

Initial stage of the degradation of three common neonicotinoids:
Theoretical prediction of charge transfer sites.
Electronic Supplementary Information

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Table 1: Relative energies, in kcal/mol, of the eight minima found for the imidacloprid. Relative energies with the ZPE are reported in parenthesis.

6-311G(3df,3pd)						6-311G(2d,2p)					
	HF	MP2	B3LYP	PBE0	PBE		HF	MP2	B3LYP	PBE0	PBE
IMI-1	0.0 (0.0)	0.0	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	IMI-1	0.0 (0.0)	0.0	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
IMI-2	0.0 (0.0)	0.0	0.0 (-0.1)	0.0 (0.0)	0.0 (0.3)	IMI-2	0.0 (0.0)	0.0	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
IMI-3	1.5 (0.4)	1.5	1.3 (1.2)	1.3 (1.2)	1.2 (1.5)	IMI-3	1.5 (1.4)	1.5	1.3 (1.3)	1.4 (1.3)	1.3 (1.2)
IMI-4	1.4 (1.4)	1.5	1.3 (1.3)	1.3 (1.6)	1.2 (1.4)	IMI-4	1.5 (1.4)	1.5	1.3 (1.3)	1.4 (1.3)	1.3 (1.2)
IMI-5	0.6 (0.4)	2.4	0.5 (0.4)	0.7 (0.5)	0.6 (0.7)	IMI-5	0.6 (0.4)	2.3	0.6 (0.4)	0.7 (0.5)	0.6 (0.4)
IMI-6	0.6 (0.4)	2.4	0.5 (0.3)	0.7 (0.5)	0.6 (0.7)	IMI-6	0.6 (0.4)	2.3	0.6 (0.4)	0.7 (0.5)	0.6 (0.4)
IMI-7	1.6 (1.4)	3.0	1.3 (1.1)	1.4 (1.5)	1.3 (1.3)	IMI-7	1.5 (1.3)	2.9	1.3 (1.0)	1.3 (1.1)	1.3 (1.0)
IMI-8	1.5 (1.4)	3.0	1.3 (1.2)	1.3 (1.2)	1.2 (1.5)	IMI-8	1.5 (1.3)	2.9	1.3 (1.0)	1.3 (1.1)	1.3 (1.0)
6-311G(d,p)						6-311++G(d,p)					
	HF	MP2	B3LYP	PBE0	PBE		HF	MP2	B3LYP	PBE0	PBE
IMI-1	0.0 (0.0)	0.0	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	IMI-1	0.0 (0.0)	0.0	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
IMI-2	0.0 (0.0)	0.0	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	IMI-2	0.0 (0.0)	0.0	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
IMI-3	1.6 (1.5)	1.5	1.4 (1.3)	1.4 (1.4)	1.4 (1.2)	IMI-3	1.5 (1.4)	1.5	1.3 (1.3)	1.4 (1.3)	1.3 (1.2)
IMI-4	1.6 (1.5)	1.5	1.4 (1.3)	1.4 (1.4)	1.4 (1.2)	IMI-4	1.5 (1.4)	1.5	1.3 (1.3)	1.4 (1.3)	1.3 (1.2)
IMI-5	0.7 (0.5)	2.1	0.7 (0.4)	0.8 (0.6)	0.8 (0.5)	IMI-5	0.6 (0.4)	2.3	0.6 (0.4)	0.7 (0.5)	0.6 (0.4)
IMI-6	0.7 (0.5)	2.1	0.7 (0.4)	0.8 (0.6)	0.8 (0.5)	IMI-6	0.6 (0.4)	2.3	0.6 (0.4)	0.7 (0.5)	0.6 (0.4)
IMI-7	1.6 (1.4)	2.7	1.4 (1.1)	1.5 (1.2)	1.4 (1.1)	IMI-7	1.5 (1.3)	2.9	1.3 (1.0)	1.3 (1.1)	1.3 (1.0)
IMI-8	1.6 (1.4)	2.7	1.4 (1.1)	1.5 (1.2)	1.4 (1.1)	IMI-8	1.5 (1.3)	2.9	1.3 (1.0)	1.3 (1.1)	1.3 (1.0)

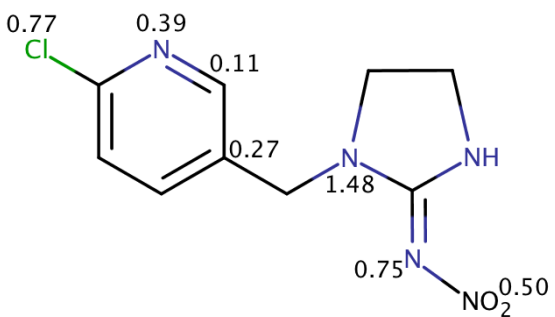
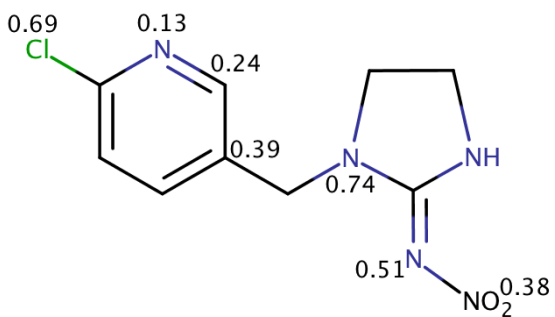
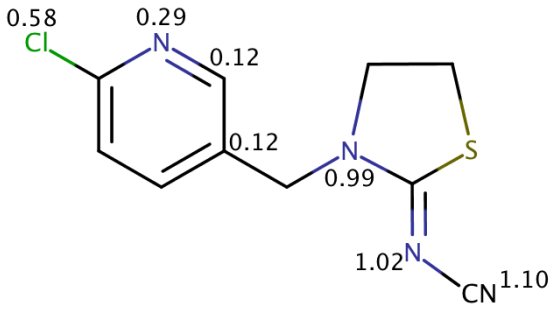
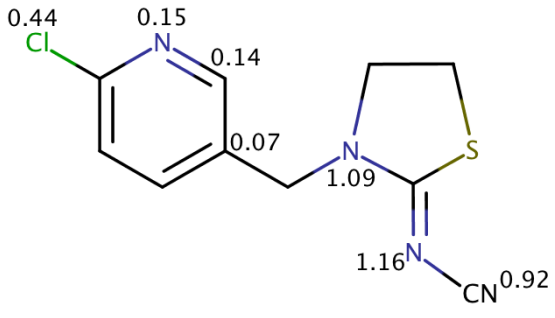
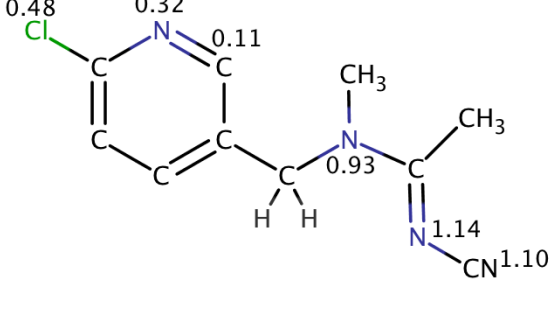
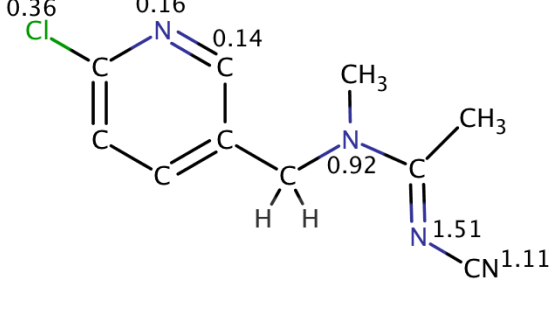
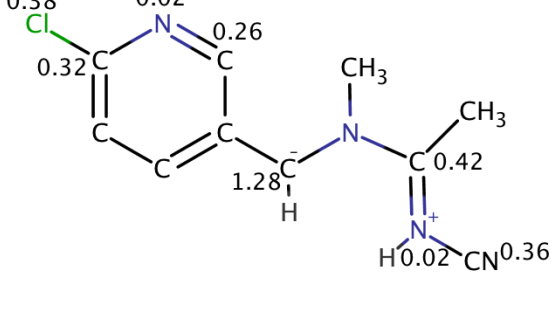
Table 2: Relative energies, in kcal/mol, for all minima found for thiacloprid and acetamiprid. Relative energies corrected by ZPE are reported in parenthesis

