

Computational Design of Thiourea-based Cyclophane Sensors for Small Anions

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Supplementary Material

Table S1. Cartesian coordinates, total energies (in Hartrees) and number of imaginary frequencies of the B3LYP/6-31G* optimized geometries of all calculated structures.

1a (-2573.66712) (0)				1b (-2573.66718) (0)			
H	3.907312	3.247127	-1.045957	H	1.630417	-3.049934	-3.753284
H	-2.853812	1.730987	-2.912199	H	3.259265	-1.050089	2.937938
C	3.655587	0.617772	1.127238	C	-1.038739	-0.924317	-3.507391
C	3.564703	-0.771191	-1.305516	C	1.051120	0.942726	-3.506326
C	3.640825	1.342488	-0.077498	C	0.290866	-1.381660	-3.506326
C	3.625118	-0.778443	1.139179	C	-1.341985	0.438932	-3.506326
C	3.581021	-1.459304	-0.090237	C	-0.281112	1.361732	-3.507391
C	3.597308	0.634319	-1.280509	C	1.319852	-0.437417	-3.507391
C	3.633412	2.857940	-0.058282	C	0.587462	-2.867254	-3.468569
C	3.600589	-1.552190	2.442077	C	-2.776845	0.924870	-3.468569
C	3.475106	-1.510509	-2.625421	C	2.189384	1.942383	-3.468569
H	4.385528	3.225591	0.650189	H	-0.039444	-3.390772	-4.200505
C	-3.162585	-0.255739	-1.276188	C	1.263655	0.579653	3.232202
C	-3.088628	0.379956	1.448696	C	-1.280176	-0.588352	3.233504
C	-3.125300	1.087221	-0.886374	C	1.149616	-0.814490	3.233504
C	-3.165048	-1.288742	-0.330347	C	0.130561	1.402840	3.233504
C	-3.126520	-0.955429	1.027576	C	-1.133822	0.804530	3.232202
C	-3.086643	1.389626	0.480592	C	-0.129832	-1.384185	3.232202
C	-3.144786	2.172657	-1.949487	C	2.407296	-1.666341	3.255559
C	-3.224782	-2.751032	-0.738625	C	0.239446	2.917949	3.255559
C	-3.066121	0.756062	2.920759	C	-2.646741	-1.251610	3.255559
H	-4.172021	2.539001	-2.093286	H	2.635185	-1.972735	4.287230
H	-2.726456	1.796106	3.016024	H	-2.539035	-2.297562	2.937938

H	3.917578	-0.905860	3.268984	H	-3.456528	0.112984	-3.753284
H	-4.087967	0.741760	3.327847	H	-3.026031	-1.295770	4.287230
H	4.313373	-2.384408	2.395197	H	-2.916772	1.729545	-4.200505
H	-2.898559	-3.369580	0.108263	H	-0.720229	3.347649	2.937938
H	-4.266950	-3.044561	-0.933082	H	0.390846	3.268504	4.287230
H	4.194158	-1.088937	-3.338201	H	2.956217	1.661226	-4.200505
H	3.743897	-2.564095	-2.485183	H	1.826112	2.936949	-3.753284
H	3.715549	1.157427	2.071214	H	-1.849756	-1.650804	-3.533120
H	3.582845	-2.548385	-0.094193	H	-0.504760	2.427337	-3.533120
H	-3.033858	2.425610	0.806136	H	-0.243085	-2.465219	3.209848
H	-3.104026	-1.756828	1.761880	H	-2.013398	1.443127	3.209848
H	-3.167843	-0.491423	-2.337534	H	2.256485	1.022090	3.209848
H	3.611756	1.182098	-2.221703	H	2.354516	-0.776534	-3.533120
S	-0.601401	-2.873325	3.750261	S	-4.219610	2.078645	0.737544
C	-0.052747	-1.324948	3.351800	C	-3.549579	0.618934	0.211052
N	-0.824922	-0.206350	3.400064	N	-3.362628	-0.466802	1.008662
N	1.235670	-1.091854	2.954533	N	-3.149664	0.431269	-1.083924
H	-0.372725	0.686584	3.238354	H	-3.038278	-1.322578	0.572524
H	1.419580	-0.229452	2.452795	H	-2.499885	-0.325867	-1.267573
N	1.083179	-2.069616	-2.434650	N	1.948323	2.512054	-1.083924
C	-0.221938	-2.235163	-2.812129	C	2.310803	2.764558	0.211052
H	1.284174	-2.068957	-1.440128	H	0.967735	2.327897	-1.267573
S	-0.776180	-1.780741	-4.343056	S	3.909965	2.614966	0.737544
N	-1.005131	-2.799494	-1.854551	N	1.277053	3.145521	1.008662
H	-0.555270	-3.121879	-1.005067	H	0.373753	3.292515	0.572524
N	1.241540	3.094351	-0.595867	N	1.201342	-2.943325	-1.083924
C	-0.040796	3.567978	-0.527955	C	1.238777	-3.383494	0.211052
H	1.390612	2.221432	-1.091127	H	1.532151	-2.002032	-1.267573
S	-0.516823	4.701813	0.631677	S	0.309645	-4.693613	0.737544
N	-0.870323	3.051239	-1.473424	N	2.085576	-2.678721	1.008662
H	-0.464065	2.449361	-2.180875	H	2.664525	-1.969938	0.572524
H	2.270745	-2.741242	3.684226	H	-4.215064	1.870638	-2.141704
C	2.219582	-2.149263	2.766687	C	-3.195568	1.478553	-2.094882
H	1.906743	-2.835869	1.967061	H	-2.548901	2.321754	-1.812972
C	-2.216792	-0.147405	3.826936	C	-3.733818	-0.568143	2.413734
H	-2.585115	-1.173813	3.837607	H	-3.937236	0.446494	2.758233
H	-2.275569	0.221517	4.860738	H	-4.672967	-1.130973	2.512200
C	-2.418476	-3.126682	-1.990267	C	1.374884	3.517653	2.413734
H	-2.536096	-4.201997	-2.185485	H	1.357033	4.612394	2.512200
H	-2.778071	-2.604158	-2.877522	H	2.355294	3.186499	2.758233
C	2.082608	-1.425542	-3.275856	C	2.878250	2.028166	-2.094882
H	2.089885	-1.925468	-4.247914	H	3.727553	2.715033	-2.141704
H	1.816382	-0.375683	-3.465195	H	3.285149	1.046535	-1.812972
C	-2.271432	3.402722	-1.664226	C	2.358935	-2.949511	2.413734

H	-2.368681	4.114593	-2.496214	H	3.315935	-3.481422	2.512200
H	-2.588447	3.927958	-0.762463	H	1.581943	-3.632994	2.758233
C	2.277842	3.453637	0.362488	C	0.317319	-3.506721	-2.094882
H	2.343573	4.543794	0.408511	H	0.487512	-4.585673	-2.141704
H	2.010429	3.112519	1.372940	H	-0.736248	-3.368291	-1.812972

1c (-2573.66475) (3)

H	-2.858539	3.512337	1.938464
H	-2.858539	-3.512337	1.938464
C	0.516258	3.521967	1.290557
C	-0.518951	3.524778	-1.312381
C	-0.877080	3.524778	1.105614
C	1.396030	3.524778	0.206765
C	0.859526	3.521967	-1.092373
C	-1.375786	3.521967	-0.198186
C	-1.821908	3.566547	2.294264
C	2.897845	3.566547	0.430685
C	-1.075938	3.566547	-2.724951
H	-1.725300	4.533635	2.805505
C	-1.375786	-3.521967	-0.198186
C	1.396030	-3.524778	0.206765
C	-0.877080	-3.524778	1.105614
C	-0.518951	-3.524778	-1.312381
C	0.859526	-3.521967	-1.092373
C	0.516258	-3.521967	1.290557
C	-1.821908	-3.566547	2.294264
C	-1.075938	-3.566547	-2.724951
C	2.897845	-3.566547	0.430685
H	-1.725300	-4.533635	2.805505
H	3.108028	-3.512337	1.506334
H	3.108028	3.512337	1.506334
H	3.292288	-4.533635	0.091400
H	3.292288	4.533635	0.091400
H	-0.249491	-3.512337	-3.444800
H	-1.566990	-4.533635	-2.896907
H	-1.566990	4.533635	-2.896907
H	-0.249491	3.512337	-3.444800
H	0.921661	3.537495	2.300194
H	1.531196	3.537495	-1.948280
H	0.921661	-3.537495	2.300194
H	1.531196	-3.537495	-1.948280
H	-2.452858	-3.537495	-0.351916
H	-2.452858	3.537495	-0.351916
S	5.027424	0.000000	-1.544164

1...F⁻ (-2673.64938) (0)

H	2.881402	0.647707	-3.304896
H	-3.485313	3.172511	-1.389501
C	3.428604	1.389087	-0.028645
C	3.411098	-1.407248	0.030846
C	3.414549	0.678377	-1.236529
C	3.412529	0.733134	1.203206
C	3.425007	-0.668338	1.215004
C	3.426976	-0.716674	-1.188623
C	3.203193	1.388052	-2.562583
C	3.199561	1.528133	2.479663
C	3.195885	-2.909901	0.080009
H	4.143489	1.815469	-2.940367
C	-3.573035	0.552097	-1.276960
C	-3.560976	-0.553829	1.293118
C	-3.559023	1.400735	-0.169020
C	-3.565752	-0.842893	-1.130736
C	-3.575920	-1.377860	0.158309
C	-3.569930	0.829746	1.112315
C	-3.348005	2.888533	-0.339991
C	-3.360670	-1.737808	-2.332410
C	-3.351765	-1.149226	2.667459
H	-4.074560	3.461994	0.253512
H	-3.490256	-0.382172	3.437796
H	2.877215	2.540424	2.207467
H	-4.077837	-1.950516	2.866699
H	4.139321	1.643268	3.039272
H	-3.504288	-2.787241	-2.051084
H	-4.085636	-1.507586	-3.126318
H	4.135219	-3.453042	-0.099436
H	2.871733	-3.180792	1.092046
H	3.357073	2.474024	-0.044296
H	3.349369	-1.196631	2.162451
H	-3.522924	1.475398	1.987468
H	-3.532578	-2.458696	0.280731
H	-3.527063	0.986634	-2.273945
H	3.352390	-1.272570	-2.120243
S	-0.013933	-0.561838	5.036720

