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SINDO1
II. Application to Ground States of Molecules Containing Carbon, Nitrogen and Oxygen 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 C, N and O atoms. Comparison is made with MINDO/3, MNDO and where possible with STO-3G results. The explicit data and an error statistics show the relative merits of SINDO1.

Key words: Application of SINDO1 to ground states of molecules – Containing C, N, O.

1. Introduction

In the preceding paper [1] we have described the details of the SINDO1 method. All pertinent information about approximations and parameters can be found there. Here we report the results on geometries, binding energies, ionization potentials and dipole moments. Results were obtained from single-determinental calculations without configuration interaction. For open shell the unrestricted Hartree–Fock scheme was used. Optimized molecular structures were obtained by a generalized Newton–Raphson procedure. We do not report here the force constants. They are usually too large by about 40%, a result which is usual for minimal basis set SCF calculations.

2. Geometries

Table 1 contains bond lengths, bond angles and a few dihedral angles of more than 110 molecules. These include closed and open shell cases, neutral molecules,

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Table 1. Molecular Geometries (A, Degrees)

Molecule	Coordinate	Exp	SINDO1	MINDO/3	MNDO	STO-3G
H_2	HH	0.742	0.710		0.663	0.712
CH	CH	1.128	1.091		1.098	1.143
$^3CH_2$	CH	1.078	1.059	1.073	1.051	1.082
	HCH	136.0	135.1	134.1	150.5	125.5
$^1CH_2$	CH	1.110	1.089	1.121	1.091	1.123
	HCH	102.4	112.0	100.2	111.1	100.5
CH_3^+	CH		1.106			1.120
	HCH		120.0			120.0
CH_3	CH	1.079[c]	1.067		1.078	1.080
	HCH	120.0	120.0		120.0	118.3
CH_3^-	CH		1.061		1.077	1.065
	HCH		120.0		120.0	120.0
CH_4	CH	1.094	1.087	1.102	1.104	1.083
$CH_5^+(C_s)$	CH^1		1.097	1.100		1.098
	CH^3		1.105	1.110		1.106
	CH^4		1.319	1.240		1.367
	CH^5		1.331	1.240		1.370
	H^1CH^2		108.7	114.8		117.7
	H^3CH^4		126.6	125.3		121.0
	H^3CH^5		88.0	83.0		83.8
$CH_5^+(C_{4v})$	CH^1		1.093			1.083
	CH^2		1.139			1.139
	H^1CH^2		109.8			113.1
$CH_5^+(D_{3h})$	CH^1		1.118			1.114
	CH^4		1.142			1.136
C_2	CC	1.242[a]	1.226		1.168	1.233
C_2H^+	CC		1.333			1.408
	CH		1.067			1.113
C_2H	CC	1.207[c]	1.228		1.291	1.221
	CH	1.061	1.055		1.054	1.067
C_2H^-	CC		1.218		1.217	1.195
	CH		1.046		1.052	1.061
C_2H_2	CC	1.203	1.218	1.191	1.194	1.168
	CH	1.060	1.052	1.076	1.051	1.065
$C_2H_3^+$	CC		1.267	1.260		1.281
	CH^1		1.106	1.102		1.106
	CH^3		1.096	1.084		1.106
	H^1CH^2		121.9	113.6		118.4
$C_2H_3^-$	CC		1.312			
	CH^1		1.089			
	CH^3		1.111			
	CCH^1		129.0			
	H^1CH^2		110.5			
	CCH^3		111.7			
C_2H_4	CC	1.337	1.324	1.308	1.335	1.306
	CH	1.086	1.076	1.098	1.089	1.082
	CCH	121.2	122.2	124.8	123.2	122.2
$C_2H_4^{2-}$	CC		1.555			
	CH		1.082			
	CCH		122.3			

Table 1 (cont.)

Molecule	Coordinate	Exp	SINDO1	MINDO/3	MNDO	STO-3G
$C_2H_5^+$	CC		1.402	1.408		1.488
	C^1H^1		1.103	1.104		1.087
	C^2H^3		1.101	1.113		1.115
	CCH^1		112.1	112.0		112.9
	CCH^3		122.7	124.3		121.6
$C_2H_5^-$	CC		1.466		1.429	
	C^1H^1		1.107			
	C^2H^3		1.062			
	CCH^1		112.1			
	CCH^3		121.0			
C_2H_6	CC	1.536	1.520	1.486	1.521	1.538
	CH	1.091	1.092	1.108	1.109	1.086
	CCH	110.9	110.5	112.8	111.2	110.7
$C_2H_7^+$	CC		2.234	1.760		2.362
	C^1H^1		1.093	1.100		1.094
	C^1H^2		1.099	1.100		1.097
	C^1H^4		1.230	1.220		1.251
	CCH^1		92.5	92.0		89.5
	CCH^2		114.1			115.6
	CH^4C		131.7	92.3		141.4
C_3H_3	C^1C^2		1.249			
	C^2C^3		1.392			
	C^1H^1		1.052			
	C^3H^2		1.073			
	$C^2C^3H^2$		120.3			
$C_3H_4\equiv -$	C^1C^2	1.206[b,k]	1.227	1.206	1.196	1.170
	C^2C^3	1.459	1.469	1.437	1.445	1.484
	C^1H^1	1.056	1.050	1.071	1.050	1.064
	C^3H^2	1.105	1.093	1.111	1.111	1.088
	CCH	110.2	109.4	112.7	111.0	110.4
$C_3H_4{=}{=}$	CC	1.308[j]	1.317	1.311	1.306	1.288
	CH	1.087	1.073	1.099	1.090	1.083
	HCH	118.2	119.0	118.4	114.2	116.2
C_3H_4 	C^1C^2	1.296	1.310	1.317	1.328	1.277
	C^1C^3	1.509	1.501	1.481	1.512	1.493
	C^1H^1	1.072	1.064	1.084	1.062	1.075
	C^3H^3	1.088	1.085	1.114	1.097	1.087
	$C^2C^1H^1$	149.9	149.5	153.1	151.6	150.3
	$H^3C^3H^4$	114.6	111.6	105.2	111.0	112.5
	$C^1C^3C^2$	50.9	51.7	52.8	52.0	50.6
$C_3H_5^+$	CC		1.383			1.385
	C^1H^1		1.092			1.100
	C^1H^2		1.095			1.101
	C^2H^3		1.093			1.084
	CCC		124.6			118.9
	$C^2C^1H^1$		123.7			122.0
	$C^2C^1H^2$		120.9			121.4
C_3H_5 	CC		1.400		1.383	1.405
	C^1H^1		1.074			1.080
	C^2H^3		1.084			1.084

Table 1 (cont.)

