SUPPORTING INFOPMATION

Evaluating the Role of Triborane(7) as Catalyst in the Pyrolysis of Tetraborane(10)

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S-1. Rate law deviation:

$B_4H_{10} + B_3H_7 \rightleftarrows B_7H_{17}$ k_1, k_{-1}, K_1 (2e)

$B_7H_{17} \rightleftarrows B_7H_{15} + H_2$ k_2, k_{-2}, K_2 (2f)

$B_7H_{15} \rightarrow B_4H_8 + B_3H_7$ k_3 (2g)

$B_4H_{10} + B_4H_8 \rightarrow B_3H_7 + B_5H_{11}$ k_4 (1c)

$$\frac{d(B_4H_{10})}{dt} = -k_1[B_4H_{10}][B_3H_7]+k_{-1}[B_7H_{17}]-k_4[B_4H_{10}][B_4H_8] \quad \text{(S1-1)}$$

$$\frac{d(B_4H_8)}{dt} = k_3[B_7H_{15}]-k_4[B_4H_{10}][B_4H_8] = 0 \quad \text{(S1-2)}$$

$$\frac{d(B_7H_{17})}{dt} = k_1[B_4H_{10}][B_3H_7]-k_{-1}[B_7H_{17}]-k_2[B_7H_{17}]+k_{-2}[B_7H_{15}][H_2] = 0 \quad \text{(S1-3)}$$

$$\frac{d(B_7H_{15})}{dt} = k_2[B_7H_{17}]-k_{-2}[B_7H_{15}][H_2]-k_3[B_7H_{15}] = 0 \quad \text{(S1-4)}$$

Insert (S1-2), (S1-3), and (S1-4) into (S1-1):

$$\frac{d(B_4H_{10})}{dt} = -2k_3[B_7H_{15}] \quad \text{(S1-5)}$$

From (S1-1), (S1-2) and (S1-3),

$[B_7H_{15}]=K_1k_2[B_4H_{10}][B_3H_7]/\{k_{-2}[H_2]+k_3+k_2k_3/k_{-1}\}$ (S1-6)

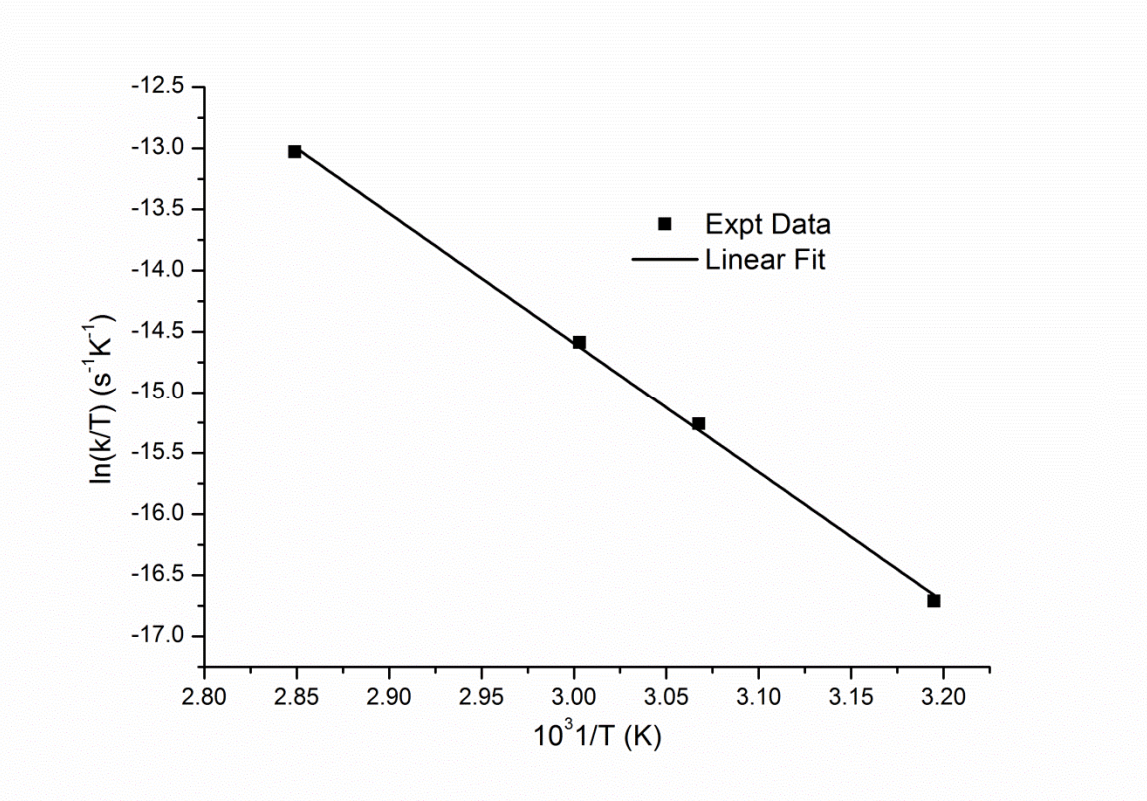
$k_{-2}[H_2] >> k_3+k_2k_3/k_{-1}$

Therefore, $k_3[B_7H_{15}]=k_3K_1K_2[B_4H_{10}][B_3H_7]/[H_2]$ (S1-7)

$$\frac{d(B_4H_{10})}{dt} = -2k_3K_1K_2[B_4H_{10}][B_3H_7]/[H_2] \quad \text{(S1-8)}$$

We assume that the ratio $[B_3H_7]/[H_2] \approx$ constant

S-2. Plot for the pyrolysis of B_4H_{10}.



The experiment data from reference (4b) has been re-plotted according to the following equation:

$$k = \boldsymbol{K}(k_B T/h)\cdot\exp(\Delta S^{\ddagger}/R)\cdot\exp(-\Delta H^{\ddagger}/RT) \qquad \text{(S2-1)}$$

Thus, the experimentally observed activation free energy is 25.3 kcal/mol.

S-3. Estimated ratio of B_3H_7 to H_2. Transition state theory was applied (Equation S3-1).

$$k = (k_B T/h)\exp(-\Delta G^{\ddagger}/RT) \qquad \text{(S3-1)}$$

$$k_{expt} = k = -2k_3K_1K_2[B_4H_{10}][B_3H_7]/[H_2] \qquad \text{(S3-2)}$$

Therefore:

$$\exp(-\Delta G^{\ddagger}_{expt}/RT) = 2\exp(-\Delta G^{\ddagger}_{3}/RT)\cdot\exp(-\Delta G_1/RT)\cdot\exp(-\Delta G_2/RT)[B_3H_7]/[H_2] \qquad \text{(S3-3)}$$

$\Delta G^{\ddagger}_{expt}$ is the experimentally observed activation free energy which is 25.3 kcal/mol. $\Delta G^{\ddagger}_{3}$, ΔG_1, and ΔG_2 are activation free energy of reaction (2g) and the reaction free energies of (2e) and (2f) the in S-1, respectively. Insert $\Delta G^{\ddagger}_{3} + \Delta G_1 + \Delta G_2$ at 333 K (19.2 kcal/mol) into equation (S3-3) to estimated the ratio of B_3H_7 to H_2 as 1.2×10^{-4}.