C	3.811940	0.000000	-0.372700	C	0.013929	-0.289366	3.353528
N	3.286953	-1.149607	0.134320	N	-0.872765	-0.822668	2.476391
N	3.286953	1.149607	0.134320	N	0.953265	0.501787	2.759549
H	2.512449	-1.097224	0.784865	H	-0.698920	-0.619108	1.482239
H	2.512449	1.097224	0.784865	H	0.950400	0.484545	1.735371
N	-1.527153	1.149607	-2.913746	N	0.950103	-2.637362	-0.949420
C	-2.228739	0.000000	-3.114888	C	0.007190	-2.763756	-1.927017
H	-0.576512	1.097224	-2.568279	H	0.949093	-1.737110	-0.459606
S	-3.850998	0.000000	-3.581796	S	-0.021942	-4.091841	-2.996486
N	-1.527153	-1.149607	-2.913746	N	-0.882101	-1.739657	-1.952065
H	-0.576512	-1.097224	-2.568279	H	-0.709945	-0.979849	-1.278728
N	-1.759802	1.149607	2.779425	N	0.956740	2.141951	-1.813876
C	-1.583203	0.000000	3.487587	C	0.016523	3.051109	-1.426122
H	-1.935939	1.097224	1.783412	H	0.953677	1.262723	-1.287707
S	-1.176428	0.000000	5.125959	S	-0.012307	4.644972	-2.032433
N	-1.759802	-1.149607	2.779425	N	-0.869225	2.558051	-0.524995
H	-1.935939	-1.097224	1.783412	H	-0.695961	1.593987	-0.207034
H	4.765280	2.611064	-0.110056	H	1.940110	1.617769	4.239844
C	3.694814	2.479010	-0.301712	C	2.175637	0.901171	3.444700
H	3.565906	2.562162	-1.387254	H	2.612525	0.030502	3.951335
C	3.694814	-2.479010	-0.301712	C	-1.933106	-1.751118	2.814713
H	3.565906	-2.562162	-1.387254	H	-1.843540	-2.625957	2.156971
H	4.765280	-2.611064	-0.110056	H	-1.773982	-2.078810	3.844665
C	-2.108698	-2.479010	-3.048948	C	-1.941141	-1.570987	-2.926849
H	-2.477952	-2.611064	-4.071827	H	-1.782957	-2.303356	-3.721856
H	-2.984351	-2.562162	-2.394539	H	-1.849544	-0.565874	-3.359814
C	-2.108698	2.479010	-3.048948	C	2.172951	-3.429681	-0.947318
H	-2.477952	2.611064	-4.071827	H	1.937954	-4.477258	-0.727493
H	-2.984351	2.562162	-2.394539	H	2.611099	-3.429655	-1.954276
C	-1.586118	-2.479010	3.350658	C	-1.929552	3.315028	0.109843
H	-2.287330	-2.611064	4.181882	H	-1.768868	4.371110	-0.118997
H	-0.581557	-2.562162	3.781792	H	-1.841444	3.180033	1.196086
C	-1.586118	2.479010	3.350658	C	2.179819	2.537539	-2.499867
H	-2.287330	2.611064	4.181882	H	1.945660	2.871944	-3.516902
H	-0.581557	2.562162	3.781792	H	2.617031	3.409116	-1.994685
				F	0.123840	-0.001338	-0.007946

1...CF⁻ (-3034.02002) (0)

H	3.465901	2.078401	-2.737658
H	-3.466426	2.082684	-2.736157
C	3.616755	1.255340	0.589480
C	3.606836	-1.283582	-0.590031
C	3.611049	1.150251	-0.809008
C	3.609551	0.123623	1.407816

1...Br⁻ (-5145.23239) (0)

H	3.493695	2.097747	-2.732368
H	-3.492602	2.097563	-2.733974
C	3.596900	1.254207	0.594338
C	3.591585	-1.278113	-0.600377
C	3.592311	1.158772	-0.805445
C	3.591903	0.117783	1.407113

C	3.611154	-1.140051	0.799343	C	3.594374	-1.142319	0.790205
C	3.613674	-0.124538	-1.379752	C	3.595648	-0.113560	-1.382903
C	3.573637	2.387053	-1.691067	C	3.575706	2.402026	-1.682237
C	3.573380	0.270656	2.920024	C	3.575623	0.256307	2.921913
C	3.565078	-2.666394	-1.219861	C	3.574297	-2.658880	-1.238965
H	4.530600	2.924966	-1.618556	H	4.533369	2.934138	-1.583915
C	-3.613491	-0.122514	-1.381722	C	-3.594983	-0.113809	-1.384643
C	-3.610608	0.121273	1.406234	C	-3.592604	0.117426	1.405383
C	-3.611199	1.151370	-0.808980	C	-3.592035	1.158501	-0.807135
C	-3.606886	-1.282809	-0.593816	C	-3.591196	-1.278392	-0.602161
C	-3.611809	-1.141456	0.795771	C	-3.594668	-1.142653	0.788425
C	-3.617534	1.254266	0.589677	C	-3.597309	1.253881	0.592651
C	-3.573507	2.389609	-1.688992	C	-3.575114	2.401792	-1.683868
C	-3.564790	-2.664575	-1.225882	C	-3.573481	-2.659131	-1.240796
C	-3.575193	0.265870	2.918684	C	-3.577067	0.255890	2.920196
H	-4.530103	2.927977	-1.615071	H	-4.532857	2.933837	-1.585959
H	-3.472586	1.327013	3.174932	H	-3.498051	1.317964	3.180812
H	3.469452	1.332109	3.174454	H	3.496362	1.318383	3.182446
H	-4.531393	-0.069894	3.346918	H	-4.534035	-0.097290	3.331745
H	4.529818	-0.063249	3.349181	H	4.532434	-0.096745	3.333936
H	-3.440979	-3.415624	-0.436705	H	-3.489898	-3.416428	-0.452390
H	-4.526018	-2.878949	-1.716425	H	-4.531254	-2.841539	-1.750081
H	4.526979	-2.882058	-1.708518	H	4.532344	-2.841239	-1.747752
H	3.439726	-3.416028	-0.429582	H	3.490367	-3.416150	-0.450570
H	3.598658	2.239218	1.054101	H	3.583867	2.235337	1.064832
H	3.588269	-2.033904	1.419610	H	3.578927	-2.039931	1.405317
H	-3.599804	2.237418	1.055852	H	-3.584592	2.234994	1.063189
H	-3.589193	-2.036282	1.414651	H	-3.579441	-2.040287	1.403509
H	-3.593307	-0.209286	-2.466285	H	-3.580783	-0.197600	-2.469447
H	3.593842	-0.213025	-2.464177	H	3.581977	-0.197395	-2.467710
S	-0.000886	-0.864094	5.505654	S	-0.001281	-0.941764	5.519413
C	-0.000770	-0.376865	3.873285	C	-0.000926	-0.371177	3.916874
N	-1.142360	-0.151307	3.164472	N	-1.143412	-0.104599	3.220636
N	1.140999	-0.149087	3.165461	N	1.141867	-0.104450	3.221198
H	-1.032185	-0.039620	2.153316	H	-1.032964	0.030851	2.212488
H	1.031529	-0.037713	2.154203	H	1.031901	0.030983	2.212995
N	1.141646	-2.637656	-1.741828	N	1.142590	-2.735329	-1.706857
C	0.000800	-3.143707	-2.287294	C	0.000694	-3.205344	-2.286418
H	1.033161	-1.817325	-1.140322	H	1.031141	-1.931438	-1.083906
S	0.001369	-4.328455	-3.511807	S	0.001062	-4.305023	-3.584224
N	-1.140469	-2.636246	-1.744024	N	-1.141527	-2.735391	-1.707447
H	-1.032079	-1.816095	-1.142238	H	-1.030441	-1.931494	-1.084439
N	1.142042	2.811108	-1.440627	N	1.142788	2.843591	-1.512230
C	0.000383	3.537916	-1.598347	C	0.000244	3.579245	-1.632022

H	1.033489	1.879922	-1.031547	H	1.032464	1.903098	-1.125026
S	0.000719	5.194836	-1.993086	S	0.000257	5.251724	-1.943400
N	-1.141489	2.811764	-1.439142	N	-1.142302	2.843511	-1.512729
H	-1.032899	1.880473	-1.030293	H	-1.032079	1.903034	-1.125460
H	2.507773	-0.330383	4.708203	H	2.541386	-0.338911	4.730981
C	2.465087	-0.521425	3.633925	C	2.465680	-0.517317	3.656210
H	2.630148	-1.602857	3.504527	H	2.599644	-1.601257	3.512267
C	-2.466199	-0.526090	3.631655	C	-2.467386	-0.517637	3.654991
H	-2.629884	-1.607485	3.500189	H	-2.601156	-1.601587	3.510933
H	-2.509516	-0.337014	4.706249	H	-2.543627	-0.339289	4.729734
C	-2.467999	-2.871923	-2.284026	C	-2.465911	-2.904179	-2.281161
H	-2.501883	-3.897937	-2.656398	H	-2.541543	-3.922885	-2.667535
H	-2.652614	-2.220140	-3.152639	H	-2.602322	-2.234566	-3.145071
C	2.469876	-2.875117	-2.279354	C	2.467279	-2.904053	-2.279886
H	2.503841	-3.901858	-2.649731	H	2.543181	-3.922771	-2.666174
H	2.656210	-2.225150	-3.148953	H	2.604085	-2.234471	-3.143758
C	-2.466201	3.402918	-1.352895	C	-2.467032	3.425416	-1.377248
H	-2.506745	4.240528	-2.052341	H	-2.540713	4.267264	-2.069075
H	-2.634381	3.827133	-0.350342	H	-2.605440	3.842052	-0.367083
C	2.467157	3.401655	-1.356224	C	2.467417	3.425590	-1.376168
H	2.507893	4.237925	-2.057270	H	2.541362	4.267413	-2.067999
H	2.636136	3.827722	-0.354596	H	2.605335	3.842281	-0.365960
Cl	-0.000004	-0.013048	0.013918	Br	-0.000007	-0.002588	0.000527

1...NO₃⁻ (-2854.10514) (0)

H	-3.511945	-1.869708	2.899632
H	3.512639	-1.867908	2.899250
C	-3.523533	0.981881	0.983311
C	-3.526008	-0.994565	-1.002218
C	-3.525005	-0.369926	1.363246
C	-3.523793	1.366228	-0.360437
C	-3.525051	0.361273	-1.341201
C	-3.526037	-1.341295	0.358477
C	-3.557973	-0.776157	2.829222
C	-3.554755	2.838743	-0.742637
C	-3.557963	-2.062084	-2.086046
H	-4.521661	-0.475802	3.265497
C	3.523963	-1.340521	0.357789
C	3.525063	1.366719	-0.362199
C	3.523989	-0.368736	1.362178
C	3.524715	-0.994341	-1.003073
C	3.525455	0.361367	-1.342574
C	3.524097	0.982932	0.981698
C	3.557377	-0.774333	2.828322

1...AcO⁻ (-2802.27700) (0)

H	-3.358105	-2.114606	2.924369
H	3.727640	-2.371188	2.259127
C	-3.429834	0.967576	1.414333
C	-3.574124	-0.729086	-0.813188
C	-3.432824	-0.420642	1.608630
C	-3.506725	1.530106	0.136275
C	-3.591804	0.663717	-0.965632
C	-3.508613	-1.250195	0.486269
C	-3.339308	-1.020766	3.000546
C	-3.506942	3.043560	-0.033711
C	-3.614046	-1.636878	-2.036788
H	-4.223938	-0.730638	3.585622
C	3.443305	-1.477822	-0.157473
C	3.537086	1.303168	-0.486998
C	3.647127	-0.664426	0.960405
C	3.268260	-0.939106	-1.439685
C	3.329573	0.453244	-1.585663
C	3.693537	0.724281	0.776377
C	3.789500	-1.279369	2.341592