Conf.	6-311G(d,p)		6-311++G(d,p)		Conf.	6-311G(d,p)		6-311++G(d,p)	
	PBE0	MP2	PBE0	MP2		PBE0	MP2	PBE0	MP2
THIA-1	0.0 (0.0)	0.0	0.0 (0.0)	0.0	ACE-1	0.0(0.0)	0.0	0.0 (0.0)	0.0
THIA-2	0.3 (0.2)	1.4	0.3 (0.3)	1.4	ACE-2	0.0(0.0)	0.0	0.0 (0.2)	0.0
THIA-3	1.0 (0.8)	2.0	1.0 (0.9)	2.0	ACE-3	1.2(1.1)	0.9	1.2 (1.5)	1.3
THIA-4	1.3 (1.2)	1.3	1.3 (1.2)	1.3	ACE-4	1.2(1.1)	0.9	1.2 (1.2)	1.3

Table 3: Ionization potential and electron affinity obtained for the eight conformers of the imidacloprid. All quantities are in eV.

Conformer	I		A		Conformer	I		A	
	6-311G(3df,3pd)					6-311G(2d,2p)			
	PBE	PBE0	PBE	PBE0		PBE	PBE0	PBE	PBE0
IMI-1	8.15	8.83	0.34	0.03	IMI-1	8.13	8.80	0.30	-0.03
IMI-2	8.28	8.83	0.34	0.03	IMI-2	8.13	8.80	0.30	-0.03
IMI-3	8.14	8.80	0.26	-0.09	IMI-3	8.12	8.77	0.22	-0.14
IMI-4	8.21	8.80	0.26	-0.07	IMI-4	8.12	8.77	0.22	-0.14
IMI-5	8.15	8.84	0.38	0.04	IMI-5	8.14	8.81	0.33	-0.03
IMI-6	8.15	8.84	0.38	0.04	IMI-6	8.15	8.81	0.33	-0.03
IMI-7	8.07	8.77	0.37	0.02	IMI-7	8.07	8.74	0.32	-0.04
IMI-8	8.15	8.77	0.26	0.02	IMI-8	8.06	8.74	0.32	-0.04
	6-311G(d,p)					6-311++G(d,p)			
	PBE	PBE0	PBE	PBE0		PBE	PBE0	PBE	PBE0
IMI-1	8.19	8.87	0.32	0.00	IMI-1	8.32	8.96	0.67	0.30
IMI-2	8.19	8.87	0.32	0.00	IMI-2	8.32	8.96	0.67	0.30
IMI-3	8.18	8.84	0.26	-0.10	IMI-3	8.30	8.92	0.62	0.25
IMI-4	8.18	8.84	0.26	-0.10	IMI-4	8.30	8.92	0.62	0.25
IMI-5	8.19	8.88	0.38	0.02	IMI-5	8.31	8.96	0.63	0.23
IMI-6	8.19	8.88	0.38	0.02	IMI-6	8.31	8.96	0.63	0.23
IMI-7	8.12	8.81	0.36	0.00	IMI-7	8.23	8.88	0.69	0.30
IMI-8	8.12	8.81	0.36	0.00	IMI-8	8.23	8.88	0.69	0.30

Table 4: Sites where $\omega_{\Omega}^{-} > 0$ for imidacloprid (IMI), thiacloprid (THIA) and acetamiprid (ACE), free and solvated.

 IMI_free	 IMI_sol
 THIA_free	 THIA_sol
 ACE_free	 ACE_sol
	 ACE-Tautomer

IMI-1				IMI-2			
Cl	-3.97684269	1.85722284	-2.37629833	Cl	0.83540005	2.95238201	-3.91615144
C	-2.38161201	1.62015996	-1.72131908	C	0.18474738	2.26249846	-2.45646253
N	-1.85932981	2.62769205	-1.06130379	N	0.03529027	3.07468991	-1.43591251
C	-0.63867405	2.4540095	-0.55334249	C	-0.45981797	2.55420082	-0.31246391
C	0.09880071	1.282725	-0.67655707	C	-0.81620644	1.21963555	-0.16116518
C	-0.484498	0.23249252	-1.39157163	C	-0.65060164	0.38429972	-1.26988074
C	-1.74860619	0.39585662	-1.92902191	C	-0.14197707	0.90755918	-2.44505021
H	-0.22541636	3.31035938	-0.02235116	H	-0.58490593	3.25339442	0.51309612
C	1.46397571	1.15061471	-0.05076051	C	-1.34523652	0.69708665	1.15027619
H	0.05777786	-0.69948154	-1.52082614	H	-0.92318875	-0.66466645	-1.20120114
H	-2.23455829	-0.38903618	-2.4948457	H	-0.00352527	0.29778644	-3.32900197
H	1.88052533	2.14156826	0.1535812	H	-2.17277432	0.00625629	0.9815933
N	1.46439792	0.41162686	1.19999127	N	-0.35419252	-0.01544588	1.93801514
H	2.14625751	0.63174065	-0.72585767	H	-1.71656601	1.52514416	1.76158332
C	0.8200919	0.92313358	2.40047735	C	0.79782304	0.65572323	2.52135765
C	1.05161848	-0.2200035	3.38939011	C	1.53570528	-0.50925201	3.18226073
N	1.17048708	-1.35484624	2.49038994	N	1.09155695	-1.62694305	2.36763655
H	1.41700249	-2.29845472	2.75646944	H	1.29417685	-2.60251733	2.53835896
C	1.51617725	-0.94588223	1.25529116	C	-0.06599269	-1.33047116	1.74776421
H	-0.25077577	1.09357972	2.22476804	H	0.48545243	1.42020499	3.23597151
H	1.27810681	1.86113343	2.72149943	H	1.40877819	1.12902665	1.74070903
H	0.2221599	-0.34830358	4.085962	H	1.22475938	-0.63764661	4.22619014
H	1.97721746	-0.07314754	3.95918931	H	2.61986956	-0.39541759	3.14596954
N	1.82951771	-1.61475192	0.16162857	N	-0.87759252	-2.05741925	1.00308868
N	1.98014481	-2.96868697	0.26641444	N	-0.6268467	-3.39745216	0.91233215
O	2.11613708	-3.55500609	-0.78333839	O	-1.29962339	-3.99412653	0.10264091
O	1.98862139	-3.53185968	1.36580245	O	0.22073899	-3.94314654	1.62627639

