SUPPORTING INFORMATION FOR

Polarized Molecular Orbital Model Chemistry. I. Ab Initio Foundations

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Supplemental Table S1 on the following pages gives the full set of polarizabilities calculated for the present work. Notice that for PM6 we give two values, the second calculated directly, as for the other NDDO methods, and the first containing a post-SCF empirical correction based on additional atomic parameters (see

http://www.openmopac.net/Polarizability_table.html (accessed Nov. 6, 2010)

for an explanation). The post-SCF correction is not relevant to the question of including polarization effects self-consistently in an NDDO calculation for modeling induction interactions by molecular orbital theory, and hence only the results without atomic corrections are included in the article proper. Since standard computer codes that include PM6 print polarizabilities containing the empirical corrections, the reader should be forewarned that this is not the result calculated directly from the NDDO wave function.

The Hartree-Fock calculations and the semiempirical molecular orbital calculations were all carried out with consistently optimized geometries. That is, for example, the HF/STO-3G(,P) polarizabilities were calculated at geometries optimized by HF/STO-3G(,P), and the AM1 polarizabilities were calculated at geometries optimized by AM1. The MP2 reference calculations were carried out at HF/STO-3G geometries for consistency with the basis set tests.

Supplemental Table S1. Calculated polarizabilities using various basis sets with Hartree-Fock theory and using various semiempirical theories. All polarizabilities are given in Å^3.

	Water	Methanol	Propylene	Methylamine	Acetone	Acetamide	Ethanol
Hartree-Fock with the following basis sets:							
STO-3G	0.40	1.18	2.47	1.41	2.56	2.36	1.99
STO-3G+	0.76	1.89	4.38	2.30	4.24	4.10	3.19
STO-3G++	0.83	1.96	4.65	2.44	4.33	4.18	3.26
STO-3G(,P)	0.81	2.42	4.85	3.00	4.62	3.97	3.96
STO-3G+(,P)	1.25	2.86	5.67	3.47	5.47	5.02	4.51
STO-3G++(,P)	1.27	2.87	5.74	3.50	5.49	5.06	4.50
STO-3G(,p)	0.50	1.44	2.90	1.74	2.98	2.69	2.39
STO-3G(,pP)	0.84	2.50	4.99	3.10	4.75	4.08	4.09
STO-3G(D,P)	1.01	2.62	5.16	3.21	5.18	4.67	4.22
STO-3G(P,P)	0.91	2.71	5.34	3.23	5.35	4.83	4.33
STO-3G(S,P)	1.02	2.62	5.34	3.30	5.17	4.59	4.26
3-21G	0.60	2.05	4.29	2.54	4.52	3.86	3.54
3-21+G	0.82	2.35	5.07	2.91	5.18	4.71	3.95
3-21++G	0.86	2.41	5.16	3.01	5.27	4.77	4.04
3-21G(,P)	0.93	2.54	5.09	3.19	5.09	4.46	4.19
3-21+G(,P)	1.15	2.78	5.61	3.46	5.62	5.09	4.48
3-21++G(,P)	1.16	2.80	5.64	3.49	5.64	5.11	4.50
3-21G(,p)	0.70	2.20	4.49	2.73	4.70	4.04	3.73
3-21G(,pP)	0.97	2.60	5.15	3.26	5.15	4.53	4.26
3-21G(D,P)	1.10	2.74	5.43	3.36	5.48	4.96	4.40
STO-3G(d)	0.50	1.33	2.65	1.56	2.83	2.64	2.20
3-21G(d)	0.70	2.13	4.32	2.59	*N/A*	3.97	*N/A*
3-21+G(d)	0.91	2.42	5.11	2.95	5.22	4.78	4.01
3-(21,3,3)G	0.41	1.27	2.70	1.50	2.82	2.60	2.13
cc-pVDZ	0.79	2.33	4.81	2.88	5.02	4.39	3.94
aug-cc-pVDZ	1.26	2.94	5.76	3.60	5.84	5.38	4.65
3-(21,21,3)G	0.48	1.46	3.30	1.78	3.53	3.19	2.57
3-(21,3,21)G	0.80	2.32	4.35	2.85	5.18	4.77	3.89
3-(21,3,3)G(,P)	1.15	3.23	5.69	3.84	6.28	5.65	5.19
3-(3,21,21)G	0.89	2.81	5.32	2.61	6.29	4.63	4.85
aug'-cc-pVDZ	1.16	2.85	5.70	3.49	5.79	5.32	4.56
aug''-cc-pVDZ	0.87	2.41	5.17	3.02	5.28	4.82	4.04
STO-3G(,P!)	0.81	1.41	2.47	2.02	2.56	2.96	2.25
STO-3G(,P*)	0.81	1.41	3.84	2.02	2.56	2.96	2.25
STO-3G(,P')	0.83	2.36	4.80	2.95	4.53	4.08	3.85
STO-3G(,P'')	0.82	2.43	4.87	3.01	4.62	4.01	3.96
Semiempirical methods:							
MNDO	0.43	1.72	3.77	2.10	3.87	3.57	2.89
AM1	0.50	1.82	3.86	2.17	4.00	3.67	3.04
PM3	0.50	1.62	3.44	2.01	3.63	3.66	2.70
RM1	0.50	1.74	3.68	2.13	3.81	3.59	2.90
PM6 (with empirical correction)	1.35	3.25	6.04	3.79	6.39	5.84	5.06
PM6 (no empirical correction)	0.30	1.18	2.64	1.42	2.84	2.82	1.99
Reference Polarizability:	1.45	3.23	6.26	4.01	6.33	5.67	5.11