C	3.556272	-2.062321	-2.086515	C	3.018960	-1.833289	-2.649362
C	3.557784	2.839000	-0.745147	C	3.618433	2.817397	-0.640753
H	4.520795	-0.472733	3.264332	H	4.784819	-1.049574	2.748239
H	3.509199	3.448310	0.165493	H	3.743685	3.266051	0.352219
H	-3.503573	3.447448	0.168266	H	-3.421707	3.511822	0.954303
H	4.522193	3.066819	-1.221868	H	4.524385	3.071679	-1.210065
H	-4.519630	3.068456	-1.217511	H	-4.476909	3.359405	-0.444373
H	3.507455	-1.578612	-3.069657	H	2.537379	-1.240999	-3.436555
H	4.520368	-2.589696	-2.045795	H	3.984653	-2.164495	-3.062696
H	-4.522099	-2.589377	-2.045347	H	-4.655914	-1.927605	-2.243790
H	-3.509255	-1.578006	-3.069013	H	-3.275259	-1.068177	-2.911002
H	-3.518590	1.753012	1.750946	H	-3.351356	1.627630	2.275615
H	-3.521614	0.640632	-2.392732	H	-3.647687	1.081456	-1.969751
H	3.519987	1.754359	1.749036	H	3.837576	1.372604	1.638338
H	3.522589	0.640367	-2.394202	H	3.193128	0.883674	-2.576093
H	3.520020	-2.390721	0.642291	H	3.395059	-2.554525	-0.013676
H	-3.523242	-2.391600	0.642586	H	-3.490745	-2.327152	0.634790
S	0.000679	4.688658	-3.032737	S	-0.043368	5.110905	-2.282025
C	0.001083	3.611909	-1.718775	C	0.024548	3.920817	-1.071667
N	1.140676	3.151987	-1.131593	N	1.196199	3.376100	-0.627646
N	-1.138141	3.152124	-1.130595	N	-1.084200	3.419935	-0.451900
H	1.016222	2.369106	-0.490594	H	1.082296	2.530907	-0.055263
H	-1.012914	2.369294	-0.489652	H	-0.919910	2.558398	0.080589
N	-1.140515	-2.552108	-2.161338	N	-1.388846	-2.717284	-1.675633
C	-0.000883	-3.290420	-2.266783	C	-0.334452	-3.198420	-2.389970
H	-1.016613	-1.605379	-1.803872	H	-1.147925	-2.142274	-0.862326
S	-0.000995	-4.966611	-2.544423	S	-0.493356	-4.148059	-3.796262
N	1.138781	-2.552238	-2.161282	N	0.864580	-2.828264	-1.857190
H	1.014878	-1.605444	-1.804150	H	0.814396	-2.257464	-1.006864
N	-1.140166	-0.602363	3.292955	N	-0.868597	-1.004524	3.176229
C	-0.000295	-0.323842	3.984526	C	0.336032	-0.939430	3.807765
H	-1.016546	-0.765796	2.294265	H	-0.825373	-0.945378	2.154844
S	-0.000135	0.275757	5.574100	S	0.497938	-0.707376	5.486070
N	1.139432	-0.602235	3.292730	N	1.401021	-1.107220	2.974211
H	1.015495	-0.766408	2.294251	H	1.182338	-1.033212	1.977792
H	-2.610992	4.362637	-1.957300	H	-2.594818	4.717157	-1.054955
C	-2.458410	3.307343	-1.714152	C	-2.429574	3.640028	-0.958942
H	-2.528847	2.759184	-2.665895	H	-2.531716	3.228036	-1.974867
C	2.460679	3.308770	-1.715290	C	2.448769	3.518972	-1.354976
H	2.531071	2.762273	-2.667994	H	2.344160	3.135276	-2.381344
H	2.612837	4.364541	-1.956713	H	2.678629	4.584035	-1.456221
C	2.458669	-3.136652	-2.006787	C	2.177084	-3.104698	-2.406342
H	2.608887	-3.874065	-2.800285	H	2.029281	-3.629642	-3.352639
H	2.530269	-3.687991	-1.056951	H	2.720109	-3.791618	-1.740306

C	-2.460419	-3.136533	-2.006916	C	-2.793647	-2.941229	-1.953239
H	-2.610780	-3.873579	-2.800725	H	-2.857196	-3.472085	-2.905570
H	-2.531882	-3.688295	-1.057313	H	-3.223212	-3.604432	-1.186918
C	2.458697	-0.173669	3.721295	C	2.761540	-0.796156	3.377683
H	2.611573	-0.495037	4.755462	H	2.954651	-1.277478	4.339700
H	2.526527	0.924836	3.727606	H	2.876891	0.285885	3.545183
C	-2.459595	-0.174891	3.722180	C	-2.107051	-0.598210	3.816351
H	-2.611819	-0.496862	4.756247	H	-2.147740	-1.057353	4.807250
H	-2.528297	0.923553	3.729016	H	-2.118595	0.490493	3.980674
O	-0.000986	-1.122927	0.570590	O	-0.009383	-1.095631	0.293214
N	0.000641	0.000683	0.000061	O	0.122953	1.095208	0.691853
O	-0.000138	0.067919	-1.258327	C	0.025393	0.123388	-0.101129
O	0.002549	1.056644	0.687401	C	-0.100658	0.399244	-1.603139
				H	0.466193	1.285420	-1.888875
				H	0.223856	-0.447798	-2.206431
				H	-1.152451	0.591906	-1.833448

1...HSO₄⁻ (-3273.39761) (0)

H	3.623556	2.070601	-2.780162
H	-3.639683	2.127629	-2.693763
C	3.733739	1.199885	0.545377
C	3.583562	-1.329289	-0.656273
C	3.675841	1.110504	-0.853864
C	3.650669	0.070308	1.364800
C	3.609888	-1.192158	0.743122
C	3.614960	-0.160922	-1.434969
C	3.619438	2.363300	-1.722555
C	3.545124	0.219054	2.881826
C	3.481343	-2.715001	-1.285455
H	4.538891	2.944188	-1.561289
C	-3.624050	-0.122641	-1.372829
C	-3.801897	0.069390	1.418302
C	-3.733888	1.140245	-0.780711
C	-3.601462	-1.296773	-0.604233
C	-3.702635	-1.178583	0.786233
C	-3.866468	1.213075	0.614288
C	-3.637319	2.401427	-1.630830
C	-3.441347	-2.676604	-1.233838
C	-3.736960	0.191011	2.939544
H	-4.535734	3.014539	-1.469646
H	-3.754390	1.252956	3.214920
H	3.542385	1.286311	3.134484
H	-4.641035	-0.254895	3.380585
H	4.452369	-0.200693	3.340467

1...H₂PO₄⁻ (-3217.30793) (0)

H	3.626884	2.155861	-2.683498
H	-3.651323	1.947116	-2.854102
C	3.905902	1.188569	0.604465
C	3.575656	-1.301241	-0.630930
C	3.740739	1.132730	-0.786504
C	3.818425	0.041542	1.400241
C	3.682638	-1.197531	0.760198
C	3.604101	-0.121080	-1.389431
C	3.613522	2.405101	-1.614292
C	3.763421	0.153976	2.922173
C	3.410460	-2.672242	-1.273269
H	4.493241	3.040180	-1.437040
C	-3.642324	-0.239792	-1.470568
C	-3.626965	0.021359	1.324477
C	-3.696630	1.036815	-0.907117
C	-3.590096	-1.397883	-0.676763
C	-3.587568	-1.246548	0.717172
C	-3.736741	1.140579	0.493079
C	-3.655209	2.269462	-1.804897
C	-3.483288	-2.779902	-1.306381
C	-3.506338	0.183830	2.839983
H	-4.583875	2.842113	-1.667111
H	-3.494971	1.253071	3.084967
H	3.781907	1.214759	3.201833
H	-4.415133	-0.224339	3.306213
H	4.669824	-0.293425	3.357586

H	-3.118334	-3.380427	-0.457960	H	-3.188326	-3.501959	-0.535535
H	-4.421825	-3.034770	-1.586291	H	-4.470531	-3.101862	-1.672100
H	4.476209	-3.030565	-1.635837	H	4.393860	-3.046889	-1.600070
H	3.186267	-3.432291	-0.510425	H	3.050473	-3.377464	-0.514959
H	3.736417	2.182663	1.010585	H	3.974943	2.160539	1.090822
H	3.570409	-2.090340	1.358965	H	3.604046	-2.103480	1.358637
H	-3.918008	2.190271	1.092383	H	-3.749556	2.127793	0.948491
H	-3.636876	-2.080038	1.392846	H	-3.510817	-2.135446	1.341670
H	-3.517932	-0.184623	-2.454554	H	-3.603899	-0.331906	-2.553805
H	3.555758	-0.239292	-2.518327	H	3.480820	-0.169869	-2.469889
S	-0.068660	-1.435894	5.246479	S	0.097630	-1.456450	5.244568
C	-0.089672	-0.334490	3.952601	C	0.123336	-0.362273	3.943022
N	-1.250486	0.126610	3.394010	N	-1.036282	0.172693	3.426930
N	1.065288	0.174445	3.416684	N	1.278281	0.072215	3.364968
H	-1.179481	0.492476	2.443912	H	-0.945786	0.693168	2.559983
H	0.986116	0.744714	2.575664	H	1.214131	0.467266	2.417376
N	1.161992	-2.442192	-2.187000	N	1.110132	-2.361657	-2.232416
C	0.013031	-3.128694	-2.453215	C	-0.002084	-3.111955	-2.446179
H	1.041630	-1.469938	-1.907774	H	0.954990	-1.397119	-1.936867
S	-0.008631	-4.704009	-3.099335	S	0.031340	-4.725153	-2.989326
N	-1.109833	-2.423181	-2.140339	N	-1.160175	-2.434816	-2.167522
H	-0.967022	-1.471118	-1.811400	H	-1.045440	-1.432467	-1.997379
N	1.157901	2.847086	-1.935325	N	1.120770	2.816215	-1.860999
C	0.003250	3.558752	-1.738728	C	-0.051651	3.505234	-1.699905
H	1.048513	1.836459	-1.871154	H	1.024556	1.803764	-1.934574
S	0.003268	5.232123	-1.457745	S	-0.094731	5.113349	-1.147442
N	-1.152272	2.825506	-1.817101	N	-1.192398	2.810086	-2.006332
H	-1.043028	1.815200	-1.783481	H	-1.072324	1.794251	-2.027608
H	2.584818	-0.475301	4.684970	H	2.756648	-0.479034	4.729254
C	2.363456	-0.472101	3.613401	C	2.578598	-0.533871	3.650798
H	2.303787	-1.529583	3.317886	H	2.555495	-1.604663	3.402920
C	-2.549394	-0.493776	3.666743	C	-2.325271	-0.510513	3.571626
H	-2.516573	-1.562112	3.410555	H	-2.237295	-1.553781	3.237872
H	-2.730869	-0.446462	4.744528	H	-2.564508	-0.552817	4.637748
C	-2.480478	-2.805950	-2.434215	C	-2.499727	-2.896389	-2.489544
H	-2.457724	-3.846110	-2.765470	H	-2.418728	-3.941327	-2.795507
H	-2.854038	-2.207102	-3.279149	H	-2.885490	-2.335366	-3.354250
C	2.516291	-2.866265	-2.483143	C	2.480525	-2.763784	-2.497978
H	2.472368	-3.915960	-2.781583	H	2.447432	-3.796872	-2.849333
H	2.902605	-2.301840	-3.346187	H	2.879920	-2.153262	-3.321143
C	-2.441618	3.347438	-1.361316	C	-2.511324	3.289267	-1.586384
H	-2.618049	4.292964	-1.881252	H	-2.747246	4.194939	-2.154918
H	-2.390950	3.587231	-0.290171	H	-2.481343	3.593396	-0.532496
C	2.453034	3.352616	-1.480521	C	2.391296	3.312718	-1.321240

H	2.667829	4.279174	-2.020635	H	2.571926	4.297496	-1.761391
H	2.398657	3.615774	-0.415910	H	2.300181	3.464208	-0.238150
S	0.118507	0.297430	0.117322	O	-0.186568	0.221289	-1.442066
O	0.220041	0.182116	-1.383701	O	-0.536065	-0.994317	0.767867
O	0.553950	-1.178240	0.675855	O	-1.102804	1.509488	0.651086
O	-1.258409	0.434642	0.580914	O	1.263945	0.802980	0.675299
O	1.039347	1.296052	0.691727	H	-1.305409	-1.375631	0.309889
H	1.528764	-1.259417	0.589936	H	-0.589919	2.330565	0.761783
				P	-0.033152	0.377376	0.073790