IMI-3				IMI-4			
Cl	1.62944258	2.6923636	-3.85259716	Cl	-2.53090906	0.64843267	-4.23312818
C	0.59098257	1.94256296	-2.67347984	C	-1.691979	0.95294304	-2.73843073
N	0.85169931	0.6914065	-2.36723668	N	-0.59308031	0.26389559	-2.52674726
C	0.06922244	0.10128619	-1.46505438	C	0.0616758	0.48166804	-1.38729217
C	-0.99775405	0.73899411	-0.83207883	C	-0.35860533	1.39012629	-0.41581438
C	-1.2494912	2.06213295	-1.18845404	C	-1.52292613	2.1087251	-0.67866914
C	-0.44765189	2.69020458	-2.12792244	C	-2.21442752	1.89739999	-1.86066427
H	0.29851029	-0.9363227	-1.23365657	H	0.97252859	-0.09340815	-1.23770355
C	-1.82870825	0.01702402	0.20000249	C	0.41907668	1.5686697	0.86491257
H	-2.07927938	2.60233602	-0.73975974	H	-1.88706339	2.84276334	0.03567141
H	-0.61472201	3.71523142	-2.43388687	H	-3.11990051	2.43952109	-2.10239255
H	-2.04958555	-0.99999276	-0.12815989	H	0.13942838	2.51280629	1.34288822
N	-1.18237161	-0.09544461	1.49442879	N	0.20855868	0.50402663	1.82830983
H	-2.77982564	0.53896938	0.3450138	H	1.49086453	1.59871062	0.66200304
C	-0.82801294	1.07088303	2.28811516	C	-1.09638797	0.23193375	2.41041571
C	-0.14694955	0.43104954	3.49889436	C	-0.79893322	-0.98065075	3.29380182
N	0.32777886	-0.81862621	2.93222159	N	0.35035876	-1.5528753	2.61568446
H	0.76823652	-1.57335119	3.44079964	H	0.9034258	-2.33512718	2.93893451
C	-0.3762577	-1.13923633	1.83071337	C	0.96797556	-0.6249765	1.86110751
H	-1.71639987	1.6468451	2.55714355	H	-1.82855418	-0.00956507	1.62786569
H	-0.13764685	1.7223171	1.73511724	H	-1.45924144	1.09127916	2.97892963
H	-0.86337517	0.2471614	4.30886142	H	-1.63037218	-1.6856276	3.33357388
H	0.6772651	1.03282776	3.88412429	H	-0.54008263	-0.67634371	4.31532613
N	-0.37658216	-2.21362523	1.0663852	N	2.09196388	-0.65438844	1.17241833
N	0.35100057	-3.29261787	1.48524458	N	2.89496821	-1.75204388	1.31183961
O	0.41675767	-4.20764591	0.69777482	O	3.85168904	-1.78850004	0.57356339
O	0.8823919	-3.3154927	2.60077664	O	2.64945369	-2.62545369	2.15098758

IMI-5				IMI-6			
Cl	-3.58538506	3.43642794	-2.23648818	Cl	0.90628653	3.6418524	-3.94531316
C	-2.23284478	2.59921735	-1.52981087	C	0.34174436	2.6583191	-2.62486119
N	-1.44246398	3.30104151	-0.75335131	N	-0.28070478	3.27686684	-1.65012964
C	-0.40485908	2.66647127	-0.20433113	C	-0.71392627	2.53116965	-0.63179854
C	-0.1193624	1.32293388	-0.40587452	C	-0.54434813	1.15592476	-0.54723295
C	-0.98179892	0.60586031	-1.23777662	C	0.12303551	0.52991825	-1.60212723
C	-2.06148307	1.24513645	-1.81746638	C	0.57814741	1.28427093	-2.66713304
H	0.23494184	3.27405972	0.433149	H	-1.22881195	3.07062729	0.16115699
C	1.07394079	0.66808375	0.23472857	C	-1.06573145	0.3700198	0.62480881
H	-0.80173351	-0.44794683	-1.42970819	H	0.27989787	-0.54474672	-1.58565522
H	-2.75030336	0.72774666	-2.47332432	H	1.09431606	0.83765494	-3.50762126
H	1.64484609	1.41237417	0.80731757	H	-1.77034511	-0.39763035	0.29575896
N	0.69231047	-0.4281599	1.09894836	N	-0.00614736	-0.31650623	1.33212327
H	1.74197714	0.25097891	-0.52277223	H	-1.60077614	1.03864957	1.31357278
C	0.07275152	-0.1945774	2.39377607	C	0.93143207	0.40240275	2.18009001
C	-0.06099922	-1.61560418	2.94094341	C	1.77892776	-0.73527206	2.74938669
N	1.00253281	-2.29942023	2.22613102	N	0.85548653	-1.85291216	2.6607948
H	1.19422911	-3.2920036	2.25100371	H	1.06879737	-2.81929986	2.8686189
C	1.32480814	-1.63383804	1.10100066	C	-0.09610233	-1.61260991	1.73907531
H	-0.88695661	0.31459543	2.28721888	H	0.39168343	0.94025401	2.97318006
H	0.73045014	0.42116196	3.02457374	H	1.51472813	1.12264459	1.60329827
H	-1.03874784	-2.04710699	2.69435794	H	2.08953443	-0.55412997	3.77919587
H	0.08602195	-1.66655197	4.0205617	H	2.66996986	-0.91411913	2.13534401
N	2.11515951	-1.93772786	0.09121334	N	-1.04192629	-2.37439775	1.22739362
N	2.65991063	-3.19067328	0.0621041	N	-1.05239748	-3.6966643	1.57225864
O	3.45390153	-3.38844963	-0.82774891	O	-1.99438915	-4.33126931	1.1583566
O	2.33662965	-4.05157011	0.88847241	O	-0.14303709	-4.19207876	2.24765447

