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H-4385-m1

Table S1 Total Energies (a.u.)[a].

Molecule	SCF	MP2	CCSD(T)
H_2	−1.1313335893	−1.1576600037	−1.165157382
CH_4	−40.2017047901	−40.3698547645	−40.388168534
SiH_2	−4.8562707434	−4.9383257559	−4.966003129
GeH_2	−4.7533735343	−4.8330419992	−4.859085068
SnH_2	−4.3684240588	−4.4424294541	−4.467364414
PbH_2	−4.4565789125	−4.5304344664	−4.553628373
SiH_4	−6.0964164240	−6.2059342505	−6.234639280
GeH_4	−5.9561792796	−6.0636064053	−6.091882131
SnH_4	−5.5377913046	−5.6367146372	−5.664705680
PbH_4	−5.5846471072	−5.6854909725	−5.713685238
SiH_3CH_3	−45.1474446930	−45.4055369385	−45.445365987†
GeH_3CH_3	−45.0035558201	−45.2603789104	−45.299562430†
SnH_3CH_3	−44.5839489970	−44.8332500590	−44.872007222†
PbH_3CH_3	−44.6281376260	−44.8799026225	−44.918698974†
eclipsed	−44.6274361186	−44.8790784539	−44.917919189†
$PbHCH_3$	−43.4983988953	−43.7247482263	−43.758148825
$PbHCH_3$(TS)	−43.4976447135	−43.7238999473	−43.757342527
SiH_4(TS)	−5.9711570341	−6.0978705951	−6.130364333†
GeH_4(TS)	−5.8411663043	−5.9657156708	−5.997876031†
SnH_4(TS)	−5.4255272255	−5.5429377408	−5.576349478†
PbH_4(TS)	−5.4850407872	−5.6043115667	−5.637897232†

a) SCF and MP2 values at optimized SCF geometry. CCSD(T) values at optimized CCSD(T) geometries, except for the transition structures (†), where the CCSD(T) energy is calculated at the SCF optimized geometry.

H-4385-m2

Table S2 Calculated Harmonic Force Constants in Symmetry Coordinates. [a,b]

	SiH_2	GeH_2	SnH_2	PbH_2
F_{11}	2.912	2.429	1.928	1.651
F_{22}	0.829	0.788	0.718	0.684
F_{12}	0.103	0.088	0.054	0.024
F_{33}	2.866	2.418	1.190	1.643
	SiH_4	GeH_4	SnH_4	PbH_4
F_{11}	3.427	3.032	2.424	2.248
F_{22}	0.489	0.465	0.396	0.383
F_{33}	3.277	2.917	2.317	2.136
F_{34}	-0.113	-0.134	-0.115	-0.149
F_{44}	0.623	0.587	0.540	0.511
	SiH_3CH_3	GeH_3CH_3	SnH_3CH_3	PbH_3CH_3
F_{11}	3.229	2.860	2.325	2.131
F_{22}	3.342	2.952	2.356	2.164
F_{33}	5.830	5.879	5.896	5.941
F_{44}	0.634	0.592	0.538	0.505
F_{55}	0.573	0.570	0.548	0.549
F_{12}	0.084	0.073	0.059	0.059
F_{13}	0.052	0.043	0.037	0.031
F_{14}	-0.140	-0.132	-0.097	-0.107
F_{15}	-0.184	-0.197	-0.198	-0.213
F_{23}	0.011	0.010	0.008	0.009
F_{24}	0.062	0.073	0.063	0.082
F_{25}	-0.219	-0.025	-0.023	-0.032
F_{34}	-0.019	-0.021	-0.020	-0.024
F_{35}	0.141	0.153	0.168	0.177
F_{45}	0.022	0.026	0.025	0.034
F_{66}	3.219	2.858	2.272	2.082
F_{77}	5.717	5.772	5.795	5.848
F_{88}	0.585	0.548	0.484	0.460
F_{99}	0.658	0.647	0.643	0.638
F_{1010}	0.631	0.575	0.491	0.453
F_{1111}	0.486	0.491	0.447	0.465
F_{67}	-0.011	-0.012	-0.010	-0.014
F_{68}	-0.084	-0.096	-0.082	-0.104
F_{69}	0.001	0.001	0.001	0.002
F_{610}	0.081	0.091	0.082	0.103
F_{611}	0.031	0.034	0.026	0.030
F_{78}	-0.015	-0.012	-0.009	-0.007
F_{79}	-0.154	-0.156	-0.159	-0.158
F_{710}	0.043	0.032	0.021	0.015
F_{711}	0.140	0.119	0.107	0.086
F_{89}	-0.008	-0.006	-0.006	-0.005
F_{810}	-0.095	-0.081	-0.085	-0.073
F_{811}	-0.029	-0.029	-0.032	-0.029
F_{910}	-0.002	-0.000	-0.000	+0.000
F_{911}	0.022	0.021	0.024	0.020
F_{1011}	0.196	0.190	0.171	0.162
F_{1212}	0.005	0.004	0.002	0.001

a) For the definition of the symmetry coordinates of MH_2, MH_4, and H_3MCH_3 see refs 35, 36, and 20, respectively.

b) In aJ $Å^{-m}rad^{-n}$ for m stretching and n bending coordinates. aJ = mdyn Å .

Table S3 Spectroscopic Constants for H_3PbCH_3.

Rotational constants:

$A_e = 1.5199\ cm^{-1}$
$B_e = 0.2126\ cm^{-1}$

Centrifugal distortion constants:

$D_j = 0.138\ (0.146) \cdot 10^{-6}\ cm^{-1}$
$D_{jk} = 0.984\ (0.125) \cdot 10^{-6}\ cm^{-1}$
$D_k = 3.637\ (4.209) \cdot 10^{-6}\ cm^{-1}$

Coriolis constants:

$\zeta_7 =$ 0.056 (0.057)
$\zeta_8 =$ -0.087 (-0.080)
$\zeta_9 =$ -0.280 (-0.281)
$\zeta_{10} =$ 0.242 (0.239)
$\zeta_{11} =$ -0.133 (-0.134)
$\zeta_{12} =$ 0.272 (0.270)

The values above refer to the unscaled (scaled) force fields.