1...H₂O (-2650.10138) (0)

H	3.744593	2.858911	-1.897361
H	-3.080285	1.115415	-3.339331
C	3.605128	0.948616	0.941618
C	3.646166	-1.066399	-1.004561
C	3.599528	1.303084	-0.416395
C	3.635792	-0.388445	1.345339
C	3.655214	-1.384670	0.355208
C	3.629161	0.288062	-1.374475
C	3.512755	2.758322	-0.828181
C	3.578557	-0.757958	2.814019
C	3.580638	-2.150958	-2.060806
H	4.265853	3.351681	-0.294952
C	-3.300239	-0.513507	-1.341007
C	-3.243131	0.637938	1.213940
C	-3.288847	0.880493	-1.218436
C	-3.289380	-1.347674	-0.212968
C	-3.267272	-0.755997	1.053941
C	-3.252944	1.442011	0.067813
C	-3.325974	1.740587	-2.470456
C	-3.270187	-2.861092	-0.346299
C	-3.169392	1.283110	2.590023
H	-4.350423	2.098891	-2.647353
H	-2.825649	2.317866	2.474044
H	3.712786	0.140546	3.426072
H	-4.175302	1.341426	3.027992
H	4.397891	-1.445700	3.062654
H	-2.979536	-3.298173	0.617859
H	-4.282336	-3.236718	-0.550271
H	4.391261	-2.021267	-2.790179
H	3.721017	-3.131650	-1.593409
H	3.583940	1.729339	1.699655
H	3.671200	-2.431774	0.651653
H	-3.203699	2.520925	0.187307

NO₃⁻ (-280.32964) (0)

N	0.000000	0.000000	0.000000
O	0.000000	1.263940	0.000000
O	1.094600	-0.631970	0.000000
O	-1.094600	-0.631970	0.000000

AcO⁻ (-228.49314) (0)

C	1.353097	0.008587	-0.015346
H	1.753066	1.006371	-0.240882
H	1.755685	-0.722982	-0.729059
H	1.724497	-0.274514	0.982490
C	-0.221347	0.002409	-0.010208
O	-0.758504	1.099534	0.286892
O	-0.749073	-1.109056	-0.269026

HSO₄⁻ (-699.67832) (0)

S	0.145939	-0.008541	0.055042
O	-1.324299	0.142471	-0.806841
H	-1.969288	-0.009702	-0.096860
O	0.828548	1.281618	-0.172112
O	0.807742	-1.179021	-0.557526
O	-0.357821	-0.223216	1.439309

H₂PO₄⁻ (-643.57870) (0)

P	-0.073341	-0.127022	0.103716
O	0.055239	0.041770	1.592834
O	1.490045	-0.006574	-0.503140
O	-0.763568	-1.268660	-0.591082
O	-0.759974	1.271099	-0.529337
H	-1.303286	0.932511	-1.257702
H	2.000126	0.274456	0.272222

TU (-548.20984) (0)

N	0.238394	-1.032245	1.146925
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H	-3.240206	-1.396849	1.931792	H	0.048233	-0.533482	2.004608
H	-3.302271	-0.954294	-2.334929	H	0.008404	-2.019044	1.153854
H	3.642186	0.551365	-2.431702	N	0.086629	-1.055756	-1.147929
S	-0.111549	-0.917379	5.266050	H	0.613463	-1.921496	-1.155651
C	0.027829	-0.390027	3.666187	H	0.118065	-0.520379	-2.004264
N	-0.941443	0.346961	3.055342	C	0.048414	-0.311718	-0.000021
N	1.101175	-0.636623	2.859570	S	-0.209613	1.342545	0.000538
H	-0.815826	0.547013	2.068715				
H	0.985711	-0.420015	1.872498	TU^{...}F⁻ (-648.10337) (0)			
N	1.111602	-2.295372	-1.951080	N	-0.456192	-1.124039	0.175932
C	-0.066908	-2.885835	-2.315115	H	0.009834	-1.988217	-0.051617
H	1.057325	-1.622383	-1.187408	H	-1.513846	-0.937049	0.104822
S	-0.355859	-3.578328	-3.828269	N	-0.451438	1.125940	0.163080
N	-1.008747	-2.860290	-1.329865	H	-1.512123	0.942655	0.095959
H	-0.711425	-2.574998	-0.404423	H	0.020538	1.987034	-0.063908
N	1.069712	2.711619	-1.256277	C	0.282885	-0.000718	0.055813
C	-0.218900	3.234081	-1.276929	S	1.992678	-0.006360	-0.184298
H	1.379498	2.314659	-2.140569	F	-2.692349	0.009816	0.017284
S	-0.719102	4.411217	-0.190797				
N	-1.018440	2.658389	-2.215520	TU^{...}Cl⁻ (-1008.51619) (0)			
H	-0.617315	1.939756	-2.807998	N	0.159990	-1.137085	0.180303
H	2.220918	-1.598894	4.296152	H	0.632282	-2.001077	-0.031095
C	2.254685	-1.440780	3.216509	H	-0.870366	-1.075637	0.146717
H	2.187689	-2.429722	2.738104	N	0.167338	1.137001	0.172177
C	-2.272776	0.558068	3.605719	H	-0.863425	1.082068	0.138936
H	-2.707530	-0.405088	3.901960	H	0.645356	1.996468	-0.044727
H	-2.204837	1.153386	4.522172	C	0.880162	-0.002778	0.052431
C	-2.354304	-3.401332	-1.455578	S	2.574500	-0.009160	-0.195880
H	-2.340302	-4.498877	-1.416875	Cl	-2.841654	0.009529	0.008370
H	-2.730174	-3.137841	-2.447544				
C	2.252539	-2.153893	-2.841737	TU^{...}Br⁻ (-3119.73097) (0)			
H	2.226317	-2.986524	-3.546703	N	0.920242	-1.140552	0.191590
H	2.167754	-1.232261	-3.439051	H	1.391383	-2.003209	-0.028665
C	-2.420585	2.982672	-2.458221	H	-0.109916	-1.085818	0.158776
H	-2.513309	3.504275	-3.420074	N	0.928017	1.135860	0.183507
H	-2.714167	3.687689	-1.679860	H	-0.102483	1.087987	0.151149
C	2.150468	3.406020	-0.533563	H	1.405052	1.993703	-0.042778
H	2.166284	4.466903	-0.811216	C	1.638567	-0.005257	0.055995
H	1.926576	3.359100	0.534562	S	3.329185	-0.011941	-0.207863
H	-0.782139	0.113029	-0.321793	Br	-2.246292	0.007508	0.003591
O	0.143515	0.051185	-0.027373				
H	0.561847	0.887945	-0.321303				

2 (-4726.86001) (0)

TU^{...}NO₃⁻ (-828.60141) (0)

C	-3.389745	0.956813	-1.008328	N	0.917425	-1.138028	-0.013596
C	-3.372404	-1.001948	0.990423	H	1.420441	-2.006022	-0.095351
C	-3.402668	1.328793	0.341328	H	-0.112627	-1.116464	-0.086608
C	-3.369935	-0.398358	-1.352578	N	0.926320	1.136292	0.004989
C	-3.356445	-1.381010	-0.355386	H	-0.103457	1.122418	0.081577
C	-3.390593	0.352923	1.342856	H	1.436218	1.999873	0.090903
C	3.759134	0.967406	1.041210	C	1.644383	-0.003822	-0.003619
C	3.784892	-0.905927	-1.037684	S	3.357982	-0.010414	-0.002624
C	3.750389	1.398209	-0.286403	O	-1.920163	1.071466	0.270884
C	3.771944	-0.404175	1.333542	N	-2.560437	0.006549	0.004360
C	3.794142	-1.338048	0.296381	O	-1.928038	-1.061664	-0.267970
C	3.772454	0.459294	-1.327883	O	-3.804017	0.009704	0.009949
H	-3.391469	1.704728	-1.793037				
H	-3.332787	-2.434316	-0.611240				
H	3.790249	0.790755	-2.361029	TU⁺AcO⁻ (-776.77884) (0)			
H	3.829551	-2.398069	0.525742	N	-0.980725	-1.115043	-0.077687
H	3.766714	1.696847	1.844589	H	-1.526123	-1.961187	-0.070524
H	-3.393691	0.658316	2.383128	H	0.057021	-1.145015	0.029801
S	-0.487226	-4.107204	-1.658239	N	-0.917838	1.161950	-0.170186
C	-0.100405	-2.720521	-2.540224	H	0.120337	1.143379	-0.061493
N	1.182214	-2.261993	-2.645783	H	-1.416456	2.034295	-0.232762
N	-1.012955	-1.955508	-3.205748	C	-1.661104	0.040816	-0.180279
H	1.390915	-1.558464	-3.345338	S	-3.377207	0.082480	-0.321596
H	-0.705327	-1.090543	-3.635980	H	4.398944	0.461074	-0.397133
N	-1.031470	-1.815719	3.287423	C	3.919204	-0.083520	0.425603
C	-0.132194	-0.845378	3.619939	H	4.307110	-1.105926	0.464615
H	-0.711233	-2.617728	2.756157	H	4.186071	0.441081	1.352053
S	-0.540580	0.611043	4.369816	C	2.383863	-0.066555	0.242361
N	1.157198	-1.156059	3.292715	O	1.864660	1.079279	0.132182
H	1.379147	-2.113790	3.045155	O	1.803662	-1.186802	0.226566
N	-1.093890	3.748222	-0.076803	TU⁺HSO₄⁻ (-1247.93909) (0)			
C	-0.184677	3.562590	-1.076776	N	1.621139	-1.142557	-0.055336
H	-0.783518	3.680943	0.886095	H	2.149336	-1.999159	-0.073549
S	-0.578431	3.496619	-2.717341	H	0.596488	-1.171300	-0.132535
N	1.100678	3.430129	-0.634984	N	1.600659	1.143490	-0.029152
H	1.314349	3.680246	0.324001	H	0.573122	1.155512	-0.027058
H	-2.674355	-2.598650	-4.331042	H	2.110449	2.008630	0.040146
C	-2.424022	-2.251640	-3.320903	C	2.323082	0.006424	-0.012407
H	-2.657780	-3.051993	-2.618816	S	4.034933	0.020817	0.057823
C	2.328147	-3.027556	-2.177568	H	-3.626022	-0.553692	1.252668
H	2.177671	-3.307226	-1.134505	O	-2.743699	-0.181128	1.420808
H	2.463283	-3.951041	-2.754152	S	-2.086408	-0.028490	-0.122119
C	2.288690	-0.350221	3.726266	O	-1.250128	-1.244744	-0.308608
H	2.415635	-0.381464	4.815468	O	-1.287263	1.216167	-0.013019

