)**

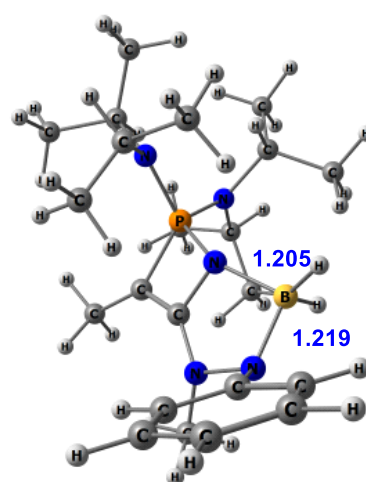
**Fig. S19** Optimized geometries of the transition states (TS) involved in the activation of *ortho* C–H bond of C<sub>6</sub>H<sub>5</sub>F by **4-7** and **9** (bond lengths are given in Å) at M06-D3/Def2-TZVP (Toluene) level of theory.



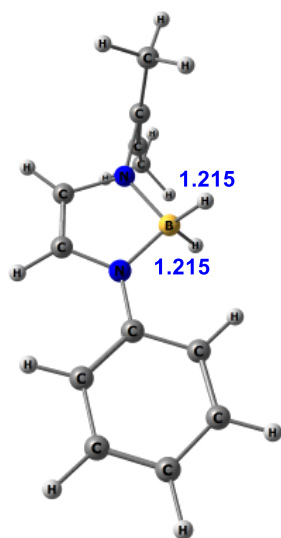
4P<sup>H-H</sup>



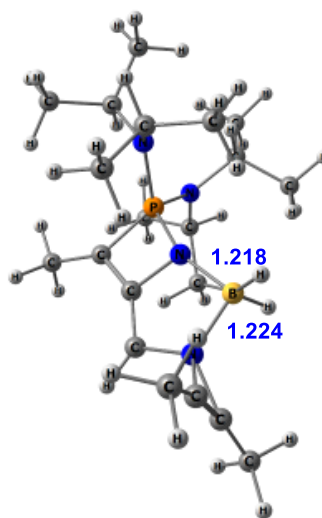
5P<sup>H-H</sup>



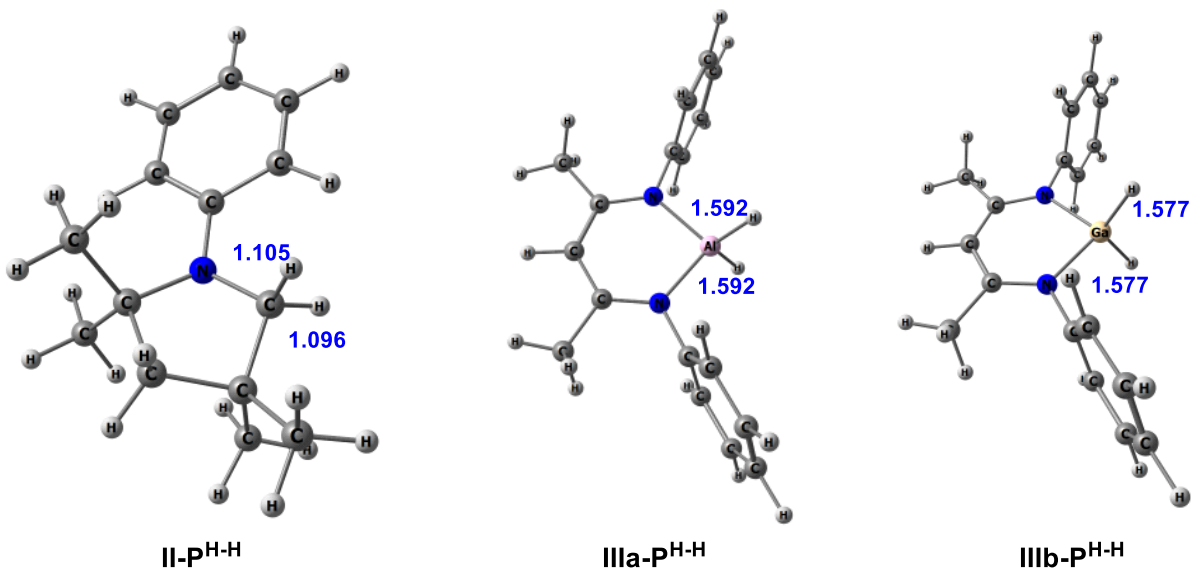
6P<sup>H-H</sup>



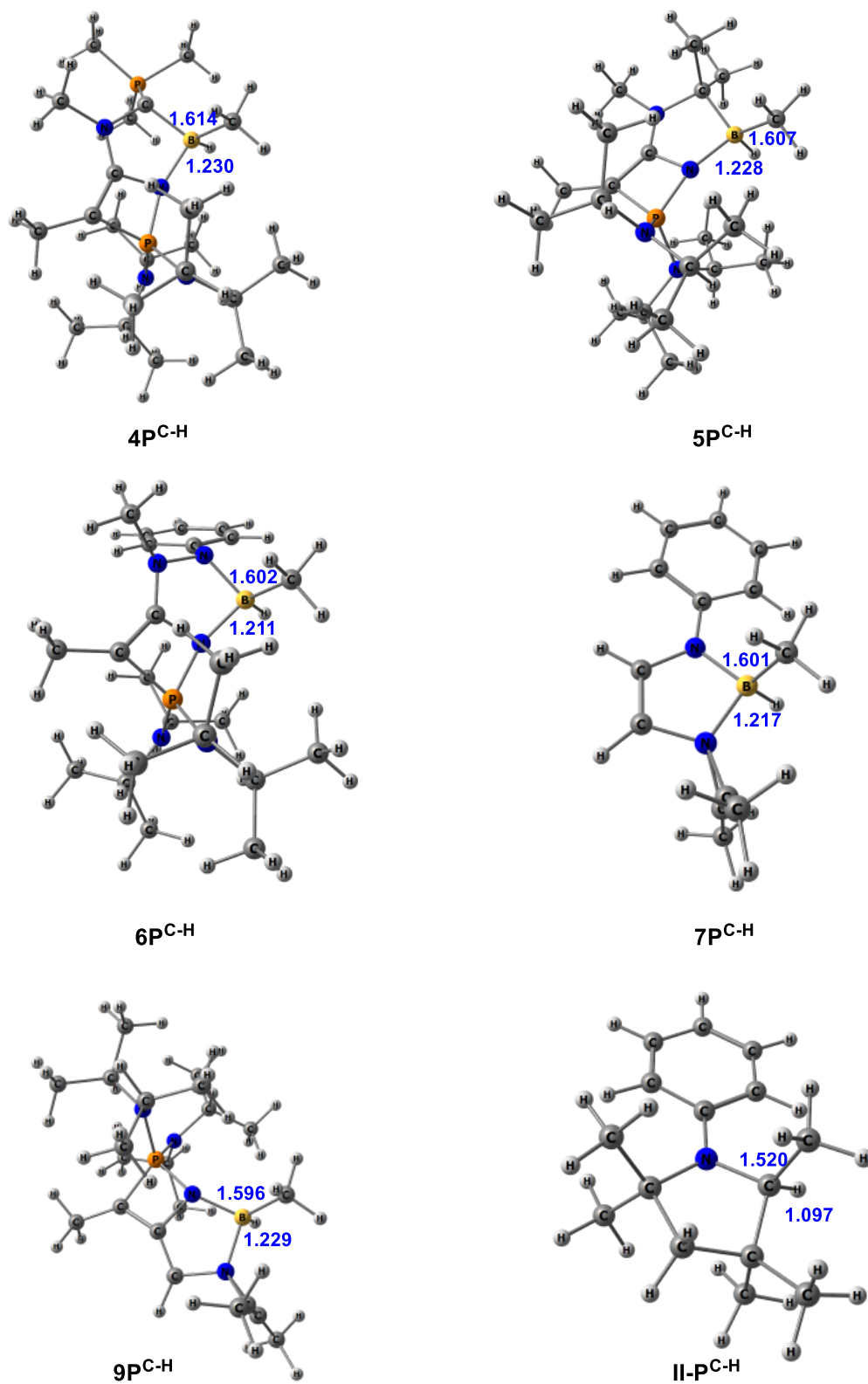
7P<sup>H-H</sup>



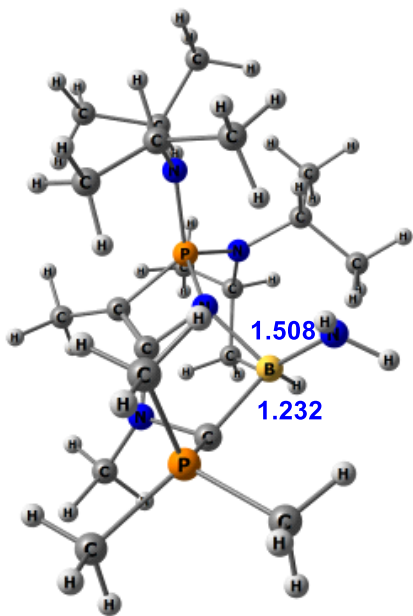
9P<sup>H-H</sup>



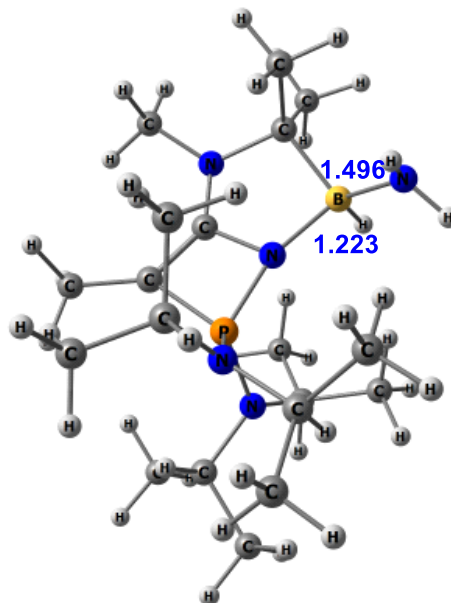
**Fig. S20** Optimized geometries of the H–H splitting product obtained for the molecules **4-7**, **9**, **II**, **IIIa** and **IIIb** at M06-D3/Def2-TZVP (Toluene) level of theory.



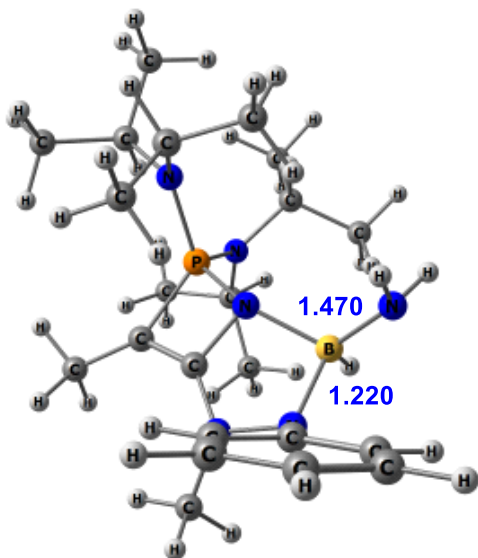
**Fig. S21** Optimized geometries of the C-H splitting product obtained for the molecules **4-7, 9** and **II** at M06-D3/Def2-TZVP (Toluene) level of theory.



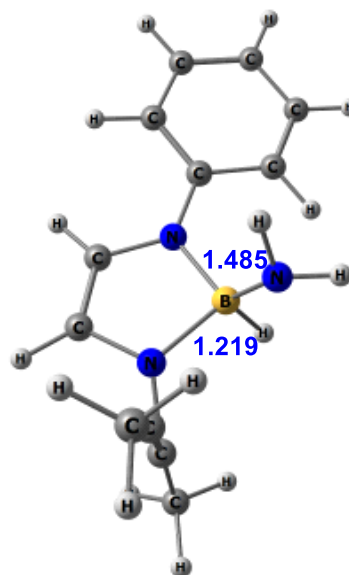
4P<sup>N</sup>-H



5P<sup>N</sup>-H

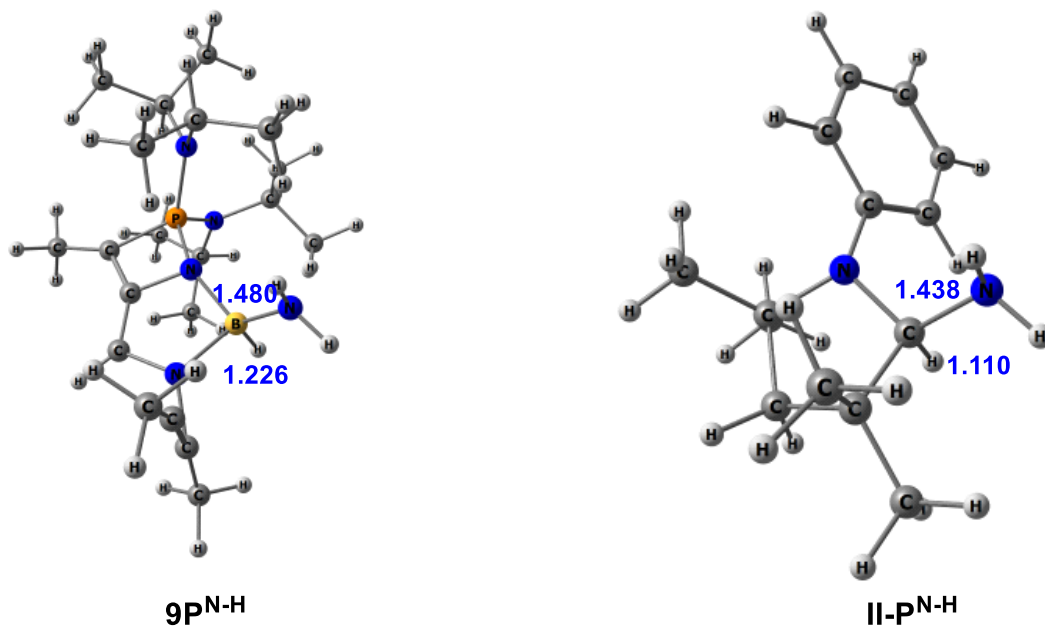


6P<sup>N</sup>-H

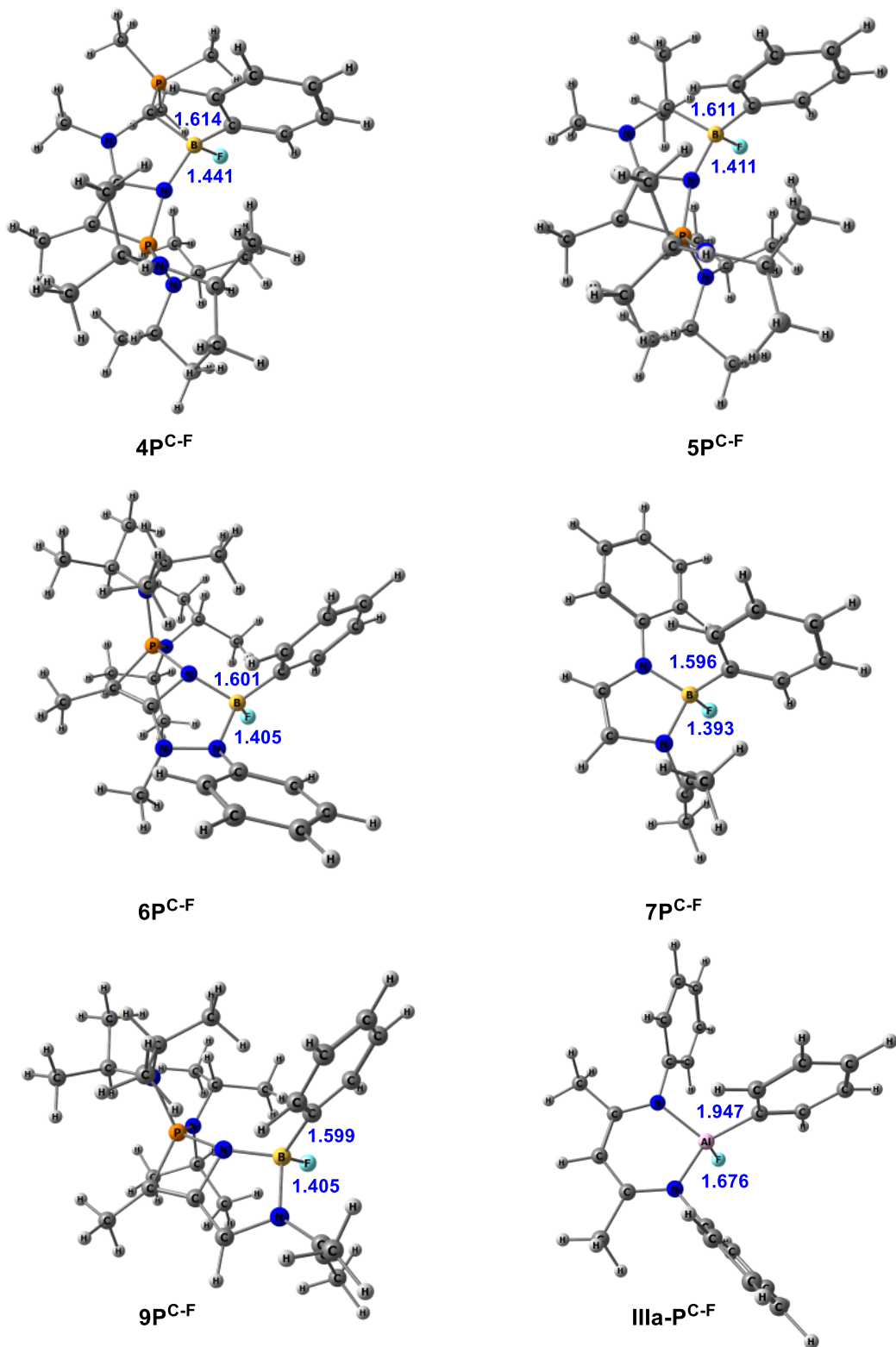


7P<sup>N</sup>-H

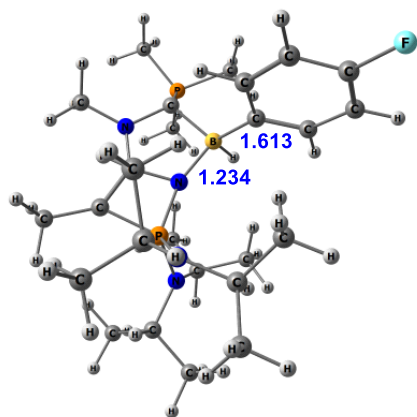




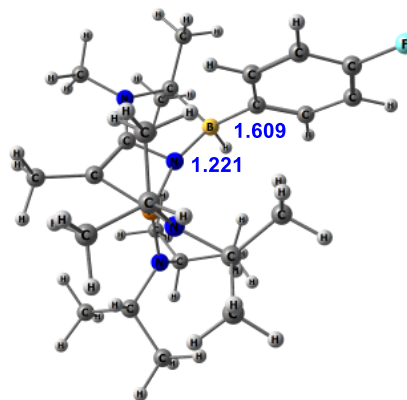
**Fig. S22** Optimized geometries of the N–H splitting product obtained for the molecules **4-7**, **9** and **II** at M06-D3/Def2-TZVP (Toluene) level of theory.



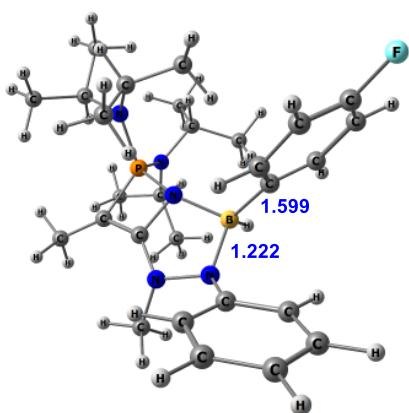
**Fig. S23** Optimized geometries of the C-F splitting product obtained for the molecules **4-7, 9** and **IIIa** at M06-D3/Def2-TZVP (Toluene) level of theory.



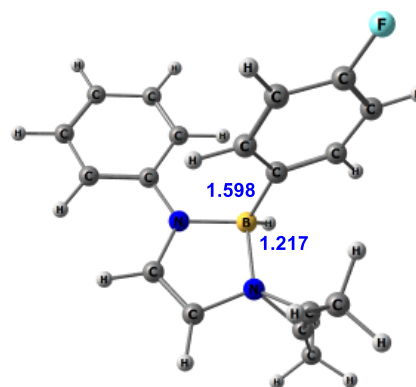
**4P<sub>p</sub>(C-H)**



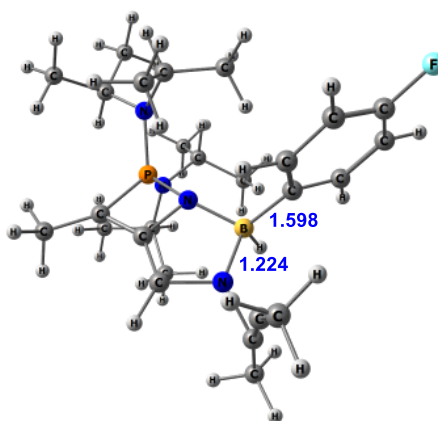
**5P<sub>p</sub>(C-H)**



**6P<sub>p</sub>(C-H)**

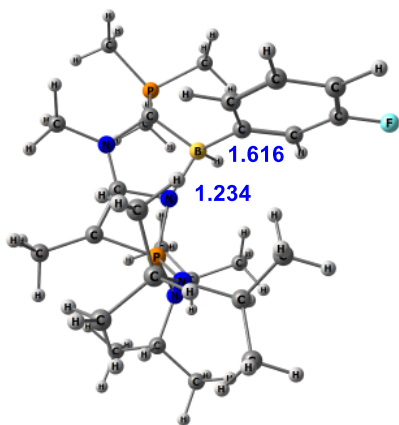


**7P<sub>p</sub>(C-H)**

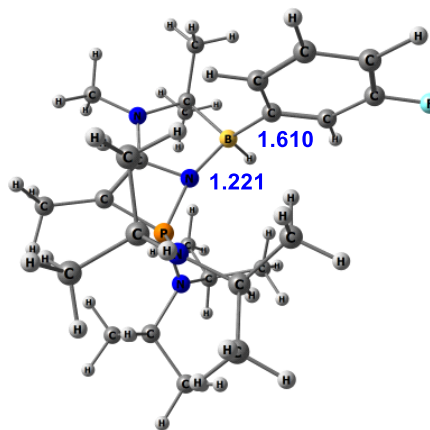


**9P<sub>p</sub>(C-H)**

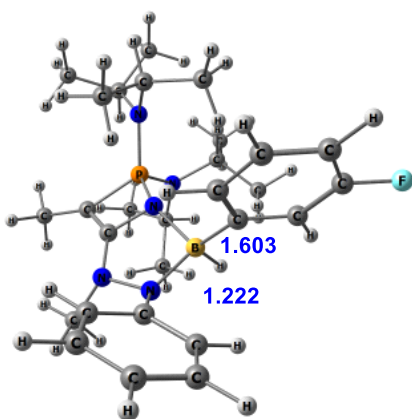
**Fig. S24** Optimized geometries of the *para* C–H splitting product obtained for the molecules **4-7** and **9** at M06-D3/Def2-TZVP (Toluene) level of theory.



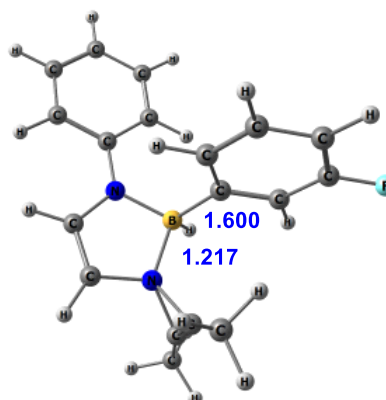
**4pm(C-H)**



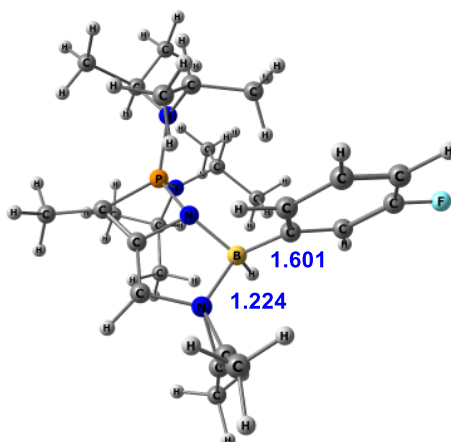
**5pm(C-H)**



**6pm(C-H)**

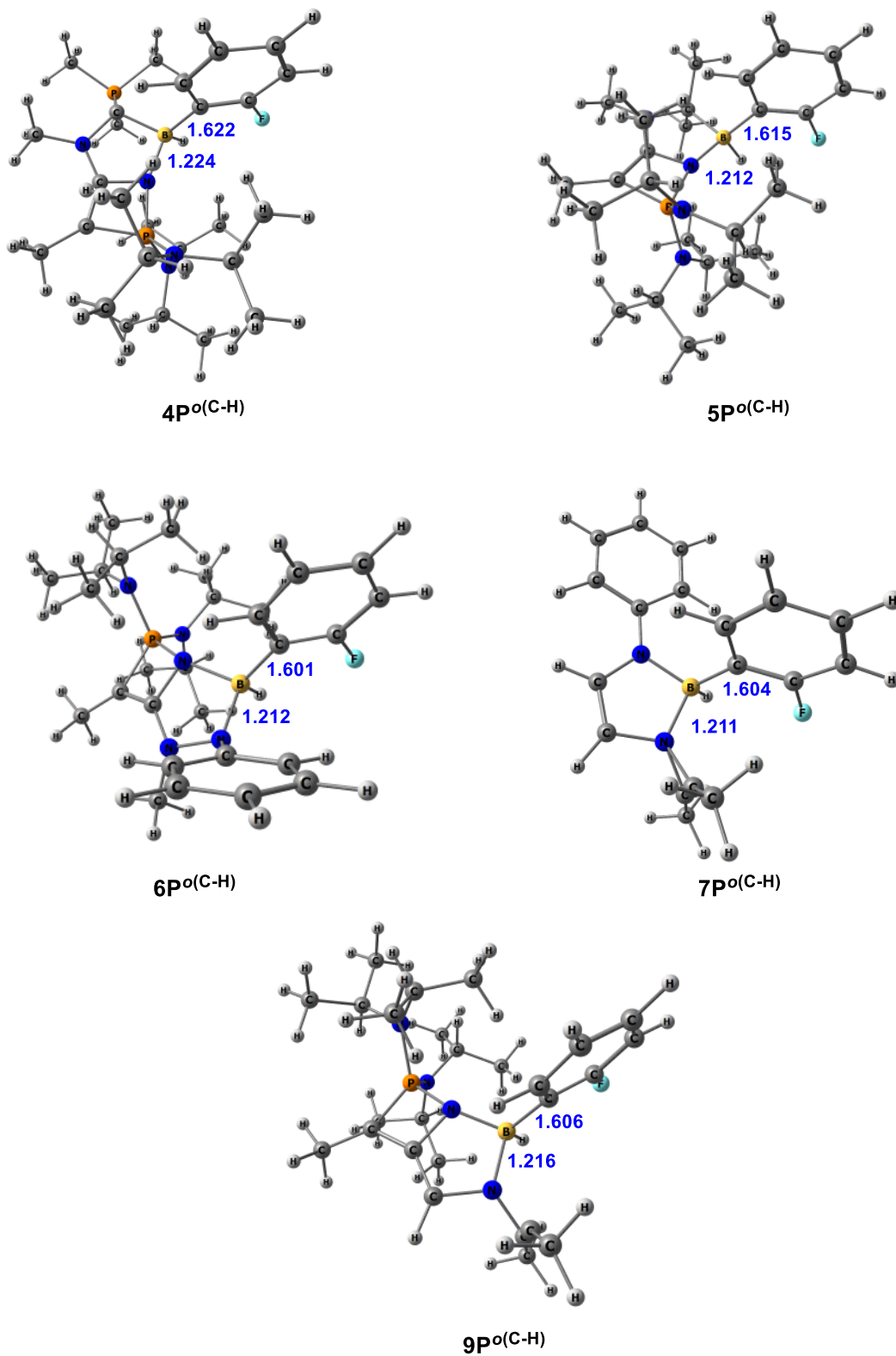


**7pm(C-H)**



**9pm(C-H)**

**Fig. S25** Optimized geometries of the *meta* C–H splitting product obtained for the molecules **4-7** and **9** at M06-D3/Def2-TZVP (Toluene) level of theory.



**Fig. S26** Optimized geometries of the *ortho* C-H splitting product obtained for the molecules **4-7** and **9** at M06-D3/Def2-TZVP (Toluene) level of theory.

Cartesian coordinates of **1-9** in their optimized singlet (S) and triplet (T) state, along with their total energies (in hartrees) including zero point vibrational correction.

**1-S** (TE= -943.221706)

6	0.490856000	1.343441000	-0.270313000
6	-1.258406000	-0.021109000	-0.188154000
7	1.011334000	0.124075000	-0.125480000
7	-0.825225000	1.324758000	-0.291490000
6	-1.632928000	2.505371000	-0.487513000
1	-2.338922000	2.625696000	0.338608000
1	-0.996995000	3.388459000	-0.523907000
1	-2.192723000	2.436585000	-1.423078000
15	-2.867642000	-0.510224000	0.114631000
6	-4.142879000	0.256736000	-0.915415000
1	-5.101420000	-0.230049000	-0.725566000
1	-4.244557000	1.319068000	-0.693446000
1	-3.879239000	0.134709000	-1.966565000
6	-3.457128000	-0.236727000	1.803237000
1	-4.488513000	-0.576128000	1.920732000
1	-2.805642000	-0.788034000	2.483006000
1	-3.397597000	0.824785000	2.049630000
6	-3.015310000	-2.268890000	-0.170599000
1	-4.014706000	-2.595578000	0.126684000
1	-2.846347000	-2.478657000	-1.226466000
1	-2.240064000	-2.776180000	0.403608000
6	2.411237000	-0.052761000	-0.029847000
6	3.222741000	0.895677000	0.581172000
6	2.982500000	-1.207843000	-0.547904000
6	4.592104000	0.699952000	0.652190000
1	2.779842000	1.777081000	1.032306000
6	4.349045000	-1.398974000	-0.469303000
1	2.322458000	-1.943918000	-0.992309000
6	5.162274000	-0.446014000	0.125714000
1	5.213342000	1.444117000	1.137593000
1	4.785024000	-2.302662000	-0.880106000
1	6.233153000	-0.600760000	0.186594000
1	1.046665000	2.263576000	-0.410145000
5	-0.069305000	-0.964750000	-0.027486000

**1-T** (TE= -943.196703)

6	0.485623000	1.504041000	0.145099000
6	-1.293168000	0.065296000	-0.152893000
7	1.032484000	0.226928000	-0.068819000
7	-0.912248000	1.429685000	0.112652000

6	-1.609349000	2.505191000	-0.545250000
1	-2.657827000	2.533807000	-0.235027000
1	-1.161776000	3.458919000	-0.259623000
1	-1.574987000	2.413654000	-1.643093000
15	-2.861614000	-0.543036000	0.080088000
6	-4.096888000	-0.052079000	-1.147965000
1	-5.060721000	-0.517114000	-0.930160000
1	-4.218470000	1.031704000	-1.146176000
1	-3.754295000	-0.361588000	-2.135843000
6	-3.618278000	-0.077011000	1.652523000
1	-4.639268000	-0.455951000	1.723822000
1	-3.015849000	-0.473954000	2.469644000
1	-3.634559000	1.011151000	1.733087000
6	-2.803805000	-2.332864000	0.007275000
1	-3.815975000	-2.735676000	0.068995000
1	-2.344226000	-2.638355000	-0.933053000
1	-2.201245000	-2.712347000	0.832122000
6	2.395620000	-0.019177000	-0.021207000
6	3.310747000	0.983524000	0.309279000
6	2.880559000	-1.298068000	-0.312118000
6	4.667494000	0.704112000	0.341856000
1	2.953010000	1.972920000	0.566360000
6	4.232101000	-1.562614000	-0.275418000
1	2.165792000	-2.075088000	-0.570142000
6	5.142557000	-0.561962000	0.049898000
1	5.362230000	1.494716000	0.604543000
1	4.584435000	-2.562190000	-0.505537000
1	6.205145000	-0.771551000	0.074739000
1	0.956060000	2.368638000	-0.320981000
5	-0.044837000	-0.716555000	-0.241662000

**2-S (TE= -562.014638)**

6	-0.685290000	0.923800000	-0.351961000
6	-2.275224000	-0.621258000	0.222841000
7	0.043313000	-0.128714000	0.014071000
7	-1.970685000	0.768841000	-0.273180000
6	-2.946410000	1.770426000	-0.631597000
1	-3.596919000	1.982202000	0.218872000
1	-2.447493000	2.692132000	-0.928362000
1	-3.563849000	1.420908000	-1.461296000
6	1.461514000	-0.062780000	0.014418000
6	2.127780000	1.093987000	0.394304000
6	2.183630000	-1.187813000	-0.355011000
6	3.512146000	1.130493000	0.380743000
1	1.567864000	1.959161000	0.733433000
6	3.565193000	-1.145826000	-0.359853000

1	1.634988000	-2.084227000	-0.618989000
6	4.235218000	0.012755000	0.002271000
1	4.025903000	2.034962000	0.684876000
1	4.124361000	-2.027389000	-0.651063000
1	5.318356000	0.040516000	-0.000872000
1	-0.254925000	1.854796000	-0.718448000
5	-0.823791000	-1.315345000	0.422735000
6	-3.028382000	-0.514958000	1.535499000
1	-3.994907000	-0.013409000	1.411563000
1	-3.213345000	-1.518042000	1.920646000
1	-2.446721000	0.024747000	2.288207000
6	-3.092072000	-1.341126000	-0.833289000
1	-3.260183000	-2.368357000	-0.508160000
1	-4.067726000	-0.867065000	-0.990489000
1	-2.563458000	-1.381299000	-1.790026000

**2-T** (TE= -562.001152)

6	-0.692436000	1.117136000	-0.065680000
6	-2.286854000	-0.634386000	0.135131000
7	0.062415000	-0.044971000	0.048520000
7	-2.021440000	0.830524000	0.122458000
6	-3.012611000	1.767490000	-0.326487000
1	-3.982800000	1.525869000	0.110672000
1	-2.741581000	2.772487000	0.004204000
1	-3.122720000	1.786292000	-1.420657000
6	1.471366000	-0.028050000	0.028531000
6	2.183184000	1.149447000	0.213161000
6	2.156734000	-1.219890000	-0.177449000
6	3.568542000	1.128646000	0.189073000
1	1.652881000	2.075011000	0.402894000
6	3.536968000	-1.233027000	-0.191413000
1	1.584069000	-2.130133000	-0.329116000
6	4.251825000	-0.057089000	-0.011950000
1	4.115961000	2.052489000	0.336564000
1	4.060467000	-2.168485000	-0.351227000
1	5.335002000	-0.068021000	-0.029530000
1	-0.358284000	1.968425000	-0.647621000
5	-0.787152000	-1.144756000	0.266288000
6	-2.879655000	-1.094234000	-1.196621000
1	-2.943086000	-2.184279000	-1.222562000
1	-3.889514000	-0.696412000	-1.342563000
1	-2.258852000	-0.770334000	-2.037212000
6	-3.207587000	-1.001669000	1.282943000
1	-4.189667000	-0.529815000	1.170495000
1	-3.362696000	-2.082480000	1.310541000
1	-2.787103000	-0.691950000	2.241389000



**3-S** (TE= -730.417201)

6	0.724582000	1.272322000	-0.438740000
7	1.221177000	0.093831000	-0.091921000
7	-0.584721000	1.267321000	-0.457898000
6	-1.431187000	2.284092000	-1.045990000
1	-2.121627000	2.699173000	-0.313600000
1	-0.795001000	3.077888000	-1.432019000
1	-2.005354000	1.850965000	-1.866243000
6	2.616235000	-0.114210000	0.041698000
6	3.450709000	0.892616000	0.506214000
6	3.143267000	-1.352852000	-0.293201000
6	4.812660000	0.666472000	0.612177000
1	3.034443000	1.844980000	0.816421000
6	4.503087000	-1.572255000	-0.178594000
1	2.464065000	-2.127280000	-0.629120000
6	5.343664000	-0.564746000	0.269275000
1	5.458039000	1.455016000	0.981070000
1	4.910470000	-2.541000000	-0.443300000
1	6.408595000	-0.742633000	0.359874000
1	1.287989000	2.151454000	-0.723143000
5	0.112359000	-0.930830000	0.154005000
7	-1.001517000	-0.033827000	-0.124967000
6	-2.386721000	-0.252724000	0.058509000
6	-2.992939000	-1.305560000	-0.612800000
6	-3.134527000	0.536075000	0.923400000
6	-4.339090000	-1.559918000	-0.424925000
1	-2.384890000	-1.922059000	-1.263680000
6	-4.485222000	0.286932000	1.094000000
1	-2.647013000	1.324219000	1.486751000
6	-5.091629000	-0.760346000	0.420818000
1	-4.804737000	-2.387464000	-0.947144000
1	-5.061570000	0.903834000	1.773543000
1	-6.147102000	-0.959608000	0.563031000

**3-T** (TE= -730.394338)

6	0.713723000	1.529130000	0.151482000
7	1.213246000	0.236818000	-0.054045000
7	-0.683864000	1.536925000	-0.033293000
6	-1.131891000	2.354496000	-1.160449000
1	-2.218973000	2.327625000	-1.230872000
1	-0.821864000	3.383723000	-0.980752000
1	-0.697215000	2.002337000	-2.104999000
6	2.567593000	-0.091281000	0.042434000
6	3.507415000	0.836996000	0.478750000
6	2.985858000	-1.374194000	-0.305650000
6	4.843989000	0.480656000	0.557564000

1	3.190793000	1.827967000	0.780237000
6	4.318275000	-1.718516000	-0.219755000
1	2.245734000	-2.091848000	-0.647939000
6	5.259542000	-0.791701000	0.209436000
1	5.566470000	1.211633000	0.902304000
1	4.627997000	-2.720275000	-0.494399000
1	6.306215000	-1.063302000	0.272422000
1	1.262644000	2.394099000	-0.202481000
5	0.100492000	-0.627628000	-0.236733000
7	-1.061061000	0.170454000	-0.187499000
6	-2.397954000	-0.188440000	0.002414000
6	-2.815585000	-1.446571000	-0.425441000
6	-3.307439000	0.663418000	0.618549000
6	-4.120591000	-1.848275000	-0.224159000
1	-2.100436000	-2.098002000	-0.917947000
6	-4.616654000	0.252199000	0.803653000
1	-2.975716000	1.632503000	0.969917000
6	-5.032751000	-1.000325000	0.387296000
1	-4.431666000	-2.831312000	-0.558459000
1	-5.317104000	0.922493000	1.288706000
1	-6.058763000	-1.314447000	0.535034000

**4-S** (TE= -1713.496545)

6	0.867080000	-0.426819000	1.002512000
6	2.719972000	-0.474972000	-0.305535000
7	0.503643000	0.002153000	-0.287613000
7	2.170887000	-0.625729000	1.061251000
6	2.813338000	-1.310801000	2.151026000
1	3.578225000	-0.688127000	2.626659000
1	2.078824000	-1.578961000	2.911730000
1	3.292250000	-2.225560000	1.787149000
15	4.287450000	0.144462000	-0.529529000
6	5.621847000	-0.768187000	0.296567000
1	6.589758000	-0.345323000	0.019946000
1	5.516818000	-0.711834000	1.380506000
1	5.582114000	-1.814777000	-0.007691000
6	4.589828000	1.848219000	0.030410000
1	5.634615000	2.145430000	-0.087618000
1	3.944320000	2.513976000	-0.545003000
1	4.312280000	1.924842000	1.084559000
6	4.730184000	0.112057000	-2.265264000
1	5.733834000	0.527383000	-2.385968000
1	4.706588000	-0.917749000	-2.620774000
1	3.993642000	0.686496000	-2.824718000
15	-1.079295000	-0.061320000	0.239764000
6	-0.326791000	-0.557764000	1.721783000

7	-1.838320000	1.398143000	0.115937000
7	-2.072616000	-1.132853000	-0.519124000
6	-0.706536000	-3.233038000	-0.148850000
1	-0.096275000	-2.942316000	-1.006654000
1	-0.161998000	-2.966845000	0.759669000
1	-0.825586000	-4.318919000	-0.164026000
6	-2.889245000	-2.848522000	1.055993000
1	-3.900577000	-2.447843000	0.955296000
1	-2.961778000	-3.923169000	1.239558000
1	-2.425663000	-2.391460000	1.932396000
6	-4.110629000	-1.140819000	-1.929852000
1	-4.677138000	-0.745563000	-1.083122000
1	-4.536882000	-0.728063000	-2.846891000
1	-4.260779000	-2.222942000	-1.964304000
6	-1.823994000	-1.315362000	-2.985375000
1	-0.783683000	-0.978010000	-2.916398000
1	-1.834579000	-2.409058000	-3.004189000
1	-2.235354000	-0.967547000	-3.935739000
6	-4.194862000	2.141901000	-0.095154000
1	-5.170834000	2.106185000	0.393695000
1	-3.967593000	3.192855000	-0.290211000
1	-4.275230000	1.629142000	-1.055287000
6	-3.045616000	2.187846000	2.139647000
1	-2.302367000	1.700508000	2.774881000
1	-2.763815000	3.238460000	2.031252000
1	-4.009803000	2.158235000	2.651865000
6	-0.670027000	-0.900229000	3.123182000
1	-0.574920000	-1.970691000	3.353932000
1	-0.045234000	-0.361796000	3.844261000
1	-1.704980000	-0.626393000	3.347467000
6	-2.077122000	-2.577938000	-0.194144000
6	-2.644511000	-0.764399000	-1.836341000
1	-2.609516000	-3.040641000	-1.029529000
1	-2.583552000	0.325959000	-1.884128000
6	-3.146349000	1.496288000	0.791700000
1	-3.466945000	0.461333000	0.974883000
6	-1.154789000	2.664507000	-0.231643000
1	-1.905936000	3.435402000	-0.031382000
6	-0.825512000	2.717895000	-1.709105000
1	-1.729244000	2.591917000	-2.311422000
1	-0.382775000	3.685112000	-1.959943000
1	-0.100445000	1.940479000	-1.983964000
6	0.049518000	2.993146000	0.636770000
1	-0.185390000	2.892168000	1.698411000
1	0.898598000	2.347183000	0.403451000
1	0.355874000	4.025401000	0.451843000

5 1.627788000 -0.000411000 -1.284221000

**4-T** (TE= -1713.438930)

6 -0.923976000 -0.666796000 -0.923832000  
6 -2.773161000 -0.914372000 0.457962000  
7 -0.583444000 0.036895000 0.256220000  
7 -2.163337000 -1.131354000 -0.876160000  
6 -2.678081000 -2.102439000 -1.804690000  
1 -3.669090000 -1.807218000 -2.161089000  
1 -2.016327000 -2.194938000 -2.667686000  
1 -2.768900000 -3.076082000 -1.313721000  
15 -4.062790000 0.253243000 0.467690000  
6 -5.544238000 -0.124360000 -0.522972000  
1 -6.396080000 0.485559000 -0.213286000  
1 -5.341946000 0.068559000 -1.578050000  
1 -5.793008000 -1.178955000 -0.393451000  
6 -3.763209000 2.038220000 0.151575000  
1 -4.568650000 2.678815000 0.520303000  
1 -2.835053000 2.297973000 0.671045000  
1 -3.634697000 2.204161000 -0.919681000  
6 -4.665038000 0.265268000 2.169095000  
1 -5.486862000 0.975232000 2.283237000  
1 -4.991517000 -0.737160000 2.447134000  
1 -3.828820000 0.553966000 2.812119000  
15 0.994063000 -0.059223000 -0.271316000  
6 0.253180000 -0.747289000 -1.676239000  
7 1.699436000 1.433748000 -0.219281000  
7 1.990777000 -1.034094000 0.604879000  
6 0.996043000 -3.313819000 0.161068000  
1 0.287850000 -3.092190000 0.965472000  
1 0.476909000 -3.150098000 -0.785321000  
1 1.274039000 -4.369356000 0.218447000  
6 3.157019000 -2.576899000 -0.924969000  
1 4.105877000 -2.065397000 -0.745735000  
1 3.368460000 -3.627024000 -1.139688000  
1 2.698711000 -2.142448000 -1.816384000  
6 3.856816000 -0.690919000 2.202833000  
1 4.417455000 -0.161113000 1.429745000  
1 4.110388000 -0.249446000 3.169106000  
1 4.202422000 -1.727812000 2.221910000  
6 1.575492000 -1.339408000 3.039985000  
1 0.496559000 -1.245718000 2.866625000  
1 1.828236000 -2.403248000 3.063464000  
1 1.810590000 -0.925560000 4.023384000  
6 3.907902000 2.444881000 0.282945000  
1 4.969332000 2.379175000 0.033540000

1	3.619415000	3.494872000	0.192592000
1	3.783672000	2.146574000	1.325882000
6	3.229499000	1.976919000	-2.094804000
1	2.686575000	1.288540000	-2.748256000
1	2.829451000	2.981978000	-2.254003000
1	4.277672000	1.986959000	-2.401632000
6	0.575850000	-1.220767000	-3.043630000
1	0.670464000	-2.312148000	-3.129581000
1	-0.184453000	-0.907899000	-3.766306000
1	1.522466000	-0.796580000	-3.390777000
6	2.243396000	-2.453733000	0.277606000
6	2.359358000	-0.599561000	1.972955000
1	2.800045000	-2.832961000	1.139454000
1	2.076711000	0.457165000	2.032262000
6	3.106225000	1.549899000	-0.643627000
1	3.522363000	0.539713000	-0.560906000
6	0.903881000	2.683427000	-0.180186000
1	1.634673000	3.475363000	-0.372709000
6	0.335392000	2.928500000	1.205049000
1	1.133829000	2.950897000	1.950672000
1	-0.182430000	3.890768000	1.233640000
1	-0.381505000	2.150265000	1.490933000
6	-0.150616000	2.798429000	-1.267777000
1	0.273895000	2.606279000	-2.255312000
1	-0.972114000	2.099513000	-1.103110000
1	-0.563700000	3.810364000	-1.264193000
5	-1.569286000	-0.435416000	1.310922000

**5-S** (TE= -1332.311847)

6	-1.677494000	-0.112228000	0.694307000
6	-3.388163000	-0.217892000	-0.882479000
7	-1.065434000	-0.251003000	-0.580326000
7	-2.986047000	-0.164066000	0.583242000
6	-3.885738000	0.113826000	1.672763000
1	-4.785689000	-0.497338000	1.583096000
1	-3.409614000	-0.125956000	2.624115000
1	-4.188375000	1.166533000	1.691848000
15	0.402029000	-0.015325000	0.197672000
6	-0.639842000	0.073730000	1.592281000
7	1.446792000	-1.269418000	-0.002845000
7	1.242899000	1.335893000	-0.211784000
6	-0.576815000	3.056565000	0.167824000
1	-0.962727000	2.814909000	-0.824960000
1	-1.193952000	2.543594000	0.909410000
1	-0.690197000	4.131174000	0.326290000
6	1.426166000	2.900469000	1.694837000