Diethylamine	Acetaldehyde	Isopropanol	Methane	Methane thiol CH3SH	Dimethyl sulfide DMS	Dimethyl ether DME	CO2	HCN	Acetylene C2H2	Methyl acetylene CH3CCH
3.86	1.76	2.75	0.82	1.73	2.63	1.99	0.97	0.86	1.06	1.99
3.86	3.06	4.50	1.17	3.63	5.29	3.20	1.95	1.73	2.41	3.70
6.41	3.08	4.61	1.34	3.84	5.61	3.26	1.95	1.76	2.54	3.86
7.75	3.15	5.35	2.00	3.48	5.17	4.11	0.97	1.17	1.96	3.72
8.49	3.93	6.05	2.25	4.87	6.83	4.56	1.95	1.92	*2.91*	4.51
7.93	3.92	6.05	2.26	4.92	6.95	4.54	1.95	1.93	2.77	4.59
4.64	2.03	3.29	1.10	2.00	3.06	2.41	0.97	0.92	1.22	2.30
8.00	3.23	5.52	2.08	3.57	5.31	4.25	0.97	1.19	2.01	3.82
8.13	3.59	5.75	2.03	4.24	5.98	4.23	1.61	1.84	2.60	4.39
8.24	3.73	5.84	2.03	4.23	6.26	4.48	1.72	1.58	2.26	4.18
8.24	3.55	5.78	2.20	3.90	5.69	4.34	1.25	1.48	2.34	4.17
7.01	3.11	4.91	1.70	3.51	5.10	3.51	1.47	1.50	1.84	3.47
7.77	3.64	5.54	1.81	4.04	5.78	3.92	1.94	1.93	2.47	4.14
7.93	3.69	5.65	1.88	4.15	5.92	4.02	1.94	1.93	2.47	4.20
8.22	3.50	5.74	2.19	4.23	5.88	4.22	1.47	1.63	2.15	4.02
8.64	3.94	6.13	2.28	4.68	6.46	4.49	1.94	2.00	*2.65*	4.48
8.66	3.96	6.14	2.30	4.75	6.54	4.52	1.94	2.00	2.61	4.50
7.38	3.23	5.17	1.84	3.66	5.32	3.71	1.47	1.53	1.93	3.62
8.34	3.55	5.83	2.23	4.28	5.95	4.27	1.47	1.64	2.18	4.08
8.44	3.86	6.00	2.23	4.69	6.40	4.44	2.01	2.13	2.99	4.76
4.22	1.95	3.04	0.89	1.93	2.87	2.19	1.16	0.98	1.22	2.22
N/A	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	3.57	1.61	1.57	1.94	4.50
7.78	3.70	5.59	1.82	*N/A*	*N/A*	3.97	2.06	2.01	2.59	4.27
4.14	1.94	2.95	0.88	3.51	5.10	2.16	1.15	1.08	1.34	2.35
7.76	3.49	5.48	1.90	3.87	5.58	3.92	1.77	1.82	2.32	4.04
8.80	4.18	6.32	2.34	5.08	6.86	4.66	2.36	2.43	3.25	5.06
5.12	2.43	3.65	0.99	2.69	4.05	2.44	1.47	1.45	1.75	2.89
7.76	3.51	5.52	1.65	3.41	5.06	3.93	1.61	1.59	1.86	3.63
10.04	4.34	7.04	2.32	4.54	6.47	5.32	1.61	1.81	2.44	4.63
8.63	4.22	6.82	2.13	3.81	5.95	4.68	1.90	1.68	2.28	4.58
8.70	4.13	6.24	2.28	5.00	6.77	4.58	2.36	2.43	3.25	5.03
7.94	3.71	5.67	1.86	4.13	5.91	4.02	1.97	1.95	2.51	4.22
4.21	1.76	3.01	0.82	2.28	2.63	1.99	0.97	0.86	1.06	1.99
4.21	2.20	3.01	0.82	2.28	2.63	1.99	0.97	1.17	1.96	2.55
7.48	2.99	5.16	1.82	3.57	5.23	3.94	0.98	1.13	1.99	3.67
7.76	3.13	5.35	1.98	3.52	5.22	4.11	0.98	1.17	1.98	3.74

