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SINDO1
III. Application to Ground States of Molecules Containing Fluorine, Boron, Beryllium and Lithium Atoms

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Molecular geometries, binding energies, ionization potentials and dipole moments are calculated by the SINDO1 method for a large number of molecules containing F, B, Be and Li atoms. Comparison is made with MINDO/3, MNDO and where possible with STO-3G results. The explicit data and an error statistics show that SINDO1 is the most reliable except for ionization potentials.

Key words: Application of SINDO1 to ground state of molecules – containing F, B, Be, Li.

1. Introduction

In two preceding papers [1, 2] we described the SINDO1 method and its application to molecules containing carbon, nitrogen and oxygen atoms. Here we wish to present an application to the rest of first-row elements. Fluorine, boron, beryllium and lithium containing compounds are investigated with respect to their geometries, binding energies, ionization potentials and dipole moments. MINDO/3 papers [3] contain only fluorine and boron, MNDO papers [4, 5] do not contain lithium.

2. Geometries

Table 1 contains theoretical and experimental data on geometries. Besides MINDO/3 and MNDO, some STO-3G results [6–10, 22] are listed. Experimental data are usually from Dewar's papers, those with a superscript are from various

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Table 1. Molecular Geometries (A, Degrees)

Molecule	Coordinate	Exp	SINDO1	MINDO/3	MNDO	STO-3G
FH	FH	0.917^{e}	0.910	0.913	0.956	0.956
FH_2	FH	(0.920^{a})	1.013			
	HFH	180.0	180.0			
CF	CF	1.267^{c}	1.265		1.340	1.293
HCF	CF	1.314	1.289		1.285	1.311
	CH	1.121	1.109		1.120	1.142
	HCF	101.6	108.8		111.1	102.3
CH_3F	CF	$1.384^{b,d}$	1.364	1.378	1.347	1.384
	CH	1.097	1.092	1.102	1.118	1.097
	HCF	108.5	109.0	107.3	110.6	108.3
C_2HF	CC	$1.198^{b,d}$	1.228	1.199	1.192	1.168
	CF	1.279	1.319	1.331	1.277	1.318
	CH	1.053^{b}	1.050	1.072		1.062
^3NF	NF	1.51^{c}	1.283		1.215	1.342
FCN	CN	$1.159^{b,d}$	1.158		1.159	1.160
	CF	1.262	1.311		1.273	1.316
OF	OF	1.30^{c}	1.310		1.226	
HOF	OF	1.442	1.341		1.277	1.354
	OH	0.966	0.986		0.964	1.006
	HOF	96.8	102.7		107.9	101.4
FCO	CO	1.18^{c}	1.176			1.224
	CF	1.34	1.332			1.349
	FCO	135	134.2			125.4
HFCO	CO	$1.183^{b,d}$	1.202		1.222	1.210
	CF	1.341	1.340		1.328	1.351
	CH	1.100	1.090			1.108
	FCO	122.7	122.4		117.9	122.1
	HCO	129.0	126.2			125.6
FNO	NO	1.136^{d}	1.165		1.161	1.222
	NF	1.514	1.352		1.305	1.381
	FNO	110.1	113.2		113.8	108.2
FNO_2	NO	$1.23^{b,d}$	1.234			
	NF	1.35	1.358			
	ONO	(125)	131.8			
F_2	FF	1.418	1.306	1.446	1.266	1.315
CF_2	CF	$1.300^{b,d}$	1.304		1.304	1.323
	FCF	104.9	108.3		108.3	102.7
CH_2F_2	CF	1.358	1.355		1.352	1.378
	CH	1.092	1.098		1.129	1.109
	FCF	108.3	108.5		106.8	108.7
	HCH	111.9	109.4		108.2	108.8
C_2F_2	CC	1.20^{c}	1.240			1.167
	CF	1.28	1.324			1.323
NF_2	NF	1.350^{d}	1.314		1.271	1.365
	FNF	103.3	106.5		109.7	102.0
N_2F_2(cis)	NN	$1.214^{b,d,f}$	1.192		1.240	1.277
	NF	1.384	1.347		1.281	1.373
	NNF	114.5	116.3		121.6	111.5
N_2F_2(trans)	NN	1.231^{f}	1.196		1.261	1.283
	NF	1.396	1.352		1.277	1.371
	NNF	105.5	107.7		112.1	106.2