IMI-7				IMI-8			
Cl	-3.17450071	1.18648686	-4.25247197	Cl	1.36585062	3.51896702	-3.91433892
C	-2.07459911	1.17701233	-2.90359369	C	0.57372126	2.4713202	-2.77256033
N	-1.67681663	0.00047615	-2.47297914	N	1.33599516	1.61939983	-2.12371538
C	-0.83542837	-0.02343861	-1.44104803	C	0.74469515	0.8116654	-1.24535711
C	-0.36540744	1.11660446	-0.79433202	C	-0.62064664	0.82531834	-0.9728434
C	-0.81038696	2.34564822	-1.27501967	C	-1.39716911	1.7428063	-1.67644081
C	-1.67869183	2.39192069	-2.35353976	C	-0.80219367	2.58527971	-2.60124142
H	-0.52072994	-1.00893072	-1.10647701	H	1.39757936	0.11549809	-0.72459
C	0.60847536	1.02247069	0.35093091	C	-1.23380277	-0.13489011	0.01259428
H	-0.47879627	3.26914537	-0.80806885	H	-2.46846593	1.80038518	-1.50369242
H	-2.04535233	3.32835169	-2.75449713	H	-1.37353133	3.31027828	-3.16699735
H	0.67317834	1.99478456	0.86101496	H	-1.31904275	-1.13502149	-0.42149875
N	0.24948359	-0.01103631	1.29486796	N	-0.44208326	-0.27287988	1.21327793
H	1.61157303	0.77985436	-0.01066882	H	-2.25135711	0.1967145	0.26639266
C	-0.92582745	0.11329867	2.14376656	C	-0.32282558	0.81631845	2.17097626
C	-0.82084738	-1.14087011	3.01007007	C	0.50023268	0.16753674	3.282924
N	0.6106775	-1.38409654	2.98532044	N	0.16115117	-1.23350545	3.10712354
H	1.08714655	-2.17987383	3.38801671	H	0.56281067	-2.01216361	3.61185504
C	1.17446985	-0.80174947	1.91052681	C	-0.2786309	-1.46464225	1.8561041
H	-1.84092439	0.14723868	1.54996019	H	-1.31761354	1.11963436	2.52918748
H	-0.86286117	1.02901525	2.75005886	H	0.16964932	1.682172	1.72495221
H	-1.36918951	-1.97964436	2.56426928	H	0.22227664	0.52409292	4.27560367
H	-1.18163688	-0.98198841	4.02710622	H	1.57383048	0.33368778	3.13233287
N	2.39507946	-0.85094365	1.41907631	N	-0.58036742	-2.57624271	1.21813694
N	3.27693399	-1.72640247	1.98991154	N	-0.31259351	-3.76258308	1.84360565
O	4.41237737	-1.6554526	1.58191127	O	-0.70813912	-4.74980353	1.26951008
O	2.91253451	-2.53517931	2.85070232	O	0.30527317	-3.79920693	2.91350676

ACE-1				ACE-2			
C	-0.95348331	0.09332387	-0.56452018	C	-0.05787279	0.93193276	-0.60400936
C	0.10430477	0.99019192	-0.38805529	C	-1.05797495	0.07919768	-0.12749526
C	0.61077672	1.60550563	-1.52583325	C	-2.02272793	-0.33705336	-1.03614824
N	0.15611313	1.38703574	-2.76079407	N	-2.04485379	0.02009561	-2.32126765
C	-0.83409354	0.53646806	-2.89279125	C	-1.08979477	0.81738906	-2.73790132
C	-1.43917878	-0.14439658	-1.83683374	C	-0.06550789	1.31431441	-1.93251204
C	0.67287399	1.27898663	0.97484813	C	-1.09103882	-0.37097356	1.30792538
N	1.40677359	0.14782861	1.537646	N	-0.00741707	-1.29264432	1.64132256
C	0.83597456	-0.64268723	2.46750737	C	1.08288459	-0.85551741	2.30127023
C	1.6583829	-1.73134308	3.09025574	C	2.12517869	-1.85331171	2.7103823
C	2.75040414	-0.03640809	1.0318793	C	-0.20489521	-2.6637746	1.22169352
N	-0.41401855	-0.41900309	2.77623873	N	1.17598112	0.42447133	2.54783798
C	-1.00981421	-1.13960282	3.70659562	C	2.20453633	0.89991058	3.22299129
N	-1.61049875	-1.73168305	4.50646427	N	3.07892347	1.40074076	3.80246264
Cl	-1.41610946	0.25584718	-4.50895917	Cl	-1.12613226	1.27308985	-4.41733735
H	1.42595943	2.32297467	-1.44565297	H	-2.83256584	-0.99105985	-0.71653673
H	-1.39054575	-0.40277726	0.29671892	H	0.71099818	1.29361939	0.07192922
H	-2.26035486	-0.82652233	-2.01777279	H	0.68633965	1.97749383	-2.34151432
H	-0.12297993	1.5342127	1.67551784	H	-2.03656964	-0.8839319	1.51372643
H	1.36491925	2.12580356	0.91583121	H	-1.01141525	0.48467014	1.97948777
H	2.73953845	0.04915318	-0.05860076	H	-0.56005047	-2.6761042	0.1871406
H	3.42944909	0.72537913	1.43333494	H	0.72276461	-3.22940824	1.26054352
H	3.13892857	-1.02016986	1.28340779	H	-0.95081868	-3.16391987	1.85101136
H	1.10157014	-2.18288119	3.91139093	H	2.86333521	-1.36694153	3.34815877
H	1.87899236	-2.515168	2.35926103	H	1.68445814	-2.6919172	3.25409646
H	2.6061831	-1.34696939	3.47372777	H	2.64485081	-2.25088584	1.83329694

