Supporting Information Available

Evaluation of Computational Chemistry Methods: Crystallographic and Cheminformatics Analysis of Aminothiazole Methoximes

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Table S1. Experimental Bond Lengths (in angstroms) of ATMO-containing Structures in the Cambridge Structural Database

CSD code	N2-C1	C1-N1	N1-C2	C2-C3	C3-S1	S1-C1	C2-C4	C4-N3	N3-O1	C4-C5	C5-O2
BAGSAD	1.301	1.348	1.388	1.337	1.735	1.718	1.476	1.290	1.377	1.522	1.212
BAGSEH1	1.317	1.322	1.388	1.351	1.726	1.735	1.447	1.291	1.395	1.524	1.244
BAGSEH2	1.319	1.342	1.406	1.334	1.727	1.728	1.459	1.270	1.402	1.531	1.233
CFTXIM	1.335	1.304	1.388	1.353	1.714	1.755	1.457	1.280	1.406	1.511	1.195
EAMTHZ	1.322	1.341	1.388	1.345	1.722	1.707	1.466	1.285	1.387	1.521	1.193
EATZAC	1.343	1.308	1.391	1.345	1.715	1.737	1.458	1.288	1.382	1.505	1.187
FAJMAE	1.341	1.329	1.399	1.332	1.728	1.727	1.487	1.288	1.406	1.465	1.241
FAJMEI	1.331	1.326	1.407	1.331	1.731	1.723	1.467	1.290	1.402	1.501	1.215
FUPKOQ	1.345	1.304	1.385	1.341	1.716	1.751	1.454	1.282	1.401	1.518	1.190
GAFTIQ	1.341	1.304	1.385	1.364	1.733	1.756	1.453	1.294	1.399	1.513	1.234
GOHRAW	1.336	1.316	1.422	1.334	1.729	1.724	1.462	1.273	1.397	1.516	1.226
VENWIU	1.281	1.342	1.396	1.311	1.744	1.725	1.442	1.278	1.428	1.566	1.228
Mean	1.326	1.324	1.395	1.340	1.727	1.732	1.461	1.284	1.399	1.516	1.217
Std Dev	0.019	0.017	0.011	0.013	0.009	0.015	0.012	0.008	0.013	0.023	0.021
Std Err	0.006	0.005	0.003	0.004	0.003	0.004	0.004	0.002	0.004	0.007	0.006

Table S2. Experimental Bond Angles (in degrees) of ATMO-containing Structures in the Cambridge Structural Database

CSD code	N2-C1-N1	C1-N1-C2	N1-C2-C3	C2-C3-S1	C3-S1-C1	S1-C1-N1	C2-C4-C5
BAGSAD	124.60	114.92	112.29	111.58	90.99	110.21	120.99
BAGSEH1	126.14	114.72	112.31	111.54	90.30	111.12	118.19
BAGSEH2	125.10	112.58	113.03	112.23	90.00	112.15	116.66
CFTXIM	125.29	110.39	115.88	110.37	89.07	114.28	118.30
EAMTHZ	124.17	114.03	111.87	112.08	90.91	111.51	117.65
EATZAC	124.03	109.96	115.53	110.75	88.90	114.85	118.22
FAJMAE	122.25	109.10	116.61	110.16	89.45	114.64	118.71
FAJMEI	123.94	113.46	113.32	110.97	90.89	111.34	120.41
FUPKOQ	125.20	109.96	115.45	111.57	87.91	115.10	118.21
GAFTIQ	124.51	110.95	114.31	111.72	87.48	115.52	123.28
GOHRAW	124.99	112.80	112.39	112.08	89.96	112.76	116.88
VENWIU	126.51	115.00	112.39	112.15	90.46	109.96	115.72
Mean	124.73	112.32	113.78	111.43	89.69	112.79	118.60
Std Dev	1.11	2.16	1.68	0.71	1.16	2.01	2.08
Std Err	0.32	0.62	0.49	0.21	0.34	0.58	0.60
CSD code	N1-C2-C4	C4-C5-O2	C2-C4-N3	C5-C4-N3	C4-N3-O1	N2-C1-S1	C3-C2-C4
BAGSAD	118.91	120.12	127.05	111.96	112.83	125.19	128.76
BAGSEH1	120.55	115.84	116.81	124.99	110.19	122.70	127.14
BAGSEH2	120.99	115.84	117.36	125.90	110.43	122.74	125.96
CFTXIM	120.01	123.38	119.37	122.33	110.12	120.43	124.07
EAMTHZ	120.80	123.37	129.13	113.17	112.90	124.31	127.33
EATZAC	116.65	124.60	131.01	110.76	111.66	121.09	127.80
FAJMAE	119.02	121.11	114.78	126.51	109.90	123.09	124.37
FAJMEI	118.37	119.96	116.86	122.67	111.11	124.72	128.31
FUPKOQ	119.29	125.30	120.66	121.05	110.12	119.69	124.95
GAFTIQ	118.45	119.59	116.52	120.06	110.03	119.90	127.21