S-4. To calculate the activation energy the Arrhenius equation and the estimated ratio of B_3H_7 to H_2 are used.

$$k_{expt} = -2k_3K_1K_2[B_3H_7]/[H_2] \quad \text{(S4-1)}$$

According to the Arrhenius equation:

$$k = A\cdot\exp(-E_a/RT) \quad \text{(S4-2)}$$

$$A_{calc}\cdot\exp(-E_{calc}/RT)$$

$$= 2A_3\cdot\exp(-(\Delta H^{\ddagger}_{3}+RT))/RT)\cdot A_1\cdot\exp(\Delta H_1/RT)\cdot A_2\cdot\exp(\Delta H_2/RT)[B_3H_7]/[H_2] \quad \text{(S4-3)}$$

$$= 2A_3A_1A_2\exp(-(\Delta H^{\ddagger}_{3} + RT + \Delta H_1 + \Delta H_2)[B_3H_7]/[H_2] \quad \text{(S4-4)}$$

Insert $\Delta H^{\ddagger}_{3}+RT+\Delta H_1+\Delta H_2$ at 333 K (14.6 kcal/mol),

$[B_3H_7]/[H_2] = \exp(-6.6(kcal/mol)/RT)$

Thus, $E_{calc} = 14.6 + 6.6 = 21.2$ kcal/mol

$\Delta H^{\ddagger}_{3}$, ΔH_1, and ΔH_2 is the activation enthalpy of reaction (2g) and the reaction enthalpies of (2e) and (2f) in S-1, respectively.

S–5. Free Radical Mechanism for Formation of H_2 from B_4H_{10}

		$\bullet G^{\ddagger}$(373K) G4
(a) Initiation	$B_4H_{10} \rightarrow H + B_4H_9$	75.6
(b) Propagation	$B_4H_{10} + H \rightarrow H_2 + B_4H_9$	13.3
(c) Propagation	$B_4H_9 \rightarrow H + B_4H_8$	33.0
(d) Termination	$H + H \rightarrow H_2$	0.0

According to steady state approximation,

(*i*) $d[H]/dt = k_d[B_4H_{10}] - k_b[B_4H_{10}][H] + k_c[B_4H_9] - 2k_d[H]^2 = 0$

(*ii*) $d[B_4H_9]/dt = k_b[B_4H_{10}][H] - k_c[B_4H_9] = 0$

i.e. (i)+(*ii*) $\rightarrow$

and hence the steady-state concentration of the H radical is:

$[H] = (k_a/2k_d)^{1/2}[B_4H_{10}]^{1/2}$

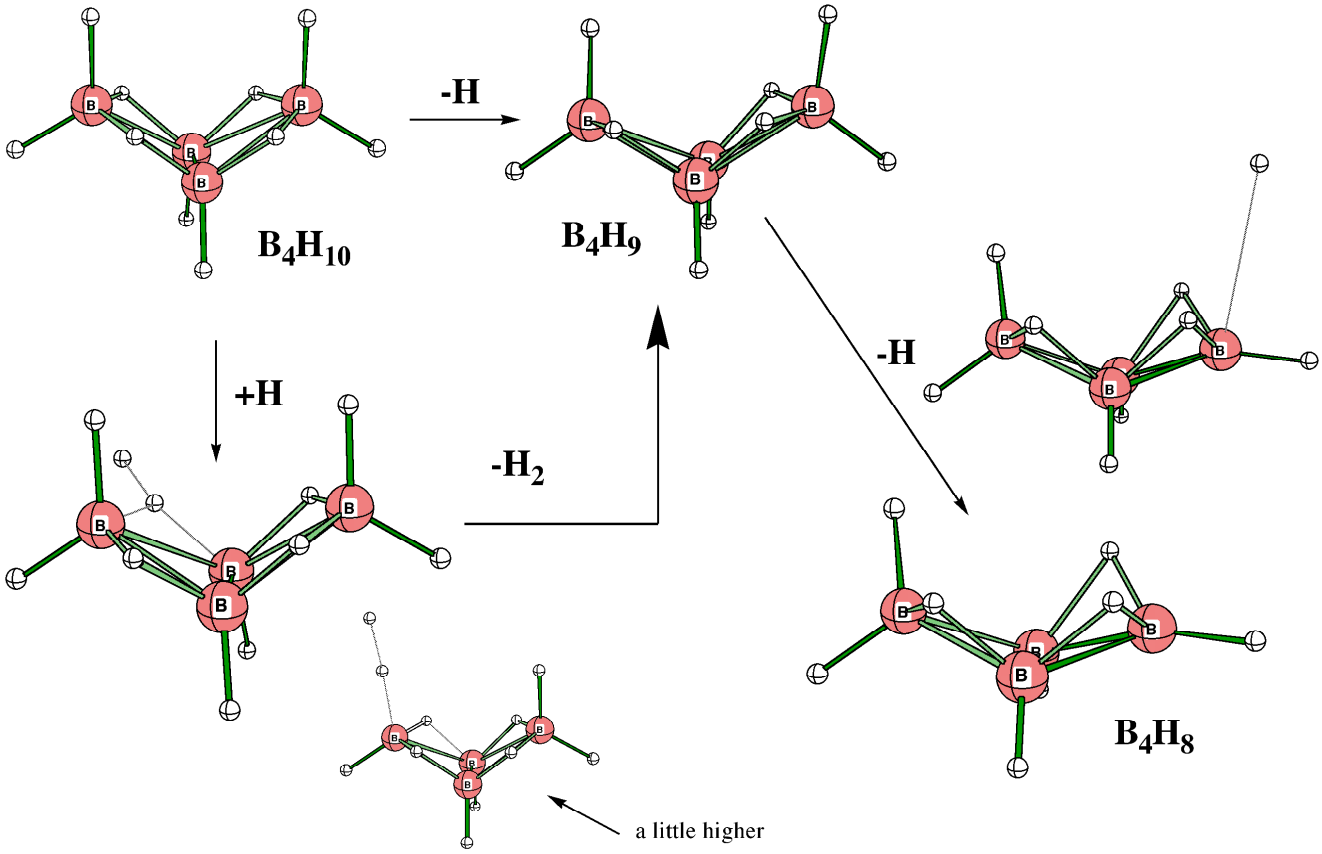
i.e. from equation (b), the rate of formation of H_2 (i.e. the rate of the overall reaction) is given by:

$d[H_2]/dt = k_b[B_4H_{10}][H] = k_b(k_d/2k_d)^{1/2}[B_4H_{10}]^{3/2}$

Eyring eq $k = (k_BT/h)\cdot e^{-\bullet G/RT}$ $\bullet G^{\ddagger}(373K) = \bullet G_b + (\bullet G_a - \bullet G_d)/2 = 51.1$ kcal/mol

The BDE of B_4H_{10} is large (75.6 kcal/mol. If H atoms are produced with a lower barrier, then the reaction to form H_2 might via a free radical mechanism would be 3/2 order in B_4H_{10}.