ACE-3				ACE-4			
C	-1.2742886	-0.67916588	-1.95855634	C	0.24016395	1.04615796	-2.12464698
C	-0.78988133	-0.34202234	-0.6975301	C	0.25353752	0.65105742	-0.78966868
C	-0.00859641	0.80887099	-0.60440579	C	-0.97513936	0.34713726	-0.20529429
N	0.30003565	1.58078357	-1.64369163	N	-2.13727917	0.40499992	-0.85120928
C	-0.17170158	1.23212982	-2.82081388	C	-2.11379962	0.77953602	-2.11172382
C	-0.96953719	0.11695858	-3.051702	C	-0.96156335	1.11976414	-2.81174764
C	-1.10129313	-1.16439935	0.52564561	C	1.52906866	0.567555	0.00745022
N	0.09540235	-1.63450163	1.21255665	N	1.7476353	-0.75032258	0.59060971
C	0.43375212	-1.1382357	2.42149169	C	1.66966545	-0.93293375	1.92588294
C	1.61454331	-1.73028575	3.13129451	C	2.01001103	-2.28340509	2.48156876
C	0.81271805	-2.70693074	0.55604758	C	2.14300219	-1.78911165	-0.33719142
N	-0.28219197	-0.16055626	2.90535418	N	1.29217534	0.07574825	2.66239728
C	-0.00482238	0.34581161	4.091169	C	1.21758299	-0.04702392	3.97346394
N	0.17358717	0.84495725	5.12549478	N	1.12744329	-0.07361643	5.13189906
Cl	0.24676886	2.25525486	-4.16520857	Cl	-3.64498766	0.84523994	-2.93658863
H	0.38417254	1.12654582	0.35866823	H	-1.02451258	0.04600817	0.83854012
H	-1.89345616	-1.56267091	-2.08955543	H	1.16794763	1.30046186	-2.63028079
H	-1.32812662	-0.11294922	-4.04703341	H	-1.01144579	1.4228494	-3.84990477
H	-1.6987744	-2.03824227	0.24123916	H	1.5145354	1.28541421	0.82916553
H	-1.67683457	-0.57876011	1.24427875	H	2.38378875	0.80414671	-0.63679785
H	0.85013882	-2.50230397	-0.5170999	H	1.56691441	-1.67573867	-1.25899403
H	1.8373035	-2.77888274	0.91400651	H	3.21029185	-1.72177931	-0.58308352
H	0.31448874	-3.6725149	0.70904194	H	1.93481596	-2.77982948	0.0611887
H	1.68542017	-1.30860084	4.1338972	H	2.02270102	-2.23639937	3.57047999
H	1.53031241	-2.81677694	3.20841671	H	1.26167048	-3.02354703	2.18203261
H	2.54171273	-1.4983691	2.59840951	H	2.98566542	-2.626063	2.12931798

THIA-1				THIA-2			
C	1.56534437	-1.15178541	1.13576609	C	1.88808839	-1.24236391	0.94257829
N	1.37574775	0.18584237	1.10085774	N	0.6855124	-1.24325553	0.32232243
C	0.68072867	0.73172658	2.25218401	C	-0.32056684	-2.08858447	0.93622672
C	1.08489457	-0.13742051	3.43041719	C	-0.01422724	-2.0931251	2.42316837
S	1.24847427	-1.81580096	2.73864296	S	1.80413792	-2.01497133	2.52718319
C	1.43678633	0.92893054	-0.1498993	C	0.54152582	-0.82927083	-1.06280778
C	0.0937696	1.0933523	-0.81241788	C	-0.54888214	0.19151592	-1.23735411
C	-0.56457647	2.31674767	-0.80523581	C	-1.66110146	-0.06400753	-2.02826741
N	-1.75995535	2.52672559	-1.35716955	N	-2.6550722	0.80430364	-2.22292591
C	-2.33812259	1.50371529	-1.94238792	C	-2.56208561	1.96811402	-1.62464602
C	-1.78691379	0.2258697	-2.0283865	C	-1.50039255	2.35442653	-0.80610907
C	-0.54707635	0.02669458	-1.44925745	C	-0.48145755	1.4404197	-0.61544593
Cl	-3.89924646	1.7889103	-2.65464918	Cl	-3.86624506	3.08965122	-1.88226409
N	1.9246523	-1.82258574	0.08850218	N	2.94114641	-0.72732591	0.39833908
C	2.17634674	-3.11640381	0.18116769	C	4.08439894	-0.68960197	1.05859447
N	2.40489888	-4.25488095	0.17308904	N	5.12513544	-0.62110887	1.56896654
H	-0.10542259	3.18498975	-0.33502056	H	-1.76348165	-1.01938513	-2.53995991
H	-0.06917645	-0.94745677	-1.49050738	H	0.36869595	1.69291898	0.01183015
H	-2.31532608	-0.57127192	-2.53594673	H	-1.48415522	3.33520155	-0.34775252
H	1.87032361	1.91038423	0.0657328	H	1.50880892	-0.42463365	-1.36970109
H	2.12559732	0.38889284	-0.80213505	H	0.33740034	-1.7091498	-1.68679693
H	-0.40581513	0.70504497	2.09339295	H	-0.26591774	-3.10406817	0.5176933
H	0.98099748	1.77245811	2.40326206	H	-1.31584031	-1.68342214	0.7346055
H	0.33141652	-0.14397237	4.2172583	H	-0.36551712	-2.99938452	2.91522274
H	2.04708953	0.166788	3.84658104	H	-0.43336293	-1.21866082	2.92430108

THIA-3				THIA-4			
C	1.45162483	-1.50969377	1.30840796	C	1.7778063	-0.94777297	1.02936774
N	0.23875881	-1.07084557	0.89185618	N	1.03416767	0.10775235	1.43279991
C	-0.71771432	-0.83721617	1.95782734	C	0.01648333	-0.20548853	2.41824249
C	0.09577069	-0.36975838	3.15092957	C	0.58212509	-1.34193161	3.25235147
S	1.65300906	-1.31177175	3.04981655	S	1.54824233	-2.3471391	2.07878559
C	-0.2257468	-1.32063768	-0.45980322	C	0.95296679	1.32594205	0.64161928
C	-0.89909374	-0.1178886	-1.06535533	C	-0.26669379	1.38627163	-0.24347184
C	-0.28593077	1.13284288	-1.05016206	C	-0.36797973	0.58599436	-1.38122962
N	-0.82123884	2.22894996	-1.58238476	N	-1.4250972	0.58348431	-2.19050905
C	-1.99584766	2.11050802	-2.16211133	C	-2.42073033	1.38931523	-1.89417825
C	-2.71189421	0.92143492	-2.25448005	C	-2.4433813	2.24650201	-0.7986292
C	-2.14225009	-0.20682071	-1.68641218	C	-1.33754642	2.23215123	0.03604629
Cl	-2.67797803	3.55513273	-2.84968662	Cl	-3.79079434	1.36682679	-2.96593917
N	2.31787123	-2.0092876	0.49099555	N	2.54246272	-0.89144626	-0.01206259
C	3.51418968	-2.36782559	0.92143347	C	3.31752553	-1.91490167	-0.32488931
N	4.581384	-2.71369523	1.22070171	N	4.02196836	-2.77070525	-0.6705227
H	0.68702197	1.2594677	-0.58073649	H	0.44528477	-0.08258542	-1.65392633
H	-2.66691091	-1.15742409	-1.72926634	H	-1.30661138	2.88803559	0.90223205
H	-3.67586491	0.89100647	-2.74635055	H	-3.29253343	2.89303344	-0.61669926
H	0.65306574	-1.61161458	-1.04125766	H	0.95564228	2.17693987	1.33032887
H	-0.91492981	-2.1763358	-0.46377249	H	1.86579603	1.36984091	0.04459814
H	-1.26065446	-1.76547547	2.18908424	H	-0.91830491	-0.50325724	1.92418065
H	-1.44089775	-0.07968803	1.64481879	H	-0.18425762	0.67708974	3.03263146
H	-0.39651407	-0.58633614	4.09833281	H	-0.19936526	-1.95767345	3.69628317
H	0.32332366	0.69618514	3.09127259	H	1.24938494	-0.97601488	4.03500137

