

LiH, BeH₂, BH₃, CH₄, NH₃, H₂O, HF

	LiH	BeH2	BH3	CH4	Property
R<Z> Å	0.2967	0.2197	0.1729	0.1415	Radius of He core
R<Z-H> Å	1.0619	0.8406	0.7328	0.6545	Radius of Z-H cloud
R<Z-L> Å	-	-	-	-	Radius of lone pair
d<Z-H> Å	1.5942	1.3329	1.1890	1.0787	distance Z-H
< HZH °	-	180.0000	120.0000	109.4712	angle H-Z-H
< LZL °	-	-	-	-	angle LoneP-Z-LoneP
kcal/mol	56.6	69.4	88.4	98.2	Mean Thermod.BondEn.

	CH4	NH3	H2O	HF	Property
R<Z> Å	0.1415	0.1128	0.0932	0.0821	Radius of He core
R<Z-H> Å	0.6545	0.5904	0.5427	0.5198	Radius of Z-H cloud
R<Z-L> Å	-	0.7137	0.5955	0.4396	Radius of lone pair
d<Z-H> Å	1.0787	1.0080	0.9505	0.9106	distance Z-H
< HZH °	109.4712	105.8262	103.2030	-	angle H-Z-H
< LZL °	-	-	120.9455	114.2797	angle LoneP-Z-LoneP
kcal/mol	98.2	92.1	109.8	136.2	Mean Thermod.BondEn.

	LiH	BeH2	BH3	CH4	Property
R<Z> Å	0.2937	0.2188	0.1723	0.1402	Radius of He core
R<Z-H> Å	1.0990	0.8411	0.7344	0.6622	Radius of Z-H cloud
R<Z-L> Å	-	-	-	-	Radius of lone pair
d<Z-H> Å	1.6397	1.3328	1.1909	1.0892	distance Z-H
< HZH °	-	180.0000	120.0000	109.4712	angle H-Z-H
< LZL °	-	-	-	-	angle LoneP-Z-LoneP
BE kcal/mol	56.3	69.2	88.3	98.2	Mean Thermod.BondEn.

	CH4	NH3	H2O	HF	Property
R<Z> Å	0.1402	0.1125	0.0943	0.0821	Radius of He core
R<Z-H> Å	0.6622	0.5935	0.5383	0.5202	Radius of Z-H cloud
R<Z-L> Å	-	0.7168	0.5954	0.4390	Radius of lone pair
d<Z-H> Å	1.0892	1.0126	0.9447	0.9109	distance Z-H
< HZH °	109.4712	105.8248	103.3440	-	angle H-Z-H
< LZL °	-	-	120.9655	114.2853	angle LoneP-Z-LoneP
BE kcal/mol	98.2	91.9	109.4	134.7	Mean Thermod.BondEn.

Upper table:
 Parametrized with G2-Energies from Curtiss, Raghavachari, Redfern & Pople, JCP 106,1063(1997).
 The atomization energies at 0 Kelvin (D0) are within 0.1 kcal/mol of the G2 values and within 0.2 kcal/mol of the experimental values (where available).
 Bondlengths are within 0.01 Angstroms, bondangles within 1-2 degrees of the experimental values.
 The parameters found can be transported to the classes of hydrocarbons, organic amines, alcohols, fluorocarbons with only small loss of precision.

Lower table is the same parametrization with G3-Theory from Curtiss,Raghavachari, Redfern & Pople, JCP 109,7764(1998).