S-6. Free Radical Mechanism



S-6. The symmetry, enthalpy (0 K), enthalpy (333 K) and free energy (333 K) of all the stationary points at G4 level of theory in kcal/mol

	P.G.[a]	ΔH(0K)	ΔH(333K)	ΔG(333K)
H_2	D_{ih}	-1.168020	-1.163365	-1.185797
BH_3	D_{3h}	-26.572791	-26.567174	-26.599396
B_2H_6	D_{2h}	-53.204881	-53.197249	-53.238019
B_3H_7(c)	C_{2V}	-78.610178	-78.600057	-78.647811
B_4H_{10}(a)	C_{2V}	-105.244686	-105.234786	-105.279649
TS(ab)	C_1	-105.200244	-105.189847	-105.236795
B_4H_{10}(b)	C_1	-105.227982	-105.217275	-105.265796
TS(ad)	C_S	-105.190765	-105.179922	-105.227137
B_4H_8(d)	C_1	-104.051379	-104.042468	-104.086033
B_5H_{13}(e)	C_1	-131.822314	-131.808055	-131.865672
TS(ef)	C_1	-131.809459	-131.796318	-131.849756
B_5H_{13}(f)	C_1	-131.817693	-131.801886	-131.865479
TS(eg)	C_S	-131.801966	-131.789200	-131.841498
B_5H_{11}(g)	C_s	-130.641641	-130.631576	-130.675755
TS(gh)	C_1	-130.627938	-130.618627	-130.660868
B_5H_{11}(h)	C_1	-130.637425	-130.627719	-130.670724
TS(hi)	C_1	-130.635574	-130.626342	-130.668283
B_5H_{11}(i)	C_1	-130.674611	-130.665626	-130.707048
B_7H_{17}(j)	C_1	-183.858977	-183.842871	-183.905951
TS(jk)	C_1	-183.844861	-183.831021	-183.884136
B_7H_{17}(k)	C_1	-183.857459	-183.843367	-183.897039
TS(kl)	C_1	-183.842060	-183.827284	-183.881907
B_7H_{15}(l)	C_1	-182.691062	-182.678453	-182.728311
TS(lm)	C_1	-182.677540	-182.664882	-182.715268
B_7H_{15}(m)	C_1	-182.686351	-182.673764	-182.722919
TS(mn)	C_1	-182.665525	-182.653456	-182.701452
B_7H_{15}(n)	C_1	-182.671863	-182.658792	-182.709003
TS(no)	C_1	-182.665744	-182.653142	-182.703075
B_7H_{15}(o)	C_1	-182.672459	-182.658578	-182.712390
TS(p)	C_1	-209.271316	-209.256408	-209.312412
B_8H_{18}(p)	C_2	-209.312415	-209.297743	-209.352015
TS(pq)	C_1	-209.269683	-209.254204	-209.312070
$B_8H_{18(}$q)	C_1	-209.298651	-209.283123	-209.341127
TS(pr)	C_1	-209.260182	-209.244628	-209.301150
B_8H_{16}(r)	C_1	-208.123180	-208.109156	-208.162960
TS(rs)	C_1	-208.088915	-208.074858	-208.128768
B_8H_{16}(s)	C_1	-208.090692	-208.075925	-208.131253
TS(s)	C_1	-208.084919	-208.069994	-208.126396

a) Point group.

S-6. Cartesian Coordinates of Geometries Optimized at the B3LYP/6-31G(2df,p) level of theory

H_2

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	0.371396
2	1	0	0.000000	0.000000	-0.371396

BH_3

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	0.000000	0.000000	0.000000
2	1	0	0.000000	1.191662	0.000000
3	1	0	1.032010	-0.595831	0.000000
4	1	0	-1.032010	-0.595831	0.000000

B_2H_6

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	0.975789
2	5	0	-0.883701	0.000000	0.000000
3	5	0	0.883701	0.000000	0.000000
4	1	0	0.000000	0.000000	-0.975790
5	1	0	-1.461761	1.038081	0.000000
6	1	0	-1.461761	-1.038081	0.000000
7	1	0	1.461761	-1.038081	0.000000
8	1	0	1.461761	1.038081	0.000000

B_3H_7(f)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	0.000000	0.867776	-0.495773
2	5	0	0.000000	-0.867776	-0.495773

3	5	0	0.000000	0.000000	1.056721
4	1	0	0.000000	1.005499	1.688589
5	1	0	-1.023888	1.481103	-0.554510
6	1	0	1.023888	1.481103	-0.554510
7	1	0	1.023888	-1.481103	-0.554510
8	1	0	-1.023888	-1.481103	-0.554510
9	1	0	0.000000	-1.005499	1.688589
10	1	0	0.000000	0.000000	-1.485016

B_4H_{10}(a)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	0.000000	1.412105	0.389718
2	5	0	0.861485	0.000000	-0.465930
3	5	0	-0.861490	0.000000	-0.465930
4	5	0	0.000000	-1.412110	0.389718
5	1	0	0.000000	-1.447780	1.582692
6	1	0	-1.317960	0.917731	0.262949
7	1	0	0.000000	2.432885	-0.218640
8	1	0	0.000000	1.447776	1.582692
9	1	0	1.317958	-0.917730	0.262949
10	1	0	0.000000	-2.432890	-0.218640
11	1	0	1.379995	0.000000	-1.528450
12	1	0	-1.380000	0.000000	-1.528450
13	1	0	1.317958	0.917731	0.262949
14	1	0	-1.317960	-0.917730	0.262949

TS(ab)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	-1.220860	-0.638360	-0.359160
2	5	0	0.160411	-0.452430	0.616445
3	5	0	-0.820240	1.005632	0.052020
4	5	0	1.721956	0.083316	-0.300490
5	1	0	1.641669	0.157703	-1.486190
6	1	0	1.126423	-1.055720	0.000085
7	1	0	-0.781530	-1.527010	0.435327
8	1	0	-2.283450	-0.250180	0.084830

9	1	0	-1.117400	-0.969440	-1.495310
10	1	0	-0.897310	1.560605	-0.996310
11	1	0	0.992294	0.942289	0.270952
12	1	0	2.765401	0.012396	0.272815
13	1	0	0.272217	-0.468490	1.798582
14	1	0	-0.924660	1.607021	1.071127

B_4H_{10}(b)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	-1.516700	-0.556900	0.138283
2	5	0	1.940997	0.036544	0.085184
3	5	0	-0.814920	1.003976	-0.072700
4	5	0	0.296116	-0.497230	-0.171850
5	1	0	-1.986220	0.651792	0.354652
6	1	0	0.242684	-1.617720	-0.576100
7	1	0	-0.345850	1.648007	0.815979
8	1	0	1.051434	-0.492490	0.897514
9	1	0	-0.931820	1.511069	-1.148530
10	1	0	1.106080	0.154026	-0.950180
11	1	0	-1.521850	-1.119330	1.195942
12	1	0	2.194446	1.132382	0.464933
13	1	0	-2.116710	-1.036770	-0.772210
14	1	0	2.780353	-0.762920	-0.176620

TS(ad)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	-0.051200	-0.102060	1.527354
2	5	0	0.616940	-0.709080	0.000000
3	5	0	-0.051200	0.844827	0.000000
4	5	0	-0.051200	-0.102060	-1.527350
5	1	0	-1.178900	-0.187600	-1.909520
6	1	0	-1.859550	1.070832	0.378711
7	1	0	0.807112	0.010294	2.342620
8	1	0	-1.178900	-0.187600	1.909521
9	1	0	0.121758	-1.368110	-1.010130
10	1	0	0.807112	0.010294	-2.342620