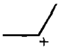
Molecule	Coordinate	Exp	SINDO1	MINDO/3	MNDO	STO-3G
	CCC		129.1		126.0	
	$C^2C^1H^1$		122.2			
	$C^2C^1H^2$		121.5			
$C_3H_5^-$	CC		1.393		1.380	
	C^1H^1		1.067			
	C^2H^3		1.093			
	CCC		135.0		130.0	
	$C^2C^1H^1$		121.7			
	$C^2C^1H^2$		121.1			
C_3H_6 	C^1C^2	1.336[b,k]	1.337	1.333	1.340	1.308
	C^2C^3	1.501	1.513	1.480	1.496	1.520
	C^1H^1	1.091	1.075	1.101	1.089	1.081
	C^1H^2	1.081	1.076	1.101	1.089	1.081
	C^2H^3	1.090	1.084	1.114	1.096	1.085
	C^3H^7	1.098	1.092	1.114	1.111	1.088
	C^3H^9	1.085	1.090		1.109	1.085
	CCC	124.3	130.1	128.9	126.9	125.1
	$C^2C^1H^1$	120.5	122.9	123.4	124.3	122.2
	$C^2C^1H^2$	121.5	121.7		122.4	121.9
	$C^1C^2H^3$	119.0	116.8		119.3	119.8
	$C^3C^2H^3$	116.7	113.1	111.4	113.8	
	$C^2C^3H^4$	107.7	109.0		110.3	
	$H^4C^3H^5$	109.0	109.0		107.7	108.5
	$C^2C^3H^6$	111.2	111.7		113.1	
	$H^4C^3H^6$	106.2	108.8		107.6	107.6
C_3H_6 	CC	1.510[i]	1.510	1.504	1.525	1.502
	CH	1.089	1.082	1.103	1.096	1.081
	HCH	115.1	111.4	108.7	110.8	113.8
$C_3H_7^+$ 	CC		1.452			1.500
	C^1H^1		1.105			1.097
	C^1H^3		1.093			1.087
	C^2H^4		1.104			1.113
	CCC		131.9			126.0
	$C^2C^1H^1$		106.8			
	$H^1C^1H^2$		106.6			106.6
	$C^2C^1H^3$		115.0			112.6
	$C^1C^2H^4$		113.9			
$C_3H_7^+$ 	CC		1.504	1.480		1.516
	C^1H^1		1.097			1.095
	C^2H^3		1.095			1.087
	C^1H^7		1.322	1.270		1.315
	CCC		72.2	71.9		75.1
	$H^1C^1H^2$		112.8	112.0		117.8
	$H^3C^2H^4$		110.5	109.0		114.0
	C^1HC^3		84.9	86.4		89.3
C_3H_8 	CC	1.526[k]	1.543	1.497	1.530	1.541
	C^1H^1	1.094	1.092	1.110	1.109	1.086
	C^1H^3	1.089	1.091	1.118	1.110	1.086
	C^2H^4	1.096	1.096		1.115	1.089
	CCC	112.6	117.8	119.6	115.4	112.4

Table 1 (cont.)

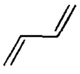
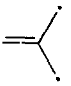
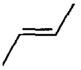
Molecule	Coordinate	Exp	SINDO1	MINDO/3	MNDO	STO-3G
	$C^2C^1H^1$		110.8			
	$C^2C^1H^3$	111.8	110.0		110.3	110.7
	$C^1C^2H^4$		107.8			
	$H^4C^2H^5$	106.1	107.9	102.5	106.0	107.2
	$H^1C^1H^2$	107.3	108.3		107.9	108.2
C_4H_2≡ — ≡	C^1C^2	1.205[j]	1 230	1.206	1.199	1.175
	C^2C^3	1.376	1.419	1.397	1.368	1.408
	C^1H^1	1.046	1.052	1.077	1.051	1.066
C_4H_4 	C^1C^2		1.337	1.342	1.357	1.313
	C^2C^3		1.579	1.533	1.534	1.569
	CH		1.071		1.071	1.081
	$C^2C^1H^1$		136.8		138.1	136.2
C_4H_6—≡—	C^1C^2	1.467[i,k]	1.471	1.433	1.444	1.483
	C^2C^3	1.213	1.235	1.216	1.199	1.171
	C^1H^1	1.115	1.093	1.105	1.111	1.088
	$C^2C^1H^1$	110.7	109.5	112.7	111.0	110.7
C_4H_6 	C^1C^2	1.341[i,k]	1.339	1.330	1.344	1.313
	C^2C^3	1.463	1.509	1.464	1.465	1.488
	C^1H^1	1.083	1.076	1.099	1.089	1.080
	C^2H^3	1.083	1.083	1.112	1.096	1.085
	CCC	123.3	128.5	131.0	125.7	124.2
	$C^2C^1H^1$	120.0	121.5	124.1	122.2	121.9
	$C^2C^1H^2$	122.4	123.5	125.5	124.3	122.1
	$C^1C^2H^3$	119.8	117.2	115.8	118.6	120.2
C_4H_6 	C^1C^2	1.342[k]	1.343	1.345	1.355	1.314
	C^2C^3	1.517	1.542	1.512	1.525	1.526
	C^3C^4	1.566	1.579	1.535	1.568	1.565
	C^1H^1	1.083	1.074	1.099	1.075	1.082
	C^3H^3	1.094	1.088	1.116	1.104	1.089
	$C^1C^2C^3$	94.2	94.6	93.6	94.0	94.7
	$C^2C^1H^1$	133.5	134.2	134.7	135.8	134.2
	$H^3C^3H^4$	109.2	109.9		108.4	109.0
$^3C_4H_6$ 	CC		1.443			
	CH		1.075			
	HCH		115.6			
C_8H_8 	C^1C^2	1.508[i]	1.514	1.464	1.497	
	C^2C^3	1.347	1.352	1.339	1.346	
	C^1H^1		1.092	1.111		
	C^2H^4		1.083	1.103		
	CCC	123.8	129.9	129.6	126.3	124.5
	$C^2C^1H^1$		111.0	114.3		
	$C^3C^2H^4$		117.2	117.9		
C_4H_8 	C^1C^2		1.511	1.473		1.520
	C^2C^3		1.352	1.339		1.312
	C^1H^1		1.022	1.111		1.087
	C^2H^4		1.085	1.112		1.085
	CCC	127.8	132.8	134.8		128.0
	$C^2C^1H^1$		111.3	113.0		112.3
	$C^3C^2H^4$		115.2	114.8		118.1

Table 1 (cont.)

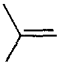
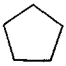
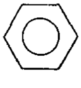
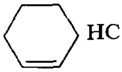
Molecule	Coordinate	Exp	SINDO1	MINDO/3	MNDO	STO-3G
C_4H_8 	C^1C^2	1.507[b,k]	1.545	1.505	1.508	1.526
	C^2C^3	1.330	1.352	1.339	1.348	1.311
	C^1H^1	1.095	1.092	1.101		1.085
	C^3H^4	1.088	1.076	1.112		1.080
	CCC	122.4	122.8		121.9	122.2
	$C^2C^1H^1$	110.7	111.2			111.1
	$C^2C^3H^4$	123.0	122.0			122.0
C_4H_8 	CC	1.548[l]	1.561	1.525	1.549	1.554
	CH	1.133	1.087	1.104	1.103	1.087
	HCH	108.1	108.4		107.6	108.7
	CCCC		0.		0.	6.9
C_5H_6 	C^1C^2	1.469[b,k]	1.531	1.492	1.477	
	C^2C^3	1.342	1.355	1.352	1.362	
	C^3C^4	1.509	1.554	1.515	1.521	
	C^1H^1		1.074	1.102		
	C^3H^3		1.074	1.103		
	C^4H^4		1.089	1.116		
	$C^1C^2C^3$	109.1	107.6	109.2		
	$C^2C^3C^4$	109.2	111.4			
	$C^3C^4C^5$	102.8	102.0	103.6		
	$C^2C^1H^1$		123.4			
	$C^2C^3H^3$		126.3			
	$H^4C^4H^5$		109.2			
$C_5H_9^-$ 	C^1C^2		1.573			
	C^2C^3		1.580			
	C^3C^4		1.550			
	C^1H^1		1.095			
	C^3H^5		1.100			
	C^4H^7		1.094			
	$C^1C^2C^3$		107.0			
	$C^2C^3C^4$		110.3			
	$C^5C^3C^4H^7$		120.5			
C_5H_{10} 	CC	1.546	1.572	1.522	1.549	
	CH	1.114	1.092	1.111	1.111	
	CCH	111.7	110.4		110.7	
C_5H_{12} 	CC	1.539[i]	1.598	1.537	1.554	1.549
	CH	1.120	1.092	1.110	1.109	1.086
	CCH	110.0	110.6	113.7	111.7	110.6
C_6H_6 	CC	1.397	1.419	1.398	1.407	1.390
	CH	1.084	1.080	1.102	1.090	1.080
C_6H_{10} 	C^1C^2	1.335	1.349	1.353	1.346	
	C^2C^3	1.504	1.539	1.499	1.504	
	C^3C^4	1.515	1.572	1.530	1.541	
	C^4C^5	1.550	1.566	1.229	1.539	
	C^1H^1	1.093	1.093		1.093	
	C^3H^3	1.093	1.081		1.114	
	C^4H^6	1.093	1.094		1.114	
	$C^1C^2C^3$	123.5	124.1		123.9	