Table 1 (*cont.*)

Molecule	Coordinate	Exp	SINDO1	MINDO/3	MNDO	STO-3G
OF_2	OF	$1.405^{b,d}$	1.333	1.439	1.281	1.358
	FOF	103.1	105.3	55.2	109.1	102.4
F_2CO	CO	$1.174^{b,d}$	1.204		1.219	1.209
	CF	1.311	1.333		1.316	1.347
	OCF	126.0	125.2		124.1	125.0
CF_3	CF	1.33	1.326		1.312	1.352
	FCF	112.0	114.0		115.4	111.9
CHF_3	CF	$1.332^{b,d}$	1.349		1.353	1.371
	CH	1.098	1.099		1.136	1.119
	FCF	108.8	109.8			108.6
	HCF	110.5	109.8		111.5	
NF_3	NF	$1.365^{b,d}$	1.343		1.315	1.386
	FNF	102.3	104.3		106.1	102.1
CF_3CN	CC	$1.461^{b,d}$	1.525		1.498	
	CN	1.153	1.155		1.158	
	CF	1.335	1.360		1.355	
	CCF	111.4	111.3		111.9	
CF_4	CF	1.321	1.344	1.303	1.347	1.366
C_2F_4	CC	1.311^{f}	1.379	1.313	1.381	1.332
	CF	1.319	1.347	1.294	1.318	1.353
	CCF	123.8	123.8	115.4	124.2	123.4
N_2F_4(trans)	NN		1.395			
	NF		1.352			
	NNF^1		105.0			
	NNF^2		110.6			
	FNNF		190.0			
N_2F_4(gauche)	NN	$1.47^{b,d,f}$	1.406		1.519	
	NF	1.37	1.352		1.302	
	NNF	104	104.0		106.2	
	FNNF	65	72.0		66.5	
CF_3OF	CO	1.395	1.395		1.443	
	CF	1.319	1.351		1.342	
	OF	1.421	1.348		1.274	
	FCF	109.4	109.5		110.7	
	COF	104.8	107.1		110.7	
C_2F_6	CC	1.545	1.629	1.475	1.674	
	CF	1.326	1.359	1.327	1.346	
	CCF	109.8	110.6	107.6	110.7	
BH	BH	1.233^{a}	1.209		1.178	1.213
BH_2	BH	1.180^{a}	1.152		1.159	1.161
	HBH	131.0	139.1		126.6	123.5
BH_3	BH	1.180^{a}	1.163			1.160
BC	BC		1.405			
^3BN	BN	1.281^{a}	1.302			1.305
BO	BO	1.205^{a}	1.220		1.169	1.190
HBO	BO	1.20^{c}	1.211			1.176
	BH	(1.23)	1.136			1.142
BO_2	BO	1.25^{a}	1.279		1.238	1.229
BO_2H	BO^1	1.40^{c}	1.354			1.347
	BO^2	(1.34)	1.224			1.187
	O^1H	1.0	0.978			0.983

Table 1 (*cont.*)

