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Absolute energies in hartrees, zero-point vibrational energies in kcal/mol, and number of imaginary frequencies (NIMAG). Compound numbers as in Figures 1 and 2. MP2 = MP2(fc)/6-31+G*//MP2(fc)/6-31+G*; B3L//MP2 = Becke3LYP/6-311++G**//MP2(fc)/6-31+G*; B3L//B3L = Becke3LYP/6-311+G**//Becke3LYP/6-311+G**; ZPE at HF/6-31+G*, unscaled; (N) = NIMAG.

	MP2	B3L//MP2	B3L//B3L	ZPE (N)
1	-78.29118	-78.61539	-78.61551	34.3 (0)
2	-116.82753	-117.31400	-117.31403	42.6 (0)
3	-124.32715	-124.86496	-124.86529	45.7 (0)
4a	-142.16169	-142.76418	-142.76421	49.8 (0)
4b	-142.14733	-142.74961		48.5 (1)
5a	-149.64964	-150.30299	-150.30334	52.6 (0)
5b	-149.64430	-150.29842		52.0 (1)
6	-132.85637	-133.35798	-133.35807	34.8 (0)
7	-140.34836	-140.90166	-140.90224	37.8 (0)
8	-195.15139	-195.94128	-195.93924	83.1 (0)
9	-195.15096	-195.94059	-195.93918	83.1 (0)
10	-202.65038	-203.48788	-203.48821	86.0 (0)
11	-202.65227	-203.48979	-203.49016	86.0 (0)
12	-220.56307	-221.46250	-221.46247	91.6 (0)
13	-220.48356	-221.38527		89.6 (1)
14	-220.47164	-221.37490		89.4 (1)
15	-228.03307	-228.98624	-228.98711	94.1 (0)
16	-228.02385	-228.97482		93.3 (1)
17	-227.97154	-228.92273		92.5 (1)
18	-228.02433	-228.97680	-228.97774	93.4 (0)
19	-227.96796	-228.92218		92.3 (1)
20	-211.20722	-212.01079	-212.00901	75.8 (0)
21	-218.71430	-219.56781	-219.56869	79.2 (0)

Absolute energies in hartrees, zero-point vibrational energies (ZPE) in kcal/mol (unscaled), and number of imaginary frequencies (NIMAG). Compound numbers as in Figures 3 and 5. MP2 = MP2(fc)/6-31+G*//MP2(fc)/6-31+G*; B3L//MP2 = Becke3LYP/6-311++G**// MP2(fc)/ 6-31+G*; B3L//B3L = Becke3LYP/6-311+G**//Becke3LYP/6-311+G**; HF = HF/ 6-31+G*; B3L = Becke3LYP/6-311+G**; (N) = NIMAG.

	absolute energies				ZPE's	
	MP2	B3L//MP2	B3L//B3L	HF	MP2	B3L
22	-195.10727	-195.90077	-195.90051	79.3	75.2	73.7
23	-220.45829	-221.37470	-221.37309	86.5	81.7	80.4
24	-211.15384	-211.96652	-211.96359	71.8	67.5	66.5
25	-202.63920	-203.49629		81.1		
26	-227.96291	-228.93464		88.0		
27	-218.66197	-219.53394		73.2		
28	-202.58277	-203.43171	-203.43199	83.0	79.1	77.2
29	-227.93751	-228.90165	-228.90175	90.4	85.9	84.2
30	-218.64663	-219.50816	-219.50860	75.5	71.6	70.2
31	-202.57661	-203.42273	-203.42328	81.8	77.8	76.2
32	-227.92030	-228.88379	-228.88382	89.3	84.7	82.9
33	-218.62241	-219.48532	-219.48608	73.8	69.8	68.6

	CID/6-31+G*//CID/6-31+G*				
	abs. energy	ZPE		abs. energy	ZPE
22	-195.00808	77.5	28	-202.48894	81.3

	MP2	B3L//MP2	B3L//B3L	ZPE HF (N)
34	-195.11412	-195.91783	-195.91844	78.8 (1)
35	-195.11431	-195.92132	-195.92080	78.8 (1)
36	-195.12412	-195.92205	-195.92141	80.5 (0)
37	-195.12616	-195.92559	-195.92549	80.7 (0)
38	-195.11318	-195.90877	-195.90820	80.5 (1)

Absolute energies in hartrees, zero-point vibrational energies in kcal/mol, and number of imaginary frequencies (NIMAG). Compound numbers as in Figures 6 - 8. MP2 = MP2(fc)/6-31+G*//MP2(fc)/6-31+G*; B3L//MP2 = Becke3LYP/6-311++G**//MP2(fc)/ 6-31+G*; B3L//B3L = Becke3LYP/6-311+G**//Becke3LYP/6-311+G**; ZPE = HF/6-31+G*, unscaled; (N) = NIMAG.

	B3L//B3L	ZPE (N)		B3L//B3L	ZPE (N)
39	-221.37370	86.1 (1)	**40**	-221.37151	86.0 (1)
41	-221.38462	88.0 (0)	**42**	-221.38136	87.9 (0)
43	-221.38433	87.9 (1)	**44**	-211.96818	71.3 (1)
45	-211.96734	71.2 (1)	**46**	-211.97294	73.5 (0)
47	-211.97192	73.3 (0)	**48**	-211.97137	73.4 (1)

	MP2	B3L//MP2	ZPE (N)		MP2	B3L//MP2	ZPE (N)
49	-202.61119	-203.46772	82.2 (1)	**50**	-202.64030	-203.48709	84.0 (0)
51	-202.62829	-203.47560	83.7 (0)	**52**	-202.59297	-203.44070	83.6 (1)
53	-227.93468	-228.90593	89.2 (1)	**54**	-227.96343	-228.92531	91.1 (0)
55	-227.95593	-228.91797	90.9 (0)	**56**	-227.95560	-228.92419	91.7 (1)
57	-218.64879	-219.51211	74.3 (1)	**58**	-218.68259	-219.54271	76.9 (0)
59	-218.65751	-219.51784	76.3 (0)	**60**	-218.65862	-219.52114	77.1 (1)

	B3L//MP2	ZPE (N)
methylborane	-65.96809	37.0
methane	-40.53400	29.9
cyclopentane C_2	-196.61153	94.3
cyclopentane C_s	-196.61149	94.3
propene	-117.94547	53.5
cyclopentylborane	-222.04453	100.9
2-borylpropene	-143.38772	60.8
pyrrolidine	-212.64619	87.4
2-azapropene	-133.98353	46.1