GOHRAW	118.51	120.05	117.92	125.00	110.55	122.25	129.09
VENWIU	117.82	116.45	116.55	127.69	108.90	123.46	129.62
Mean	119.11	120.47	120.33	121.01	110.73	122.46	127.05
Std Dev	1.29	3.28	5.53	5.91	1.20	1.85	1.85
Std Err	0.37	0.95	1.60	1.71	0.35	0.54	0.53

Table S3. Experimental Dihedral Angles (in degrees) of ATMO-containing Structures in the Cambridge Structural Database

CSD code	N2-C1-N1-C2	C1-N1-C2-C3	N1-C2-C3-S1	C2-C3-S1-C1	C3-S1-C1-N1	S1-C1-N1-C2
BAGSAD	-179.60	0.53	-1.08	1.06	0.75	0.29
BAGSEH1	-177.80	0.50	-0.77	0.66	-0.38	0.01
BAGSEH2	178.61	0.61	-0.62	0.37	-0.02	-0.32
CFTXIM	179.07	1.08	-1.26	0.82	-0.24	-0.40
EAMTHZ	-179.96	-1.17	0.82	-0.24	-0.42	0.98
EATZAC	-178.08	0.32	-0.75	0.72	-0.58	0.27
FAJMAE	-176.55	-1.75	0.69	0.40	-1.46	2.02
FAJMEI	178.73	1.87	-0.86	-0.19	1.25	-1.97
FUPKOQ	179.64	-0.74	-0.02	0.55	-1.02	1.17
GAFTIQ	178.43	-1.61	1.08	-0.23	-0.71	1.43
GOHRAW	178.11	1.03	-0.05	-0.66	1.27	-1.53
VENWIU	-176.99	-1.32	1.50	-1.05	0.29	0.49
CSD code	C1-N1-C2-C4	N1-C2-C4-C5	N1-C2-C4-N3	C2-C4-N3-O1	C2-C4-C5-O2	C5-C4-N3-O1
BAGSAD	-177.22	1.52	-177.38	-3.54	174.42	177.47
BAGSEH1	-179.35	-175.62	4.86	-179.64	79.69	0.88
BAGSEH2	-178.04	172.37	-4.53	178.88	-86.41	2.29
CFTXIM	-176.78	-163.64	16.63	177.34	101.71	-2.38
EAMTHZ	179.39	178.11	0.84	-1.87	-4.84	-179.24
EATZAC	-178.13	12.43	-167.57	-1.03	-103.30	178.97
FAJMAE	178.63	-162.87	16.95	179.49	-60.36	-0.70
FAJMEI	-177.88	169.18	-8.01	177.69	85.31	0.57
FUPKOQ	-174.66	35.44	-147.81	-172.61	-89.00	4.06
GAFTIQ	176.48	171.54	-4.18	178.27	-84.11	2.40
GOHRAW	-179.64	175.60	0.40	177.94	-92.54	3.16
VENWIU	-176.97	175.71	-2.26	-179.52	-66.03	2.79

CSD code	N2-C1-S1-C3	O2-C5-C4-N3
BAGSAD	179.14	-6.53
BAGSEH1	177.52	-100.84
BAGSEH2	-178.98	90.19
CFTXIM	-179.73	-78.56
EAMTHZ	-179.48	172.85
EATZAC	177.82	76.70
FAJMAE	177.10	119.84
FAJMEI	-179.46	-97.67
FUPKOQ	-179.58	94.25
GAFTIQ	-177.86	91.46
GOHRAW	-178.38	82.28
VENWIU	177.86	111.67

Table S4. Optimized Bond Lengths (in angstroms) from Computational Chemistry Methods