11	1	0	1.803779	−0.720440	0.000000
12	1	0	0.098730	2.011450	0.000000
13	1	0	0.121758	−1.368110	1.010134
14	1	0	−1.859550	1.070832	−0.378710

B_4H_8(d)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	−0.112020	−0.832310	−0.338460
2	5	0	0.018880	0.865657	−0.242050
3	5	0	−1.405780	−0.011100	0.190198
4	5	0	1.414191	−0.126460	0.197885
5	1	0	−0.893190	−1.008530	0.835023
6	1	0	1.596824	−0.632530	1.265726
7	1	0	−2.581540	0.043439	0.129777
8	1	0	2.337140	0.032450	−0.537060
9	1	0	−0.163940	−1.802400	−1.008450
10	1	0	0.010015	1.705612	−1.076260
11	1	0	1.049069	1.096085	0.591974
12	1	0	−0.940180	1.092488	0.727895

B_5H_{13}(e)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	2.750432	−1.011320	−0.917560
2	5	0	2.881851	0.558099	0.094609
3	5	0	2.118366	−0.802430	0.833684
4	5	0	1.118721	0.730009	0.584327
5	1	0	−1.556360	1.474959	0.026034
6	1	0	1.953135	−1.727120	−0.003600
7	1	0	3.767609	−1.618830	−0.988810
8	1	0	1.970691	−1.064350	−1.817760
9	1	0	2.069146	1.492177	−0.133250
10	1	0	0.861182	1.376385	1.538654
11	1	0	3.836605	0.983292	0.645243
12	1	0	2.609128	−1.196870	1.833545
13	1	0	3.102050	0.335669	−1.124160
14	1	0	0.886338	−0.610950	1.006994

15	5	0	−0.687940	1.694705	−0.763160
16	1	0	−0.067780	2.713402	−0.668250
17	1	0	−0.727150	1.157361	−1.832650
18	1	0	0.323207	0.608679	−0.342490

TS(ef)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	−1.109500	0.699553	−0.756750
2	5	0	−1.557320	−1.026210	−0.084870
3	5	0	−0.728720	0.345461	0.919181
4	5	0	0.895317	0.660899	0.119757
5	1	0	1.214578	−0.196320	−0.788090
6	1	0	−1.196660	1.096109	1.704490
7	1	0	−1.961530	1.529169	−0.777350
8	1	0	−0.255250	0.867402	−1.586730
9	1	0	−0.868720	−1.956990	−0.370620
10	1	0	1.181568	1.802938	0.069795
11	1	0	−2.700780	−1.215440	0.181538
12	1	0	−1.047820	−0.828360	1.224611
13	1	0	−1.586290	−0.379590	−1.265720
14	1	0	0.465696	0.132957	1.284107
15	5	0	2.323921	−0.517660	−0.145020
16	1	0	2.293091	0.194801	0.862540
17	1	0	3.174388	−0.147560	−0.890740
18	1	0	2.149818	−1.670660	0.096055

B_5H_{13}(f)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	−1.798970	0.609851	−0.864790
2	5	0	−1.876620	−1.020110	−0.273070
3	5	0	−1.550150	0.306349	0.874925
4	5	0	1.851997	0.585372	0.559787
5	1	0	1.825577	0.022614	−0.625420
6	1	0	−1.424290	1.460123	1.122681
7	1	0	−2.792930	1.264054	−0.969760
8	1	0	−0.783590	1.069765	−1.296900

9	1	0	−0.917960	−1.732180	−0.280140
10	1	0	2.073973	1.745726	0.444556
11	1	0	−2.927400	−1.497810	0.035465
12	1	0	−1.507220	−0.432170	1.803344
13	1	0	−2.007810	−0.529310	−1.487650
14	1	0	0.924900	0.191678	1.197893
15	5	0	2.910985	−0.598990	−0.205330
16	1	0	2.935731	−0.025680	0.982655
17	1	0	3.841726	−0.214210	−0.834850
18	1	0	2.671480	−1.754610	−0.074890

TS(eg)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	−1.020140	1.517686	0.000000
2	5	0	−1.025050	−0.120810	−0.862650
3	5	0	−1.025050	−0.120810	0.862652
4	5	0	0.448157	−0.915460	0.000000
5	1	0	2.614403	−0.949650	1.056157
6	1	0	−0.897470	1.036395	1.334822
7	1	0	−2.053820	2.102458	0.000000
8	1	0	−0.007880	2.153439	0.000000
9	1	0	0.082969	−0.524580	−1.304630
10	1	0	0.325547	−2.096470	0.000000
11	1	0	−1.927390	−0.684980	−1.377260
12	1	0	−1.927390	−0.684980	1.377257
13	1	0	−0.897470	1.036395	−1.334820
14	1	0	0.082969	−0.524580	1.304628
15	5	0	2.221919	−0.560980	0.000000
16	1	0	2.614403	−0.949650	−1.056160
17	1	0	2.551357	0.663878	0.000000
18	1	0	1.494536	0.441926	0.000000

B_5H_{11}(g)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	1	0	2.034027	0.706696	0.000000
2	5	0	0.831583	0.676200	0.000000

3	1	0	−0.919040	−0.895040	1.345157
4	5	0	0.238516	−0.880220	0.862078
5	5	0	−1.382090	−1.077230	0.000000
6	5	0	0.238516	2.260080	0.000000
7	5	0	0.238516	−0.880220	−0.862080
8	1	0	0.475038	0.285962	1.290733
9	1	0	−1.835890	−2.178580	0.000000
10	1	0	0.074977	2.871327	1.017719
11	1	0	−0.919040	−0.895040	−1.345160
12	1	0	0.922492	−1.701980	−1.376080
13	1	0	0.922492	−1.701980	1.376084
14	1	0	−2.130300	−0.141650	0.000000
15	1	0	0.475038	0.285962	−1.290730
16	1	0	0.074977	2.871327	−1.017720

TS(gh)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	1.631511	−0.709500	−0.285830
2	5	0	0.687961	0.998114	−0.278010
3	5	0	0.236135	−0.161440	0.990262
4	5	0	−1.037610	0.785584	−0.117250
5	1	0	0.766479	−1.260780	0.555471
6	1	0	2.694970	−0.519790	0.201404
7	1	0	1.507351	−1.580640	−1.093960
8	1	0	−0.236990	1.168572	−1.149870
9	1	0	−1.474630	1.766238	0.396460
10	1	0	1.298021	1.979240	−0.033570
11	1	0	0.679874	0.177794	2.037826
12	1	0	1.353625	0.270183	−1.129550
13	1	0	−0.803430	−0.805120	1.179018
14	5	0	−1.820040	−0.664710	−0.343000
15	1	0	−2.811640	−0.894460	0.284353
16	1	0	−1.391150	−1.542000	−1.033440

B_5H_{11}(h)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z

1	5	0	1.693018	−0.670800	−0.161520
2	5	0	0.813217	1.058691	−0.062030
3	5	0	−0.176730	−0.564600	0.631807
4	5	0	−0.841650	0.932493	0.053451
5	1	0	0.673744	−1.411240	0.091210
6	1	0	2.427354	−0.503230	0.754494
7	1	0	2.073589	−1.346530	−1.072350
8	1	0	−0.068240	1.363366	−0.981630
9	1	0	−1.307090	1.875238	0.596873
10	1	0	1.467800	1.960119	0.331163
11	1	0	−0.150930	−0.721250	1.805035
12	1	0	1.514793	0.369425	−0.928520
13	1	0	−1.068880	−1.515790	0.135889
14	5	0	−1.718010	−0.497880	−0.343340
15	1	0	−2.758050	−0.608190	0.228833
16	1	0	−1.647380	−0.724080	−1.519480