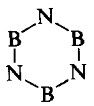
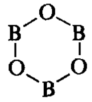
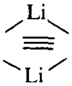
Molecule	Coordinate	Exp	SINDO1	MINDO/3	MNDO	STO-3G
$B(OH)_2$	BO	1.27^{c}	1.363			
	OH	0.97	0.977			
	OBO	(180)	123.7			
	BOH	105	106.3			
$B(OH)_3$	BO		1.383		1.371	1.365
	OH		0.968		0.945	0.981
	BOH		109.4		116.5	109.8
BF	BF	1.262^{a}	1.301			1.243
BOF	BO	1.20^{c}	1.218			1.188
	BF	1.30	1.323			1.295
BF_2	BF	1.295^{c}	1.326		1.291	1.305
	FBF	120	125.0		125.6	116.9
BHF_2	BF	$1.311^{b,d}$	1.334		1.316	1.303
	BH	1.189	1.154			1.169
	FBF	118.3	117.0		114.8	118.2
BOF_2	BO	1.40^{c}	1.358			
	BF	1.30	1.342			
	FBO	117	120.2			
BF_2OH	BO	1.36^{c}	1.357			1.358
	BF	1.30	1.345			1.313
	OH	0.96	0.969			0.981
	F^1BO	120	118.7			119.0
	F^2BO	120	123.7			121.4
	BOH	105	109.3			110.6
BF_3	BF	1.310	1.334		1.316	1.309
$^3B_2$	BB	1.589^{a}	1.538			1.531
B_2H_6	BB	1.775^{c}	1.836		1.753	1.805
	BH^1	1.196	1.170		1.164	1.154
	BH^5	1.339	1.385		1.350	1.327
	H^1BH^2	120.2	114.6			122.6
	BBH^5	42.1	38.4		41.1	38.5
B_2O_3	BO^1	1.36^{c}	1.361		1.341	
	BO^2	1.20	1.225		1.181	
	BOB	120	114.8		123.2	
	OBO	(180)	175			
B_2F_4	BB	1.67^{c}	1.768		1.747	
	BF	1.32	1.348		1.316	
	BBF	120	122.6		123.9	
$B_3N_3H_6$ 	BN	1.435	1.459		1.429	
	BH	1.258	1.167		1.172	
	NH	1.050	0.989		0.998	
	BNB	121.1	120.4		123.6	
$B_3O_3H_3$ 	BO	$1.36^{b,d}$	1.404		1.380	

Table 1 (*cont.*)

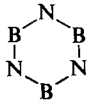
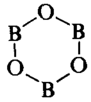
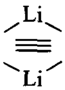
Molecule	Coordinate	Exp	SINDO1	MINDO/3	MNDO	STO-3G
	BH	1.18	1.159		1.171	
	BOB	120	122.0		123.4	
BeH	BeH	1.343	1.296		1.291	1.301
BeH_2	BeH	1.343[a]	1.270		1.278	1.291
BeB	BeB		1.762			1.495
BeC	BeC		1.542			
BeN	BeN	1.406[c]	1.435			
BeO	BeO	1.331	1.308		1.335	1.269
BeOH	BeO	1.4[c]	1.422			
	OH	0.96	0.980			
	BeOH	(120)	107.3			
$Be(OH)_2$	BeO	1.35	1.427		1.487	
	OH	0.97	0.972		0.920	
	BeOH	100	104.2		152.4	
BeF	BeF	1.361	1.375		1.458	1.297
BeF_2	BeF	1.36[a]	1.374		1.459	1.329
$^3Be_2O$	BeO	1.4[c]	1.403			
LiH	LiH	1.594[b,d]	1.518			1.510
LiBe	LiBe		2.422			2.6
^3LiB	LiB		2.139			1.707
LiC	LiC		1.985			1.648
^3LiN	LiN	1.71[c]	1.750			2.347
LiO	LiO	1.62[c]	1.646			1.422
LiOH	LiO	1.60[c]	1.628			1.432
	OH	0.96	0.955			0.971
	LiOH	(110)	122.9			180.0
LiF	LiF	1.564[b,d]	1.549			1.407
Li_2	LiLi	2.672[a]	2.737			2.696
CH_2Li_2	LiC		1.948			1.923
	CH		1.080			1.091
	LiCLi		116.7			119.8
	HCH		107.3			106.7
C_2Li_2 	CC		1.235			
	LiC		2.038			
	CCLi		72.3			
$C_2H_2Li_2$	CC		1.335			
	LiC		1.961			
	CH		1.124			
	CCLi		82.8			
	CCH		127.0			
Li_2O	LiO	1.59[c]	1.599			
Li_3N	LiN		1.711			