Table 1 (cont.)

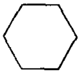
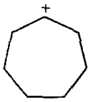
Molecule	Coordinate	Exp	SINDO1	MINDO/3	MNDO	STO-3G
	$C^2C^3C^4$	112.1	109.3		113.9	
	$C^3C^4C^5$	111.0	113.9		114.3	
	$C^1C^2C^4C^5$	28.3	24.0		21.8	
C_6H_{12} 	CC	1.536[i]	1.565	1.517	1.539	
	CH	1.121	1.094	1.123	1.114	
	CCC	111.4	114.3		114.1	
	HCH	107.5	108.6		105.7	
	CCCC	54.9	45.8	62.7	46.3	
$C_7H_{11}^+$ 	C^1C^2		1.347			
	C^2C^3		1.533			
	C^3C^4		1.577			
	C^4C^5		1.466			
	C^1H^1		1.095			
	C^3H^3		1.087			
	C^4H^5		1.107			
	C^5H^7		1.105			
	$C^1C^2C^3$		133.0			
	$C^2C^3C^4$		122.6			
	$C^3C^4C^5$		125.6			
	$C^1C^2C^4C^6$		8.3			
^3NH	NH	1.038[a]	1.003		0.993	1.079
NH_2	NH	1.024[a]	1.015		1.002	1.058
	HNH	103.3	106.1		104.4	100.2
NH_3	NH	1.014[b,k]	1.017	1.032	1.007	1.003
	HNH	107.1	106.7	104.6	105.3	104.2
$^3CN^+$	CN	1.29[c]	1.230			
CN	CN	1.172	1.160		1.153	1.235
HCN	CN	1.153[b,k]	1.149	1.148	1.160	1.153
	CH	1.066	1.056	1.096	1.055	1.070
HNC	CN		1.170			1.170
	NH		0.995			1.011
CH_3NH_2	CN	1.474[k]	1.444	1.404	1.460	
	CH	1.093	1.094	1.111		
	NH	1.011	1.020	1.026	1.008	
	NCH	112.0	109.7	112.5	109.8	
	HNH	105.5	107.8		105.6	
CH_3CN	CC	1.458[b,k]	1.469	1.453	1.451	1.489
	CN	1.157	1.157	1.165	1.162	1.154
	CH	1.104	1.091	1.118	1.110	1.088
	CCH	109.5	109.1		110.6	109.9
C_2H_5N 	CC	1.481	1.461	1.464	1.516	1.490
	CN	1.475	1.461	1.454	1.479	
	CH^1	1.084	1.091	1.113	1.100	1.084
	CH^2	1.083	1.089	1.112	1.100	1.084
	NH	1.016	1.021	1.037	1.008	1.042
	CNC	60.3	60.1	60.5	61.7	
	NCH^1	118.3	118.7	123.6	120.3	
	NCH^2	114.3	111.9	116.2	115.5	
	HNCC	112.5	101.5	117.5	117.9	

Table 1 (cont.)

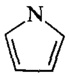
Molecule	Coordinate	Exp	SINDO1	MINDO/3	MNDO	STO-3G
$(CH_3)_2NH$	CN	$1.466^{b,k}$	1.461	1.393	1.462	1.484
	CH	1.091	1.095	1.122	1.114	1.092
	NH	1.022	1.019	1.021	1.009	1.033
	CNC	112.2	117.6	129.4	117.6	110.5
	CNH	108.8	104.7		109.5	
	NCH^1	109.7	107.8		109.0	
	NCH^2	113.8	115.3			
	NCH^3	108.2	108.3		110.3	
$(CH_3)_3N$	CN	1.451^j	1.489	1.416	1.464	
	CH	1.090	1.094	1.121		
	CNC	110.9	112.0	119.8	116.0	
C_4H_5N 	C^1C^2	$1.417^{b,k}$	1.475	1.433	1.437	
	C^2C^3	1.382	1.392	1.391	1.394	
	CN	1.370	1.420	1.368	1.398	
	C^1H^1	1.077	1.072	1.097	1.080	
	C^3H^3	1.076	1.074	1.103	1.082	
	NH	0.996	1.003	1.000	0.993	
	$C^1C^2C^3$		108.5			
	C^2C^3N		104.3			
	$C^2C^1H^1$		125.3			
	$C^3C^2H^2$	130.8	133.9		131.2	
	$C^2C^3H^3$	125.5	126.2		126.5	
N_2	NN	1.094	1.089	1.097	1.103	1.134
N_2H_2(trans)	NN		1.185			1.267
	NH		1.033			1.061
	NNH		107.2			105.3
N_2H_4	NN	1.449^i	1.388	1.311	1.397	1.458
	NH^1	1.022	1.029	1.055	1.021	1.037
	HNH	106.0	103.6		103.1	104.6
	NNH^1	112.0	103.3	115.5	107.2	105.4
	NNH^2	112.0	109.8	115.5	107.2	109.0
	HNNH	90.0	119.7		189.0	
NH_2CN	CN^1	$1.346^{e,k}$	1.376	1.321	1.376	1.398^h
	CN^2	1.160	1.160	1.164	1.162	1.158
	NH	1.001	1.022	1.011	1.011	1.030
	HNH	113.5	106.4	112.7	107.7	
CH_2N_2	NN	1.32^i	1.344	1.274	1.310	1.282^h
	CN	1.12	1.129	1.113	1.141	1.190
	CH	1.08	1.065	1.099	1.086	1.079
	HCH	127.0	125.6	122.7	120.7	121.6
$(CN)_2$	CC	1.389	1.431	1.421	1.377	1.412
	CN	1.154	1.159	1.159	1.161	1.160
C_4N_2	C^1C^2	1.19^c	1.237			
	C^2C^3	1.37	1.422			
	C^3N	1.14	1.161			
N_3^-	NN		1.175			
HN_3	N^1N^2	$1.133^{b,k}$	1.114			1.176
	N^2N^3	1.237	1.329			1.285
	N^3H	0.975	1.016			1.057

Table 1 (cont.)