Method	N2-C1	C1-N1	N1-C2	C2-C3	C3-S1	S1-C1	C2-C4	C4-N3	N3-O1	C4-C5	C5-O2
AM1	1.398	1.347	1.394	1.391	1.664	1.750	1.467	1.306	1.318	1.521	1.242
PM3	1.410	1.341	1.411	1.369	1.730	1.776	1.468	1.295	1.407	1.512	1.220
MNDO	1.425	1.346	1.394	1.401	1.719	1.736	1.478	1.311	1.299	1.517	1.228
MMFF94 (Spartan)	1.336	1.309	1.395	1.384	1.712	1.714	1.460	1.308	1.402	1.529	1.222
Sybyl (Spartan)	1.299	1.264	1.441	1.341	1.799	1.773	1.482	1.277	1.406	1.480	1.221
Tripos (SYBYL)	1.331	1.265	1.440	1.340	1.799	1.773	1.481	1.276	1.406	1.474	1.221
MMFF94 (SYBYL)	1.342	1.310	1.400	1.383	1.711	1.714	1.464	1.305	1.402	1.533	1.223
MMFF94s (SYBYL)	1.336	1.310	1.400	1.384	1.711	1.714	1.465	1.306	1.402	1.533	1.223
AMBER*	1.421	1.282	1.391	1.320	1.704	1.728	1.490	1.279	1.410	1.509	1.230
OPLS/A	1.412	1.281	1.420	1.393	1.709	1.725	1.489	1.278	1.408	1.490	1.229
OPLS-AA	1.372	1.329	1.416	1.376	1.756	1.745	1.522	1.487	1.405	1.434	1.235
MMFF94 (MMod)	1.343	1.309	1.399	1.384	1.712	1.713	1.464	1.305	1.401	1.530	1.223
MMFF94s (MMod)	1.336	1.310	1.400	1.384	1.711	1.714	1.465	1.306	1.402	1.533	1.223
DFT 6-31G*	1.376	1.299	1.396	1.372	1.742	1.764	1.479	1.294	1.381	1.539	1.224
DFT 6-31G*/SCRF	1.365	1.307	1.394	1.368	1.742	1.771	1.478	1.296	1.380	1.532	1.239
DFT 6-31G**	1.374	1.300	1.396	1.372	1.742	1.764	1.479	1.294	1.381	1.540	1.224
DFT 6-31+G*	1.378	1.300	1.397	1.373	1.742	1.761	1.480	1.294	1.381	1.539	1.227
DFT 6-311G*	1.374	1.296	1.395	1.368	1.740	1.763	1.478	1.289	1.378	1.540	1.217
DFT 6-311+G**	1.374	1.296	1.395	1.368	1.740	1.761	1.479	1.288	1.379	1.540	1.219
HF STO-3G	1.433	1.303	1.437	1.339	1.734	1.743	1.503	1.296	1.406	1.543	1.220
HF 3-21G(*)	1.349	1.287	1.405	1.345	1.732	1.743	1.476	1.266	1.419	1.539	1.219
HF3-21G(*)/SCRF	1.337	1.297	1.406	1.345	1.729	1.747	1.470	1.268	1.419	1.536	1.234
HF 6-31G*	1.372	1.273	1.383	1.338	1.736	1.747	1.481	1.258	1.354	1.517	1.198
HF 6-31G**	1.369	1.274	1.383	1.338	1.736	1.748	1.481	1.258	1.355	1.517	1.198
HF 6-31+G*	1.372	1.274	1.383	1.339	1.736	1.745	1.481	1.258	1.354	1.518	1.200
HF 6-311G*	1.373	1.270	1.382	1.336	1.736	1.746	1.481	1.256	1.349	1.519	1.192
LMP2 6-31G*	1.388	1.308	1.400	1.377	1.731	1.748	1.482	1.304	1.402	1.532	1.234

Table S5. Optimized Bond Angles (in degrees) from Computational Chemistry Methods

Method	N2-C1-N1	C1-N1-C2	N1-C2-C3	C2-C3-S1	C3-S1-C1	S1-C1-N1	C2-C4-C5
AM1	126.631	109.433	114.994	111.325	90.688	113.561	114.535
PM3	120.382	110.809	114.420	112.070	88.854	113.847	116.197
MNDO	124.624	110.121	115.051	109.892	90.401	114.478	117.688
MMFF94 (Spartan)	123.134	110.694	113.790	110.408	89.713	115.395	118.548
Sybyl (Spartan)	123.936	117.516	108.459	114.134	86.790	113.045	119.064
Tripos (SYBYL)	124.510	117.631	108.516	114.076	86.904	112.873	117.573
MMFF94 (SYBYL)	123.134	110.465	113.790	110.408	89.771	115.510	118.605
MMFF94s (SYBYL)	123.191	110.522	113.790	110.465	89.771	115.452	118.834
AMBER*	120.898	109.318	113.561	113.790	86.102	117.172	120.038
OPLS/A	119.866	109.204	112.127	112.643	87.191	118.892	120.497
OPLS-AA	123.076	110.236	112.070	113.962	86.217	117.516	126.516
MMFF94 (MMod)	123.076	110.580	113.675	110.465	89.713	115.510	118.204
MMFF94s (MMod)	123.191	110.522	113.790	110.465	89.771	115.452	118.834
DFT 6-31G*	124.166	112.013	114.134	110.866	88.510	114.478	123.707
DFT 6-31G*/SCRF	124.510	111.726	115.051	110.408	88.854	113.962	123.535
DFT 6-31G**	124.166	112.070	114.191	110.809	88.510	114.420	123.822
DFT 6-31+G*	124.051	112.013	114.076	110.809	88.567	114.478	123.707
DFT 6-311G*	124.223	112.185	114.134	110.866	88.452	114.363	123.478
DFT 6-311+G**	124.223	112.127	114.248	110.752	88.567	114.363	123.363
HF STO-3G	122.446	108.745	114.707	111.841	87.994	116.713	121.127
HF 3-21G(*)	124.108	112.529	113.503	111.153	88.968	113.847	123.191
HF 3-21G(*)/SCRF	124.854	112.242	114.076	110.866	89.427	113.389	122.962
HF 6-31G*	123.994	110.866	116.255	109.548	88.338	114.994	117.229
HF 6-31G**	123.994	110.866	116.312	109.490	88.395	114.994	117.229
HF 6-31+G*	123.936	110.981	116.140	109.490	88.452	114.936	117.057
HF 6-311G*	123.994	110.981	116.140	109.490	88.338	114.994	117.229
LMP2 6-31G*	123.478	110.981	114.306	110.694	88.854	115.051	123.248