[a] Ref. [11]
[b] Ref. [12]
[c] Ref. [13]
[d] microwave spectra
[e] infrared spectra
[f] electron diffraction

Table 2. Binding energies (Hartree)[c] and heats of formation (kcal/mol)

Molecule	E_B (Hartree) Exp	SINDO1	ΔE_B (kcal/mol) SINDO1	$\Delta\Delta Hf^0_{298}$ (kcal/mol) MINDO/3	MNDO	ΔHf^0_{298} (kcal/mol) Exp
FH	0.221	0.2225	−0.9	1.1	5.3	−65.1
FH_2		0.2195				
CF	0.207	0.2226	−9.8			60.1^b
HCF	0.347	0.3361	−6.8		−8.5	30.0
CH_3F	0.672	0.6655	4.1	5.6	−4.1	−56.7
C_2HF	0.624	0.6207	2.1	11.1	10.0	5.0
^3NF	0.116	0.1222	−3.9		−27.9	59.5
FCN	0.475	0.4836	−5.4		−11.3	8.6
OF	0.084	0.0817	1.4		6.4	26.1
HOF	0.268	0.2457	14.0		4.8	−23.5
FCO	0.467	0.4917	−15.5			-41^b
HFCO		0.6139			1.1	−90.0
FNO	0.335	0.3218	8.3		−9.8	−15
FNO_2	0.449	0.4012	29.9		26.6	−26.0
F_2	0.060	0.0598	0.1	−2.5	7.3	0
CF_2	0.421	0.4134	4.8	−46.1	−20.2	−45.0
CH_2F_2		0.6899		1.2	−4.1	−111.8
C_2F_2	0.604	0.5950	5.6	−35.5	−3.8	4.65^b
NF_2	0.227	0.2215	3.4		−24.8	10.1
N_2F_2(cis)	0.4004	0.4085	−5.1		−18.6	−2.2
N_2F_2(trans)	0.3930	0.4041	−7.0		−16.9	2.5
OF_2	0.148	0.1478	0.1	−24.4	12.3	5.9
F_2CO	0.679	0.6582	13.0	−8.1	13.9	−152.7
CF_3	0.548	0.5844	−22.8	−55.3	−24.8	−112.4
CHF_3	0.731	0.7265	2.8	−0.8	2.7	−163.9
NF_3	0.325	0.3050	12.5	−3.2	−2.7	−31.8
CF_3CN	1.017	1.0331	−10.1		4.7	−118.4
CF_4	0.756	0.7743	−11.5	−0.8	8.7	−223.0
C_2F_4	0.928	0.9285	−0.3	−0.8	−18.4	−157.4
N_2F_4(trans)		0.5172			−16.3	−2.0
N_2F_4(gauche)	0.493	0.5149	−13.7			
CF_3OF	0.791	0.8129	−13.7		19.3	−182.8
C_2F_6	1.254	1.2354	11.7	−4.3	21.3	−321.3
BH	0.130	0.1038	16.4	−54.8	−36.1	108.2
BH_2	0.283	0.2592	14.9		20.8	45.7
BH_3	0.445	0.4347	6.5		−12.1	23.8
BC	0.171	0.1529	11.4			196^b
^3BN	0.212	0.1678	27.7			11.3^b
BO	0.307	0.2831	15.0		−19.9	18.4
HBO	(0.431)	0.4740				$-20^b \pm 20$
BO_2	0.514	0.5080	3.8		6.6	−75.3
BO_2H	0.714	0.6925	13.5		1.0	−134.1
$B(OH)_2$	0.767	0.7674	−0.3			112^b
$B(OH)_3$	1.155	1.1753	−12.7	−4.2	0.7	−237.0
BF	0.288	0.2705	11.0			28.4
BOF	0.571	0.5465	15.4		3.5	−144.0
BF_2	0.499	0.4702	18.1		−6.8	−130.0