IMI-(12-water)-1			
Cl	-5.29049135	1.73049686	-1.53108694
C	-3.63752861	1.20797618	-1.68697611
N	-2.7278365	2.15292193	-1.77720486
C	-1.45383125	1.76895518	-1.88014056
C	-1.05114286	0.44163508	-1.89583236
C	-2.03873419	-0.53935556	-1.81145192
C	-3.36366694	-0.15725696	-1.70443005
H	-0.7334563	2.58239762	-1.94371132
C	0.41040026	0.09040622	-1.92330956
H	-1.77677014	-1.59297117	-1.82238055
H	-4.15694666	-0.8867225	-1.60878297
H	0.98652717	0.91726009	-2.35040699
N	0.94083423	-0.16486402	-0.59252262
H	0.59043705	-0.80326392	-2.52224805
C	0.94701166	0.86345777	0.44819643
C	1.60060581	0.11975455	1.61062799
N	1.27277959	-1.2735131	1.28834687
H	1.78008074	-2.02858656	1.72668542
C	1.03888688	-1.3782542	-0.03972017
H	-0.08127877	1.15609489	0.67941167
H	1.512731	1.73812486	0.12841924
H	1.19774688	0.40752439	2.58030816
H	2.68653449	0.25016918	1.61636907
N	0.79523765	-2.45981029	-0.78382633
N	1.16593407	-3.64625172	-0.28978271
O	0.61164864	-4.62558983	-0.77469575
O	2.04898286	-3.75950802	0.57216373
O	1.4705237	3.51284827	2.39754315
H	1.29458871	2.89624677	3.13219996
H	2.25861231	3.20155622	1.9267398
O	3.71114117	2.69840418	0.86173945
H	3.99380314	1.92985507	0.33320646
H	4.38116329	3.37246723	0.7407056
O	-1.5174531	4.82427762	-1.26405088
H	-2.26679121	4.26201004	-1.49423756
H	-1.29028473	4.54265578	-0.3657756
O	0.42753473	1.70717607	4.20597359
H	-0.474819	1.68420474	3.79184807
H	0.2952745	1.83758264	5.14567976
O	6.66807019	-1.22892547	-0.31185409
H	6.23517724	-0.39978731	-0.55869297
H	7.51030488	-0.99096955	0.07838959
O	-3.29926704	-2.69440619	0.38268825
H	-3.75654392	-3.3106233	0.9564
H	-2.86615074	-3.23083436	-0.31083441
O	4.37349168	0.47493719	-0.68713079
H	3.97558001	0.47971694	-1.56039136
H	4.09928165	-0.37690222	-0.27093746
O	4.15509783	-1.84429822	0.6036603
H	3.65034458	-2.65937063	0.47572865
H	5.0943166	-2.03426823	0.45058022
O	-1.96766025	-3.96710715	-1.63866157
H	-2.30521898	-4.67514462	-2.18935013
H	-1.03646085	-4.18816436	-1.45100171
O	-0.96852465	3.99455123	1.43883381
H	-0.02378935	3.8762339	1.70745497
H	-1.26781978	4.77457777	1.91187115
O	-1.84243957	1.71247757	2.84731595
H	-1.97616727	0.90482229	2.31950045
H	-1.73042045	2.45451318	2.2286366
O	-1.74601249	-0.68057595	1.46542228
H	-2.35935833	-1.33964856	1.08767284
H	-0.99051987	-1.18380681	1.78196984

IMI-(12-water)-2			
Cl	-3.0955844	1.52250304	-2.93211732
C	-1.74299625	0.96637176	-1.98797022
N	-0.97619591	1.89868617	-1.45877634
C	0.06979991	1.50568698	-0.72718982
C	0.39017384	0.17373412	-0.50988889
C	-0.44267208	-0.78641642	-1.08049188
C	-1.53155781	-0.39580186	-1.838373
H	0.67575172	2.29691395	-0.30220915
C	1.59471053	-0.20456695	0.31519982
H	-0.24908488	-1.84298508	-0.93770302
H	-2.18159274	-1.11819395	-2.3120745
H	2.14274093	0.68994045	0.61605718
N	1.21955551	-0.92168861	1.52227704
H	2.27650419	-0.83325989	-0.25920616
C	0.49936673	-0.23476004	2.59719171
C	0.31656291	-1.35041354	3.61462857
N	0.36036395	-2.54064526	2.75564599
H	0.50114277	-3.47411405	3.12163922
C	1.05988944	-2.24159015	1.62364209
H	-0.46035864	0.12362158	2.21491691
H	1.07655905	0.61883126	2.95134611
H	-0.634472	-1.26675459	4.13952172
H	1.13631991	-1.37797262	4.34063833
N	1.50702137	-3.04902474	0.65976688
N	1.45446183	-4.39587011	0.85407041
O	1.83861258	-5.05984529	-0.09050293
O	1.05783006	-4.88875191	1.90939156
O	1.59452934	2.70300937	2.29634453
H	2.04671438	2.90293143	1.46500015
H	0.64491565	2.80099216	2.12490429
O	2.15228535	-0.26676919	-3.45837789
H	2.53233291	-0.96896395	-2.91358423
H	1.33751368	-0.67537172	-3.78666332
O	2.38731597	2.35376741	-2.74489317
H	2.29729257	1.41586254	-3.01986651
H	1.6038121	2.80022537	-3.07130228
O	-2.14512067	-2.37973678	1.14344765
H	-1.46920818	-2.63249933	1.78946829
H	-2.82094758	-3.0589326	1.18488804
O	-1.24799614	2.70697418	2.00881494
H	-1.53340672	3.59853397	1.70799511
H	-1.70310465	2.0598375	1.44403946
O	0.2046934	-2.32696545	-3.78137962
H	0.87805253	-2.71136068	-3.19206105
H	0.14403437	-2.91831393	-4.53322827
O	2.32894992	-2.77445789	-2.02419512
H	2.0413003	-2.8508357	-1.08780862
H	2.88617794	-3.54698422	-2.14897593
O	-2.06624329	1.09100004	4.0456085
H	-1.73468215	1.84998304	3.52195809
H	-2.55065307	1.47187099	4.77940006
O	-1.57380055	4.6073798	-1.5947441
H	-1.37245189	3.64193802	-1.60341871
H	-2.33337056	4.71146539	-2.17098684
O	-1.84047472	5.16366698	1.03593537
H	-1.22175881	5.85559251	1.27542486
H	-1.76663051	5.06320836	0.06089308
O	-2.73945503	0.42677761	1.37055908
H	-2.83847303	0.43354355	2.3339774
H	-2.58716431	-0.50208685	1.14355584
O	3.06197969	2.8227726	-0.16754498
H	3.90081301	3.28501348	-0.1465453
H	2.85372061	2.6831263	-1.11753755