1	2.498458000	2.696598000	1.735847000
1	1.261205000	3.933619000	2.009086000
1	0.926423000	2.251779000	2.416009000
6	3.443297000	1.952391000	-1.176170000
1	3.934186000	1.519160000	-0.301461000
1	4.090064000	1.794090000	-2.041857000
1	3.368054000	3.032055000	-1.024135000
6	1.379348000	1.901954000	-2.627588000
1	0.428227000	1.389563000	-2.806154000
1	1.179016000	2.969262000	-2.497265000
1	2.000776000	1.792825000	-3.519016000
6	3.912836000	-1.529647000	0.107250000
1	4.776143000	-1.406613000	0.764489000
1	3.938589000	-2.553425000	-0.273455000
1	4.029476000	-0.850179000	-0.738740000
6	2.478846000	-2.173703000	2.068813000
1	1.565290000	-1.947455000	2.623718000
1	2.439913000	-3.221807000	1.761334000
1	3.328906000	-2.062089000	2.745131000
6	-0.556766000	0.253681000	3.063619000
1	-1.006106000	1.193425000	3.408151000
1	-1.046369000	-0.559059000	3.608735000
1	0.484578000	0.262718000	3.394688000
6	0.890765000	2.684664000	0.294485000
6	2.093195000	1.310443000	-1.428820000
1	1.434398000	3.366839000	-0.364109000
1	2.266486000	0.252577000	-1.640513000
6	2.635595000	-1.248326000	0.875867000
1	2.705424000	-0.221555000	1.260937000
6	1.101867000	-2.556575000	-0.651094000
1	1.964172000	-3.196957000	-0.441507000
6	1.003425000	-2.397918000	-2.153785000
1	1.939754000	-2.010233000	-2.563570000
1	0.802727000	-3.364747000	-2.621052000
1	0.186292000	-1.720312000	-2.431699000
6	-0.112740000	-3.251660000	-0.059628000
1	-0.048929000	-3.308181000	1.028985000
1	-1.038911000	-2.741014000	-0.329075000
1	-0.172219000	-4.269532000	-0.450874000
5	-1.977374000	-0.280120000	-1.723689000
6	-4.242633000	-1.447819000	-1.109673000
1	-5.153278000	-1.435861000	-0.497970000
1	-4.542554000	-1.495142000	-2.157788000
1	-3.686843000	-2.362693000	-0.883531000
6	-4.151953000	1.051171000	-1.212906000
1	-4.402676000	1.058594000	-2.274441000

1	-5.085177000	1.132171000	-0.642035000
1	-3.545165000	1.940568000	-1.010717000

**5-T** (TE= -1332.261627)

6	-1.612750000	-0.334356000	0.692806000
6	-3.373926000	-0.399995000	-0.886275000
7	-0.963517000	-0.551060000	-0.530600000
7	-2.928748000	-0.277129000	0.556294000
6	-3.822922000	0.044173000	1.636660000
1	-4.681678000	-0.631952000	1.643026000
1	-3.304080000	-0.060532000	2.589340000
1	-4.196599000	1.070314000	1.558628000
15	0.428678000	-0.062557000	0.248579000
6	-0.605827000	-0.078244000	1.634619000
7	1.642349000	-1.143162000	-0.020307000
7	1.027384000	1.396142000	-0.223031000
6	-0.906251000	2.900548000	0.417163000
1	-1.381934000	2.572757000	-0.514461000
1	-1.373129000	2.353127000	1.238866000
1	-1.113032000	3.964185000	0.559616000
6	1.263357000	2.902024000	1.715448000
1	2.351096000	2.863602000	1.618346000
1	0.987877000	3.877118000	2.124000000
1	0.957494000	2.140927000	2.436504000
6	2.999528000	2.245532000	-1.460263000
1	3.647019000	1.840278000	-0.679207000
1	3.530079000	2.176455000	-2.412434000
1	2.843425000	3.307650000	-1.254663000
6	0.769189000	2.037387000	-2.615283000
1	-0.157661000	1.451934000	-2.674844000
1	0.499546000	3.078900000	-2.418578000
1	1.268275000	2.005749000	-3.586796000
6	4.112348000	-1.100122000	-0.245085000
1	5.026928000	-0.780746000	0.259115000
1	4.244167000	-2.149414000	-0.519861000
1	4.008707000	-0.519270000	-1.163490000
6	3.041826000	-1.719263000	1.945248000
1	2.193475000	-1.533815000	2.608913000
1	3.077159000	-2.790617000	1.730523000
1	3.959276000	-1.460387000	2.478139000
6	-0.574923000	0.122872000	3.103066000
1	-1.024014000	1.070446000	3.432145000
1	-1.089434000	-0.679967000	3.641915000
1	0.455970000	0.124978000	3.467619000
6	0.598024000	2.681107000	0.372654000
6	1.690929000	1.482734000	-1.545868000

1	0.995988000	3.437870000	-0.309050000
1	1.928613000	0.451215000	-1.822159000
6	2.921369000	-0.900153000	0.673211000
1	2.905192000	0.158666000	0.961440000
6	1.401201000	-2.507246000	-0.548159000
1	2.357864000	-3.020927000	-0.409663000
6	1.117780000	-2.477404000	-2.037404000
1	1.922246000	-1.970125000	-2.575601000
1	1.041241000	-3.496290000	-2.424136000
1	0.171562000	-1.968059000	-2.257567000
6	0.361221000	-3.307718000	0.217007000
1	0.552607000	-3.284620000	1.291777000
1	-0.645589000	-2.927263000	0.034468000
1	0.392895000	-4.348545000	-0.112809000
5	-1.941050000	-0.295843000	-1.632474000
6	-4.059764000	-1.751128000	-1.052065000
1	-4.952379000	-1.855144000	-0.418764000
1	-4.371345000	-1.876311000	-2.091786000
1	-3.365052000	-2.561004000	-0.813559000
6	-4.337000000	0.723057000	-1.226563000
1	-4.540252000	0.697192000	-2.299338000
1	-5.299107000	0.637299000	-0.704097000
1	-3.891064000	1.695523000	-0.999831000

**6-S (TE= -1500.702804)**

6	-0.743526000	0.187032000	1.055171000
7	-0.386575000	-0.156925000	-0.262945000
7	-2.064453000	0.342296000	1.146613000
6	-2.601920000	1.394120000	1.989226000
1	-3.636085000	1.184087000	2.258225000
1	-2.007802000	1.451329000	2.901539000
1	-2.560826000	2.356556000	1.468594000
15	1.204974000	-0.017136000	0.231392000
6	0.432741000	0.321361000	1.765317000
7	2.042887000	-1.400471000	-0.040058000
7	2.066249000	1.193173000	-0.457428000
6	0.736396000	3.206100000	0.303768000
1	0.060192000	3.018468000	-0.533756000
1	0.267028000	2.825093000	1.212391000
1	0.849671000	4.286728000	0.414043000
6	3.006810000	2.675203000	1.275262000
1	4.015407000	2.335100000	1.030223000
1	3.068333000	3.707996000	1.625378000
1	2.633249000	2.066511000	2.101751000
6	3.972377000	1.396792000	-2.029656000
1	4.607075000	0.885212000	-1.302508000



1	4.311313000	1.120915000	-3.030311000
1	4.129899000	2.472944000	-1.922206000
6	1.605101000	1.728620000	-2.838634000
1	0.571477000	1.383117000	-2.729628000
1	1.632585000	2.812908000	-2.698529000
1	1.926112000	1.522574000	-3.861767000
6	4.391472000	-2.002213000	-0.568366000
1	5.418619000	-1.898588000	-0.212547000
1	4.217047000	-3.065252000	-0.750074000
1	4.306168000	-1.476902000	-1.521208000
6	3.531484000	-2.168186000	1.790069000
1	2.857733000	-1.727490000	2.529047000
1	3.276434000	-3.226068000	1.688031000
1	4.550947000	-2.111723000	2.177069000
6	0.762080000	0.598459000	3.183632000
1	0.711219000	1.662973000	3.447050000
1	0.085856000	0.066526000	3.858727000
1	1.773850000	0.262142000	3.425374000
6	2.099376000	2.578343000	0.066391000
6	2.515532000	1.012334000	-1.862652000
1	2.568484000	3.154797000	-0.735163000
1	2.430191000	-0.060288000	-2.061417000
6	3.432784000	-1.439162000	0.463112000
1	3.716541000	-0.393654000	0.637166000
6	1.415662000	-2.701532000	-0.388767000
1	2.225474000	-3.425408000	-0.259011000
6	1.003396000	-2.733402000	-1.845501000
1	1.858505000	-2.526072000	-2.493620000
1	0.614361000	-3.721393000	-2.101945000
1	0.216317000	-2.000751000	-2.056401000
6	0.296791000	-3.135228000	0.541840000
1	0.591436000	-3.047216000	1.589761000
1	-0.612486000	-2.553432000	0.382871000
1	0.054581000	-4.181492000	0.344319000
5	-1.515635000	-0.051835000	-1.219468000
7	-2.563448000	0.261016000	-0.232701000
6	-3.937045000	0.012036000	-0.344036000
6	-4.602681000	0.407527000	-1.504613000
6	-4.661986000	-0.626264000	0.659682000
6	-5.952508000	0.161986000	-1.652514000
1	-4.028171000	0.892121000	-2.284290000
6	-6.019641000	-0.857185000	0.505307000
1	-4.150319000	-0.968886000	1.551547000
6	-6.675746000	-0.467184000	-0.647856000
1	-6.450179000	0.473515000	-2.564246000
1	-6.564138000	-1.360347000	1.296909000

1 -7.736858000 -0.651391000 -0.766371000

**6-T** (TE= -1500.635324)

6 0.762283000 -0.495113000 0.971294000  
7 0.443304000 0.187426000 -0.217371000  
7 2.049683000 -0.910481000 0.991513000  
6 2.322332000 -2.242922000 1.509759000  
1 3.390637000 -2.358870000 1.687426000  
1 1.791617000 -2.379596000 2.452176000  
1 1.990245000 -2.998423000 0.788855000  
15 -1.154402000 0.008006000 0.248462000  
6 -0.406816000 -0.663087000 1.680009000  
7 -1.905850000 1.466913000 0.184035000  
7 -2.047012000 -1.025006000 -0.653943000  
6 -1.181241000 -3.314180000 -0.046571000  
1 -0.429845000 -3.163815000 -0.827523000  
1 -0.700917000 -3.119799000 0.913786000  
1 -1.500524000 -4.359261000 -0.059975000  
6 -3.352541000 -2.433455000 0.897019000  
1 -4.280841000 -1.916399000 0.643305000  
1 -3.598765000 -3.461879000 1.169950000  
1 -2.925704000 -1.951854000 1.780772000  
6 -3.783183000 -0.690668000 -2.402588000  
1 -4.381290000 -0.099470000 -1.706980000  
1 -3.943321000 -0.294423000 -3.407329000  
1 -4.166299000 -1.714278000 -2.396436000  
6 -1.477597000 -1.463715000 -3.033807000  
1 -0.411454000 -1.399916000 -2.785901000  
1 -1.773171000 -2.516524000 -3.022098000  
1 -1.625720000 -1.093433000 -4.050553000  
6 -4.099913000 2.429069000 -0.462574000  
1 -5.174920000 2.308434000 -0.312572000  
1 -3.868251000 3.484356000 -0.302098000  
1 -3.871260000 2.184547000 -1.501828000  
6 -3.598423000 1.885433000 1.945259000  
1 -3.096784000 1.178245000 2.612157000  
1 -3.233577000 2.889048000 2.178920000  
1 -4.667887000 1.863138000 2.164958000  
6 -0.727739000 -1.128016000 3.049706000  
1 -0.931189000 -2.204098000 3.115802000  
1 0.097622000 -0.912176000 3.733117000  
1 -1.607242000 -0.612841000 3.446846000  
6 -2.382556000 -2.413121000 -0.266953000  
6 -2.304641000 -0.640949000 -2.065737000  
1 -2.916211000 -2.809978000 -1.135071000  
1 -1.976128000 0.401679000 -2.153124000

6	-3.348758000	1.522883000	0.493846000
1	-3.722927000	0.506028000	0.338776000
6	-1.163821000	2.754902000	0.221363000
1	-1.940400000	3.501926000	0.409603000
6	-0.549113000	3.071937000	-1.127713000
1	-1.309381000	3.058306000	-1.912135000
1	-0.099470000	4.067222000	-1.107899000
1	0.235560000	2.355268000	-1.389952000
6	-0.164187000	2.879147000	1.356841000
1	-0.607022000	2.589829000	2.312620000
1	0.722574000	2.268597000	1.182816000
1	0.159981000	3.919081000	1.434509000
5	1.465437000	-0.319197000	-1.213377000
7	2.600720000	-0.633382000	-0.301414000
6	3.883294000	-0.132095000	-0.331610000
6	4.388326000	0.298131000	-1.570147000
6	4.714113000	-0.048447000	0.791436000
6	5.669969000	0.800517000	-1.665301000
1	3.745480000	0.222640000	-2.442027000
6	5.997173000	0.453417000	0.674266000
1	4.336333000	-0.335378000	1.764986000
6	6.493117000	0.879947000	-0.550306000
1	6.035203000	1.133110000	-2.631346000
1	6.616458000	0.523486000	1.562398000
1	7.501255000	1.267398000	-0.633653000

**7-S** (TE= -598.842606)

6	-1.531063000	0.863603000	1.201690000
6	-0.201168000	0.851424000	1.230551000
1	-2.251515000	1.331126000	1.855256000
1	0.425242000	1.335469000	1.967817000
6	-3.235111000	-0.666332000	0.098900000
6	-3.203384000	0.357978000	-0.646211000
7	-1.921152000	0.057976000	0.074170000
7	0.341333000	0.083733000	0.199549000
5	-0.666931000	-0.522649000	-0.679424000
6	1.739234000	-0.009728000	0.036062000
6	2.579154000	1.045384000	0.376212000
6	2.294961000	-1.173567000	-0.485880000
6	3.949160000	0.932382000	0.208503000
1	2.160330000	1.973333000	0.748998000
6	3.661949000	-1.275099000	-0.659750000
1	1.629867000	-1.985552000	-0.754469000
6	4.499349000	-0.226592000	-0.309762000
1	4.588230000	1.766545000	0.475235000
1	4.079086000	-2.189429000	-1.066540000

1	5.571182000	-0.312098000	-0.443504000
6	-3.539781000	1.400024000	-1.599590000
1	-2.897119000	1.302528000	-2.478341000
1	-4.582482000	1.321156000	-1.903531000
1	-3.368350000	2.386188000	-1.162354000
6	-3.639869000	-1.883562000	0.779086000
1	-4.687004000	-2.105560000	0.578901000
1	-3.019751000	-2.712417000	0.427609000
1	-3.494907000	-1.785504000	1.857143000

**7-T** (TE= -598.801965)

6	-1.472279000	1.792047000	-0.283827000
6	-0.141142000	1.767747000	-0.294953000
1	-2.164263000	2.607140000	-0.417438000
1	0.526770000	2.598950000	-0.456637000
6	-3.296580000	0.201750000	0.680846000
6	-3.313603000	-0.010355000	-0.659357000
7	-1.964866000	0.472485000	-0.066052000
7	0.340818000	0.458092000	-0.093020000
5	-0.790425000	-0.384068000	0.053788000
6	1.699872000	0.106178000	-0.034389000
6	2.702934000	1.055554000	0.112810000
6	2.044400000	-1.240348000	-0.112799000
6	4.028607000	0.658684000	0.173118000
1	2.458066000	2.106853000	0.198131000
6	3.367304000	-1.627081000	-0.043262000
1	1.255605000	-1.977253000	-0.233589000
6	4.370351000	-0.679435000	0.096582000
1	4.800488000	1.410667000	0.288765000
1	3.618090000	-2.679590000	-0.106047000
1	5.408681000	-0.983654000	0.145714000
6	-3.371622000	-1.263202000	-1.454072000
1	-2.883851000	-2.110765000	-0.945769000
1	-4.421940000	-1.526596000	-1.595831000
1	-2.925713000	-1.153433000	-2.443965000
6	-3.329430000	-0.743882000	1.824818000
1	-4.374709000	-0.952578000	2.062569000
1	-2.844385000	-1.705911000	1.592556000
1	-2.865248000	-0.333467000	2.723028000

**8-S** (TE= -811.621275)

6	1.294502000	0.036224000	-1.515723000
6	-0.046943000	0.046000000	-1.570969000
1	2.047498000	0.047491000	-2.291838000
1	-0.591400000	0.063958000	-2.511860000
6	2.968667000	-0.651503000	0.246455000

6	2.992111000	0.615506000	0.265626000
7	1.676687000	0.012873000	-0.118263000
5	0.424955000	0.010433000	0.852599000
6	3.397210000	1.999650000	0.439776000
1	2.791977000	2.451791000	1.230333000
1	4.450568000	2.066233000	0.708942000
1	3.227344000	2.564160000	-0.479940000
6	3.317861000	-2.055423000	0.377801000
1	4.371778000	-2.174143000	0.625989000
1	2.707185000	-2.502516000	1.167029000
1	3.108011000	-2.586866000	-0.553321000
6	-0.626910000	0.035825000	-0.251363000
15	-2.280457000	0.003789000	0.137335000
6	-2.805848000	-1.495513000	0.991368000
1	-2.179218000	-1.609938000	1.877704000
1	-3.857547000	-1.439314000	1.280635000
1	-2.645487000	-2.355320000	0.339976000
6	-3.349316000	0.133857000	-1.308302000
1	-4.396809000	0.119249000	-1.003756000
1	-3.142624000	1.065639000	-1.836415000
1	-3.163309000	-0.703433000	-1.982291000
6	-2.776370000	1.332969000	1.245244000
1	-3.823002000	1.230936000	1.539438000
1	-2.130892000	1.285568000	2.124019000
1	-2.618581000	2.291838000	0.750694000

**8-T** (TE= -811.590734)

6	-1.132338000	-1.827409000	0.000979000
6	0.204201000	-1.738520000	0.000648000
1	-1.789045000	-2.684160000	0.000527000
1	0.861939000	-2.602056000	-0.000827000
6	-3.075909000	-0.263735000	-0.681766000
6	-3.076663000	-0.262117000	0.682675000
7	-1.717847000	-0.521299000	0.001316000
5	-0.605982000	0.455662000	0.001983000
6	-3.208824000	0.867414000	1.640041000
1	-2.726008000	0.663654000	2.598160000
1	-2.795040000	1.810092000	1.243554000
1	-4.270925000	1.030891000	1.838001000
6	-3.207574000	0.862080000	-1.643372000
1	-2.795170000	1.806619000	-1.249960000
1	-2.723128000	0.654898000	-2.599942000
1	-4.269487000	1.023850000	-1.843708000
6	0.638004000	-0.343477000	0.002384000
15	2.238490000	0.218877000	0.000469000
6	2.259798000	2.009822000	0.020395000

1	1.744903000	2.365247000	0.913389000
1	3.287767000	2.374577000	0.016317000
1	1.731921000	2.383528000	-0.857586000
6	3.198127000	-0.306080000	-1.433076000
1	4.230438000	0.042246000	-1.367842000
1	3.190272000	-1.396455000	-1.483936000
1	2.731907000	0.085304000	-2.337576000
6	3.211813000	-0.342743000	1.410699000
1	4.244910000	0.002393000	1.341241000
1	2.758167000	0.029699000	2.329476000
1	3.200269000	-1.434104000	1.436903000

**9-S** (TE= -1369.118146)

6	-1.360034000	0.024481000	1.202707000
7	-0.959420000	-0.111596000	-0.197243000
15	0.626408000	0.006325000	0.317568000
6	-0.109597000	0.120847000	1.858516000
7	1.535013000	-1.307028000	-0.129996000
7	1.482680000	1.290936000	-0.271667000
6	-0.113613000	3.115815000	0.457228000
1	-0.695890000	2.941766000	-0.450698000
1	-0.610955000	2.601283000	1.281936000
1	-0.123752000	4.187568000	0.669375000
6	2.132831000	2.814870000	1.560146000
1	3.177996000	2.545564000	1.390634000
1	2.096922000	3.850325000	1.907269000
1	1.741135000	2.181600000	2.358242000
6	3.479960000	1.783229000	-1.660404000
1	4.111021000	1.313883000	-0.901952000
1	3.927799000	1.594344000	-2.638738000
1	3.502077000	2.864133000	-1.499421000
6	1.167702000	1.859883000	-2.667423000
1	0.173260000	1.401903000	-2.647271000
1	1.056079000	2.935911000	-2.505202000
1	1.589843000	1.721285000	-3.665381000
6	3.949220000	-1.760490000	-0.481179000
1	4.927708000	-1.714984000	0.001965000
1	3.819502000	-2.779022000	-0.855610000
1	3.960168000	-1.083837000	-1.337486000
6	2.867805000	-2.301137000	1.721800000
1	2.093657000	-2.008910000	2.434804000
1	2.695097000	-3.342818000	1.438905000
1	3.836206000	-2.255034000	2.224898000
6	0.252857000	0.285389000	3.285058000
1	-0.039905000	1.261452000	3.697736000
1	-0.212255000	-0.477732000	3.918849000

1	1.333180000	0.194373000	3.430447000
6	1.324210000	2.652951000	0.288903000
6	2.070948000	1.223114000	-1.629012000
1	1.771588000	3.310619000	-0.461553000
1	2.136704000	0.158231000	-1.863200000
6	2.863261000	-1.385118000	0.510157000
1	3.084379000	-0.369511000	0.866559000
6	0.975972000	-2.565766000	-0.667211000
1	1.806414000	-3.276341000	-0.605211000
6	0.619294000	-2.418477000	-2.132733000
1	1.493001000	-2.110183000	-2.712802000
1	0.263644000	-3.371105000	-2.533099000
1	-0.177150000	-1.679558000	-2.276245000
6	-0.161624000	-3.163836000	0.146677000
1	0.094836000	-3.223765000	1.206003000
1	-1.081209000	-2.583207000	0.049172000
1	-0.366553000	-4.174988000	-0.212906000
5	-2.008698000	-0.100776000	-1.176733000
6	-2.705622000	0.043443000	1.264262000
1	-3.395562000	0.157910000	2.084830000
6	-4.517104000	-0.674708000	-0.380108000
6	-4.502248000	0.595452000	-0.447352000
7	-3.199490000	-0.036519000	-0.117674000
6	-4.925020000	-2.069137000	-0.387618000
1	-6.001040000	-2.170900000	-0.522307000
1	-4.407366000	-2.593353000	-1.196010000
1	-4.636620000	-2.542371000	0.554744000
6	-4.879780000	1.990076000	-0.603389000
1	-4.355056000	2.412237000	-1.465242000
1	-5.953984000	2.100557000	-0.745115000
1	-4.575532000	2.555863000	0.281147000

**9-T** (TE= -1369.067729)

6	1.241946000	-0.346294000	1.423133000
7	0.967587000	-0.114416000	-0.000244000
15	-0.666837000	-0.059973000	0.380358000
6	-0.085725000	-0.343976000	1.953619000
7	-1.313587000	1.381917000	-0.126365000
7	-1.599510000	-1.186602000	-0.378761000
6	-0.452787000	-3.271398000	0.477548000
1	0.249440000	-3.206545000	-0.356424000
1	0.030734000	-2.853412000	1.361768000
1	-0.655222000	-4.328005000	0.667058000
6	-2.727543000	-2.580137000	1.319655000
1	-3.680616000	-2.128607000	1.034300000
1	-2.916602000	-3.606513000	1.642175000

1	-2.329422000	-2.030684000	2.174913000
6	-3.428941000	-1.318760000	-2.054782000
1	-4.077657000	-0.769907000	-1.368359000
1	-3.695154000	-1.032313000	-3.074625000
1	-3.648226000	-2.384276000	-1.951660000
6	-1.040905000	-1.772307000	-2.723102000
1	0.000919000	-1.481627000	-2.558690000
1	-1.122080000	-2.852510000	-2.575354000
1	-1.291609000	-1.563821000	-3.765411000
6	-3.522860000	2.222933000	-0.886064000
1	-4.576773000	2.284319000	-0.606479000
1	-3.192465000	3.236931000	-1.124619000
1	-3.446798000	1.619034000	-1.792224000
6	-2.842853000	2.448746000	1.522193000
1	-2.283160000	1.993487000	2.342525000
1	-2.467888000	3.465370000	1.377973000
1	-3.890108000	2.526434000	1.821804000
6	-0.590229000	-0.480775000	3.338624000
1	-0.495066000	-1.500353000	3.737582000
1	-0.061746000	0.181736000	4.032563000
1	-1.649941000	-0.217099000	3.399428000
6	-1.756022000	-2.560386000	0.157719000
6	-1.967618000	-1.002677000	-1.800939000
1	-2.221970000	-3.118888000	-0.658849000
1	-1.820881000	0.060738000	-2.004768000
6	-2.721821000	1.622296000	0.254062000
1	-3.145715000	0.632173000	0.465688000
6	-0.497521000	2.576528000	-0.440219000
1	-1.221335000	3.396833000	-0.465774000
6	0.098819000	2.483910000	-1.832593000
1	-0.682887000	2.326072000	-2.579479000
1	0.625476000	3.408747000	-2.079779000
1	0.820073000	1.663998000	-1.915904000
6	0.533894000	2.955928000	0.610631000
1	0.087423000	3.009220000	1.604968000
1	1.369173000	2.254446000	0.654107000
1	0.943345000	3.939456000	0.368775000
5	2.176275000	-0.093794000	-0.691380000
6	2.570279000	-0.440838000	1.604352000
1	3.175180000	-0.600532000	2.479967000
6	4.533652000	0.543062000	0.177039000
6	4.610055000	-0.808273000	-0.003003000
7	3.239906000	-0.254751000	0.314154000
6	4.631949000	1.674037000	-0.783748000
1	4.329744000	1.395939000	-1.808267000
1	4.025549000	2.530315000	-0.475701000



1	5.669708000	2.012011000	-0.830565000
6	4.839648000	-1.626658000	-1.221126000
1	4.436007000	-1.150967000	-2.131482000
1	5.914865000	-1.750642000	-1.367896000
1	4.403604000	-2.624805000	-1.141223000

Cartesian coordinates of **II**, **IIIa**, **IIIb**, H<sub>2</sub>, NH<sub>3</sub>, CH<sub>4</sub> and C<sub>6</sub>H<sub>5</sub>F in their optimized state, along with their total energies (in hartrees) including zero point vibrational correction.

**II-S** (TE= -599.083898)

6	-0.834585000	1.167201000	0.341199000
6	-2.293293000	0.876531000	0.002692000
6	-2.379777000	-0.637795000	-0.265835000
6	-0.961484000	-1.104996000	-0.493753000
7	-0.188744000	-0.103925000	-0.170043000
1	-2.574729000	1.427875000	-0.899825000
1	-2.963780000	1.202257000	0.802694000
6	1.236861000	-0.235451000	-0.150921000
6	2.004567000	0.269970000	-1.186767000
6	3.381242000	0.125557000	-1.154641000
6	3.989454000	-0.520136000	-0.091000000
6	3.217058000	-1.032677000	0.938670000
6	1.840981000	-0.891886000	0.909035000
1	1.517347000	0.756237000	-2.023832000
1	3.980518000	0.513092000	-1.970098000
1	5.066926000	-0.633039000	-0.069312000
1	3.687244000	-1.551120000	1.765941000
1	1.216659000	-1.302416000	1.695532000
6	-3.240019000	-0.950948000	-1.478000000
1	-3.270742000	-2.027135000	-1.660692000
1	-4.263354000	-0.594879000	-1.322982000
1	-2.844966000	-0.467494000	-2.375411000
6	-2.908332000	-1.409082000	0.941289000
1	-3.937926000	-1.107012000	1.154801000
1	-2.894467000	-2.483104000	0.744868000
1	-2.309401000	-1.226873000	1.837423000
6	-0.308045000	2.388649000	-0.383421000
1	0.745924000	2.572122000	-0.162935000
1	-0.428939000	2.287613000	-1.464517000
1	-0.873016000	3.266981000	-0.061554000
6	-0.576639000	1.299441000	1.831927000
1	-1.076535000	2.192862000	2.213271000
1	-0.954721000	0.435964000	2.383126000
1	0.491234000	1.399276000	2.040949000

**II-T (TE= -599.015824)**

6	-0.889815000	1.254200000	-0.065375000
6	-2.334901000	0.735235000	-0.244249000
6	-2.353149000	-0.791062000	-0.002604000
6	-0.940599000	-1.055786000	-0.364985000
7	-0.091672000	-0.003278000	-0.177627000
1	-2.655979000	0.920864000	-1.272819000
1	-3.025738000	1.263219000	0.420341000
6	1.276693000	-0.161782000	-0.091089000
6	2.183872000	0.895215000	0.056380000
6	3.541055000	0.646346000	0.136863000
6	4.043456000	-0.643607000	0.070004000
6	3.151588000	-1.694932000	-0.084411000
6	1.794864000	-1.465213000	-0.168374000
1	1.840759000	1.917889000	0.112507000
1	4.218002000	1.485388000	0.254064000
1	5.109118000	-0.825918000	0.131881000
1	3.518419000	-2.713723000	-0.144697000
1	1.104084000	-2.292831000	-0.297395000
6	-3.354403000	-1.484997000	-0.908256000
1	-3.318862000	-2.567704000	-0.767687000
1	-4.370828000	-1.151048000	-0.680239000
1	-3.145075000	-1.269946000	-1.958207000
6	-2.655033000	-1.143197000	1.454566000
1	-3.658256000	-0.803020000	1.731537000
1	-2.610864000	-2.224784000	1.599565000
1	-1.937139000	-0.686889000	2.138196000
6	-0.567096000	2.231511000	-1.183137000
1	0.412728000	2.696507000	-1.077798000
1	-0.606415000	1.723817000	-2.149480000
1	-1.314215000	3.029736000	-1.187122000
6	-0.710726000	1.897116000	1.301388000
1	-1.355545000	2.776960000	1.368432000
1	-0.991840000	1.210761000	2.101310000
1	0.314511000	2.219375000	1.480675000

**IIIa-S (TE= -1009.409742)**

13	0.000000000	0.000000000	1.110506000
7	0.000000000	1.386940000	-0.292988000
7	0.000000000	-1.386940000	-0.292988000
6	0.000000000	1.245033000	-1.614298000
6	0.000000000	-1.245033000	-1.614298000
6	0.000000000	0.000000000	-2.238800000
1	0.000000000	0.000000000	-3.320264000

6	0.000000000	2.702141000	0.255590000
6	1.199517000	3.330234000	0.562679000
6	-1.199517000	3.330234000	0.562679000
6	1.197849000	4.585900000	1.145554000
6	-1.197849000	4.585900000	1.145554000
6	0.000000000	5.218642000	1.434713000
1	2.138872000	5.069007000	1.381637000
1	-2.138872000	5.069007000	1.381637000
1	0.000000000	6.199265000	1.895485000
6	0.000000000	-2.702141000	0.255590000
6	-1.199517000	-3.330234000	0.562679000
6	1.199517000	-3.330234000	0.562679000
6	-1.197849000	-4.585900000	1.145554000
6	1.197849000	-4.585900000	1.145554000
6	0.000000000	-5.218642000	1.434713000
1	-2.138872000	-5.069007000	1.381637000
1	2.138872000	-5.069007000	1.381637000
1	0.000000000	-6.199265000	1.895485000
6	0.000000000	-2.456392000	-2.492692000
1	0.000000000	-2.178613000	-3.544638000
1	0.875113000	-3.078819000	-2.293080000
1	-0.875113000	-3.078819000	-2.293080000
6	0.000000000	2.456392000	-2.492692000
1	0.000000000	2.178613000	-3.544638000
1	-0.875113000	3.078819000	-2.293080000
1	0.875113000	3.078819000	-2.293080000
1	2.131074000	-2.819532000	0.341262000
1	-2.131074000	-2.819532000	0.341262000
1	-2.131074000	2.819532000	0.341262000
1	2.131074000	2.819532000	0.341262000

**IIIa-T (TE= -1009.355372)**

13	0.916948000	-0.000011000	0.433110000
7	0.323817000	1.437161000	-0.492460000
7	0.323807000	-1.437176000	-0.492468000
6	-0.183808000	1.266332000	-1.790231000
6	-0.183810000	-1.266336000	-1.790243000
6	-0.374284000	0.000001000	-2.329309000
1	-0.679812000	0.000006000	-3.370593000
6	0.219174000	2.659410000	0.191383000
6	1.307705000	3.127396000	0.929984000
6	-0.970609000	3.390602000	0.231127000
6	1.210059000	4.282641000	1.686239000
6	-1.054476000	4.553958000	0.971447000
6	0.031920000	5.009035000	1.704996000
1	2.070145000	4.624969000	2.250354000

1	-1.988848000	5.103756000	0.991309000
1	-0.042175000	5.920194000	2.286083000
6	0.219166000	-2.659425000	0.191377000
6	-0.970631000	-3.390592000	0.231183000
6	1.307716000	-3.127424000	0.929941000
6	-1.054489000	-4.553940000	0.971515000
6	1.210081000	-4.282662000	1.686207000
6	0.031930000	-5.009036000	1.705018000
1	-1.988872000	-5.103718000	0.991424000
1	2.070185000	-4.625002000	2.250290000
1	-0.042157000	-5.920188000	2.286115000
6	-0.338754000	-2.472733000	-2.655775000
1	-0.420707000	-2.172761000	-3.700497000
1	0.526525000	-3.137359000	-2.557158000
1	-1.218497000	-3.079925000	-2.421149000
6	-0.338778000	2.472746000	-2.655734000
1	-0.420755000	2.172798000	-3.700461000
1	-1.218520000	3.079927000	-2.421070000
1	0.526499000	3.137375000	-2.557121000
1	2.247349000	-2.584419000	0.878519000
1	-1.839360000	-3.016878000	-0.298173000
1	-1.839318000	3.016905000	-0.298275000
1	2.247330000	2.584374000	0.878603000

**IIIb-S (TE= -2691.803645)**

7	-0.020994000	1.429672000	-0.441933000
7	-0.020994000	-1.429672000	-0.441933000
6	0.044433000	1.254883000	-1.752143000
6	0.044433000	-1.254883000	-1.752143000
6	0.067408000	0.000000000	-2.362804000
1	0.106832000	0.000000000	-3.443925000
6	-0.018067000	2.737817000	0.098698000
6	1.177908000	3.413711000	0.315229000
6	-1.210659000	3.321956000	0.510161000
6	1.176348000	4.664666000	0.906844000
6	-1.208411000	4.573539000	1.102666000
6	-0.016535000	5.250881000	1.299244000
1	2.114924000	5.182185000	1.069093000
1	-2.145148000	5.019569000	1.416584000
1	-0.015529000	6.228548000	1.766233000
6	-0.018067000	-2.737817000	0.098698000
6	-1.210659000	-3.321956000	0.510161000
6	1.177908000	-3.413711000	0.315229000
6	-1.208411000	-4.573539000	1.102666000
6	1.176348000	-4.664666000	0.906844000
6	-0.016535000	-5.250881000	1.299244000

1	-2.145148000	-5.019569000	1.416584000
1	2.114924000	-5.182185000	1.069093000
1	-0.015529000	-6.228548000	1.766234000
6	0.083324000	-2.451203000	-2.655930000
1	0.045512000	-2.156002000	-3.702582000
1	0.993611000	-3.032075000	-2.492295000
1	-0.754584000	-3.120021000	-2.446366000
6	0.083324000	2.451203000	-2.655930000
1	0.045512000	2.156002000	-3.702582000
1	-0.754584000	3.120021000	-2.446366000
1	0.993611000	3.032075000	-2.492295000
1	2.107942000	-2.941409000	0.015342000
1	-2.138371000	-2.780381000	0.356053000
1	-2.138371000	2.780381000	0.356053000
1	2.107942000	2.941409000	0.015342000
31	-0.124814000	0.000000000	1.090861000

**IIIb-T** (TE= -2691.716936)

7	-0.326046000	1.436277000	-0.654512000
7	-0.326047000	-1.436275000	-0.654512000
6	0.189898000	1.272769000	-1.934278000
6	0.189902000	-1.272768000	-1.934275000
6	0.393121000	0.000000000	-2.464834000
1	0.731919000	0.000000000	-3.496254000
6	-0.243689000	2.642245000	0.036908000
6	0.957737000	3.358822000	0.099162000
6	-1.335894000	3.124705000	0.763878000
6	1.050888000	4.509020000	0.856279000
6	-1.228512000	4.271647000	1.529964000
6	-0.038625000	4.977154000	1.577556000
1	1.995757000	5.039426000	0.897859000
1	-2.092876000	4.624603000	2.080980000
1	0.041695000	5.881203000	2.168668000
6	-0.243693000	-2.642243000	0.036907000
6	-1.335897000	-3.124702000	0.763880000
6	0.957731000	-3.358825000	0.099156000
6	-1.228516000	-4.271645000	1.529965000
6	1.050881000	-4.509023000	0.856271000
6	-0.038630000	-4.977155000	1.577552000
1	-2.092879000	-4.624599000	2.080983000
1	1.995749000	-5.039432000	0.897848000
1	0.041688000	-5.881204000	2.168663000
6	0.386336000	-2.472902000	-2.803991000
1	0.447351000	-2.172033000	-3.850085000
1	1.293348000	-3.041507000	-2.577051000
1	-0.449165000	-3.172392000	-2.697132000

6	0.386316000	2.472902000	-2.803999000
1	0.447342000	2.172029000	-3.850092000
1	-0.449198000	3.172378000	-2.697148000
1	1.293317000	3.041524000	-2.577057000
1	1.828672000	-2.974902000	-0.418562000
1	-2.285731000	-2.603332000	0.693454000
1	-2.285728000	2.603337000	0.693449000
1	1.828679000	2.974897000	-0.418552000
31	-1.404788000	0.000001000	0.059146000

H<sub>2</sub> (TE= -1.160836)

1	0.000000000	0.000000000	0.373457000
1	0.000000000	0.000000000	-0.373457000

NH<sub>3</sub> (TE= -56.509166)

7	0.000000000	0.000000000	0.114416000
1	0.000000000	0.938276000	-0.266971000
1	-0.812571000	-0.469138000	-0.266971000
1	0.812571000	-0.469138000	-0.266971000

CH<sub>4</sub> (TE= -40.448443)

6	0.000000000	0.000000000	0.000000000
1	0.628315000	0.628315000	0.628315000
1	-0.628315000	-0.628315000	0.628315000
1	-0.628315000	0.628315000	-0.628315000
1	0.628315000	-0.628315000	-0.628315000

C<sub>6</sub>H<sub>5</sub>F (TE= -331.304540)

6	-1.125631000	-1.198877000	0.000002000
6	0.259400000	-1.208049000	-0.000003000
6	0.925405000	-0.000023000	-0.000007000
6	0.259399000	1.208038000	-0.000002000
6	-1.125598000	1.198903000	-0.000001000
6	-1.820232000	0.000003000	0.000002000
1	-1.664248000	-2.139173000	0.000008000
1	0.825356000	-2.131391000	-0.000007000
1	0.825436000	2.131333000	-0.000001000
1	-1.664245000	2.139181000	0.000007000
1	-2.903359000	0.000035000	0.000004000
9	2.260512000	0.000005000	0.000006000

Cartesian coordinates of the transition states involved in the activation of hydrogen by **4-7**, **9**, **II**, **IIIa** and **IIIb**, along with their total energies (in hartrees) including zero point vibrational correction.

**4TS<sup>H-H</sup>** (TE= -1714.647074)

6	-0.824802000	-0.584687000	1.020779000
6	-2.690115000	-0.747905000	-0.281247000
7	-0.435128000	-0.362348000	-0.311966000
7	-2.125530000	-0.801579000	1.080084000
6	-2.824703000	-1.226108000	2.260587000
1	-3.301777000	-2.196581000	2.089784000
1	-2.129481000	-1.318318000	3.094991000
1	-3.601382000	-0.508820000	2.547138000
15	-4.209474000	-0.018582000	-0.529924000
6	-4.386658000	1.671970000	0.103014000
1	-5.388003000	2.069548000	-0.075286000
1	-4.180673000	1.687140000	1.175291000
1	-3.644415000	2.288352000	-0.413728000
6	-5.630076000	-0.886302000	0.186329000
1	-6.557814000	-0.377733000	-0.083862000
1	-5.650301000	-1.909523000	-0.190047000
1	-5.552060000	-0.914175000	1.274082000
6	-4.517242000	0.096386000	-2.287632000
1	-5.535183000	0.457864000	-2.447871000
1	-3.799776000	0.808830000	-2.709474000
1	-4.389611000	-0.880746000	-2.750497000
15	1.101793000	-0.082186000	0.274344000
6	0.335435000	-0.435472000	1.790555000
7	2.216538000	-1.108586000	-0.371997000
7	1.704463000	1.428851000	0.034616000
6	-0.294820000	2.741116000	0.866266000
1	-0.751289000	2.641489000	-0.123838000
1	-0.742979000	1.997610000	1.530108000
1	-0.544707000	3.729657000	1.258849000
6	1.862102000	2.654306000	2.175755000
1	2.949988000	2.592469000	2.092890000
1	1.607865000	3.591295000	2.676728000
1	1.517714000	1.834989000	2.808852000
6	3.607222000	2.568616000	-1.065486000
1	4.274091000	2.099140000	-0.337878000
1	4.142153000	2.653857000	-2.013967000
1	3.392521000	3.584623000	-0.724842000
6	1.378767000	2.375117000	-2.242438000
1	0.500236000	1.741702000	-2.396896000
1	1.026621000	3.352283000	-1.900799000

1	1.870515000	2.523259000	-3.206659000
6	4.681900000	-1.067975000	-0.660190000
1	5.624213000	-0.984303000	-0.114781000
1	4.739486000	-1.972975000	-1.269793000
1	4.600695000	-0.211451000	-1.331758000
6	3.649053000	-2.291178000	1.278002000
1	2.818513000	-2.303379000	1.987688000
1	3.658863000	-3.246322000	0.746488000
1	4.582646000	-2.218744000	1.840030000
6	0.658458000	-0.560401000	3.232497000
1	0.468556000	-1.564822000	3.628102000
1	1.719209000	-0.359725000	3.404671000
1	0.100823000	0.145160000	3.862718000
6	1.216807000	2.598414000	0.806567000
6	2.349267000	1.745623000	-1.263100000
1	1.584041000	3.461153000	0.244712000
1	2.653002000	0.782518000	-1.678166000
6	3.522726000	-1.122781000	0.317390000
1	3.555988000	-0.198651000	0.912352000
6	1.890520000	-2.253845000	-1.250340000
1	2.834778000	-2.801325000	-1.334318000
6	1.513024000	-1.780902000	-2.639272000
1	2.312872000	-1.175322000	-3.073411000
1	1.339943000	-2.637534000	-3.294739000
1	0.590353000	-1.188791000	-2.621028000
6	0.870636000	-3.223947000	-0.676008000
1	1.118355000	-3.499319000	0.351062000
1	-0.137683000	-2.806357000	-0.691195000
1	0.859949000	-4.134526000	-1.279315000
5	-1.581241000	-0.331602000	-1.260601000
1	-1.753039000	0.910057000	-2.128912000
1	-1.989828000	1.911336000	-2.244105000

**5TS<sup>H-H</sup>** (TE= -1333.460884)

6	-1.654180000	0.047067000	0.703338000
6	-3.415969000	-0.165240000	-0.825040000
7	-1.050919000	-0.194010000	-0.553607000
7	-2.966360000	0.107705000	0.598601000
6	-3.859135000	0.305735000	1.708551000
1	-4.462547000	-0.586161000	1.903600000
1	-3.287015000	0.534306000	2.607862000
1	-4.537094000	1.140691000	1.515646000
15	0.415469000	-0.007888000	0.210033000
6	-0.607644000	0.172002000	1.607700000
7	1.403262000	-1.310146000	0.002842000
7	1.320430000	1.289705000	-0.240199000



6	-0.251843000	3.168895000	0.407632000
1	-0.771308000	3.015435000	-0.543338000
1	-0.841217000	2.686826000	1.189590000
1	-0.226551000	4.240911000	0.616947000
6	1.863736000	2.710589000	1.702391000
1	2.919126000	2.443902000	1.612490000
1	1.799634000	3.721943000	2.110363000
1	1.401096000	2.032869000	2.423275000
6	3.456241000	1.744518000	-1.423928000
1	3.994617000	1.259248000	-0.606774000
1	3.994431000	1.540833000	-2.352060000
1	3.491914000	2.824735000	-1.262296000
6	1.256477000	1.908021000	-2.644893000
1	0.277528000	1.439227000	-2.775888000
1	1.110344000	2.972400000	-2.441592000
1	1.800825000	1.824934000	-3.588086000
6	3.847867000	-1.713773000	-0.140939000
1	4.788039000	-1.569292000	0.395596000
1	3.791493000	-2.769486000	-0.416794000
1	3.885948000	-1.125329000	-1.059432000
6	2.617214000	-2.113839000	2.014653000
1	1.792829000	-1.780764000	2.649980000
1	2.475107000	-3.176976000	1.804091000
1	3.547592000	-2.012246000	2.577445000
6	-0.508917000	0.361856000	3.075900000
1	-0.751218000	1.380898000	3.405138000
1	-1.168250000	-0.319225000	3.622071000
1	0.505668000	0.153720000	3.426341000
6	1.169726000	2.636766000	0.357164000
6	2.035578000	1.225605000	-1.537863000
1	1.717106000	3.294363000	-0.323362000
1	2.094454000	0.162056000	-1.786920000
6	2.684353000	-1.295082000	0.738396000
1	2.851111000	-0.249553000	1.025003000
6	0.940353000	-2.620727000	-0.510419000
1	1.784654000	-3.292825000	-0.328634000
6	0.712939000	-2.568549000	-2.006828000
1	1.621626000	-2.250511000	-2.524434000
1	0.438649000	-3.558019000	-2.380156000
1	-0.097472000	-1.877011000	-2.266394000
6	-0.246753000	-3.201883000	0.236238000
1	-0.083045000	-3.194428000	1.315608000
1	-1.161668000	-2.648106000	0.021082000
1	-0.402562000	-4.235798000	-0.079044000
5	-2.027648000	-0.120030000	-1.682815000
6	-4.001763000	-1.571650000	-0.865820000

1	-4.833361000	-1.687083000	-0.160034000
1	-4.379527000	-1.780819000	-1.868499000
1	-3.247140000	-2.328125000	-0.633904000
6	-4.480496000	0.835310000	-1.227646000
1	-4.647708000	0.757019000	-2.304396000
1	-5.438962000	0.642671000	-0.731224000
1	-4.173126000	1.859640000	-1.008471000
1	-2.040731000	1.731841000	-1.906165000
1	-1.918676000	1.053259000	-2.475629000

**6TS<sup>H-H</sup>** (TE= -1501.845351)

6	0.711428000	-0.296516000	1.069384000
7	0.377747000	0.111004000	-0.232832000
7	2.023294000	-0.520562000	1.167451000
6	2.530063000	-1.547152000	2.053681000
1	3.575447000	-1.358025000	2.295400000
1	1.950619000	-1.532643000	2.976194000
1	2.448244000	-2.532440000	1.583453000
15	-1.221913000	0.004714000	0.241126000
6	-0.475876000	-0.418731000	1.765040000
7	-2.008926000	1.421727000	0.016742000
7	-2.119307000	-1.150176000	-0.497760000
6	-0.760033000	-3.201307000	0.103431000
1	-0.091876000	-2.940566000	-0.720895000
1	-0.286822000	-2.892995000	1.037411000
1	-0.863466000	-4.288176000	0.126199000
6	-3.021900000	-2.762873000	1.137707000
1	-4.032485000	-2.401038000	0.936318000
1	-3.082071000	-3.820819000	1.402591000
1	-2.634379000	-2.225318000	2.005445000
6	-4.069443000	-1.288731000	-2.026561000
1	-4.694962000	-0.846102000	-1.248123000
1	-4.441634000	-0.948294000	-2.995047000
1	-4.201550000	-2.373010000	-1.994518000
6	-1.721613000	-1.498855000	-2.924795000
1	-0.691041000	-1.144233000	-2.820668000
1	-1.719903000	-2.590874000	-2.866691000
1	-2.076694000	-1.224916000	-3.920363000
6	-4.364608000	2.080847000	-0.391276000
1	-5.370733000	2.036766000	0.030554000
1	-4.152593000	3.128620000	-0.616609000
1	-4.364133000	1.525035000	-1.330489000
6	-3.374697000	2.256557000	1.914116000
1	-2.666387000	1.816036000	2.619824000
1	-3.110072000	3.308223000	1.779245000
1	-4.371023000	2.222843000	2.359519000