Method	N1-C2-C4	C4-C5-O2	C2-C4-N3	C5-C4-N3	C4-N3-O1	N2-C1-S1	C3-C2-C4
AM1	120.669	120.841	128.809	116.599	117.520	119.580	124.338
PM3	119.465	122.790	126.917	116.885	118.950	125.484	126.115
MNDO	117.631	122.675	128.121	114.191	118.150	120.898	127.318
MMFF94 (Spartan)	120.153	120.439	125.943	115.510	113.450	121.471	126.057
Sybyl (Spartan)	120.554	117.287	125.541	115.395	110.010	122.962	130.987
Tripes (SYBYL)	120.955	120.038	126.172	116.255	109.720	122.618	130.586
MMFF94 (SYBYL)	120.153	120.038	125.369	116.025	113.730	121.357	126.000
MMFF94s (SYBYL)	120.325	120.096	125.255	115.911	113.730	121.357	125.885
AMBER*	122.904	119.924	121.471	118.490	125.830	121.930	123.478
OPLS/A	124.280	120.325	121.070	118.376	125.250	121.242	123.535
OPLS-AA	119.408	121.815	112.127	121.127	108.570	119.408	128.522
MMFF94 (MMod)	119.924	119.981	126.000	115.796	113.850	121.414	126.401
MMFF94s (MMod)	120.325	120.153	125.255	115.911	113.730	121.357	125.885
DFT 6-31G*	119.350	120.726	126.631	109.662	114.710	121.242	126.459
DFT 6-31G*/SCRF	119.121	120.210	125.771	110.694	114.540	121.471	125.828
DFT 6-31G**	119.350	120.669	126.516	109.662	114.710	121.299	126.459
DFT 6-31+G*	119.465	120.783	126.344	109.949	114.940	121.299	126.401
DFT 6-311G*	119.580	120.726	126.631	109.892	114.990	121.299	126.287
DFT 6-311+G**	119.580	120.841	126.401	110.236	115.050	121.299	126.172
HF STO-3G	117.917	121.758	126.573	112.299	113.160	120.669	127.376
HF 3-21G(*)	120.268	119.924	126.459	110.350	115.800	121.987	126.229
HF 3-21G(*)/SCRF	120.153	119.465	126.745	110.293	115.680	121.758	125.771
HF 6-31G*	117.000	120.325	127.834	114.936	115.220	120.955	126.745
HF 6-31G**	116.943	120.325	127.834	114.879	115.170	120.955	126.745
HF 6-31+G*	116.656	120.153	128.006	114.936	115.220	121.070	127.204
HF 6-311G*	117.000	120.268	127.777	114.936	115.450	120.955	126.860
LMP2 6-31G*	118.949	120.611	126.745	109.949	113.220	121.299	126.745

TABLE S6. Single-Point Energies (in eV) for Variation of the C6-O1-N3-C4 Dihedral Angle in 30° Increments

