Supplementary Information for

Inner Reorganization Limiting Electron Transfer during Electrochemically Controlled Hydrogen Bonding: Intra vs Intermolecular Effects

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Internal coordinates obtained for the minimum energy conformers for the neutral and anion radicals of Metronidazole at the BHandHLYP/6-311++G(2d,2p) level considering solvation by the Cramer and Truhlar model in Z-matrix

Conformer A, Oxidized Species

Atom Number	Symbol	NA	Bond	NB	Angle	NC	Dihedral
1	C						
2	N	1	1.3786256				
3	N	1	2.2053741	2	71.9529657		
4	C	3	1.3238289	1	70.6215763	2	0.0097733
5	C	3	1.3399138	1	35.7557852	2	-179.928803
6	H	5	1.0684411	3	123.244465	1	179.753043
7	N	1	1.397828	5	126.419655	3	178.695524
8	O	7	1.2171153	1	119.630323	5	-178.044437
9	O	7	1.2141543	1	117.246234	5	1.5330409
10	C	2	1.4606301	1	129.88435	5	-178.730432
11	H	10	1.0794315	2	107.288217	1	-151.008064
12	H	10	1.0756163	2	108.510482	1	-34.6526376
13	C	4	1.4789519	3	124.223552	1	-179.492044
14	H	13	1.0837872	4	110.951615	3	115.914889
15	H	13	1.0824828	4	111.324294	3	-123.814766
16	H	13	1.0791078	4	108.715534	3	-3.6980391
17	C	10	1.5131564	2	112.957769	1	89.0329196
18	H	17	1.0808815	10	110.299262	2	57.9794697
19	H	17	1.0861596	10	107.366298	2	175.316082
20	O	17	1.4068845	10	113.65058	2	-61.4419025
21	H	20	0.9523915	17	109.198891	10	-53.4411201

Conformer A, Reduced Species

Atom Number	Symbol	NA	Bond	NB	Angle	NC	Dihedral
1	C						
2	N	1	1.3816531				
3	N	2	2.2063235	1	72.893768		
4	C	3	1.3046771	2	34.8891704	1	179.996068
5	C	3	1.3665296	2	71.5309494	1	0.0422071
6	H	5	1.0668978	3	123.002315	2	-179.750616
7	N	1	1.3723397	5	127.956573	3	-179.533413
8	O	7	1.2985133	1	120.555561	5	172.649113
9	O	7	1.2762598	1	117.926538	5	-4.05966
10	C	2	1.4561613	1	129.417988	5	178.758128
11	H	10	1.0799105	2	107.618606	1	-152.3643
12	H	10	1.0766255	2	108.332982	1	-35.7513368
13	C	4	1.4836649	3	124.852713	2	-178.566712
14	H	13	1.0845439	4	111.493129	3	114.546945
15	H	13	1.0831874	4	111.990442	3	-124.710689
16	H	13	1.0800169	4	108.599283	3	-4.7805473
17	C	10	1.5148899	2	113.805832	1	87.3630095
18	H	17	1.0849477	10	109.700926	2	60.1019438
19	H	17	1.088452	10	106.931803	2	176.175696
20	O	17	1.4020185	10	113.850372	2	-61.4417155
21	H	20	0.9741326	17	108.400791	10	-17.2381477

Conformer B, Oxidized Species

Atom number	Symbol	NA	Bond	NB	Angle	NC	Dihedral
1	C						
2	N	1	1.3791218				
3	N	1	2.2044369	2	71.9463923		
4	C	3	1.3233567	1	70.6992703	2	0.0767602
5	C	3	1.3406977	1	35.7469073	2	-179.808886
6	H	5	1.0684652	3	123.208459	1	-179.926352
7	N	1	1.3981413	5	127.014386	3	179.643498
8	O	7	1.2148611	1	119.160402	5	179.491888
9	O	7	1.2148912	1	117.355717	5	-0.4332788
10	C	2	1.4579328	1	129.71133	5	-178.873292
11	H	10	1.0794023	2	106.997143	1	-157.757454
12	H	10	1.0759029	2	109.136212	1	-40.7328193
13	C	4	1.4793746	3	124.12199	1	-179.796244
14	H	13	1.0834899	4	111.067439	3	116.704899
15	H	13	1.0826353	4	111.32074	3	-122.894968
16	H	13	1.0791205	4	108.676709	3	-2.8997354
17	C	10	1.5180085	2	111.6788	1	81.8898689
18	H	17	1.0801124	10	110.197065	2	-63.6557985
19	H	17	1.0849147	10	109.877498	2	55.4263684
20	O	17	1.4068759	10	110.658976	2	178.558014
21	H	20	0.9523743	17	109.272353	10	-72.1088562