5.75	2.72	4.01	1.28	2.70	3.94	3.04	1.68	1.36	1.75	3.22
5.97	2.83	4.16	1.31	2.93	4.31	3.17	1.66	1.40	1.77	3.34
5.28	2.60	3.69	1.12	2.69	3.96	2.76	1.69	1.50	1.75	3.11
5.82	2.70	3.95	1.19	3.09	4.36	2.98	1.65	1.32	1.78	3.27
9.35	4.58	6.86	2.67	5.59	7.61	5.16	2.75	2.47	3.32	5.40
3.95	2.03	2.78	0.76	2.23	3.24	2.08	1.58	1.15	1.46	2.52

9.61	4.59	7.61	2.59	5.49	7.39	5.16	2.91	2.59	3.33	6.18

Ethylene C2H4	HCl	Acetyl chloride CH3Cl	Acetyl chloride CH3C(O)Cl	Acetonitrile CH3CN	Glycine HO2CCH2NH2	*s-trans*-butadiene C4H6	Benzene C6H6	Toluene C6H5CH3	Water dimer H2O .. H2O	Pyridine C5H5N
1.59	0.42	1.34	2.39	1.72	2.70	3.72	4.75	5.71	0.87	4.39
3.02	0.97	2.36	4.43	2.98	4.62	7.04	8.85	10.14	1.65	8.05
3.07	1.00	2.48	4.46	3.06	4.66	7.42	9.30	10.61	1.77	8.29
3.22	0.74	2.37	3.40	2.71	4.26	6.62	7.82	9.55	1.83	6.91
3.94	1.41	3.21	5.10	3.67	5.47	8.07	9.73	11.48	2.49	8.82
3.95	1.41	3.28	5.09	3.69	5.51	8.17	9.85	11.61	2.52	8.88
1.87	0.47	1.54	2.59	1.93	3.01	4.18	5.19	6.31	1.09	4.75
3.31	0.76	2.44	3.47	2.78	4.36	6.78	7.96	9.74	1.86	7.03
3.46	1.57	3.25	4.85	3.44	5.18	7.22	8.86	10.67	2.18	8.10
3.51	0.89	2.89	4.70	3.35	5.25	7.72	9.39	11.16	2.10	8.58
3.63	0.98	2.68	4.09	3.15	4.86	7.39	8.84	10.59	2.19	7.83
2.73	0.95	2.66	4.29	3.01	4.16	5.93	7.19	8.83	1.27	6.63
3.38	1.22	3.04	5.12	3.53	5.14	7.35	8.95	10.62	1.77	8.22
3.43	1.24	3.09	5.17	3.57	5.19	7.39	8.98	10.70	1.83	8.25
3.36	1.29	3.05	4.58	3.32	4.80	6.92	8.24	10.09	1.97	7.46
3.86	1.58	3.40	5.37	3.78	5.52	7.89	9.44	11.24	2.33	8.65