TS(hi)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	1.671399	−0.685820	−0.161410
2	5	0	0.831881	1.039385	−0.048070
3	5	0	−0.121990	−0.480910	0.644347
4	5	0	−0.848720	0.910525	0.022700
5	1	0	0.608330	−1.387100	0.048206
6	1	0	2.437154	−0.617000	0.741475
7	1	0	1.991214	−1.335080	−1.115540
8	1	0	−0.005280	1.374622	−0.980090
9	1	0	−1.391320	1.858331	0.472631
10	1	0	1.438813	1.956017	0.384182
11	1	0	−0.134860	−0.701770	1.805444
12	1	0	1.575334	0.398918	−0.899220
13	1	0	−1.190140	−1.652770	−0.068770
14	5	0	−1.710660	−0.559200	−0.283260
15	1	0	−2.751310	−0.532310	0.298334
16	1	0	−1.683850	−0.477530	−1.490870

B_5H_{11}(i)

Center	Atomic	Atomic	Coordinates(Angstroms)

Number	Number	Type	X	Y	Z
1	1	0	-0.028550	-0.234460	1.975680
2	5	0	-0.004940	-0.261430	0.793577
3	1	0	-0.019580	1.369891	-1.003850
4	5	0	0.912771	0.874237	-0.141970
5	5	0	-0.880960	0.966755	-0.089280
6	5	0	1.577212	-0.736270	-0.151970
7	5	0	-1.535560	-0.746940	-0.187370
8	1	0	1.463704	1.783655	0.374796
9	1	0	-1.385860	1.907204	0.416099
10	1	0	2.616523	-0.744460	0.426029
11	1	0	-2.503740	-0.862990	0.490375
12	1	0	1.332806	-1.618520	-0.911210
13	1	0	-1.451180	-1.432010	-1.165030
14	1	0	1.641122	0.317707	-1.044550
15	1	0	-1.662220	0.429897	-0.929560
16	1	0	-0.352480	-1.365300	0.311542

B_7H_{11}(j)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	-2.412160	1.300053	-0.197570
2	5	0	-2.689240	-0.531090	-0.419710
3	5	0	-1.866660	-0.016270	1.004201
4	5	0	-0.939030	-1.103680	-0.177050
5	1	0	-0.087770	-0.605200	-0.856380
6	1	0	-1.611680	1.214957	0.961525
7	1	0	-3.376840	1.905128	0.140957
8	1	0	-1.590420	1.843032	-0.870840
9	1	0	-1.914890	-1.141910	-1.201260
10	1	0	-0.814440	-2.236220	0.157614
11	1	0	-3.685790	-1.144000	-0.250350
12	1	0	-2.368970	-0.316620	2.031120
13	1	0	-2.870970	0.428964	-1.211290
14	1	0	-0.653930	-0.353430	0.984977
15	5	0	2.690152	1.088811	-0.174580
16	5	0	2.850954	-0.298330	0.855978
17	5	0	2.404895	-0.536420	-0.854280
18	1	0	2.191781	-0.107550	-1.940520
19	1	0	3.645897	1.538501	-0.732970

20	1	0	1.662957	1.693928	−0.248970
21	1	0	2.991773	0.986096	1.102500
22	1	0	1.938876	−0.689540	1.522243
23	1	0	3.916732	−0.813050	1.017457
24	1	0	2.384491	−1.718180	−0.748670

TS(jk)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	−2.106170	1.224118	−0.080840
2	5	0	−2.043270	−0.540960	−0.644810
3	5	0	−1.692480	−0.217360	1.010512
4	5	0	−0.388060	−1.098710	0.001817
5	1	0	1.111841	−1.103030	0.234425
6	1	0	−1.561430	1.014605	1.219608
7	1	0	−3.219920	1.601459	0.079311
8	1	0	−1.275710	2.012358	−0.411230
9	1	0	−0.976140	−0.920220	−1.232660
10	1	0	−0.426490	−2.266820	0.218343
11	1	0	−2.938700	−1.272450	−0.885520
12	1	0	−2.375740	−0.737010	1.821423
13	1	0	−2.098770	0.517912	−1.317810
14	1	0	−0.468310	−0.457300	1.244122
15	5	0	2.067657	1.200996	0.024499
16	5	0	2.738549	−0.500460	0.299062
17	5	0	1.191361	−0.269610	−0.672600
18	1	0	0.657148	0.809000	−0.450020
19	1	0	2.433476	1.881562	−0.882530
20	1	0	1.612660	1.747215	0.986218
21	1	0	3.214075	0.684086	0.488056
22	1	0	2.642775	−0.935860	1.412750
23	1	0	3.525215	−1.015290	−0.431120
24	1	0	1.298604	−0.611970	−1.801890

B_7H_{17}(k)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	−2.139940	1.239287	0.085706

2	5	0	-2.138120	-0.425860	-0.703930
3	5	0	-1.792680	-0.336200	0.979327
4	5	0	-0.453660	-1.075030	-0.143360
5	1	0	1.714762	-1.101900	0.362179
6	1	0	-1.670690	0.845115	1.383655
7	1	0	-3.217710	1.697267	0.286426
8	1	0	-1.237360	1.986167	-0.142050
9	1	0	-1.078520	-0.724930	-1.333350
10	1	0	-0.520830	-2.262230	-0.072420
11	1	0	-3.051140	-1.108270	-1.017100
12	1	0	-2.495520	-0.960550	1.695970
13	1	0	-2.215850	0.704225	-1.241950
14	1	0	-0.567630	-0.604670	1.163953
15	5	0	2.124300	1.276063	-0.170860
16	5	0	2.881182	-0.511190	0.432670
17	5	0	1.112815	-0.446720	-0.576480
18	1	0	0.908987	0.797967	-0.289840
19	1	0	2.687849	1.565873	-1.168560
20	1	0	1.745789	2.152139	0.554163
21	1	0	2.855611	0.744481	0.763955
22	1	0	3.021783	-0.859450	1.571352
23	1	0	3.697736	-0.823370	-0.362350
24	1	0	1.461698	-0.680540	-1.684270

TS(kg)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	-2.493200	1.072825	-0.116340
2	5	0	-2.218310	-0.712370	-0.492860
3	5	0	-1.751260	-0.139790	1.059122
4	5	0	-0.389000	-0.883340	-0.032650
5	1	0	1.808534	-0.281960	0.201957
6	1	0	-1.834580	1.108861	1.154378
7	1	0	-3.622270	1.359422	0.119621
8	1	0	-1.790840	1.887324	-0.633270
9	1	0	-1.177650	-0.970270	-1.175780
10	1	0	-0.197180	-2.006250	0.313322
11	1	0	-2.996060	-1.602660	-0.516480
12	1	0	-2.249500	-0.673210	1.989357
13	1	0	-2.566410	0.214328	-1.262540
14	1	0	-0.488120	-0.133040	1.139279