6	-0.834985000	-0.756367000	3.163066000
1	-0.755840000	-1.827368000	3.389779000
1	-0.201683000	-0.225736000	3.879470000
1	-1.864933000	-0.462666000	3.381017000
6	-2.131127000	-2.570536000	-0.071867000
6	-2.618111000	-0.879901000	-1.871254000
1	-2.603917000	-3.094164000	-0.906474000
1	-2.568204000	0.205637000	-1.991717000
6	-3.367173000	1.505838000	0.595595000
1	-3.669771000	0.470241000	0.802816000
6	-1.336154000	2.695266000	-0.349007000
1	-2.123619000	3.447698000	-0.243198000
6	-0.918013000	2.679149000	-1.805139000
1	-1.787932000	2.544407000	-2.453136000
1	-0.434826000	3.621819000	-2.068966000
1	-0.201709000	1.878849000	-2.010886000
6	-0.212370000	3.099218000	0.588076000
1	-0.524826000	3.030275000	1.632403000
1	0.684056000	2.493517000	0.437866000
1	0.069239000	4.134359000	0.383886000
5	1.546799000	0.023099000	-1.130909000
7	2.554285000	-0.497599000	-0.178959000
6	3.906198000	-0.151257000	-0.285368000
6	4.585622000	-0.508518000	-1.447161000
6	4.572206000	0.578541000	0.694356000
6	5.905213000	-0.140649000	-1.620823000
1	4.052080000	-1.067284000	-2.207439000
6	5.903159000	0.921928000	0.520094000
1	4.034897000	0.896757000	1.580155000
6	6.577309000	0.567941000	-0.634662000
1	6.419484000	-0.420674000	-2.533353000
1	6.409491000	1.490883000	1.291951000
1	7.615936000	0.845149000	-0.770235000
1	1.955545000	1.133460000	-1.802994000
1	2.268522000	2.066450000	-1.374338000

**7TS<sup>H-H</sup>** (TE= -599.985495)

6	-1.524979000	-0.994735000	1.115611000
6	-0.189746000	-1.038476000	1.109224000
1	-2.248170000	-1.555421000	1.687161000
1	0.412935000	-1.680091000	1.737150000
6	-3.131570000	-0.357061000	-0.744076000
6	-3.292061000	0.546982000	0.136441000
7	-1.938920000	-0.044639000	0.108423000
7	0.383512000	-0.159643000	0.214076000
5	-0.666728000	0.664770000	-0.461246000

6	1.763068000	-0.038376000	0.053477000
6	2.653473000	-1.036972000	0.447706000
6	2.277408000	1.124776000	-0.520302000
6	4.015946000	-0.868384000	0.279368000
1	2.284338000	-1.965109000	0.867697000
6	3.639910000	1.278330000	-0.693705000
1	1.584747000	1.895297000	-0.839102000
6	4.521849000	0.287917000	-0.291659000
1	4.688878000	-1.660044000	0.589624000
1	4.016855000	2.190206000	-1.143425000
1	5.589636000	0.413682000	-0.424493000
6	-3.867634000	1.612410000	0.942770000
1	-3.379466000	2.562822000	0.714046000
1	-4.934818000	1.706062000	0.749422000
1	-3.709141000	1.407135000	2.004231000
6	-3.301424000	-1.284662000	-1.846479000
1	-4.308464000	-1.227126000	-2.256265000
1	-2.577898000	-1.042371000	-2.629980000
1	-3.108992000	-2.307556000	-1.513633000
1	-0.757767000	1.977856000	0.748367000
1	-0.716611000	2.000290000	-0.172315000

**9TS<sup>H-H</sup>** (TE= -1370.262716)

6	-1.334628000	0.093127000	1.199323000
7	-0.923932000	-0.071247000	-0.188858000
15	0.653090000	0.010390000	0.335544000
6	-0.091054000	0.146898000	1.871581000
7	1.525081000	-1.323969000	-0.125072000
7	1.537544000	1.270609000	-0.258986000
6	0.090184000	3.160417000	0.599579000
1	-0.556444000	3.020463000	-0.272669000
1	-0.389089000	2.671721000	1.449816000
1	0.151986000	4.230394000	0.813161000
6	2.360767000	2.677511000	1.590269000
1	3.384109000	2.373248000	1.357323000
1	2.386660000	3.692801000	1.993190000
1	1.977552000	2.018598000	2.372295000
6	3.471942000	1.680105000	-1.756952000
1	4.115431000	1.146122000	-1.053738000
1	3.846705000	1.497264000	-2.766598000
1	3.573133000	2.751206000	-1.564265000
6	1.115330000	1.946151000	-2.611953000
1	0.095306000	1.556593000	-2.557002000
1	1.079217000	3.018487000	-2.401510000
1	1.474884000	1.824663000	-3.636279000
6	3.880284000	-1.867115000	-0.686586000

1	4.904218000	-1.800804000	-0.312155000
1	3.707049000	-2.907378000	-0.973397000
1	3.805392000	-1.251205000	-1.584735000
6	3.008023000	-2.256712000	1.638424000
1	2.329772000	-1.890773000	2.412860000
1	2.760064000	-3.302357000	1.437404000
1	4.026358000	-2.231123000	2.032528000
6	0.259887000	0.279269000	3.303763000
1	0.078421000	1.284885000	3.709454000
1	-0.307610000	-0.420012000	3.927229000
1	1.318246000	0.059821000	3.473260000
6	1.487930000	2.618183000	0.352989000
6	2.032711000	1.211804000	-1.652385000
1	1.945684000	3.273036000	-0.393774000
1	2.010818000	0.153586000	-1.926203000
6	2.907889000	-1.406748000	0.383769000
1	3.186131000	-0.381580000	0.658613000
6	0.904664000	-2.590320000	-0.570735000
1	1.713164000	-3.325527000	-0.508017000
6	0.487576000	-2.504665000	-2.025632000
1	1.340632000	-2.241454000	-2.655935000
1	0.096373000	-3.466820000	-2.365833000
1	-0.297371000	-1.754685000	-2.171192000
6	-0.213055000	-3.110489000	0.319263000
1	0.088630000	-3.131821000	1.368202000
1	-1.116543000	-2.503053000	0.235902000
1	-0.466228000	-4.129105000	0.015751000
5	-2.008872000	-0.008305000	-1.133329000
6	-2.682587000	0.138025000	1.263430000
1	-3.367637000	0.261666000	2.086619000
6	-4.456193000	-0.735231000	-0.344407000
6	-4.549381000	0.533987000	-0.415159000
7	-3.199253000	0.024440000	-0.103702000
6	-4.732497000	-2.161142000	-0.323761000
1	-5.792836000	-2.366558000	-0.462722000
1	-4.162559000	-2.655918000	-1.115558000
1	-4.410243000	-2.582461000	0.632505000
6	-5.089690000	1.880380000	-0.534045000
1	-6.171259000	1.855491000	-0.658317000
1	-4.843110000	2.452666000	0.364388000
1	-4.631819000	2.394319000	-1.381787000
1	-2.209286000	1.992588000	-1.764982000
1	-2.150582000	0.999249000	-2.048684000

**II-TS<sup>H-H</sup>** (TE= -600.210632)

6	-0.845676000	1.214313000	0.348005000
6	-2.310395000	0.854412000	0.056643000
6	-2.353989000	-0.657975000	-0.216142000
6	-0.937440000	-0.976954000	-0.601787000
7	-0.153599000	-0.033100000	-0.100821000
1	-2.641267000	1.382850000	-0.842618000
1	-2.968235000	1.154854000	0.877207000
6	1.259831000	-0.183050000	-0.097220000
6	2.035766000	0.370825000	-1.105311000
6	3.409068000	0.189270000	-1.091267000
6	4.005742000	-0.542415000	-0.078486000
6	3.227335000	-1.104714000	0.921322000
6	1.855803000	-0.928245000	0.910146000
1	1.558118000	0.923302000	-1.905510000
1	4.014723000	0.617490000	-1.881275000
1	5.080488000	-0.680909000	-0.071011000
1	3.690621000	-1.684675000	1.710803000
1	1.224203000	-1.366688000	1.676284000
6	-3.393337000	-1.045614000	-1.247496000
1	-3.309720000	-2.106781000	-1.496618000
1	-4.398470000	-0.871312000	-0.853354000
1	-3.273825000	-0.472330000	-2.168154000
6	-2.622579000	-1.446347000	1.071044000
1	-3.598176000	-1.167878000	1.478915000
1	-2.625712000	-2.519778000	0.869536000
1	-1.865720000	-1.252726000	1.834700000
6	-0.402304000	2.404416000	-0.481519000
1	0.636747000	2.675481000	-0.280786000
1	-0.516040000	2.193266000	-1.548644000
1	-1.027418000	3.267973000	-0.240818000
6	-0.560219000	1.465585000	1.816682000
1	-1.067634000	2.375456000	2.144874000
1	-0.905432000	0.639012000	2.441308000
1	0.511273000	1.599781000	1.986548000
1	-0.703789000	-1.401803000	-1.714481000
1	-0.945183000	-0.753933000	-2.538839000

**IIIa-TS<sup>H-H</sup>** (TE= -1010.518206)

13	0.913095000	-0.188334000	0.000000000
7	-0.340422000	-0.189231000	1.414797000
7	-0.340422000	-0.189231000	-1.414797000
6	-1.654855000	-0.116001000	1.253844000
6	-1.654855000	-0.116001000	-1.253844000
6	-2.270949000	-0.106728000	0.000000000
1	-3.352149000	-0.085549000	0.000000000

6	0.245953000	-0.068139000	2.707607000
6	0.363645000	1.182136000	3.299319000
6	0.768330000	-1.187263000	3.341261000
6	0.975822000	1.305175000	4.534936000
6	1.378036000	-1.058632000	4.577266000
6	1.480635000	0.186265000	5.176906000
1	1.064744000	2.282453000	4.994788000
1	1.778744000	-1.935542000	5.071982000
1	1.962009000	0.285367000	6.142561000
6	0.245953000	-0.068139000	-2.707607000
6	0.768330000	-1.187263000	-3.341261000
6	0.363645000	1.182136000	-3.299319000
6	1.378036000	-1.058632000	-4.577266000
6	0.975822000	1.305175000	-4.534936000
6	1.480635000	0.186265000	-5.176906000
1	1.778744000	-1.935542000	-5.071982000
1	1.064744000	2.282453000	-4.994788000
1	1.962009000	0.285367000	-6.142561000
6	-2.537116000	-0.053912000	-2.458367000
1	-3.576391000	-0.227284000	-2.187534000
1	-2.466595000	0.926400000	-2.935084000
1	-2.231775000	-0.789508000	-3.204967000
6	-2.537116000	-0.053912000	2.458367000
1	-3.576391000	-0.227284000	2.187534000
1	-2.231775000	-0.789508000	3.204967000
1	-2.466595000	0.926400000	2.935084000
1	-0.017573000	2.051001000	-2.772276000
1	0.687220000	-2.153993000	-2.855537000
1	0.687220000	-2.153993000	2.855537000
1	-0.017573000	2.051001000	2.772276000
1	1.153570000	1.770135000	0.000000000
1	2.073772000	0.900002000	0.000000000

**IIIb-TS<sup>H-H</sup>** (TE= -2692.887142)

7	1.448309000	0.440048000	-0.191299000
7	-1.448315000	0.440069000	-0.191275000
6	1.259845000	1.747996000	-0.143920000
6	-1.259843000	1.748015000	-0.143990000
6	0.000006000	2.353617000	-0.157557000
1	0.000012000	3.435138000	-0.160669000
6	2.736783000	-0.137063000	-0.034722000
6	3.377270000	-0.708536000	-1.125653000
6	3.322117000	-0.199609000	1.222971000
6	4.614159000	-1.309046000	-0.963725000
6	4.558988000	-0.800643000	1.378962000
6	5.208634000	-1.353003000	0.286794000

1	5.114191000	-1.747399000	-1.819428000
1	5.013706000	-0.845208000	2.361694000
1	6.175298000	-1.826159000	0.412115000
6	-2.736793000	-0.137032000	-0.034699000
6	-3.322153000	-0.199502000	1.222988000
6	-3.377245000	-0.708597000	-1.125603000
6	-4.559001000	-0.800576000	1.378997000
6	-4.614110000	-1.309153000	-0.963654000
6	-5.208603000	-1.353048000	0.286858000
1	-5.013739000	-0.845082000	2.361722000
1	-5.114106000	-1.747585000	-1.819337000
1	-6.175246000	-1.826242000	0.412196000
6	-2.452918000	2.649074000	-0.083892000
1	-2.900483000	2.626564000	0.912222000
1	-2.173037000	3.676509000	-0.306957000
1	-3.224476000	2.325902000	-0.784965000
6	2.452918000	2.649040000	-0.083541000
1	2.173183000	3.676389000	-0.307187000
1	2.899876000	2.626959000	0.912857000
1	3.224892000	2.325555000	-0.784008000
1	-2.896054000	-0.671432000	-2.097269000
1	-2.788331000	0.214905000	2.072079000
1	2.788242000	0.214688000	2.072080000
1	2.896098000	-0.671317000	-2.097326000
31	-0.000012000	-0.862070000	-0.215776000
1	0.000009000	-2.072948000	0.762763000
1	0.000060000	-1.097477000	1.764810000

Cartesian coordinates of the transition states involved in the activation of N-H bond of NH<sub>3</sub> by **4**-, **7**, **9** and **II**, along with their total energies (in hartrees) including zero point vibrational correction.

**4TS<sup>N-H</sup>** (TE= -1770.002380)

6	-0.699444000	-0.893750000	-0.898148000
6	-2.619425000	-0.586635000	0.275249000
7	-0.403192000	-0.031281000	0.169846000
7	-1.990453000	-1.172595000	-0.917729000
6	-2.556747000	-2.212251000	-1.735000000
1	-3.334586000	-1.823266000	-2.399610000
1	-1.780925000	-2.664109000	-2.353813000
1	-2.999631000	-2.987684000	-1.102049000
15	-4.237576000	-0.040129000	0.241497000
6	-5.460045000	-1.284856000	-0.249496000
1	-6.463929000	-0.867816000	-0.148798000
1	-5.314356000	-1.589791000	-1.286194000
1	-5.364734000	-2.159856000	0.394401000



6	-4.579116000	1.350659000	-0.869745000
1	-5.644402000	1.586995000	-0.917927000
1	-4.028168000	2.210116000	-0.478979000
1	-4.215139000	1.111960000	-1.871697000
6	-4.711271000	0.521459000	1.868377000
1	-5.778361000	0.754639000	1.861541000
1	-4.499914000	-0.255571000	2.602010000
1	-4.123296000	1.425515000	2.082407000
15	1.203896000	-0.200581000	-0.263185000
6	0.526018000	-1.200844000	-1.504373000
7	1.902778000	1.248450000	-0.608929000
7	2.187697000	-0.918299000	0.842432000
6	0.900588000	-3.077787000	1.159648000
1	0.241823000	-2.539145000	1.844330000
1	0.391482000	-3.165119000	0.197788000
1	1.050930000	-4.086081000	1.552023000
6	3.123999000	-3.030347000	-0.031962000
1	4.116768000	-2.574751000	-0.041817000
1	3.238215000	-4.098633000	0.166370000
1	2.687836000	-2.921718000	-1.026571000
6	4.171995000	-0.372740000	2.224038000
1	4.756059000	-0.253980000	1.308241000
1	4.550685000	0.335618000	2.964023000
1	4.354198000	-1.376429000	2.616227000
6	1.853553000	-0.278566000	3.219170000
1	0.805940000	-0.037102000	3.014179000
1	1.901966000	-1.299522000	3.608204000
1	2.210516000	0.389240000	4.006208000
6	4.236482000	2.092272000	-0.640739000
1	5.216883000	1.933736000	-1.094669000
1	3.977607000	3.143749000	-0.786728000
1	4.323545000	1.910433000	0.431812000
6	3.103346000	1.399622000	-2.775274000
1	2.381940000	0.712279000	-3.223045000
1	2.784327000	2.420925000	-2.999021000
1	4.072004000	1.245619000	-3.255539000
6	0.931743000	-1.998357000	-2.686696000
1	0.863559000	-3.084375000	-2.532455000
1	0.328625000	-1.762320000	-3.570082000
1	1.969999000	-1.788919000	-2.958083000
6	2.247988000	-2.388066000	1.023992000
6	2.700352000	-0.108628000	1.973032000
1	2.755304000	-2.518852000	1.983651000
1	2.606595000	0.931545000	1.651703000
6	3.215647000	1.169437000	-1.279254000
1	3.568760000	0.139421000	-1.126620000

6	1.185294000	2.543443000	-0.653137000
1	1.909201000	3.233379000	-1.098452000
6	0.882956000	3.039561000	0.745377000
1	1.801442000	3.127612000	1.331293000
1	0.408948000	4.023254000	0.705342000
1	0.186988000	2.373450000	1.264105000
6	-0.039793000	2.560148000	-1.553613000
1	0.187736000	2.147707000	-2.538952000
1	-0.868129000	1.994702000	-1.121935000
1	-0.376003000	3.591494000	-1.684111000
5	-1.590607000	0.258155000	1.026430000
1	-1.944232000	1.570925000	1.649405000
7	-2.518915000	2.841559000	1.729222000
1	-2.037423000	3.308044000	2.500171000
1	-2.148538000	3.315067000	0.902323000

**5TS<sup>N-H</sup>** (TE= -1388.810179)

6	-1.509697000	-0.485186000	0.887018000
6	-3.369810000	-0.272025000	-0.505448000
7	-1.009281000	-0.182628000	-0.402434000
7	-2.822710000	-0.591943000	0.865413000
6	-3.633957000	-0.751793000	2.044061000
1	-4.445972000	-1.456623000	1.854178000
1	-3.029469000	-1.144419000	2.861488000
1	-4.072834000	0.198816000	2.363396000
15	0.520017000	-0.136023000	0.291267000
6	-0.402860000	-0.526281000	1.717976000
7	1.541549000	-1.238265000	-0.368746000
7	1.309477000	1.298036000	0.263325000
6	-0.549511000	2.770225000	1.142814000
1	-0.943296000	2.828814000	0.125671000
1	-1.135767000	2.033111000	1.697008000
1	-0.697552000	3.740139000	1.621962000
6	1.485493000	2.258170000	2.540975000
1	2.557815000	2.052595000	2.512378000
1	1.326816000	3.167105000	3.125651000
1	0.992147000	1.438348000	3.065182000
6	3.487788000	2.229053000	-0.466099000
1	3.992838000	1.571732000	0.245931000
1	4.136265000	2.348428000	-1.336596000
1	3.382766000	3.214864000	-0.006363000
6	1.423198000	2.535829000	-1.889711000
1	0.502643000	2.071011000	-2.256076000
1	1.156824000	3.502487000	-1.451744000
1	2.062831000	2.737417000	-2.751749000
6	4.014167000	-1.490426000	-0.430235000

1	4.896635000	-1.574793000	0.207105000
1	4.038437000	-2.330500000	-1.128171000
1	4.098382000	-0.567508000	-1.006284000
6	2.644594000	-2.789012000	1.227346000
1	1.750252000	-2.779803000	1.854623000
1	2.595683000	-3.664298000	0.574671000
1	3.517152000	-2.909595000	1.872681000
6	-0.180700000	-0.843651000	3.151152000
1	-0.664672000	-0.130156000	3.828333000
1	-0.540469000	-1.842224000	3.418686000
1	0.886287000	-0.826306000	3.386005000
6	0.930680000	2.433340000	1.142500000
6	2.157787000	1.650169000	-0.906206000
1	1.438778000	3.292966000	0.698813000
1	2.364579000	0.703421000	-1.408683000
6	2.761079000	-1.506620000	0.424766000
1	2.842482000	-0.673577000	1.138329000
6	1.177543000	-2.205313000	-1.429178000
1	2.064439000	-2.839527000	-1.523579000
6	0.976089000	-1.503912000	-2.756970000
1	1.875096000	-0.953391000	-3.044840000
1	0.760943000	-2.234862000	-3.539324000
1	0.131755000	-0.806154000	-2.722440000
6	0.019418000	-3.121435000	-1.071090000
1	0.156622000	-3.572064000	-0.086188000
1	-0.932703000	-2.588532000	-1.079078000
1	-0.047730000	-3.925590000	-1.806869000
5	-2.045311000	0.026804000	-1.400736000
6	-4.147118000	-1.468843000	-1.022613000
1	-5.009060000	-1.703645000	-0.387028000
1	-4.520351000	-1.254972000	-2.025705000
1	-3.514258000	-2.358326000	-1.086396000
6	-4.264147000	0.951539000	-0.413422000
1	-4.594840000	1.234315000	-1.414205000
1	-5.155449000	0.762116000	0.196149000
1	-3.727801000	1.806386000	0.009146000
1	-1.913065000	1.014630000	-2.392475000
7	-1.851060000	2.373838000	-2.784565000
1	-2.836626000	2.594480000	-2.944870000
1	-1.616283000	2.933780000	-1.960810000

**6TS<sup>N-H</sup>** (TE= -1557.196122)

6	0.619661000	-0.551096000	1.082912000
7	0.318593000	0.094907000	-0.120287000
7	1.927540000	-0.840666000	1.146068000
6	2.398174000	-2.017278000	1.846304000

1	3.441624000	-1.889704000	2.168371000
1	1.775640000	-2.170649000	2.739023000
1	2.335137000	-2.907670000	1.195681000
15	-1.323470000	-0.086208000	0.288317000
6	-0.586395000	-0.780926000	1.736676000
7	-2.125713000	1.363764000	0.282602000
7	-2.178906000	-1.101492000	-0.703633000
6	-0.937136000	-3.276793000	-0.334489000
1	-0.205060000	-2.925662000	-1.080537000
1	-0.504055000	-3.126061000	0.666699000
1	-1.074282000	-4.360641000	-0.477121000
6	-3.243535000	-2.881456000	0.637237000
1	-4.240621000	-2.461657000	0.427158000
1	-3.350152000	-3.970470000	0.766889000
1	-2.895169000	-2.467096000	1.597763000
6	-3.994726000	-0.877990000	-2.382608000
1	-4.666519000	-0.516073000	-1.587000000
1	-4.272802000	-0.370147000	-3.319841000
1	-4.189684000	-1.953468000	-2.531420000
6	-1.584868000	-1.101391000	-3.122497000
1	-0.542154000	-0.821642000	-2.887100000
1	-1.638720000	-2.197658000	-3.237285000
1	-1.840809000	-0.656812000	-4.097243000
6	-4.432292000	2.144915000	-0.214219000
1	-5.489580000	2.002095000	0.060518000
1	-4.224309000	3.225501000	-0.147596000
1	-4.308396000	1.839579000	-1.265182000
6	-3.701255000	1.741780000	2.167986000
1	-3.070486000	1.119637000	2.824669000
1	-3.420254000	2.796159000	2.328886000
1	-4.748825000	1.627800000	2.489132000
6	-0.977248000	-1.364458000	3.045565000
1	-0.985779000	-2.472209000	3.061327000
1	-0.299832000	-1.034454000	3.851326000
1	-1.987941000	-1.037658000	3.341586000
6	-2.273859000	-2.563955000	-0.486374000
6	-2.538901000	-0.595296000	-2.055358000
1	-2.723569000	-2.943241000	-1.419830000
1	-2.419314000	0.501219000	-1.999148000
6	-3.542083000	1.334088000	0.712183000
1	-3.859625000	0.276701000	0.624958000
6	-1.438256000	2.683633000	0.253847000
1	-2.242219000	3.400627000	0.497738000
6	-0.942483000	3.012877000	-1.141529000
1	-1.769503000	2.972354000	-1.869486000
1	-0.513184000	4.027673000	-1.165540000

1	-0.129697000	2.345429000	-1.471123000
6	-0.371407000	2.855704000	1.323772000
1	-0.754182000	2.596066000	2.323960000
1	0.520084000	2.242573000	1.119391000
1	-0.041529000	3.906663000	1.345712000
5	1.485497000	0.089026000	-1.033731000
7	2.481809000	-0.572553000	-0.151086000
6	3.850025000	-0.271315000	-0.187159000
6	4.532191000	-0.430751000	-1.401337000
6	4.541049000	0.228211000	0.924294000
6	5.874452000	-0.087955000	-1.499459000
1	3.977855000	-0.812581000	-2.263554000
6	5.892001000	0.553953000	0.817933000
1	4.004688000	0.393678000	1.863326000
6	6.567197000	0.402074000	-0.390243000
1	6.390270000	-0.210100000	-2.456728000
1	6.417199000	0.948899000	1.693211000
1	7.625521000	0.665588000	-0.470172000
1	1.809092000	1.124260000	-1.784485000
7	2.289846000	2.514178000	-1.432287000
1	3.291107000	2.305399000	-1.301653000
1	1.990575000	2.689337000	-0.461645000

**7TS<sup>N-H</sup> (TE= -655.337819)**

6	1.442994000	-1.492691000	-0.942778000
6	0.111327000	-1.476027000	-0.968693000
1	2.158432000	-2.107409000	-1.465743000
1	-0.522215000	-2.121439000	-1.560277000
6	3.174517000	-0.492214000	0.663393000
6	3.139380000	0.302748000	-0.324426000
7	1.857690000	-0.437925000	-0.055112000
7	-0.422285000	-0.484660000	-0.149598000
5	0.617476000	0.263384000	0.533414000
6	-1.810768000	-0.270074000	-0.027372000
6	-2.726684000	-1.294440000	-0.235081000
6	-2.266320000	0.998431000	0.321514000
6	-4.083767000	-1.050168000	-0.107857000
1	-2.384329000	-2.294853000	-0.473920000
6	-3.623071000	1.227325000	0.453940000
1	-1.549718000	1.799834000	0.479118000
6	-4.539824000	0.210050000	0.236878000
1	-4.787120000	-1.858995000	-0.269938000
1	-3.966827000	2.219447000	0.723191000
1	-5.602002000	0.398360000	0.338343000
6	3.453266000	1.298524000	-1.332870000
1	2.733654000	2.119240000	-1.246197000

1	4.463864000	1.678766000	-1.194391000
1	3.365789000	0.867373000	-2.332758000
6	3.591651000	-1.243421000	1.834144000
1	4.627718000	-1.018071000	2.081450000
1	2.953648000	-0.980985000	2.681449000
1	3.493221000	-2.316216000	1.654085000
1	0.631008000	1.605941000	0.774286000
7	0.594211000	2.947452000	0.235714000
1	1.553993000	3.296839000	0.261491000
1	0.359993000	2.912919000	-0.759045000

**9TS<sup>N-H</sup>** (TE= -1425.612576)

6	-1.140694000	-0.430544000	1.374260000
7	-0.823024000	-0.291352000	-0.041286000
15	0.781777000	-0.110370000	0.399603000
6	0.137852000	-0.339803000	1.970984000
7	1.752779000	-1.233305000	-0.330811000
7	1.465543000	1.335544000	0.007072000
6	-0.272404000	2.837211000	1.067445000
1	-0.866634000	2.758070000	0.153129000
1	-0.686699000	2.146395000	1.804922000
1	-0.382057000	3.852109000	1.456392000
6	2.035057000	2.595185000	2.058257000
1	3.092280000	2.451527000	1.823156000
1	1.923699000	3.557652000	2.563209000
1	1.729868000	1.815222000	2.757505000
6	3.353511000	2.243055000	-1.318726000
1	4.050484000	1.703422000	-0.672904000
1	3.777005000	2.274388000	-2.325094000
1	3.290654000	3.274943000	-0.963716000
6	1.005898000	2.296178000	-2.240585000
1	0.050476000	1.768288000	-2.313655000
1	0.802819000	3.308087000	-1.877106000
1	1.410648000	2.392085000	-3.250481000
6	4.165901000	-1.392761000	-0.889958000
1	5.168315000	-1.346334000	-0.459031000
1	4.094049000	-2.333133000	-1.442199000
1	4.063329000	-0.572490000	-1.602516000
6	3.283601000	-2.431017000	1.221824000
1	2.540501000	-2.347462000	2.018144000
1	3.173175000	-3.412193000	0.752781000
1	4.277848000	-2.394065000	1.672184000
6	0.580403000	-0.398064000	3.383100000
1	0.210487000	0.442146000	3.986928000
1	0.250768000	-1.316191000	3.881626000
1	1.671490000	-0.379593000	3.453360000

6	1.197260000	2.561265000	0.796581000
6	1.997838000	1.564158000	-1.358787000
1	1.549195000	3.375780000	0.158211000
1	2.141408000	0.568807000	-1.784303000
6	3.125211000	-1.308827000	0.211063000
1	3.288682000	-0.361438000	0.743864000
6	1.255125000	-2.409236000	-1.075527000
1	2.142056000	-3.036650000	-1.208437000
6	0.777662000	-2.013220000	-2.458437000
1	1.576522000	-1.518489000	-3.016042000
1	0.468148000	-2.897965000	-3.019788000
1	-0.081315000	-1.336686000	-2.409203000
6	0.236514000	-3.259299000	-0.331203000
1	0.574365000	-3.490653000	0.680549000
1	-0.736140000	-2.767812000	-0.262676000
1	0.095202000	-4.200694000	-0.867153000
5	-1.956583000	-0.215700000	-0.895227000
6	-2.479607000	-0.534159000	1.515699000
1	-3.117127000	-0.607465000	2.381671000
6	-4.394508000	-0.984382000	-0.132579000
6	-4.396486000	0.276111000	0.048296000
7	-3.069798000	-0.386765000	0.181257000
6	-4.795875000	-2.361815000	-0.365878000
1	-5.875544000	-2.445752000	-0.479718000
1	-4.308438000	-2.740928000	-1.268009000
1	-4.476166000	-2.984946000	0.473523000
6	-4.783535000	1.667459000	0.211342000
1	-4.267798000	2.268876000	-0.544230000
1	-5.860153000	1.794662000	0.110939000
1	-4.470667000	2.022254000	1.197069000
1	-2.195495000	0.588208000	-1.986379000
7	-2.433564000	1.890427000	-2.586632000
1	-3.451008000	1.977374000	-2.643387000
1	-2.157858000	2.617880000	-1.921260000

**II-TS<sup>N-H</sup> (TE= -655.559058)**

6	-0.766491000	1.319131000	-0.570683000
6	-2.244444000	0.916049000	-0.498115000
6	-2.330552000	-0.312146000	0.421317000
6	-0.932541000	-0.846016000	0.398681000
7	-0.111945000	0.092015000	-0.019646000
1	-2.591066000	0.636411000	-1.497426000
1	-2.869932000	1.743240000	-0.152481000
6	1.300526000	-0.048255000	0.101010000
6	2.089736000	-0.323000000	-1.004989000
6	3.457583000	-0.468269000	-0.848833000

6	4.034400000	-0.342655000	0.403736000
6	3.241013000	-0.079387000	1.508838000
6	1.874155000	0.066186000	1.358510000
1	1.629328000	-0.446743000	-1.977611000
1	4.073911000	-0.693058000	-1.711017000
1	5.105168000	-0.459792000	0.520885000
1	3.687707000	0.009891000	2.491876000
1	1.231307000	0.265423000	2.210060000
6	-3.387172000	-1.302759000	-0.024806000
1	-3.354257000	-2.208324000	0.585465000
1	-4.381299000	-0.858818000	0.077727000
1	-3.242905000	-1.589995000	-1.067313000
6	-2.606257000	0.086409000	1.876195000
1	-3.576647000	0.585930000	1.942725000
1	-2.628332000	-0.796794000	2.517946000
1	-1.845609000	0.765532000	2.268316000
6	-0.335623000	1.565422000	-2.003810000
1	0.715636000	1.853556000	-2.070395000
1	-0.500018000	0.673123000	-2.613842000
1	-0.932338000	2.378923000	-2.423441000
6	-0.418546000	2.518509000	0.291660000
1	-0.905778000	3.411332000	-0.105890000
1	-0.746094000	2.383617000	1.324388000
1	0.659524000	2.697287000	0.293937000
1	-0.637408000	-1.962459000	0.342914000
7	-0.617569000	-2.871499000	-0.902983000
1	-1.543768000	-3.020352000	-1.302925000
1	-0.095252000	-2.406852000	-1.647739000

Cartesian coordinates of the transition states involved in the activation of C-H bond of CH<sub>4</sub> by **4-7**, **9** and **II** via  $\sigma_{\text{CH}_2}$  approach, along with their total energies (in hartrees) including zero point vibrational correction.

**4TS $_{\sigma}^{\text{C-H}}$**  (TE= -1753.915941)

6	-0.710348000	-0.815853000	-0.948535000
6	-2.617071000	-0.604473000	0.266273000
7	-0.413859000	0.014442000	0.146760000
7	-1.997634000	-1.114270000	-0.966594000
6	-2.542693000	-2.167253000	-1.781904000
1	-3.369729000	-1.808452000	-2.402326000
1	-1.773007000	-2.562924000	-2.445284000
1	-2.914281000	-2.978290000	-1.146582000
15	-4.228855000	-0.054718000	0.261044000
6	-5.479941000	-1.266762000	-0.236856000
1	-6.476061000	-0.839919000	-0.103218000



1	-5.358979000	-1.541131000	-1.285367000
1	-5.381949000	-2.162087000	0.377914000
6	-4.586426000	1.363470000	-0.812044000
1	-5.638957000	1.652689000	-0.775113000
1	-3.958130000	2.195881000	-0.487510000
1	-4.322761000	1.100465000	-1.839315000
6	-4.666560000	0.434048000	1.924685000
1	-5.686327000	0.824979000	1.926892000
1	-4.597417000	-0.430090000	2.584493000
1	-3.968246000	1.206980000	2.249851000
15	1.196306000	-0.178815000	-0.268900000
6	0.512878000	-1.108390000	-1.561706000
7	1.946848000	1.259027000	-0.539686000
7	2.138973000	-0.975239000	0.819670000
6	0.793640000	-3.115203000	1.000985000
1	0.132351000	-2.593664000	1.696499000
1	0.304556000	-3.143662000	0.024839000
1	0.910943000	-4.144579000	1.347272000
6	3.047431000	-3.064885000	-0.133806000
1	4.052332000	-2.638682000	-0.093019000
1	3.126369000	-4.144973000	0.010816000
1	2.643503000	-2.891881000	-1.132880000
6	4.114895000	-0.544375000	2.252817000
1	4.715290000	-0.393100000	1.352517000
1	4.498545000	0.116498000	3.033128000
1	4.268256000	-1.570869000	2.595525000
6	1.786101000	-0.446017000	3.221299000
1	0.745902000	-0.174380000	3.013957000
1	1.809866000	-1.485000000	3.562223000
1	2.145192000	0.176758000	4.043560000
6	4.300818000	2.040041000	-0.480167000
1	5.288036000	1.874917000	-0.916786000
1	4.071238000	3.102758000	-0.589094000
1	4.356654000	1.812944000	0.585919000
6	3.206734000	1.461879000	-2.668363000
1	2.478787000	0.813291000	-3.161111000
1	2.922079000	2.499710000	-2.859856000
1	4.183201000	1.298838000	-3.129540000
6	0.917264000	-1.879511000	-2.761818000
1	0.841502000	-2.968825000	-2.636044000
1	0.317359000	-1.616500000	-3.639494000
1	1.957377000	-1.669739000	-3.025979000
6	2.159866000	-2.452828000	0.930500000
6	2.653189000	-0.234012000	1.995930000
1	2.638870000	-2.642676000	1.894705000
1	2.587005000	0.822815000	1.725423000

6	3.273547000	1.170393000	-1.180235000
1	3.595308000	0.125996000	-1.060665000
6	1.259233000	2.570968000	-0.556325000
1	2.013009000	3.262663000	-0.945862000
6	0.920289000	3.013474000	0.851608000
1	1.823071000	3.062163000	1.465991000
1	0.460317000	4.004055000	0.839270000
1	0.204608000	2.334116000	1.323396000
6	0.070250000	2.648062000	-1.500553000
1	0.332456000	2.279623000	-2.494728000
1	-0.782356000	2.077038000	-1.127427000
1	-0.248341000	3.688976000	-1.593393000
5	-1.590121000	0.231607000	1.046973000
1	-1.948196000	1.572387000	1.574499000
6	-2.397352000	3.043797000	1.492368000
1	-3.458386000	3.270502000	1.663701000
1	-1.805766000	3.552867000	2.262397000
1	-2.111020000	3.449340000	0.512813000

**5TS<sub>σ</sub><sup>C-H</sup> (TE= -1372.729032)**

6	-1.562117000	-0.080944000	0.807028000
6	-3.390486000	-0.181659000	-0.653646000
7	-1.018045000	-0.018124000	-0.497471000
7	-2.880506000	-0.120557000	0.775957000
6	-3.695229000	-0.322783000	1.944719000
1	-3.921548000	-1.381373000	2.113529000
1	-3.183215000	0.065349000	2.826509000
1	-4.638639000	0.215466000	1.840569000
15	0.488102000	-0.041937000	0.218744000
6	-0.478285000	-0.094513000	1.671371000
7	1.383349000	-1.348519000	-0.256812000
7	1.473309000	1.247603000	-0.035617000
6	0.248222000	3.093795000	1.170367000
1	-0.268161000	3.353631000	0.244955000
1	-0.418853000	2.464448000	1.762774000
1	0.433262000	4.014399000	1.728473000
6	2.310626000	2.024605000	2.151649000
1	3.309132000	1.646319000	1.921764000
1	2.417989000	2.892611000	2.805693000
1	1.774209000	1.253944000	2.711033000
6	3.578323000	1.719883000	-1.285622000
1	4.113277000	1.019202000	-0.641694000
1	4.019402000	1.661982000	-2.282807000
1	3.759002000	2.731610000	-0.914500000
6	1.350254000	2.399786000	-2.228238000
1	0.321179000	2.074700000	-2.388867000

1	1.334296000	3.391812000	-1.766922000
1	1.834734000	2.495853000	-3.202232000
6	3.739761000	-1.881368000	-0.827209000
1	4.761652000	-1.813220000	-0.447465000
1	3.584760000	-2.912260000	-1.153806000
1	3.658163000	-1.232590000	-1.701310000
6	2.846221000	-2.382070000	1.469701000
1	2.177250000	-2.038551000	2.263215000
1	2.578512000	-3.412652000	1.222963000
1	3.864902000	-2.392515000	1.863215000
6	-0.313897000	-0.286000000	3.132990000
1	-0.354386000	0.648824000	3.706625000
1	-1.085050000	-0.946603000	3.538646000
1	0.646674000	-0.754927000	3.365994000
6	1.567228000	2.402565000	0.885595000
6	2.097682000	1.398212000	-1.373451000
1	2.187220000	3.126811000	0.349964000
1	1.997867000	0.419696000	-1.855242000
6	2.763445000	-1.470210000	0.259431000
1	3.047079000	-0.467574000	0.590297000
6	0.783557000	-2.597338000	-0.785453000
1	1.608973000	-3.315150000	-0.776021000
6	0.354975000	-2.433854000	-2.228872000
1	1.201003000	-2.113108000	-2.842110000
1	-0.008939000	-3.386085000	-2.622515000
1	-0.443937000	-1.693179000	-2.338640000
6	-0.300274000	-3.190123000	0.096245000
1	0.046205000	-3.312531000	1.124919000
1	-1.198028000	-2.572774000	0.112717000
1	-0.582304000	-4.172718000	-0.288604000
5	-2.070781000	0.199614000	-1.536102000
6	-3.803348000	-1.619810000	-0.950975000
1	-4.543486000	-1.985196000	-0.228006000
1	-4.254067000	-1.667444000	-1.944204000
1	-2.950834000	-2.303187000	-0.948660000
6	-4.606094000	0.710083000	-0.804545000
1	-4.820625000	0.837326000	-1.867850000
1	-5.495847000	0.267430000	-0.341280000
1	-4.451630000	1.699574000	-0.372700000
1	-2.074718000	1.360886000	-2.209310000
6	-2.275900000	2.593538000	-1.500039000
1	-2.335623000	2.564510000	-0.411804000
1	-1.413905000	3.177084000	-1.823852000
1	-3.195307000	2.987573000	-1.932768000

6TS<sub>σ</sub><sup>C-H</sup> (TE= -1541.114966)

6	-0.601783000	-0.469834000	-1.091492000
7	-0.300048000	0.140052000	0.136876000
7	-1.906477000	-0.747515000	-1.176048000
6	-2.346022000	-1.924844000	-1.898359000
1	-3.396098000	-1.833009000	-2.172235000
1	-1.755672000	-2.019157000	-2.809046000
1	-2.219144000	-2.820731000	-1.282040000
15	1.311781000	-0.061236000	-0.268264000
6	0.599835000	-0.684449000	-1.738674000
7	2.139857000	1.349716000	-0.218431000
7	2.155103000	-1.124007000	0.652345000
6	0.787229000	-3.223130000	0.278184000
1	0.090129000	-2.842962000	1.028945000
1	0.358596000	-3.044014000	-0.709258000
1	0.873612000	-4.303582000	0.411126000
6	3.093778000	-2.952898000	-0.713231000
1	4.102746000	-2.582631000	-0.519365000
1	3.143059000	-4.037447000	-0.833195000
1	2.751916000	-2.529918000	-1.660046000
6	4.046179000	-1.078661000	2.259619000
1	4.706469000	-0.750217000	1.453814000
1	4.388060000	-0.616597000	3.188037000
1	4.162199000	-2.158905000	2.376526000
6	1.663683000	-1.142688000	3.086721000
1	0.642639000	-0.796844000	2.893183000
1	1.649328000	-2.232519000	3.175825000
1	1.983562000	-0.739692000	4.049829000
6	4.507280000	1.983502000	0.172879000
1	5.523401000	1.831963000	-0.196788000
1	4.340471000	3.061712000	0.229321000
1	4.448331000	1.577509000	1.184073000
6	3.588647000	1.870852000	-2.164449000
1	2.886911000	1.358768000	-2.827072000
1	3.355874000	2.938471000	-2.182590000
1	4.596029000	1.747581000	-2.567209000
6	0.990501000	-1.237277000	-3.057559000
1	0.909731000	-2.330205000	-3.118518000
1	0.378202000	-0.821756000	-3.862581000
1	2.027274000	-0.984186000	-3.293468000
6	2.159928000	-2.588642000	0.422042000
6	2.607868000	-0.678899000	1.996042000
1	2.591050000	-3.000100000	1.337976000
1	2.570470000	0.413447000	1.970081000
6	3.516869000	1.309293000	-0.756915000
1	3.786795000	0.245836000	-0.809478000

6	1.510818000	2.681965000	-0.037063000
1	2.326686000	3.387812000	-0.219730000
6	1.064510000	2.869595000	1.398405000
1	1.911004000	2.760527000	2.081021000
1	0.643113000	3.867841000	1.534677000
1	0.290531000	2.150637000	1.678470000
6	0.422998000	2.992554000	-1.047924000
1	0.779699000	2.839734000	-2.068515000
1	-0.465389000	2.381548000	-0.886984000
1	0.117653000	4.036176000	-0.944138000
5	-1.484144000	0.137062000	1.026505000
7	-2.458753000	-0.556763000	0.146029000
6	-3.829921000	-0.291590000	0.199095000
6	-4.480730000	-0.461453000	1.419679000
6	-4.553051000	0.178098000	-0.893367000
6	-5.819257000	-0.149205000	1.544268000
1	-3.905544000	-0.820050000	2.265633000
6	-5.899028000	0.475667000	-0.760313000
1	-4.046576000	0.355954000	-1.834742000
6	-6.541429000	0.318250000	0.455009000
1	-6.307186000	-0.276576000	2.504127000
1	-6.445145000	0.852350000	-1.618070000
1	-7.593095000	0.558447000	0.555320000
1	-1.900147000	1.207886000	1.640272000
6	-2.495890000	2.567953000	0.981650000
1	-3.493356000	2.629837000	1.423948000
1	-1.859127000	3.387612000	1.323336000
1	-2.570903000	2.567332000	-0.109897000

**7TS<sub>σ</sub><sup>C-H</sup> (TE= -639.259172)**

6	1.475993000	-0.902587000	-1.299257000
6	0.140966000	-0.906838000	-1.324679000
1	2.195357000	-1.310031000	-1.992408000
1	-0.457291000	-1.357165000	-2.103960000
6	3.040655000	-0.788013000	0.695742000
6	3.267310000	0.289168000	0.059091000
7	1.889465000	-0.228698000	-0.090416000
7	-0.430631000	-0.265971000	-0.243761000
5	0.623775000	0.331122000	0.630192000
6	-1.809504000	-0.172760000	-0.052621000
6	-2.728722000	-0.898294000	-0.811239000
6	-2.296459000	0.679852000	0.940444000
6	-4.087179000	-0.763537000	-0.586951000
1	-2.392264000	-1.588217000	-1.575232000
6	-3.654829000	0.800843000	1.160208000
1	-1.582587000	1.230266000	1.542029000

6	-4.564490000	0.085727000	0.397282000
1	-4.780339000	-1.339946000	-1.189598000
1	-4.006369000	1.469011000	1.938659000
1	-5.629352000	0.186354000	0.569009000
6	3.942567000	1.472918000	-0.453364000
1	3.487358000	2.375852000	-0.040461000
1	4.998479000	1.451584000	-0.188099000
1	3.847714000	1.521302000	-1.540636000
6	3.132901000	-1.966615000	1.536445000
1	4.128991000	-2.066538000	1.964369000
1	2.398256000	-1.889717000	2.342593000
1	2.902359000	-2.862114000	0.953562000
1	0.660231000	1.634587000	0.828908000
6	0.643119000	2.453351000	-0.354656000
1	1.047094000	2.028412000	-1.273515000
1	-0.403267000	2.726961000	-0.477447000
1	1.240940000	3.297188000	-0.008163000

**9TS<sub>o</sub><sup>C-H</sup>** (TE= -1409.533453)

6	-1.211692000	0.000248000	1.277791000
7	-0.845481000	0.016722000	-0.132511000
15	0.744317000	-0.024055000	0.350602000
6	0.050363000	0.001635000	1.915495000
7	1.537476000	-1.360022000	-0.241749000
7	1.704541000	1.228487000	-0.136101000
6	0.413904000	3.131122000	0.916486000
1	-0.201389000	3.207107000	0.018337000
1	-0.139606000	2.550472000	1.657082000
1	0.563239000	4.138421000	1.312627000
6	2.634158000	2.375573000	1.841209000
1	3.627148000	2.004119000	1.577100000
1	2.750121000	3.344186000	2.333100000
1	2.190990000	1.686442000	2.563100000
6	3.650880000	1.690958000	-1.611612000
1	4.276946000	1.102025000	-0.937268000
1	4.018396000	1.544205000	-2.629752000
1	3.789589000	2.747482000	-1.369313000
6	1.297756000	2.097137000	-2.421738000
1	0.275692000	1.709216000	-2.409565000
1	1.268990000	3.143850000	-2.104428000
1	1.660821000	2.074613000	-3.451755000
6	3.880404000	-1.950569000	-0.806434000
1	4.890044000	-2.017027000	-0.394980000
1	3.646474000	-2.921517000	-1.250482000
1	3.886472000	-1.206330000	-1.604866000
6	2.917071000	-2.594072000	1.422548000

1	2.217936000	-2.310992000	2.212756000
1	2.650153000	-3.595594000	1.074930000
1	3.918418000	-2.654620000	1.854506000
6	0.443683000	-0.079286000	3.340773000
1	0.312224000	0.865888000	3.886283000
1	-0.134433000	-0.838444000	3.879493000
1	1.497085000	-0.355960000	3.446097000
6	1.763085000	2.508045000	0.608105000
6	2.197540000	1.263476000	-1.530210000
1	2.272098000	3.197084000	-0.071872000
1	2.141965000	0.230765000	-1.883909000
6	2.896538000	-1.582683000	0.289222000
1	3.216281000	-0.618841000	0.705691000
6	0.855081000	-2.532585000	-0.827120000
1	1.628337000	-3.306613000	-0.864196000
6	0.430549000	-2.257769000	-2.256138000
1	1.291471000	-1.970841000	-2.865381000
1	-0.015329000	-3.152818000	-2.697676000
1	-0.316621000	-1.457678000	-2.304040000
6	-0.277666000	-3.099171000	0.014196000
1	0.040372000	-3.275893000	1.043463000
1	-1.139976000	-2.430502000	0.034743000
1	-0.602614000	-4.051719000	-0.411816000
5	-1.982994000	0.086885000	-1.027951000
6	-2.556644000	-0.046214000	1.394519000
1	-3.208184000	-0.078385000	2.252934000
6	-4.256218000	-1.010376000	-0.240409000
6	-4.549810000	0.228027000	-0.152337000
7	-3.123743000	-0.079713000	0.043851000
6	-4.310462000	-2.458210000	-0.351813000
1	-5.332796000	-2.811123000	-0.479701000
1	-3.706395000	-2.788524000	-1.201531000
1	-3.890297000	-2.908614000	0.552327000
6	-5.344747000	1.445625000	-0.053368000
1	-5.134457000	2.120766000	-0.885669000
1	-6.407855000	1.208436000	-0.042046000
1	-5.088197000	1.974586000	0.868133000
1	-2.235896000	1.054537000	-1.887028000
6	-2.447039000	2.486568000	-1.459190000
1	-1.579777000	3.025199000	-1.843778000
1	-3.350714000	2.757177000	-2.009383000
1	-2.566463000	2.648655000	-0.385812000

**II-TS<sub>o</sub><sup>C-H</sup> (TE= -639.483317)**

6	0.741029000	-1.340687000	0.358587000
6	2.223897000	-0.951173000	0.269685000

6	2.288618000	0.393616000	-0.471989000
6	0.918398000	0.967750000	-0.248024000
7	0.084732000	-0.042790000	0.026447000
1	2.813896000	-1.731847000	-0.219089000
1	2.626605000	-0.822447000	1.279008000
6	-1.318669000	0.118871000	-0.080047000
6	-1.869080000	0.381740000	-1.328956000
6	-3.233059000	0.555872000	-1.468194000
6	-4.061222000	0.466377000	-0.359573000
6	-3.515504000	0.213010000	0.886962000
6	-2.147966000	0.043658000	1.031563000
1	-1.203595000	0.447370000	-2.183780000
1	-3.653270000	0.757939000	-2.446578000
1	-5.130989000	0.600973000	-0.467566000
1	-4.156167000	0.158707000	1.759417000
1	-1.717057000	-0.120630000	2.011656000
6	2.414919000	0.183751000	-1.986307000
1	2.462237000	1.146792000	-2.499557000
1	3.328793000	-0.373747000	-2.212099000
1	1.568184000	-0.369305000	-2.397870000
6	3.440432000	1.267536000	-0.018932000
1	4.390844000	0.828269000	-0.335037000
1	3.366494000	2.261754000	-0.468002000
1	3.463519000	1.385604000	1.064504000
6	0.333223000	-2.399256000	-0.652607000
1	-0.747259000	-2.563272000	-0.626241000
1	0.609273000	-2.116559000	-1.670110000
1	0.821666000	-3.347656000	-0.417554000
6	0.392759000	-1.821515000	1.757885000
1	1.024193000	-2.677045000	2.012531000
1	0.569928000	-1.035844000	2.496345000
1	-0.647456000	-2.146049000	1.829432000
1	0.753927000	2.011298000	0.247682000
6	1.022726000	2.144385000	1.775970000
1	-0.012457000	2.297918000	2.083685000
1	1.473449000	1.311114000	2.312520000
1	1.619107000	3.052573000	1.865441000



Cartesian coordinates of the transition states involved in the activation of C-H bond of CH<sub>4</sub> by **4-7**, **9** and **II** via inverted  $\pi_{\text{CH}_2}$  approach, along with their total energies (in hartrees) including zero point vibrational correction.