H	2.123689	0.689126	3.441157	O	-3.274971	0.035673	-0.993151
C	-2.445627	-1.781736	3.588448				
H	-2.695730	-2.491579	4.386542	TU ⁺ H ₂ PO ₄ ⁻ (-1191.84893) (0)			
H	-2.690538	-0.778351	3.936906	N	-1.550152	-1.160197	0.110082
C	2.239440	3.415929	-1.541595	H	-2.069523	-2.021081	0.162560
H	2.354205	4.374337	-2.062646	H	-0.517125	-1.188655	0.056860
H	2.094089	2.643393	-2.297138	N	-1.580706	1.120889	-0.092866
C	-2.508206	3.981015	-0.269706	H	-0.548138	1.175554	-0.053794
H	-2.770920	5.023993	-0.053674	H	-2.122554	1.968432	-0.134016
H	-2.740797	3.782651	-1.315928	C	-2.273225	-0.028618	0.014817
S	-3.502489	-0.786856	-3.098238	S	-3.991721	-0.050324	0.029414
S	-3.573673	3.030747	0.879806	H	2.925156	-0.809480	-1.729818
S	3.810890	3.159732	-0.638450	O	3.041695	0.052000	-1.299768
S	3.886649	-2.089807	-2.385871	P	1.996151	0.025139	-0.013878
S	3.862349	-0.978468	3.033924	O	3.053365	0.024542	1.262639
S	-3.508873	-2.322147	2.196901	O	1.242111	1.333351	0.059535
				O	1.274461	-1.301514	-0.080793
				H	2.919746	0.883166	1.693427
2...F⁻ (-4826.88355) (0)				2...Cl⁻ (-5187.22747) (0)			
C	-3.671624	-1.379822	-0.190470	C	-3.688134	-1.325566	0.130869
C	-3.665154	1.404570	0.110857	C	-3.625217	1.466856	-0.044288
C	-3.650874	-0.557500	-1.321906	C	-3.685520	-0.702924	-1.121538
C	-3.675618	-0.817549	1.093837	C	-3.645971	-0.551471	1.296637
C	-3.685111	0.573683	1.239828	C	-3.627521	0.844351	1.209721
C	-3.660276	0.835737	-1.167183	C	-3.668482	0.694275	-1.209387
C	3.683215	0.097212	-1.352283	C	3.760834	-0.037430	-1.444377
C	3.652916	-0.119307	1.440033	C	3.786625	-0.118201	1.354770
C	3.668264	-1.166599	-0.752451	C	3.734420	-1.269246	-0.782696
C	3.670813	1.255853	-0.563030	C	3.787898	1.157313	-0.711524
C	3.668620	1.143439	0.831363	C	3.814573	1.113442	0.686031
C	3.665498	-1.270747	0.645567	C	3.760524	-1.306779	0.618386
H	-3.652763	-2.457419	-0.316038	H	-3.672622	-2.407188	0.212838
H	-3.676943	1.004161	2.235851	H	-3.565350	1.455146	2.103985
H	3.642266	-2.245809	1.121218	H	3.735609	-2.255236	1.144939
H	3.648787	2.043019	1.437743	H	3.831866	2.043653	1.244398
H	3.673501	0.172605	-2.434717	H	3.735861	-0.018322	-2.528989
H	-3.633240	1.482917	-2.037678	H	-3.639403	1.163112	-2.187235
S	-0.051162	-1.737898	4.707259	S	0.045481	0.198126	5.600912
C	-0.031884	-1.152044	3.124899	C	0.008424	0.096943	3.907400
N	0.769900	-0.130453	2.692196	N	1.058711	0.417618	3.100062
N	-0.814324	-1.639371	2.113962	N	-1.097285	-0.304167	3.217396
H	0.724483	0.074558	1.688008	H	0.911272	0.362830	2.089208
H	-0.744230	-1.141375	1.218952	H	-1.067845	-0.227950	2.198981

N	-0.794664	2.664986	0.355349	N	-1.088231	2.963679	-1.302467
C	0.006899	3.282920	-0.565636	C	0.000092	3.343385	-2.031666
H	-0.737045	1.640689	0.377822	H	-1.058724	2.040856	-0.864366
S	0.013817	4.945226	-0.855633	S	0.027487	4.756263	-2.971385
N	0.804927	2.384384	-1.220577	N	1.041680	2.469684	-1.935971
H	0.739205	1.413503	-0.895681	H	0.899150	1.624803	-1.376847
N	-0.763001	-1.009792	-2.497032	N	-1.214105	-2.586868	-1.878385
C	0.024681	-2.126703	-2.563438	C	-0.142863	-3.431004	-1.870930
H	-0.706503	-0.478466	-1.621078	H	-1.150277	-1.743846	-1.304616
S	0.037268	-3.204104	-3.861707	S	-0.173789	-4.956814	-2.613316
N	0.799072	-2.262507	-1.443022	N	0.932568	-2.928670	-1.201447
H	0.730967	-1.498854	-0.761281	H	0.826910	-2.012973	-0.757381
H	-1.929101	-3.212875	1.389576	H	-2.304288	-0.927804	4.795927
C	-1.869352	-2.582477	2.278712	C	-2.400263	-0.413486	3.837111
H	-1.684668	-3.190265	3.165288	H	-2.839194	0.571367	4.038757
C	1.816302	0.466704	3.452998	C	2.334411	0.886617	3.549342
H	1.891444	1.523976	3.191408	H	2.546259	1.872007	3.125085
H	1.609290	0.351424	4.517519	H	2.316736	0.957799	4.638423
C	1.869506	2.727010	-2.103253	C	2.293702	2.596286	-2.618410
H	1.682039	3.707403	-2.542842	H	2.272944	3.506629	-3.220375
H	1.946705	1.967699	-2.883762	H	2.458968	1.734148	-3.270758
C	-1.853025	3.294008	1.072656	C	-2.388364	3.573840	-1.477171
H	-1.931579	2.843231	2.063776	H	-2.276564	4.659576	-1.518300
H	-1.656838	4.363641	1.155077	H	-2.863362	3.259916	-2.414797
C	1.849242	-3.212517	-1.284582	C	2.179250	-3.606298	-1.011839
H	1.660107	-4.080023	-1.917937	H	2.120949	-4.585075	-1.491470
H	1.905940	-3.510812	-0.236064	H	2.381727	-3.736793	0.054978
C	-1.807092	-0.688098	-3.411905	C	-2.536501	-3.019788	-2.275393
H	-1.872255	0.396936	-3.512815	H	-2.467388	-3.596733	-3.200276
H	-1.605142	-1.149283	-4.379393	H	-2.996334	-3.669211	-1.520441
F	-0.010858	0.000095	0.002487	Cl	-0.068774	0.004758	-0.006487
S	-3.577864	-1.847735	2.559200	S	-3.576218	-1.427628	2.862119
S	-3.520219	-1.310002	-2.944841	S	-3.661767	-1.624584	-2.662039
S	3.562856	-2.624708	-1.791753	S	3.658351	-2.771387	-1.766362
S	3.522783	-0.289393	3.220951	S	3.774124	-0.219541	3.148748
S	3.565800	2.885063	-1.306531	S	3.782918	2.762890	-1.518497
S	-3.552506	3.187476	0.273274	S	-3.524798	3.259143	-0.072702

2...Br⁻ (-7298.44119) (0)

C	-3.701336	-1.336778	-0.380629
C	-3.687850	1.374779	0.313511
C	-3.679033	-0.359033	-1.381290
C	-3.704846	-0.959935	0.967691
C	-3.710775	0.395723	1.313860

2...NO₃⁻ (-5007.31232) (0)

C	-3.546842	0.652952	1.244565
C	-3.547853	-0.654608	-1.232065
C	-3.543116	-0.745209	1.194110
C	-3.540203	1.401712	0.059263
C	-3.549169	0.746394	-1.176888

C	-3.683187	0.997116	-1.033604	C	-3.552598	-1.397898	-0.046604
C	3.789813	0.678868	-1.179756	C	3.549988	-1.403378	-0.057731
C	3.748935	-0.717344	1.247152	C	3.542796	1.396187	0.049146
C	3.772342	-0.719956	-1.180822	C	3.545751	-0.751106	1.183235
C	3.774284	1.383725	0.031051	C	3.542625	-0.659679	-1.242923
C	3.765876	0.683731	1.242281	C	3.546557	0.741305	-1.187246
C	3.764196	-1.416092	0.035243	C	3.552054	0.647016	1.234180
H	-3.675592	-2.390869	-0.635163	H	-3.521298	1.175969	2.194347
H	-3.691927	0.702335	2.354150	H	-3.524544	1.306749	-2.105177
H	3.745677	-2.500637	0.050776	H	3.530501	1.169705	2.184246
H	3.747468	1.239791	2.173511	H	3.519793	1.302075	-2.115225
H	3.790238	1.208010	-2.126773	H	3.526263	-2.487407	-0.080051
H	-3.643010	1.744693	-1.818543	H	-3.530831	-2.481975	-0.068669
S	-0.077598	-2.031161	5.334330	S	0.002642	5.668708	-1.152366
C	-0.066080	-1.468741	3.733125	C	0.001433	3.973331	-1.163383
N	1.044321	-0.989432	3.103376	N	1.131164	3.210645	-1.194477
N	-1.179221	-1.443581	2.945133	N	-1.129457	3.212230	-1.192413
H	0.927455	-0.616557	2.158390	H	1.000311	2.199031	-1.170787
H	-1.093668	-1.008039	2.024422	H	-0.999967	2.200425	-1.169254
N	-1.126051	3.289565	-0.224797	N	-1.135832	-2.630911	-2.188751
C	0.000255	3.966424	-0.591011	C	-0.006845	-2.985658	-2.866020
H	-1.056434	2.273271	-0.140319	H	-1.003822	-2.106344	-1.323631
S	0.014026	5.631666	-0.917609	S	-0.009741	-3.820286	-4.341952
N	1.100740	3.165774	-0.675092	N	1.124752	-2.632708	-2.192172
H	0.967897	2.163480	-0.522087	H	0.996132	-2.107709	-1.326790
N	-1.130089	-1.833785	-2.738166	N	-1.125392	-0.572132	3.378833
C	-0.008906	-2.500826	-3.136588	C	0.005486	-0.979275	4.022643
H	-1.060092	-1.256754	-1.897334	H	-0.995991	-0.087852	2.490043
S	0.002272	-3.605893	-4.424543	S	0.006915	-1.835492	5.485909
N	1.089236	-2.192732	-2.389337	N	1.135181	-0.574734	3.375139
H	0.958817	-1.559015	-1.597605	H	1.004050	-0.090017	2.486854
H	-2.490758	-2.403148	4.235925	H	-2.433999	4.802677	-1.151573
C	-2.515924	-1.641916	3.453787	C	-2.470565	3.712501	-1.208903
H	-2.922024	-0.725349	3.898248	H	-2.982954	3.425707	-2.132644
C	2.340103	-0.846660	3.699604	C	2.472935	3.709064	-1.214943
H	2.599147	0.210072	3.817609	H	2.982086	3.422007	-2.140408
H	2.325219	-1.318601	4.683579	H	2.438057	4.799267	-1.157028
C	2.405106	3.590050	-1.092410	C	2.465558	-2.906181	-2.612711
H	2.406616	4.678031	-1.178806	H	2.429362	-3.402756	-3.584891
H	2.662278	3.157379	-2.064136	H	2.970519	-3.565536	-1.899619
C	-2.453579	3.848939	-0.325116	C	-2.478342	-2.902939	-2.604780
H	-2.416146	4.906928	-0.058195	H	-2.445959	-3.399761	-3.576965
H	-2.848348	3.780144	-1.346118	H	-2.981710	-3.561526	-1.889847
C	2.388143	-2.779907	-2.541887	C	2.477449	-0.805064	3.816765