Table 2 (*cont.*)

Molecule	E_B (Hartree) Exp	SINDO1	ΔE_B (kcal/mol) SINDO1	$\Delta\Delta Hf^0_{298}$ (kcal/mol) MINDO/3	MNDO	ΔHf^0_{298} (kcal/mol) Exp
BHF_2	0.647	0.6480	−0.6		−1.7	−175.4
BOF_2	0.691	0.7111	−12.6			−199[b]
BF_2OH	0.881	0.8974	−10.3		5.6	−259.0
BF_3	0.741	0.7515	−6.6		10.0	−271.4
$^3B_2$	0.113	0.1042	5.5			193.5
B_2H_6	0.952	0.9668	−9.3	4.5	−10.2	8.4
B_2O_3	1.038	1.0218	10.2	44.8	0.7	−199.2
B_2F_4	1.101	1.0788	13.9		2.8	−342.2
$B_3N_3H_6$ 	1.936	1.9360	0	−85.8	−8.9	−122.2
$B_3O_3H_3$ 	1.671	1.6926	−13.6		18.3	−290.0
BeH	0.089	0.0739	9.5		−15.8	76[b]
BeH_2	0.254	0.2354	11.7		17.6	−8
BeB		0.1088				
BeC		0.1061				
BeN		0.1141				
BeO	0.173	0.1651	5.0		7.2	31
BeOH	0.354	0.3497	2.7			−25[b]
$Be(OH)_2$	0.751	0.7698	−11.8		19.8	−156.4
BeF	0.221	0.2078	8.3		−4.9	−48
BeF_2	0.491	0.4931	−1.3		−2.0	−190.3
$^3Be_2O$	0.373	0.3662	4.2			−15.4
LiH	0.092	0.0812	7.0			33.65[b]
LiBe		0.0642				
^3LiB		0.0834				
LiC		0.0872				
^3LiN	0.114	0.1063	4.8			80[b]
LiO	0.124	0.1283	2.7			20[b]
LiOH	0.343	0.3275	9.7			−58.1[b]
LiF	0.222	0.2222	0.1			−81.4[a]
Li_2	0.039	0.0581	−12.0			50.3[b]
CH_2Li_2		0.5747				
C_2Li_2 		0.7279				−14.2[b]
$C_2H_2Li_2$		0.869				
Li_2O	0.2829	0.2903	−4.6			−39.6[b]
Li_3N		0.4193				

[a] Ref. [11]
[b] Ref. [13]
[c] 1 Hartree = 627.46 kcal/mol = 2625.3 kJ/mol

data tables [11–13]. A study of this table shows that bond lengths calculated by SINDO1 and bond angles calculated by STO-3G are the best. Actually there are too few bond angles for a good statistics. Also MINDO/3 and STO-3G values for geometries are insufficient for a final assessment. So the comparison is really between SINDO1 and MNDO. SINDO1 bond lengths in the fluorine compounds NF, FNO, F_2, OF_2 and C_2F_6 are poor, but MNDO is even less satisfactory. STO-3G results are often not available but they can be quite poor as N_2F_2 reveals. Experimental data for boron and beryllium compounds are often unreliable and many of them are estimated values.

A few trends can be recognized. BH and BeH bonds tend to be too short. It is not clear, though, that the BH length in HBO is really so much underestimated. In this case STO-3G gives a similar result as SINDO1. The experimental geometry of B_2O_3 is uncertain. The BB bond of B_2F_4 is too long in SINDO1 as well as in MNDO. Lithium compounds are well reproduced in SINDO1.