Method	0°	30°	60°	90°	120°	150°	180°	210°	240°	270°
AM1	ND	17.446	8.3141	1.3212	0.926	0.8182	0.7648	0.8083	0.9169	1.018
PM3	2.95172	2.005	1.2125	0.9711	0.8736	0.7802	0.7424	0.781	0.8695	0.9994
MNDO	2.82215	2.2145	0.9453	0.2594	0.0325	-0.1077	-0.1623	-0.1081	0.0262	0.248
MMFF94 (Spartan)	118.015	73.105	140.94	4.0607	1.6124	1.4531	1.4057	1.4541	1.5583	1.7069
Sybyl (Spartan)	191819	86366	329496	27.754	0.5125	0.5095	0.5264	0.514	0.483	0.4745
AMBER*	330.259	155.46	101.05	6.6581	4.337	4.1136	4.0056	4.0988	4.2958	4.4055
OPLS/A	613.995	6140.8	163.27	5.552	1.3673	1.2298	1.1699	1.2254	1.3434	1.4436
OPLS-AA	16.5336	4.1348	2.6357	2.2045	2.103	2.0826	2.0978	2.1884	111.62	92.819
MMFF94 (MMod)	23.5839	47.097	16.435	5.4088	4.5174	4.3747	4.3226	4.3699	4.4849	4.6892
MMFF94s (MMod)	23.3579	41.76	17.634	6.0331	4.8753	4.7256	4.6736	4.7209	4.8345	5.0241
Tripes	191779	86301.4	345006	28.248	0.524	0.5204	0.5373	0.5249	0.4939	0.4852
MMFF94 (SYBYL)	121.115	73.371	144.22	4.4131	1.6744	1.4992	1.4455	1.4932	1.6048	1.7715
MMFF94s (SYBYL)	122.819	74.344	146.49	4.4799	1.6687	1.4926	1.4386	1.4856	1.5954	1.7594
Method	300°	330°								
AM1	1.3552	7.1375								
PM3	1.5603	2.6167								
MNDO	0.9843	2.1892								
MMFF94 (Spartan)	2.8441	20.349								
Sybyl (Spartan)	3.2695	3372								
AMBER*	4.5118	17.488								
OPLS/A	2.162	27.245								
OPLS-AA	55.067	140.71								
MMFF94 (MMod)	5.9342	14.913								
MMFF94s (MMod)	6.1129	13.642								
Tripes	3.2392	3350								
MMFF94 (SYBYL)	2.9243	19.932								
MMFF94s (SYBYL)	2.9168	20.054								

Method	0°	30°	60°	90°	120°	150°
HF STO-3G	-27828.4012	-27823.2861	-27847.3877	-27856.9494	-27857.5962	-27857.7831
HF 3-21G(*)	-28011.6674	-28014.2663	-28045.7694	-28048.6102	-28048.9118	-28049.0832
HF 3-21G(*)/SCRF	-28012.1636	-28013.0287	-28046.6635	-28049.7436	-28049.9663	-28050.0659
HF 6-31G*	-28179.9008	-28189.739	-28195.3541	-28196.0786	-28196.2157	-28196.3357
HF 6-31G**	-28180.7015	-28190.3679	-28195.9883	-28196.7095	-28196.8461	-28196.9661
HF 6-31+G*	-28179.9383	-28189.8323	-28195.7796	-28196.5603	-28196.7124	-28196.8386
HF 6-311G*	-28183.9946	-28193.9741	-28199.7123	-28200.4531	-28200.5911	-28200.714
DFT 6-31G*	-28295.8203	-28300.5323	-28316.7051	-28318.009	-28318.2377	-28318.4368
DFT 6-31G*/SCRF	ND	-28251.6092	-28310.7402	-28314.1868	-28314.5209	-28314.65
DFT 6-31G**	-28296.5497	-28301.0088	-28317.2703	-28318.5541	-28318.7828	-28318.9821
DFT 6-311G*	-28301.4916	-28307.3059	-28321.7598	-28322.958	-28323.1868	-28323.3884
DFT 6-31+G*	-28297.5881	-28303.5886	-28317.6012	-28318.7826	-28319.0209	-28319.2291
DFT 6-311+G**	-28303.3171	-28310.7243	-28322.8972	-28323.9471	-28324.1823	-28324.3869
LMP2 6-31G*	ND	-28179.8915	-28241.2151	-28244.9035	-28245.2221	-28245.3799
Method	180°	210°	240°	270°	300°	330°
HF STO-3G	-27857.8689	-27857.8044	-27857.6421	-27857.4687	-27856.3942	-27844.5295
HF 3-21G(*)	-28049.1535	-28049.0845	-28048.9144	-28048.6159	-28045.8208	-28012.175
HF 3-21G(*)/SCRF	-28050.1132	-28050.0652	-28049.9741	-28049.7851	-28047.3591	-28017.4358
HF 6-31G*	-28196.3811	-28196.3123	-28196.1591	-28195.5614	-28187.7933	-28182.0586
HF 6-31G**	-28197.0117	-28196.9432	-28196.79	-28196.2065	-28188.645	-28182.7535
HF 6-31+G*	-28196.8868	-28196.8158	-28196.6614	-28196.1272	-28188.9884	-28182.1034
HF 6-311G*	-28200.759	-28200.6869	-28200.5295	-28199.9572	-28192.4177	-28186.1915
DFT 6-31G*	-28318.5131	-28318.4075	-28318.1792	-28317.8206	-28313.8811	-28285.6481
DFT 6-31G*/SCRF	-28314.7013	-28314.6475	-28314.5167	-28314.181	-28310.7173	-28251.5436
DFT 6-31G**	-28319.0584	-28318.9522	-28318.7225	-28318.3666	-28314.5802	-28286.1034
DFT 6-311G*	-28323.461	-28323.3492	-28323.1135	-28322.733	-28318.4064	-28291.8371
DFT 6-31+G*	-28319.3037	-28319.1901	-28318.9477	-28318.5495	-28314.0466	-28287.5868

