Supporting Information

Table 1 (extended). Optimized geometries for Group VI dihydrides.

Molecule	Method		∠(H-X-H)	R(X-H) (Å)
(116)H_2				
	DFT/HF-exch	SO	98.330	2.058
	DFT/HF-exch		90.495	1.808
	DFT/B3LYP	SO	94.733	2.047
	DFT/B3LYP		90.073	1.836
	HF-SCF		90.507	1.808
	HF-MP2		88.657	1.803
	HF-CCSD		89.112	1.824
	HF-CCSD(T)		89.327	1.819
	KR-SCF	SO	98.940	2.060
	KR-MP2	SO	94.240	2.038
	KR-CCSD(T)	SO	94.701	2.059
	KR-CCSD	SO	94.222	2.051
PoH_2				
	DFT/HF-exch	SO	90.670	1.742
	DFT/HF-exch		91.180	1.726
	DFT/B3LYP	SO	89.360	1.808
	DFT/B3LYP		89.710	1.789
	HF-SCF		91.180	1.726
	HF-MP2		89.030	1.734
	HF-CCSD(T)		89.109	1.747
	HF-CCSD		89.301	1.744
TeH_2				
	DFT/HF-exch	SO	92.107	1.645
	DFT/HF-exch		92.103	1.645
	DFT/B3LYP	SO	90.052	1.690
	DFT/B3LYP		90.050	1.690
	HF-SCF		92.107	1.645
	HF-MP2		90.166	1.645
	HF-CCSD(T)		90.149	1.655
	HF-CCSD		90.307	1.653
	Expt		90.260	1.659
SeH_2				
	DFT/HF-exch	SO	93.448	1.431
	DFT/HF-exch		93.435	1.430
	DFT/B3LYP	SO	91.181	1.467
	DFT/B3LYP		91.213	1.467
	HF-SCF		93.435	1.430

	HF-MP2		91.635	1.423
	HF-CCSD(T)		91.624	1.430
	HF-CCSD		91.726	1.430
	Expt.		90.570	1.460
H_2S				
	DFT/HF-exch	SO	94.801	1.331
	DFT/HF-exch		94.790	1.331
	DFT/B3LYP	SO	92.777	1.352
	DFT/B3LYP		92.777	1.352
	HF-SCF		94.800	1.331
	HF-MP2		92.570	1.331
	HF-CCSD(T)		92.502	1.336
	HF-CCSD		92.615	1.335
	Expt.		92.120	1.336
H_2O				
	DFT (SO)	HF-exch	106.757	0.950
	DFT	HF-exch	106.755	0.950
	DFT (SO)	B3LYP	105.099	0.971
	DFT	B3LYP	105.103	0.971
	HF	SCF	106.756	0.950
	HF	MP2	103.145	0.968
	HF	CCSD(T)	103.544	0.967
	HF	CCSD	103.534	0.967
	Expt.		104.520	0.957

SO=calculation includes the spin-orbit interaction
DFT=based on density functional theory
KR=based on a Kramers'-restricted two-component *ab initio* wavefunction
HF=based on a Hartree-Fock wavefunction
HF-exch= the Hartree-Fock exchange only potential was used
Experimental data are from Reference 1.

Uncontracted Cartesian basis set for Element 116

```
S   20.38        1.0
     9.94        1.0
     1.520638    1.0
     0.182956    1.0
     0.076570    1.0
D,S
    15.555105    1.0
     3.367447    1.0
     1.505696    1.0
     0.538240    1.0
```

0.126942 1.0
0.042631 1.0

P

14.176438 1.0
4.063696 1.0
3.699851 1.0
1.541538 1.0
0.644783 1.0
0.249799 1.0
0.081662 1.0

F,P

0.820928 1.0
0.060148 1.0

Uncontracted Cartesian basis set used for Po

S

1.817818 1.0
0.963673 1.0
0.379815 1.0
0.166737 1.0
0.079820 1.0

P

9.44088 1.0
0.700806 1.0
0.445134 1.0
0.157003 1.0
0.061235 1.0

D,S

11.93660 1.0
1.95180 1.0
0.97140 1.0
0.64840 1.0
0.28760 1.0