15	5	0	2.493072	1.138293	0.123609
16	5	0	3.066988	-0.683580	0.268597
17	5	0	0.868624	-0.017170	-0.844560
18	1	0	0.889754	1.192111	-0.696870
19	1	0	2.939225	1.723276	-0.802400
20	1	0	2.073677	1.660086	1.101971
21	1	0	3.590507	0.432153	0.571681
22	1	0	2.938367	-1.293430	1.281662
23	1	0	3.538523	-1.133280	-0.717310
24	1	0	1.307438	-0.390380	-1.884160

TS(kl)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	2.580859	-0.367490	0.901612
2	5	0	1.969948	-0.525230	-0.826700
3	5	0	1.800772	0.999150	-0.054340
4	5	0	0.204141	0.164197	-0.661940
5	1	0	-1.530220	-1.524470	-0.313780
6	1	0	2.087636	0.960459	1.164759
7	1	0	3.763121	-0.283110	0.993574
8	1	0	1.972112	-0.882890	1.787728
9	1	0	0.814329	-1.044490	-0.949710
10	1	0	-0.069280	0.663271	-1.713730
11	1	0	2.581132	-0.545770	-1.838830
12	1	0	2.307178	1.925513	-0.587260
13	1	0	2.352190	-1.426900	-0.044390
14	1	0	0.567039	1.190311	0.191233
15	5	0	-2.386510	0.719974	0.575827
16	5	0	-2.683330	-0.901810	-0.190950
17	5	0	-1.059420	-0.487390	0.332382
18	1	0	-1.928080	1.589816	-0.923880
19	1	0	-1.756640	1.420142	1.299627
20	1	0	-2.555670	1.939821	-0.676470
21	1	0	-3.565900	0.879470	0.640754
22	1	0	-3.061580	-0.701130	-1.305580
23	1	0	-3.368610	-1.553630	0.534471
24	1	0	-0.778950	-0.875300	1.429024

B_7H_{15}(l)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	-2.412160	1.300053	-0.197570
2	5	0	-2.689240	-0.531090	-0.419710
3	5	0	-1.866660	-0.016270	1.004201
4	5	0	-0.939030	-1.103680	-0.177050
5	1	0	-0.087770	-0.605200	-0.856380
6	1	0	-1.611680	1.214957	0.961525
7	1	0	-3.376840	1.905128	0.140957
8	1	0	-1.590420	1.843032	-0.870840
9	1	0	-1.914890	-1.141910	-1.201260
10	1	0	-0.814440	-2.236220	0.157614
11	1	0	-3.685790	-1.144000	-0.250350
12	1	0	-2.368970	-0.316620	2.031120
13	1	0	-2.870970	0.428964	-1.211290
14	1	0	-0.653930	-0.353430	0.984977
15	5	0	2.690152	1.088811	-0.174580
16	5	0	2.850954	-0.298330	0.855978
17	5	0	2.404895	-0.536420	-0.854280
18	1	0	2.191781	-0.107550	-1.940520
19	1	0	3.645897	1.538501	-0.732970
20	1	0	1.662957	1.693928	-0.248970
21	1	0	2.991773	0.986096	1.102500
22	1	0	1.938876	-0.689540	1.522243
23	1	0	3.916732	-0.813050	1.017457
24	1	0	2.384491	-1.718180	-0.748670

TS(lm)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	-2.130040	-1.063160	-0.105030
2	5	0	-1.476880	0.219664	1.038692
3	5	0	-1.794870	0.679368	-0.591970
4	5	0	-0.057290	0.943249	0.051279
5	1	0	1.267624	-1.993900	0.221430
6	1	0	-2.047600	-0.303410	-1.327130
7	1	0	-3.283720	-1.304640	0.042020
8	1	0	-1.401820	-1.929400	-0.482440
9	1	0	-0.205910	0.191701	1.198163

10	1	0	0.010664	2.085297	0.393763
11	1	0	-2.031400	0.827780	1.886035
12	1	0	-2.559570	1.563286	-0.763500
13	1	0	-1.580640	-1.015190	1.221639
14	1	0	-0.672920	0.879532	-1.172870
15	5	0	1.601605	0.629260	-0.505610
16	5	0	2.692604	-0.207140	0.533379
17	5	0	1.361503	-1.041780	-0.479350
18	1	0	1.864775	1.169411	-1.531320
19	1	0	2.453086	1.090919	0.374554
20	1	0	2.409061	-0.416930	1.671523
21	1	0	3.799472	-0.450490	0.158802
22	1	0	0.962420	-1.162970	-1.594350

B_7H_{15}(m)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	1.182499	1.311008	0.106804
2	5	0	1.501936	-0.234600	0.992670
3	5	0	1.812515	-0.188830	-0.698900
4	5	0	0.390214	-1.311070	-0.120090
5	1	0	-1.924210	1.927962	-0.340840
6	1	0	1.483689	0.911471	-1.220590
7	1	0	1.860398	2.273392	0.255359
8	1	0	-0.002170	1.582545	-0.082030
9	1	0	0.463886	-0.908270	1.214379
10	1	0	0.719393	-2.454870	-0.089160
11	1	0	2.405446	-0.539680	1.690611
12	1	0	2.908618	-0.468200	-1.040840
13	1	0	0.990829	0.836781	1.422817
14	1	0	0.926578	-0.839580	-1.316110
15	5	0	-1.259470	-0.860730	-0.400430
16	5	0	-2.213070	0.089239	0.711726
17	5	0	-1.365750	0.924433	-0.660540
18	1	0	-1.816480	-1.400800	-1.309640
19	1	0	-1.926410	-1.203760	0.669725
20	1	0	-1.736550	0.485377	1.735220
21	1	0	-3.392060	0.194616	0.565568
22	1	0	-1.018100	0.894508	-1.796200

TS(mn)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	1.117119	-1.304090	-0.147630
2	5	0	1.491066	0.171816	-0.996040
3	5	0	1.833008	0.071211	0.654517
4	5	0	0.642037	1.340657	0.068237
5	1	0	-2.013920	-1.732830	0.307907
6	1	0	1.427489	-0.945980	1.271914
7	1	0	1.568896	-2.385840	-0.305360
8	1	0	-0.136820	-1.457540	0.152223
9	1	0	-0.090680	0.798715	-0.745760
10	1	0	0.877365	2.497377	0.041614
11	1	0	2.320106	0.408983	-1.803740
12	1	0	2.920389	0.362051	1.010088
13	1	0	0.726600	-0.739920	-1.432140
14	1	0	0.844735	0.821529	1.238482
15	5	0	-1.212210	0.896071	0.343697
16	5	0	-2.274780	-0.094130	-0.629050
17	5	0	-1.280880	-0.860300	0.691125
18	1	0	-1.577090	1.572517	1.247823
19	1	0	-1.941470	1.242353	-0.651480
20	1	0	-1.900030	-0.501130	-1.687120
21	1	0	-3.441380	-0.084110	-0.394670
22	1	0	-1.086680	-0.907130	1.862665

B_7H_{15}(n)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	-1.027970	-1.337590	0.189869
2	5	0	-1.663530	0.035438	0.946712
3	5	0	-1.781790	-0.023090	-0.792110
4	5	0	-0.936790	1.356281	0.161330
5	1	0	2.128115	-1.468880	-0.056550
6	1	0	-1.313970	-0.728170	-1.655520
7	1	0	-1.328170	-2.482180	0.190428
8	1	0	0.247670	-1.382370	-0.127490
9	1	0	0.302276	1.171362	0.510547
10	1	0	-1.170750	2.516265	0.219061