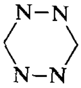
Molecule	Coordinate	Exp	SINDO1	MINDO/3	MNDO	STO-3G
	NNN	(180.0)	170.5			170.0
	NNH	114.8	103.8			103.0
$C_2H_2N_4$ 	CN		1.342			
	NN		1.267			
	CH		1.083			
	NCN		117.8			
OH	OH	0.971[a]	0.971	0.948	0.937	0.968
H_2O	OH	0.957[k]	0.978	0.950	0.943	0.990
	HOH	104.5	105.2	103.5	106.8	100.0
H_3O^+	OH		1.017	0.965	0.964	0.990
	HOH		110.8	109.6	115.3	113.9
H_4O^+	OH		1.075			
	HOH		109.5			
CO^+	CO		1.150	1.101	1.142	1.206
CO	CO	1.128[b,k]	1.142	1.134	1.163	1.146
HCO^+	CO	(1.090[c])	1.138			1.138
	CH	(1.029)	1.112			1.129
	HCO	180.0	180.0			180.0
H_2CO	CO	1.208[k]	1.202	1.180	1.216	1.217
	CH	1.116	1.090	1.119	1.106	1.101
	HCH	116.5	113.4	108.2	113.0	114.5
CH_3OH	CO	1.425	1.394	1.340	1.391	1.473
	CH	1.094	1.098	1.119 1.124	1.115 1.119	1.118
	OH	0.945	0.977	0.952	0.946	0.995
	H^1CO	107.0	105.4	107.9	108.1	
	H^2CH^3	108.6	108.3	104.9	107.4	
	COH	108.5	108.4	110.7		
^3CCO	CC		1.345			
	CO		1.178			
H_2C_2O	CC	1.314[b,k]	1.341	1.310	1.319	1.300
	CO	1.161	1.181	1.167	1.186	1.183
	CH	1.083	1.061	1.084	1.085	1.075
	HCH	122.6	122.0	122.5	116.5	119.6
CH_3CHO	CC	1.501[b,k]	1.520	1.479	1.517	1.534
	CO	1.216	1.215	1.193	1.221	1.218
	CH^1	1.086	1.088	1.111	1.108	1.087
	CH^4	1.114	1.097	1.140	1.112	1.104
	CCO	123.9	127.5	130.1	125.0	
	H^1CH^2	108.3	109.8	105.5	108.2	
	CCH^4	117.5	113.4	120.6	114.0	
C_2H_4O 	CC	1.470[j]	1.486	1.447	1.513	
	CO	1.435	1.412	1.389	1.417	
	CH	1.084	1.085	1.114	1.102	1.087
	COC	61.6	63.5	62.8	64.5	
	HCH	116.3	113.0	107.4	111.7	
$(CH_3)_2O$	CO	1.410[b,k]	1.410	1.347	1.396	1.433
	CH^1	1.091	1.097	1.117	1.120	1.092
	CH^2	1.100	1.097	1.117	1.124	1.095
	COC	111.7	120.2	123.4	120.0	

Table 1 (cont.)

Molecule	Coordinate	Exp	SINDO1	MINDO/3	MNDO	STO-3G
C_4H_4O 	C^1C^2	$1.431^{b,k}$	1.479	1.455	1.444	
	C^2C^3	1.361	1.384	1.367	1.390	
	CO	1.362	1.394	1.343	1.367	
	C^1H^1	1.077	1.072	1.096	1.079	
	C^3H^3	1.075	1.077	1.104	1.084	
	CCC	106.1	105.8	105.5	105.9	
	CCO	110.7	111.1	110.0	110.3	
	$C^2C^1H^1$	128.0	126.4	126.5	126.6	
	OCH^3	115.9	116.1		117.1	
	$C^2C^3H^3$	133.8	132.8	135.8	132.6	
NO^+	NO		1.095			1.133
NO	NO	$1.151^{b,k}$	1.134		1.122	1.306
HNO	NO	1.239^{c}	1.170			1.231
	NH	1.020	1.039			1.082
	HNO	114.4	113.0			107.6
H_3NO	NO		1.387			
	NH		1.039			
	HNO		113.1			
$^3NCO^+$	CN		1.338			
	CO		1.163			
NCO^-	CN		1.172			1.177
	CO		1.262			1.257
NH_2CHO	CN	$1,376^{b,k}$	1.409	1.334	1.408	1.403
	CO	1.193	1.211	1.208	1.225	1.218
	CH	1.102	1.099	1.140	1.108	1.105
	NH^2	1.002	1.014	1.016	1.000	1.013
	NH^3	1.014	1.014	1.017	1.001	1.014
	OCN	123.5	121.5	126.6	121.2	124.3
	HCO	122.6	126.6	123.4	124.3	124.3
	H^2NC	120.4	109.4	123.9	115.7	121.6
	H^3NC	117.9	109.6	125.8	117.9	120.5
	H^2NCH	(−12 ± 5)	−47.6	0.0	−28.1	
	H^3NCO	(7 ± 5)	21.2	0.0	17.0	
N_2O	NN	$1.129^{b,k}$	1.118	1.093	1.127	1.154
	NO	1.188	1.274	1.197	1.181	1.275
$^3O_2$	OO	$1.208^{b,k}$	1.181	1.206	1.135	1.217
O_2^-	OO		1.274			1.308
H_2O_2	OO	$1.467^{g,j}$	1.347	1.380	1.295	1.396
	OH	0.965	0.985	0.964	0.961	1.001
	OOH	98.5	107.0	107.3	107.3	101.1
	HOOH	120.0	91.0	84.6	180.0	125 ± 2
CO_2	CO	1.162	1.190	1.180	1.186	1.188
HCOOH	CO^1	$1.343^{b,k}$	1.351	1.319	1.354	1.386
	CO^2	1.202	1.210	1.203	1.227	1.214
	CH	1.097	1.097	1.138	1.105	1.104
	O^1H	0.972	0.977	0.953	0.949	0.991
	OCO	124.9	128.5	134.7	120.6	
	HCO^1	124.1	123.2	123.1	126.7	
	HO^1C	106.3	110.3	118.4	116.3	

Table 1 (cont.)

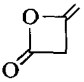
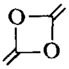
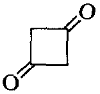
Molecule	Coordinate	Exp	SINDO1	MINDO/3	MNDO	STO-3G
C_3O_2	CC	(1.28[c])	1.358			
	CO	1.16	1.176			
	CCC	(180.0)	108.0			125.0[f]
	CCO	180	174.5			
$C_4H_4O_2$ 	C^1C^2	1.52[d,i]	1.576			
	C^2C^3	1.52	1.553			
	C^3C^4	1.31	1.348			
	C^1O^1	1.19	1.163			
	C^1O^2	1.41	1.415			
	C^3O^2	1.41	1.422			
	C^2H^1	1.09	1.083			
	C^4H^3	1.09	1.071			
	$C^1O^2C^3$	89	91.6			
	$O^2C^1C^2$		93.1			
	$O^2C^3C^2$		94.1			
	$C^2C^1O^1$	145	139.0			
	$C^2C^3C^4$	136	139.2			
	$H^1C^2H^2$		110.7			
	$H^3C^4H^4$		118.1			
$C_4H_4O_2$ 	CC		1.352			
	CO		1.387			
	CH		1.067			
	CCO		135.0			
	HCH		119.8			
$C_4H_4O_2$ 	CC		1.561			
	CO		1.213			
	CH		1.085			
	CCO		134.0			
	HCH		110.4			
NO_2	NO	1.193[b,k]	1.198		1.174	1.249
	ONO	134.4	137.8		133.0	130.2
NO_2^-	NO		1.242			
	ONO		122.3			
HNO_2(cis)	NO^1		1.178			1.226
	NO^2		1.329			1.402
	O^2H		0.982			1.001
	ONO		120.8			
	NOH		114.8			
HNO_2(trans)	NO^1	1.163[k]	1.178	1.197	1.166	1.224
	NO^2	1.433	1.342	1.373	1.312	1.415
	O^2H	0.954	0.980	0.954	0.958	0.995
	ONO	110.7	113.3	122.2	113.3	
	NOH	102.1	106.0	112.1	110.0	
N_2O_2(cis)	NN		1.398			
	NO		1.178			
	NNO		120.8			
N_2O_2(trans)	NN		1.352			
	NO		1.191			
	NNO		121.5			

Table 1 (cont.)