**4TS $\pi^{\text{C-H}}$  (inverted) (TE= -1753.868017)**

6	0.809244000	-0.474412000	1.132891000
6	2.782721000	-0.912474000	-0.003313000
7	0.470912000	-0.335937000	-0.232807000
7	2.091752000	-0.733814000	1.305264000
6	2.647462000	-1.140195000	2.568758000
1	3.471359000	-0.488512000	2.872472000
1	1.884736000	-1.107225000	3.348561000
1	3.037088000	-2.159949000	2.490160000
15	4.059343000	0.156144000	-0.379008000
6	5.327835000	0.332746000	0.916012000
1	6.205176000	0.853356000	0.527455000
1	4.927229000	0.909718000	1.751669000
1	5.623081000	-0.654967000	1.273199000
6	3.797383000	1.900493000	-0.878813000
1	4.715736000	2.347498000	-1.266353000
1	3.027204000	1.916369000	-1.652927000
1	3.455134000	2.479763000	-0.019634000
6	4.962087000	-0.514301000	-1.787037000
1	5.796937000	0.138934000	-2.052693000
1	5.329351000	-1.510173000	-1.537502000
1	4.262969000	-0.592402000	-2.621014000
15	-1.068247000	-0.000642000	0.281358000
6	-0.382601000	-0.292461000	1.847115000
7	-1.577733000	1.515125000	-0.163470000
7	-2.298556000	-0.988319000	-0.211124000
6	-1.403647000	-3.222004000	0.538433000
1	-0.951587000	-3.376686000	-0.443637000
1	-0.638074000	-2.835342000	1.214096000
1	-1.733472000	-4.192489000	0.916682000
6	-3.263857000	-2.076620000	1.794207000
1	-4.133466000	-1.422320000	1.695185000
1	-3.601079000	-3.034702000	2.196496000
1	-2.576699000	-1.634317000	2.517159000
6	-4.419983000	-0.835110000	-1.493013000
1	-4.810888000	-0.154489000	-0.733532000
1	-4.828224000	-0.533145000	-2.460219000
1	-4.802885000	-1.836539000	-1.281354000
6	-2.344489000	-1.766497000	-2.568663000
1	-1.260583000	-1.658771000	-2.640617000
1	-2.570443000	-2.805877000	-2.314297000

1	-2.775636000	-1.566757000	-3.552123000
6	-3.731670000	2.638860000	-0.670152000
1	-4.719629000	2.856783000	-0.258110000
1	-3.309728000	3.585744000	-1.015840000
1	-3.861396000	1.990243000	-1.538130000
6	-2.676875000	2.907757000	1.586595000
1	-2.067137000	2.434019000	2.358964000
1	-2.196144000	3.847251000	1.301842000
1	-3.648190000	3.155779000	2.020327000
6	-0.686566000	0.025779000	3.266792000
1	-0.587562000	-0.835955000	3.937962000
1	-0.049763000	0.823458000	3.671006000
1	-1.719792000	0.370328000	3.367747000
6	-2.589864000	-2.279723000	0.451813000
6	-2.903530000	-0.797462000	-1.546281000
1	-3.323358000	-2.761795000	-0.200816000
1	-2.608719000	0.207608000	-1.858697000
6	-2.859916000	1.989557000	0.390538000
1	-3.381124000	1.091071000	0.744157000
6	-0.648362000	2.544673000	-0.672610000
1	-1.252110000	3.456817000	-0.724775000
6	-0.198150000	2.218737000	-2.082390000
1	-1.063157000	2.107329000	-2.741900000
1	0.426081000	3.025502000	-2.475977000
1	0.390878000	1.292956000	-2.112412000
6	0.517787000	2.841023000	0.255145000
1	0.177989000	3.048819000	1.271936000
1	1.213894000	2.001613000	0.288269000
1	1.063896000	3.715324000	-0.108683000
5	1.650317000	-0.884611000	-1.118222000
1	1.397285000	-2.185606000	-0.824256000
6	1.313167000	-2.455367000	-2.060360000
1	2.311549000	-2.717774000	-2.400841000
1	0.801651000	-3.405014000	-1.762391000
1	0.739930000	-2.092352000	-2.909805000

**5TS<sub>π</sub><sup>C-H</sup> (inverted)** (TE= -1372.694836)

6	1.528882000	0.041933000	0.862784000
6	3.427476000	0.178857000	-0.527350000
7	1.000873000	-0.006833000	-0.440621000
7	2.851239000	0.003494000	0.878212000
6	3.603680000	0.201023000	2.091134000
1	3.795261000	1.260234000	2.296075000
1	3.061595000	-0.220986000	2.938675000
1	4.564639000	-0.311207000	2.019937000
15	-0.496382000	0.050801000	0.258933000

6	0.437699000	0.096126000	1.727308000
7	-1.407925000	1.344063000	-0.205847000
7	-1.490866000	-1.256109000	0.060585000
6	0.159145000	-3.092868000	0.580283000
1	0.438858000	-3.141324000	-0.474387000
1	0.898700000	-2.485253000	1.106176000
1	0.204970000	-4.104535000	0.989885000
6	-1.666822000	-2.489801000	2.208204000
1	-2.680625000	-2.093664000	2.303227000
1	-1.649369000	-3.492604000	2.641453000
1	-0.994442000	-1.862178000	2.793634000
6	-3.816019000	-1.762000000	-0.635106000
1	-4.179324000	-1.148472000	0.192603000
1	-4.516322000	-1.659151000	-1.467168000
1	-3.841230000	-2.808057000	-0.319740000
6	-1.894644000	-2.161940000	-2.216280000
1	-0.925277000	-1.782485000	-2.548418000
1	-1.771180000	-3.210618000	-1.932054000
1	-2.581695000	-2.129914000	-3.064755000
6	-3.827084000	1.913483000	-0.058983000
1	-4.650416000	2.025503000	0.649668000
1	-3.788243000	2.828091000	-0.655195000
1	-4.064938000	1.083341000	-0.726140000
6	-2.197716000	2.844322000	1.605971000
1	-1.277006000	2.656812000	2.162711000
1	-2.069461000	3.768371000	1.036076000
1	-3.006986000	3.008500000	2.320961000
6	0.258339000	0.336561000	3.182612000
1	0.607593000	-0.493568000	3.809105000
1	0.773343000	1.238997000	3.530369000
1	-0.800198000	0.472454000	3.419807000
6	-1.245141000	-2.542973000	0.753143000
6	-2.432870000	-1.321012000	-1.075245000
1	-1.914354000	-3.250763000	0.256279000
1	-2.519478000	-0.296386000	-1.440347000
6	-2.529656000	1.677713000	0.693469000
1	-2.678854000	0.789717000	1.325289000
6	-0.994682000	2.353936000	-1.201514000
1	-1.799874000	3.095360000	-1.180712000
6	-0.943037000	1.759880000	-2.594965000
1	-1.903494000	1.318768000	-2.874695000
1	-0.699267000	2.535729000	-3.324309000
1	-0.151775000	1.001577000	-2.660594000
6	0.300754000	3.069218000	-0.863402000
1	0.343664000	3.347614000	0.191963000
1	1.155057000	2.432821000	-1.101650000

1	0.387753000	3.978647000	-1.462494000
5	2.133031000	-0.120876000	-1.491746000
6	3.933791000	1.615437000	-0.611546000
1	4.730658000	1.822126000	0.116822000
1	4.331840000	1.797909000	-1.611092000
1	3.125564000	2.330437000	-0.441398000
6	4.604719000	-0.760633000	-0.711719000
1	4.950204000	-0.706498000	-1.746663000
1	5.456102000	-0.489556000	-0.077475000
1	4.339512000	-1.799405000	-0.494979000
1	2.304333000	-1.456262000	-1.241763000
6	2.108012000	-1.719868000	-2.452052000
1	1.186861000	-1.582465000	-3.010030000
1	2.952889000	-1.595168000	-3.120069000
1	2.102647000	-2.797858000	-2.142030000

**6TS $\pi$ <sup>C-H</sup> (inverted)** (TE= -1541.071366)

6	0.626787000	-0.707144000	1.062161000
7	0.302538000	-0.466943000	-0.285348000
7	1.895946000	-1.100669000	1.194532000
6	2.296024000	-2.090091000	2.165563000
1	3.350883000	-1.969275000	2.415248000
1	1.702515000	-1.968820000	3.072957000
1	2.139595000	-3.100029000	1.767969000
15	-1.170341000	0.044515000	0.264881000
6	-0.505343000	-0.438156000	1.809327000
7	-1.422423000	1.635362000	-0.070430000
7	-2.513455000	-0.743937000	-0.260859000
6	-1.890202000	-3.116439000	0.334071000
1	-1.434629000	-3.239151000	-0.651063000
1	-1.101148000	-2.889960000	1.055007000
1	-2.342782000	-4.069109000	0.617835000
6	-3.603824000	-1.838472000	1.671788000
1	-4.393352000	-1.085425000	1.615520000
1	-4.046648000	-2.774633000	2.018782000
1	-2.873832000	-1.519752000	2.417700000
6	-4.588509000	-0.275770000	-1.537803000
1	-4.909036000	0.378462000	-0.723821000
1	-4.951068000	0.147651000	-2.476952000
1	-5.080036000	-1.243353000	-1.410865000
6	-2.601781000	-1.342837000	-2.667425000
1	-1.509914000	-1.347412000	-2.718132000
1	-2.944162000	-2.366694000	-2.493068000
1	-2.986912000	-1.027759000	-3.639432000
6	-3.423485000	3.075198000	-0.357315000
1	-4.308168000	3.456090000	0.157261000

1	-2.884022000	3.937352000	-0.756718000
1	-3.756261000	2.464846000	-1.198577000
6	-2.127864000	3.118599000	1.793055000
1	-1.527439000	2.532340000	2.492239000
1	-1.534254000	3.979440000	1.475344000
1	-3.000816000	3.500901000	2.326283000
6	-0.740538000	-0.221136000	3.259348000
1	-0.842811000	-1.155319000	3.823730000
1	0.068060000	0.352991000	3.725717000
1	-1.664220000	0.340504000	3.422686000
6	-2.955764000	-2.035419000	0.316584000
6	-3.077487000	-0.394934000	-1.584583000
1	-3.738235000	-2.381848000	-0.363983000
1	-2.677727000	0.595020000	-1.818459000
6	-2.566215000	2.277520000	0.607890000
1	-3.184435000	1.455421000	0.994987000
6	-0.391993000	2.521668000	-0.664507000
1	-0.838925000	3.519201000	-0.607181000
6	-0.176745000	2.199057000	-2.128644000
1	-1.116975000	2.259591000	-2.683368000
1	0.524445000	2.911590000	-2.569035000
1	0.254738000	1.198528000	-2.253825000
6	0.919313000	2.576697000	0.102119000
1	0.753741000	2.686366000	1.176452000
1	1.521310000	1.682790000	-0.069751000
1	1.503254000	3.433841000	-0.240029000
5	1.398867000	-1.099448000	-1.172818000
7	2.510564000	-1.159027000	-0.125263000
6	3.671191000	-0.385103000	-0.190489000
6	4.341634000	-0.303364000	-1.416496000
6	4.220386000	0.290989000	0.901441000
6	5.499881000	0.434486000	-1.542177000
1	3.906020000	-0.819254000	-2.264269000
6	5.386261000	1.028883000	0.762202000
1	3.715045000	0.270432000	1.858701000
6	6.038571000	1.109888000	-0.454208000
1	5.992023000	0.484120000	-2.507818000
1	5.780557000	1.555077000	1.625312000
1	6.949644000	1.687364000	-0.556740000
1	0.990917000	-2.388843000	-0.873683000
6	1.065325000	-2.651987000	-2.111619000
1	0.583811000	-3.628424000	-1.845100000
1	0.491151000	-2.287764000	-2.960056000
1	2.074949000	-2.883896000	-2.437062000

**7TS<sub>π</sub><sup>C-H</sup> (inverted) (TE= -639.222716)**

6	-1.465107000	-1.344996000	0.928337000
6	-0.123291000	-1.353608000	0.956215000
1	-2.172082000	-2.055970000	1.328780000
1	0.468900000	-2.139438000	1.406014000
6	-3.013858000	-0.500690000	-0.894898000
6	-3.311828000	0.195584000	0.132279000
7	-1.915073000	-0.238995000	0.106301000
7	0.450750000	-0.295988000	0.303044000
5	-0.648486000	0.629949000	-0.234506000
6	1.815851000	-0.165578000	0.100626000
6	2.763294000	-0.914717000	0.808600000
6	2.282421000	0.771742000	-0.828392000
6	4.114414000	-0.740768000	0.578291000
1	2.447240000	-1.631592000	1.557003000
6	3.636299000	0.931508000	-1.052376000
1	1.544443000	1.336707000	-1.388778000
6	4.568655000	0.181144000	-0.353028000
1	4.824823000	-1.334662000	1.143302000
1	3.967160000	1.656833000	-1.788148000
1	5.629756000	0.315324000	-0.524851000
6	-4.089991000	1.010528000	1.059819000
1	-3.710910000	2.035151000	1.089663000
1	-5.137669000	1.035746000	0.763842000
1	-4.017448000	0.601513000	2.070879000
6	-2.975429000	-1.200899000	-2.161651000
1	-3.900931000	-1.083640000	-2.723142000
1	-2.141942000	-0.796351000	-2.746463000
1	-2.788245000	-2.266113000	-1.999452000
1	-0.792895000	1.268004000	0.985262000
6	-0.668734000	2.357502000	0.382549000
1	-0.687689000	2.813991000	1.403880000
1	0.271094000	2.694849000	-0.050313000
1	-1.507092000	2.784266000	-0.158601000

**9TS<sub>π</sub><sup>C-H</sup> (inverted) (TE= -1409.488243)**

6	-1.170660000	-0.103070000	1.314341000
7	-0.783369000	-0.437806000	-0.040102000
15	0.747271000	0.009660000	0.375954000
6	0.067773000	0.183627000	1.942047000
7	1.860903000	-1.181750000	0.037641000
7	1.408835000	1.340185000	-0.374357000
6	-0.454185000	2.942638000	0.200378000
1	-1.016273000	2.533080000	-0.643488000
1	-0.828074000	2.471547000	1.112077000
1	-0.655831000	4.015066000	0.262916000

6	1.846298000	3.186390000	1.208029000
1	2.916367000	3.086464000	1.011562000
1	1.633572000	4.236104000	1.425872000
1	1.607901000	2.605604000	2.100055000
6	3.261115000	1.967854000	-1.898551000
1	3.978958000	1.691038000	-1.122606000
1	3.706166000	1.741612000	-2.870445000
1	3.114983000	3.050332000	-1.854660000
6	0.943421000	1.560584000	-2.807459000
1	0.020403000	0.985192000	-2.672447000
1	0.685384000	2.623613000	-2.786020000
1	1.349912000	1.344047000	-3.798559000
6	4.311708000	-1.285830000	-0.323543000
1	5.275659000	-1.048909000	0.132318000
1	4.336322000	-2.342767000	-0.601832000
1	4.212868000	-0.697265000	-1.237580000
6	3.345164000	-1.774757000	1.943181000
1	2.534226000	-1.545110000	2.637780000
1	3.344202000	-2.852772000	1.760066000
1	4.294510000	-1.525711000	2.422765000
6	0.368921000	0.721909000	3.288025000
1	-0.113453000	1.691706000	3.489822000
1	0.049701000	0.042783000	4.086486000
1	1.444167000	0.869114000	3.424602000
6	1.036978000	2.716499000	0.016164000
6	1.960663000	1.202976000	-1.739021000
1	1.335348000	3.336352000	-0.834349000
1	2.193299000	0.141925000	-1.852422000
6	3.186432000	-0.990778000	0.651749000
1	3.246353000	0.076796000	0.905437000
6	1.495586000	-2.549336000	-0.368570000
1	2.423216000	-3.125225000	-0.282738000
6	1.094906000	-2.569230000	-1.831753000
1	1.940345000	-2.289858000	-2.465617000
1	0.752753000	-3.562996000	-2.132565000
1	0.286390000	-1.858968000	-2.019950000
6	0.481886000	-3.240324000	0.530569000
1	0.795336000	-3.205237000	1.575228000
1	-0.504571000	-2.779474000	0.464216000
1	0.390254000	-4.288821000	0.235858000
5	-1.990985000	-0.536133000	-0.945423000
6	-2.518280000	-0.029305000	1.438077000
1	-3.120074000	0.342894000	2.254474000
6	-4.551826000	-0.380617000	-0.011698000
6	-4.209845000	0.833119000	-0.232485000
7	-3.117139000	-0.113777000	0.100715000

6	-5.372367000	-1.569313000	0.197985000
1	-5.061192000	-2.061159000	1.124165000
1	-6.427558000	-1.309700000	0.274418000
1	-5.250651000	-2.291299000	-0.613952000
6	-4.208229000	2.257996000	-0.512374000
1	-3.537333000	2.452995000	-1.354417000
1	-5.203643000	2.628241000	-0.753278000
1	-3.824675000	2.805650000	0.353880000
1	-2.238274000	-1.853577000	-0.609410000
6	-2.450643000	-2.060134000	-1.850779000
1	-1.756002000	-2.055280000	-2.686031000
1	-2.524130000	-3.140439000	-1.554515000
1	-3.434486000	-1.775161000	-2.212468000

**II-TS<sub>π</sub><sup>C-H</sup> (inverted) (TE= -639.448690)**

6	0.776206000	1.423576000	-0.117489000
6	2.251005000	0.994379000	0.046800000
6	2.254609000	-0.502301000	0.399509000
6	0.939022000	-0.988886000	-0.190509000
7	0.069836000	0.106812000	-0.141682000
1	2.764729000	1.615509000	0.787463000
1	2.780445000	1.129930000	-0.903622000
6	-1.303059000	-0.084987000	-0.008347000
6	-1.789537000	-1.351015000	0.347669000
6	-3.143142000	-1.584361000	0.483325000
6	-4.068186000	-0.575780000	0.261500000
6	-3.601739000	0.674339000	-0.103749000
6	-2.247124000	0.921136000	-0.244318000
1	-1.067315000	-2.138243000	0.527963000
1	-3.479178000	-2.574879000	0.770946000
1	-5.130063000	-0.763010000	0.364646000
1	-4.301809000	1.480649000	-0.293990000
1	-1.934289000	1.908621000	-0.550488000
6	2.164170000	-0.713872000	1.909307000
1	2.194678000	-1.780670000	2.141071000
1	2.997720000	-0.220297000	2.419518000
1	1.231102000	-0.316128000	2.314462000
6	3.489392000	-1.206909000	-0.121611000
1	4.384484000	-0.806789000	0.361890000
1	3.445166000	-2.278364000	0.090827000
1	3.614592000	-1.075286000	-1.200917000
6	0.345421000	2.284673000	1.061350000
1	-0.701690000	2.580851000	1.012087000
1	0.501183000	1.758841000	2.005540000
1	0.947793000	3.196048000	1.079852000
6	0.617322000	2.181123000	-1.430566000



1	1.312218000	3.025146000	-1.458440000
1	0.851530000	1.529544000	-2.277765000
1	-0.388249000	2.576084000	-1.577588000
1	1.405135000	-0.802597000	-1.413955000
6	0.912703000	-1.873094000	-1.796222000
1	-0.154464000	-2.078354000	-1.788700000
1	1.163029000	-1.542342000	-2.828106000
1	1.492014000	-2.760080000	-1.570815000

Cartesian coordinates of the transition states involved in the activation of C-F bond of C<sub>6</sub>H<sub>5</sub>F by **4-7**, **9** and **IIIa**, along with their total energies (in hartrees) including zero point vibrational correction.

**4TS<sup>C-F</sup>** (TE= -2044.789841)

6	0.053330000	-1.830065000	-0.553082000
6	2.241413000	-1.213140000	-0.636463000
7	0.115495000	-0.452675000	-0.268873000
7	1.267761000	-2.319263000	-0.722653000
6	1.533230000	-3.640275000	-1.225307000
1	2.121433000	-3.578989000	-2.146029000
1	2.089399000	-4.245209000	-0.501175000
1	0.596347000	-4.153749000	-1.442774000
15	3.761120000	-1.491962000	0.079176000
6	4.794641000	-2.743809000	-0.728164000
1	5.779252000	-2.770159000	-0.256898000
1	4.344601000	-3.733438000	-0.645471000
1	4.902476000	-2.491993000	-1.783794000
6	3.753425000	-2.044240000	1.810294000
1	4.756700000	-2.283570000	2.169600000
1	3.321016000	-1.246004000	2.416982000
1	3.119398000	-2.929617000	1.899674000
6	4.737399000	0.005505000	0.045013000
1	5.675918000	-0.168371000	0.575494000
1	4.944646000	0.278269000	-0.989465000
1	4.171040000	0.812844000	0.511604000
15	-1.549113000	-0.524457000	-0.059428000
6	-1.300668000	-2.175875000	-0.536346000
7	-1.958257000	-0.148817000	1.498103000
7	-2.522466000	0.395715000	-1.011368000
6	-1.728237000	-0.290336000	-3.295263000
1	-1.010550000	0.531566000	-3.268550000
1	-1.208914000	-1.205456000	-3.004786000
1	-2.078340000	-0.409614000	-4.323232000
6	-3.918666000	-1.147546000	-2.378856000
1	-4.751876000	-0.920709000	-1.708977000
1	-4.320248000	-1.290778000	-3.384691000

1	-3.466880000	-2.088985000	-2.066526000
6	-4.311860000	2.056378000	-0.586389000
1	-4.801988000	1.373108000	0.108786000
1	-4.498131000	3.077741000	-0.246595000
1	-4.792386000	1.947898000	-1.562364000
6	-2.160304000	2.781409000	-1.636194000
1	-1.102126000	2.558730000	-1.771896000
1	-2.642707000	2.774554000	-2.616932000
1	-2.245896000	3.796892000	-1.242765000
6	-3.952290000	0.724821000	2.685634000
1	-5.025918000	0.570781000	2.815302000
1	-3.512655000	0.791708000	3.683528000
1	-3.802307000	1.683138000	2.186172000
6	-3.519864000	-1.744082000	2.611908000
1	-3.110270000	-2.570431000	2.027217000
1	-3.019759000	-1.733613000	3.583525000
1	-4.578557000	-1.943202000	2.791786000
6	-2.024836000	-3.471836000	-0.495215000
1	-2.067806000	-3.981793000	-1.465507000
1	-1.582265000	-4.176619000	0.220010000
1	-3.062048000	-3.322927000	-0.183012000
6	-2.909340000	-0.017729000	-2.383525000
6	-2.816605000	1.808945000	-0.673897000
1	-3.425355000	0.856414000	-2.788318000
1	-2.379417000	1.973688000	0.316634000
6	-3.359003000	-0.420300000	1.884802000
1	-3.919887000	-0.495248000	0.944561000
6	-0.984890000	-0.050896000	2.614162000
1	-1.614958000	-0.008038000	3.507486000
6	-0.203546000	1.242817000	2.548374000
1	-0.880983000	2.100409000	2.508960000
1	0.428282000	1.348067000	3.434420000
1	0.458211000	1.265602000	1.674847000
6	-0.080010000	-1.261516000	2.780781000
1	-0.647084000	-2.195047000	2.772717000
1	0.677093000	-1.305318000	1.996358000
1	0.442362000	-1.189156000	3.737963000
6	1.754966000	2.479629000	-0.864988000
6	1.018970000	3.232402000	0.067936000
6	3.120798000	2.776359000	-1.020153000
6	1.686331000	3.942580000	1.037895000
1	-0.060414000	3.132026000	0.096692000
6	3.771339000	3.500646000	-0.049207000
1	3.656083000	2.335371000	-1.853555000
6	3.076964000	4.043194000	1.032088000
1	3.594726000	4.612357000	1.794271000

9	1.097860000	2.087757000	-2.002237000
5	1.511892000	0.079957000	-0.256520000
1	4.843333000	3.654129000	-0.133483000
1	1.113241000	4.436458000	1.817234000

**5TS<sup>C-F</sup>** (TE= -1663.604788)

6	-0.225404000	1.937562000	-0.707015000
6	2.075407000	2.111669000	-0.351804000
7	0.231460000	0.664488000	-0.264000000
7	0.786236000	2.769430000	-0.822604000
6	0.650825000	4.169977000	-1.127193000
1	-0.314283000	4.359341000	-1.596999000
1	0.724320000	4.787470000	-0.226425000
1	1.432613000	4.484537000	-1.821770000
15	-1.380039000	0.195801000	-0.206691000
6	-1.600109000	1.818685000	-0.812314000
7	-1.673845000	-1.136700000	-1.120588000
7	-1.944359000	-0.153333000	1.292584000
6	-1.617792000	2.068840000	2.452841000
1	-0.590845000	1.764521000	2.667242000
1	-1.601960000	2.744446000	1.595372000
1	-1.991815000	2.628571000	3.312840000
6	-3.914210000	1.244976000	1.792641000
1	-4.556726000	0.362892000	1.744573000
1	-4.347670000	1.946078000	2.509220000
1	-3.923085000	1.726534000	0.812574000
6	-2.641701000	-2.189822000	2.525987000
1	-3.447423000	-2.341238000	1.804511000
1	-2.296201000	-3.170130000	2.860563000
1	-3.057935000	-1.680397000	3.398848000
6	-0.364309000	-1.184069000	2.912632000
1	0.476616000	-0.663307000	2.444479000
1	-0.701175000	-0.603824000	3.775973000
1	0.002033000	-2.141755000	3.289298000
6	-3.124331000	-3.147099000	-1.023588000
1	-4.163752000	-3.466551000	-0.923389000
1	-2.712470000	-3.654563000	-1.898961000
1	-2.576386000	-3.489594000	-0.143799000
6	-3.805677000	-1.145532000	-2.389301000
1	-3.784104000	-0.054106000	-2.445763000
1	-3.368353000	-1.540767000	-3.309771000
1	-4.848685000	-1.467023000	-2.356184000
6	-2.689950000	2.728879000	-1.243272000
1	-2.906192000	3.522816000	-0.517466000
1	-2.461626000	3.213565000	-2.196434000
1	-3.621172000	2.177394000	-1.394574000

6	-2.509351000	0.862444000	2.209504000
6	-1.484150000	-1.421197000	1.919671000
1	-2.592082000	0.341072000	3.166810000
1	-1.073363000	-2.022313000	1.101037000
6	-3.064804000	-1.637854000	-1.160143000
1	-3.561042000	-1.209407000	-0.281795000
6	-0.762072000	-1.611005000	-2.193800000
1	-1.364880000	-2.330601000	-2.754761000
6	0.419126000	-2.352786000	-1.607503000
1	0.086526000	-3.183879000	-0.979818000
1	1.049392000	-2.757500000	-2.403047000
1	1.046821000	-1.692838000	-1.000877000
6	-0.337162000	-0.540467000	-3.183151000
1	-1.193364000	0.024283000	-3.558031000
1	0.377355000	0.158159000	-2.743710000
1	0.155709000	-1.017206000	-4.032776000
5	1.630028000	0.613306000	0.094504000
6	3.060613000	2.074247000	-1.503513000
1	3.300847000	3.078841000	-1.870752000
1	3.989489000	1.601909000	-1.177839000
1	2.669802000	1.484349000	-2.338124000
6	2.619402000	2.896865000	0.826342000
1	3.509464000	2.400453000	1.216020000
1	2.898446000	3.919904000	0.548162000
1	1.887895000	2.944486000	1.639906000
6	3.265068000	-0.847078000	1.138106000
6	2.878241000	-2.186188000	0.923599000
6	4.497942000	-0.432549000	0.593747000
6	3.481346000	-2.916481000	-0.072184000
1	2.023289000	-2.574976000	1.468045000
6	5.081229000	-1.172639000	-0.408778000
1	4.909268000	0.524121000	0.898388000
6	4.552970000	-2.401210000	-0.801598000
1	3.113951000	-3.915609000	-0.288731000
1	5.982196000	-0.797316000	-0.884994000
1	5.024431000	-2.984046000	-1.583067000
9	2.946258000	-0.315720000	2.360141000

**6TS<sup>C-F</sup> (TE= -1831.992915)**

6	0.227637000	-1.923573000	0.025124000
7	0.098156000	-0.543423000	0.282066000
7	1.513680000	-2.253045000	-0.138187000
6	1.846501000	-3.250601000	-1.139233000
1	1.729329000	-2.837269000	-2.146946000
1	2.872703000	-3.590714000	-1.010361000
1	1.178429000	-4.103399000	-1.018202000

15	-1.556081000	-0.758642000	0.028823000
6	-1.049233000	-2.427800000	-0.092493000
7	-2.483834000	-0.218584000	1.267330000
7	-2.040495000	-0.023346000	-1.348993000
6	-1.416503000	-1.580712000	-3.226686000
1	-0.489527000	-1.014429000	-3.334881000
1	-1.191456000	-2.485845000	-2.660722000
1	-1.752192000	-1.880064000	-4.222276000
6	-3.744221000	-1.553752000	-2.260520000
1	-4.550609000	-0.910125000	-1.900966000
1	-4.089600000	-2.063760000	-3.161950000
1	-3.557246000	-2.322344000	-1.504209000
6	-2.893804000	2.272037000	-1.847073000
1	-3.716054000	2.155159000	-1.139597000
1	-2.592659000	3.322037000	-1.839389000
1	-3.270725000	2.052182000	-2.849363000
6	-0.563589000	1.632422000	-2.482122000
1	0.319673000	1.049583000	-2.207342000
1	-0.867349000	1.379141000	-3.502130000
1	-0.267108000	2.683471000	-2.464609000
6	-3.996896000	1.696294000	1.668459000
1	-4.959665000	2.125715000	1.382647000
1	-3.970455000	1.653639000	2.760085000
1	-3.206639000	2.374021000	1.334380000
6	-4.919048000	-0.646421000	1.464135000
1	-4.794192000	-1.607801000	0.958327000
1	-4.917126000	-0.826310000	2.541958000
1	-5.901861000	-0.249020000	1.202175000
6	-1.641122000	-3.781682000	-0.187952000
1	-2.665649000	-3.782949000	0.195837000
1	-1.684111000	-4.181251000	-1.208778000
1	-1.080218000	-4.498130000	0.418668000
6	-2.494556000	-0.748578000	-2.551789000
6	-1.692676000	1.415835000	-1.493999000
1	-2.776765000	0.043552000	-3.251890000
1	-1.327228000	1.738206000	-0.510197000
6	-3.838144000	0.327933000	1.037318000
1	-3.923795000	0.448585000	-0.043234000
6	-2.121568000	-0.465241000	2.692738000
1	-3.041144000	-0.245254000	3.241005000
6	-1.058920000	0.489570000	3.194122000
1	-1.382552000	1.526008000	3.087465000
1	-0.871614000	0.304983000	4.254145000
1	-0.116374000	0.366436000	2.657098000
6	-1.775050000	-1.909382000	3.001351000
1	-2.528108000	-2.594954000	2.605935000

1	-0.802411000	-2.195325000	2.598108000
1	-1.733537000	-2.037602000	4.084727000
5	1.361245000	0.171468000	0.027801000
7	2.224419000	-0.973282000	-0.216626000
6	3.615137000	-1.033524000	-0.064797000
6	4.386585000	-0.028435000	-0.644916000
6	4.246541000	-2.046582000	0.649794000
6	5.758530000	-0.029852000	-0.492561000
1	3.882110000	0.749761000	-1.206606000
6	5.625659000	-2.047385000	0.781478000
1	3.650800000	-2.817368000	1.124842000
6	6.390043000	-1.041580000	0.217393000
1	6.343655000	0.763636000	-0.943797000
1	6.103462000	-2.840471000	1.345842000
1	7.467741000	-1.044095000	0.328000000
6	1.673431000	2.425950000	0.799847000
6	2.611277000	3.096535000	-0.012635000
6	0.398707000	3.013211000	0.932132000
6	2.208609000	4.120377000	-0.836579000
1	3.637440000	2.746143000	-0.013899000
6	0.016762000	4.047690000	0.103335000
1	-0.292705000	2.602536000	1.658583000
6	0.896449000	4.597866000	-0.821408000
1	2.939687000	4.582467000	-1.492915000
1	-0.990034000	4.448073000	0.197409000
1	0.594341000	5.417839000	-1.461099000
9	2.174845000	1.830224000	1.932620000

**7TSC<sup>C-F</sup> (TE= -930.130844)**

6	1.593767000	-2.456420000	-0.401038000
6	0.265835000	-2.544634000	-0.403847000
1	2.353498000	-3.173662000	-0.670555000
1	-0.319263000	-3.409529000	-0.685352000
6	3.131080000	-0.965525000	0.976184000
6	3.265966000	-0.549890000	-0.214781000
7	1.925244000	-1.140951000	0.085920000
7	-0.339248000	-1.377957000	0.060695000
5	0.625233000	-0.343118000	0.384261000
6	-1.740491000	-1.245105000	0.130528000
6	-2.572912000	-1.865624000	-0.793599000
6	-2.295350000	-0.435118000	1.113737000
6	-3.943014000	-1.677865000	-0.729568000
1	-2.147773000	-2.468042000	-1.588362000
6	-3.662528000	-0.242659000	1.163462000
1	-1.629598000	0.054192000	1.817292000
6	-4.494889000	-0.864923000	0.246052000

1	-4.581331000	-2.160657000	-1.460563000
1	-4.081065000	0.401553000	1.928282000
1	-5.566894000	-0.713870000	0.288920000
6	3.843114000	-0.006502000	-1.433484000
1	3.344042000	0.924126000	-1.708791000
1	4.908351000	0.172786000	-1.296094000
1	3.699511000	-0.710714000	-2.256166000
6	3.347585000	-1.324164000	2.366068000
1	4.372560000	-1.106294000	2.662445000
1	2.659447000	-0.763098000	3.002585000
1	3.152471000	-2.389302000	2.512022000
6	0.370369000	1.548777000	-0.652664000
6	-1.008846000	1.814164000	-0.788304000
6	1.186944000	2.589761000	-0.148110000
6	-1.568171000	2.853518000	-0.077075000
1	-1.626416000	1.124982000	-1.354230000
6	0.609745000	3.618052000	0.550366000
1	2.265722000	2.484997000	-0.195364000
6	-0.779820000	3.738376000	0.648729000
1	-2.645458000	2.986308000	-0.105862000
1	1.247579000	4.359614000	1.020889000
1	-1.226249000	4.556785000	1.199377000
9	0.922492000	0.808051000	-1.708223000

**9TSC<sup>C-F</sup> (TE= -1700.409789)**

6	0.123575000	2.049868000	0.829845000
7	-0.145788000	0.755905000	0.202454000
15	1.498633000	0.448185000	0.277871000
6	1.523026000	1.991874000	1.020724000
7	1.823823000	-0.954699000	1.095150000
7	2.191275000	0.217386000	-1.200271000
6	1.981435000	2.529442000	-2.187129000
1	0.996887000	2.244164000	-2.563761000
1	1.836067000	3.105578000	-1.272172000
1	2.456205000	3.177033000	-2.928100000
6	4.181484000	1.661247000	-1.308786000
1	4.831253000	0.784158000	-1.258320000
1	4.692395000	2.434611000	-1.886810000
1	4.043543000	2.042839000	-0.293705000
6	2.979261000	-1.724458000	-2.534476000
1	3.695097000	-1.984231000	-1.752248000
1	2.648412000	-2.649752000	-3.010769000
1	3.504561000	-1.140213000	-3.294643000
6	0.780582000	-0.629749000	-3.063095000
1	-0.107235000	-0.150847000	-2.638927000
1	1.213426000	0.032716000	-3.817473000

1	0.462156000	-1.540406000	-3.575863000
6	3.288680000	-2.956364000	0.983818000
1	4.329759000	-3.264433000	0.863853000
1	2.900297000	-3.465217000	1.869267000
1	2.726965000	-3.308995000	0.116478000
6	3.983134000	-0.931974000	2.313507000
1	3.978492000	0.161633000	2.333787000
1	3.551785000	-1.288680000	3.252701000
1	5.021529000	-1.268776000	2.277943000
6	2.470854000	2.923944000	1.671497000
1	3.382965000	2.410282000	1.990523000
1	2.787452000	3.758409000	1.029760000
1	2.031424000	3.365830000	2.571565000
6	2.852326000	1.307404000	-1.945279000
6	1.782356000	-0.976543000	-1.977721000
1	3.072025000	0.875538000	-2.926197000
1	1.274200000	-1.636293000	-1.263313000
6	3.215845000	-1.446583000	1.108936000
1	3.687551000	-1.023654000	0.217469000
6	0.945438000	-1.461558000	2.179116000
1	1.587423000	-2.130831000	2.759174000
6	-0.185554000	-2.292357000	1.611963000
1	0.197473000	-3.103656000	0.988574000
1	-0.780101000	-2.733218000	2.416156000
1	-0.858723000	-1.690151000	0.995432000
6	0.446077000	-0.409442000	3.154874000
1	1.262997000	0.207558000	3.535331000
1	-0.301674000	0.249192000	2.706813000
1	-0.025514000	-0.914298000	4.001153000
5	-1.484928000	0.544357000	-0.222315000
6	-1.041511000	2.717603000	0.954380000
1	-1.287825000	3.696196000	1.333004000
6	-3.426642000	1.808817000	1.069320000
6	-3.387119000	2.430405000	-0.040456000
7	-2.092776000	1.854550000	0.392954000
6	-3.830410000	1.186821000	2.318230000
1	-4.875862000	1.390030000	2.546387000
1	-3.680919000	0.103830000	2.244612000
1	-3.206944000	1.560299000	3.134755000
6	-3.767737000	3.191594000	-1.219143000
1	-3.624892000	2.571547000	-2.108069000
1	-4.808947000	3.505365000	-1.163151000
1	-3.132735000	4.075184000	-1.317299000
6	-2.970455000	-1.059917000	-1.195919000
6	-2.233888000	-2.234195000	-1.461151000
6	-4.080641000	-1.176327000	-0.333660000



6	-2.438535000	-3.366419000	-0.708087000
1	-1.456434000	-2.198731000	-2.216586000
6	-4.258987000	-2.316367000	0.420833000
1	-4.748600000	-0.328065000	-0.229868000
6	-3.426149000	-3.420962000	0.273925000
1	-1.817399000	-4.237708000	-0.894371000
1	-5.088546000	-2.356541000	1.121085000
1	-3.579031000	-4.317414000	0.861591000
9	-3.137069000	-0.200049000	-2.255730000

**IIIa-TS<sup>C-F</sup> (TE= -1340.688970)**

13	-0.000088000	-0.152275000	0.717365000
7	1.399797000	-1.397178000	0.245098000
7	-1.400015000	-1.397186000	0.245229000
6	1.249130000	-2.684584000	-0.039225000
6	-1.249369000	-2.684608000	-0.039069000
6	-0.000119000	-3.301642000	-0.117288000
1	-0.000115000	-4.366283000	-0.307966000
6	2.679687000	-0.781415000	0.184792000
6	3.287337000	-0.340566000	1.354003000
6	3.275461000	-0.510076000	-1.041371000
6	4.488324000	0.347229000	1.295731000
6	4.478447000	0.171264000	-1.094299000
6	5.088261000	0.601939000	0.073800000
1	4.954799000	0.688343000	2.212385000
1	4.934258000	0.380365000	-2.054994000
1	6.025634000	1.143436000	0.030119000
6	-2.679840000	-0.781318000	0.184895000
6	-3.275988000	-0.510706000	-1.041256000
6	-3.286999000	-0.339503000	1.353997000
6	-4.478855000	0.170824000	-1.094251000
6	-4.487853000	0.348519000	1.295651000
6	-5.088174000	0.602469000	0.073754000
1	-4.934952000	0.379339000	-2.054938000
1	-4.953929000	0.690390000	2.212226000
1	-6.025445000	1.144138000	0.030011000
6	-2.454789000	-3.537517000	-0.278155000
1	-2.195877000	-4.593668000	-0.233933000
1	-3.234854000	-3.327065000	0.455868000
1	-2.883956000	-3.335540000	-1.261998000
6	2.454536000	-3.537375000	-0.278764000
1	2.195844000	-4.593561000	-0.234080000
1	2.882980000	-3.335582000	-1.262968000
1	3.235072000	-3.326558000	0.454646000
1	-2.804815000	-0.537817000	2.305086000
1	-2.771817000	-0.819110000	-1.951104000

1	2.770924000	-0.817788000	-1.951256000
1	2.805423000	-0.539439000	2.305112000
6	0.000041000	1.985227000	-0.235808000
6	1.212500000	2.685183000	-0.257668000
6	-1.212185000	2.685566000	-0.257549000
6	1.196872000	4.053285000	-0.084688000
1	2.149249000	2.144696000	-0.342272000
6	-1.196143000	4.053659000	-0.084570000
1	-2.149081000	2.145343000	-0.342046000
6	0.000477000	4.752855000	0.022646000
1	2.141307000	4.585330000	-0.043161000
1	-2.140413000	4.585988000	-0.042954000
1	0.000652000	5.827259000	0.156297000
9	-0.000311000	0.747294000	-1.134218000

Cartesian coordinates of the transition states involved in the activation of C-H bond (*para*, *meta* and *ortho*) of C<sub>6</sub>H<sub>5</sub>F by **4-7** and **9**, along with their total energies (in hartrees) including zero point vibrational correction.