11	1	0	−2.617450	−0.034950	1.644393
12	1	0	−2.921340	0.240933	−0.999100
13	1	0	−0.772450	−0.812140	1.407136
14	1	0	−1.027750	1.075065	−1.114840
15	5	0	1.277160	0.951924	−0.319010
16	5	0	2.414917	−0.113220	0.568910
17	5	0	1.293932	−0.776190	−0.652440
18	1	0	1.395880	1.653597	−1.263490
19	1	0	2.107054	1.337180	0.527910
20	1	0	2.158532	−0.359390	1.705496
21	1	0	3.557228	−0.047710	0.234706
22	1	0	1.298414	−1.070830	−1.799710

TS(no)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	1.282807	1.330932	0.096095
2	5	0	1.688265	−0.026230	0.980777
3	5	0	1.928462	−0.043510	−0.707390
4	5	0	0.961293	−1.332170	0.116531
5	1	0	−2.228620	1.375390	0.382648
6	1	0	1.258194	0.923041	−1.245360
7	1	0	1.433714	2.498161	0.101063
8	1	0	−0.400960	1.350160	−0.299140
9	1	0	−0.263880	−1.095830	0.310434
10	1	0	1.223458	−2.484940	0.171457
11	1	0	2.436497	−0.022450	1.895628
12	1	0	2.969449	−0.160030	−1.255370
13	1	0	0.703838	0.785346	1.216374
14	1	0	1.132022	−1.021420	−1.164130
15	5	0	−1.369380	−0.918550	−0.478640
16	5	0	−2.424310	0.047221	0.673239
17	5	0	−1.522000	0.874319	−0.557240
18	1	0	−1.199410	−1.200680	−1.618510
19	1	0	−2.030670	−1.748850	0.084683
20	1	0	−1.990930	−0.068880	1.778248
21	1	0	−3.589610	−0.115700	0.489388
22	1	0	−1.934830	1.283700	−1.594890

B_7H_{15}(o)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	-2.027410	-1.249550	0.049150
2	5	0	-1.808990	0.095251	0.931595
3	5	0	-1.964400	0.258066	-0.767500
4	5	0	-0.775170	1.251482	0.096997
5	1	0	2.357046	-1.553590	0.090293
6	1	0	-1.550310	-0.969200	-1.160730
7	1	0	-2.558190	-2.299250	0.015140
8	1	0	0.866858	-1.162720	-1.165640
9	1	0	0.296807	0.773437	0.469496
10	1	0	-0.919730	2.424681	0.135142
11	1	0	-2.289340	0.285951	1.991655
12	1	0	-2.839870	0.682626	-1.439460
13	1	0	-1.085690	-1.094390	0.937876
14	1	0	-0.837120	0.891576	-1.167600
15	5	0	1.646947	0.931124	-0.143730
16	5	0	2.384843	-0.450470	0.814460
17	5	0	1.938123	-0.730650	-0.840860
18	1	0	1.539152	1.405370	-1.229260
19	1	0	2.034685	1.704027	0.675910
20	1	0	1.647992	-0.665180	1.732646
21	1	0	3.529087	-0.222440	1.059266
22	1	0	2.781551	-0.691400	-1.683000

TS(p)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	2.343718	1.082189	0.709632
2	5	0	2.444615	-0.684370	0.160154
3	5	0	1.858288	0.472901	-0.974250
4	5	0	0.786603	-0.984150	-0.590670
5	1	0	-0.558240	-1.199390	-0.464770
6	1	0	1.628395	1.579090	-0.426960
7	1	0	3.410239	1.607714	0.697577
8	1	0	1.531279	1.445396	1.505003
9	1	0	1.470546	-1.452370	0.497576
10	1	0	0.873126	-1.801570	-1.451890
11	1	0	3.401234	-1.318310	-0.132280

12	1	0	2.446540	0.592995	-1.994910
13	1	0	2.524328	-0.203200	1.315381
14	1	0	0.617770	0.248867	-1.199340
15	5	0	-1.903830	0.595266	0.792203
16	5	0	-2.487620	-0.773690	-0.002070
17	5	0	-2.484100	0.951831	-0.787380
18	5	0	-0.817750	-0.846200	0.723282
19	1	0	-1.672060	1.667482	0.129203
20	1	0	-0.541710	-1.593820	1.603975
21	1	0	-3.489770	1.590130	-0.870910
22	1	0	-0.459280	0.334678	0.997146
23	1	0	-2.313740	0.863784	1.873838
24	1	0	-3.359950	-1.267400	0.650200
25	1	0	-2.470060	-1.112690	-1.156000
26	1	0	-1.738270	0.949719	-1.727360

B_8H_{18}(p)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	-0.283630	2.366528	1.156689
2	5	0	-0.677740	2.404280	-0.636540
3	5	0	-1.626970	1.386842	0.376775
4	5	0	-0.677740	0.544934	-1.039230
5	1	0	-0.053650	-1.677620	-1.377030
6	1	0	-1.197540	1.316687	1.550609
7	1	0	-0.648500	3.319151	1.771544
8	1	0	0.708055	1.803324	1.518611
9	1	0	0.053650	1.677615	-1.377030
10	1	0	-1.452600	0.377775	-1.933120
11	1	0	-1.273450	3.219154	-1.259680
12	1	0	-2.797290	1.580166	0.366269
13	1	0	0.300406	2.917305	-0.047350
14	1	0	-1.337440	0.175039	0.121643
15	5	0	1.626974	-1.386840	0.376775
16	5	0	0.677737	-2.404280	-0.636540
17	5	0	0.283632	-2.366530	1.156689
18	5	0	0.677737	-0.544930	-1.039230
19	1	0	1.197536	-1.316690	1.550609
20	1	0	1.452598	-0.377780	-1.933120
21	1	0	0.648502	-3.319150	1.771544
22	1	0	1.337439	-0.175040	0.121643

23	1	0	2.797286	−1.580170	0.366269
24	1	0	1.273454	−3.219150	−1.259680
25	1	0	−0.300410	−2.917310	−0.047350
26	1	0	−0.708060	−1.803320	1.518611

B_8H_{18}(q)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	−2.010260	−1.029540	0.480012
2	5	0	−1.931500	0.623359	−0.352330
3	5	0	−3.476740	−0.356590	−0.180680
4	5	0	−0.338090	1.373908	−0.202540
5	1	0	1.976193	1.494586	−0.093420
6	1	0	−3.215680	−1.465770	0.522287
7	1	0	−1.692130	−0.852160	1.617672
8	1	0	−1.380590	−1.811750	−0.166870
9	1	0	−0.836980	0.450114	−1.038380
10	1	0	−0.306710	2.403667	−0.799700
11	1	0	−2.667470	1.287893	−1.016200
12	1	0	−4.200730	0.306553	0.496571
13	1	0	−1.424660	1.402514	0.567002
14	1	0	−3.855220	−0.712570	−1.251760
15	5	0	1.871182	−0.811600	0.737273
16	5	0	2.731022	0.487798	0.010405
17	5	0	2.285985	−0.955140	−1.052760
18	5	0	1.018902	0.862802	0.710805
19	1	0	1.505631	−1.673990	−0.097660
20	1	0	1.131655	1.395662	1.773341
21	1	0	3.180226	−1.692680	−1.314090
22	1	0	0.684226	−0.453350	0.995424
23	1	0	2.384455	−1.319950	1.672745
24	1	0	3.766925	0.765187	0.508285
25	1	0	2.848310	0.351910	−1.230260
26	1	0	1.407877	−0.814420	−1.850950