DFT 6-311+G**	-28324.2536	-28324.338	-28324.0951	-28323.6812	-28318.7657	-28294.1522
LMP2 6-31G*	-28245.4483	-28245.3737	-28245.213	-28244.8942	-28241.1849	-28179.8353

ND stands for no data as explained in the text.

Table S7. Single-Point Energies (in eV) for Variation of the N1-C2-C4-N3 Dihedral Angle in 30° Increments

Method	0°	30°	60°	90°	120°	150°	180°	210°
AM1	0.93693	0.8628	0.8317	0.8283	0.7982	0.7652	0.7964	0.8503
PM3	0.87433	0.8079	0.7462	0.7483	0.7707	0.8139	0.8778	0.8664
MNDO	0.06962	-0.0161	-0.131	-0.163	-0.132	-0.0343	0.0746	0.0161
MMFF94 (Spartan)	1.50152	1.4672	1.4976	1.5415	1.4614	1.417	1.6089	1.5853
Sybyl (Spartan)	63.9101	2.8812	0.603	0.637	0.5685	0.495	0.6738	0.5187
AMBER*	7.56648	2.2678	2.0362	2.0921	2.0418	2.0054	2.2552	2.0323
OPLS/A	1.43886	0.3791	0.2529	0.2728	0.2069	0.2685	0.9161	0.3253
OPLS-AA	3.02911	3.0261	3.2668	3.2894	2.8539	2.3025	2.0843	2.3984
MMFF94 (MMod)	1.84054	1.7408	1.7321	1.6991	1.5386	1.4432	1.5894	1.6015
MMFF94s (MMod)	1.90084	1.7343	1.7069	1.667	1.5104	1.451	1.6466	1.6154
Tripos	64.2686	2.9669	0.6141	0.6479	0.5797	0.506	0.684	0.5304
MMFF94 (SYBYL)	1.97276	1.7719	1.7345	1.688	1.5221	1.4575	1.6592	1.6478
MMFF94s (SYBYL)	1.90179	1.7346	1.7071	1.6668	1.5101	1.4512	1.4737	1.6158
Method	240°	270°	300°	330°				
AM1	0.921	0.934	0.9221	0.9414				
PM3	0.8375	0.8085	0.7981	0.8397				
MNDO	-0.058	-0.088	-0.073	0.0079				
MMFF94 (Spartan)	1.6327	1.6941	1.6165	1.5172				
Sybyl (Spartan)	0.575	0.6373	0.5861	1.447				
AMBER*	2.0392	2.0943	2.0392	2.1693				
OPLS/A	0.2629	0.3232	0.321	0.6967				
OPLS-AA	3.0187	3.4091	3.361	3.1462				
MMFF94 (MMod)	1.736	1.9043	2.0136	2.0115				
MMFF94s (MMod)	1.7204	1.8883	2.0648	2.2383				
Tripos	0.5864	0.6482	0.5965	1.4389				
MMFF94 (SYBYL)	1.7613	1.9318	2.1257	2.4143				
MMFF94s (SYBYL)	1.7201	1.8883	2.0649	2.2403				