**4TSP<sup>(C-F)</sup>** (TE= -2044.791479)

6	0.381796000	-2.141863000	0.378924000
6	-1.696325000	-2.275838000	-0.527768000
7	0.134366000	-0.940623000	-0.307397000
7	-0.674070000	-2.933573000	0.296897000
6	-0.704638000	-4.299664000	0.740220000
1	-0.889106000	-4.970459000	-0.104994000
1	0.248407000	-4.566198000	1.197427000
1	-1.492236000	-4.460750000	1.484283000
15	-3.357755000	-2.451854000	-0.209494000
6	-3.896069000	-2.050328000	1.477602000
1	-4.963397000	-2.232743000	1.619786000
1	-3.332548000	-2.656299000	2.190274000
1	-3.673020000	-0.998436000	1.666892000
6	-4.042027000	-4.112123000	-0.458164000
1	-5.122359000	-4.105158000	-0.299262000
1	-3.824717000	-4.436149000	-1.476490000
1	-3.591951000	-4.820827000	0.238610000
6	-4.276614000	-1.374617000	-1.304302000
1	-5.344380000	-1.508122000	-1.116634000
1	-3.990543000	-0.329676000	-1.145877000
1	-4.047693000	-1.638788000	-2.336788000
15	1.656674000	-0.445612000	0.183547000
6	1.664659000	-2.016660000	0.924513000
7	2.637913000	-0.111943000	-1.093965000
7	1.742423000	0.860515000	1.178532000
6	-0.183411000	0.303279000	2.707900000

1	-0.855397000	0.817680000	2.016673000
1	-0.250924000	-0.770196000	2.514929000
1	-0.535348000	0.480774000	3.726843000
6	2.203033000	0.098289000	3.501082000
1	3.222205000	0.466454000	3.359143000
1	1.918037000	0.271745000	4.541363000
1	2.196035000	-0.978156000	3.329521000
6	3.032249000	2.961251000	1.380219000
1	3.953657000	2.374706000	1.416081000
1	3.248523000	3.906598000	0.877589000
1	2.741696000	3.200858000	2.406277000
6	0.647019000	3.007328000	0.558061000
1	-0.120914000	2.462582000	0.000211000
1	0.244024000	3.235360000	1.548683000
1	0.818677000	3.959890000	0.051611000
6	4.816123000	1.064138000	-1.350602000
1	5.840846000	1.081637000	-0.973934000
1	4.874564000	1.019807000	-2.440502000
1	4.336433000	2.004498000	-1.073763000
6	4.736779000	-1.438994000	-1.189036000
1	4.208695000	-2.292643000	-0.758361000
1	4.744973000	-1.552853000	-2.276087000
1	5.773989000	-1.464145000	-0.847828000
6	2.575663000	-2.906028000	1.685712000
1	2.141979000	-3.260931000	2.628953000
1	2.883416000	-3.793517000	1.120243000
1	3.493705000	-2.373549000	1.948132000
6	1.240782000	0.813020000	2.574594000
6	1.940891000	2.223204000	0.629601000
1	1.221776000	1.860366000	2.886077000
1	2.288258000	2.075709000	-0.393854000
6	4.080447000	-0.133843000	-0.778573000
1	4.145044000	-0.059644000	0.317597000
6	2.226047000	-0.159175000	-2.513875000
1	3.140708000	0.082920000	-3.064850000
6	1.209693000	0.922324000	-2.825208000
1	1.602754000	1.912989000	-2.581463000
1	0.962838000	0.908739000	-3.889123000
1	0.274601000	0.764742000	-2.275629000
6	1.771687000	-1.531485000	-2.984369000
1	2.493488000	-2.303740000	-2.711616000
1	0.801274000	-1.799792000	-2.563864000
1	1.671159000	-1.528981000	-4.072170000
5	-1.218227000	-0.880716000	-0.916596000
1	-2.000175000	0.486572000	-1.243329000
6	-2.559176000	1.755615000	-1.040794000

6	-2.905493000	2.004897000	0.283677000
6	-2.321655000	2.878566000	-1.832290000
6	-3.045306000	3.282741000	0.809730000
1	-3.054870000	1.153861000	0.957785000
6	-2.427270000	4.176703000	-1.342792000
1	-2.035495000	2.753544000	-2.877688000
6	-2.794958000	4.352170000	-0.025316000
1	-3.331223000	3.465093000	1.841350000
1	-2.232843000	5.048696000	-1.960051000
9	-2.902583000	5.603714000	0.464340000

**4TS<sup>m</sup>(C-F) (TE= -2044.794230)**

6	0.094735000	-2.173190000	0.239911000
6	-1.998784000	-1.957528000	-0.613389000
7	-0.005449000	-0.893578000	-0.333673000
7	-1.054708000	-2.814595000	0.115184000
6	-1.251492000	-4.202366000	0.429377000
1	-1.530023000	-4.760903000	-0.470121000
1	-0.333730000	-4.627816000	0.835467000
1	-2.043299000	-4.335351000	1.174315000
15	-3.666049000	-1.973992000	-0.279350000
6	-4.142352000	-1.699998000	1.451488000
1	-5.223175000	-1.773884000	1.589990000
1	-3.650628000	-2.440298000	2.086017000
1	-3.800261000	-0.707105000	1.749924000
6	-4.541458000	-3.507104000	-0.690713000
1	-5.612041000	-3.392349000	-0.509151000
1	-4.372318000	-3.740034000	-1.742561000
1	-4.171529000	-4.335199000	-0.084402000
6	-4.460672000	-0.685267000	-1.232164000
1	-5.533687000	-0.707485000	-1.029313000
1	-4.046223000	0.295921000	-0.976424000
1	-4.281606000	-0.867199000	-2.291696000
15	1.575336000	-0.643584000	0.158605000
6	1.389024000	-2.260691000	0.764598000
7	2.576378000	-0.333764000	-1.109728000
7	1.844855000	0.552029000	1.254180000
6	-0.110189000	0.128346000	2.789094000
1	-0.719368000	0.799177000	2.178620000
1	-0.330745000	-0.899904000	2.492099000
1	-0.411428000	0.244927000	3.832856000
6	2.239660000	-0.468213000	3.488172000
1	3.297413000	-0.235878000	3.340680000
1	2.006488000	-0.344751000	4.548287000
1	2.075207000	-1.514759000	3.231373000
6	3.382302000	2.461866000	1.580183000

1	4.225591000	1.767749000	1.543364000
1	3.701963000	3.411479000	1.145267000
1	3.144317000	2.651906000	2.629916000
6	1.002672000	2.857122000	0.840572000
1	0.158947000	2.449992000	0.275029000
1	0.658442000	3.057333000	1.858880000
1	1.272998000	3.817562000	0.395380000
6	4.882239000	0.579447000	-1.310732000
1	5.907575000	0.430517000	-0.966065000
1	4.913150000	0.630385000	-2.401484000
1	4.534527000	1.543289000	-0.935295000
6	4.489967000	-1.899430000	-1.357836000
1	3.865324000	-2.714842000	-0.986286000
1	4.469543000	-1.921728000	-2.450440000
1	5.520201000	-2.081242000	-1.044251000
6	2.188435000	-3.324355000	1.420368000
1	1.723524000	-3.708032000	2.337056000
1	2.374517000	-4.187175000	0.769882000
1	3.169415000	-2.938097000	1.709496000
6	1.367800000	0.449892000	2.656181000
6	2.193823000	1.922323000	0.808422000
1	1.500198000	1.458292000	3.056184000
1	2.498118000	1.819204000	-0.234156000
6	4.007877000	-0.562458000	-0.826129000
1	4.092366000	-0.591172000	0.270706000
6	2.150784000	-0.227069000	-2.522385000
1	3.086156000	-0.074764000	-3.070715000
6	1.290386000	1.001366000	-2.743055000
1	1.814432000	1.909381000	-2.433115000
1	1.040873000	1.099007000	-3.801901000
1	0.344722000	0.931127000	-2.193577000
6	1.509512000	-1.488198000	-3.079042000
1	2.116462000	-2.370231000	-2.865390000
1	0.510069000	-1.646768000	-2.670595000
1	1.412044000	-1.397782000	-4.163369000
5	-1.350631000	-0.605754000	-0.892701000
1	-2.003145000	0.861795000	-1.035323000
6	-2.410251000	2.134932000	-0.668023000
6	-2.713529000	2.289626000	0.684093000
6	-1.998582000	3.277963000	-1.351664000
6	-2.650452000	3.513329000	1.331644000
1	-2.996763000	1.405924000	1.264967000
6	-1.916321000	4.490638000	-0.698274000
1	-1.727921000	3.244143000	-2.407627000
6	-2.239715000	4.642811000	0.635161000
1	-2.913699000	3.602206000	2.382713000

1	-2.160742000	5.616447000	1.103761000
9	-1.502051000	5.580664000	-1.377908000

**4TS<sup>o</sup>(C-F)** (TE= -2044.798112)

6	0.010132000	-2.152367000	0.166025000
6	-2.100877000	-1.791778000	-0.589482000
7	-0.063966000	-0.825298000	-0.290642000
7	-1.167897000	-2.738545000	0.036337000
6	-1.411503000	-4.137655000	0.250996000
1	-1.735261000	-4.616168000	-0.678950000
1	-0.502066000	-4.627264000	0.599607000
1	-2.190210000	-4.294113000	1.005345000
15	-3.751004000	-1.752811000	-0.182621000
6	-4.143351000	-1.538091000	1.577960000
1	-5.218732000	-1.574114000	1.765446000
1	-3.653838000	-2.327354000	2.152942000
1	-3.743537000	-0.575809000	1.903807000
6	-4.710237000	-3.226312000	-0.623724000
1	-5.766677000	-3.074893000	-0.393341000
1	-4.592966000	-3.419429000	-1.690589000
1	-4.353956000	-4.095226000	-0.068695000
6	-4.536251000	-0.393522000	-1.045452000
1	-5.605536000	-0.404377000	-0.821909000
1	-4.095574000	0.558901000	-0.743900000
1	-4.381298000	-0.516784000	-2.117041000
15	1.547655000	-0.676614000	0.136620000
6	1.322569000	-2.330671000	0.618986000
7	2.492989000	-0.298681000	-1.155361000
7	1.925528000	0.410594000	1.311718000
6	0.020463000	-0.042122000	2.898753000
1	-0.576154000	0.707243000	2.372907000
1	-0.269243000	-1.029052000	2.529741000
1	-0.229007000	0.002276000	3.961559000
6	2.363461000	-0.812772000	3.433115000
1	3.424684000	-0.618466000	3.257638000
1	2.180884000	-0.770486000	4.509393000
1	2.135591000	-1.824151000	3.096060000
6	3.578808000	2.203759000	1.721923000
1	4.379771000	1.472282000	1.589334000
1	3.932562000	3.168510000	1.351347000
1	3.396450000	2.317141000	2.793662000
6	1.195221000	2.782646000	1.130041000
1	0.309717000	2.471534000	0.568022000
1	0.900134000	2.907054000	2.175781000
1	1.501219000	3.764012000	0.760623000
6	4.824534000	0.531419000	-1.419162000

1	5.856455000	0.319669000	-1.131866000
1	4.811835000	0.658884000	-2.503950000
1	4.532264000	1.478436000	-0.962694000
6	4.317012000	-1.914718000	-1.644709000
1	3.676384000	-2.732415000	-1.307203000
1	4.237258000	-1.842110000	-2.732403000
1	5.353293000	-2.164701000	-1.406763000
6	2.110370000	-3.475529000	1.137987000
1	1.679711000	-3.918710000	2.044533000
1	2.225625000	-4.286136000	0.408693000
1	3.120605000	-3.151784000	1.402465000
6	1.506639000	0.214563000	2.721797000
6	2.330424000	1.793661000	0.965145000
1	1.710409000	1.177974000	3.196279000
1	2.583275000	1.763886000	-0.095534000
6	3.925578000	-0.609092000	-0.977602000
1	4.069302000	-0.733854000	0.106461000
6	1.992153000	-0.035641000	-2.523113000
1	2.899765000	0.144936000	-3.108437000
6	1.161373000	1.231837000	-2.568038000
1	1.732846000	2.091288000	-2.207206000
1	0.849077000	1.441107000	-3.593191000
1	0.248703000	1.133988000	-1.969639000
6	1.276810000	-1.216203000	-3.160179000
1	1.866957000	-2.130876000	-3.077432000
1	0.301413000	-1.390276000	-2.702685000
1	1.112039000	-1.012601000	-4.220697000
5	-1.415808000	-0.440497000	-0.771893000
1	-1.915511000	1.143209000	-0.931347000
6	-2.184605000	2.417457000	-0.558072000
6	-2.429548000	2.498979000	0.806961000
6	-1.849103000	3.608731000	-1.157566000
6	-2.370496000	3.686638000	1.522108000
1	-2.645282000	1.565551000	1.340594000
6	-1.741737000	4.819509000	-0.496819000
6	-2.013687000	4.854954000	0.863283000
1	-2.585069000	3.707112000	2.586609000
1	-1.456314000	5.715697000	-1.039053000
9	-1.601402000	3.625478000	-2.494430000
1	-1.941593000	5.792448000	1.403695000

**5TS<sup>p(C-F)</sup> (TE= -1663.599852)**

6	-1.405495000	1.790259000	0.516126000
6	0.054167000	3.344236000	-0.424875000
7	-0.520280000	1.053495000	-0.312467000
7	-1.142579000	3.078857000	0.453454000
6	-1.848162000	4.091592000	1.193551000
1	-2.376592000	4.776111000	0.524551000
1	-2.578823000	3.627088000	1.855245000
1	-1.156872000	4.676328000	1.805878000
15	-1.318833000	-0.332222000	0.214478000
6	-2.226740000	0.851038000	1.115391000
7	-2.028767000	-1.155307000	-1.017471000
7	-0.457642000	-1.432815000	1.069187000
6	0.703103000	0.118169000	2.681726000
1	1.506881000	0.241956000	1.951780000
1	0.029888000	0.975412000	2.606623000
1	1.144557000	0.129638000	3.680591000
6	-1.169823000	-1.390310000	3.450398000
1	-1.680767000	-2.338270000	3.266028000
1	-0.784927000	-1.403147000	4.472537000
1	-1.901107000	-0.584438000	3.384326000
6	-0.077827000	-3.879944000	1.042347000
1	-1.155023000	-4.043970000	1.121749000
1	0.347156000	-4.692023000	0.448400000
1	0.352193000	-3.954570000	2.044272000
6	1.724848000	-2.302898000	0.259056000
1	1.929931000	-1.335566000	-0.207907000
1	2.229932000	-2.323270000	1.228563000
1	2.180231000	-3.079644000	-0.359155000
6	-2.905381000	-3.468088000	-1.278494000
1	-3.600485000	-4.188232000	-0.842110000
1	-3.129629000	-3.409705000	-2.345993000
1	-1.893933000	-3.860563000	-1.164646000
6	-4.468100000	-1.569351000	-0.776698000
1	-4.582963000	-0.611132000	-0.265095000
1	-4.705448000	-1.423570000	-1.833542000
1	-5.202126000	-2.267668000	-0.369277000
6	-3.413455000	0.917014000	2.005715000
1	-3.184586000	1.317171000	3.000003000
1	-4.215466000	1.532101000	1.584976000
1	-3.833251000	-0.079877000	2.160303000
6	-0.030575000	-1.192807000	2.472112000
6	0.236365000	-2.551528000	0.382469000
1	0.695171000	-1.986008000	2.666446000
1	-0.176733000	-2.574591000	-0.627717000
6	-3.066696000	-2.122564000	-0.596132000



1	-2.908215000	-2.280553000	0.480558000
6	-1.999890000	-0.756991000	-2.442974000
1	-2.664975000	-1.476649000	-2.930090000
6	-0.616845000	-0.946037000	-3.031159000
1	-0.286498000	-1.982033000	-2.921767000
1	-0.623619000	-0.701699000	-4.095581000
1	0.115563000	-0.285857000	-2.552617000
6	-2.569238000	0.624080000	-2.721715000
1	-3.541345000	0.758606000	-2.243423000
1	-1.899591000	1.413904000	-2.377274000
1	-2.699725000	0.751544000	-3.798429000
5	0.454209000	1.881731000	-1.006615000
1	1.847965000	1.525589000	-1.103670000
6	3.132077000	0.993632000	-0.670594000
6	3.815930000	0.923968000	0.537630000
6	3.553552000	0.150264000	-1.688508000
6	4.875271000	0.042624000	0.734021000
1	3.535043000	1.571379000	1.369837000
6	4.622610000	-0.724557000	-1.541067000
1	3.009841000	0.163460000	-2.637850000
6	5.257827000	-0.764642000	-0.317056000
1	5.408895000	-0.024255000	1.677158000
1	4.963254000	-1.374732000	-2.340923000
9	6.283359000	-1.619340000	-0.141842000
6	1.191294000	3.884474000	0.427527000
1	2.088674000	3.987989000	-0.185600000
1	0.956900000	4.866159000	0.854887000
1	1.430981000	3.198249000	1.246038000
6	-0.325948000	4.331397000	-1.511211000
1	-0.608481000	5.306682000	-1.097435000
1	0.525046000	4.484679000	-2.176992000
1	-1.158031000	3.958901000	-2.115603000

**5TS<sup>m(C-F)</sup> (TE= -1663.602360)**

6	-1.298189000	1.877187000	0.366757000
6	0.295176000	3.292982000	-0.573073000
7	-0.411545000	1.046351000	-0.366665000
7	-0.971321000	3.146314000	0.233649000
6	-1.586117000	4.215125000	0.977382000
1	-1.729723000	5.088799000	0.338688000
1	-2.562690000	3.900126000	1.344438000
1	-0.974189000	4.513277000	1.834611000
15	-1.311071000	-0.261579000	0.197875000
6	-2.196815000	1.021056000	0.977295000
7	-2.000745000	-1.120714000	-1.020359000

7	-0.556516000	-1.349812000	1.161696000
6	0.588714000	0.230810000	2.759714000
1	1.439896000	0.276742000	2.075982000
1	-0.033836000	1.114982000	2.602139000
1	0.971505000	0.273361000	3.781713000
6	-1.400431000	-1.141207000	3.489822000
1	-1.946904000	-2.073081000	3.326436000
1	-1.076501000	-1.113701000	4.532582000
1	-2.085039000	-0.306815000	3.336013000
6	-0.279332000	-3.809409000	1.283084000
1	-1.365170000	-3.924747000	1.316679000
1	0.137550000	-4.667856000	0.751914000
1	0.099062000	-3.849978000	2.307479000
6	1.625248000	-2.345877000	0.518434000
1	1.889297000	-1.411758000	0.016035000
1	2.079138000	-2.333717000	1.513053000
1	2.083149000	-3.167667000	-0.036844000
6	-2.969513000	-3.404262000	-1.196035000
1	-3.721116000	-4.065891000	-0.760614000
1	-3.133324000	-3.396811000	-2.276073000
1	-1.985852000	-3.835435000	-1.004701000
6	-4.465426000	-1.413637000	-0.880036000
1	-4.558631000	-0.422150000	-0.431509000
1	-4.646988000	-1.322154000	-1.953809000
1	-5.249419000	-2.052784000	-0.468662000
6	-3.426499000	1.203648000	1.789679000
1	-3.234951000	1.687584000	2.753963000
1	-4.184423000	1.799899000	1.271317000
1	-3.887927000	0.238039000	2.009770000
6	-0.198134000	-1.052577000	2.573082000
6	0.123919000	-2.531822000	0.573559000
1	0.473775000	-1.867728000	2.851747000
1	-0.236912000	-2.593594000	-0.455055000
6	-3.101508000	-2.015946000	-0.598514000
1	-3.002713000	-2.117520000	0.491959000
6	-1.888699000	-0.802963000	-2.462223000
1	-2.570011000	-1.512810000	-2.941150000
6	-0.493694000	-1.094991000	-2.974930000
1	-0.224683000	-2.139023000	-2.796146000
1	-0.441039000	-0.909249000	-4.049820000
1	0.251694000	-0.448675000	-2.497552000
6	-2.370157000	0.588124000	-2.839563000

1	-3.347484000	0.804307000	-2.403696000
1	-1.668198000	1.359516000	-2.518748000
1	-2.459410000	0.658083000	-3.925705000
5	0.648316000	1.778085000	-1.041664000
1	2.045300000	1.376506000	-1.043603000
6	3.271062000	0.846311000	-0.478158000
6	3.822742000	0.889962000	0.798712000
6	3.712321000	-0.146298000	-1.341926000
6	4.784144000	-0.027357000	1.205330000
1	3.506246000	1.655871000	1.508151000
6	4.679620000	-1.040932000	-0.937301000
1	3.276721000	-0.245943000	-2.339742000
6	5.225906000	-1.009990000	0.330511000
1	5.200090000	0.015647000	2.208640000
6	1.399629000	3.830433000	0.322249000
1	2.341830000	3.844366000	-0.228850000
1	1.189799000	4.849814000	0.666209000
1	1.543156000	3.191885000	1.200468000
6	0.043877000	4.223805000	-1.743347000
1	-0.224970000	5.234666000	-1.415007000
1	0.950073000	4.300145000	-2.346826000
1	-0.754407000	3.846645000	-2.388424000
1	5.974181000	-1.740611000	0.613889000
9	5.102729000	-1.996156000	-1.789544000

**5TS<sup>o</sup>(C-F)** (TE= -1663.608242)

6	-1.732641000	1.616472000	0.286351000
6	-0.392895000	3.400209000	-0.387815000
7	-0.524801000	1.055142000	-0.202782000
7	-1.720644000	2.927110000	0.153804000
6	-2.764560000	3.796509000	0.630287000
1	-2.996293000	4.558393000	-0.116943000
1	-3.670798000	3.220725000	0.818017000
1	-2.477465000	4.301412000	1.557593000
15	-1.164752000	-0.456563000	0.189637000
6	-2.482103000	0.546758000	0.741632000
7	-1.377694000	-1.397989000	-1.137086000
7	-0.386052000	-1.369026000	1.304099000
6	0.258819000	0.423828000	2.945896000
1	1.196723000	0.561619000	2.402683000
1	-0.444156000	1.196248000	2.624365000
1	0.451779000	0.576871000	4.009892000
6	-1.610260000	-1.182340000	3.469375000

1	-2.028774000	-2.166793000	3.246332000
1	-1.442328000	-1.118679000	4.546709000
1	-2.347161000	-0.423617000	3.205301000
6	0.141580000	-3.764976000	1.627375000
1	-0.912978000	-4.012395000	1.483620000
1	0.740733000	-4.589312000	1.234447000
1	0.334306000	-3.709640000	2.701766000
6	1.974821000	-2.122419000	1.080265000
1	2.223263000	-1.206675000	0.537291000
1	2.250921000	-1.980523000	2.128756000
1	2.599963000	-2.926976000	0.686523000
6	-1.927263000	-3.806916000	-1.456532000
1	-2.655007000	-4.571809000	-1.178352000
1	-1.828946000	-3.836819000	-2.543847000
1	-0.965202000	-4.079391000	-1.020412000
6	-3.723820000	-2.066859000	-1.619683000
1	-4.072274000	-1.096799000	-1.258986000
1	-3.630679000	-2.015403000	-2.707341000
1	-4.485576000	-2.814961000	-1.390300000
6	-3.855542000	0.384062000	1.282991000
1	-4.020932000	0.962105000	2.198201000
1	-4.630020000	0.680477000	0.567735000
1	-4.045739000	-0.661730000	1.536015000
6	-0.303307000	-0.968183000	2.733003000
6	0.514589000	-2.482261000	0.910260000
1	0.421095000	-1.664959000	3.160844000
1	0.339760000	-2.633127000	-0.155701000
6	-2.405105000	-2.449672000	-0.974211000
1	-2.576347000	-2.531416000	0.110065000
6	-0.903005000	-1.080409000	-2.503090000
1	-1.230557000	-1.935985000	-3.102125000
6	0.609527000	-1.036181000	-2.558420000
1	1.045702000	-1.986951000	-2.241239000
1	0.946187000	-0.836782000	-3.577480000
1	1.019403000	-0.240027000	-1.929620000
6	-1.540663000	0.158813000	-3.109235000
1	-2.626627000	0.145448000	-3.001028000
1	-1.158182000	1.071135000	-2.648495000
1	-1.304770000	0.205924000	-4.174450000
5	0.442619000	2.030217000	-0.658297000
1	1.933315000	1.508057000	-0.962623000
6	3.167575000	0.910504000	-0.653024000

6	3.449983000	1.241112000	0.665563000
6	4.016201000	-0.017227000	-1.208459000
6	4.502397000	0.688796000	1.383904000
1	2.788303000	1.965806000	1.155919000
6	5.071110000	-0.618297000	-0.545195000
6	5.313734000	-0.255337000	0.772110000
1	4.690949000	0.982827000	2.412276000
6	0.295676000	4.257100000	0.660434000
1	1.283694000	4.550822000	0.301109000
1	-0.270109000	5.170754000	0.876605000
1	0.433899000	3.706560000	1.596495000
6	-0.617868000	4.186910000	-1.665371000
1	-1.201322000	5.097897000	-1.488740000
1	0.345752000	4.483779000	-2.082788000
1	-1.136280000	3.587181000	-2.418663000
1	6.136417000	-0.709575000	1.313563000
1	5.689319000	-1.353558000	-1.051060000
9	3.827053000	-0.399911000	-2.501771000

**6TS<sup>p(C-F)</sup> (TE= -1831.987262)**

6	-0.011149000	1.557895000	1.008809000
7	-0.104727000	0.815106000	-0.179943000
7	1.244133000	1.995099000	1.200992000
6	1.797834000	1.908427000	2.544419000
1	2.675405000	2.544783000	2.640129000
1	1.041511000	2.243972000	3.253648000
1	2.080721000	0.874812000	2.771466000
15	-1.713003000	0.545530000	0.229074000
6	-1.253254000	1.536439000	1.599782000
7	-2.704643000	1.112162000	-0.943663000
7	-2.158980000	-0.991941000	0.537491000
6	-0.630003000	-1.556712000	2.468941000
1	0.135842000	-1.824129000	1.736283000
1	-0.410923000	-0.557890000	2.851860000
1	-0.555857000	-2.257098000	3.303458000
6	-3.107267000	-1.176123000	2.811768000
1	-4.096341000	-1.357907000	2.385716000
1	-3.039384000	-1.713936000	3.759809000
1	-3.020498000	-0.109896000	3.029713000
6	-3.706650000	-2.654726000	-0.460614000
1	-4.543000000	-1.972640000	-0.291616000
1	-3.908610000	-3.220078000	-1.372619000
1	-3.679138000	-3.372551000	0.362747000

6	-1.218453000	-2.830585000	-0.833486000
1	-0.288606000	-2.269094000	-0.956664000
1	-1.083832000	-3.530497000	-0.004262000
1	-1.374088000	-3.423797000	-1.736917000
6	-4.980916000	0.544330000	-1.757459000
1	-6.018363000	0.434844000	-1.435240000
1	-4.981196000	1.201093000	-2.630455000
1	-4.616107000	-0.435730000	-2.069393000
6	-4.631612000	2.486834000	-0.198243000
1	-4.043281000	2.866198000	0.640703000
1	-4.560836000	3.208125000	-1.016129000
1	-5.678193000	2.440473000	0.109091000
6	-1.830343000	2.169659000	2.808627000
1	-1.608381000	1.623179000	3.733675000
1	-1.456347000	3.189259000	2.936244000
1	-2.918382000	2.239686000	2.735363000
6	-2.019754000	-1.640932000	1.866276000
6	-2.396579000	-1.907458000	-0.611111000
1	-2.200888000	-2.698878000	1.662157000
1	-2.481303000	-1.260615000	-1.489039000
6	-4.150598000	1.112450000	-0.622764000
1	-4.265696000	0.440121000	0.237475000
6	-2.268580000	1.937690000	-2.099105000
1	-3.207973000	2.284075000	-2.539258000
6	-1.567430000	1.090696000	-3.140846000
1	-2.210347000	0.271760000	-3.471626000
1	-1.319201000	1.700424000	-4.012207000
1	-0.631865000	0.670655000	-2.757457000
6	-1.482117000	3.182989000	-1.728824000
1	-1.974794000	3.742624000	-0.931193000
1	-0.464458000	2.947680000	-1.413761000
1	-1.410024000	3.832494000	-2.603457000
5	1.217078000	0.628627000	-0.795501000
1	1.809983000	-0.557161000	-1.362908000
6	2.314879000	-1.949944000	-1.073826000
6	2.483059000	-2.215083000	0.282099000
6	2.181542000	-3.060130000	-1.905733000
6	2.531608000	-3.503676000	0.803990000
1	2.576580000	-1.377544000	0.981508000
6	2.217032000	-4.365117000	-1.425569000
1	2.034723000	-2.922884000	-2.977544000
6	2.392451000	-4.559815000	-0.071152000

1	2.671694000	-3.701128000	1.862634000
1	2.113138000	-5.227291000	-2.077323000
9	2.424875000	-5.817783000	0.410343000
7	2.025382000	1.406467000	0.137822000
6	3.308665000	1.923167000	-0.071771000
6	4.239160000	1.112281000	-0.721024000
6	3.672460000	3.208354000	0.316982000
6	5.508890000	1.591045000	-0.973772000
1	3.946167000	0.107733000	-1.016073000
6	4.955082000	3.670198000	0.067425000
1	2.942223000	3.855704000	0.788453000
6	5.879921000	2.868846000	-0.577188000
1	6.223403000	0.951812000	-1.480117000
1	5.225656000	4.674547000	0.373884000
1	6.881229000	3.234399000	-0.771137000

**6TS<sup>m(C-F)</sup> (TE= -1831.989890)**

6	-0.091723000	-1.666624000	0.886747000
7	0.020885000	-0.780470000	-0.197901000
7	-1.368628000	-2.046933000	1.062583000
6	-1.881320000	-2.084452000	2.424836000
1	-2.803128000	-2.660928000	2.471937000
1	-1.136508000	-2.559574000	3.062937000
1	-2.077728000	-1.067854000	2.782875000
15	1.652999000	-0.666516000	0.190400000
6	1.162680000	-1.798466000	1.435504000
7	2.575903000	-1.142741000	-1.074168000
7	2.210367000	0.784607000	0.682647000
6	0.746228000	1.178771000	2.706950000
1	-0.018634000	1.568817000	2.030567000
1	0.483524000	0.153351000	2.974728000
1	0.723819000	1.777423000	3.620036000
6	3.203250000	0.632675000	2.940893000
1	4.193699000	0.808918000	2.515922000
1	3.183058000	1.054858000	3.947897000
1	3.058075000	-0.445455000	3.031915000
6	3.838595000	2.480258000	-0.115941000
1	4.639641000	1.741995000	-0.036869000
1	4.066407000	3.139801000	-0.955721000
1	3.849923000	3.095026000	0.787207000
6	1.361076000	2.824571000	-0.438882000
1	0.404920000	2.327773000	-0.621107000
1	1.260636000	3.420672000	0.472306000

1	1.541074000	3.518321000	-1.262899000
6	4.895816000	-0.654721000	-1.810175000
1	5.940545000	-0.711040000	-1.498190000
1	4.822571000	-1.141496000	-2.785455000
1	4.633563000	0.397030000	-1.935148000
6	4.368648000	-2.793802000	-0.597658000
1	3.740618000	-3.259583000	0.165387000
1	4.246242000	-3.354309000	-1.527753000
1	5.411892000	-2.891686000	-0.291064000
6	1.726631000	-2.610824000	2.538948000
1	1.548717000	-2.178005000	3.531233000
1	1.302960000	-3.618919000	2.544240000
1	2.808339000	-2.723079000	2.432206000
6	2.127238000	1.267508000	2.085446000
6	2.492079000	1.823891000	-0.344794000
1	2.360236000	2.332259000	2.010572000
1	2.542169000	1.288008000	-1.296793000
6	4.014913000	-1.329500000	-0.776966000
1	4.189704000	-0.827322000	0.184225000
6	2.058607000	-1.742420000	-2.330291000
1	2.962091000	-2.077514000	-2.847829000
6	1.399921000	-0.697043000	-3.206217000
1	2.092809000	0.118235000	-3.427178000
1	1.091512000	-1.145442000	-4.152995000
1	0.503744000	-0.280361000	-2.735129000
6	1.190629000	-2.973195000	-2.133045000
1	1.654073000	-3.680471000	-1.442518000
1	0.197937000	-2.719295000	-1.758411000
1	1.057660000	-3.475098000	-3.093535000
5	-1.299998000	-0.436756000	-0.741909000
1	-1.848498000	0.850390000	-1.143773000
6	-2.232736000	2.213476000	-0.688381000
6	-2.336119000	2.332833000	0.696943000
6	-1.974552000	3.381229000	-1.403184000
6	-2.206928000	3.549117000	1.352867000
1	-2.517596000	1.434524000	1.295440000
6	-1.835522000	4.586138000	-0.744767000
1	-1.863919000	3.378120000	-2.487711000
6	-1.945885000	4.702633000	0.626661000
1	-2.303631000	3.610653000	2.434090000
7	-2.134235000	-1.279963000	0.106900000
6	-3.452840000	-1.685758000	-0.126109000



6	-4.341022000	-0.746765000	-0.650298000
6	-3.893191000	-2.982415000	0.119631000
6	-5.644211000	-1.111114000	-0.922265000
1	-3.990503000	0.265658000	-0.834413000
6	-5.208206000	-3.329426000	-0.146816000
1	-3.198314000	-3.725969000	0.492120000
6	-6.090868000	-2.400886000	-0.667856000
1	-6.324727000	-0.372492000	-1.330708000
1	-5.538120000	-4.343896000	0.047685000
1	-7.117682000	-2.677083000	-0.875673000
1	-1.829802000	5.671100000	1.098337000
9	-1.573124000	5.701833000	-1.456613000

**6TS<sup>o</sup>(C-F)** (TE= -1831.994624)

6	-0.167548000	-1.336279000	1.075582000
7	0.024526000	-0.681312000	-0.152235000
7	-1.456767000	-1.673845000	1.236024000
6	-2.045096000	-1.494205000	2.554996000
1	-3.000676000	-2.010969000	2.618953000
1	-1.367561000	-1.916769000	3.296635000
1	-2.199190000	-0.429978000	2.763468000
15	1.642171000	-0.549398000	0.279653000
6	1.048281000	-1.352896000	1.719754000
7	2.584368000	-1.366436000	-0.782313000
7	2.273731000	0.945661000	0.431174000
6	0.620038000	1.957613000	2.047106000
1	-0.011129000	2.230638000	1.198610000
1	0.218851000	1.044100000	2.494120000
1	0.539454000	2.753557000	2.790691000
6	2.967166000	1.351503000	2.768788000
1	4.010180000	1.311322000	2.446553000
1	2.893118000	2.051599000	3.603585000
1	2.683796000	0.364960000	3.139869000
6	4.064804000	2.329840000	-0.586259000
1	4.804903000	1.631669000	-0.187916000
1	4.433112000	2.705765000	-1.543009000
1	4.000770000	3.184622000	0.090935000
6	1.657953000	2.593855000	-1.312908000
1	0.720953000	2.060871000	-1.493736000
1	1.449583000	3.408402000	-0.613355000
1	1.975843000	3.043730000	-2.255485000
6	4.974518000	-1.207702000	-1.438923000
1	5.993058000	-1.279716000	-1.052510000

1	4.904140000	-1.883613000	-2.294302000
1	4.818714000	-0.188935000	-1.797378000
6	4.212933000	-2.982511000	0.170169000
1	3.503657000	-3.228899000	0.963637000
1	4.107258000	-3.726044000	-0.623724000
1	5.223846000	-3.074290000	0.572097000
6	1.543725000	-1.951270000	2.982412000
1	1.262018000	-1.372823000	3.870358000
1	1.165264000	-2.968136000	3.122333000
1	2.634338000	-2.016626000	2.982068000
6	2.069254000	1.795934000	1.634066000
6	2.724983000	1.654544000	-0.796538000
1	2.411148000	2.784765000	1.319307000
1	2.867234000	0.873592000	-1.547207000
6	3.985426000	-1.575459000	-0.349666000
1	4.147389000	-0.881997000	0.487555000
6	2.083755000	-2.202054000	-1.901849000
1	2.984865000	-2.692708000	-2.281408000
6	1.531673000	-1.344910000	-3.021677000
1	2.282082000	-0.632816000	-3.373200000
1	1.240785000	-1.975165000	-3.864661000
1	0.641904000	-0.791471000	-2.705225000
6	1.126645000	-3.307987000	-1.489757000
1	1.504942000	-3.863923000	-0.629716000
1	0.135162000	-2.922095000	-1.247048000
1	1.009108000	-4.007580000	-2.319840000
5	-1.259264000	-0.375298000	-0.801305000
1	-1.720443000	0.937180000	-1.267150000
6	-2.099510000	2.264798000	-0.754132000
6	-2.627357000	2.304231000	0.533333000
6	-1.640918000	3.470497000	-1.230098000
6	-2.700818000	3.472369000	1.282283000
1	-2.991613000	1.376631000	0.981318000
6	-1.666414000	4.659993000	-0.524593000
6	-2.208283000	4.655111000	0.752454000
1	-3.132445000	3.462320000	2.278543000
1	-1.278815000	5.569703000	-0.972552000
7	-2.157596000	-1.069710000	0.124898000
6	-3.447615000	-1.540680000	-0.137535000
6	-4.304376000	-0.732171000	-0.885403000
6	-3.892959000	-2.786111000	0.295655000
6	-5.577569000	-1.170532000	-1.187787000

1	-3.952519000	0.238005000	-1.220554000
6	-5.177867000	-3.208122000	-0.006573000
1	-3.221789000	-3.436340000	0.844247000
6	-6.028153000	-2.407564000	-0.747150000
1	-6.231307000	-0.531365000	-1.770449000
1	-5.509055000	-4.182233000	0.335976000
1	-7.031621000	-2.741799000	-0.981720000
1	-2.247798000	5.574760000	1.325599000
9	-1.116180000	3.525115000	-2.483326000

**7TS<sup>p(C-F)</sup> (TE= -930.126443)**

6	-0.287835000	2.213749000	-1.439893000
6	-1.346027000	1.405321000	-1.455521000
1	0.133403000	2.844051000	-2.207295000
1	-2.002211000	1.248873000	-2.299276000
6	1.776755000	2.416380000	0.015046000
6	0.990047000	3.298801000	0.478967000
7	0.321666000	2.103197000	-0.138662000
7	-1.531097000	0.741520000	-0.249259000
5	-0.499208000	1.107435000	0.727851000
6	-2.563159000	-0.188576000	-0.045388000
6	-3.675621000	-0.260622000	-0.879336000
6	-2.472280000	-1.066722000	1.033585000
6	-4.667841000	-1.196061000	-0.642418000
1	-3.787546000	0.425888000	-1.709714000
6	-3.470884000	-1.993863000	1.262847000
1	-1.605755000	-1.017013000	1.680958000
6	-4.574102000	-2.069071000	0.427698000
1	-5.527540000	-1.233621000	-1.301839000
1	-3.379975000	-2.671071000	2.104429000
1	-5.353559000	-2.798952000	0.610240000
6	0.427411000	4.482521000	1.103049000
1	-0.187076000	4.187119000	1.956976000
1	1.216628000	5.152066000	1.440994000
1	-0.211898000	5.013706000	0.393662000
6	2.976914000	1.720727000	-0.421851000
1	3.852474000	2.347247000	-0.258361000
1	3.094883000	0.778711000	0.119450000
1	2.898790000	1.483095000	-1.485906000
6	1.071951000	-0.909946000	0.759137000
6	2.198434000	-1.177609000	1.521702000
6	1.023328000	-1.383791000	-0.541700000
6	3.254349000	-1.926478000	1.015086000

1	2.271625000	-0.795411000	2.539535000
6	2.069156000	-2.123906000	-1.081515000
1	0.151391000	-1.184092000	-1.166645000
6	3.166559000	-2.380496000	-0.285652000
1	4.134906000	-2.161566000	1.603781000
1	2.046547000	-2.505153000	-2.096991000
1	0.186895000	0.123522000	1.344782000
9	4.183017000	-3.094415000	-0.792851000

**7TS<sup>m(C-F)</sup> (TE= -930.128150)**

6	0.415129000	2.347994000	1.286467000
6	1.492074000	1.565016000	1.291423000
1	0.056213000	3.064923000	2.008131000
1	2.237493000	1.522486000	2.072420000
6	-1.795570000	2.321012000	0.044926000
6	-1.090695000	3.151452000	-0.607058000
7	-0.320606000	2.058993000	0.081931000
7	1.566779000	0.753732000	0.164567000
5	0.433698000	0.973835000	-0.734078000
6	2.609769000	-0.167549000	-0.034266000
6	3.838840000	-0.039552000	0.605054000
6	2.408120000	-1.234555000	-0.907275000
6	4.841948000	-0.966802000	0.381666000
1	4.029750000	0.798586000	1.264680000
6	3.418093000	-2.152167000	-1.125905000
1	1.446864000	-1.343918000	-1.395100000
6	4.639862000	-2.028095000	-0.483557000
1	5.794668000	-0.848723000	0.885261000
1	3.242870000	-2.979699000	-1.803831000
1	5.427871000	-2.750803000	-0.657933000
6	-0.637214000	4.256861000	-1.431684000
1	-0.116751000	3.868476000	-2.310483000
1	-1.479764000	4.867189000	-1.752646000
1	0.063073000	4.881490000	-0.871927000
6	-2.919158000	1.658287000	0.686895000
1	-3.827061000	2.242918000	0.546446000
1	-3.061364000	0.656951000	0.272664000
1	-2.722004000	1.549957000	1.756386000
6	-1.126199000	-1.086031000	-0.434874000
6	-2.316043000	-1.425800000	-1.062309000
6	-0.961470000	-1.396918000	0.907254000
6	-3.293275000	-2.090189000	-0.347181000
1	-2.504024000	-1.185310000	-2.108069000

6	-1.958222000	-2.054604000	1.616989000
1	-0.037124000	-1.128219000	1.420544000
6	-3.143014000	-2.408200000	0.988683000
1	-1.819468000	-2.298566000	2.666130000
1	-0.295411000	-0.096415000	-1.163145000
1	-3.939829000	-2.924062000	1.510652000
9	-4.436174000	-2.439608000	-0.960753000

**7TS<sup>o</sup>(C-F)** (TE= -930.131475)

6	-0.110048000	2.373609000	-1.310447000
6	-1.272444000	1.725117000	-1.303776000
1	0.308688000	3.073105000	-2.016909000
1	-2.043237000	1.797061000	-2.057558000
6	2.121898000	1.998961000	-0.159710000
6	1.565279000	2.894046000	0.546112000
7	0.619996000	1.948423000	-0.144532000
7	-1.403211000	0.884401000	-0.200360000
5	-0.230284000	0.933968000	0.662533000
6	-2.547587000	0.089800000	0.008578000
6	-3.780506000	0.420337000	-0.542694000
6	-2.439957000	-1.051296000	0.799518000
6	-4.884026000	-0.384302000	-0.315307000
1	-3.892720000	1.320878000	-1.134994000
6	-3.548909000	-1.844639000	1.023871000
1	-1.476012000	-1.317695000	1.218189000
6	-4.776565000	-1.520046000	0.467897000
1	-5.838791000	-0.110621000	-0.749635000
1	-3.448179000	-2.732992000	1.636727000
1	-5.642319000	-2.146581000	0.645791000
6	1.307387000	4.017293000	1.428972000
1	0.773390000	3.669747000	2.316585000
1	2.241889000	4.486713000	1.732032000
1	0.682741000	4.758567000	0.925210000
6	3.111752000	1.203440000	-0.866860000
1	4.095295000	1.660519000	-0.769462000
1	3.142299000	0.184681000	-0.471790000
1	2.846320000	1.139595000	-1.924970000
6	1.117021000	-1.354587000	0.398345000
6	2.305674000	-1.833570000	0.897250000
6	0.865816000	-1.621475000	-0.941589000
6	3.220665000	-2.560757000	0.158271000
6	1.750509000	-2.349792000	-1.728423000
1	-0.054138000	-1.248078000	-1.396744000
6	2.932519000	-2.817579000	-1.174800000
1	1.522085000	-2.552926000	-2.769708000

1	0.419470000	-0.267219000	1.063906000
1	3.633159000	-3.385488000	-1.776301000
9	2.622049000	-1.579632000	2.188854000
1	4.134683000	-2.919552000	0.620267000

**9TS<sup>p(C-F)</sup> (TE= -1700.402680)**

6	-0.377733000	1.489170000	1.369883000
7	-0.187887000	0.921724000	0.038842000
15	-1.450340000	-0.127296000	0.380899000
6	-1.439039000	0.709250000	1.876680000
7	-2.673426000	0.023930000	-0.732121000
7	-1.075140000	-1.729199000	0.334335000
6	0.465760000	-1.948632000	2.315026000
1	1.316691000	-1.785249000	1.650712000
1	0.226522000	-0.999756000	2.798599000
1	0.766605000	-2.662312000	3.085780000
6	-1.937528000	-2.720870000	2.422032000
1	-2.726980000	-3.235778000	1.869115000
1	-1.678000000	-3.329372000	3.291226000
1	-2.340494000	-1.773920000	2.789068000
6	-1.531977000	-3.629870000	-1.207181000
1	-2.608248000	-3.479702000	-1.106211000
1	-1.336363000	-3.998068000	-2.216556000
1	-1.232510000	-4.419956000	-0.513652000
6	0.740273000	-2.570524000	-1.133953000
1	1.299449000	-1.645703000	-0.978243000
1	1.119615000	-3.320672000	-0.434146000
1	0.956024000	-2.929043000	-2.142898000
6	-4.325476000	-1.358102000	-1.970403000
1	-5.072612000	-2.143626000	-1.836090000
1	-4.802195000	-0.551599000	-2.532658000
1	-3.513051000	-1.761740000	-2.577957000
6	-4.934367000	-0.313580000	0.238343000
1	-4.562494000	-0.058788000	1.234803000
1	-5.357383000	0.591282000	-0.206256000
1	-5.746032000	-1.035687000	0.351283000
6	-2.206270000	0.811688000	3.138410000
1	-1.751189000	0.273093000	3.981342000
1	-2.304525000	1.857658000	3.446968000
1	-3.223342000	0.422478000	3.029305000
6	-0.720555000	-2.500127000	1.545459000
6	-0.750584000	-2.349934000	-0.971841000
1	-0.419378000	-3.480824000	1.166163000

1	-1.060833000	-1.620503000	-1.729167000
6	-3.822851000	-0.897019000	-0.615473000
1	-3.442798000	-1.779227000	-0.093608000
6	-2.932792000	1.278545000	-1.478037000
1	-3.974595000	1.192932000	-1.800351000
6	-2.081490000	1.353304000	-2.729998000
1	-2.234278000	0.470107000	-3.354554000
1	-2.348794000	2.236363000	-3.316365000
1	-1.016109000	1.419950000	-2.485659000
6	-2.858199000	2.551158000	-0.650904000
1	-3.471449000	2.479267000	0.249993000
1	-1.837091000	2.790736000	-0.347173000
1	-3.229532000	3.384731000	-1.251896000
5	0.834896000	1.558891000	-0.728960000
6	0.472623000	2.523977000	1.540870000
1	0.650447000	3.189338000	2.369971000
6	1.520783000	4.047419000	-0.221999000
6	2.509822000	3.426882000	0.287216000
7	1.235357000	2.673544000	0.298643000
6	0.647818000	5.046174000	-0.815030000
1	1.180938000	5.976185000	-1.006784000
1	0.233614000	4.667383000	-1.753780000
1	-0.187374000	5.249209000	-0.138673000
6	3.841174000	3.156074000	0.812319000
1	4.278293000	2.297754000	0.296887000
1	4.483601000	4.026667000	0.688322000
1	3.776631000	2.910873000	1.875695000
1	1.976588000	1.032040000	-1.304458000
6	3.137050000	0.176418000	-0.895180000
6	3.748581000	-0.552624000	-1.908862000
6	3.292707000	-0.291449000	0.405308000
6	4.506790000	-1.688580000	-1.649408000
1	3.629076000	-0.244729000	-2.947500000
6	4.042136000	-1.424493000	0.702676000
1	2.803642000	0.224782000	1.235082000
6	4.637155000	-2.102678000	-0.340014000
1	4.990799000	-2.255954000	-2.437943000
1	4.163473000	-1.790318000	1.717557000
9	5.361231000	-3.203864000	-0.073055000

**9TS<sup>m(C-F)</sup>** (TE= -1700.404645)

6	-0.441034000	1.639353000	1.288048000
7	-0.156142000	0.931415000	0.043926000
15	-1.497082000	-0.026406000	0.361221000
6	-1.588292000	0.963758000	1.757105000
7	-2.595901000	0.052302000	-0.880366000
7	-1.205875000	-1.638668000	0.520395000
6	0.201605000	-1.676755000	2.610400000
1	1.098840000	-1.618387000	1.990794000
1	-0.031480000	-0.671491000	2.966481000
1	0.424918000	-2.305092000	3.476013000
6	-2.227917000	-2.371227000	2.644087000
1	-3.002561000	-2.908350000	2.091534000
1	-2.045879000	-2.903428000	3.580484000
1	-2.612583000	-1.380461000	2.895683000
6	-1.656888000	-3.699439000	-0.798629000
1	-2.729756000	-3.502393000	-0.757154000
1	-1.439406000	-4.187467000	-1.751169000
1	-1.412000000	-4.413869000	-0.008491000
6	0.648919000	-2.708019000	-0.733266000
1	1.230193000	-1.786572000	-0.657176000
1	0.965217000	-3.377277000	0.071914000
1	0.904624000	-3.192383000	-1.678268000
6	-4.215500000	-1.410692000	-2.065319000
1	-5.038768000	-2.109184000	-1.899277000
1	-4.557035000	-0.676682000	-2.799179000
1	-3.382136000	-1.964774000	-2.501549000
6	-4.964543000	0.018258000	-0.133314000
1	-4.674712000	0.427200000	0.838308000
1	-5.277457000	0.850106000	-0.769935000
1	-5.832327000	-0.628717000	0.012323000
6	-2.450472000	1.208454000	2.935402000
1	-2.060850000	0.774211000	3.866806000
1	-2.573149000	2.281792000	3.113725000
1	-3.455035000	0.798706000	2.794509000
6	-0.952724000	-2.278405000	1.830458000
6	-0.839436000	-2.426175000	-0.680929000
1	-0.659571000	-3.302154000	1.580973000
1	-1.085884000	-1.787709000	-1.536327000
6	-3.819925000	-0.765363000	-0.750640000
1	-3.566101000	-1.571746000	-0.055936000
6	-2.683415000	1.193313000	-1.821426000
1	-3.689764000	1.118779000	-2.243991000



6	-1.705306000	1.030644000	-2.967990000
1	-1.865289000	0.079260000	-3.480541000
1	-1.838456000	1.835959000	-3.695061000
1	-0.668435000	1.062740000	-2.617792000
6	-2.603548000	2.568706000	-1.180451000
1	-3.302491000	2.661915000	-0.346654000
1	-1.601925000	2.796372000	-0.811271000
1	-2.860177000	3.322980000	-1.928079000
5	0.970464000	1.434935000	-0.672195000
6	0.453563000	2.637763000	1.448553000
1	0.591818000	3.372563000	2.224831000
6	1.779488000	3.914461000	-0.324289000
6	2.666296000	3.284455000	0.337948000
7	1.343175000	2.618285000	0.284260000
6	1.045873000	4.909597000	-1.087718000
1	1.663735000	5.781145000	-1.299019000
1	0.699887000	4.475768000	-2.030022000
1	0.165635000	5.228059000	-0.522064000
6	3.916627000	2.977129000	1.018403000
1	4.340511000	2.051253000	0.621844000
1	4.628675000	3.791454000	0.892349000
1	3.730263000	2.829710000	2.085420000
1	2.138756000	0.798927000	-1.109388000
6	3.223405000	-0.081878000	-0.596568000
6	3.839233000	-0.922341000	-1.516782000
6	3.270658000	-0.446978000	0.746294000
6	4.489448000	-2.060571000	-1.084365000
1	3.817964000	-0.715334000	-2.586346000
6	3.926755000	-1.594449000	1.171207000
1	2.767209000	0.169435000	1.494966000
6	4.549043000	-2.420808000	0.247266000
1	3.951325000	-1.858574000	2.225195000
1	5.067052000	-3.326642000	0.538368000
9	5.090250000	-2.859813000	-1.985957000

**9TS<sup>o</sup>(C-F)** (TE= -1700.408961)

6	-0.264272000	1.594074000	1.379176000
7	-0.034085000	0.896820000	0.117754000
15	-1.479887000	0.084194000	0.378206000
6	-1.492731000	1.040314000	1.801360000
7	-2.531095000	0.322958000	-0.883021000
7	-1.371146000	-1.554074000	0.492758000
6	0.008119000	-1.797127000	2.587510000

1	0.912409000	-1.816425000	1.975500000
1	-0.123146000	-0.783549000	2.971049000
1	0.157726000	-2.468629000	3.436364000
6	-2.479910000	-2.240146000	2.588788000
1	-3.301736000	-2.672626000	2.013107000
1	-2.362854000	-2.821361000	3.506258000
1	-2.760022000	-1.223753000	2.873868000
6	-2.057980000	-3.513523000	-0.875108000
1	-3.099704000	-3.192109000	-0.817992000
1	-1.905243000	-3.995416000	-1.843229000
1	-1.895145000	-4.274908000	-0.107958000
6	0.348619000	-2.802668000	-0.791303000
1	1.037369000	-1.959780000	-0.700219000
1	0.584691000	-3.520704000	-0.000877000
1	0.542632000	-3.295315000	-1.746587000
6	-4.302473000	-0.910126000	-2.111627000
1	-5.210868000	-1.499290000	-1.967227000
1	-4.534522000	-0.132218000	-2.843057000
1	-3.538730000	-1.562097000	-2.539710000
6	-4.899858000	0.590210000	-0.182268000
1	-4.581774000	0.952243000	0.798903000
1	-5.089047000	1.459433000	-0.817814000
1	-5.846585000	0.059238000	-0.061371000
6	-2.342912000	1.330521000	2.978200000
1	-2.005531000	0.835663000	3.899719000
1	-2.370516000	2.404758000	3.187768000
1	-3.378390000	1.017654000	2.815145000
6	-1.195533000	-2.254411000	1.784597000
6	-1.096189000	-2.348676000	-0.728455000
1	-1.006542000	-3.294922000	1.505995000
1	-1.264986000	-1.665298000	-1.567141000
6	-3.852785000	-0.330316000	-0.783777000
1	-3.718754000	-1.167526000	-0.091279000
6	-2.449837000	1.476332000	-1.809894000
1	-3.445582000	1.531600000	-2.259505000
6	-1.468393000	1.205040000	-2.932763000
1	-1.735989000	0.290549000	-3.467050000
1	-1.475250000	2.031549000	-3.647971000
1	-0.446328000	1.096657000	-2.555723000
6	-2.217497000	2.823896000	-1.146617000
1	-2.922805000	2.993925000	-0.330619000
1	-1.206245000	2.919675000	-0.746946000

1	-2.356610000	3.613004000	-1.889300000
5	1.168938000	1.259705000	-0.550731000
6	0.744770000	2.465702000	1.592410000
1	0.957086000	3.151682000	2.396111000
6	2.273919000	3.607178000	-0.110290000
6	3.053437000	2.852138000	0.554739000
7	1.657115000	2.361304000	0.449339000
6	1.696575000	4.704261000	-0.867668000
1	2.423953000	5.498082000	-1.031270000
1	1.336889000	4.339960000	-1.834016000
1	0.840940000	5.114088000	-0.323821000
6	4.233399000	2.363869000	1.253314000
1	4.565816000	1.420998000	0.812031000
1	5.038338000	3.095512000	1.200449000
1	3.990756000	2.175881000	2.302370000
1	2.297665000	0.460954000	-1.027575000
6	3.255558000	-0.552699000	-0.626634000
6	3.794192000	-1.463067000	-1.506092000
6	3.226720000	-0.959150000	0.703647000
6	4.297728000	-2.699256000	-1.145355000
6	3.728576000	-2.184012000	1.126605000
1	2.770920000	-0.302801000	1.450899000
6	4.264188000	-3.058981000	0.194015000
1	3.692213000	-2.462042000	2.175722000
1	4.653332000	-4.022495000	0.503462000
9	3.838596000	-1.150390000	-2.824807000
1	4.708317000	-3.363066000	-1.899508000

Cartesian coordinates of the H–H splitting product obtained from **4-7**, **9**, **II**, **IIIa** and **IIIb**, along with their total energies (in hartrees) including zero point vibrational correction.