Conformer B, Reduced Species

Atom number	Symbol	NA	Bond	NB	Angle	NC	Dihedral
1	C						
2	N	1	1.3831265				
3	N	2	2.2060102	1	73.0308247		
4	C	3	1.3036573	2	34.9503356	1	-179.71157
5	C	3	1.3682967	2	71.4982701	1	0.1468454
6	H	5	1.0668075	3	122.943259	2	179.82598
7	N	1	1.3700176	5	128.328915	3	179.865078
8	O	7	1.2845498	1	120.61784	5	-178.938567
9	O	7	1.2859062	1	117.311692	5	0.8438581
10	C	2	1.4520501	1	129.252519	5	-177.904676
11	H	10	1.0797791	2	107.788411	1	-156.904682
12	H	10	1.0761098	2	108.752928	1	-38.8880023
13	C	4	1.4834565	3	124.936865	2	-179.575873
14	H	13	1.0842564	4	111.720773	3	117.257988
15	H	13	1.0837348	4	111.84694	3	-121.973297
16	H	13	1.0800747	4	108.608527	3	-2.2394214
17	C	10	1.5161293	2	111.934096	1	82.4972317
18	H	17	1.0828934	10	109.683436	2	-58.4874742
19	H	17	1.0820814	10	110.190722	2	60.8165554
20	O	17	1.4114537	10	110.963941	2	178.558244
21	H	20	0.952243	17	108.854567	10	71.475069

Conformer C, Oxidized Species

Atom number	Symbol	NA	Bond	NB	Angle	NC	Dihedral
1	C						
2	N	1	1.37972				
3	N	1	2.2037567	2	71.9982036		
4	C	3	1.3240979	1	70.7315694	2	-0.1647119
5	C	3	1.3401577	1	35.7596604	2	179.941017
6	H	5	1.0685474	3	123.252482	1	179.791511
7	N	1	1.3976836	5	126.837844	3	178.544098
8	O	7	1.215098	1	119.223273	5	-178.752938
9	O	7	1.2149724	1	117.32375	5	1.1196288
10	C	2	1.4602324	1	129.536937	5	-179.803971
11	H	10	1.0781285	2	106.519179	1	-160.280639
12	H	10	1.0770971	2	109.080193	1	-43.6448083
13	C	4	1.4802653	3	123.839478	1	-179.178136
14	H	13	1.0836074	4	111.053081	3	116.676627
15	H	13	1.0817319	4	111.331988	3	-122.888553
16	H	13	1.07925	4	108.521398	3	-2.7379911
17	C	10	1.5141401	2	113.258498	1	79.1104686
18	H	17	1.0819671	10	107.38094	2	176.543389
19	H	17	1.082158	10	110.672294	2	-65.8668327
20	O	17	1.4100673	10	112.673901	2	58.5581579
21	H	20	0.9512786	17	109.352215	10	-86.7476866

Conformer C, Reduced Species

Atom number	Symbol	NA	Angle	NB	Bond	NC	Dihedral
1	C						
2	N	1			1.3788461		
3	N	2	72.5807643	1	2.2057777		
4	C	3	34.848522	2	1.3061228	1	179.595037
5	C	1	106.477197	2	1.3525931	4	0.3917429
6	H	5	127.499676	1	1.0688762	2	178.911706
7	N	1	128.616528	5	1.4064017	3	-176.685029
8	O	7	116.851985	1	1.3105366	5	104.481663
9	O	7	117.165786	1	1.2789181	5	-49.8744238
10	C	2	131.018322	1	1.4636911	5	168.569549
11	H	10	106.479848	2	1.0794795	1	154.058967
12	H	10	108.601254	2	1.0846666	1	-89.9194904
13	C	4	124.588296	3	1.4838615	2	-178.065987
14	H	13	111.606196	4	1.0840733	3	116.615172
15	H	13	111.954557	4	1.0834913	3	-122.586768
16	H	13	108.508703	4	1.0800445	3	-2.8178376
17	C	10	116.797206	2	1.5114483	1	32.9259736
18	H	17	105.928184	10	1.0839912	2	177.512343
19	H	17	110.762612	10	1.0839408	2	-66.5976049
20	O	17	113.391705	10	1.3979922	2	58.5581981
21	H	20	104.393252	17	0.9750533	10	-85.5810684

Values of the total energies required for calculation of the inner reorganization component $\lambda_{i,j}$ for the obtained conformers.

	Zero Point Corrected Energies / eV *			
Conformer	**N as N**	**A as N**	**N as A**	**A as A**
A	-16349.0315	-16351.6285	-16348.6133	-16352.1553
B	-16349.0153	-16351.5684	-16348.6732	-16351.9399
C	-16349.0248	-16351.5761	-16347.8187	-16351.8535

* Notation represents values of single point calculations of a given electronic configuration in a reference optimized structure, N: neutral, A: Anion.