3.87	1.60	3.44	5.38	3.80	5.53	7.91	9.47	11.27	2.34	8.67
2.87	1.01	2.77	4.38	3.11	4.35	6.14	7.39	9.10	1.47	6.79
3.39	1.30	3.09	4.61	3.36	4.88	6.98	8.28	10.15	2.03	7.50
3.71	2.11	3.82	5.62	3.81	5.42	7.58	9.28	11.09	2.27	8.52
1.70	0.69	1.64	2.82	1.91	3.06	3.94	5.14	6.19	1.09	4.78
2.78	*N/A*	*N/A*	*N/A*	3.08	4.34	5.98	7.39	9.02	1.48	6.83
3.42	*N/A*	*N/A*	*N/A*	3.62	5.27	7.41	9.17	10.85	1.96	8.47
1.75	0.95	2.66	4.29	2.02	2.93	4.12	5.19	6.23	0.88	4.84
3.15	1.29	3.03	4.81	3.42	4.78	6.70	8.24	9.99	1.66	7.61
4.01	2.34	4.12	6.13	4.18	5.90	8.10	9.95	11.79	2.56	9.19
2.13	0.74	2.16	3.81	2.54	3.60	5.03	6.33	7.60	1.00	5.91
2.69	1.28	2.93	4.98	3.16	5.24	5.88	7.45	9.25	1.99	7.00
3.65	1.74	3.64	5.51	3.75	6.49	7.62	9.13	11.37	2.78	8.46
3.20	0.69	2.87	5.08	3.68	5.24	6.97	8.53	10.88	2.10	7.57
3.96	2.28	4.07	6.10	4.15	5.84	8.05	9.91	11.72	2.39	9.15
3.48	1.22	3.07	5.20	3.58	5.24	7.42	9.03	10.74	1.88	8.31
1.59	0.74	1.34	2.39	1.72	3.58	3.72	4.75	5.71	1.83	4.39
3.22	0.74	1.34	2.39	1.72	3.58	6.62	7.82	8.40	1.83	6.91
3.25	0.64	2.23	3.37	2.59	4.33	6.92	8.19	9.85	1.94	7.16
3.25	0.72	2.36	3.41	2.70	4.29	6.72	7.92	9.65	1.86	6.98

2.43	0.67	1.99	3.77	2.67	3.95	5.73	7.23	8.62	0.86	6.70
2.47	0.60	1.98	3.82	2.80	4.15	5.73	7.22	8.66	1.03	6.76
2.22	0.80	2.08	4.12	2.76	3.96	5.22	6.76	8.02	1.12	6.46
2.35	0.59	2.03	3.88	2.62	4.08	5.54	6.94	8.31	1.02	6.54
4.12	2.34	4.34	6.73	4.44	6.47	8.17	10.17	12.13	2.40	9.38
1.73	0.47	1.46	3.21	2.11	3.31	4.29	5.31	6.27	0.67	5.07