3. Binding energies

Table 2 shows the experimental and SINDO1 binding energies, errors in the SINDO1 binding energies (ΔE_B) and the errors in the heats of formation ($\Delta\Delta Hf^0_{298}$) given by MINDO/3 and MNDO. Unlike SINDO1, MINDO/3 and MNDO have been calibrated for heats of formation at 25°C. The experimental thermochemical data are taken from Dewar's papers and data tables [13–16]. For about 70 compounds experimental binding energies estimated from the available heats of formation at 0°K and energies of zero point vibration [17–19] can be compared with the predictions based on SINDO1. SINDO1 errors are not larger than 29.9 kcal/mol. The largest errors are in FNO_2, BN and HBO. MINDO/3 leads to high errors in many fluorine and boron compounds, the maximum errors in them being 55.3 kcal/mol and 85.8 kcal/mol respectively. Maximum MNDO errors in these compounds are reduced to 27.8 kcal/mol in NF and 36.1 kcal/mol in BH.

Similar to MNDO SINDO1 predicts cis-N_2F_2 to be stabler than the trans form and trans-N_2F_4 stabler than the gauche conformer. This result for N_2F_4 is, however, in variance with the experimental finding [11].

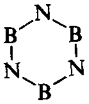
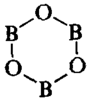
4. Ionization potentials

Available experimental data on the first ionization potential for over 40 compounds are compared with the values calculated via Koopmans' theorem in Table 3. The unlabelled data are from Dewar's papers, the labelled ones from data tables [11, 16]. Here MNDO results are superior to SINDO1 results. The SINDO1 values are mostly too large, quite a few of them being in error by more than 1 ev. MINDO/3 data are insufficient, but would probably be less reliable than SINDO1 results. STO-3G would probably be of not much help either. The only available value, 10.36 ev for FH[8] is too small by almost 6 ev.

Table 3. Ionization potentials (ev)

Molecule	Exp	SINDO1	MINDO/3	MNDO	STO-3G
FH	16.03	17.21	14.80	14.82	10.36
FH_2		9.33			
CF	8.91^c	9.99			
HCF		10.85			
CH_3F	13.31	14.14	12.05	13.05	
C_2HF	11.30	11.32	10.43	11.07	
^3NF		13.23			
FCN		13.00			
OF		13.73		14.11	
HOF	13.0	13.90		12.75	
FCO		10.43			
HFCO		12.35			
FNO	12.94	11.54		12.93	
FNO_2	13.51	12.10		12.99	
F_2	15.83	16.34	13.66	15.25	
CF_2	11.7^c	11.55		12.18	
CH_2F_2	12.71^c	14.04			
C_2F_2	11.4^c	11.00			
NF_2	12.10	13.10		12.23	
N_2F_2(cis)	13.4	12.72		13.00	
N_2F_2(trans)		12.58			
OF_2	13.26	13.93		13.52	
F_2CO	13.62	13.45		13.60	
CF_3	9.25^c	11.32		11.20	
CHF_3	13.73	14.62		13.93	
NF_3	13.0^c	13.38			
CF_3CN		13.90			
CF_4	16.23	16.29	13.49	16.81	
C_2F_4	10.54	10.70		10.75	
N_2F_4	12.84	12.81		13.02	
CF_3OF	13.64	14.51		14.23	
C_2F_6	14.6	13.00	12.62	14.50	
BH	9.7^a	9.45		10.1	
BH_2	9.8^c	9.43			
BH_3	(11.4–14.0^c)	14.74			
BC	10.00^c	9.39			
^3BN		11.24			
BO	12.8^c	12.19			
HBO		14.22			
BO_2		11.88			
BO_2H	12.6^c	12.30			
$B(OH)_2$		7.97			
$B(OH)_3$	13.5^c	13.12			
BF	11.11^c	10.80			
BOF	13.4^c	13.71			
BF_2		9.80			
BHF_2		14.46			
BOF_2		14.71			
BF_2OH		14.80			
BF_3	16.22	16.31		15.95	

Table 3 (*cont.*)