Method	0°	30°	60°	90°	120°	150°
HF STO-3G	-27856.6266	-27857.3208	-27857.6541	-27857.6748	-27857.7609	-27857.8684
HF 3-21G(*)	-28047.6816	-28048.3739	-28048.6345	-28048.641	-28048.7654	-28049.0223
HF 3-21G(*)/SCRF	ND	-27951.6799	-28035.0766	-28040.9491	-28043.3098	-28044.489
HF 6-31G*	-28196.1387	-28196.1925	-28196.2349	-28196.217	-28196.1646	-28196.0809
HF 6-31G**	-28196.7677	-28196.8193	-28196.8634	-28196.8461	-28196.793	-28196.7107
HF 6-31+G*	-28196.6042	-28196.6659	-28196.7245	-28196.7023	-28196.6399	-28196.5777
HF 6-311G*	-28200.5073	-28200.5587	-28200.608	-28200.5921	-28200.5358	-28200.4602
DFT 6-31G*	-28317.8339	-28317.8541	-28318.148	-28318.1711	-28318.2418	-28318.4046
DFT 6-31G*/SCRF	ND	-28228.1222	-28307.0277	-28311.9923	-28313.7025	-28314.6084
DFT 6-31G**	-28318.3601	-28318.4091	-28318.6961	-28318.7151	-28318.7844	-28318.9485
DFT 6-311G*	-28322.8154	-28322.7775	-28323.0838	-28323.1309	-28323.2056	-28323.3565
DFT 6-31+G*	-28318.6653	-28318.6617	-28318.9722	-28319.0282	-28319.0944	-28319.2154
DFT 6-311+G**	-28323.8296	-28323.8064	-28324.1206	-28324.1813	-28324.2467	-28324.3645
LMP2 6-31G*	ND	-28155.6585	-28237.2165	-28242.4597	-28244.4923	-28245.4115
Method	180°	210°	240°	270°	300°	330°
HF STO-3G	-27857.7324	-27857.619	-27857.6338	-27857.62	-27857.6342	-27857.4182
HF 3-21G(*)	-28049.1535	-28049.0189	-28048.763	-28048.6402	-28048.6331	-28048.3664
HF 3-21G(*)/SCRF	-28044.8086	-28044.5052	-28043.3393	-28040.9874	-28034.1015	-27887.4518
HF 6-31G*	-28196.1869	-28196.3706	-28196.3499	-28196.2986	-28196.3274	-28196.2755
HF 6-31G**	-28196.819	-28197.0017	-28196.98	-28196.9286	-28196.9571	-28196.9068
HF 6-31+G*	-28196.7102	-28196.8798	-28196.8537	-28196.8017	-28196.8233	-28196.7626
HF 6-311G*	-28200.5764	-28200.7517	-28200.7231	-28200.6719	-28200.7	-28200.6491
DFT 6-31G*	-28318.5055	-28318.4709	-28318.2854	-28318.1601	-28318.1856	-28318.1634
DFT 6-31G*/SCRF	-28314.7016	-28314.6275	-28313.7428	-28312.0087	-28306.1715	-28167.7551
DFT 6-31G**	-28319.0502	-28319.0143	-28318.8266	-28318.7032	-28318.7303	-28318.7022
DFT 6-311G*	-28323.4512	-28323.2558	-28323.1291	-28323.1428	-28323.1155	-28323.1155
DFT 6-31+G*	-28319.2916	-28319.2826	-28319.136	-28319.0313	-28319.0371	-28318.9814

DFT 6-311+G**	-28324.4401	-28324.4437	-28324.2983	-28324.1893	-28324.1935	-28324.1353
LMP2 6-31G*	-28245.4483	-28245.4234	-28244.5179	-28242.4956	-28236.3646	-28093.0216

ND stands for no data as explained in the text.

Table S8. Single-Point Energies (in eV) for Variation of the O2-C4-C5-C2 Dihedral Angle in 30° Increments

Method	0°	30°	60°	90°	120°	150°	180°	210°	240°	270°
AM1	1.17737	1.1166	0.9016	0.854	0.8557	1.0455	1.7218	1.5082	0.8506	0.777
PM3	0.88748	0.8903	0.8604	0.8328	0.8405	0.9065	0.9101	0.8449	0.7783	0.7451
MNDO	0.07682	0.0466	-0.035	-0.065	-0.008	0.1045	0.1601	0.0781	-0.086	-0.161
MMFF94 (Spartan)	1.54037	1.5977	1.5846	1.576	1.5893	1.6281	1.6023	1.5096	1.4712	1.4331
Sybyl (Spartan)	0.48665	0.543	0.6518	0.7093	0.6471	0.5351	0.4932	0.5367	0.6455	0.7091
AMBER*	1.61324	1.6805	1.7924	1.8579	1.8019	1.6865	1.6375	1.6865	1.7846	1.8345
OPLS/A	0.20995	0.2789	0.3566	0.3978	0.36	0.2711	0.1969	0.2013	0.2746	0.3141
OPLS-AA	1.85095	1.8514	1.9551	2.1212	2.1824	2.1173	2.0861	2.1598	2.2097	2.1212
MMFF94 (MMod)	1.58201	1.6024	1.5768	1.5868	1.6332	1.723	1.7507	1.5547	1.4419	1.4454
MMFF94s (MMod)	1.5391	1.5764	1.5673	1.5729	1.5989	1.6471	1.6263	1.4814	1.4393	1.4406
Tripes	0.49989	0.55628	0.6646	0.72155	0.65874	0.54613	0.50432	0.54817	0.6574	0.72129
MMFF94 (SYBYL)	1.58366	1.5986	1.5761	1.5849	1.6238	1.6909	1.6923	1.5162	1.4467	1.4676
MMFF94s (SYBYL)	1.5385	1.5763	1.5676	1.5733	1.5991	1.6472	1.6263	1.4812	1.4391	1.4403
Method	300°	330°								
AM1	0.8162	0.9481								
PM3	0.7517	0.814								
MNDO	-0.133	-0.024								
MMFF94 (Spartan)	1.4059	1.4397								
Sybyl (Spartan)	0.6505	0.5349								
AMBER*	1.7664	1.6492								
OPLS/A	0.2724	0.2078								
OPLS-AA	1.959	1.8648								
MMFF94 (MMod)	1.454	1.5005								
MMFF94s (MMod)	1.4345	1.4649								
Tripes	0.66282	0.54756								
MMFF94 (SYBYL)	1.4799	1.5188								
MMFF94s (SYBYL)	1.4341	1.4643								