**4P<sup>H-H</sup>** (TE= -1714.746663)

6	0.930073000	-0.653873000	0.883547000
6	2.811308000	-0.936245000	-0.441532000
7	0.584358000	-0.010808000	-0.318462000
7	2.181956000	-1.096670000	0.886053000
6	2.624007000	-2.108202000	1.813128000
1	3.606511000	-1.866080000	2.225086000
1	1.919099000	-2.197780000	2.641819000
1	2.704789000	-3.071959000	1.300255000
15	4.060874000	0.220160000	-0.469675000
6	5.334104000	-0.049660000	0.788083000

1	6.153072000	0.661703000	0.665548000
1	4.895977000	0.093418000	1.778126000
1	5.716470000	-1.067883000	0.711816000
6	3.721557000	2.011399000	-0.265614000
1	4.621372000	2.621246000	-0.378899000
1	2.978904000	2.312892000	-1.007339000
1	3.303076000	2.178628000	0.729477000
6	4.892755000	0.136491000	-2.062373000
1	5.668048000	0.901590000	-2.131359000
1	5.331361000	-0.852727000	-2.189251000
1	4.151502000	0.294447000	-2.846766000
15	-0.980146000	-0.055543000	0.241488000
6	-0.234285000	-0.712244000	1.658069000
7	-1.666898000	1.451687000	0.203020000
7	-2.053823000	-1.016021000	-0.564206000
6	-1.022287000	-3.290952000	-0.157343000
1	-0.357475000	-3.087996000	-1.000437000
1	-0.460195000	-3.106120000	0.760354000
1	-1.300182000	-4.347599000	-0.177413000
6	-3.145323000	-2.576456000	1.005728000
1	-4.101308000	-2.065424000	0.870169000
1	-3.346696000	-3.629310000	1.217346000
1	-2.651960000	-2.150322000	1.881939000
6	-4.067997000	-0.705239000	-1.980967000
1	-4.574615000	-0.216511000	-1.146101000
1	-4.419260000	-0.244183000	-2.906793000
1	-4.382590000	-1.751831000	-2.003272000
6	-1.850965000	-1.250470000	-3.033910000
1	-0.770672000	-1.098991000	-2.974024000
1	-2.041685000	-2.327544000	-3.043304000
1	-2.211504000	-0.846024000	-3.982550000
6	-3.912450000	2.454198000	-0.125375000
1	-4.944203000	2.409457000	0.230466000
1	-3.610831000	3.504364000	-0.108941000
1	-3.894482000	2.112477000	-1.162043000
6	-3.013788000	2.089628000	2.191827000
1	-2.400617000	1.441492000	2.822948000
1	-2.617970000	3.106280000	2.263424000
1	-4.028462000	2.103093000	2.595907000
6	-0.543225000	-1.134505000	3.045669000
1	-0.627464000	-2.223038000	3.173178000
1	0.215943000	-0.788195000	3.754235000
1	-1.493595000	-0.708839000	3.380855000
6	-2.278614000	-2.439565000	-0.230264000
6	-2.559621000	-0.566435000	-1.881199000
1	-2.859593000	-2.825857000	-1.072637000

1	-2.321733000	0.500430000	-1.937417000
6	-3.024994000	1.594421000	0.756579000
1	-3.449407000	0.583548000	0.761014000
6	-0.865618000	2.687686000	0.069130000
1	-1.574755000	3.498058000	0.265487000
6	-0.369398000	2.863008000	-1.353430000
1	-1.207854000	2.870554000	-2.054351000
1	0.165625000	3.810918000	-1.453597000
1	0.310827000	2.055805000	-1.636568000
6	0.248928000	2.824626000	1.091915000
1	-0.129255000	2.715742000	2.110213000
1	1.021261000	2.072361000	0.927885000
1	0.710585000	3.811304000	1.001245000
5	1.572439000	-0.603293000	-1.448501000
1	1.805220000	0.235404000	-2.310768000
1	1.061444000	-1.596760000	-1.954510000

**5P<sup>H-H</sup>** (TE= -1333.582679)

6	-1.620748000	-0.131047000	0.692164000
6	-3.424612000	-0.269450000	-0.799204000
7	-1.005292000	-0.375161000	-0.541320000
7	-2.937665000	-0.074389000	0.605327000
6	-3.802938000	0.182825000	1.724364000
1	-4.582856000	-0.580332000	1.798963000
1	-3.226867000	0.168709000	2.648943000
1	-4.290444000	1.158644000	1.637511000
15	0.423295000	-0.030798000	0.220715000
6	-0.595058000	0.068539000	1.619918000
7	1.527919000	-1.238707000	0.017168000
7	1.215206000	1.346479000	-0.227326000
6	-0.631016000	3.020465000	0.243246000
1	-1.075209000	2.734393000	-0.713590000
1	-1.186832000	2.515142000	1.036340000
1	-0.760233000	4.097131000	0.376274000
6	1.457278000	2.922761000	1.657153000
1	2.540080000	2.780608000	1.632577000
1	1.252140000	3.941368000	1.995005000
1	1.039943000	2.237164000	2.396819000
6	3.339534000	2.026171000	-1.312971000
1	3.889088000	1.624387000	-0.458548000
1	3.946319000	1.875586000	-2.208627000
1	3.234718000	3.105019000	-1.172873000
6	1.209981000	1.882775000	-2.654981000
1	0.271105000	1.337496000	-2.782991000
1	0.969479000	2.941392000	-2.522226000
1	1.793411000	1.792053000	-3.574006000

6	4.003295000	-1.399244000	0.040644000
1	4.885034000	-1.217378000	0.658768000
1	4.061502000	-2.432521000	-0.310224000
1	4.055678000	-0.742264000	-0.829425000
6	2.669818000	-2.051980000	2.068113000
1	1.768452000	-1.848422000	2.650929000
1	2.662361000	-3.108198000	1.786351000
1	3.538902000	-1.890262000	2.709452000
6	-0.530351000	0.305628000	3.083078000
1	-0.938938000	1.277939000	3.391100000
1	-1.059733000	-0.462288000	3.656445000
1	0.506835000	0.281187000	3.428066000
6	0.851548000	2.686445000	0.288570000
6	2.000568000	1.334049000	-1.482899000
1	1.338470000	3.381317000	-0.401186000
1	2.203710000	0.280077000	-1.689644000
6	2.743279000	-1.150475000	0.848818000
1	2.783944000	-0.112885000	1.207577000
6	1.211093000	-2.549431000	-0.589437000
1	2.111263000	-3.149376000	-0.421526000
6	1.026063000	-2.423375000	-2.088428000
1	1.913820000	-1.986873000	-2.553001000
1	0.859518000	-3.407475000	-2.532501000
1	0.160424000	-1.800059000	-2.328756000
6	0.058935000	-3.290294000	0.067532000
1	0.171580000	-3.321383000	1.152755000
1	-0.896465000	-2.818622000	-0.167831000
1	0.028929000	-4.317779000	-0.302168000
5	-2.043210000	-0.083658000	-1.691402000
6	-4.018186000	-1.662881000	-0.910934000
1	-4.855533000	-1.822221000	-0.219656000
1	-4.390758000	-1.825450000	-1.925383000
1	-3.258359000	-2.424724000	-0.712925000
6	-4.467480000	0.779372000	-1.124022000
1	-4.713649000	0.720460000	-2.187121000
1	-5.400848000	0.646516000	-0.562279000
1	-4.082979000	1.785256000	-0.932733000
1	-1.932931000	1.063750000	-2.107447000
1	-1.954639000	-0.889494000	-2.602208000

**6P<sup>H-H</sup>** (TE= -1501.960707)

6	0.732103000	-0.916026000	0.813482000
7	0.466443000	-0.220986000	-0.374078000
7	1.930118000	-1.499757000	0.777288000
6	2.313329000	-2.645969000	1.557334000
1	3.359750000	-2.566997000	1.859168000

1	1.692005000	-2.694020000	2.452295000
1	2.182446000	-3.564046000	0.976577000
15	-1.072621000	-0.026612000	0.223453000
6	-0.397426000	-0.832447000	1.612033000
7	-1.477002000	1.570067000	0.213534000
7	-2.287585000	-0.799037000	-0.568178000
6	-1.762727000	-3.228507000	-0.116270000
1	-1.109837000	-3.205404000	-0.991504000
1	-1.133078000	-3.136671000	0.770865000
1	-2.259790000	-4.200723000	-0.079667000
6	-3.641342000	-2.036438000	1.080192000
1	-4.471877000	-1.339282000	0.947671000
1	-4.053131000	-3.014210000	1.339837000
1	-3.041439000	-1.694660000	1.927040000
6	-4.160714000	-0.115456000	-2.048299000
1	-4.566716000	0.495182000	-1.239333000
1	-4.386172000	0.381755000	-2.994038000
1	-4.692007000	-1.070549000	-2.052692000
6	-2.096697000	-1.173191000	-3.018554000
1	-1.011559000	-1.262830000	-2.933963000
1	-2.526660000	-2.178472000	-2.998268000
1	-2.333616000	-0.736465000	-3.991065000
6	-3.475774000	2.984081000	-0.184021000
1	-4.515199000	3.123397000	0.121016000
1	-2.986016000	3.958318000	-0.117262000
1	-3.466961000	2.670379000	-1.229750000
6	-2.781685000	2.385308000	2.159907000
1	-2.349783000	1.602995000	2.789852000
1	-2.189239000	3.293969000	2.295266000
1	-3.792222000	2.594348000	2.517242000
6	-0.700916000	-1.201140000	3.015470000
1	-1.027189000	-2.242127000	3.139442000
1	0.170887000	-1.057284000	3.660014000
1	-1.495607000	-0.571934000	3.426032000
6	-2.808376000	-2.128593000	-0.182389000
6	-2.660748000	-0.301774000	-1.913697000
1	-3.488589000	-2.397328000	-0.995586000
1	-2.193751000	0.685359000	-2.001733000
6	-2.814753000	1.949197000	0.706988000
1	-3.419282000	1.037447000	0.650847000
6	-0.462703000	2.652246000	0.136677000
1	-1.021675000	3.559041000	0.386003000
6	0.056694000	2.816848000	-1.277868000
1	-0.767947000	2.972437000	-1.977627000
1	0.719853000	3.683051000	-1.334735000
1	0.624271000	1.938426000	-1.593575000

6	0.663079000	2.545463000	1.150361000
1	0.279879000	2.368300000	2.157643000
1	1.359884000	1.745489000	0.894042000
1	1.225362000	3.481690000	1.160568000
5	1.358776000	-0.967958000	-1.459603000
7	2.547232000	-1.300439000	-0.481603000
6	3.661967000	-0.460054000	-0.413437000
6	4.370763000	-0.202614000	-1.592508000
6	4.129951000	0.111319000	0.771353000
6	5.489143000	0.603648000	-1.582689000
1	4.022764000	-0.650969000	-2.515440000
6	5.259718000	0.914613000	0.769642000
1	3.596264000	-0.061533000	1.698199000
6	5.948664000	1.171618000	-0.401165000
1	6.015931000	0.788392000	-2.512746000
1	5.597995000	1.349206000	1.704395000
1	6.830744000	1.800647000	-0.397274000
1	0.807761000	-1.994029000	-1.821652000
1	1.685247000	-0.253056000	-2.373881000

**7P<sup>H-H</sup>** (TE= -600.111808)

6	-1.523341000	-1.490932000	-0.001390000
6	-0.184988000	-1.524343000	-0.001481000
1	-2.242431000	-2.295628000	-0.002396000
1	0.390557000	-2.440322000	-0.002399000
6	-3.234897000	0.271148000	-0.637601000
6	-3.234788000	0.270011000	0.638262000
7	-1.958408000	-0.114907000	-0.000113000
7	0.418706000	-0.301437000	-0.000327000
5	-0.656373000	0.820259000	0.000626000
6	1.781464000	-0.096011000	-0.000107000
6	2.720190000	-1.135455000	-0.000569000
6	2.263986000	1.218717000	0.000656000
6	4.074663000	-0.862576000	-0.000334000
1	2.396396000	-2.169128000	-0.001068000
6	3.621019000	1.476814000	0.000896000
1	1.554114000	2.037287000	0.001041000
6	4.542963000	0.442150000	0.000394000
1	4.776801000	-1.689424000	-0.000702000
1	3.961632000	2.506592000	0.001486000
1	5.606482000	0.647380000	0.000583000
6	-3.637532000	0.419174000	2.027428000
1	-2.979827000	1.136103000	2.525259000
1	-4.666772000	0.766384000	2.102060000
1	-3.544938000	-0.535052000	2.551854000
6	-3.637683000	0.422797000	-2.026487000



1	-4.666863000	0.770316000	-2.100505000
1	-2.979852000	1.140470000	-2.523078000
1	-3.545269000	-0.530533000	-2.552574000
1	-0.653250000	1.499018000	1.008895000
1	-0.653322000	1.500695000	-1.006518000

**9p<sup>H-H</sup>** (TE= -1370.379621)

6	-1.324350000	0.093865000	1.139981000
7	-0.899858000	-0.123113000	-0.224985000
15	0.644200000	0.015771000	0.312959000
6	-0.097717000	0.170869000	1.846879000
7	1.553568000	-1.315250000	-0.105195000
7	1.557468000	1.275962000	-0.269360000
6	0.010693000	3.139590000	0.457165000
1	-0.579545000	2.965365000	-0.445733000
1	-0.495834000	2.641378000	1.286208000
1	0.024640000	4.213735000	0.658295000
6	2.245529000	2.775198000	1.564929000
1	3.287082000	2.493028000	1.393208000
1	2.223422000	3.806263000	1.926525000
1	1.843178000	2.135689000	2.352849000
6	3.552588000	1.716865000	-1.676840000
1	4.176737000	1.237661000	-0.919001000
1	3.989203000	1.510571000	-2.656923000
1	3.602074000	2.797910000	-1.522845000
6	1.239453000	1.849637000	-2.666131000
1	0.232420000	1.424308000	-2.642252000
1	1.154086000	2.927835000	-2.503438000
1	1.653345000	1.700684000	-3.666233000
6	3.956669000	-1.818833000	-0.453247000
1	4.937518000	-1.782038000	0.026142000
1	3.809558000	-2.840921000	-0.811914000
1	3.975914000	-1.155633000	-1.320207000
6	2.868764000	-2.309966000	1.757272000
1	2.100398000	-1.994155000	2.466571000
1	2.676712000	-3.352230000	1.488382000
1	3.838362000	-2.275019000	2.259245000
6	0.217092000	0.342078000	3.283103000
1	-0.026478000	1.342690000	3.671264000
1	-0.317536000	-0.377834000	3.913542000
1	1.283498000	0.186456000	3.472880000
6	1.436255000	2.639430000	0.290551000
6	2.129861000	1.191483000	-1.627689000
1	1.903930000	3.288329000	-0.455856000
1	2.169671000	0.124490000	-1.860411000
6	2.877467000	-1.410084000	0.533143000

1	3.116132000	-0.394055000	0.875600000
6	0.966789000	-2.566466000	-0.621227000
1	1.782910000	-3.295169000	-0.571259000
6	0.588986000	-2.422375000	-2.082779000
1	1.455303000	-2.122874000	-2.678022000
1	0.216701000	-3.371471000	-2.476574000
1	-0.198974000	-1.676418000	-2.212514000
6	-0.175328000	-3.136635000	0.206282000
1	0.091995000	-3.203183000	1.262430000
1	-1.072975000	-2.520845000	0.119670000
1	-0.413115000	-4.142224000	-0.149834000
5	-2.049007000	0.170071000	-1.193396000
6	-2.672055000	0.190437000	1.226840000
1	-3.323624000	0.355646000	2.071019000
6	-4.454529000	-0.743607000	-0.323359000
6	-4.601070000	0.525249000	-0.377890000
7	-3.236215000	0.069771000	-0.111473000
6	-4.689615000	-2.177764000	-0.316484000
1	-5.745184000	-2.416017000	-0.440327000
1	-4.119211000	-2.651070000	-1.120865000
1	-4.338766000	-2.599345000	0.629621000
6	-5.209415000	1.844645000	-0.483226000
1	-4.773962000	2.393610000	-1.321613000
1	-6.286902000	1.774145000	-0.624708000
1	-5.006762000	2.418578000	0.424829000
1	-2.056337000	1.303290000	-1.656259000
1	-2.228709000	-0.671370000	-2.055465000

**II-P<sup>H-H</sup>** (TE= -600.325466)

6	-0.836577000	1.216716000	0.224198000
6	-2.259154000	0.707244000	0.518746000
6	-2.369445000	-0.697062000	-0.066468000
6	-0.950329000	-1.191846000	0.151062000
7	-0.112048000	-0.039614000	-0.109202000
1	-3.022065000	1.389500000	0.132449000
1	-2.400915000	0.643556000	1.603275000
6	1.262885000	-0.188794000	-0.078014000
6	2.146567000	0.869987000	-0.339954000
6	3.514129000	0.681880000	-0.333709000
6	4.068167000	-0.561668000	-0.074803000
6	3.212237000	-1.616517000	0.183541000
6	1.840061000	-1.440209000	0.189004000
1	1.765338000	1.854407000	-0.567137000
1	4.157730000	1.529159000	-0.544276000
1	5.141885000	-0.702943000	-0.075933000
1	3.612702000	-2.602175000	0.394740000

1	1.211371000	-2.291711000	0.411202000
6	-2.709205000	-0.690217000	-1.551030000
1	-2.832493000	-1.714179000	-1.914944000
1	-3.645299000	-0.154594000	-1.732775000
1	-1.925354000	-0.222295000	-2.148435000
6	-3.386362000	-1.541670000	0.676053000
1	-4.394879000	-1.141375000	0.539186000
1	-3.386032000	-2.570790000	0.305159000
1	-3.175020000	-1.566954000	1.748363000
6	-0.868425000	2.207650000	-0.934990000
1	0.121124000	2.566664000	-1.214929000
1	-1.326927000	1.767769000	-1.821371000
1	-1.463293000	3.078364000	-0.646243000
6	-0.277423000	1.883579000	1.474538000
1	-0.959034000	2.673641000	1.800210000
1	-0.189912000	1.154042000	2.284668000
1	0.703120000	2.333140000	1.315868000
1	-0.830728000	-1.559651000	1.186708000
1	-0.699732000	-2.020715000	-0.520414000

**IIIa-P<sup>H-H</sup>** (TE= -1010.628621)

13	0.000000000	0.000000000	0.949504000
7	0.000000000	1.408395000	-0.335952000
7	0.000000000	-1.408395000	-0.335952000
6	0.000000000	1.251492000	-1.651690000
6	0.000000000	-1.251492000	-1.651690000
6	0.000000000	0.000000000	-2.272088000
1	0.000000000	0.000000000	-3.353330000
6	0.000000000	2.710673000	0.239599000
6	1.201152000	3.330852000	0.557153000
6	-1.201152000	3.330852000	0.557153000
6	1.198667000	4.576427000	1.161027000
6	-1.198667000	4.576427000	1.161027000
6	0.000000000	5.202914000	1.460875000
1	2.139174000	5.057114000	1.403744000
1	-2.139174000	5.057114000	1.403744000
1	0.000000000	6.176121000	1.937220000
6	0.000000000	-2.710673000	0.239599000
6	-1.201152000	-3.330852000	0.557153000
6	1.201152000	-3.330852000	0.557153000
6	-1.198667000	-4.576427000	1.161027000
6	1.198667000	-4.576427000	1.161027000
6	0.000000000	-5.202914000	1.460875000
1	-2.139174000	-5.057114000	1.403744000
1	2.139174000	-5.057114000	1.403744000
1	0.000000000	-6.176121000	1.937220000

6	0.000000000	-2.461048000	-2.529947000
1	0.000000000	-2.183214000	-3.581387000
1	0.875545000	-3.082684000	-2.329263000
1	-0.875545000	-3.082684000	-2.329263000
6	0.000000000	2.461048000	-2.529947000
1	0.000000000	2.183214000	-3.581387000
1	-0.875545000	3.082684000	-2.329263000
1	0.875545000	3.082684000	-2.329263000
1	2.131453000	-2.821844000	0.327575000
1	-2.131453000	-2.821844000	0.327575000
1	-2.131453000	2.821844000	0.327575000
1	2.131453000	2.821844000	0.327575000
1	1.357826000	0.000000000	1.781693000
1	-1.357826000	0.000000000	1.781693000

**IIIb-P<sup>H-H</sup>** (TE= -2692.983213)

7	-0.000044000	-0.439596000	-1.444195000
7	-0.000044000	-0.439596000	1.444195000
6	-0.000022000	-1.747161000	-1.258536000
6	-0.000022000	-1.747161000	1.258536000
6	-0.000017000	-2.356726000	0.000000000
1	-0.000035000	-3.438044000	0.000000000
6	-0.000039000	0.123244000	-2.746968000
6	1.200867000	0.436251000	-3.370918000
6	-1.200945000	0.436436000	-3.370827000
6	1.198415000	1.031473000	-4.620630000
6	-1.198502000	1.031658000	-4.620536000
6	-0.000044000	1.327677000	-5.249440000
1	2.139050000	1.269707000	-5.103488000
1	-2.139138000	1.270039000	-5.103319000
1	-0.000044000	1.796844000	-6.226126000
6	-0.000039000	0.123244000	2.746968000
6	-1.200945000	0.436436000	3.370827000
6	1.200867000	0.436251000	3.370918000
6	-1.198502000	1.031658000	4.620536000
6	1.198415000	1.031473000	4.620630000
6	-0.000044000	1.327677000	5.249440000
1	-2.139138000	1.270039000	5.103319000
1	2.139050000	1.269707000	5.103488000
1	-0.000044000	1.796844000	6.226126000
6	-0.000044000	-2.644554000	2.456589000
1	-0.000046000	-3.691822000	2.163282000
1	0.875717000	-2.453579000	3.080882000
1	-0.875834000	-2.453561000	3.080839000

6	-0.000044000	-2.644554000	-2.456589000
1	-0.000046000	-3.691822000	-2.163282000
1	-0.875834000	-2.453561000	-3.080839000
1	0.875717000	-2.453579000	-3.080882000
1	2.131381000	0.208732000	2.861145000
1	-2.131450000	0.209054000	2.860977000
1	-2.131450000	0.209054000	-2.860977000
1	2.131381000	0.208732000	-2.861145000
31	0.000148000	0.907438000	0.000000000
1	1.377846000	1.675228000	0.000000000
1	-1.377189000	1.675827000	0.000000000

Cartesian coordinates of the N–H splitting product obtained from **4-7**, **9** and **II**, along with their total energies (in hartrees) including zero point vibrational correction.

**4P<sup>N-H</sup>** (TE= -1770.102805)

6	-0.840595000	-0.669287000	-0.960749000
6	-2.759477000	-0.903950000	0.313866000
7	-0.519876000	-0.011345000	0.235811000
7	-2.101853000	-1.096643000	-0.993455000
6	-2.500277000	-2.161164000	-1.882294000
1	-3.473891000	-1.959276000	-2.334270000
1	-1.769629000	-2.277729000	-2.684977000
1	-2.576808000	-3.101147000	-1.325522000
15	-4.050694000	0.198126000	0.252580000
6	-5.221924000	-0.142330000	-1.085764000
1	-6.075501000	0.535554000	-1.022790000
1	-4.727496000	0.010976000	-2.047106000
1	-5.566801000	-1.174495000	-1.020741000
6	-3.802930000	2.007937000	0.016599000
1	-4.744884000	2.562891000	0.007786000
1	-3.158583000	2.400940000	0.805730000
1	-3.293865000	2.159604000	-0.938380000
6	-5.005016000	0.093232000	1.776618000
1	-5.772478000	0.868762000	1.805947000
1	-5.468791000	-0.890977000	1.836837000
1	-4.329728000	0.210044000	2.624466000
15	1.056126000	-0.065336000	-0.294028000
6	0.335890000	-0.752855000	-1.711727000
7	1.735423000	1.446133000	-0.272921000
7	2.107999000	-1.009402000	0.555381000
6	1.228074000	-3.326693000	0.071930000

1	0.543432000	-3.192795000	0.912295000
1	0.665212000	-3.137168000	-0.844263000
1	1.565822000	-4.365937000	0.056203000
6	3.330478000	-2.457309000	-1.024061000
1	4.253909000	-1.900423000	-0.848319000
1	3.593934000	-3.490418000	-1.262830000
1	2.836355000	-2.030331000	-1.899970000
6	4.013803000	-0.587385000	2.087899000
1	4.523643000	-0.029731000	1.300059000
1	4.279569000	-0.138277000	3.047432000
1	4.407360000	-1.607419000	2.090081000
6	1.804902000	-1.352623000	3.001891000
1	0.720925000	-1.296698000	2.883630000
1	2.103541000	-2.404970000	2.995748000
1	2.071143000	-0.942861000	3.978911000
6	3.931311000	2.511860000	0.159086000
1	4.987680000	2.468113000	-0.115820000
1	3.614548000	3.553090000	0.061076000
1	3.839494000	2.226430000	1.208929000
6	3.212633000	1.988142000	-2.194055000
1	2.668892000	1.279357000	-2.824279000
1	2.791662000	2.983129000	-2.362500000
1	4.253947000	2.011320000	-2.523069000
6	0.660261000	-1.187151000	-3.091997000
1	0.795432000	-2.272635000	-3.201266000
1	-0.119588000	-0.889954000	-3.800191000
1	1.586370000	-0.722338000	-3.443172000
6	2.429733000	-2.405208000	0.194289000
6	2.505864000	-0.566627000	1.911239000
1	3.016869000	-2.775397000	1.039907000
1	2.170937000	0.473693000	1.991023000
6	3.127603000	1.583706000	-0.733173000
1	3.567928000	0.584981000	-0.643628000
6	0.921241000	2.682765000	-0.249183000
1	1.626726000	3.480570000	-0.501360000
6	0.403407000	2.961558000	1.148083000
1	1.233140000	3.063544000	1.851988000
1	-0.170307000	3.892228000	1.161454000
1	-0.239125000	2.149939000	1.499595000
6	-0.178739000	2.738389000	-1.295605000
1	0.208841000	2.528171000	-2.294708000
1	-0.969529000	2.020760000	-1.072615000
1	-0.619852000	3.738464000	-1.303276000
5	-1.520813000	-0.651891000	1.365971000
1	-1.042016000	-1.725879000	1.732741000
7	-1.624930000	0.261870000	2.561189000

1	-2.158771000	1.116121000	2.469256000
1	-1.881875000	-0.188546000	3.426422000

**5P<sup>N-H</sup>** (TE= -1388.940330)

6	-1.495673000	-0.186804000	0.859543000
6	-3.424766000	-0.180962000	-0.457950000
7	-0.972278000	-0.211169000	-0.433286000
7	-2.815392000	-0.316076000	0.899146000
6	-3.546952000	-0.062517000	2.115217000
1	-4.529442000	-0.532800000	2.060703000
1	-3.016672000	-0.490690000	2.966011000
1	-3.687609000	1.009884000	2.298981000
15	0.511720000	-0.031061000	0.269853000
6	-0.421590000	-0.015468000	1.733603000
7	1.549373000	-1.272055000	-0.064273000
7	1.363347000	1.331902000	-0.110120000
6	-0.385391000	3.056583000	0.501965000
1	-0.829214000	2.927080000	-0.487376000
1	-0.970375000	2.473101000	1.217111000
1	-0.467243000	4.110317000	0.777856000
6	1.699370000	2.752814000	1.884594000
1	2.765696000	2.518813000	1.846251000
1	1.583871000	3.765519000	2.277830000
1	1.222476000	2.067623000	2.587116000
6	3.488960000	1.986708000	-1.209781000
1	4.039970000	1.502301000	-0.400418000
1	4.064111000	1.868243000	-2.130802000
1	3.441518000	3.057337000	-0.995489000
6	1.318255000	2.038182000	-2.490634000
1	0.352004000	1.542383000	-2.622012000
1	1.136708000	3.096108000	-2.280919000
1	1.865251000	1.980977000	-3.434317000
6	4.010994000	-1.569039000	-0.128142000
1	4.918913000	-1.477696000	0.471888000
1	3.998390000	-2.579334000	-0.544519000
1	4.077982000	-0.861842000	-0.956807000
6	2.704186000	-2.271552000	1.898854000
1	1.832397000	-2.058399000	2.521619000
1	2.632867000	-3.306870000	1.555371000
1	3.598861000	-2.193713000	2.520349000
6	-0.257107000	0.048935000	3.207862000
1	-0.721628000	0.934865000	3.660386000
1	-0.665879000	-0.828264000	3.720650000
1	0.803320000	0.086112000	3.471044000
6	1.077604000	2.647013000	0.507060000
6	2.113700000	1.371430000	-1.384864000

1	1.597550000	3.365624000	-0.132462000
1	2.258105000	0.326347000	-1.670581000
6	2.790996000	-1.301938000	0.733787000
1	2.900582000	-0.292505000	1.152524000
6	1.138911000	-2.529647000	-0.724081000
1	2.004815000	-3.189885000	-0.610585000
6	0.934438000	-2.311657000	-2.210128000
1	1.850980000	-1.938420000	-2.673990000
1	0.659399000	-3.249012000	-2.698953000
1	0.128825000	-1.597704000	-2.395745000
6	-0.037927000	-3.232086000	-0.067677000
1	0.118347000	-3.342460000	1.007252000
1	-0.971994000	-2.693207000	-0.233467000
1	-0.150538000	-4.229508000	-0.498950000
5	-2.161842000	-0.480873000	-1.501578000
6	-4.534260000	-1.193663000	-0.638027000
1	-5.407447000	-0.995381000	-0.003423000
1	-4.873365000	-1.166824000	-1.677642000
1	-4.173547000	-2.204981000	-0.434388000
6	-3.975415000	1.229033000	-0.597595000
1	-4.361972000	1.374613000	-1.608389000
1	-4.794376000	1.428282000	0.103693000
1	-3.194330000	1.978317000	-0.424685000
1	-2.133571000	-1.662639000	-1.817889000
7	-2.171400000	0.364610000	-2.735913000
1	-2.051937000	1.362247000	-2.618444000
1	-1.583944000	0.053639000	-3.494805000

**6P<sup>N-H</sup>** (TE= -1557.321446)

6	-0.672258000	-0.822215000	-0.941994000
7	-0.426924000	-0.175103000	0.273734000
7	-1.861031000	-1.414092000	-0.949415000
6	-2.301564000	-2.419661000	-1.874660000
1	-3.308873000	-2.195752000	-2.235163000
1	-1.621840000	-2.443878000	-2.726869000
1	-2.312243000	-3.400531000	-1.391567000
15	1.134102000	-0.007332000	-0.280936000
6	0.475392000	-0.721236000	-1.720389000
7	1.617739000	1.567160000	-0.190494000
7	2.304190000	-0.864786000	0.498913000
6	1.670623000	-3.245054000	-0.071439000
1	0.992482000	-3.227556000	0.784482000
1	1.073654000	-3.084966000	-0.971210000
1	2.120758000	-4.238425000	-0.136638000
6	3.650215000	-2.107155000	-1.153620000
1	4.509083000	-1.459477000	-0.963095000



1	4.022125000	-3.094390000	-1.437023000
1	3.101388000	-1.702595000	-2.007035000
6	4.191944000	-0.315947000	2.014166000
1	4.624577000	0.319260000	1.238837000
1	4.432299000	0.122325000	2.985203000
1	4.685474000	-1.290187000	1.969541000
6	2.082293000	-1.328598000	2.930761000
1	0.997953000	-1.393129000	2.817456000
1	2.488980000	-2.342783000	2.888742000
1	2.308107000	-0.927583000	3.921239000
6	3.709344000	2.841719000	0.204670000
1	4.743166000	2.941216000	-0.133267000
1	3.272580000	3.843199000	0.207225000
1	3.720768000	2.473211000	1.232293000
6	2.902107000	2.409575000	-2.138715000
1	2.398616000	1.691556000	-2.791194000
1	2.364642000	3.359402000	-2.202904000
1	3.910733000	2.575194000	-2.523330000
6	0.817949000	-1.095347000	-3.113783000
1	1.079241000	-2.154931000	-3.239162000
1	-0.009324000	-0.885332000	-3.797972000
1	1.671552000	-0.517233000	-3.478061000
6	2.767218000	-2.203864000	0.074362000
6	2.686735000	-0.436662000	1.863578000
1	3.402916000	-2.542549000	0.897355000
1	2.259081000	0.563982000	1.989403000
6	2.958404000	1.894349000	-0.712241000
1	3.510372000	0.947663000	-0.725263000
6	0.675532000	2.699365000	-0.022126000
1	1.273964000	3.584423000	-0.257990000
6	0.237418000	2.821496000	1.423161000
1	1.101293000	2.945788000	2.080627000
1	-0.416259000	3.687510000	1.550536000
1	-0.313215000	1.931415000	1.738475000
6	-0.501108000	2.706635000	-0.982330000
1	-0.176044000	2.550313000	-2.013097000
1	-1.232582000	1.938320000	-0.726092000
1	-1.001937000	3.675780000	-0.927663000
5	-1.374233000	-0.965314000	1.352832000
7	-2.526952000	-1.280648000	0.285028000
6	-3.647167000	-0.439378000	0.196821000
6	-4.555186000	-0.434585000	1.261060000
6	-3.917575000	0.375580000	-0.903629000
6	-5.672257000	0.374152000	1.229805000
1	-4.354046000	-1.075685000	2.109817000
6	-5.051367000	1.173132000	-0.931121000

1	-3.230945000	0.389587000	-1.742636000
6	-5.934217000	1.185536000	0.132956000
1	-6.359262000	0.361376000	2.069208000
1	-5.238501000	1.796430000	-1.799164000
1	-6.819538000	1.809835000	0.108178000
1	-0.810085000	-2.000878000	1.664358000
7	-1.823020000	-0.198248000	2.524154000
1	-1.256586000	-0.245056000	3.354415000
1	-2.167762000	0.740667000	2.383700000

**7P<sup>N-H</sup>** (TE= -655.474823)

6	-1.457003000	-1.619211000	-0.084594000
6	-0.118853000	-1.623023000	-0.101500000
1	-2.154541000	-2.437411000	-0.181523000
1	0.476529000	-2.520948000	-0.203488000
6	-3.190666000	0.172676000	-0.541941000
6	-3.209951000	0.014175000	0.723395000
7	-1.916110000	-0.266379000	0.075133000
7	0.463972000	-0.396704000	0.046940000
5	-0.620658000	0.724859000	0.226134000
6	1.831228000	-0.196193000	0.053377000
6	2.746406000	-1.160700000	-0.385793000
6	2.343471000	1.024945000	0.509452000
6	4.106296000	-0.914436000	-0.353576000
1	2.395486000	-2.109053000	-0.774717000
6	3.704109000	1.260491000	0.532229000
1	1.654947000	1.784949000	0.857582000
6	4.602573000	0.295421000	0.103935000
1	4.788182000	-1.682524000	-0.702475000
1	4.067765000	2.215283000	0.896568000
1	5.669029000	0.484038000	0.122804000
6	-3.644267000	-0.021971000	2.111407000
1	-3.028362000	0.654443000	2.709209000
1	-4.688828000	0.271410000	2.203131000
1	-3.520844000	-1.028539000	2.518654000
6	-3.612935000	0.427958000	-1.910848000
1	-4.679963000	0.642739000	-1.955312000
1	-3.052908000	1.273010000	-2.314690000
1	-3.402542000	-0.445529000	-2.533496000
1	-0.658732000	1.187842000	1.352975000
7	-0.659192000	1.783236000	-0.815596000
1	-0.397587000	2.709763000	-0.519490000
1	-0.187491000	1.574377000	-1.684998000

**9P<sup>N-H</sup>** (TE= -1425.743700)

6	-1.205477000	0.098223000	1.256336000
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7	-0.832375000	-0.202809000	-0.109161000
15	0.732117000	0.025625000	0.363715000
6	0.042146000	0.226032000	1.914895000
7	1.696234000	-1.280016000	-0.010537000
7	1.561945000	1.292690000	-0.320241000
6	0.030649000	3.157337000	0.434157000
1	-0.605666000	2.955504000	-0.430723000
1	-0.422864000	2.670465000	1.299792000
1	0.040814000	4.235639000	0.612422000
6	2.334545000	2.867603000	1.414062000
1	3.369175000	2.598555000	1.188242000
1	2.314109000	3.910248000	1.740863000
1	1.995121000	2.249925000	2.247834000
6	3.466913000	1.712227000	-1.854538000
1	4.141815000	1.281044000	-1.111440000
1	3.854251000	1.469679000	-2.846906000
1	3.500764000	2.800069000	-1.752386000
6	1.100527000	1.762553000	-2.716379000
1	0.108757000	1.311359000	-2.626957000
1	0.996781000	2.843627000	-2.584988000
1	1.467906000	1.589130000	-3.730669000
6	4.113475000	-1.678410000	-0.393406000
1	5.102488000	-1.562224000	0.055724000
1	4.010255000	-2.727249000	-0.683786000
1	4.076417000	-1.071360000	-1.299994000
6	3.108440000	-2.077226000	1.875304000
1	2.341360000	-1.754507000	2.582782000
1	2.965541000	-3.143779000	1.681404000
1	4.086545000	-1.958903000	2.347143000
6	0.387207000	0.519736000	3.323994000
1	0.112170000	1.537730000	3.639928000
1	-0.104490000	-0.168341000	4.021176000
1	1.462653000	0.419495000	3.497970000
6	1.451073000	2.672408000	0.197605000
6	2.059983000	1.163103000	-1.704617000
1	1.861142000	3.300950000	-0.598500000
1	2.108514000	0.088010000	-1.896564000
6	3.039206000	-1.261890000	0.594903000
1	3.232247000	-0.214639000	0.862939000
6	1.175743000	-2.594259000	-0.431377000
1	2.024371000	-3.276909000	-0.317347000
6	0.812230000	-2.576390000	-1.903003000
1	1.688278000	-2.338749000	-2.512094000
1	0.437119000	-3.554170000	-2.217715000
1	0.037962000	-1.832887000	-2.112951000
6	0.059298000	-3.157372000	0.435391000

1	0.332834000	-3.142027000	1.492178000
1	-0.865524000	-2.588485000	0.316833000
1	-0.132645000	-4.194151000	0.147635000
5	-1.977252000	0.158970000	-1.072950000
6	-2.546634000	0.222820000	1.397248000
1	-3.145503000	0.464983000	2.262682000
6	-4.417192000	-0.699008000	-0.050073000
6	-4.516311000	0.573751000	-0.130533000
7	-3.161180000	0.077513000	0.091525000
6	-4.751732000	-2.108805000	0.089875000
1	-5.827444000	-2.261707000	0.173600000
1	-4.379733000	-2.685421000	-0.760463000
1	-4.267979000	-2.499431000	0.989940000
6	-5.084124000	1.912910000	-0.217728000
1	-4.694939000	2.432600000	-1.096686000
1	-6.171425000	1.883586000	-0.273149000
1	-4.787899000	2.493158000	0.660330000
1	-1.998878000	1.326628000	-1.447901000
7	-2.158208000	-0.774029000	-2.207257000
1	-2.243252000	-1.758719000	-1.994174000
1	-2.821348000	-0.513433000	-2.919982000

**II-P<sup>N-H</sup>** (TE= -655.652774)

6	-0.664109000	1.346511000	-0.321000000
6	-2.138854000	0.987363000	-0.594809000
6	-2.390305000	-0.383481000	0.023085000
6	-0.999681000	-1.017466000	-0.151367000
7	-0.108113000	0.069275000	0.206275000
1	-2.303716000	0.929854000	-1.676012000
1	-2.821904000	1.749236000	-0.207938000
6	1.284645000	-0.140472000	0.131711000
6	1.859129000	-1.014506000	-0.789052000
6	3.231484000	-1.177656000	-0.847859000
6	4.063110000	-0.468101000	0.003171000
6	3.502021000	0.394977000	0.929579000
6	2.128520000	0.546575000	1.001851000
1	1.224772000	-1.576000000	-1.464320000
1	3.655613000	-1.865293000	-1.571200000
1	5.137833000	-0.597351000	-0.046369000
1	4.136685000	0.942021000	1.617786000
1	1.690188000	1.186429000	1.758525000
6	-3.455362000	-1.160719000	-0.723710000
1	-3.575461000	-2.166279000	-0.308055000
1	-4.424826000	-0.660167000	-0.650363000
1	-3.206539000	-1.258236000	-1.784243000
6	-2.779897000	-0.271500000	1.489175000

1	-3.688493000	0.328524000	1.587546000
1	-2.990078000	-1.253853000	1.921187000
1	-1.996354000	0.199970000	2.085786000
6	0.016129000	1.763170000	-1.618454000
1	1.057977000	2.049450000	-1.455509000
1	-0.003581000	0.949777000	-2.349321000
1	-0.507127000	2.619601000	-2.051836000
6	-0.547914000	2.475409000	0.690084000
1	-1.060909000	3.363402000	0.310630000
1	-1.000620000	2.199947000	1.645036000
1	0.493755000	2.749559000	0.866399000
1	-0.913172000	-1.299511000	-1.221912000
7	-0.677640000	-2.194008000	0.610449000
1	-0.797677000	-2.022150000	1.602035000
1	-1.259592000	-2.976434000	0.340639000

Cartesian coordinates of the C–H splitting product obtained from **4-7**, **9** and **II**, along with their total energies (in hartrees) including zero point vibrational correction.

