## LiH, BeH<sub>2</sub>, BH<sub>3</sub>, CH<sub>4</sub>, NH<sub>3</sub>, H<sub>2</sub>O, HF

	LiH	BeH2	BH3	CH4	Property
R(Z) A	0.2967	0.2197	0.1729	0.1415	Radius of He core
R(Z-H) A	1.0619	0.8406	0.7328	0.6545	Radius of Z-H cloud
R(Z-L) A		-	4 4000	4 0000	Radius of lone pair
d(Z-H) A ( HZH º	1.5942	1.3329 180.0000	1.1890 120.0000	1.0787 109.4712	distance Z-H angle H-Z-H
₹ LZL °		100.0000	120.0000	107.4712	angle LoneP-Z-LoneF
kcal/mol	56.6	69.4	88.4	98.2	Mean Thermod.BondEn
	CH4	NH3	H20	HF	Property
R(Z) A	0.1415	0.1128	0.0932	0.0821	Radius of He core
R(Z-H) A	0.6545	0.5904	0.5427	0.5198	Radius of Z-H cloud
R(Z-L) A		0.7137	0.5955	0.4396	Radius of lone pair
d(Z-H) A	1.0787	1.0080	0.9505	0.9106	distance Z-H
< HZH °	109.4712	105.8262	103.2030	_	angle H-Z-H
< LZL o	_	_	120.9455	114.2797	angle LoneP-Z-LoneI
kcal/mol	98.2	92.1	109.8	136.2	Mean Thermod.BondEn
		D 110	PHO	011.4	
	LiH	BeH2	ВНЗ	CH4	Property
R(Z) A					
R(Z) 8 R(Z-H) 8	LiH 0.2937 1.0990	BeH2 0.2188 0.8411	BH3 0.1723 0.7344	CH4 0.1402 0.6622	Radius of He core Radius of Z-H cloud
R(Z-H) A R(Z-L) A	0.2937 1.0990	0.2188 0.8411	0.1723 0.7344	0.1402 0.6622	Radius of He core Radius of Z-H cloud Radius of lone pair
R(Z-H) A R(Z-L) A d(Z-H) A	0.2937	0.2188 0.8411 1.3328	0.1723 0.7344 - 1.1909	0.1402 0.6622 1.0892	Radius of He core Radius of Z-H cloud Radius of lone pair distance Z-H
R(Z-H) 8 R(Z-L) 8 d(Z-H) 8 ( HZH °	0.2937 1.0990	0.2188 0.8411	0.1723 0.7344	0.1402 0.6622	Radius of He core Radius of Z-H cloud Radius of lone pair distance Z-H angle H-Z-H
R(Z-H) A R(Z-L) A d(Z-H) A < HZH ° < LZL °	0.2937 1.0990 1.6397	0.2188 0.8411 - 1.3328 180.0000	0.1723 0.7344 - 1.1909 120.0000	0.1402 0.6622 - 1.0892 109.4712	Radius of He core Radius of Z-H cloud Radius of lone pair distance Z-H angle H-Z-H angle LoneP-Z-LoneP
R(Z-H) 8 R(Z-L) 8 d(Z-H) 8 ( HZH °	0.2937 1.0990	0.2188 0.8411 1.3328	0.1723 0.7344 - 1.1909	0.1402 0.6622 1.0892	Radius of He core Radius of Z-H cloud Radius of lone pair distance Z-H angle H-Z-H angle LoneP-Z-LoneP
R(Z-H) A R(Z-L) A d(Z-H) A < HZH ° < LZL °	0.2937 1.0990 1.6397 - - 56.3	0.2188 0.8411 - 1.3328 180.0000 - 69.2	0.1723 0.7344 - 1.1909 120.0000 - 88.3	0.1402 0.6622 1.0892 109.4712 98.2	Radius of He core Radius of Z-H cloud Radius of lone pair distance Z-H angle H-Z-H angle LoneP-Z-LoneP Mean Thermod.BondEn
R(Z-H) A R(Z-L) A d(Z-H) A < HZH O < LZL O BE kc/mol	0.2937 1.0990 1.6397	0.2188 0.8411 - 1.3328 180.0000	0.1723 0.7344 - 1.1909 120.0000	0.1402 0.6622 - 1.0892 109.4712	Radius of He core Radius of Z-H cloud Radius of lone pair distance Z-H angle H-Z-H angle LoneP-Z-LoneP