H	2.388057	-3.396787	-3.442241	H	2.443899	-1.395392	4.735185
H	2.633212	-3.409756	-1.681355	H	2.987211	0.140944	4.025486
C	-2.458377	-2.173021	-3.190684	C	-2.466745	-0.800069	3.824427
H	-2.412418	-2.469975	-4.240334	H	-2.431535	-1.390135	4.742952
H	-2.877438	-3.015312	-2.627029	H	-2.974277	0.146879	4.034277
Br	-0.047519	-0.000446	0.000598	O	-0.000620	-1.240999	0.212926
S	-3.689819	-2.275342	2.191624	N	0.000214	0.001011	-0.001688
S	-3.631705	-0.761430	-3.131803	O	-0.000985	0.436472	-1.184612
S	3.770329	-1.565187	-2.767535	O	0.002264	0.807854	0.966797
S	3.718157	-1.669304	2.771754	S	-3.518111	3.187790	0.225507
S	3.771791	3.180596	0.090943	S	-3.521406	-1.779758	2.659371
S	-3.652726	3.091716	0.841168	S	3.526933	-1.786097	2.648227
				S	3.524019	3.182231	0.216033
				S	3.524662	-1.409346	-2.872450
				S	-3.536554	-1.404891	-2.861360

2...AcO⁻ (-4955.49236) (0)

C	-3.589454	-1.370579	-0.334953
C	-3.592337	1.399248	0.108231
C	-3.620452	-0.486030	-1.417349
C	-3.571058	-0.868159	0.973253
C	-3.575668	0.514481	1.196722
C	-3.645058	0.893532	-1.193783
C	3.524815	0.494550	-1.203432
C	3.810888	-0.453329	1.412460
C	3.672515	-0.877527	-0.970621
C	3.520585	1.400756	-0.132885
C	3.669302	0.920308	1.176818
C	3.829501	-1.347829	0.339098
H	-3.542618	-2.442269	-0.494443
H	-3.530128	0.909064	2.206838
H	3.944418	-2.408524	0.533730
H	3.656139	1.616937	2.009599
H	3.397974	0.834905	-2.224974
H	-3.640566	1.558060	-2.050008
S	-0.147770	-1.042046	5.564387
C	0.040610	-1.286584	3.896724
N	1.241326	-1.216754	3.247342
N	-1.007939	-1.574629	3.073385
H	1.181781	-1.175492	2.222656
H	-0.823298	-1.533653	2.068367
N	-1.299556	3.171316	-1.290978
C	-0.126027	3.842667	-1.469609
H	-1.230643	2.146279	-1.262638

2...HSO₄⁻ (-5426.62400) (0)

C	-3.686760	0.738692	-1.921813
C	-3.899780	-0.728067	0.461674
C	-3.813609	1.402881	-0.697333
C	-3.611953	-0.658770	-1.949418
C	-3.744508	-1.388830	-0.763990
C	-3.938166	0.671981	0.489515
C	3.356942	0.449005	1.958012
C	4.062990	-0.648017	-0.520153
C	3.796873	1.279613	0.920131
C	3.274700	-0.934858	1.760618
C	3.642830	-1.480688	0.521137
C	4.180648	0.730898	-0.306573
H	-3.561960	1.302269	-2.840511
H	-3.676945	-2.472136	-0.779096
H	4.480928	1.378000	-1.124000
H	3.552468	-2.551085	0.361252
H	3.048306	0.905203	2.891445
H	-4.033364	1.211648	1.425550
S	0.778082	-4.083335	-3.739466
C	0.632980	-2.502972	-3.133411
N	1.720834	-1.789071	-2.712276
N	-0.562472	-1.846340	-3.050298
H	1.572015	-0.928010	-2.183366
H	-0.611197	-1.003189	-2.476405
N	-1.839529	-0.477749	3.131682
C	-0.861941	-1.065144	3.879720
H	-1.534347	0.110427	2.356285

S	0.018198	5.529528	-1.457352	S	-1.150215	-2.208571	5.090519
N	0.918149	2.987827	-1.703226	N	0.385992	-0.580152	3.576732
H	0.705999	1.988724	-1.622487	H	0.438657	0.108128	2.824636
N	-1.097105	-2.043957	-2.569173	N	-1.018861	3.450117	-0.315473
C	-0.027303	-2.876518	-2.682066	C	0.219721	3.988794	-0.541263
H	-0.986997	-1.186499	-2.015735	H	-1.047434	2.599595	0.242001
S	0.007646	-4.176838	-3.776585	S	0.501369	5.215364	-1.675122
N	0.979741	-2.576112	-1.814892	N	1.213332	3.470682	0.245366
H	0.757127	-1.954137	-1.023786	H	0.998555	2.595530	0.719222
H	-2.537018	-2.070007	4.411518	H	-1.774177	-3.239203	-4.012844
C	-2.381686	-1.454092	3.521999	C	-1.829314	-2.550412	-3.168143
H	-2.626974	-0.422881	3.802098	H	-2.042455	-3.140382	-2.269451
C	2.406908	-0.617010	3.859259	C	3.008682	-2.435553	-2.511384
H	2.347367	0.478816	3.855053	H	2.959145	-3.193412	-1.721125
H	2.473878	-0.942653	4.899183	H	3.306775	-2.951275	-3.427296
C	2.286018	3.374813	-1.842865	C	1.614181	-1.062664	4.127388
H	2.329597	4.445501	-2.050416	H	1.381382	-1.734110	4.956266
H	2.747285	2.827550	-2.667738	H	2.225870	-0.236299	4.497475
C	-2.576613	3.782255	-1.057426	C	-3.246940	-0.727596	3.256913
H	-2.426525	4.849739	-0.878726	H	-3.415303	-1.301081	4.170092
H	-3.239622	3.668205	-1.921527	H	-3.785565	0.220954	3.327621
C	2.278397	-3.162381	-1.845983	C	2.614166	3.669595	-0.095512
H	2.291814	-3.968579	-2.581881	H	2.814765	4.738501	-0.186696
H	2.541804	-3.559348	-0.862699	H	2.863440	3.195848	-1.051104
C	-2.391865	-2.403279	-3.107823	C	-2.105945	3.612911	-1.268389
H	-2.298018	-2.699514	-4.156999	H	-2.154646	4.661300	-1.565739
H	-2.819124	-3.258137	-2.570183	H	-1.939505	3.008451	-2.166793
O	-0.345710	0.464723	-1.037243	S	-3.276397	-1.465358	-3.526675
O	0.298772	-1.001507	0.519088	S	-3.769526	3.202301	-0.593087
S	-3.594151	-2.081605	2.301408	S	3.782038	3.061240	1.192621
S	-3.584526	-1.016668	-3.128655	S	4.395167	-1.273410	-2.174818
S	3.654137	-2.005628	-2.364950	S	2.664729	-2.098516	2.990413
S	3.989995	-1.124099	3.073258	S	-4.031845	-1.755307	1.928243
S	3.364466	3.178298	-0.334167	S	0.081969	0.119782	-0.094009
S	-3.468288	3.158131	0.444407	O	1.386094	0.380502	-0.727233
C	0.016873	1.298851	1.190022	O	0.072376	-1.442757	0.411977
H	0.834871	1.988016	0.955154	O	-0.125174	0.940894	1.157923
H	-0.907159	1.880705	1.159197	O	-1.055481	0.176464	-1.015708
H	0.166631	0.917330	2.200199	H	0.859658	-1.614630	0.967617
C	-0.016524	0.173889	0.155913				

2...H₂PO₄⁻ (-5370.53721) (0)

C	-3.621596	0.647958	-1.827071
C	-4.155637	-0.852622	0.486079

2...H₂O (-4803.29742) (0)

C	3.400698	0.999274	1.225112
C	2.146361	2.889389	-0.435318

C	-3.843058	1.297872	-0.605815	C	2.552761	1.970613	1.775871
C	-3.646284	-0.752136	-1.896373	C	3.588303	0.949442	-0.163966
C	-3.926979	-1.501798	-0.741351	C	2.961926	1.893595	-0.987662
C	-4.151999	0.547254	0.535892	C	1.924043	2.914252	0.948003
C	3.569000	0.690558	1.914220	C	-3.667483	-1.519858	0.443639
C	3.997920	-0.453432	-0.609267	C	-2.447920	-2.416007	-1.917405
C	3.872597	1.504991	0.817812	C	-2.791783	-2.607050	0.476519
C	3.446687	-0.692179	1.745584	C	-3.918002	-0.855740	-0.766405
C	3.700764	-1.263876	0.492463	C	-3.315358	-1.312218	-1.943632
C	4.087846	0.935142	-0.443290	C	-2.190919	-3.064393	-0.704026
H	-3.381589	1.217503	-2.718054	H	3.915425	0.285500	1.858400
H	-3.918773	-2.586934	-0.780181	H	3.100128	1.834236	-2.062136
H	4.292764	1.565982	-1.302133	H	-1.521383	-3.918198	-0.688373
H	3.601748	-2.336566	0.366858	H	-3.515651	-0.801961	-2.880557
H	3.369102	1.155241	2.873259	H	-4.149019	-1.189724	1.358531
H	-4.297894	1.065173	1.477696	H	1.282127	3.666880	1.393593
S	0.740604	-4.218847	-3.509892	S	2.493349	-2.660179	-3.614944
C	0.621850	-2.562224	-3.166616	C	1.662111	-1.822574	-2.425170
N	1.703466	-1.777899	-2.899127	N	0.414307	-1.273773	-2.597377
N	-0.574134	-1.889391	-3.152625	N	2.143859	-1.601766	-1.160336
H	1.491162	-0.866086	-2.480497	H	-0.003045	-0.823271	-1.786728
H	-0.547070	-0.954534	-2.739709	H	1.557504	-1.047818	-0.542617
N	-1.931367	-0.761393	2.966504	N	-0.962169	3.232337	-0.671969
C	-0.893191	-1.152053	3.764284	C	-2.201754	3.220280	-0.080299
H	-1.703558	-0.356790	2.057245	H	-0.764750	2.499466	-1.344656
S	-1.088345	-2.038623	5.191971	S	-2.938356	4.604952	0.520440
N	0.322668	-0.728665	3.282014	N	-2.729368	1.962488	-0.012722
H	0.331639	-0.012951	2.540508	H	-2.091314	1.180301	-0.149701
N	-0.901228	3.340178	-0.236397	N	0.896897	-0.171459	3.705216
C	0.273296	4.025005	-0.468199	C	0.854576	-1.391099	3.101454
H	-0.791040	2.457189	0.256302	H	0.044071	0.373836	3.770524
S	0.372855	5.396454	-1.459371	S	2.178034	-2.395598	2.889876
N	1.342618	3.512055	0.194912	N	-0.414976	-1.728256	2.631641
H	1.235465	2.560797	0.570390	H	-1.188702	-1.320196	3.154572
H	-1.831932	-3.339188	-3.956507	H	3.498107	-2.084757	0.313593
C	-1.838436	-2.600428	-3.152403	C	3.495824	-1.795725	-0.738020
H	-2.007231	-3.145953	-2.215203	H	3.960911	-2.569590	-1.349995
C	2.977723	-2.368902	-2.525683	C	-0.463009	-1.567433	-3.686547
H	2.876972	-3.006504	-1.640737	H	-1.061748	-0.683630	-3.917285
H	3.350793	-2.994976	-3.339533	H	0.125831	-1.859409	-4.557228
C	1.577228	-0.879609	3.971905	C	-4.073816	1.656800	0.394685
H	1.412694	-1.472026	4.874085	H	-4.635040	2.589820	0.471288
H	1.976398	0.097711	4.255894	H	-4.091524	1.162299	1.371209
C	-3.328449	-0.944330	3.242843	C	-0.188250	4.449661	-0.834603