**4P<sup>C-H</sup>** (TE= -1754.021281)

6	0.822297000	-0.633822000	0.959111000
6	2.802892000	-0.768008000	-0.226711000
7	0.433026000	-0.286816000	-0.339182000
7	2.122359000	-0.851678000	1.062856000
6	2.722964000	-1.408558000	2.244690000
1	3.445937000	-0.721617000	2.695698000
1	1.954896000	-1.628500000	2.987254000
1	3.249800000	-2.331710000	1.985726000
15	4.110795000	0.291028000	-0.423793000
6	5.461909000	0.086099000	0.769218000
1	6.343570000	0.631542000	0.426440000
1	5.169543000	0.485922000	1.741495000
1	5.704356000	-0.971495000	0.874639000
6	3.967043000	2.127963000	-0.462927000
1	4.921954000	2.610542000	-0.687275000
1	3.234477000	2.403041000	-1.225222000
1	3.608147000	2.482745000	0.505372000
6	4.822980000	-0.064837000	-2.039191000
1	5.647459000	0.618278000	-2.251812000
1	5.174730000	-1.095711000	-2.060712000
1	4.043182000	0.055573000	-2.792850000
15	-1.092281000	-0.105980000	0.272857000
6	-0.346332000	-0.650541000	1.739669000
7	-1.610903000	1.466077000	0.133349000
7	-2.341082000	-0.987246000	-0.349790000
6	-1.420921000	-3.313898000	-0.055029000

1	-0.989854000	-3.274980000	-1.056471000
1	-0.638246000	-3.053119000	0.660584000
1	-1.738237000	-4.340302000	0.144507000
6	-3.244990000	-2.435326000	1.443075000
1	-4.118316000	-1.780503000	1.494253000
1	-3.567069000	-3.453781000	1.672067000
1	-2.535056000	-2.129399000	2.213506000
6	-4.503249000	-0.642044000	-1.523179000
1	-4.885431000	-0.158398000	-0.621217000
1	-4.946234000	-0.143528000	-2.388396000
1	-4.857851000	-1.675498000	-1.532251000
6	-2.429847000	-1.262536000	-2.814513000
1	-1.354336000	-1.087230000	-2.897092000
1	-2.596093000	-2.342314000	-2.762645000
1	-2.909409000	-0.896880000	-3.725376000
6	-3.803078000	2.624422000	0.005588000
1	-4.745516000	2.770707000	0.538027000
1	-3.405122000	3.615774000	-0.225144000
1	-4.020953000	2.119775000	-0.937089000
6	-2.558462000	2.525331000	2.178893000
1	-1.878906000	1.940364000	2.802095000
1	-2.111238000	3.509803000	2.018199000
1	-3.488080000	2.675756000	2.732234000
6	-0.603365000	-0.602662000	3.202888000
1	-0.463292000	-1.568416000	3.703501000
1	0.030646000	0.125552000	3.725587000
1	-1.638846000	-0.309401000	3.398142000
6	-2.611035000	-2.382856000	0.067358000
6	-2.990804000	-0.546414000	-1.602646000
1	-3.361163000	-2.739912000	-0.643928000
1	-2.736727000	0.511364000	-1.704865000
6	-2.842382000	1.819864000	0.863796000
1	-3.333015000	0.866836000	1.100793000
6	-0.732280000	2.582769000	-0.267646000
1	-1.331412000	3.480892000	-0.085800000
6	-0.436180000	2.536668000	-1.753440000
1	-1.363443000	2.559411000	-2.331746000
1	0.168175000	3.399236000	-2.046411000
1	0.122027000	1.634429000	-2.016782000
6	0.531223000	2.724041000	0.565022000
1	0.309869000	2.704257000	1.634523000
1	1.237462000	1.922759000	0.342042000
1	1.017414000	3.675693000	0.334470000
5	1.615556000	-0.686576000	-1.367463000
1	1.770323000	0.215249000	-2.190463000
6	1.363515000	-2.106992000	-2.092525000

1	1.270017000	-2.917977000	-1.358704000
1	0.479421000	-2.147060000	-2.741789000
1	2.228404000	-2.354538000	-2.720001000

**5P<sup>C-H</sup>** (TE= -1372.860331)

6	-1.499460000	-0.203503000	0.859546000
6	-3.429111000	-0.158923000	-0.457832000
7	-0.979984000	-0.190256000	-0.437101000
7	-2.817618000	-0.342066000	0.897051000
6	-3.547764000	-0.136549000	2.123217000
1	-4.533373000	-0.597108000	2.047407000
1	-3.021415000	-0.606082000	2.954524000
1	-3.680781000	0.927558000	2.354312000
15	0.507924000	-0.034326000	0.263269000
6	-0.422370000	-0.049160000	1.730608000
7	1.535853000	-1.276040000	-0.095923000
7	1.371123000	1.330290000	-0.077710000
6	-0.390043000	3.047822000	0.515415000
1	-0.809127000	2.931658000	-0.486364000
1	-0.992777000	2.455980000	1.208806000
1	-0.477714000	4.097711000	0.803965000
6	1.656366000	2.721249000	1.948713000
1	2.720771000	2.475667000	1.938100000
1	1.541263000	3.731724000	2.347776000
1	1.151662000	2.035644000	2.630915000
6	3.540163000	1.987865000	-1.087212000
1	4.062196000	1.474038000	-0.276927000
1	4.142623000	1.892415000	-1.993328000
1	3.494677000	3.051795000	-0.841305000
6	1.416779000	2.094159000	-2.439936000
1	0.450647000	1.615617000	-2.617960000
1	1.239070000	3.148735000	-2.211408000
1	1.995922000	2.052987000	-3.365014000
6	3.995948000	-1.597742000	-0.142600000
1	4.898213000	-1.526201000	0.468543000
1	3.979700000	-2.599185000	-0.579533000
1	4.077841000	-0.874644000	-0.955927000
6	2.662805000	-2.336478000	1.852563000
1	1.787426000	-2.131340000	2.472808000
1	2.585467000	-3.361906000	1.481988000
1	3.552447000	-2.282484000	2.483748000
6	-0.248249000	-0.043509000	3.205168000
1	-0.737615000	0.806681000	3.697253000
1	-0.624159000	-0.954647000	3.683345000
1	0.812288000	0.018467000	3.462811000
6	1.071814000	2.636640000	0.553578000

6	2.165869000	1.391561000	-1.324710000
1	1.609515000	3.363628000	-0.061174000
1	2.308509000	0.352340000	-1.630954000
6	2.769707000	-1.338714000	0.713141000
1	2.885433000	-0.341364000	1.158458000
6	1.120076000	-2.513197000	-0.790511000
1	1.984034000	-3.178916000	-0.696087000
6	0.915880000	-2.252536000	-2.269462000
1	1.833335000	-1.867491000	-2.721819000
1	0.640322000	-3.175432000	-2.784772000
1	0.111362000	-1.533167000	-2.436946000
6	-0.058440000	-3.229415000	-0.152218000
1	0.097319000	-3.368569000	0.919511000
1	-0.991633000	-2.685111000	-0.304850000
1	-0.173204000	-4.215083000	-0.609332000
5	-2.150465000	-0.437581000	-1.487865000
6	-4.542349000	-1.162553000	-0.666998000
1	-5.416288000	-0.978687000	-0.029085000
1	-4.882529000	-1.107753000	-1.705502000
1	-4.185343000	-2.180214000	-0.492407000
6	-3.981608000	1.255591000	-0.537805000
1	-4.396059000	1.442291000	-1.531354000
1	-4.785787000	1.429847000	0.187352000
1	-3.196818000	1.998363000	-0.360745000
1	-2.156031000	-1.622130000	-1.812485000
6	-2.082036000	0.506704000	-2.786374000
1	-1.997982000	1.574910000	-2.548537000
1	-1.236897000	0.256065000	-3.438241000
1	-2.982502000	0.386831000	-3.401232000

**6P<sup>C-H</sup>** (TE= -1541.239119)

6	0.637698000	-0.829037000	0.936596000
7	0.330754000	-0.436491000	-0.365193000
7	1.890850000	-1.277830000	1.041911000
6	2.307940000	-2.269088000	2.000533000
1	3.347347000	-2.103250000	2.288788000
1	1.680478000	-2.193660000	2.889178000
1	2.216894000	-3.274230000	1.575782000
15	-1.148283000	0.007949000	0.234221000
6	-0.487916000	-0.619216000	1.720386000
7	-1.364664000	1.629440000	0.033890000
7	-2.514604000	-0.693634000	-0.349717000
6	-2.075637000	-3.114742000	0.218561000
1	-1.576441000	-3.241994000	-0.743150000
1	-1.308737000	-2.957052000	0.980687000
1	-2.604933000	-4.040412000	0.455511000



6	-3.760350000	-1.753079000	1.504967000
1	-4.519895000	-0.971935000	1.428179000
1	-4.249684000	-2.674447000	1.828358000
1	-3.048995000	-1.466086000	2.281841000
6	-4.557212000	-0.043595000	-1.609266000
1	-4.858660000	0.569515000	-0.757157000
1	-4.884550000	0.459801000	-2.521462000
1	-5.096624000	-0.992196000	-1.555101000
6	-2.612437000	-1.131429000	-2.787211000
1	-1.521879000	-1.170951000	-2.845475000
1	-2.985382000	-2.152317000	-2.664969000
1	-2.992966000	-0.752358000	-3.738109000
6	-3.336422000	3.133034000	-0.098948000
1	-4.217624000	3.467231000	0.452667000
1	-2.789048000	4.027205000	-0.406665000
1	-3.674202000	2.616136000	-0.998789000
6	-2.024554000	2.942602000	2.034826000
1	-1.435080000	2.276273000	2.668581000
1	-1.410648000	3.815026000	1.796908000
1	-2.884407000	3.293379000	2.609428000
6	-0.740310000	-0.631752000	3.182300000
1	-0.975136000	-1.629659000	3.573921000
1	0.118011000	-0.255313000	3.748392000
1	-1.588214000	0.009409000	3.438244000
6	-3.064707000	-1.966433000	0.175874000
6	-3.052888000	-0.232475000	-1.649924000
1	-3.833191000	-2.248224000	-0.548966000
1	-2.607118000	0.751858000	-1.816216000
6	-2.489502000	2.229401000	0.778020000
1	-3.124066000	1.388822000	1.090172000
6	-0.333937000	2.553270000	-0.494621000
1	-0.765129000	3.546864000	-0.338554000
6	-0.152909000	2.371449000	-1.988057000
1	-1.098470000	2.513944000	-2.517247000
1	0.564415000	3.100764000	-2.370925000
1	0.236591000	1.376697000	-2.218833000
6	0.993594000	2.529054000	0.244624000
1	0.850583000	2.532066000	1.327617000
1	1.586504000	1.653826000	-0.024263000
1	1.574015000	3.414775000	-0.023047000
5	1.410751000	-1.133534000	-1.321563000
7	2.545729000	-1.237834000	-0.211613000
6	3.668340000	-0.416315000	-0.225075000
6	4.414893000	-0.338231000	-1.407655000
6	4.115914000	0.310727000	0.881055000
6	5.546559000	0.445775000	-1.478831000

1	4.085043000	-0.910247000	-2.267469000
6	5.259625000	1.088905000	0.798581000
1	3.549322000	0.285160000	1.804288000
6	5.985193000	1.168279000	-0.376117000
1	6.101746000	0.489068000	-2.409777000
1	5.580075000	1.647118000	1.672048000
1	6.878830000	1.777897000	-0.434646000
1	1.747353000	-0.384393000	-2.211859000
6	0.970055000	-2.595593000	-1.805921000
1	0.758452000	-3.254402000	-0.953206000
1	0.083287000	-2.601055000	-2.448887000
1	1.780009000	-3.064846000	-2.374454000

**7P<sup>C-H</sup>** (TE= -639.391135)

6	-1.462912000	-1.296909000	-0.904630000
6	-0.123724000	-1.301139000	-0.935639000
1	-2.171001000	-1.968704000	-1.365672000
1	0.456426000	-2.038249000	-1.474967000
6	-3.288535000	0.299761000	-0.183702000
6	-3.069826000	-0.430687000	0.839689000
7	-1.912406000	-0.216398000	-0.062305000
7	0.471359000	-0.307485000	-0.217947000
5	-0.620589000	0.674016000	0.336033000
6	1.836322000	-0.165870000	-0.069749000
6	2.770818000	-0.953069000	-0.754638000
6	2.328661000	0.808366000	0.808356000
6	4.127081000	-0.769465000	-0.563353000
1	2.442298000	-1.712737000	-1.453293000
6	3.686693000	0.981432000	0.990129000
1	1.625337000	1.422371000	1.357556000
6	4.603451000	0.196989000	0.308019000
1	4.823697000	-1.394439000	-1.111820000
1	4.032542000	1.743724000	1.679940000
1	5.667968000	0.336404000	0.451265000
6	-3.223497000	-1.179196000	2.075701000
1	-2.534734000	-0.790731000	2.830210000
1	-4.242594000	-1.114217000	2.453583000
1	-2.972360000	-2.229583000	1.907453000
6	-3.984711000	1.096756000	-1.185250000
1	-5.054859000	1.121629000	-0.984378000
1	-3.601185000	2.118880000	-1.201345000
1	-3.818719000	0.667218000	-2.176695000
1	-0.601858000	0.777923000	1.548772000
6	-0.669709000	2.064392000	-0.457427000
1	0.251288000	2.640786000	-0.335884000
1	-0.804252000	1.902616000	-1.535038000

1 -1.488390000 2.706048000 -0.113118000

**9P<sup>C-H</sup>** (TE= -1409.660060)

6 1.206844000 -0.130993000 1.259714000  
7 0.840702000 0.179433000 -0.108636000  
15 -0.725729000 -0.024737000 0.367697000  
6 -0.040374000 -0.226370000 1.921240000  
7 -1.668722000 1.288797000 -0.040610000  
7 -1.557837000 -1.288234000 -0.319958000  
6 -0.238709000 -3.227386000 0.605008000  
1 0.436524000 -3.138060000 -0.249079000  
1 0.232443000 -2.723442000 1.450825000  
1 -0.349375000 -4.286636000 0.850954000  
6 -2.536368000 -2.658174000 1.481070000  
1 -3.541522000 -2.341934000 1.191574000  
1 -2.601231000 -3.666222000 1.897839000  
1 -2.184394000 -1.992756000 2.272361000  
6 -3.363988000 -1.582761000 -1.996021000  
1 -4.042419000 -1.001991000 -1.368032000  
1 -3.625925000 -1.397980000 -3.040434000  
1 -3.545903000 -2.642935000 -1.800357000  
6 -0.972517000 -2.009984000 -2.628407000  
1 0.067458000 -1.723665000 -2.456219000  
1 -1.064625000 -3.083658000 -2.441219000  
1 -1.210205000 -1.841438000 -3.681386000  
6 -3.996018000 1.817210000 -0.719507000  
1 -5.041376000 1.654060000 -0.447069000  
1 -3.858234000 2.894302000 -0.844134000  
1 -3.816886000 1.338519000 -1.684443000  
6 -3.329641000 1.897011000 1.704811000  
1 -2.705813000 1.435200000 2.474356000  
1 -3.103531000 2.966737000 1.684943000  
1 -4.375955000 1.787486000 1.999166000  
6 -0.382156000 -0.456433000 3.342674000  
1 -0.269115000 -1.502718000 3.665818000  
1 0.248739000 0.145529000 4.005767000  
1 -1.416803000 -0.173670000 3.560490000  
6 -1.600526000 -2.631926000 0.288399000  
6 -1.913860000 -1.204961000 -1.750242000  
1 -2.048304000 -3.270208000 -0.479715000  
1 -1.795085000 -0.150115000 -2.021889000  
6 -3.087736000 1.245527000 0.353810000  
1 -3.334613000 0.183448000 0.454740000  
6 -1.106173000 2.635126000 -0.277405000  
1 -1.951368000 3.317337000 -0.141965000  
6 -0.644734000 2.772873000 -1.714151000

1	-1.465437000	2.571134000	-2.406538000
1	-0.275139000	3.783544000	-1.906115000
1	0.163307000	2.071192000	-1.925940000
6	-0.041051000	3.085588000	0.709573000
1	-0.373091000	2.953087000	1.741158000
1	0.891213000	2.532349000	0.576069000
1	0.164468000	4.147007000	0.549727000
5	1.998675000	-0.275695000	-1.032491000
6	2.546645000	-0.272150000	1.396580000
1	3.151443000	-0.522308000	2.254885000
6	4.378512000	0.723891000	-0.040414000
6	4.545117000	-0.541624000	-0.116708000
7	3.162044000	-0.118897000	0.088139000
6	4.612617000	2.154928000	0.073422000
1	5.672060000	2.384843000	0.182560000
1	4.224501000	2.680160000	-0.803055000
1	4.074676000	2.531050000	0.948677000
6	5.182806000	-1.848757000	-0.206241000
1	4.828857000	-2.380862000	-1.092778000
1	6.267145000	-1.759735000	-0.253402000
1	4.911722000	-2.450912000	0.664932000
1	1.959875000	-1.479056000	-1.282197000
6	2.292455000	0.618668000	-2.322139000
1	1.505179000	0.503751000	-3.075240000
1	2.359964000	1.689362000	-2.091840000
1	3.229154000	0.326235000	-2.809750000

**II-PC<sup>H</sup>** (TE= -639.594566)

6	-0.759442000	1.353558000	0.189102000
6	-2.231198000	0.909383000	0.240675000
6	-2.297817000	-0.501704000	-0.332439000
6	-0.954765000	-1.076909000	0.133924000
7	-0.049174000	0.064675000	0.016371000
1	-2.880233000	1.607993000	-0.295308000
1	-2.574377000	0.892496000	1.280205000
6	1.316716000	-0.113694000	-0.044323000
6	1.868825000	-1.402436000	-0.174185000
6	3.232418000	-1.601828000	-0.266965000
6	4.119881000	-0.540492000	-0.227948000
6	3.597326000	0.733444000	-0.090595000
6	2.235540000	0.949131000	0.001964000
1	1.225345000	-2.270589000	-0.206383000
1	3.602564000	-2.616346000	-0.369248000
1	5.188312000	-0.702020000	-0.297705000
1	4.260582000	1.590907000	-0.051030000
1	1.893337000	1.965961000	0.111478000

6	-2.335572000	-0.503429000	-1.857462000
1	-2.480662000	-1.522086000	-2.228173000
1	-3.162708000	0.108890000	-2.227862000
1	-1.408657000	-0.126356000	-2.292183000
6	-3.512184000	-1.257985000	0.173453000
1	-4.423694000	-0.804877000	-0.226487000
1	-3.491623000	-2.300982000	-0.156709000
1	-3.587660000	-1.246599000	1.262204000
6	-0.548583000	2.306862000	-0.985432000
1	0.494615000	2.584268000	-1.128068000
1	-0.907702000	1.872823000	-1.918954000
1	-1.113742000	3.224901000	-0.804686000
6	-0.409983000	2.053403000	1.500839000
1	-1.125606000	2.860740000	1.678785000
1	-0.473256000	1.352844000	2.336664000
1	0.586936000	2.492784000	1.505448000
1	-0.652627000	-1.858111000	-0.574667000
6	-0.952700000	-1.661400000	1.537207000
1	0.067032000	-1.890535000	1.851331000
1	-1.369473000	-0.959307000	2.263547000
1	-1.533262000	-2.584936000	1.586321000

Cartesian coordinates of the C–F splitting product obtained from **4-7**, **9** and **IIIa**, along with their total energies (in hartrees) including zero point vibrational correction.

**4P<sup>C-F</sup>** (TE= -2044.969784)

6	-0.410589000	-1.245041000	1.036056000
6	-2.537266000	-0.476513000	0.588648000
7	-0.204958000	-0.308174000	0.017292000
7	-1.686528000	-1.407913000	1.326591000
6	-2.131010000	-2.141732000	2.477835000
1	-2.778002000	-2.979676000	2.195422000
1	-1.276248000	-2.545155000	3.020846000
1	-2.699029000	-1.480093000	3.140673000
15	-4.015270000	-1.026605000	-0.026157000
6	-5.257486000	-1.507882000	1.206665000
1	-6.206724000	-1.721624000	0.710503000
1	-4.941096000	-2.401543000	1.745530000
1	-5.390288000	-0.694152000	1.919896000
6	-4.074794000	-2.448596000	-1.176945000
1	-5.091382000	-2.688895000	-1.498062000
1	-3.455799000	-2.210068000	-2.042827000
1	-3.645796000	-3.320019000	-0.675663000
6	-4.772434000	0.330028000	-0.931225000
1	-5.759787000	0.026327000	-1.282798000
1	-4.863851000	1.195264000	-0.274718000

1	-4.143559000	0.593329000	-1.781222000
15	1.423251000	-0.541562000	0.259144000
6	0.863116000	-1.651752000	1.461386000
7	2.185872000	-1.074217000	-1.108834000
7	2.337387000	0.734264000	0.766843000
6	1.116061000	1.324317000	2.894179000
1	0.466433000	1.991031000	2.323604000
1	0.592518000	0.375936000	3.036856000
1	1.286901000	1.770252000	3.876912000
6	3.379911000	0.210968000	2.951596000
1	4.352176000	0.149241000	2.457343000
1	3.536250000	0.587003000	3.965464000
1	2.970540000	-0.796977000	3.031341000
6	4.286271000	2.034128000	-0.051616000
1	4.881286000	1.118371000	-0.064344000
1	4.625410000	2.670706000	-0.872005000
1	4.500966000	2.566244000	0.878681000
6	1.964864000	2.999365000	-0.179351000
1	0.909545000	2.765480000	-0.334720000
1	2.059385000	3.530985000	0.771987000
1	2.281910000	3.684032000	-0.969447000
6	4.512411000	-1.073279000	-1.975874000
1	5.535630000	-1.361840000	-1.725315000
1	4.289095000	-1.495440000	-2.958738000
1	4.474992000	0.014194000	-2.057949000
6	3.597353000	-3.099162000	-0.809807000
1	2.923421000	-3.457035000	-0.028285000
1	3.307407000	-3.572614000	-1.751508000
1	4.609736000	-3.433864000	-0.572883000
6	1.367436000	-2.669157000	2.415546000
1	1.279436000	-2.373240000	3.470625000
1	0.851221000	-3.629815000	2.308777000
1	2.427996000	-2.871260000	2.240732000
6	2.445588000	1.129503000	2.190090000
6	2.806513000	1.739561000	-0.213548000
1	2.922859000	2.112928000	2.162671000
1	2.666622000	1.278303000	-1.195109000
6	3.556585000	-1.584461000	-0.913200000
1	3.892254000	-1.178281000	0.050341000
6	1.492579000	-1.481842000	-2.349758000
1	2.270591000	-1.973630000	-2.942425000
6	1.043156000	-0.263755000	-3.131838000
1	1.902637000	0.352550000	-3.407496000
1	0.528045000	-0.565560000	-4.046867000
1	0.343493000	0.341909000	-2.553811000
6	0.389725000	-2.511206000	-2.158894000

1	0.742379000	-3.355691000	-1.562898000
1	-0.490265000	-2.081358000	-1.680286000
1	0.082280000	-2.890972000	-3.136428000
5	-1.577300000	0.310711000	-0.482919000
6	-1.590019000	1.923862000	-0.441261000
6	-1.472145000	2.704495000	-1.590974000
6	-1.693585000	2.604484000	0.772195000
6	-1.436544000	4.091309000	-1.534647000
6	-1.651121000	3.986719000	0.845926000
6	-1.518128000	4.738826000	-0.313091000
9	-1.810440000	-0.096094000	-1.845964000
1	-1.408043000	2.209044000	-2.555606000
1	-1.822030000	2.017187000	1.678760000
1	-1.729289000	4.483741000	1.807837000
1	-1.488805000	5.821876000	-0.263381000
1	-1.343757000	4.669846000	-2.448345000
<b>5P<sup>C-F</sup></b> (TE= -1663.798624)			
6	-0.396297000	-1.552321000	0.956222000
6	-2.549954000	-1.966381000	0.120141000
7	-0.467682000	-0.666886000	-0.122151000
7	-1.530956000	-2.196556000	1.185833000
6	-1.636359000	-3.239166000	2.173652000
1	-1.376776000	-4.224090000	1.770121000
1	-0.973205000	-3.022531000	3.011852000
1	-2.656783000	-3.284886000	2.556501000
15	1.092612000	-0.225935000	0.255021000
6	0.885766000	-1.438072000	1.486997000
7	2.119285000	-0.455353000	-1.015974000
7	1.399974000	1.311856000	0.764922000
6	0.052617000	1.435579000	2.896576000
1	-0.794501000	1.862911000	2.357997000
1	-0.110455000	0.360244000	2.997605000
1	0.076156000	1.873043000	3.897255000
6	2.571038000	1.272005000	2.944658000
1	3.490065000	1.595724000	2.451281000
1	2.566733000	1.682282000	3.957028000
1	2.593470000	0.184526000	3.028663000
6	2.701473000	3.279941000	-0.027658000
1	3.614219000	2.689572000	0.076108000
1	2.822938000	3.942433000	-0.887407000
1	2.604787000	3.916343000	0.855346000
6	0.201504000	3.200710000	-0.305416000
1	-0.650141000	2.556062000	-0.534534000
1	-0.005756000	3.712611000	0.639081000
1	0.274423000	3.963967000	-1.083444000
6	4.343962000	0.448039000	-1.663640000

1	5.362196000	0.589986000	-1.295138000
1	4.419825000	-0.028200000	-2.643985000
1	3.889991000	1.430975000	-1.798553000
6	4.158124000	-1.787009000	-0.535236000
1	3.599006000	-2.381282000	0.191082000
1	4.158115000	-2.325192000	-1.486672000
1	5.194739000	-1.714964000	-0.198833000
6	1.626791000	-2.115896000	2.580041000
1	1.398433000	-1.726716000	3.581565000
1	1.423741000	-3.190356000	2.599346000
1	2.706792000	-2.012292000	2.443527000
6	1.351334000	1.746529000	2.179977000
6	1.484563000	2.398042000	-0.239845000
1	1.413161000	2.837019000	2.130174000
1	1.610732000	1.896075000	-1.202779000
6	3.556410000	-0.401113000	-0.682289000
1	3.618409000	0.091837000	0.296516000
6	1.757263000	-1.047813000	-2.321250000
1	2.716784000	-1.176075000	-2.831834000
6	0.943077000	-0.070659000	-3.146526000
1	1.521922000	0.833204000	-3.352296000
1	0.661052000	-0.520993000	-4.100819000
1	0.017569000	0.209532000	-2.639473000
6	1.130343000	-2.426994000	-2.232314000
1	1.724124000	-3.086310000	-1.595650000
1	0.115666000	-2.377969000	-1.842698000
1	1.081335000	-2.869061000	-3.230031000
5	-1.917395000	-0.680950000	-0.767196000
6	-2.641408000	-3.220683000	-0.737921000
1	-2.996869000	-4.077951000	-0.154514000
1	-3.345141000	-3.063933000	-1.557365000
1	-1.676856000	-3.482511000	-1.179142000
6	-3.908784000	-1.708501000	0.744039000
1	-4.608959000	-1.394777000	-0.034433000
1	-4.326857000	-2.607415000	1.211873000
1	-3.878773000	-0.915948000	1.492950000
6	-2.628275000	0.756595000	-0.613304000
6	-3.031709000	1.492682000	-1.725651000
6	-2.811565000	1.356013000	0.633502000
6	-3.576981000	2.763894000	-1.604062000
1	-2.903142000	1.058212000	-2.712043000
6	-3.356646000	2.620190000	0.772723000
1	-2.502248000	0.816015000	1.525206000
6	-3.740154000	3.334668000	-0.353231000
1	-3.874257000	3.312908000	-2.491653000
1	-3.477701000	3.054533000	1.760271000



1	-4.164574000	4.327602000	-0.254023000
9	-1.857416000	-1.028168000	-2.133652000

**6P<sup>C-F</sup>** (TE= -1832.183239)

6	-0.089860000	-1.631555000	-0.387210000
7	-0.036978000	-0.288226000	-0.012785000
7	-1.299942000	-2.163754000	-0.195463000
6	-1.453819000	-3.565146000	0.130436000
1	-2.462375000	-3.895874000	-0.119159000
1	-0.741668000	-4.147644000	-0.453699000
1	-1.279466000	-3.730659000	1.198359000
15	1.614594000	-0.407501000	-0.266520000
6	1.185950000	-2.019858000	-0.759935000
7	2.145561000	0.717158000	-1.344720000
7	2.599266000	-0.274532000	1.039064000
6	1.837550000	-2.251108000	2.424159000
1	1.036036000	-1.618382000	2.809588000
1	1.417272000	-2.896029000	1.649706000
1	2.196569000	-2.890892000	3.233536000
6	4.059963000	-2.259631000	1.226569000
1	4.933786000	-1.655114000	0.973811000
1	4.382382000	-3.063504000	1.892192000
1	3.686130000	-2.719869000	0.309616000
6	4.347865000	1.305989000	1.816982000
1	4.930359000	1.093881000	0.918081000
1	4.518229000	2.348683000	2.093547000
1	4.739663000	0.689257000	2.629713000
6	2.048732000	1.348282000	2.838547000
1	0.985436000	1.186179000	2.653264000
1	2.348701000	0.702830000	3.668833000
1	2.196060000	2.382255000	3.157856000
6	4.291933000	1.878077000	-1.808327000
1	5.347409000	1.701533000	-2.026090000
1	3.913544000	2.559891000	-2.573590000
1	4.223019000	2.380741000	-0.842324000
6	3.617387000	-0.133385000	-3.153945000
1	3.098641000	-1.094534000	-3.131216000
1	3.168745000	0.474634000	-3.943732000
1	4.659314000	-0.310711000	-3.428462000
6	1.764600000	-3.251359000	-1.348837000
1	1.945479000	-4.046709000	-0.613930000
1	1.115619000	-3.669055000	-2.124016000
1	2.724932000	-3.042690000	-1.827811000
6	2.992269000	-1.418916000	1.896739000
6	2.865646000	1.075969000	1.591412000
1	3.454220000	-0.950244000	2.769662000

1	2.534963000	1.779036000	0.821005000
6	3.541359000	0.559571000	-1.805582000
1	4.028793000	-0.092586000	-1.069913000
6	1.270810000	1.593456000	-2.159370000
1	1.941730000	2.010914000	-2.916178000
6	0.758623000	2.753623000	-1.330533000
1	1.592450000	3.343228000	-0.942210000
1	0.128329000	3.409082000	-1.935888000
1	0.153440000	2.410371000	-0.488188000
6	0.177581000	0.864578000	-2.920193000
1	0.590870000	0.039799000	-3.504878000
1	-0.586927000	0.466611000	-2.252974000
1	-0.307799000	1.560728000	-3.607995000
5	-1.243412000	-0.026218000	0.981919000
7	-2.115685000	-1.252686000	0.517203000
6	-3.430006000	-1.184639000	0.071524000
6	-4.373639000	-0.560053000	0.893144000
6	-3.856123000	-1.707239000	-1.150488000
6	-5.683729000	-0.427791000	0.484132000
1	-4.050668000	-0.172235000	1.853173000
6	-5.179189000	-1.582800000	-1.543032000
1	-3.137519000	-2.187881000	-1.804344000
6	-6.101756000	-0.938290000	-0.738171000
1	-6.393508000	0.072275000	1.133826000
1	-5.486411000	-1.990283000	-2.500298000
1	-7.134264000	-0.841328000	-1.051415000
6	-1.888819000	1.423225000	0.765143000
6	-2.495796000	1.793073000	-0.436299000
6	-1.774951000	2.405414000	1.745194000
6	-2.958283000	3.077663000	-0.655524000
1	-2.610340000	1.053879000	-1.225474000
6	-2.224119000	3.702127000	1.534463000
1	-1.318410000	2.147397000	2.695679000
6	-2.816197000	4.043117000	0.331059000
1	-3.429420000	3.330447000	-1.599423000
1	-2.114637000	4.447456000	2.315243000
1	-3.172201000	5.053529000	0.162747000
9	-0.824201000	-0.211655000	2.310729000

**7P<sup>C-F</sup>** (TE= -930.333576)

6	-0.946974000	-2.161881000	-1.210326000
6	0.382133000	-2.043880000	-1.108469000
1	-1.542440000	-2.835278000	-1.807652000
1	1.086981000	-2.633774000	-1.679892000
6	-2.909885000	-0.692764000	-0.555808000
6	-2.867648000	-1.596015000	0.343872000

7	-1.566456000	-1.257070000	-0.278561000
7	0.812463000	-1.132203000	-0.184391000
5	-0.391176000	-0.468337000	0.530221000
6	2.137101000	-0.738007000	-0.055090000
6	3.099510000	-0.992789000	-1.035049000
6	2.529842000	-0.036596000	1.088616000
6	4.408089000	-0.578330000	-0.862177000
1	2.822535000	-1.497735000	-1.953019000
6	3.835679000	0.384344000	1.243417000
1	1.797376000	0.164441000	1.861600000
6	4.790242000	0.112699000	0.275064000
1	5.134958000	-0.788731000	-1.639086000
1	4.112471000	0.926826000	2.140592000
1	5.814856000	0.440085000	0.402867000
6	-3.273761000	-2.567753000	1.348326000
1	-2.826192000	-2.323992000	2.313291000
1	-4.358032000	-2.587781000	1.448371000
1	-2.925181000	-3.563082000	1.062097000
6	-3.399623000	0.300203000	-1.500970000
1	-4.487564000	0.285572000	-1.548889000
1	-3.065636000	1.300135000	-1.211960000
1	-2.993877000	0.090966000	-2.494165000
6	-0.552073000	1.099198000	0.274980000
6	-1.212972000	1.918482000	1.187400000
6	-0.144097000	1.673647000	-0.929075000
6	-1.465855000	3.253779000	0.909998000
1	-1.537155000	1.497120000	2.134408000
6	-0.388007000	3.006166000	-1.215606000
1	0.378161000	1.058985000	-1.659364000
6	-1.055462000	3.800427000	-0.295068000
1	-1.982182000	3.871690000	1.636816000
1	-0.055829000	3.430071000	-2.157049000
1	-1.248411000	4.844609000	-0.514473000
9	-0.520939000	-0.828791000	1.870095000

**9P<sup>C-F</sup>** (TE= -1700.603096)

6	-0.251529000	-1.263452000	-1.426483000
7	-0.336258000	-0.288462000	-0.361362000
15	1.319184000	-0.207490000	-0.425641000
6	1.124372000	-1.270502000	-1.752079000
7	1.901294000	1.340105000	-0.617732000
7	2.149846000	-0.737480000	0.910483000
6	1.210901000	-3.086393000	0.997599000
1	0.346669000	-2.697295000	1.539913000
1	0.924977000	-3.204947000	-0.049835000
1	1.456120000	-4.073943000	1.396569000

6	3.607178000	-2.650148000	0.349009000
1	4.485444000	-2.032425000	0.550458000
1	3.850665000	-3.685054000	0.602000000
1	3.399170000	-2.608450000	-0.721623000
6	3.701086000	0.115906000	2.653547000
1	4.447826000	0.306241000	1.879435000
1	3.804422000	0.886679000	3.420957000
1	3.937462000	-0.841544000	3.124970000
6	1.245614000	-0.134563000	3.145692000
1	0.237950000	-0.046043000	2.733658000
1	1.348196000	-1.141737000	3.560178000
1	1.348479000	0.573076000	3.971780000
6	4.033340000	2.518452000	-0.144644000
1	5.110166000	2.484551000	-0.325037000
1	3.686756000	3.512147000	-0.439814000
1	3.863710000	2.405374000	0.927534000
6	3.596095000	1.567255000	-2.427012000
1	3.102570000	0.768682000	-2.985241000
1	3.231725000	2.525235000	-2.807576000
1	4.668286000	1.520980000	-2.630769000
6	1.893028000	-2.064807000	-2.736928000
1	1.888662000	-3.145147000	-2.526375000
1	1.507882000	-1.941547000	-3.755272000
1	2.941710000	-1.755139000	-2.764184000
6	2.414619000	-2.172645000	1.153947000
6	2.293811000	0.147572000	2.085933000
1	2.699166000	-2.224632000	2.208886000
1	2.116925000	1.158757000	1.711508000
6	3.339428000	1.424730000	-0.936320000
1	3.773588000	0.467091000	-0.620217000
6	1.072051000	2.503383000	-0.985038000
1	1.791248000	3.279767000	-1.266560000
6	0.322272000	3.022349000	0.226514000
1	1.024885000	3.327446000	1.006123000
1	-0.294929000	3.884919000	-0.036746000
1	-0.341343000	2.261689000	0.642036000
6	0.182716000	2.283526000	-2.197503000
1	0.775067000	2.005917000	-3.071389000
1	-0.548559000	1.495639000	-2.020100000
1	-0.358452000	3.204967000	-2.427861000
5	-1.648680000	-0.433975000	0.414416000
6	-1.444480000	-1.858825000	-1.663224000
1	-1.699299000	-2.681522000	-2.314546000
6	-3.843010000	-1.542936000	-0.877386000
6	-3.339782000	-2.443428000	-0.122667000
7	-2.388416000	-1.437115000	-0.640462000

6	-4.797493000	-0.857648000	-1.740148000
1	-5.708731000	-1.443817000	-1.854982000
1	-5.053796000	0.124803000	-1.337548000
1	-4.347183000	-0.705879000	-2.725080000
6	-3.162349000	-3.661429000	0.655030000
1	-2.998328000	-3.423793000	1.707646000
1	-4.023081000	-4.323079000	0.565018000
1	-2.271095000	-4.182413000	0.293534000
6	-2.483262000	0.911880000	0.638922000
6	-2.911507000	1.678605000	-0.445034000
6	-2.751866000	1.405288000	1.912520000
6	-3.565525000	2.885777000	-0.273518000
1	-2.708427000	1.325874000	-1.454458000
6	-3.398120000	2.619154000	2.100091000
1	-2.433943000	0.829390000	2.776392000
6	-3.805593000	3.364329000	1.006790000
1	-3.881916000	3.461597000	-1.136968000
1	-3.584862000	2.985091000	3.104143000
1	-4.309789000	4.313691000	1.149240000
9	-1.525289000	-1.161878000	1.610065000

**IIIa-PC-F** (TE= -1340.868236)

13	0.000020000	-0.166564000	0.767955000
7	1.407629000	-1.214325000	0.067264000
7	-1.407519000	-1.214410000	0.067244000
6	1.252304000	-2.447313000	-0.402719000
6	-1.252118000	-2.447382000	-0.402754000
6	0.000112000	-3.041770000	-0.569861000
1	0.000146000	-4.067452000	-0.913055000
6	2.688291000	-0.594010000	0.103939000
6	3.259257000	-0.283293000	1.330931000
6	3.323132000	-0.202643000	-1.068370000
6	4.467392000	0.392252000	1.381641000
6	4.530435000	0.468772000	-1.011940000
6	5.107557000	0.766043000	0.212835000
1	4.906967000	0.630145000	2.343126000
1	5.016960000	0.774727000	-1.930728000
1	6.050023000	1.298781000	0.254546000
6	-2.688215000	-0.594163000	0.103920000
6	-3.323035000	-0.202739000	-1.068382000
6	-3.259232000	-0.283555000	1.330915000
6	-4.530366000	0.468625000	-1.011942000
6	-4.467396000	0.391938000	1.381635000
6	-5.107538000	0.765787000	0.212836000
1	-5.016874000	0.774626000	-1.930724000
1	-4.907011000	0.629747000	2.343123000

1	-6.050025000	1.298486000	0.254555000
6	-2.453076000	-3.259116000	-0.769011000
1	-2.192237000	-4.311879000	-0.855955000
1	-3.245208000	-3.143488000	-0.027205000
1	-2.865668000	-2.934714000	-1.726678000
6	2.453311000	-3.258986000	-0.768955000
1	2.192560000	-4.311788000	-0.855692000
1	2.865762000	-2.934717000	-1.726729000
1	3.245512000	-3.143157000	-0.027257000
1	-2.743722000	-0.573190000	2.240270000
1	-2.849517000	-0.410736000	-2.022172000
1	2.849649000	-0.410723000	-2.022159000
1	2.743734000	-0.572890000	2.240290000
6	-0.000061000	1.643819000	0.050182000
6	-0.000215000	2.791454000	0.844917000
6	-0.000013000	1.834406000	-1.334571000
6	-0.000317000	4.063031000	0.291146000
1	-0.000256000	2.690808000	1.927390000
6	-0.000112000	3.098125000	-1.902296000
1	0.000094000	0.967044000	-1.995243000
6	-0.000265000	4.217866000	-1.085326000
1	-0.000345000	5.210553000	-1.522091000
9	-0.000007000	-0.240768000	2.442424000
1	-0.000438000	4.936918000	0.934108000
1	-0.000071000	3.213400000	-2.981131000

Cartesian coordinates of the C–H (*para*, *meta* and *ortho*) splitting product obtained from **4-7** and **9**, along with their total energies (in hartrees) including zero point vibrational correction.

**4P<sup>p</sup>(C-F)** (TE= -2044.899005)

6	-0.305468000	-1.291933000	1.126576000
6	-2.503530000	-0.858033000	0.548989000
7	-0.181077000	-0.435889000	0.027466000
7	-1.562346000	-1.564767000	1.418132000
6	-1.954971000	-2.274102000	2.602864000
1	-2.405250000	-3.244530000	2.363716000
1	-1.089417000	-2.451341000	3.241978000
1	-2.693634000	-1.682878000	3.153233000
15	-3.763010000	-1.737158000	-0.165865000
6	-4.979738000	-2.460015000	0.968705000
1	-5.828207000	-2.848684000	0.401648000
1	-4.537908000	-3.281645000	1.533522000
1	-5.323763000	-1.695183000	1.665183000
6	-3.426276000	-3.151613000	-1.286213000
1	-4.338093000	-3.602607000	-1.685148000
1	-2.803079000	-2.798598000	-2.110247000

1	-2.866849000	-3.909182000	-0.731024000
6	-4.693468000	-0.587279000	-1.188043000
1	-5.549571000	-1.094538000	-1.636156000
1	-5.031950000	0.248114000	-0.575442000
1	-4.039634000	-0.204261000	-1.973059000
15	1.456679000	-0.524681000	0.257812000
6	0.998117000	-1.550846000	1.575482000
7	2.223032000	-1.132490000	-1.078954000
7	2.293436000	0.851052000	0.617134000
6	1.138198000	1.533698000	2.753176000
1	0.421057000	2.115075000	2.170302000
1	0.684648000	0.567942000	2.987802000
1	1.325304000	2.061347000	3.691411000
6	3.473922000	0.577241000	2.774717000
1	4.426189000	0.550519000	2.240006000
1	3.644430000	1.034983000	3.751980000
1	3.145282000	-0.449578000	2.942098000
6	4.079128000	2.231627000	-0.413956000
1	4.747967000	1.368400000	-0.389381000
1	4.319815000	2.823018000	-1.300264000
1	4.296062000	2.854811000	0.457398000
6	1.678124000	2.990509000	-0.477644000
1	0.640569000	2.655929000	-0.547293000
1	1.779062000	3.605455000	0.421245000
1	1.889199000	3.630873000	-1.337192000
6	4.506595000	-1.035302000	-2.047152000
1	5.559271000	-1.210045000	-1.814040000
1	4.287252000	-1.572750000	-2.973082000
1	4.370988000	0.031257000	-2.234759000
6	3.802707000	-3.001725000	-0.652882000
1	3.190643000	-3.329454000	0.190503000
1	3.514306000	-3.587146000	-1.530042000
1	4.846945000	-3.234500000	-0.432805000
6	1.586254000	-2.439589000	2.607129000
1	1.520701000	-2.040388000	3.629310000
1	1.113487000	-3.427796000	2.619385000
1	2.648695000	-2.611875000	2.411948000
6	2.442397000	1.368763000	1.996462000
6	2.623586000	1.805637000	-0.464199000
1	2.849377000	2.375354000	1.866147000
1	2.473931000	1.254827000	-1.397153000
6	3.636217000	-1.512396000	-0.898739000
1	3.972378000	-0.988705000	0.005726000
6	1.521261000	-1.700997000	-2.248630000
1	2.307953000	-2.203112000	-2.820662000
6	0.966017000	-0.596982000	-3.126944000

1	1.768985000	0.055270000	-3.479076000
1	0.461068000	-1.019317000	-3.999248000
1	0.233697000	0.006810000	-2.585570000
6	0.486604000	-2.764381000	-1.916950000
1	0.906199000	-3.529911000	-1.260595000
1	-0.389497000	-2.332572000	-1.431960000
1	0.157204000	-3.250050000	-2.839102000
5	-1.603739000	0.018277000	-0.523260000
1	-1.739129000	-0.336471000	-1.697856000
6	-1.796815000	1.618799000	-0.460583000
6	-1.820512000	2.408163000	-1.607850000
6	-1.921082000	2.286933000	0.758820000
6	-1.935640000	3.792389000	-1.560261000
1	-1.742195000	1.920614000	-2.577524000
6	-2.025709000	3.664999000	0.844636000
1	-1.944192000	1.694413000	1.671241000
6	-2.026858000	4.396840000	-0.326882000
1	-1.954384000	4.400612000	-2.457567000
1	-2.115854000	4.178774000	1.795450000
9	-2.133563000	5.734575000	-0.258677000

**4P<sup>m</sup>(C-F)** (TE= -2044.899966)

6	-0.332236000	-1.403890000	1.013236000
6	-2.521061000	-0.811910000	0.562889000
7	-0.198772000	-0.409068000	0.038857000
7	-1.592380000	-1.669072000	1.297904000
6	-1.989008000	-2.521137000	2.382681000
1	-2.499311000	-3.422184000	2.022879000
1	-1.116419000	-2.833651000	2.956938000
1	-2.677326000	-1.979931000	3.039772000
15	-3.863955000	-1.509492000	-0.194993000
6	-5.082416000	-2.289713000	0.899304000
1	-5.975056000	-2.555198000	0.329026000
1	-4.674314000	-3.198464000	1.343389000
1	-5.349019000	-1.594812000	1.695901000
6	-3.676421000	-2.788859000	-1.498401000
1	-4.634224000	-3.128667000	-1.899877000
1	-3.069905000	-2.374057000	-2.305810000
1	-3.145011000	-3.643854000	-1.072427000
6	-4.748487000	-0.178934000	-1.019761000
1	-5.647738000	-0.569279000	-1.499315000
1	-5.015711000	0.585823000	-0.290653000
1	-4.094593000	0.266593000	-1.771123000
15	1.439469000	-0.585212000	0.211093000
6	0.970042000	-1.767488000	1.386526000
7	2.153919000	-1.029554000	-1.215435000



7	2.335163000	0.697624000	0.734130000
6	1.260805000	1.112718000	2.979352000
1	0.545900000	1.784611000	2.500445000
1	0.783434000	0.137784000	3.101036000
1	1.491119000	1.507025000	3.971977000
6	3.559742000	0.088278000	2.796656000
1	4.497174000	0.105599000	2.236051000
1	3.770312000	0.399384000	3.822590000
1	3.198843000	-0.940859000	2.829708000
6	4.153350000	2.140440000	-0.145084000
1	4.787445000	1.258242000	-0.255914000
1	4.398700000	2.838725000	-0.948433000
1	4.413227000	2.629429000	0.797266000
6	1.785210000	2.989763000	-0.041989000
1	0.733528000	2.707931000	-0.127819000
1	1.930532000	3.471764000	0.929125000
1	2.004433000	3.732816000	-0.812144000
6	4.427587000	-0.902044000	-2.204111000
1	5.472778000	-1.160676000	-2.020625000
1	4.168349000	-1.287745000	-3.193186000
1	4.344996000	0.185679000	-2.232831000
6	3.645546000	-3.012896000	-1.092137000
1	3.026789000	-3.430278000	-0.294584000
1	3.320681000	-3.451758000	-2.039325000
1	4.679498000	-3.322922000	-0.925260000
6	1.546951000	-2.808051000	2.272072000
1	1.517280000	-2.550656000	3.340437000
1	1.039358000	-3.772594000	2.161687000
1	2.598057000	-2.986709000	2.027838000
6	2.537614000	1.012888000	2.166664000
6	2.681275000	1.779272000	-0.214944000
1	2.976337000	2.014591000	2.164448000
1	2.490493000	1.368293000	-1.210317000
6	3.549076000	-1.497506000	-1.119028000
1	3.922132000	-1.125606000	-0.155682000
6	1.408862000	-1.396759000	-2.437389000
1	2.165750000	-1.835544000	-3.095307000
6	0.877379000	-0.159107000	-3.132963000
1	1.696106000	0.510410000	-3.407837000
1	0.339705000	-0.433659000	-4.043822000
1	0.178695000	0.384176000	-2.492399000
6	0.342429000	-2.461866000	-2.238641000
1	0.741841000	-3.322901000	-1.698395000
1	-0.513449000	-2.071722000	-1.687375000
1	-0.012669000	-2.806002000	-3.213324000
5	-1.612106000	0.164511000	-0.405762000

1	-1.791086000	-0.016578000	-1.613380000
6	-1.733054000	1.749853000	-0.116996000
6	-1.749932000	2.678568000	-1.154745000
6	-1.789746000	2.251891000	1.185566000
6	-1.796599000	4.031767000	-0.883467000
1	-1.720333000	2.347736000	-2.190268000
6	-1.825159000	3.609893000	1.446145000
1	-1.814070000	1.542851000	2.010163000
6	-1.825242000	4.526443000	0.401480000
1	-1.859072000	3.970685000	2.469221000
1	-1.859262000	5.595947000	0.570270000
9	-1.809071000	4.901004000	-1.909013000