Molecule	Exp	SINDO1	MINDO/3	MNDO	STO-3G
$^3B_2$		8.75			
B_2H_6	11.4[b]	13.25			
B_2O_3	13.7[b]	12.17		13.14	
B_2F_4	12.07[b]	12.16		13.46	
$B_3N_3H_6$ 	10.09	10.90		10.96	
$B_3O_3H_3$ 		11.77			
BeH	8.6[a]	7.86			
BeH_2		12.82		12.26	
BeB		8.46			
BeC		9.11			
BeN		9.73			
BeO	10.1[b]	11.80		11.25	
BeOH		7.89			
$Be(OH)_2$		12.16		11.19	
BeF	9.1[b]	8.47			
BeF_2	14.5[b]	14.96		14.45	
$^3Be_2O$	(10.5[b])	7.31			
LiH	6.5[a]	9.46			
LiBe		5.75			
^3LiB		6.94			
LiC		6.48			
^3LiN		7.09			
LiO	8.6[b]	8.82			
LiOH		9.70			
LiF	11.3[b]	10.89			
Li_2	5.15[b]	6.02			
CH_2Li_2		6.98			
C_2Li_2 		8.80			
$C_2H_2Li_2$		5.86			
Li_2O	(6.3-7.0[b])	8.41			
Li_3N		6.93			

[a] Ref. [11]
[b] Ref. [16]

5. Dipole moments

Table 4 presents a study on dipole moments. The available experimental values for 25 compounds are taken from Dewar's papers and other sources [11, 20]. SINDO1 results are in good accord with experiment and are better than those given by MNDO. The largest SINDO1 error of about 1 Debye occurs in CF_3CN

Table 4. Dipole moments (Debye)

Molecule	Exp	SINDO1	MINDO/3	MNDO	STO-3G
FH	1.83	1.44	1.84	1.99	1.25
CF	0.65[a]	0.28			0.61
HCF		1.29			1.14
CH_3F	1.86	1.55	1.71	1.76	1.15
C_2HF	0.73	0.70	0.60	1.57	0.61
^3NF		0.36			0.19
FCN	2.12[c]	1.51		0.89	1.84
OF		0.29			
HOF	2.23	1.51		1.81	1.47
FCO		0.38			0.73
HFCO	2.02	1.61		2.50	1.52
FNO	1.81	0.71		0.60	0.21
FNO_2	0.47	0.57		0.65	
CF_2	0.47	0.15		0.04	0.58
CH_2F_2	1.96	1.73		2.21	1.30
NF_2	0.14	0.37		0.01	
N_2F_2	0.16	0.42		0.02	0.90
OF_2	0.30[b]	0.25			0.21
F_2CO	0.95	0.63		0.81	0.90
CF_3		0.45			0.34
CHF_3	1.65	1.45		2.23	1.13
NF_3	0.24	0.20		0.20	0.40
CF_3CN	1.26	0.20		0.35	
N_2F_4(gauche)		0.03			
N_2F_4(trans)		0.07			
CF_3OF	0.33	0.18		0.09	
BH	1.27[a]	1.52		0.49	0.99
BH_2		0.28			0.21
BC		0.63			
^3BN		1.70			2.06
BO		1.80			1.64
HBO		1.61			1.58
BO_2H		2.44		2.71	2.51
$B(OH)_2$		2.58			
BF	0.5[a]	0.70			1.18
BOF		1.13			1.43
BF_2		0.80			0.54
BHF_2	0.97	1.02		1.33	0.31
BOF_2		0.41			
BF_2OH	1.86	2.05		2.10	1.47
B_2O_3		1.03		0.81	
BeH		0.30		1.38	0.59
BeB		0.34			0.83
BeC		3.58			
BeN		2.26			
BeO		5.25		5.32	4.20
BeOH		1.63			
BeF		1.03		1.63	
LiH	5.90	5.70			4.84
LiBe		4.26			0.31