H	-3.430781	-1.544608	4.149792	H	-0.651614	5.156299	-1.534277
H	-3.820588	0.020482	3.400134	H	-0.103396	4.956297	0.128293
C	2.697407	3.931028	-0.109684	C	-0.694543	-3.131675	2.264737
H	2.777656	5.018552	-0.041773	H	-0.368779	-3.815854	3.055152
H	2.984016	3.642128	-1.127588	H	-0.144711	-3.380453	1.357329
C	-2.000950	3.400535	-1.176116	C	2.099007	0.481253	4.182732
H	-2.036594	4.411067	-1.583996	H	2.064241	0.615331	5.269364
H	-1.859358	2.694217	-2.001343	H	2.944253	-0.162089	3.940462
S	-3.304972	-1.532100	-3.487083	S	4.614103	-0.300773	-0.940866
S	-3.672294	3.081511	-0.443229	S	2.316626	2.188812	3.543324
S	3.939214	3.285563	1.084379	S	-2.482541	-3.427067	2.048002
S	4.304776	-1.124514	-2.253042	S	-1.635139	-3.003011	-3.404563
S	2.910532	-1.806475	3.059192	S	-4.979238	0.591808	-0.819428
S	-4.305315	-1.877754	1.957730	S	1.446116	4.083087	-1.570923
O	0.823362	-1.547188	0.061574	H	-0.385256	-0.524431	0.902535
O	-1.341891	-0.236257	0.238921	O	-0.226314	0.075194	0.141627
O	0.671069	0.894233	0.991600	H	0.309689	0.811432	0.488594
O	0.406501	0.340695	-1.577013				
H	-1.814289	-0.850708	-0.347189				
P	0.242614	-0.035767	-0.129689				
H	0.925221	-1.788376	1.001022				

3 (-2633.28348) (0)

H	3.404168	-3.476922	-0.409082
H	-3.137750	-2.395592	-2.800801
C	3.686242	-0.084213	-0.855748
C	3.288918	-0.198068	1.913253
C	3.541861	-1.332066	-0.227286
C	3.635094	1.098806	-0.118799
C	3.435511	1.030899	1.270051
C	3.344436	-1.377937	1.152745
C	3.568177	-2.607563	-1.055739
C	3.758912	2.451906	-0.803128
C	3.038009	-0.272877	3.411646
H	4.539211	-2.730454	-1.545858
C	-3.423704	-1.242054	-0.492633
C	-3.303483	1.555203	-0.466642
C	-3.227197	-0.553710	-1.689761
C	-3.567025	-0.556349	0.725647
C	-3.499364	0.836861	0.725056
C	-3.163890	0.849854	-1.661971
C	-3.103676	-1.318237	-2.989841
C	-3.809919	-1.301203	2.020260
C	-3.261804	3.068139	-0.472495

3...F⁻ (-2733.23499) (0)

H	-3.977773	3.129589	1.061040
H	3.376167	3.285160	0.795617
C	-3.438658	1.192108	-1.706830
C	-3.903804	-0.811554	0.186397
C	-3.677774	1.550414	-0.372299
C	-3.413343	-0.142825	-2.105929
C	-3.662882	-1.135423	-1.147353
C	-3.922218	0.540808	0.556705
C	-3.565515	2.991759	0.053322
C	-3.026124	-0.530686	-3.509770
C	-4.039991	-1.883564	1.236931
H	-4.141946	3.650902	-0.605999
C	3.235026	0.835599	1.607580
C	3.525775	-1.149582	-0.342229
C	3.513803	1.202891	0.291326
C	3.097169	-0.512937	1.970222
C	3.245231	-1.492953	0.989125
C	3.657934	0.197761	-0.677139
C	3.636716	2.666535	-0.068515
C	2.775430	-0.917164	3.391330
C	3.668081	-2.206885	-1.414369

H	-3.941503	-1.086692	-3.658301	H	4.668692	2.917998	-0.344402
H	-3.049702	3.437346	-1.480743	H	3.767923	-1.731633	-2.394926
H	3.870052	2.315940	-1.884762	H	-3.062203	0.341703	-4.174640
H	-4.232890	3.484817	-0.179428	H	4.572210	-2.808262	-1.255514
H	4.639704	2.990300	-0.438829	H	-3.723331	-1.264824	-3.929791
H	-3.854592	-0.599339	2.858810	H	2.597184	-1.995608	3.440516
H	-4.772859	-1.825097	1.993040	H	3.616633	-0.699954	4.061845
H	3.847517	-0.812385	3.913348	H	-4.902482	-1.699997	1.887880
H	2.991920	0.736926	3.834750	H	-4.211321	-2.861592	0.769360
H	3.832959	-0.051137	-1.932828	H	-3.222567	1.971421	-2.436000
H	3.387529	1.955516	1.840452	H	-3.621632	-2.182586	-1.443049
H	-2.993406	1.389108	-2.590801	H	3.838816	0.483048	-1.710788
H	-3.589327	1.382561	1.661364	H	3.106135	-2.540573	1.245523
H	-3.458293	-2.328958	-0.493525	H	3.084684	1.602947	2.363313
H	3.222061	-2.334999	1.654672	H	-4.085239	0.803704	1.600745
N	1.456315	3.146776	-1.282735	N	-0.738292	-0.994569	-2.682708
H	1.476704	2.392869	-1.955881	H	-0.944908	-0.506366	-1.786538
N	0.595267	-0.327980	3.623353	N	-1.660407	-1.524419	1.821622
H	0.646501	0.620162	3.276371	H	-1.513564	-0.964319	0.955922
N	1.256583	-2.916152	-1.816411	N	-1.103278	2.728287	0.061590
H	1.065663	-3.096845	-0.840277	H	-1.197072	1.693538	-0.001880
C	2.547877	3.332234	-0.479401	C	-1.629076	-1.165283	-3.689193
C	1.752612	-1.052860	3.705312	C	-2.846112	-2.058950	2.201675
C	2.524418	-2.548803	-2.175386	C	-2.143833	3.595992	0.072247
O	2.542992	4.114907	0.465532	O	-1.386419	-1.770136	-4.736959
C	-0.496048	3.096751	0.247536	C	0.790064	-2.469690	-1.480646
H	-0.634386	2.023066	0.078608	H	0.733127	-1.822772	-0.600426
H	0.159271	3.226378	1.113096	H	-0.006752	-3.216462	-1.392941
C	0.170079	3.761522	-0.966789	C	0.569956	-1.629955	-2.743445
H	0.336964	4.820477	-0.754239	H	0.603369	-2.244070	-3.645479
H	-0.464163	3.688703	-1.855238	H	1.354457	-0.864510	-2.821868
S	-2.097927	3.837933	0.737458	S	2.327662	-3.475398	-1.468891
S	-1.626315	-0.906434	-4.019771	S	2.667556	3.212775	-1.542192
S	-2.611533	-2.655574	2.398030	S	1.370700	-0.016151	4.182028
C	-0.245730	-1.241652	-2.863235	C	0.977534	2.577046	-1.201698
H	-0.480441	-0.803100	-1.887076	H	0.979693	1.490187	-1.078099
H	0.612804	-0.708869	-3.281058	H	0.427212	2.803571	-2.121558
C	0.127882	-2.725220	-2.722804	C	0.264586	3.220497	-0.007373
H	-0.713192	-3.310179	-2.339355	H	0.799314	2.973775	0.920371
H	0.401696	-3.124726	-3.702507	H	0.226181	4.307758	-0.099149
C	-1.012033	-1.762400	2.391792	C	0.019874	-0.157918	2.944265
H	-0.250392	-2.538430	2.276134	H	-0.776899	0.468066	3.360843
H	-0.972184	-1.107662	1.514199	H	0.313690	0.278084	1.985253
C	-0.710677	-0.978665	3.678352	C	-0.511001	-1.576702	2.713668

H	-1.464040	-0.205979	3.857717	H	0.277570	-2.200569	2.270795
H	-0.717425	-1.663827	4.529579	H	-0.831029	-2.043830	3.647058
O	2.800141	-2.157342	-3.305152	O	-2.025025	4.823327	0.116360
O	1.759689	-2.254557	3.952344	O	-3.020716	-2.690349	3.247338
				F	-0.718067	0.051421	-0.176989

3...Cl⁻ (-3093.60800) (0)

H	-4.222399	3.570697	-0.339870
H	2.913486	3.065625	1.741279
C	-3.355824	0.776839	-1.984334
C	-3.907626	-0.400818	0.495475
C	-3.537677	1.597003	-0.864769
C	-3.441110	-0.618872	-1.895342
C	-3.718240	-1.188887	-0.647597
C	-3.815825	0.989744	0.366822
C	-3.471406	3.103793	-0.989525
C	-3.272476	-1.486395	-3.123801
C	-4.239529	-1.035285	1.828626
H	-3.729966	3.411115	-2.009630
C	3.162240	0.484386	1.856142
C	3.579369	-0.796944	-0.594647
C	3.425697	1.251139	0.715249
C	3.099495	-0.910165	1.791151
C	3.311595	-1.538823	0.558844
C	3.635412	0.598379	-0.502182
C	3.480249	2.763240	0.854960
C	2.819689	-1.777325	3.007037
C	3.824004	-1.441898	-1.948715
H	4.513584	3.098037	1.018222
H	3.609199	-0.716320	-2.739643
H	-3.724328	-0.998212	-3.996484
H	4.882114	-1.715559	-2.058641
H	-3.815216	-2.430647	-2.998135
H	2.427081	-2.744681	2.678084
H	3.749991	-1.988771	3.551399
H	-4.803443	-0.332149	2.452856
H	-4.900735	-1.898609	1.682635
H	-3.152911	1.235745	-2.950656
H	-3.797913	-2.271604	-0.564752
H	3.810081	1.193157	-1.395437
H	3.235206	-2.620978	0.483763
H	2.967351	0.977535	2.805587
H	-3.973555	1.615583	1.243739
N	-0.810013	-1.408123	-2.879130

3...NO₃⁻ (-2913.69277) (0)

H	4.227531	-0.749364	3.267155
H	-2.856563	0.394862	3.377622
C	3.469046	-1.385935	0.072537
C	3.480057	1.413348	-0.081087
C	3.474177	-0.637498	1.258201
C	3.469481	-0.772479	-1.187474
C	3.472167	0.628762	-1.242397
C	3.477370	0.760756	1.160109
C	3.572512	-1.330770	2.603900
C	3.565387	-1.592865	-2.459974
C	3.587207	2.924651	-0.156648
H	4.054333	-2.306934	2.489238
C	-3.352830	1.081148	0.901348
C	-3.363136	-1.051219	-0.910201
C	-3.359639	-0.235423	1.387198
C	-3.353123	1.346269	-0.468338
C	-3.358629	0.267396	-1.365879
C	-3.365000	-1.289476	0.472840
C	-3.375971	-0.439990	2.895832
C	-3.364173	2.754704	-1.046202
C	-3.383292	-2.255079	-1.841883
H	-4.408490	-0.415023	3.269178
H	-2.867540	-3.091757	-1.359177
H	4.214211	-2.462059	-2.285122
H	-4.417288	-2.586799	-2.006392
H	4.053559	-1.009750	-3.247190
H	-2.845989	2.750172	-2.010843
H	-4.395898	3.068676	-1.253943
H	4.073543	3.312381	0.744069
H	4.242146	3.202540	-0.993772
H	3.494165	-2.472351	0.134528
H	3.500320	1.118954	-2.213911
H	-3.339796	-2.310631	0.844829
H	-3.328356	0.454162	-2.436416
H	-3.318504	1.914443	1.598674
H	3.509113	1.357059	2.070183
N	1.201038	-2.313138	-2.343932