Method	0°	30°	60°	90°	120°	150°
HF STO-3G	-27857.735	-27857.6658	-27857.6473	-27857.6627	-27857.7427	-27858.0445
HF 3-21G(*)	-28048.9226	-28048.9084	-28048.8339	-28048.7738	-28048.8499	-28049.0148
HF 3-21G(*)/SCRF	ND	-27951.7909	-28030.7669	-28038.0127	-28042.2192	-28044.1478
HF 6-31G*	-28196.2529	-28196.3779	-28196.3323	-28196.2172	-28196.156	-28196.0728
HF 6-31G**	-28196.881	-28197.008	-28196.9642	-28196.8498	-28196.7879	-28196.7067
HF 6-31+G*	-28196.7192	-28196.8738	-28196.858	-28196.7474	-28196.6541	-28196.5208
HF 6-311G*	-28200.6241	-28200.7551	-28200.7165	-28200.6074	-28200.5333	-28200.4265
DFT 6-31G*	-28318.3738	-28318.4041	-28318.3811	-28318.3402	-28318.3995	-28318.5111
DFT 6-31G*/SCRF	ND	-28224.8286	-28302.9174	-28309.3836	-28312.5137	-28314.0435
DFT 6-31G**	-28318.9175	-28318.9468	-28318.9218	-28318.8793	-28318.9385	-28319.0537
DFT 6-311G*	-28323.3337	-28323.3721	-28323.3589	-28323.3283	-28323.3756	-28323.462
DFT 6-31+G*	-28319.1778	-28319.2331	-28319.2398	-28319.2091	-28319.2362	-28319.3042
DFT 6-311+G**	-28324.3349	-28324.393	-28324.3977	-28324.3639	-28324.3892	-28324.4594
LMP2 6-31G*	ND	-28152.2123	-28233.0056	-28239.9126	-28243.2612	-28244.8466
Method	180°	210°	240°	270°	300°	330°
HF STO-3G	-27857.8092	-27857.6338	-27857.6295	-27857.6618	-27857.7415	-27857.7985
HF 3-21G(*)	-28049.1535	-28049.016	-28048.8503	-28048.7746	-28048.8358	-28048.9106
HF 3-21G(*)/SCRF	-28044.811	-28044.5089	-28042.5218	-28035.8091	-28025.8653	-27952.6559
HF 6-31G*	-28196.019	-28196.1566	-28196.1637	-28196.1037	-28196.089	-28196.1124
HF 6-31G**	-28196.6482	-28196.7881	-28196.7974	-28196.7371	-28196.7208	-28196.7413
HF 6-31+G*	-28196.4655	-28196.653	-28196.6908	-28196.6341	-28196.5894	-28196.5778
HF 6-311G*	-28200.3671	-28200.5342	-28200.5511	-28200.4944	-28200.4661	-28200.4801
DFT 6-31G*	-28318.4243	-28318.3429	-28318.3142	-28318.3013	-28318.3538	-28318.3837
DFT 6-31G*/SCRF	-28314.7013	-28314.5911	-28312.9678	-28307.1073	-28298.434	-28226.0983
DFT 6-31G**	-28318.9772	-28318.8908	-28318.8575	-28318.8425	-28318.8945	-28318.9256
DFT 6-311G*	-28323.3558	-28323.2995	-28323.288	-28323.2819	-28323.3227	-28323.3395
DFT 6-31+G*	-28319.2107	-28319.1622	-28319.1614	-28319.1561	-28319.1783	-28319.1756

DFT 6-311+G**	-28324.3491	-28324.308	-28324.316	-28324.31	-28324.3283	-28324.3262
LMP2 6-31G*	-28245.4483	-28245.323	-28243.702	-28237.8767	-28228.1617	-28153.5788

ND stands for no data as explained in the text.