Molecule	Coordinate	Exp	SINDO1	MINDO/3	MNDO	STO-3G
O_3	OO	1.278^k	1.241	1.253	1.191	1.285
	OOO	116.8	122.1	126.1	117.6	116.2
NO_3	NO^1	1.27^c	1.252		1.199	
	NO^3	1.27	1.315		1.253	
	O^2NO^3	(120)	115.8		117.3	
HNO_3	NO^1	$1.199^{b,k}$	1.246	1.221	1.202	
	NO^2	1.211	1.246	1.219	1.211	
	NO^3	1.406	1.350	1.394	1.340	
	O^3H	0.964	0.982	0.958	0.962	
	O^1NO^2	130.3	127.6	130.4	126.5	
	O^2NO^3	113.9	113.0	111.5	115.1	
	NO^3H	102.2	109.7	118.7	114.1	
N_2O_3	NN		1.431			
	NO^1		1.170			
	NO^2		1.246			
	NNO^1		116.5			
	O^2NO^3		127.0			
	ONNO		92.1			

[a] Ref. [15] [b] Ref. [16] [c] Ref. [17] [d] Ref. [18] [e] Ref. [37]
[f] Ref. [20] [g] Ref. [40] [h] Ref. [41] [i] electron diffraction
[j] infrared spectra [k] microwave spectra [l] NMR

positive and negative ions, radicals and a few conformers. We compare our calculated data with experimental and other theoretical data as MINDO/3 [2–4, 36, 38], MNDO [5, 35, 36] and STO-3G [6–14, 43] results in cases where information was available. Most of the experimental data were taken from MNDO and MINDO/3 papers except for those with a superscript [15–18].

Bond lengths and bond angles are calculated with an uncertainty of the order of 0.001 Å and 0.1° respectively. However, since the experimental data are often less accurate by an order of magnitude than these values the last figure is not particularly significant for comparison. As a general observation, no method's geometries are the best, but the average differences between all four methods considered are quite small. In hydrocarbons SINDO1 produces too long single bonds between two double or triple bonds and in five or six-membered rings. MNDO shows large errors for CH_2 and C_2. Special molecules which are difficult to get in all methods are H_2O_2 and N_2H_4. Here SINDO1 produced qualitatively the orthogonal conformation, whereas MNDO obtains the trans conformation. In HN_3 and N_2O the two weaker bonds are again much too long. For HN_3 experimental evidence of a linear NNN group is now in doubt in the light of sophisticated *ab initio* calculations [19]. A critical case of this sort is also C_3O_2 where a bent C_3 group is obtained, a result similar to Christoffersen's [20] *ab initio* calculation. The reason seems to be the rather low bending frequency of the C_3 group. In NH_2CHO we do not obtain the almost planar arrangement of the NH_2C group. In other cases, O_3 or HNO_2, MNDO errors are more pronounced than

SINDO1 errors. In sterically crowded systems like $(CH_3)_4C$ and $(CH_3)_3N$ SINDO1 bond lengths are too long. In the latter case there is, however, a significant improvement in the angles. SINDO1 predicts the CNC angle of $(CH_3)_3N$ to be 112.0° versus 110.8° experimentally and 116.0° by MNDO or the planar arrangement of 119.8° by MINDO/3. We have not fully studied ions, but present only a selection for comparison. The geometries of the carbocations listed do not imply that these belong to the most stable isomers. Hydrogen bonded systems are better in SINDO1 than MINDO/3 [33, 34]. But the hydrogen bonds are still much too long.

3. Binding Energies

Table 2 shows SINDO1 binding energies for a large number of molecules together with the experimental values for over sixty molecules obtained using the available heats of formation at 0°K and the energies of zero point vibration. Unlike SINDO1, MINDO/3 and MNDO have been parametrized to reproduce heats of formation of molecules at 25°C, but employ an objectionable approach of neglecting the effects of finite temperature and zero point vibration in estimating this quantity. In Table 2 the errors in SINDO1 binding energies ($\Delta E_B = E(\text{exp}) - E(\text{SINDO1})$) are compared with the errors in the heats of formation ($\Delta\Delta Hf^0_{298} = \Delta Hf(\text{exp}) = \Delta Hf(\text{calc})$) given by MINDO/3 and MNDO. Experimental heats of formation are taken from Dewar's papers and several other sources [17, 21–23]. Zero point vibration energies are from JANAF [17], Shimanouchi [24, 25] and Herzberg [26]. SINDO1 has no error larger than 26.3 kcal/mol. The largest errors are in H_2O_2, N_2O and NH_2CHO which are also poor in geometry. SINDO1 shows also a tendency to underestimate the binding energy of larger ring compounds. STO-3G energy results can be unreliable. In CH_4, C_2H_2, C_2H_4 heats of formation are too small by 80 kcal/mol or more [27]. It is not much of a consolation that relative energies are much better [13, 28]. Pople's criticism [29] of MINDO/3 had to be based on 6–31G calculations. Because of the lack of vibrational experimental data for ions we have not fully concentrated on a study of binding energies of ions. We list only CH_5^+ where the ordering is in agreement with *ab initio* work [8] and MINDO/3 [3]. The bridged form of $C_2H_3^+$ is more stable than the classical form by 5.3 kcal/mol. The same value is obtained by MINDO/3.

For $C_2H_5^+$ the bridged form is 5.0 and 8.2 kcal/mol more stable than the classical forms compared to the MINDO/3 value of 8.0 kcal/mol [38] and the best *ab initio* value quoted there of 6.3 kcal/mol. In $C_2H_7^+$ the classical form of H_2 attached to $C_2H_5^+$ is more stable by 6.8 and 9.3 kcal/mol than the bridged forms, qualitatively in agreement with MINDO/3. For the last three cations, STO-3G predicts the opposite. In the case of $C_3H_7^+$ we find the classical form more stable by 12.7 kcal/mol versus 7.5 kcal/mol by MINDO/3 [3] and 19.1 kcal/mol by the best *ab initio* calculations [39].