IMI-(12-water)-3			
Cl	-2.70631245	2.82589756	-2.62044008
C	-1.29316365	1.95356946	-2.0809703
N	-0.31522839	2.67912153	-1.58308349
C	0.75236889	2.03533286	-1.10618743
C	0.88004414	0.65173471	-1.10774982
C	-0.15434431	-0.0878395	-1.68467697
C	-1.26967851	0.56964902	-2.18200334
H	1.53889472	2.66720383	-0.70220707
C	2.0660763	-0.0114497	-0.45573219
H	-0.0932127	-1.16885776	-1.75067588
H	-2.09475259	0.02713727	-2.62536638
H	2.93586079	0.64588381	-0.50073068
N	1.80659548	-0.32291807	0.94255533
H	2.32078266	-0.93358294	-0.97659509
C	1.67479442	0.74279283	1.94136502
C	1.18783425	-0.01787561	3.17621336
N	0.66224242	-1.23899278	2.58221784
H	0.11206597	-1.94242244	3.05062482
C	1.07858056	-1.39528619	1.32919522
H	0.94531476	1.49545914	1.61660034
H	2.62759197	1.24561453	2.1068408
H	0.42634243	0.53173735	3.72538353
H	2.01067636	-0.25370868	3.85856466
N	0.86301583	-2.36579385	0.43207909
N	0.17494794	-3.44225356	0.81786371
O	-0.06491382	-4.26393652	-0.06411651
O	-0.211399	-3.61541694	1.98069442
O	-3.04841231	-3.43970669	2.08239192
H	-2.22751443	-3.94413227	2.01031742
H	-3.20703893	-3.08783727	1.18588887
O	0.29981902	-3.2494638	-2.62844131
H	0.24443738	-3.62661099	-1.72965829
H	-0.16198445	-3.86281264	-3.20180632
O	5.08250643	-1.51634787	-2.24496726
H	5.57136957	-1.49383766	-1.42205363
H	4.80571656	-0.60211395	-2.42788756
O	1.01027294	2.86391744	3.9972172
H	0.49476765	3.2300761	3.2498194
H	1.0302775	3.55773098	4.65638518
O	3.52534848	0.65671212	-3.03665529
H	3.67061427	1.14523568	-3.848086
H	2.97071553	-0.1160039	-3.28195181
O	-2.93923955	2.76852526	1.07891937
H	-2.77982806	1.80746277	1.06058768
H	-3.20924408	3.00313407	0.18797343
O	2.51800734	-1.80102225	-3.3790837
H	1.75651167	-2.36133609	-3.14269591
H	3.30636445	-2.20449059	-2.99275965
O	0.12792858	5.1762907	-0.46602818
H	-0.16336996	4.45565486	-1.06070308
H	-0.32438576	5.97056221	-0.75241051
O	-2.10599099	0.12017566	1.10937515
H	-1.18123904	0.21701279	0.86487388
H	-2.11506768	-0.29442011	2.00921403
O	-0.35783424	3.58043719	1.77147397
H	-1.29726684	3.38302505	1.60323524
H	-0.12669083	4.26745728	1.12355324
O	-2.24774582	-1.27523584	3.38072089
H	-2.60825674	-2.11947441	2.99753002
H	-2.83504979	-1.02447922	4.09596116
O	-3.24303355	-1.98198447	-0.27912438
H	-4.09264373	-1.76405665	-0.66576588
H	-2.8939767	-1.15093994	0.09694383

THIA-(12-water)-1			
C	1.44123199	-2.36942158	0.52995537
N	1.43043222	-1.19957268	1.17797409
C	0.7472384	-1.22756059	2.46821439
C	0.94920175	-2.62582551	3.02070149
S	0.94632376	-3.7115955	1.55242955
C	1.5192739	0.06078761	0.43570562
C	0.18080502	0.4018824	-0.16316286
C	-0.77663119	1.08505745	0.57360019
N	-2.02182826	1.30031878	0.13888522
C	-2.34179062	0.86077616	-1.06153883
C	-1.46510138	0.19931885	-1.9122007
C	-0.18468936	-0.0369382	-1.43673978
Cl	-3.98551295	1.13447799	-1.56949286
N	1.77140968	-2.43987848	-0.72997148
C	1.7146721	-3.52759106	-1.43954816
N	1.66713258	-4.40628523	-2.20496836
H	-0.55023627	1.47574102	1.56197183
H	0.53124354	-0.56862035	-2.05286807
H	-1.76728567	-0.14768949	-2.8928867
H	1.85814944	0.82740616	1.13442914
H	2.2676588	-0.04845884	-0.34983961
H	-0.32307459	-1.03302511	2.33179412
H	1.16079722	-0.46435825	3.13016996
H	0.13309171	-2.91413575	3.68238895
H	1.90745944	-2.73979012	3.53120006
O	2.8060583	0.91695163	-2.53956
H	2.44131114	0.32101623	-3.23053284
H	3.68805968	1.14620172	-2.83717671
O	1.27634214	3.09797936	-1.81592085
H	0.37271764	2.88031512	-2.0521804
H	1.80888759	2.32615193	-2.09456468
O	-3.52624139	1.34462944	2.39739509
H	-3.13992097	1.48697222	1.49704354
H	-4.42568525	1.67591503	2.37040882
O	-1.55033763	2.93948451	3.63021251
H	-0.79529888	2.40541419	3.94099784
H	-2.26461117	2.32814832	3.3916802
O	-2.52265908	-1.2893332	2.69072993
H	-3.02888586	-1.83158656	2.08385333
H	-2.97560317	-0.4299813	2.69299597
O	2.57144418	2.45132964	2.60069268
H	3.44295149	2.79674739	2.79736845
H	2.18069967	3.05721594	1.901525
O	-0.98238418	-1.45354474	-4.75502563
H	-1.58160025	-1.48536554	-5.50237546
H	-0.51448778	-2.30862372	-4.74952295
O	0.94487276	-3.46033165	-4.6806723
H	1.20478001	-4.05619418	-5.38568084
H	1.15366663	-3.93061674	-3.84026774
O	0.75636874	1.58300311	4.35269738
H	1.47735098	1.95722876	3.7925379
H	1.0140018	1.74542424	5.26154028
O	1.49714548	3.9632645	0.8069508
H	1.44267917	3.67533435	-0.12444623
H	0.60572596	4.27917662	1.06143228
O	-0.98579323	4.67193771	1.6661968
H	-1.14243414	5.55742261	1.99648052
H	-1.21689109	4.06337935	2.40715927
O	1.69811508	-0.67731481	-4.42113899
H	1.80863328	-1.63748023	-4.47357874
H	0.76157859	-0.56375294	-4.64260162