4.25	2.63	4.72	6.62	4.48	6.52	8.64	10.32	12.26	2.88	9.18

Benzaldehyde PhCHO	Benzyl alcohol BzOH	Phenol PhOH	Nicotinamide C6H6N2O	Pyrimidine C4H4N2	Purine C5H4N4	Vinyl alcohol C2H3OH	Ethane C2H6	Propane C3H8
6.06	6.09	5.24	6.28	4.04	6.11	1.96	1.61	2.41
10.77	10.73	9.38	10.91	7.21	10.34	3.68	2.45	3.81
11.11	11.14	9.74	11.06	7.35	10.41	3.78	2.66	4.00
9.09	9.84	8.10	9.06	6.02	8.18	3.46	3.58	5.11
11.63	11.98	10.21	11.76	7.88	11.08	4.47	3.90	5.54
11.74	12.09	10.31	11.81	7.92	11.10	4.49	3.91	5.54
6.49	6.66	5.67	6.68	4.31	6.39	2.22	2.03	2.97
9.23	10.03	8.24	9.20	6.11	8.28	3.55	3.70	5.28
10.86	11.19	9.49	11.13	7.30	10.51	3.97	3.68	5.28
11.36	11.69	9.83	11.53	7.72	10.87	4.09	3.68	5.30
10.26	10.93	9.17	10.35	6.85	9.44	3.96	3.81	5.42
9.00	9.17	7.66	9.15	6.04	8.74	3.07	3.16	4.60
11.04	11.13	9.47	11.27	7.49	10.71	3.88	3.39	4.98
11.06	11.19	9.50	11.31	7.51	10.73	3.93	3.50	5.12
9.97	10.43	8.67	10.16	6.67	9.42	3.67	3.81	5.42
11.49	11.71	9.94	11.73	7.83	11.05	4.32	3.96	5.64
11.51	11.74	9.96	11.76	7.84	11.06	4.33	3.97	5.66
9.19	9.44	7.86	9.36	6.16	8.87	3.21	3.36	4.85
10.01	10.51	8.73	10.22	6.70	9.46	3.73	3.87	5.50
11.38	11.59	9.88	11.64	7.70	10.98	4.21	3.87	5.51
6.61	6.66	5.74	6.92	4.41	6.74	2.16	1.74	2.61
9.26	9.43	7.93	9.46	6.23	9.06	3.18	3.16	4.59
11.32	11.44	9.76	11.59	7.73	11.09	4.00	3.39	4.97
6.68	6.65	5.74	6.94	4.48	6.79	2.16	1.71	2.56
10.24	10.42	8.78	10.45	6.91	9.97	3.57	3.50	5.08
12.09	12.29	10.59	12.19	8.36	11.89	4.59	4.02	5.72
8.17	8.06	6.88	8.41	5.48	8.21	2.59	2.09	3.19
9.59	9.96	8.31	10.41	6.46	9.73	3.35	3.19	4.72
11.40	12.25	10.14	12.21	7.65	11.16	4.45	4.26	6.20
11.12	11.70	9.57	10.52	6.44	8.75	3.92	4.11	6.04
12.06	12.24	10.54	12.15	8.34	11.86	4.53	3.95	5.64
11.14	11.25	9.58	11.05	7.57	10.83	3.97	3.49	5.12
6.06	6.38	5.53	7.02	4.04	6.11	2.18	1.61	2.41
9.09	9.00	8.10	9.06	6.02	8.18	3.46	1.61	2.41
9.44	10.24	8.51	9.44	6.13	8.33	3.59	3.30	4.75
9.19	9.96	8.21	9.18	6.07	8.25	3.50	3.55	5.08

8.96	8.98	8.00	9.32	6.13	9.38	3.04	2.46	3.62
9.18	9.11	7.98	9.46	6.29	9.76	3.09	2.56	3.74
8.65	8.47	7.52	9.31	6.16	9.81	2.87	2.22	3.25
8.85	8.77	7.71	9.25	6.11	9.52	3.01	2.39	3.52
12.58	12.77	11.06	12.96	8.59	12.44	4.90	4.48	6.28
7.08	6.75	6.05	7.54	4.82	7.77	2.35	1.56	2.35

12.80	13.15	11.1	12.19	8.53	12.78	4.85	4.48	6.38