We do not consider here hydrogen bonded systems because SINDO1 is not particularly useful for them. The systems are bound but their energy of dimerization is only 1 kcal/mol and their geometry is poor. Rotational barriers will not be

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

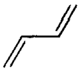
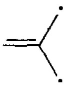
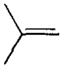
Molecule	E_B (Hartree) Exp	SINDO1	ΔE_B (kcal/mol) SINDO1	$\Delta\Delta Hf^0_{298}$ (kcal/mol) MINDO/3	MNDO	ΔHf^0_{298} (kcal/mol) Exp
H_2	0.175	0.1691	3.7	0.1	0.7	0
CH	0.134	0.1271	4.3			
$^3CH_2$	0.307	0.3082	−0.8			
$^1CH_2$		0.2642				
CH_3^+	0.610[a]	0.6066	2.1		−16.1	260
CH_3	0.489	0.4898	−0.5		9.0	34.8
CH_4	0.669	0.6556	8.4	−6.3	6.0	−17.9
$CH_5^+(C_s)$		0.8698				
$CH_5^+(C_{4v})$		0.8570				
$CH_5^+(D_{3h})$		0.8536				
C_2	0.229	0.2141	9.3			
C_2H		0.4143				
C_2H_2	0.647	0.6328	8.9	3.5	3.0	54.3
C_2H_4	0.897	0.8953	1.1	6.8	2.8	12.4
C_2H_6	1.134	1.1335	0.3	0.4	0.5	−20.2
C_3H_3≡ —·		0.9857				
C_3H_4≡ —	1.123	1.1269	−2.4	−9.3	−3.5	44.3
C_3H_4= =	1.120	1.1348	−9.3	−3.9	−1.8	45.9
C_3H_4 	1.0848	1.1009	−10.1	−6.8	2.0	66.2
C_3H_5 		1.2395				
C_3H_6 	1.371	1.3699	0.7	1.6	0	4.9
C_3H_6 	1.357	1.3805	−14.7	−4.0	−1.5	12.7
C_3H_8 	1.602	1.5991	1.8	−1.7	−0.1	−24.8
C_4H_2≡ — ≡	1.108	1.1059	1.3	−21.9	−10.8	113.0
C_4H_4 		1.2916				
C_4H_6— ≡ —	1.601	1.6190	−11.3	−22.6	−10.3	34.7
C_4H_6 	1.614	1.6049	5.7	5.8	2.9	26.1
C_4H_6 		1.5839		−4.3	−6.5	37.4
C_4H_6 		1.5646				
C_4H_8 		1.8427		−3.3	−2.1	−3.0
C_4H_8 		1.8414		−3.8	−2.1	−1.9
C_4H_8 	(1.851)	1.8287		+6.8	+2.2	−4.3

Table 2 (*cont.*)

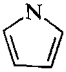
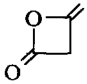
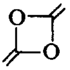
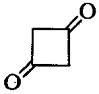
Molecule	E_B (Hartree) Exp	SINDO1	ΔE_B (kcal/mol) SINDO1	$\Delta\Delta Hf^0_{298}$ (kcal/mol) MINDO/3	MNDO	ΔHf^0_{298} (kcal/mol) Exp
C_4H_8 	1.820	1.8350	−9.4	−11.9	−18.7	6.8
C_5H_6 		1.8516		10.0	0.1	31.9
C_5H_{10} 	2.334	2.3228	7.0	−9.5	−12.1	−18.4
C_5H_{12} 		2.4869		25.7	15.7	−40.3
C_6H_6 	2.170	2.1606	5.9	9.0	1.4	19.8
C_6H_{10}  HC		2.5742		1.0	−8.9	−1.1
C_6H_{10}  HB		2.5592				
C_6H_{12} 	2.815	2.7985	11.0	−7.1	−5.3	−29.5
^3NH	0.140	0.1527	−8.0			
NH_2	0.297	0.3015	−2.8		−3.0	40.1
NH_3	0.475	0.4564	11.7	1.6	4.7	−11.0
CN	0.290	0.2802	6.1			103.2[b]
HCN	0.498	0.4835	9.1	3.1	2.6	31.2
HNC		0.4451				
CH_3NH_2	0.927	0.9232	2.4	0.6	−2.0	−5.5
CH_3CN	0.975	0.9841	−5.7	−11.4	−2.0	20.9
C_2H_5N 	1.151	1.1523	−0.8	−8.3	−5.0	30.2
$(CH_3)_2NH$	1.384	1.3759	5.1	8.8	−2.2	−4.4
C_4H_5N 	(1.670)	1.6354		4.9	6.5	24.6
N_2	0.362	0.3555	4.1	5.2	8.0	0
N_2H_2	0.4654	0.5060	−25.5	−44.7	−17.1	50.9
N_2H_4	0.696	0.7179	−13.7	−20.1	−8.5	22.8
NH_2CN		0.7712				
CH_2N_2	0.708	0.6861	13.7		−3.9	71.0
$(CN)_2$	0.793	0.8133	−12.7		−7.9	73.8
C_4N_2	1.264	1.2884	−15.3		−15.8	126.5
HN_3	0.531	0.5241	4.3		2.7	70.3
$C_2H_2N_4$ 		1.3420				
OH	0.170	0.1767	−4.2		−9.0	9.5
H_2O	0.370	0.3515	11.6	4.2	−3.1	−57.8

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
H_3O^+		0.6483				139
H_4O^+		0.6487				
CO	0.413	0.4154	−1.5	12.9	20.2	−26.4
HCO	0.465	0.4598	3.3		−10.9	10.4
H_2CO	0.597	0.5819	9.5	0.4	−7.0	−25.9
CH_3OH	0.815	0.8220	−4.4	−2.0	−9.3	−48.1
^3CCO		0.5551				
^1CCO		0.5148				
H_2C_2O	0.852	0.8476	2.8	−6.5	4.4	−14.2
CH_3CHO	1.076	1.0635	−7.8	−3.9	−2.7	−39.7
C_2H_4O 	1.035	1.0560	−13.2	−13.9	−2.9	−12.6
$(CH_3)_2O$	1.269	1.2742	−3.3	2.9	−7.2	−44.0
C_4H_4O 	1.556	1.5546	0.9	0.3	−0.4	−8.3
NO	0.243	0.2629	−12.5		−21.8	21.6
HNO	0.331	0.3538	−14.3			
H_3NO		0.4980				
HNCO	0.690	0.6746	9.7			−27.9[b]
NH_2CHO	0.905	0.8725	20.4	−6.1	4.7	−46.0
N_2O	0.431	0.3957	22.1	−61.3	11.3	19.6
$^3O_2$	0.1915	0.2073	−9.9	0.8	−9.8	22.0
H_2O_2	0.427	0.4689	−26.3	0.9	−5.7	−32.5
CO_2	0.619	0.5924	16.7	1.7	18.7	−94.0
HCOOH	0.797	0.7806	10.3	1.8	−2.1	−90.6
C_3O_2	1.057	1.0734	−10.3		(−1.7)[c]	−22.4
$C_4H_4O_2$ 		1.7100				
$C_4H_4O_2$ 		1.7032				
$C_4H_4O_2$ 		1.7072				
NO_2	0.362	0.3686	−4.1		−12.5	7.9
HNO_2(cis)		0.5330				
HNO_2(trans)	0.497	0.5297	−20.5	5.2	−21.8	−18.8
N_2O_2(cis)		0.5269				
N_2O_2(trans)		0.5209				
O_3	0.233	0.2272	3.6	5.0	14.3	34.0
NO_3	0.444	0.4440	0			18.5
HNO_3	0.616	0.6118	2.6	2.9	14.6	−32.3
N_2O_3		0.6145				

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[a] Ref. 23 [b] Ref. 17 [c] linear geometry assumed

[d] 1 Hartree = 627.46 kcal/mol = 2625.3 kJ/mol

Table 3. Ionization potentials (ev)