THIA-(12-water)-2			
C	0.69768088	-2.06190918	0.56114599
N	0.46228459	-0.78462091	0.81490192
C	-0.22558055	-0.49559775	2.07218119
C	0.14229558	-1.62665878	3.01230217
S	0.30035674	-3.09959177	1.93791981
C	0.60379677	0.25838381	-0.18955542
C	-0.72946623	0.70105832	-0.72241388
C	-1.01127579	2.05600315	-0.82200327
N	-2.18450747	2.54247191	-1.2315641
C	-3.10529909	1.67066219	-1.58386805
C	-2.93339461	0.28895485	-1.56681527
C	-1.71684416	-0.20002971	-1.11473623
Cl	-4.64756856	2.31961388	-2.07204114
N	1.21552052	-2.48566779	-0.57329161
C	1.30611174	-3.78916456	-0.7600765
N	1.37420197	-4.92395478	-1.00414377
H	-0.26105288	2.78615547	-0.53371467
H	-1.55874849	-1.27530154	-1.06314226
H	-3.72586024	-0.37349615	-1.89312828
H	1.11627725	1.1012337	0.27524306
H	1.22474839	-0.1314421	-0.99421972
H	-1.30517453	-0.44598169	1.8933607
H	0.10465872	0.4803267	2.43862731
H	-0.62981274	-1.81015552	3.75868115
H	1.10074611	-1.45653292	3.50641863
O	4.84766198	-0.62030947	-2.56736271
H	4.99483453	0.32701437	-2.4872413
H	4.77237492	-0.91252388	-1.64356984
O	-2.19967097	3.46975494	1.7014994
H	-2.38482716	2.52040904	1.56699471
H	-2.33779422	3.85199845	0.82803101
O	2.83393844	3.53706861	1.1235053
H	3.56057225	3.98340114	1.55931473
H	3.24078989	2.89192056	0.50369158
O	-3.27088282	0.88521255	1.82077368
H	-3.85257281	1.34620992	2.45421294
H	-3.82599703	0.64727509	1.07398435
O	3.71762652	-3.05814118	1.98344811
H	2.80119258	-3.35243181	2.06594122
H	4.22114827	-3.8566838	1.8073933
O	-4.3671435	2.89157026	3.33064917
H	-3.66201615	3.43003669	2.93110422
H	-4.37444628	3.10099621	4.26558167
O	1.82544543	1.72466964	-2.62735166
H	1.71575424	2.33358346	-3.35895525
H	1.84159483	0.81803717	-3.00482733
O	3.76067603	1.70564626	-0.66228691
H	3.10772857	1.76874472	-1.38723762
H	3.70969619	0.79363144	-0.33661692
O	2.19074759	-0.85063465	-3.27673434
H	3.15797264	-0.90955093	-3.12861863
H	1.78729311	-1.56109685	-2.76930877
O	-1.78358884	-3.58580062	-1.02339629
H	-1.11549474	-4.19165353	-1.3607044
H	-2.23600184	-4.08275056	-0.33922092
O	3.77992836	-1.12961121	-0.06953351
H	3.96173244	-1.6581437	0.72651053
H	2.9872094	-1.55507567	-0.43207083
O	0.52915145	2.53010989	2.26285392
H	-0.23183295	3.11245445	2.14630175
H	1.31599613	3.00587393	1.9414635

THIA-(12-water)-3			
C	0.9512689	-1.0512646	0.25389358
N	0.9011643	0.26898869	0.3065664
C	0.29836476	0.8280905	1.51191974
C	0.4799753	-0.20422668	2.6041909
S	0.38483357	-1.80822738	1.74326477
C	1.09498256	1.13326007	-0.85668972
C	-0.16471112	1.16529314	-1.68108132
C	-1.22720578	1.97014346	-1.28964086
N	-2.42694409	1.93835533	-1.87634851
C	-2.59351985	1.11813752	-2.89473036
C	-1.59066706	0.3120578	-3.4169176
C	-0.35717348	0.33669913	-2.78468459
Cl	-4.18278579	1.07299031	-3.60013357
N	1.32418611	-1.72403573	-0.81775435
C	1.40981502	-3.03145543	-0.72746075
N	1.51399746	-4.18990456	-0.7322779
H	-1.10782214	2.67549976	-0.47268546
H	0.45637512	-0.28460957	-3.14413577
H	-1.78162441	-0.31607618	-4.27771356
H	1.34526405	2.12008487	-0.46501461
H	1.93917042	0.76689528	-1.43785912
H	-0.76569878	1.02156619	1.33324158
H	0.79359568	1.77110765	1.74629169
H	-0.31582363	-0.13388436	3.34485493
H	1.46833438	-0.14916432	3.06116413
O	2.97649818	-5.43917928	1.35320818
H	2.37528296	-6.05833013	1.77033286
H	2.50530699	-5.11934016	0.56067864
O	4.02963599	-3.36886734	2.80747906
H	3.62863423	-4.11074164	2.30843153
H	4.92978175	-3.64342422	2.98846957
O	-2.47071341	1.05830815	3.40397108
H	-3.10621272	0.71800312	2.72503431
H	-2.93781117	1.02165791	4.24042843
O	0.17054019	3.93931544	0.95314387
H	-0.69340225	3.88456763	1.41647615
H	0.43972638	4.85668176	1.00568963
O	-2.2623183	3.51018607	2.04844378
H	-4.95664667	3.29767903	-0.25213683
H	-2.30729569	2.73187833	2.63277897
O	-4.06522016	0.35367331	1.39555172
H	-4.24447666	1.16322337	0.88876628
H	-3.59223935	-0.24144055	0.78946101
O	3.07296482	-0.77488932	-2.84812808
H	2.47099899	-1.204369	-2.21065484
H	3.45212288	-1.48091468	-3.37535544
O	-2.37716606	-1.27533423	-0.09994129
H	-1.70857529	-1.60236707	0.51978817
H	-2.60175352	-2.02270869	-0.65790274
O	3.40057845	1.71018653	1.24713274
H	3.47558347	0.81511892	1.63769742
H	3.88037481	2.29775711	1.83228525
O	4.76942549	0.05260628	-0.70227173
H	4.29868266	-0.11013357	-1.5339758
H	4.4129115	0.87740809	-0.34400043
O	-4.17324976	2.81725273	0.0213625
H	-2.97768766	3.39161676	1.40468292
H	-3.66095971	2.60845385	-0.79946068
O	3.60429127	-0.93773671	1.59936847
H	4.1272061	-0.92351257	0.77877364
H	3.79508996	-1.77628686	2.06212509