

Supporting Information

Tetryliumylidene ions in synthesis and catalysis

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Z-matrixes and energies of the optimized structures at the B3LYP/def2-TZVP level.
For the Sn and Pb the corresponding ECP was utilized.

[HC]⁺

C
H 1 1.1375
E(RB3LYP) = -38.09257 E_h

[HSi]⁺

Si
H 1 1.5149
E(RB3LYP) = -289.71941 E_h

[HGe]⁺

Ge
H 1 1.5925
E(RB3LYP) = -2077.29158 E_h

[HSn]⁺

Sn
H 1 1.7674
E(RB3LYP) = -214.66551 E_h

[HPb]⁺

Pb
H 1 1.8362
E(RB3LYP) = -193.24704 E_h

H₂C

C
H 1 1.1103
H 1 1.1103 2 101.870
E(RB3LYP) = -39.1505217130

H₂Si

Si
H 1 1.5236
H 1 1.5236 2 91.620
E(RB3LYP) = -290.641250885

H₂Ge

Ge
H 1 1.5996
H 1 1.5996 90.805
E(RB3LYP) = -2078.19692932

H₂Sn

Sn
H 1 1.7805
H 1 1.7805 2 90.567
E(RB3LYP) = -215.538707322

H₂Pb

Pb
H 1 1.8550
H 1 1.8550 2 90.282
E(RB3LYP) = -194.104174230