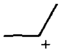
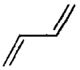
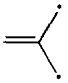
Molecule	Exp	SINDO1	MINDO/3	MNDO	STO-3G
H_2	15.98	17.78	15.63	15.74	14.57
CH	10.64[a]	11.41			8.54
$^3CH_2$	10.40[c]	11.88			8.63
$^1CH_2$		10.85			8.11
CH_3^+		28.27			
CH_3	9.84	11.76			
CH_4	14.0	15.90	13.30	13.87	11.79
$CH_5^+(C_s)$		25.69			
$CH_5^+(C_{4v})$		25.59			
$CH_5^+(D_{3h})$		25.64			
C_2	12.0[a]	12.16			
C_2H^+		23.03			
C_2H		11.65			
C_2H_2	11.40	11.66	10.83	11.03	
$C_2H_3^+$		22.30			
C_2H_4	10.51	11.78	10.42	10.18	
$C_2H_5^+$		21.88			
C_2H_6	12.1	13.48	11.79	12.70	
$C_2H_7^+$		23.57			
C_3H_3	8.68[c]	9.51			
C_3H_4≡ —	10.37	10.44	10.18	10.73	
C_3H_4= =	10.07	10.46	9.64	10.02	
C_3H_4 	9.70	9.67	9.31	9.89	
$C_3H_5^+$		20.61			
C_3H_5		9.95			
C_3H_6 	9.88	10.73	9.85	9.97	
C_3H_6 	11.0	11.90	10.33	11.43	
$C_3H_7^+$ 		20.60			
$C_3H_7^+$ 		20.91			
C_3H_8 	11.5	12.58	11.31	12.34	(0.05)
C_4H_2≡ — ≡	10.17	9.79	9.52	10.00	
C_4H_4 	8.2[c]	8.24			
C_4H_6— ≡ —	9.56[c]	9.47	10.79		
C_4H_6 	9.08	9.89	9.09	9.14	
C_4H_6 	9.43	10.21	9.56	9.77	
$^3C_4H_6$ 		10.40			

Table 3 (cont.)

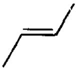
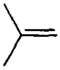
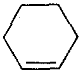
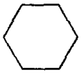
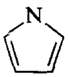
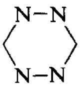
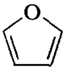
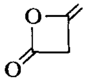
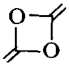
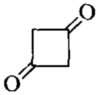
Molecule	Exp	SINDO1	MINDO/3	MNDO	STO-3G
C_4H_8 	9.12	9.88	9.44		
C_4H_8 	9.12	9.89	9.48		
C_4H_8 	9.17	10.14	9.63		
C_4H_8 	11.00	11.03	10.26	11.81	
C_5H_6 	8.57	9.24	8.81	9.04	
C_5H_{10} 	11.59	11.96	11.08		
C_5H_{12} 	11.3	11.50	10.93	12.12	
C_6H_6 	9.25	9.69	9.22	9.39	
C_6H_{10}  HC	8.94	9.98	9.43	9.75	
C_6H_{12} 	9.81	11.12	10.46		
^3NH	13.10^{a}	14.65			10.45
NH_2	11.4^{c}	13.62			7.85
NH_3	10.85	12.36	10.07	11.19	6.76
CN	14.2^{a}	13.58			
HCN	13.60	13.38	10.50	13.42	
HNC		12.85			
CH_3NH_2	9.45	11.28	9.26	10.55	
CH_3CN	12.21	11.88	10.12	12.80	
C_2H_5N 	9.8	11.26	9.23	10.68	
$(CH_3)_2NH$	8.93	10.55	8.69	10.04	
C_4H_5N 	8.21	8.66	8.20	8.57	
N_2	15.60	15.20	8.90	14.88	
N_2H_2	9.9^{c}	11.07			
N_2H_4	(9.56^{c})	10.57			
NH_2CN		11.12			
CH_2N_2	9.00^{c}	8.16			
$(CN)_2$	13.36	12.14	9.66	13.22	
C_4N_2	11.81^{b}	10.42			
HN_3	10.74^{c}	9.71			
$C_2H_2N_4$ 		9.15			

Table 3 (cont.)

Molecule	Exp	SINDO1	MINDO/3	MNDO	STO-3G
OH	13.36[a]	14.23			
H_2O	12.62[c]	14.03	12.76	12.19	
CO	14.01	13.43	10.96	13.43	
HCO	9.83[c]	9.42			
H_2CO	10.88	11.29	10.74	11.04	
CH_3OH	10.96	12.10	11.08	11.41	
^3CCO	10.60[b]	10.29			
H_2C_2O	9.60[b]	9.24	9.17	9.29	
CH_3CHO	10.21	10.46	10.29	10.88	
C_2H_4O 	10.57	11.78	10.85	11.49	
$(CH_3)_2O$	10.04	11.09	10.49	11.04	
C_4H_4O 	8.88	8.91	8.38	9.14	
NO	9.25[a]	9.59			
HNO		10.71			
H_3NO		9.18			
HNCO	11.6[c]	10.64			
NH_2CHO	10.24[c]	10.80			
N_2O	12.89[b]	11.12	11.12	11.89	
$^3O_2$	12.08[a]	11.98			
H_2O_2	10.92[c]	12.61			
CO_2	13.78	12.15	12.74	12.79	
HCOOH	11.51	11.42	11.16	11.74	
C_3O_2	10.60[c]	8.80			
$C_4H_4O_2$ 		9.87			
$C_4H_4O_2$ 		8.95			
$C_4H_4O_2$ 		9.27			
NO_2	9.78[b]	11.04			
HNO_2(cis)		10.63			
HNO_2(trans)		10.45			
N_2O_2(cis)		8.63			
N_2O_2(trans)		8.70			
O_3	12.52[b]	10.87	11.28	12.71	
NO_3		11.54			
HNO_3		11.33			
N_2O_3		9.77			

[a] Ref. [15] [b] Ref. [30] [c] Ref. [23]

Table 4. Dipole moments (Debye)

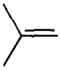
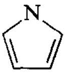
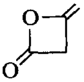
Molecule	Exp	SINDO1	MINDO/3	MNDO	STO-3G
CH	1.46[a]	1.28			1.07
$^3CH_2$		0.45			0.22
$^1CH_2$		2.07			1.54
C_2H		0.33			0.19
C_3H_3		0.13			0.01
C_3H_4≡ —	0.78	0.52	0.03	0.12	0.49
C_3H_4 	0.45	1.01	0.81	0.48	
C_3H_5		0.09			0.01
C_3H_6 	0.37	0.49	0.03	0.04	
C_3H_8 	0.08	0.003	0.01	0.00	0.02
C_4H_6 	0.13	0.09	0.13	0.08	0.05
C_4H_8 		0.15			0.13
C_4H_8 	0.36	0.80			0.40
C_5H_6 	0.42	0.31	0.17	0.18	
C_6H_{10} 	HC 0.33[a]	0.12			
^3NH	1.31[a]	1.12			1.26
NH_2		1.78			1.77
NH_3	1.47	2.16	1.63	1.76	1.87
CN	1.45[a]	1.34			1.81
HCN	2.98	2.33	1.62	2.51	2.45
HNC		3.01			2.46
CH_3NH_2	1.30[a]	1.99	1.09	1.48	1.62
CH_3CN	3.92	2.87	2.04	2.63	3.10
C_2H_5N 	1.90	1.87	1.26	1.75	1.82
$(CH_3)_2NH$	1.03	1.79	0.71	1.17	1.36
C_4H_5N 	1.74	1.65	1.99	1.81	
N_2H_4	1.75[a]	1.56	2.39		
NH_2CN	4.3[a]	3.16			3.42
CH_2N_2	1.50[a]	0.33	0.94	1.25	1.43
HN_3	0.84[a]	1.72			
OH	1.72[a]	1.30			1.23
H_2O	1.85	1.89	2.11	1.78	1.71
CO	0.11	0.53	0.49	0.19	0.12
HCO	1.36[c]	0.75			1.16
H_2CO	2.33	1.48	2.10	2.16	1.54

Table 4 (cont.)