TS(pr)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z

1	5	0	2.876145	0.815802	0.621840
2	5	0	2.183832	-0.773770	0.094912
3	5	0	1.906539	0.619877	-0.842990
4	5	0	0.684530	-0.682880	-0.856500
5	1	0	-1.614590	-1.070800	-1.038530
6	1	0	2.066615	1.669076	-0.080870
7	1	0	3.984732	1.150383	0.353836
8	1	0	2.483701	1.025799	1.731114
9	1	0	1.213106	-1.355710	1.538590
10	1	0	0.689670	-1.136020	-1.962010
11	1	0	2.818474	-1.759840	0.195674
12	1	0	2.559140	0.688014	-1.831500
13	1	0	1.668057	-0.830900	1.845477
14	1	0	0.631082	0.678972	-1.087300
15	5	0	-1.869750	0.117979	1.079707
16	5	0	-2.540090	-0.526060	-0.368390
17	5	0	-2.419530	1.300234	-0.217460
18	5	0	-0.749230	-1.036660	0.048583
19	1	0	-1.693860	1.356935	1.029908
20	1	0	-0.807150	-2.118750	0.547846
21	1	0	-3.444030	1.855816	0.015304
22	1	0	-0.624030	-0.122780	1.083122
23	1	0	-2.395660	-0.193990	2.091746
24	1	0	-3.482980	-1.228590	-0.243140
25	1	0	-2.747900	0.349603	-1.241650
26	1	0	-1.591640	1.878893	-0.854740

B_8H_{16}(r)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	2.603643	0.918034	0.598850
2	5	0	2.192930	-0.650160	0.427333
3	5	0	2.020911	0.375477	-0.931600
4	5	0	0.825349	-0.896950	-0.634470
5	1	0	-1.478350	-1.280770	-0.792420
6	1	0	1.860835	1.581868	-0.248200
7	1	0	3.416379	1.625617	1.076022
8	1	0	1.814675	0.298680	1.414898
9	1	0	0.930274	-1.685830	-1.529060
10	1	0	2.787210	-1.536670	0.931983
11	1	0	2.658489	0.519933	-1.918520

12	1	0	0.722041	0.286992	-1.252040
13	5	0	-1.753340	0.301315	1.045304
14	5	0	-2.406840	-0.599430	-0.269200
15	5	0	-2.252230	1.218352	-0.468640
16	5	0	-0.630000	-1.047630	0.287896
17	1	0	-1.557460	1.506337	0.765995
18	1	0	-0.719740	-2.009640	0.983621
19	1	0	-3.270720	1.824367	-0.375680
20	1	0	-0.515160	0.045974	1.131209
21	1	0	-2.309560	0.197474	2.083782
22	1	0	-3.369640	-1.245910	-0.036730
23	1	0	-2.575930	0.095123	-1.300400
24	1	0	-1.398810	1.653681	-1.182420

TS(rs)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	2.346456	1.145374	0.428532
2	5	0	1.964764	-0.427380	0.701576
3	5	0	2.154333	0.112206	-0.916140
4	5	0	0.901465	-1.106020	-0.487550
5	1	0	-0.501910	-0.922740	-0.782890
6	1	0	1.834370	1.436228	-0.751850
7	1	0	3.053928	2.009679	0.799420
8	1	0	1.393597	0.790473	1.205664
9	1	0	1.137616	-2.151880	-0.998710
10	1	0	2.432459	-1.049040	1.588231
11	1	0	2.995980	-0.067450	-1.727400
12	1	0	0.987622	-0.221080	-1.498460
13	5	0	-1.805710	0.425727	1.004811
14	5	0	-2.319420	-0.535940	-0.328910
15	5	0	-2.118900	1.160787	-0.683550
16	5	0	-0.807420	-1.076930	0.416905
17	1	0	-1.381950	1.553996	1.094190
18	1	0	-0.801160	-2.137600	0.940507
19	1	0	-3.081640	1.846313	-0.827080
20	1	0	-0.560430	-0.121150	1.238251
21	1	0	-2.505250	0.110728	1.912741
22	1	0	-3.324800	-1.159430	-0.269210
23	1	0	-2.218410	0.011958	-1.474870
24	1	0	-1.074710	1.566191	-1.110400

B_8H_{16}(s)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	-2.101270	1.276293	0.388288
2	5	0	-1.938090	0.361523	-0.948250
3	5	0	-2.354610	-0.406600	0.530662
4	5	0	-1.151080	-1.156300	-0.555040
5	1	0	0.001244	-0.674570	-0.534750
6	1	0	-1.834780	0.457530	1.416195
7	1	0	-2.483650	2.303280	0.814817
8	1	0	-1.102000	1.330488	-0.455460
9	1	0	-1.346130	-2.178850	-1.112530
10	1	0	-2.332940	0.664350	-2.017500
11	1	0	-3.358210	-0.904910	0.907360
12	1	0	-1.404460	-1.354810	0.716614
13	5	0	2.472319	-0.387950	-0.258600
14	5	0	1.533090	0.238111	1.017900
15	5	0	2.173424	1.298192	-0.422810
16	5	0	1.011446	-1.249450	0.254898
17	1	0	2.568329	0.315933	-1.335490
18	1	0	0.816582	-2.333840	0.683791
19	1	0	3.135135	1.994126	-0.312280
20	1	0	1.700465	-1.432350	-0.834640
21	1	0	3.498167	-0.926730	-0.006780
22	1	0	2.096921	0.188090	2.069036
23	1	0	0.542750	0.926577	1.016690
24	1	0	1.235346	1.732883	-1.026750

TS(s)

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	5	0	2.175529	1.275174	-0.452960
2	5	0	2.054628	0.405037	0.912893
3	5	0	2.472094	-0.413170	-0.532780
4	5	0	1.348284	-1.173210	0.616417
5	1	0	0.159370	-0.909590	0.629988
6	1	0	1.914621	0.427164	-1.442460

7	1	0	2.534926	2.298116	−0.910570
8	1	0	1.160962	1.318973	0.361573
9	1	0	1.691071	−2.173370	1.154909
10	1	0	2.419220	0.775883	1.971850
11	1	0	3.488223	−0.882080	−0.915930
12	1	0	1.527820	−1.372790	−0.678180
13	5	0	−2.575060	−0.353230	0.367209
14	5	0	−1.742710	0.229288	−1.002110
15	5	0	−2.178700	1.339579	0.415076
16	5	0	−1.317120	−1.278250	−0.376520
17	1	0	−2.452720	0.399104	1.412231
18	1	0	−0.989050	−2.343590	−0.755150
19	1	0	−3.151700	2.028743	0.401846
20	1	0	−1.777740	−1.402380	0.847119
21	1	0	−3.657310	−0.834240	0.283685
22	1	0	−2.269530	0.319590	−2.065090
23	1	0	−0.549660	0.460487	−0.977690
24	1	0	−1.180600	1.784544	0.897126