R(Z-H) A R(Z-L) A d(Z-H) A < HZH ° < LZL ° BE kc/mol	0.2937 1.0990 1.6397 - - 56.3 CH4 0.1402	0.2188 0.8411 1.3328 180.0000 69.2 NH3	0.1723 0.7344 1.1909 120.0000 88.3 H20 0.0943	0.1402 0.6622 1.0892 109.4712 98.2 HF	Radius of He core Radius of Z-H cloud Radius of lone pair distance Z-H angle H-Z-H angle LoneP-Z-LoneP Mean Thermod.BondEn  Property  Radius of He core
R(Z-H) A R(Z-L) A d(Z-H) A < HZH ° < LZL ° BE kc/mo1	0.2937 1.0990 1.6397 - 56.3	0.2188 0.8411 1.3328 180.0000 69.2 NH3 0.1125 0.5935	0.1723 0.7344 1.1909 120.0000 88.3 H20 0.0943 0.5383	0.1402 0.6622 1.0892 109.4712 98.2 HF 0.0821 0.5202	Radius of He core Radius of Z-H cloud Radius of lone pair distance Z-H angle H-Z-H angle LoneP-Z-LoneP Mean Thermod.BondEn  Property  Radius of He core Radius of Z-H cloud
R(Z-H) A R(Z-L) A d(Z-H) A < HZH ° < LZL ° BE kc/mo1	0.2937 1.0990 1.6397 - - 56.3 CH4 0.1402 0.6622	0.2188 0.8411 1.3328 180.0000 69.2 NH3 0.1125 0.5935 0.7168	0.1723 0.7344 - 1.1909 120.0000 - 88.3 H20 0.0943 0.5383 0.5954	0.1402 0.6622 1.0892 109.4712 98.2 HF 0.0821 0.5202 0.4390	Radius of He core Radius of Z-H cloud Radius of lone pair distance Z-H angle H-Z-H angle LoneP-Z-LoneP Mean Thermod.BondEn  Property  Radius of He core Radius of Z-H cloud Radius of lone pair
R(Z-H) A R(Z-L) A d(Z-H) A < HZH   C LZL   BE kc/mo1  R(Z) A R(Z-H) A R(Z-L) A d(Z-H) A	0.2937 1.0990 1.6397 - - 56.3 CH4 0.1402 0.6622 1.0892	0.2188 0.8411 - 1.3328 180.0000 - 69.2 NH3 0.1125 0.5935 0.7168 1.0126	0.1723 0.7344 - 1.1909 120.0000 - 88.3 H20 0.0943 0.5383 0.5954 0.9447	0.1402 0.6622 1.0892 109.4712 98.2 HF 0.0821 0.5202	Radius of He core Radius of Z-H cloud Radius of lone pair distance Z-H angle H-Z-H angle LoneP-Z-LoneP Mean Thermod.BondEn  Property  Radius of He core Radius of Z-H cloud Radius of lone pair distance Z-H
R(Z-H) A R(Z-L) A d(Z-H) A < HZH   C LZL   BE kc/mo1  R(Z) A R(Z-H) A R(Z-L) A d(Z-H) A < HZH   C	0.2937 1.0990 1.6397 - - 56.3 CH4 0.1402 0.6622	0.2188 0.8411 1.3328 180.0000 69.2 NH3 0.1125 0.5935 0.7168	0.1723 0.7344 - 1.1909 120.0000 - 88.3 H20 0.0943 0.5383 0.5954 0.9447 103.3440	0.1402 0.6622 - 1.0892 109.4712 98.2 HF 0.0821 0.5202 0.4390 0.9109	Radius of He core Radius of Z-H cloud Radius of lone pair distance Z-H angle H-Z-H angle LoneP-Z-LoneP Mean Thermod.BondEn  Property  Radius of He core Radius of Z-H cloud Radius of lone pair distance Z-H angle H-Z-H
R(Z-H) A R(Z-L) A d(Z-H) A < HZH	0.2937 1.0990 1.6397 - - 56.3 CH4 0.1402 0.6622 1.0892	0.2188 0.8411 - 1.3328 180.0000 - 69.2 NH3 0.1125 0.5935 0.7168 1.0126	0.1723 0.7344 - 1.1909 120.0000 - 88.3 H20 0.0943 0.5383 0.5954 0.9447	0.1402 0.6622 1.0892 109.4712 98.2 HF 0.0821 0.5202 0.4390	Radius of He core Radius of Z-H cloud Radius of lone pair distance Z-H angle H-Z-H angle LoneP-Z-LoneP Mean Thermod.BondEn  Property  Radius of He core Radius of Z-H cloud Radius of lone pair distance Z-H

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).