Molecule	Exp	SINDO1	MINDO/3	MNDO	STO-3G
CH_3OH	1.70	1.61	1.48	1.48	1.51
^3CCO		2,65			1.08
H_2C_2O	1.42	0.14	1.32	1.04	0.84
CH_3CHO	2.69	2.08	2.83	2.38	1.78
C_2H_4O 	1.89	1.50	1.76	1.92	1.46
$(CH_3)_2O$	1.30	1.39	0.82	1.26	1.33
C_4H_4O 	0.66	0.43	0.20	0.42	0.53
NO	0.15	0.02			0.19
HNO		0.94			1.41
H_3NO		4.74			
HNCO		1.67			1.74
NH_2CHO	3.29^a	2.44	3.87	3.09	2.32
N_2O	0.17	0.90	1.15	0.76	0.49
H_2O_2	2.07^b	1.85	1.77		1.30
HCOOH	1.41	0.79	1.86	1.49	0.63
$C_4H_4O_2$ 	2.667^a	2.45			
NO_2	0.32^a	0.57			0.23
HNO_2(cis)	1.42^a	1.18	1.09	1.56	1.68
N_2O_2(cis)		0.20			
O_3	0.53	0.81	1.37	1.18	0.49
NO_3		1.48			
HNO_3	2.16	2.44	2.38	2.78	
N_2O_3		2.04			

[a] Ref. [32] [b] Ref. [31] [c] Ref. [42]

included here because some of them are beyond the SCF level like ethylene or butadiene. Unlike the MNDO procedure for C_2H_4 which lists a value obtained without CI, we emphasize that CI and reoptimization of the geometry is necessary for proper comparison.

4. Ionization Potentials

Table 3 lists the first ionization potentials given by different methods together with experimental data for about 70 compounds which are taken from Dewar's papers or other sources [15, 23, 30]. Ionization potentials calculated by SINDO1 using Koopmans' theorem are often too large by about 1 ev. MNDO results are much better. MINDO/3 results could be assessed only using unpublished data [36]. From the statistics presented by Dewar and Thiel [5] it appears that there were problems with nitrogen compounds where the average error was 1.58 ev. This is confirmed by our statistics. MINDO/3 errors are excessively large in N_2, HCN and $(CN)_2$. SINDO1 errors are large in hydrocarbons when the ratio of hydrogen atoms is at least twice the number of carbon atoms. The error seems to be caused

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

	Type	Compounds	SINDO1	MINDO/3	MNDO	STO-3G
Bond length (A)	XY	C	0.021(40)	0.016(37)	0.012(39)	0.020(28)
		C, N	0.026(26)	0.028(17)	0.016(19)	0.029(16)
		C, N, O	0.025(33)	0.028(27)	0.033(30)	0.036(22)
		all	0.024(99)	0.022(81)	0.020(88)	0.028(66)
Bond length (A)	XH	C	0.012(39)	0.016(29)	0.013(37)	0.011(35)
		C, N	0.010(20)	0.022(15)	0.011(17)	0.023(12)
		C, N, O	0.012(23)	0.019(19)	0.012(21)	0.020(18)
		all	0.012(82)	0.018(63)	0.013(75)	0.016(65)
Bond angle (Degrees)	XYZ	C	3.0(15)	4.5(6)	2.1(9)	0.5(8)
		C,N C, N, O	3.0(14)	5.7(13)	2.7(14)	1.0(3)
		all	3.0(29)	5.3(19)	2.4(23)	0.6(11)
Bond angle (Degrees)	XYH, HXH	C	1.6(28)	3.2(18)	2.3(27)	1.4(24)
		C, N C, N, O	3.0(38)	4.9(24)	3.5(34)	4.0(16)
		all	2.4(66)	4.2(42)	2.9(61)	2.4(40)
Binding energy (kcal/mol)	E	C	5.7(23)	7.5(25)	5.1(29)	
		C, N	8.8(16)	10.9(10)	6.0(15)	
		C, N, O	9.5(26)	7.4(18)	9.8(22)	
		all	8.0(65)	8.1(53)	6.9(66)	
Ionization potential (ev)	I	C	0.73(31)	0.30(24)	0.36(19)	
		C, N	1.11(16)	1.75(10)	0.60(9)	
		C, N, O	0.84(23)	0.75(12)	0.55(13)	
		all	0.85(70)	0.73(46)	0.47(41)	
Dipole moment (Debye)	D	C	0.22(9)	0.29(6)	0.23(6)	0.17(5)
		C, N	0.58(13)	0.67(9)	0.35(8)	0.39(10)
		C, N, O	0.42(21)	0.38(16)	0.25(15)	0.38(19)
		all	0.42(43)	0.45(31)	0.27(29)	0.53(34)

by the presence of hydrogen; the hydrogen molecule has a substantial error. STO-3G ionization potentials [10] are less accurate than SINDO1 results. We do not concentrate here on higher ionization potentials. Their order seems to be properly represented, but their absolute values are mostly too high. There is an improvement over the $1a_1$ levels calculated with MNDO for CH_4, NH_3, H_2O.

5. Dipole moments

Table 4 lists dipole moments for over 40 compounds for which experimental data are available from Dewar's paper or McClellan [31–32]. They are calculated from charge and one center polarization terms. Whereas hydrocarbons do not cause any problem in any of the methods, MNDO results for nitrogen and oxygen compounds are best. SINDO1 suffers from large errors in CH_2N_2, H_2C_2O and

MINDO/3 is poor for CH_3CN and HCN. Contrary to the expectation based on the calculated geometry, SINDO1 predicts the dipole moments of H_2O_2 and N_2H_4 fairly well. STO-3G dipole moments [38] are competitive with those given by the three semiempirical methods.

6. Conclusion

In summary, an error statistics with average absolute errors $\Delta = 1/n \sum_{i=1}^{n} |\Delta_i|$ of the presented quantities for different methods considered is given in Table 5. Number of bond lengths etc. used in the statistics are in parentheses. Cases where the experimental data were uncertain were excluded. The molecules considered here have been classified into different groups as indicated in the column 3 of Table 5. The group X, Y for example, includes molecules $H_aX_bY_c$, where c is a non-zero number and a and b can be any number including zero. It appears that SINDO1 is close to MNDO in geometry and slightly superior to MINDO/3. The best angles are given by STO-3G. The average error of binding energies favors MNDO. With respect to the MINDO/3 value a few remarks are appropriate. We would find 6.4 kcal/mol if we made the statistics for the compounds in Table 2 on the basis of the data published by Bingham et al. [2]. We find 8.1 kcal/mole when we include unpublished data supplied by Thiel [36]. With a larger set of molecules Dewar and Thiel [5] find 11.0 kcal/mol as the MINDO/3 error. This clearly means that the set of molecules chosen by Bingham et al. [2] is not representative and the error increases when more compounds are included. Ionization potentials are far better by MNDO than by SINDO1. MINDO/3 results are representative only when unpublished data on compounds containing nitrogen and oxygen are included. Dipole moments are best by MNDO, and SINDO1 being slightly better than MINDO/3.

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