**4P<sup>o</sup>(C-F)** (TE= -2044.900132)

6	-0.394925000	-1.191153000	1.154055000
6	-2.558556000	-0.552847000	0.637676000
7	-0.217017000	-0.312569000	0.080174000
7	-1.665342000	-1.364927000	1.463148000
6	-2.097931000	-2.088913000	2.624521000
1	-2.624559000	-3.011493000	2.353581000
1	-1.241567000	-2.357792000	3.243755000
1	-2.782399000	-1.465420000	3.208206000
15	-3.898923000	-1.288160000	-0.092687000
6	-5.152496000	-1.961014000	1.031832000
1	-6.039965000	-2.250565000	0.465281000
1	-4.771463000	-2.842234000	1.549397000
1	-5.419356000	-1.204040000	1.769461000
6	-3.707888000	-2.666033000	-1.290934000
1	-4.662928000	-3.010425000	-1.695058000
1	-3.067365000	-2.327192000	-2.107542000
1	-3.212457000	-3.499977000	-0.786814000
6	-4.744071000	-0.010587000	-1.035575000
1	-5.632614000	-0.425967000	-1.514228000
1	-5.025713000	0.804831000	-0.369170000
1	-4.063915000	0.375587000	-1.796780000
15	1.410340000	-0.552994000	0.267383000
6	0.889526000	-1.578126000	1.563621000
7	2.090239000	-1.178424000	-1.106774000
7	2.372678000	0.731697000	0.649833000
6	1.346735000	1.444701000	2.842615000
1	0.671650000	2.112865000	2.303898000
1	0.809635000	0.518793000	3.060091000
1	1.611252000	1.917205000	3.791675000
6	3.578618000	0.269588000	2.759899000
1	4.509678000	0.172950000	2.196596000
1	3.817390000	0.672027000	3.747136000

1	3.157472000	-0.726938000	2.900648000
6	4.238815000	1.995023000	-0.390627000
1	4.833088000	1.078994000	-0.410257000
1	4.503597000	2.590764000	-1.267104000
1	4.531649000	2.571438000	0.490667000
6	1.911528000	2.954156000	-0.352615000
1	0.847199000	2.712301000	-0.393787000
1	2.093853000	3.527581000	0.560821000
1	2.148370000	3.602647000	-1.199176000
6	4.349527000	-1.236182000	-2.134251000
1	5.388895000	-1.507581000	-1.936614000
1	4.062100000	-1.718992000	-3.071543000
1	4.300951000	-0.155982000	-2.281504000
6	3.518182000	-3.186105000	-0.789079000
1	2.905928000	-3.492924000	0.061952000
1	3.155525000	-3.712877000	-1.675788000
1	4.545146000	-3.512802000	-0.610996000
6	1.416910000	-2.555878000	2.546434000
1	1.417884000	-2.190045000	3.583084000
1	0.850908000	-3.493792000	2.539408000
1	2.451915000	-2.822387000	2.313351000
6	2.607113000	1.183113000	2.040281000
6	2.751743000	1.693630000	-0.408789000
1	3.105884000	2.150212000	1.931008000
1	2.528966000	1.191506000	-1.354621000
6	3.470683000	-1.680079000	-0.978932000
1	3.871805000	-1.219265000	-0.066898000
6	1.315396000	-1.643386000	-2.276739000
1	2.044407000	-2.187321000	-2.885874000
6	0.831738000	-0.467508000	-3.102239000
1	1.676863000	0.131261000	-3.450744000
1	0.278273000	-0.817402000	-3.977130000
1	0.159011000	0.174006000	-2.528544000
6	0.204915000	-2.629535000	-1.952706000
1	0.573783000	-3.447856000	-1.330348000
1	-0.621773000	-2.142935000	-1.434106000
1	-0.184013000	-3.055913000	-2.880952000
5	-1.604053000	0.275264000	-0.427237000
1	-1.796257000	-0.034066000	-1.595542000
6	-1.656713000	1.888054000	-0.259009000
6	-1.645992000	2.802188000	-1.298325000
6	-1.688824000	2.458281000	1.015841000
6	-1.647002000	4.176525000	-1.131015000
6	-1.675365000	3.824603000	1.234713000
1	-1.731886000	1.778379000	1.864418000
6	-1.652501000	4.692679000	0.151715000

1	-1.690354000	4.216630000	2.246170000
1	-1.648385000	5.766093000	0.303483000
1	-1.636176000	4.818320000	-2.004663000
9	-1.618867000	2.361021000	-2.573492000

**5P<sup>p(C-F)</sup>** (TE= -1663.730917)

6	-0.217521000	1.784345000	0.799371000
6	1.681973000	2.781739000	-0.158048000
7	0.113225000	0.886776000	-0.216648000
7	0.665511000	2.761658000	0.940878000
6	0.459356000	3.858125000	1.851511000
1	-0.100318000	4.681364000	1.393697000
1	-0.089035000	3.513005000	2.728752000
1	1.421796000	4.245653000	2.188601000
15	-1.241147000	0.032636000	0.215052000
6	-1.403824000	1.325753000	1.370068000
7	-2.289846000	-0.134892000	-1.049475000
7	-1.076157000	-1.495303000	0.815536000
6	0.267947000	-1.079250000	2.912397000
1	1.199860000	-1.270194000	2.378122000
1	0.104667000	0.000244000	2.945456000
1	0.384050000	-1.438717000	3.937397000
6	-2.184040000	-1.668529000	3.021303000
1	-2.970764000	-2.276910000	2.569693000
1	-2.049010000	-1.999981000	4.053373000
1	-2.526428000	-0.632990000	3.048980000
6	-1.712123000	-3.811400000	0.162687000
1	-2.762563000	-3.525330000	0.247778000
1	-1.622740000	-4.532156000	-0.653021000
1	-1.424472000	-4.329821000	1.080589000
6	0.640562000	-2.983808000	-0.180102000
1	1.248300000	-2.121308000	-0.464351000
1	1.002866000	-3.351827000	0.784427000
1	0.801590000	-3.775846000	-0.914864000
6	-4.133357000	-1.702191000	-1.620267000
1	-5.065429000	-2.121688000	-1.235620000
1	-4.339583000	-1.327555000	-2.625674000
1	-3.404370000	-2.509842000	-1.702347000
6	-4.638291000	0.543436000	-0.617545000
1	-4.288261000	1.319088000	0.067412000
1	-4.798131000	1.001530000	-1.597157000
1	-5.605755000	0.180604000	-0.263623000
6	-2.311782000	1.819599000	2.435098000
1	-1.973480000	1.585353000	3.453804000
1	-2.444937000	2.903960000	2.382894000
1	-3.309693000	1.384670000	2.330319000

6	-0.885955000	-1.806446000	2.250757000
6	-0.827510000	-2.612391000	-0.125459000
1	-0.620906000	-2.867108000	2.265550000
1	-1.108295000	-2.231710000	-1.111014000
6	-3.644775000	-0.601652000	-0.696200000
1	-3.558639000	-1.034877000	0.308692000
6	-2.116273000	0.471364000	-2.385591000
1	-3.065121000	0.278153000	-2.895531000
6	-1.034450000	-0.245984000	-3.169533000
1	-1.288924000	-1.299921000	-3.305394000
1	-0.918307000	0.206073000	-4.157226000
1	-0.066479000	-0.180549000	-2.666096000
6	-1.929169000	1.977049000	-2.369908000
1	-2.692413000	2.462422000	-1.758125000
1	-0.947246000	2.246447000	-1.983226000
1	-2.007378000	2.366845000	-3.387328000
5	1.467661000	1.302685000	-0.922986000
6	1.355054000	3.935965000	-1.095054000
1	1.435395000	4.910092000	-0.596780000
1	2.054662000	3.934871000	-1.934103000
1	0.347013000	3.845967000	-1.507692000
6	3.065637000	3.009464000	0.420973000
1	3.812268000	2.879475000	-0.366725000
1	3.188477000	4.024122000	0.818121000
1	3.303901000	2.300483000	1.215336000
6	2.600066000	0.182130000	-0.698941000
6	3.218683000	-0.449904000	-1.775809000
6	2.971787000	-0.260104000	0.573019000
6	4.146517000	-1.470703000	-1.611389000
1	2.954390000	-0.138613000	-2.782974000
6	3.893306000	-1.272973000	0.775036000
1	2.509023000	0.198707000	1.443292000
6	4.465902000	-1.866254000	-0.332052000
1	4.617157000	-1.960455000	-2.456164000
1	4.169443000	-1.610168000	1.768047000
9	5.356291000	-2.854304000	-0.153923000
1	1.310635000	1.482259000	-2.120805000

**5P<sup>m</sup>(C-F)** (TE= -1663.732150)

6	-0.151547000	1.863011000	0.641007000
6	1.902372000	2.611380000	-0.218673000
7	0.212448000	0.822620000	-0.215091000
7	0.784630000	2.792797000	0.760595000
6	0.568009000	4.009402000	1.500389000
1	0.108898000	4.793972000	0.888600000
1	-0.080726000	3.812917000	2.354779000

1	1.518608000	4.385629000	1.880866000
15	-1.241314000	0.118640000	0.161824000
6	-1.421852000	1.557929000	1.126260000
7	-2.163911000	-0.142453000	-1.182160000
7	-1.257212000	-1.325952000	0.958236000
6	-0.094305000	-0.730203000	3.118566000
1	0.866901000	-1.046354000	2.710330000
1	-0.177185000	0.353005000	3.004173000
1	-0.104478000	-0.962495000	4.185937000
6	-2.583909000	-1.140454000	3.038366000
1	-3.367589000	-1.749766000	2.583031000
1	-2.576123000	-1.343516000	4.111649000
1	-2.845559000	-0.090212000	2.902397000
6	-2.004375000	-3.660326000	0.527501000
1	-3.031949000	-3.296169000	0.463537000
1	-1.892416000	-4.484134000	-0.180778000
1	-1.851123000	-4.074558000	1.527014000
6	0.429025000	-3.040078000	0.347587000
1	1.129599000	-2.263932000	0.030210000
1	0.661980000	-3.302069000	1.384029000
1	0.600473000	-3.929703000	-0.262527000
6	-4.060810000	-1.644885000	-1.752593000
1	-5.057456000	-1.946410000	-1.423253000
1	-4.134066000	-1.396643000	-2.814107000
1	-3.393818000	-2.502381000	-1.650394000
6	-4.479861000	0.746072000	-1.110733000
1	-4.140832000	1.581408000	-0.493803000
1	-4.496164000	1.077186000	-2.152428000
1	-5.506088000	0.501327000	-0.828261000
6	-2.392463000	2.242269000	2.016497000
1	-2.178446000	2.120021000	3.087126000
1	-2.434520000	3.317175000	1.818825000
1	-3.405517000	1.863261000	1.855559000
6	-1.231876000	-1.460519000	2.432761000
6	-1.003248000	-2.569510000	0.193933000
1	-1.052879000	-2.525431000	2.604337000
1	-1.152431000	-2.302843000	-0.855611000
6	-3.581849000	-0.463960000	-0.927892000
1	-3.636610000	-0.760632000	0.127719000
6	-1.803231000	0.261106000	-2.556901000
1	-2.706185000	0.061374000	-3.142177000
6	-0.705823000	-0.626280000	-3.111746000
1	-1.027137000	-1.670351000	-3.137608000
1	-0.450858000	-0.323464000	-4.129872000
1	0.206114000	-0.554288000	-2.513353000
6	-1.497933000	1.738949000	-2.715662000

1	-2.276080000	2.353940000	-2.258853000
1	-0.540315000	1.992332000	-2.262962000
1	-1.442896000	1.989852000	-3.777386000
5	1.651780000	1.065360000	-0.820976000
6	1.754161000	3.655868000	-1.316034000
1	1.861902000	4.677983000	-0.932365000
1	2.526664000	3.503439000	-2.073244000
1	0.784729000	3.579216000	-1.814997000
6	3.236270000	2.823303000	0.471970000
1	4.043823000	2.550856000	-0.212508000
1	3.394811000	3.869985000	0.757528000
1	3.342899000	2.204480000	1.364061000
6	2.673789000	-0.085804000	-0.347268000
6	3.344416000	-0.871085000	-1.281935000
6	2.885172000	-0.393076000	1.000318000
6	4.164071000	-1.904480000	-0.872258000
1	3.219646000	-0.687193000	-2.345210000
6	3.708357000	-1.429558000	1.400502000
1	2.373260000	0.195049000	1.757343000
6	4.362282000	-2.209518000	0.456241000
1	3.844066000	-1.643028000	2.455927000
1	1.625376000	1.101347000	-2.040913000
1	5.011497000	-3.031029000	0.733241000
9	4.786475000	-2.645774000	-1.802262000

**5P<sup>o(C-F)</sup>** (TE= -1663.731639)

6	0.183759000	1.717619000	0.830546000
6	2.330547000	2.217378000	0.012621000
7	0.382088000	0.714038000	-0.118016000
7	1.251933000	2.478283000	1.018255000
6	1.225438000	3.640321000	1.868734000
1	0.894441000	4.539298000	1.336839000
1	0.552552000	3.468456000	2.709643000
1	2.222146000	3.828661000	2.270100000
15	-1.168403000	0.221846000	0.203164000
6	-1.120316000	1.573130000	1.301331000
7	-2.114155000	0.239257000	-1.149796000
7	-1.419298000	-1.270952000	0.859820000
6	-0.202094000	-1.077739000	3.064667000
1	0.701505000	-1.505215000	2.626989000
1	-0.108653000	0.010572000	3.055655000
1	-0.263971000	-1.406129000	4.104742000
6	-2.723466000	-1.069041000	2.951722000
1	-3.589584000	-1.500078000	2.444739000
1	-2.761166000	-1.367343000	4.001868000
1	-2.810863000	0.017801000	2.913015000

6	-2.524397000	-3.405905000	0.215807000
1	-3.480623000	-2.878523000	0.201817000
1	-2.543323000	-4.162322000	-0.571816000
1	-2.441744000	-3.936988000	1.167270000
6	-0.022922000	-3.165289000	0.074660000
1	0.794360000	-2.485049000	-0.176564000
1	0.159272000	-3.555436000	1.080484000
1	0.007595000	-4.010723000	-0.616307000
6	-4.220012000	-0.885165000	-1.842774000
1	-5.255282000	-1.052645000	-1.538083000
1	-4.241646000	-0.530057000	-2.875805000
1	-3.700096000	-1.844349000	-1.825107000
6	-4.262364000	1.468844000	-0.969176000
1	-3.799105000	2.176776000	-0.278052000
1	-4.221852000	1.898139000	-1.973719000
1	-5.315541000	1.361719000	-0.700411000
6	-1.976652000	2.320519000	2.255735000
1	-1.797843000	2.066308000	3.309506000
1	-1.841196000	3.401594000	2.159613000
1	-3.035952000	2.127883000	2.063685000
6	-1.433481000	-1.546259000	2.314645000
6	-1.360900000	-2.460411000	-0.021234000
1	-1.430989000	-2.637433000	2.384130000
1	-1.458814000	-2.074369000	-1.039281000
6	-3.566211000	0.121061000	-0.913200000
1	-3.672383000	-0.263763000	0.109407000
6	-1.688285000	0.715906000	-2.482281000
1	-2.609402000	0.720997000	-3.073256000
6	-0.744550000	-0.274817000	-3.135942000
1	-1.229618000	-1.246057000	-3.260677000
1	-0.440785000	0.083256000	-4.122151000
1	0.166523000	-0.409544000	-2.547493000
6	-1.153198000	2.135762000	-2.496780000
1	-1.827318000	2.816422000	-1.972559000
1	-0.169129000	2.189596000	-2.033242000
1	-1.054739000	2.479368000	-3.529004000
5	1.831411000	0.803047000	-0.746080000
6	2.359994000	3.378103000	-0.971678000
1	2.635015000	4.324379000	-0.489415000
1	3.097345000	3.177018000	-1.752093000
1	1.392230000	3.512718000	-1.461322000
6	3.677111000	2.141569000	0.707553000
1	4.436718000	1.821541000	-0.010276000
1	3.995642000	3.114015000	1.101400000
1	3.680716000	1.422625000	1.528085000
6	2.665678000	-0.535361000	-0.395573000



6	3.257781000	-1.358680000	-1.339605000
6	2.780053000	-0.991824000	0.920878000
6	3.903250000	-2.547264000	-1.042277000
6	3.420782000	-2.167576000	1.267564000
1	2.324475000	-0.393658000	1.705898000
6	3.984635000	-2.956317000	0.275590000
1	3.474507000	-2.473558000	2.307017000
1	1.782607000	0.988058000	-1.942943000
1	4.486604000	-3.884077000	0.524815000
9	3.210203000	-1.021722000	-2.640747000
1	4.329465000	-3.133071000	-1.848508000

**6P<sup>p(C-F)</sup>** (TE= -1832.110292)

6	-0.204650000	-1.799043000	0.262999000
7	-0.083956000	-0.433601000	-0.013651000
7	0.912720000	-2.470167000	-0.012544000
6	0.904701000	-3.870509000	-0.365759000
1	1.853980000	-4.331553000	-0.089418000
1	0.103542000	-4.371907000	0.177078000
1	0.753750000	-3.993587000	-1.442734000
15	-1.738077000	-0.368271000	0.215788000
6	-1.519354000	-2.041686000	0.630343000
7	-2.161813000	0.760067000	1.336194000
7	-2.673757000	-0.057434000	-1.100825000
6	-2.047334000	-2.014310000	-2.582485000
1	-1.166204000	-1.445659000	-2.889456000
1	-1.733281000	-2.750136000	-1.839485000
1	-2.428239000	-2.557179000	-3.450478000
6	-4.310938000	-1.869194000	-1.477447000
1	-5.126126000	-1.193857000	-1.208768000
1	-4.687949000	-2.585667000	-2.210811000
1	-4.023505000	-2.428937000	-0.585359000
6	-4.228083000	1.720847000	-1.866471000
1	-4.879218000	1.502478000	-1.017311000
1	-4.289089000	2.791224000	-2.074475000
1	-4.624020000	1.199846000	-2.741706000
6	-1.873004000	1.616012000	-2.751338000
1	-0.838910000	1.363695000	-2.504648000
1	-2.161331000	1.038196000	-3.633908000
1	-1.917718000	2.673332000	-3.021070000
6	-4.215630000	2.068055000	1.822754000
1	-5.278821000	1.968655000	2.051075000
1	-3.778919000	2.712018000	2.589831000
1	-4.119066000	2.573721000	0.860724000
6	-3.685687000	-0.004806000	3.139665000
1	-3.233180000	-0.998423000	3.103524000

1	-3.196717000	0.561951000	3.936191000
1	-4.737181000	-0.114325000	3.413278000
6	-2.259136000	-3.222728000	1.137174000
1	-2.500586000	-3.957946000	0.358330000
1	-1.697852000	-3.748537000	1.915095000
1	-3.208052000	-2.921769000	1.588966000
6	-3.135802000	-1.100829000	-2.046917000
6	-2.788544000	1.342253000	-1.575084000
1	-3.507493000	-0.536379000	-2.906104000
1	-2.448510000	1.963284000	-0.741793000
6	-3.563166000	0.698710000	1.800307000
1	-4.098980000	0.092532000	1.057375000
6	-1.208397000	1.537223000	2.160546000
1	-1.838009000	2.027025000	2.909943000
6	-0.562227000	2.633997000	1.337782000
1	-1.319873000	3.318137000	0.947972000
1	0.136341000	3.210976000	1.948043000
1	0.002792000	2.225460000	0.496233000
6	-0.208339000	0.690168000	2.927842000
1	-0.716952000	-0.064143000	3.531965000
1	0.488985000	0.184261000	2.259553000
1	0.370129000	1.329865000	3.598392000
5	1.099222000	-0.278983000	-1.068768000
7	1.836912000	-1.638330000	-0.686179000
6	3.133716000	-1.719407000	-0.193289000
6	4.167371000	-1.171355000	-0.960946000
6	3.462503000	-2.321893000	1.023011000
6	5.469099000	-1.191220000	-0.507423000
1	3.921265000	-0.718288000	-1.914840000
6	4.776846000	-2.348840000	1.461348000
1	2.676505000	-2.743988000	1.638779000
6	5.789498000	-1.780190000	0.709340000
1	6.249009000	-0.747662000	-1.116615000
1	5.005996000	-2.815185000	2.413724000
1	6.814753000	-1.801265000	1.058588000
6	1.942141000	1.055409000	-0.809392000
6	2.570918000	1.319561000	0.410407000
6	2.005417000	2.055517000	-1.774674000
6	3.220871000	2.513004000	0.665018000
1	2.553463000	0.564900000	1.192534000
6	2.641275000	3.269620000	-1.548216000
1	1.536502000	1.881915000	-2.739324000
6	3.237913000	3.475358000	-0.325232000
1	3.710781000	2.708818000	1.611700000
1	2.682172000	4.046526000	-2.302654000
1	0.667778000	-0.316955000	-2.211959000

9 3.857831000 4.640158000 -0.088122000

**6P<sup>m</sup>(C-F)** (TE= -1832.111019)

6	-0.097255000	-1.807930000	0.105927000
7	-0.039427000	-0.414840000	0.003664000
7	1.063665000	-2.387423000	-0.200643000
6	1.126444000	-3.727448000	-0.738814000
1	2.095428000	-4.174620000	-0.513849000
1	0.347780000	-4.334493000	-0.277416000
1	0.989111000	-3.712429000	-1.824503000
15	-1.702571000	-0.456787000	0.169742000
6	-1.409544000	-2.157279000	0.382730000
7	-2.225792000	0.498554000	1.403159000
7	-2.603905000	-0.025191000	-1.136213000
6	-1.819837000	-1.743543000	-2.823187000
1	-0.958799000	-1.099155000	-3.016580000
1	-1.497353000	-2.552471000	-2.164944000
1	-2.137555000	-2.188512000	-3.768777000
6	-4.126761000	-1.850548000	-1.807377000
1	-4.987890000	-1.255421000	-1.496006000
1	-4.434851000	-2.489279000	-2.638263000
1	-3.843571000	-2.500433000	-0.977092000
6	-4.219892000	1.761727000	-1.737298000
1	-4.889456000	1.407538000	-0.950456000
1	-4.328272000	2.845811000	-1.812427000
1	-4.556156000	1.338324000	-2.686961000
6	-1.831174000	1.881564000	-2.525908000
1	-0.795621000	1.647603000	-2.267842000
1	-2.055616000	1.408266000	-3.485874000
1	-1.919764000	2.961394000	-2.662319000
6	-4.358596000	1.641972000	1.959565000
1	-5.424021000	1.467837000	2.123569000
1	-3.985311000	2.198527000	2.822525000
1	-4.247938000	2.272450000	1.075967000
6	-3.780954000	-0.559314000	3.023189000
1	-3.276799000	-1.518175000	2.882603000
1	-3.355558000	-0.078368000	3.907778000
1	-4.835846000	-0.751313000	3.230229000
6	-2.103814000	-3.427959000	0.702889000
1	-2.278320000	-4.065879000	-0.173491000
1	-1.542869000	-4.023335000	1.429107000
1	-3.082521000	-3.234568000	1.149819000
6	-2.974749000	-0.959612000	-2.225536000
6	-2.774208000	1.417139000	-1.434512000
1	-3.344581000	-0.308343000	-3.021884000
1	-2.498009000	1.941198000	-0.515433000

6	-3.639948000	0.316607000	1.791673000
1	-4.116002000	-0.210431000	0.953909000
6	-1.345280000	1.202018000	2.364054000
1	-2.028401000	1.563558000	3.138896000
6	-0.718433000	2.422021000	1.719148000
1	-1.490421000	3.119579000	1.385382000
1	-0.071868000	2.942536000	2.429279000
1	-0.101217000	2.149892000	0.859557000
6	-0.338948000	0.305521000	3.063262000
1	-0.834616000	-0.546068000	3.534133000
1	0.414172000	-0.071335000	2.371244000
1	0.174229000	0.874431000	3.842042000
5	1.174057000	-0.067817000	-0.962602000
7	1.956732000	-1.434306000	-0.744348000
6	3.257939000	-1.535239000	-0.272277000
6	4.262241000	-0.833788000	-0.949066000
6	3.621009000	-2.302536000	0.836840000
6	5.567664000	-0.871069000	-0.507861000
1	3.990637000	-0.249952000	-1.821689000
6	4.939185000	-2.343012000	1.262099000
1	2.857477000	-2.843048000	1.384382000
6	5.922229000	-1.626553000	0.602889000
1	6.323825000	-0.308130000	-1.044031000
1	5.194718000	-2.939379000	2.131614000
1	6.950668000	-1.659853000	0.941628000
6	1.950892000	1.242487000	-0.463632000
6	2.518917000	1.334763000	0.810193000
6	2.003748000	2.375840000	-1.268111000
6	3.103142000	2.501518000	1.264851000
1	2.502682000	0.465960000	1.462545000
6	2.582572000	3.538952000	-0.798939000
1	1.588552000	2.361818000	-2.271493000
6	3.135228000	3.631610000	0.458431000
1	3.539310000	2.541788000	2.256985000
1	0.795123000	0.054829000	-2.118115000
1	3.582974000	4.562082000	0.785696000
9	2.607887000	4.617273000	-1.597026000

**6P<sup>o(C-F)</sup>** (TE= -1832.109818)

6	-0.081684000	-1.738376000	-0.254020000
7	-0.006434000	-0.358547000	-0.001226000
7	1.067227000	-2.229312000	-0.709665000
6	1.177780000	-3.446803000	-1.472476000
1	2.120203000	-3.947731000	-1.243232000
1	0.355957000	-4.112419000	-1.208850000
1	1.145886000	-3.229631000	-2.544316000

15	-1.677007000	-0.431399000	0.121836000
6	-1.396839000	-2.133743000	-0.067676000
7	-2.224085000	0.219574000	1.534202000
7	-2.543275000	0.309246000	-1.063405000
6	-1.938447000	-1.068814000	-3.098541000
1	-1.054685000	-0.437858000	-3.213126000
1	-1.625638000	-2.002958000	-2.628398000
1	-2.327123000	-1.306549000	-4.091426000
6	-4.203464000	-1.259990000	-2.003861000
1	-5.019703000	-0.693132000	-1.550798000
1	-4.573800000	-1.713060000	-2.926235000
1	-3.932171000	-2.070263000	-1.323536000
6	-4.046809000	2.283358000	-1.203680000
1	-4.714459000	1.822622000	-0.473032000
1	-4.077189000	3.364786000	-1.054707000
1	-4.445759000	2.085555000	-2.201725000
6	-1.696062000	2.412615000	-2.081835000
1	-0.667499000	2.074368000	-1.943956000
1	-2.000128000	2.161847000	-3.101968000
1	-1.719250000	3.500667000	-1.991386000
6	-4.268059000	1.379315000	2.334470000
1	-5.354578000	1.285927000	2.393642000
1	-3.908378000	1.611697000	3.339672000
1	-4.033929000	2.225159000	1.685771000
6	-3.975659000	-1.088902000	2.708666000
1	-3.571498000	-2.015577000	2.294060000
1	-3.549466000	-0.950828000	3.705762000
1	-5.054890000	-1.206728000	2.826317000
6	-2.096184000	-3.441364000	-0.064565000
1	-2.310120000	-3.831032000	-1.068450000
1	-1.515634000	-4.204895000	0.460969000
1	-3.055447000	-3.370744000	0.454986000
6	-3.016217000	-0.364022000	-2.294782000
6	-2.619431000	1.790509000	-1.053702000
1	-3.378775000	0.453658000	-2.923488000
1	-2.266566000	2.096052000	-0.063341000
6	-3.671193000	0.090062000	1.802369000
1	-4.138349000	-0.110519000	0.831208000
6	-1.362406000	0.539780000	2.695408000
1	-2.063265000	0.671883000	3.525179000
6	-0.665520000	1.867363000	2.479135000
1	-1.395912000	2.674846000	2.390058000
1	0.000136000	2.098228000	3.314633000
1	-0.060043000	1.852421000	1.571156000
6	-0.420555000	-0.575354000	3.114279000
1	-0.962260000	-1.513000000	3.256892000

1	0.366284000	-0.742019000	2.378011000
1	0.052913000	-0.309359000	4.061901000
5	1.149805000	0.157739000	-0.983490000
7	1.990103000	-1.197444000	-0.983077000
6	3.207611000	-1.350373000	-0.315660000
6	4.295966000	-0.587137000	-0.749784000
6	3.397282000	-2.223502000	0.755422000
6	5.510916000	-0.659225000	-0.101776000
1	4.162058000	0.071719000	-1.600799000
6	4.627581000	-2.301331000	1.389310000
1	2.567062000	-2.826491000	1.105713000
6	5.689372000	-1.516032000	0.976956000
1	6.334538000	-0.045102000	-0.449037000
1	4.749523000	-2.981575000	2.225537000
1	6.647467000	-1.576846000	1.479104000
6	1.964017000	1.401952000	-0.389459000
6	2.381373000	1.430400000	0.944132000
6	2.366914000	2.487464000	-1.148855000
6	3.137396000	2.459387000	1.474458000
1	2.110648000	0.594985000	1.584294000
6	3.121129000	3.539248000	-0.660584000
6	3.510526000	3.522207000	0.665748000
1	3.443466000	2.429756000	2.513984000
1	0.689871000	0.353155000	-2.088355000
1	4.106452000	4.335423000	1.063922000
1	3.396745000	4.347859000	-1.327314000
9	2.041404000	2.541245000	-2.451976000

**7Pp<sup>(C-F)</sup>** (TE= -930.263069)

6	-0.154481000	-2.486009000	-1.207140000
6	1.060077000	-1.923946000	-1.198789000
1	-0.565115000	-3.246552000	-1.853506000
1	1.844595000	-2.187894000	-1.894980000
6	-2.419265000	-1.891329000	-0.242382000
6	-1.940539000	-2.755002000	0.566124000
7	-0.942406000	-1.923337000	-0.139380000
7	1.252099000	-0.981809000	-0.229928000
5	-0.055134000	-0.776320000	0.588497000
6	2.431205000	-0.285390000	-0.040662000
6	3.546146000	-0.422908000	-0.875830000
6	2.526954000	0.608452000	1.032740000
6	4.699296000	0.301486000	-0.639899000
1	3.519175000	-1.095993000	-1.723867000
6	3.685251000	1.326765000	1.256550000
1	1.676616000	0.733570000	1.692467000
6	4.784808000	1.183216000	0.425400000

1	5.545373000	0.173411000	-1.306356000
1	3.725977000	2.011055000	2.096928000
1	5.691029000	1.749252000	0.602889000
6	-1.814909000	-3.817633000	1.550377000
1	-1.290406000	-3.443072000	2.433041000
1	-2.792138000	-4.194259000	1.848060000
1	-1.225836000	-4.641250000	1.139419000
6	-3.352269000	-1.111535000	-1.043938000
1	-4.354299000	-1.535634000	-0.995587000
1	-3.383797000	-0.076124000	-0.695298000
1	-3.017670000	-1.098186000	-2.084529000
6	-0.767952000	0.635114000	0.356526000
6	-1.633557000	1.168660000	1.308931000
6	-0.638669000	1.329337000	-0.846783000
6	-2.357768000	2.329323000	1.079447000
1	-1.746025000	0.657079000	2.261458000
6	-1.344560000	2.492913000	-1.103444000
1	0.038420000	0.948532000	-1.607464000
6	-2.199313000	2.970138000	-0.130784000
1	-3.029503000	2.744908000	1.821382000
1	-1.240362000	3.034905000	-2.036063000
1	0.042743000	-1.068723000	1.765819000
9	-2.888188000	4.093630000	-0.366646000

**7P<sup>m</sup>(C-F)** (TE= -930.263769)

6	-0.163944000	-2.583560000	-0.983219000
6	1.073011000	-2.073181000	-0.965439000
1	-0.566151000	-3.416524000	-1.539236000
1	1.890763000	-2.467678000	-1.553217000
6	-2.459200000	-1.765589000	-0.289591000
6	-2.079796000	-2.515016000	0.671070000
7	-0.995987000	-1.837066000	-0.072514000
7	1.242433000	-1.004586000	-0.133054000
5	-0.103931000	-0.636179000	0.549891000
6	2.437186000	-0.332141000	0.044406000
6	3.599724000	-0.628668000	-0.676396000
6	2.499479000	0.702563000	0.985490000
6	4.766273000	0.079650000	-0.457653000
1	3.600059000	-1.414731000	-1.421456000
6	3.671508000	1.402965000	1.193432000
1	1.612253000	0.951984000	1.555318000
6	4.818492000	1.101439000	0.476622000
1	5.649871000	-0.173442000	-1.033539000
1	3.685328000	2.198957000	1.929841000
1	5.735710000	1.653521000	0.641034000
6	-2.072372000	-3.419615000	1.809105000

1	-1.587429000	-2.936263000	2.660995000
1	-3.084801000	-3.705830000	2.089217000
1	-1.501083000	-4.319706000	1.569002000
6	-3.296738000	-1.080299000	-1.263948000
1	-4.325000000	-1.434865000	-1.208304000
1	-3.279011000	-0.001234000	-1.091427000
1	-2.909156000	-1.258922000	-2.270380000
6	-0.732424000	0.756004000	0.072058000
6	-1.628299000	1.442397000	0.888002000
6	-0.493059000	1.267671000	-1.204254000
6	-2.257641000	2.578865000	0.422637000
1	-1.840926000	1.093589000	1.894694000
6	-1.130328000	2.410810000	-1.656147000
1	0.211880000	0.757215000	-1.855039000
6	-2.031121000	3.080737000	-0.841480000
1	-0.927448000	2.792051000	-2.650817000
1	-0.099126000	-0.758268000	1.760514000
9	-3.117041000	3.220339000	1.225414000
1	-2.542333000	3.979361000	-1.164581000

**7P<sup>o</sup>(C-F)** (TE= -930.264399)

6	-0.539554000	-2.415169000	-1.073732000
6	0.752022000	-2.066522000	-1.052152000
1	-1.043600000	-3.183807000	-1.639347000
1	1.515209000	-2.565541000	-1.633824000
6	-2.696388000	-1.239843000	-0.479897000
6	-2.499919000	-2.042391000	0.492482000
7	-1.278209000	-1.557719000	-0.180624000
7	1.055067000	-1.029437000	-0.218023000
5	-0.228713000	-0.527641000	0.503084000
6	2.333447000	-0.549611000	-0.002736000
6	3.445807000	-0.976737000	-0.737360000
6	2.538834000	0.416467000	0.989437000
6	4.702198000	-0.461499000	-0.480317000
1	3.335438000	-1.712321000	-1.524648000
6	3.799561000	0.924608000	1.234483000
1	1.693408000	0.763158000	1.571623000
6	4.896088000	0.492443000	0.505679000
1	5.543944000	-0.812511000	-1.067439000
1	3.924130000	1.671129000	2.011215000
1	5.883317000	0.893344000	0.700133000
6	-2.713201000	-2.910589000	1.638909000
1	-2.220586000	-2.483290000	2.516343000
1	-3.775153000	-3.028124000	1.848083000
1	-2.273662000	-3.893994000	1.456184000
6	-3.349607000	-0.428138000	-1.497571000



1	-4.420665000	-0.624611000	-1.520354000
1	-3.185394000	0.635403000	-1.306534000
1	-2.922448000	-0.656573000	-2.477655000
6	-0.664402000	0.962213000	0.098036000
6	-1.542297000	1.722372000	0.852945000
6	-0.259897000	1.537437000	-1.108023000
6	-2.011128000	2.965644000	0.474320000
6	-0.706009000	2.779960000	-1.526217000
1	0.432862000	0.981976000	-1.735137000
6	-1.587356000	3.496603000	-0.731730000
1	-0.365144000	3.192194000	-2.468879000
1	-0.211545000	-0.735270000	1.696325000
1	-1.942904000	4.471114000	-1.045665000
9	-1.994869000	1.232823000	2.021328000
1	-2.697020000	3.497122000	1.123405000

**9P<sup>p(C-F)</sup>** (TE= -1700.531383)

6	-0.177744000	1.530646000	-1.313810000
7	0.138080000	0.488943000	-0.361366000
15	-1.472394000	0.112969000	-0.378397000
6	-1.540275000	1.293844000	-1.615212000
7	-1.772592000	-1.497259000	-0.676187000
7	-2.318527000	0.374818000	1.030694000
6	-1.778886000	2.829364000	1.303043000
1	-0.838774000	2.545053000	1.783103000
1	-1.560285000	3.078360000	0.262193000
1	-2.161578000	3.726602000	1.796049000
6	-4.098518000	2.053686000	0.694136000
1	-4.849547000	1.278334000	0.862456000
1	-4.500534000	3.004345000	1.053238000
1	-3.936559000	2.144631000	-0.381245000
6	-3.584117000	-0.879915000	2.760278000
1	-4.327145000	-1.147377000	2.005611000
1	-3.502088000	-1.710888000	3.464867000
1	-3.962646000	-0.020021000	3.319028000
6	-1.189278000	-0.221432000	3.164801000
1	-0.210149000	-0.082825000	2.698747000
1	-1.451772000	0.708060000	3.678448000
1	-1.104558000	-1.003327000	3.923196000
6	-3.624154000	-3.087608000	-0.230599000
1	-4.695168000	-3.246678000	-0.375095000
1	-3.110473000	-3.971894000	-0.616356000
1	-3.430667000	-3.024735000	0.841726000
6	-3.486378000	-1.896038000	-2.437258000
1	-3.174272000	-0.978706000	-2.941470000
1	-2.974740000	-2.737682000	-2.911862000

1	-4.558180000	-2.032437000	-2.598154000
6	-2.486793000	2.007440000	-2.502009000
1	-2.647979000	3.057088000	-2.212093000
1	-2.151362000	2.017823000	-3.545146000
1	-3.469393000	1.526887000	-2.499139000
6	-2.807557000	1.716295000	1.413356000
6	-2.230250000	-0.608148000	2.130273000
1	-3.048894000	1.629535000	2.476803000
1	-1.896128000	-1.537554000	1.663254000
6	-3.184384000	-1.825243000	-0.949884000
1	-3.770626000	-0.993634000	-0.536713000
6	-0.760501000	-2.449134000	-1.172366000
1	-1.335159000	-3.325534000	-1.490095000
6	0.139783000	-2.903587000	-0.039488000
1	-0.449117000	-3.386346000	0.744501000
1	0.885535000	-3.618055000	-0.397164000
1	0.678433000	-2.063054000	0.402888000
6	0.008367000	-1.973133000	-2.393996000
1	-0.669074000	-1.737238000	-3.216638000
1	0.595145000	-1.081876000	-2.172899000
1	0.690850000	-2.759676000	-2.726585000
5	1.391801000	0.865985000	0.452841000
6	0.853049000	2.391916000	-1.483281000
1	0.909786000	3.313105000	-2.044206000
6	3.284762000	2.502895000	-0.736413000
6	2.622610000	3.222631000	0.086723000
7	1.883453000	2.092531000	-0.498499000
6	4.348807000	2.082521000	-1.639600000
1	5.126044000	2.843257000	-1.706972000
1	4.797173000	1.144029000	-1.306039000
1	3.930188000	1.914856000	-2.635896000
6	2.218884000	4.286987000	0.992942000
1	1.993042000	3.875667000	1.980100000
1	2.992546000	5.046947000	1.091666000
1	1.304765000	4.753982000	0.615257000
6	2.500078000	-0.283216000	0.540273000
6	3.017673000	-0.877000000	-0.612795000
6	2.937921000	-0.790691000	1.759642000
6	3.915003000	-1.928878000	-0.565657000
1	2.692056000	-0.512400000	-1.584973000
6	3.829710000	-1.851892000	1.843003000
1	2.557628000	-0.349774000	2.677218000
6	4.300610000	-2.403723000	0.672813000
1	4.310153000	-2.390363000	-1.463359000
1	4.160897000	-2.251637000	2.794308000
1	1.158613000	1.348657000	1.553783000

9 5.160832000 -3.429191000 0.734382000

**9P<sup>m</sup>(C-F)** (TE= -1700.532552)

6	-0.110790000	1.621582000	-1.236844000
7	0.177950000	0.473785000	-0.404819000
15	-1.455597000	0.216842000	-0.353290000
6	-1.501636000	1.510262000	-1.473021000
7	-1.891908000	-1.333545000	-0.773138000
7	-2.197412000	0.405720000	1.124131000
6	-1.458701000	2.780301000	1.577934000
1	-0.514960000	2.386155000	1.964114000
1	-1.286393000	3.113327000	0.552059000
1	-1.741109000	3.650095000	2.176466000
6	-3.861653000	2.230199000	1.053883000
1	-4.659147000	1.498285000	1.201234000
1	-4.167746000	3.169531000	1.521094000
1	-3.756567000	2.409350000	-0.017458000
6	-3.460579000	-0.915802000	2.804514000
1	-4.259257000	-1.060040000	2.073366000
1	-3.404091000	-1.812340000	3.426324000
1	-3.744869000	-0.087362000	3.458529000
6	-1.004641000	-0.467333000	3.124524000
1	-0.044119000	-0.354501000	2.614814000
1	-1.168456000	0.425269000	3.735335000
1	-0.938642000	-1.321622000	3.802271000
6	-3.819963000	-2.836570000	-0.348920000
1	-4.907307000	-2.907346000	-0.425917000
1	-3.402047000	-3.710091000	-0.855857000
1	-3.548586000	-2.895803000	0.706702000
6	-3.738422000	-1.443975000	-2.437727000
1	-3.395685000	-0.502483000	-2.872650000
1	-3.317053000	-2.264492000	-3.024725000
1	-4.825130000	-1.496191000	-2.535753000
6	-2.439348000	2.373442000	-2.226117000
1	-2.506967000	3.396718000	-1.825803000
1	-2.160072000	2.466959000	-3.281503000
1	-3.453119000	1.962998000	-2.211001000
6	-2.560558000	1.736563000	1.655114000
6	-2.124883000	-0.680732000	2.123186000
1	-2.745556000	1.567980000	2.720052000
1	-1.885824000	-1.582759000	1.555010000
6	-3.338111000	-1.540540000	-0.975363000
1	-3.835106000	-0.717135000	-0.445464000
6	-0.984715000	-2.296987000	-1.426028000
1	-1.640836000	-3.096301000	-1.786395000
6	-0.053559000	-2.922197000	-0.404930000

1	-0.627293000	-3.447238000	0.362935000
1	0.621059000	-3.638785000	-0.880255000
1	0.564697000	-2.167305000	0.084806000
6	-0.258402000	-1.754299000	-2.646134000
1	-0.965496000	-1.392816000	-3.395309000
1	0.405978000	-0.931860000	-2.381685000
1	0.342362000	-2.548532000	-3.097038000
5	1.497178000	0.686481000	0.361175000
6	0.970115000	2.422412000	-1.389024000
1	1.063037000	3.388933000	-1.861917000
6	3.437721000	2.307580000	-0.766871000
6	2.864923000	2.981028000	0.156351000
7	2.024990000	1.962842000	-0.495824000
6	4.428466000	1.913677000	-1.760767000
1	5.255755000	2.622321000	-1.787569000
1	4.819125000	0.916108000	-1.548290000
1	3.956757000	1.881964000	-2.746863000
6	2.575371000	3.968078000	1.185177000
1	2.332660000	3.467672000	2.126321000
1	3.415830000	4.641774000	1.344694000
1	1.699861000	4.552927000	0.889138000
6	2.523066000	-0.539762000	0.269824000
6	2.939042000	-1.049678000	-0.962705000
6	2.980311000	-1.181505000	1.415728000
6	3.761031000	-2.157892000	-1.052991000
1	2.588534000	-0.572159000	-1.874979000
6	3.795074000	-2.291914000	1.312746000
1	2.691708000	-0.826230000	2.400711000
6	4.196694000	-2.801362000	0.097818000
1	4.063629000	-2.537429000	-2.023038000
1	1.363822000	1.068730000	1.516377000
1	4.835303000	-3.675581000	0.063011000
9	4.210990000	-2.897199000	2.434330000

**9P<sup>o</sup>(C-F)** (TE= -1700.532219)

6	0.129306000	1.356366000	-1.434547000
7	0.278295000	0.321325000	-0.435453000
15	-1.373339000	0.223476000	-0.424817000
6	-1.256326000	1.334243000	-1.721888000
7	-1.941597000	-1.327131000	-0.635130000
7	-2.143090000	0.695193000	0.972484000
6	-1.205372000	3.038403000	1.114420000
1	-0.317288000	2.629256000	1.603494000
1	-0.963916000	3.196009000	0.060886000
1	-1.429718000	4.009836000	1.562358000
6	-3.627424000	2.624907000	0.555638000

1	-4.493747000	1.993557000	0.766240000
1	-3.863344000	3.645753000	0.866333000
1	-3.465564000	2.633615000	-0.523572000
6	-3.580761000	-0.250281000	2.762134000
1	-4.361770000	-0.434482000	2.020924000
1	-3.628551000	-1.045405000	3.509919000
1	-3.812919000	0.687417000	3.273774000
6	-1.107848000	0.034412000	3.135657000
1	-0.121025000	-0.014396000	2.668500000
1	-1.212797000	1.019965000	3.598682000
1	-1.147087000	-0.708969000	3.935276000
6	-4.014895000	-2.573705000	-0.083650000
1	-5.101416000	-2.556258000	-0.195448000
1	-3.668565000	-3.547201000	-0.440053000
1	-3.780645000	-2.499686000	0.979804000
6	-3.736791000	-1.524524000	-2.348066000
1	-3.296333000	-0.692461000	-2.901870000
1	-3.373932000	-2.457259000	-2.788179000
1	-4.820133000	-1.497613000	-2.485776000
6	-2.079607000	2.157356000	-2.636294000
1	-2.062285000	3.230607000	-2.391564000
1	-1.755985000	2.068037000	-3.679344000
1	-3.128079000	1.846676000	-2.611411000
6	-2.400771000	2.116185000	1.286720000
6	-2.204749000	-0.232285000	2.121816000
1	-2.639673000	2.124218000	2.354215000
1	-2.027157000	-1.225772000	1.703207000
6	-3.393339000	-1.434081000	-0.870848000
1	-3.827741000	-0.499992000	-0.490712000
6	-1.108697000	-2.455790000	-1.092218000
1	-1.824820000	-3.242449000	-1.352713000
6	-0.267319000	-2.990351000	0.050944000
1	-0.907129000	-3.337593000	0.866089000
1	0.352551000	-3.827437000	-0.280152000
1	0.402670000	-2.222768000	0.443479000
6	-0.300753000	-2.176327000	-2.348662000
1	-0.948152000	-1.864089000	-3.169904000
1	0.436699000	-1.391864000	-2.181612000
1	0.227676000	-3.083430000	-2.653534000
5	1.580952000	0.533149000	0.363538000
6	1.284175000	2.031816000	-1.644001000
1	1.479272000	2.911803000	-2.239185000
6	3.702764000	1.825573000	-0.866756000
6	3.140318000	2.663270000	-0.081840000
7	2.255462000	1.625956000	-0.636804000
6	4.710948000	1.228190000	-1.734129000

1	5.587764000	1.870768000	-1.809435000
1	5.018267000	0.248427000	-1.361906000
1	4.289550000	1.086025000	-2.733166000
6	2.878625000	3.802091000	0.784561000
1	2.518433000	3.454773000	1.756575000
1	3.769203000	4.411801000	0.928425000
1	2.090865000	4.419710000	0.343942000
6	2.498027000	-0.783461000	0.446400000
6	2.892360000	-1.434453000	-0.725517000
6	2.888458000	-1.403277000	1.619919000
6	3.610910000	-2.616033000	-0.724897000
1	2.601442000	-0.993205000	-1.676741000
6	3.599997000	-2.589499000	1.668895000
6	3.962377000	-3.200892000	0.483480000
1	3.889153000	-3.086982000	-1.661022000
1	1.434657000	1.091948000	1.433727000
1	4.517863000	-4.131361000	0.504070000
9	2.553131000	-0.857415000	2.801171000
1	3.855688000	-3.015188000	2.632099000