Table 4 (*cont.*)

Molecule	Exp	SINDO1	MINDO/3	MNDO	STO-3G
^{3}LiB		5.89			1.26
LiC		6.62			0.98
^{3}LiN		6.45			2.16
LiO		5.78			2.47
LiOH		4.98			1.47
LiF	6.28[a]	5.95			3.11
CH_2Li_2		5.26			3.21
$C_2H_2Li_2$		2.87			

[a] Ref. [20]
[b] Ref. [11]
[c] Ref. [21]

Table 5. Error statistics for various minimal basis set MO methods with number of values in parentheses

	Type	Compound	SINDO1	MINDO/3	MNDO	STO-3G
Bond length (A)	XY	F	0.037(47)	0.023(10)	0.052(38)	0.041(33)
		F,B	0.032(22)	—	0.019(12)	0.020(16)
		F,B,Be,Li	0.027(13)	—	0.084(4)	0.082(5)
		all	0.034(82)	—	0.047(54)	0.039(54)
Bond length (A)	XH	F	0.011(7)	0.007(4)	0.027(5)	0.021(7)
		F,B	0.026(10)	—	0.036(6)	0.019(2)
		F,B,Be,Li	0.037(6)	—	0.056(3)	0.043(1)
		all	0.024(23)	—	0.037(14)	0.024(10)
Bond angle (Degrees)	XYZ	F	1.7(18)	16.2(3)	3.1(15)	1.8(15)
		F,B	3.1(6)	—	3.7(5)	0.9(4)
		F,B,Be,Li	—	—	—	—
		all	2.0(24)	—	3.3(20)	1.6(19)
Bond angle (Degrees)	XYH, HXH	F	2.9(6)	1.2(1)	4.1(4)	1.6(3)
		F,B	4.8(4)	—	4.4(1)	4.0(4)
		F,B,Be,Li	—	—	—	—
		all	3.7(10)	—	4.1(5)	3.0(5)
Binding energy (kcal/mol)	E	F	8.3(29)	13.4(15)	12.6(29)	
		F,B	10.8(23)	38.8(5)	9.9(17)	
		F,B,Be,Li	5.7(15)	—	11.2(6)	
		all	8.6(67)	19.7(20)	11.6(52)	
Ionization potential (ev)	I	F	0.77(23)	1.71(6)	0.43(19)	
		F,B	0.60(13)	—	0.70(5)	
		F,B,Be,Li	0.74(7)	—	0.60(2)	
		all	0.71(43)	—	0.50(26)	
Dipole moment (Debye)	D	F	0.35(19)	0.10(3)	0.44(17)	0.46(15)
		F,B	0.17(4)	—	0.46(3)	0.50(4)
		F,B,Be,Li	0.27(2)	—	—	2.16(2)
		all	0.32(25)	—	0.45(20)	0.63(21)

and FNO. MNDO has a similar error in these compounds. High dipole moments observed for LiH and LiF are well reproduced in SINDO1. STO-3G dipole moments in these cases [38] are much poorer.

6. Conclusion

In summary, an error statistics with average absolute errors,

$$\Delta = \frac{1}{n} \sum_{i=1}^{n} |\Delta_i|$$

in the investigated molecular properties for different methods is given in Table 5. The number of values used in the statistics are given in parentheses. Excluded were the cases where the experimental data are uncertain. The classification of molecules into groups, indicated in column 3 of the Table, is as described in the preceding paper. Unfortunately, MINDO/3 data on various molecular properties studied here are scanty and are not properly representative for a reliable statistic. In bond lengths SINDO1 shows smaller error than MNDO and STO-3G. For bond angles also SINDO1 appears superior to MNDO, but the number of data considered here is not sufficiently large for a final assessment. For binding energies SINDO1 represents an improvement over MNDO and MINDO/3. MNDO provides a better estimate of ionization potentials compared to SINDO1 but reverse is the situation with dipole moments.

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