H	-0.951376	-0.860694	-2.026061	H	1.141717	-1.846048	-1.440202
N	-1.838396	-1.457428	2.261261	N	1.224178	3.194931	-0.837973
H	-1.635187	-0.984636	1.376270	H	1.161466	2.179102	-0.882917
N	-1.114445	3.096499	-0.229504	N	1.211563	-0.860851	3.174616
H	-1.169635	2.075077	-0.192906	H	1.152137	-0.312831	2.317471
C	-1.854280	-1.894835	-3.588882	C	2.294447	-2.171704	-3.128500
C	-3.101253	-1.558118	2.737016	C	2.322502	3.800759	-0.330492
C	-2.152489	3.846145	-0.667594	C	2.303166	-1.613710	3.443850
O	-1.744248	-2.619799	-4.578553	O	2.353963	-2.539530	-4.301744
C	1.185664	-2.616708	-2.091691	C	-0.977484	-1.624581	-3.283109
H	1.055141	-2.136894	-1.117573	H	-0.918110	-0.821409	-2.546293
H	0.678869	-3.587676	-2.067561	H	-0.629292	-1.222779	-4.240407
C	0.573968	-1.735780	-3.190259	C	-0.076976	-2.794173	-2.850165
H	0.586760	-2.244062	-4.156285	H	0.114737	-3.470315	-3.685970
H	1.144975	-0.803474	-3.274910	H	-0.558159	-3.360179	-2.045991
S	2.962959	-3.028738	-2.326908	S	-2.742538	-2.061939	-3.558302
S	2.954894	3.789978	-0.585629	S	-2.734438	-2.024426	3.582973
S	1.731409	-1.096462	4.331750	S	-2.715996	4.140751	-0.020212
C	1.244456	3.206628	-0.927089	C	-0.973486	-2.007715	3.053802
H	1.245245	2.115122	-0.991666	H	-0.922105	-1.766796	1.990256
H	1.009246	3.609137	-1.918483	H	-0.626842	-3.038940	3.178211
C	0.187306	3.666886	0.086880	C	-0.065266	-1.053027	3.848110
H	0.477040	3.344862	1.094206	H	-0.541555	-0.071473	3.941210
H	0.083819	4.753572	0.082731	H	0.129274	-1.441625	4.849964
C	0.179575	-0.680379	3.436829	C	-0.954245	3.671832	0.222511
H	-0.380967	-0.048867	4.134828	H	-0.603117	4.295276	1.051474
H	0.424021	-0.083301	2.554116	H	-0.902929	2.630620	0.546428
C	-0.674920	-1.887342	3.023531	C	-0.050375	3.879421	-1.004872
H	-0.078827	-2.566831	2.402391	H	-0.531114	3.469950	-1.899275
H	-1.032981	-2.435346	3.897153	H	0.146960	4.940626	-1.170280
O	-2.116993	5.069931	-0.802728	O	2.363317	-2.442290	4.352088
O	-3.396112	-2.049682	3.827253	O	2.391804	5.003051	-0.075175
Cl	-0.203971	0.019908	-0.068264	O	0.126276	0.703942	1.050731
				N	0.114924	0.012181	-0.002022
				O	0.120426	-1.245432	0.071563
				O	0.113745	0.578457	-1.127209

1-Nitroazo (-3424.94054) (0)

H	2.639702	-4.447665	0.933818
H	5.621872	1.413504	3.747799
C	0.257970	-2.424159	-0.495236
C	2.171812	-2.538580	-2.543407
C	1.422298	-3.184570	-0.312515
C	0.051925	-1.682047	-1.662931

1-Nitroazo...NO₃⁻ (-3705.36862) (0)

H	4.334927	-0.810531	-4.313782
H	7.010765	-1.887228	2.121605
C	1.206872	-1.185227	-2.962980
C	1.402340	1.605120	-3.054529
C	2.348482	-0.601391	-3.527547
C	0.164655	-0.409983	-2.443499

C	1.026171	-1.747874	-2.670422	C	0.279148	0.985971	-2.493869
C	2.366148	-3.237113	-1.344167	C	2.426864	0.794646	-3.566354
C	1.655137	-3.964009	0.971680	C	3.468751	-1.452549	-4.110805
C	-1.196318	-0.853714	-1.898974	C	-1.065765	-1.112596	-1.894714
C	3.125850	-2.683689	-3.717395	C	1.479184	3.124619	-3.123330
H	0.921961	-4.776944	1.058846	H	3.150871	-1.854969	-5.083761
C	6.031023	2.086800	1.275806	C	5.791145	0.374354	2.554884
C	4.074158	3.689664	0.069342	C	3.272528	0.211356	3.771350
C	4.896376	2.442646	2.006517	C	5.245641	-0.883272	2.824388
C	6.219125	2.519092	-0.048512	C	5.109328	1.559532	2.879578
C	5.231118	3.311885	-0.635695	C	3.856268	1.457305	3.487161
C	3.923245	3.248176	1.386853	C	3.981392	-0.944986	3.436475
C	4.742677	1.997287	3.450001	C	6.008888	-2.152799	2.479484
C	7.464028	2.115907	-0.815772	C	5.719281	2.918386	2.579510
C	3.019443	4.549235	-0.600511	C	1.911798	0.137295	4.444349
H	4.719710	2.877796	4.105236	H	6.146020	-2.752197	3.390648
H	2.368814	5.001044	0.156956	H	1.689430	-0.902466	4.713514
H	-2.088930	-1.488899	-1.835615	H	-0.852762	-2.184828	-1.848773
H	3.505621	5.372518	-1.138034	H	1.945252	0.706761	5.383698
H	-1.155680	-0.465937	-2.921522	H	-1.900602	-0.995890	-2.599702
H	7.499532	2.650754	-1.772291	H	5.118842	3.699985	3.059951
H	8.359802	2.410729	-0.255232	H	6.724978	2.972586	3.019195
H	2.929381	-3.637645	-4.226830	H	1.237999	3.454100	-4.144625
H	2.902455	-1.906051	-4.460956	H	0.702665	3.548517	-2.474571
H	-0.497688	-2.408619	0.284284	H	1.128342	-2.268753	-2.913710
H	0.868925	-1.183613	-3.587470	H	-0.512476	1.606198	-2.078575
H	3.046541	3.561021	1.951515	H	3.542526	-1.916782	3.655594
H	5.371813	3.670869	-1.654037	H	3.319511	2.368176	3.745766
H	6.800343	1.482233	1.752819	H	6.769593	0.435500	2.081955
H	3.253915	-3.852145	-1.214283	H	3.314644	1.257340	-3.990984
S	-0.455458	2.662565	-2.920867	S	-2.023540	0.872332	2.177925
C	0.259373	2.155703	-1.473716	C	-0.642996	0.017064	1.682324
N	1.381247	2.745009	-0.959471	N	0.472290	-0.122003	2.452750
N	-0.217128	1.141782	-0.708521	N	-0.553805	-0.621947	0.482008
H	1.834993	2.292027	-0.174313	H	1.299656	-0.433077	1.943391
H	0.260834	0.898853	0.151491	H	0.367436	-0.961161	0.211665
N	5.004322	-1.380580	-2.799358	N	3.205969	3.431251	-1.396014
C	6.202800	-1.153449	-2.187678	C	4.369293	3.823717	-0.815482
H	4.498907	-0.572664	-3.145584	H	2.724714	2.647568	-0.954694
S	7.321303	-2.368368	-1.856852	S	5.443239	4.913408	-1.552711
N	6.414081	0.155306	-1.855028	N	4.568151	3.283171	0.423805
H	5.601872	0.762233	-1.822101	H	3.952709	2.503830	0.648351
N	2.505281	-2.031990	2.264296	N	4.447794	-2.205463	-1.981691
C	2.478619	-1.001802	3.138817	C	4.877488	-3.041933	-1.001076

H	3.155548	-1.998302	1.486959	H	4.204771	-1.260287	-1.684826
S	1.304092	-0.889410	4.375958	S	5.027741	-4.719705	-1.221184
N	3.436167	-0.053027	2.985390	N	5.204446	-2.395472	0.157018
H	4.059568	-0.110763	2.187388	H	4.874116	-1.432746	0.207913
C	-1.436367	0.389094	-0.974349	C	-1.610683	-0.656592	-0.513471
H	-2.066517	1.059731	-1.565776	H	-2.024797	0.354936	-0.599197
C	2.146338	3.790207	-1.617609	C	0.735214	0.698493	3.623514
H	2.775520	3.373150	-2.419068	H	0.940529	1.738584	3.329389
H	1.441957	4.475359	-2.093914	H	-0.169451	0.714590	4.236286
C	7.557655	0.603107	-1.070791	C	5.861815	3.255347	1.083457
H	8.476434	0.366754	-1.615626	H	6.324469	4.237834	0.965528
H	7.608032	0.053951	-0.121010	H	6.529734	2.526749	0.597334
C	4.620992	-2.659250	-3.384589	C	2.832591	3.755794	-2.760598
H	5.204036	-2.857049	-4.295239	H	2.766544	4.843699	-2.872015
H	4.888942	-3.444484	-2.674443	H	3.617548	3.430010	-3.457273
C	3.472657	1.190639	3.753245	C	5.340039	-3.067629	1.436950
H	3.435735	0.944556	4.817574	H	5.944456	-3.965739	1.288873
H	2.575524	1.785319	3.538457	H	4.357405	-3.401916	1.805489
C	1.538745	-3.131633	2.255861	C	3.923485	-2.650559	-3.259889
H	1.701820	-3.767619	3.133437	H	4.698973	-3.205251	-3.800021
H	0.534052	-2.712722	2.351782	H	3.097635	-3.359181	-3.107535
O	-12.445171	-0.362934	-1.501245	O	-12.282320	2.631734	-0.620986
N	-11.971300	-0.574743	-0.384609	N	-12.087184	1.470028	-0.256256
C	-10.512806	-0.486502	-0.234026	C	-10.706499	0.985086	-0.221949
O	-12.633588	-0.855682	0.614902	O	-12.981189	0.689534	0.080443
C	-9.946308	-0.718338	1.023574	C	-10.458520	-0.331691	0.182514
C	-9.736347	-0.174684	-1.349257	C	-9.673950	1.847353	-0.593843
C	-8.569399	-0.636190	1.167134	C	-9.152193	-0.793842	0.212244
H	-10.592042	-0.957273	1.859699	H	-11.291615	-0.963926	0.464493
C	-8.356837	-0.095143	-1.195676	C	-8.367810	1.374709	-0.560656
H	-10.216414	-0.001762	-2.304259	H	-9.906647	2.860041	-0.898573
C	-7.763479	-0.323577	0.055710	C	-8.092014	0.055936	-0.162108
H	-8.094973	-0.809612	2.125792	H	-8.921958	-1.806913	0.520282
H	-7.712369	0.145014	-2.034976	H	-7.533502	2.010150	-0.839205
C	-4.436966	-0.315882	1.278791	C	-5.173998	-1.912501	0.190096
C	-3.854655	-0.535775	2.534992	C	-4.947226	-3.248124	0.558424
C	-3.609555	-0.006680	0.184429	C	-4.074655	-1.089026	-0.132640
C	-2.478926	-0.449608	2.686221	C	-3.655251	-3.749685	0.583532
H	-4.499783	-0.767979	3.376377	H	-5.799547	-3.868604	0.816875
C	-2.225005	0.075088	0.301151	C	-2.774504	-1.568252	-0.117056
H	-4.083725	0.174203	-0.775019	H	-4.261306	-0.049726	-0.378152
C	-1.663821	-0.149816	1.583743	C	-2.573637	-2.924432	0.241124
H	-2.015802	-0.615357	3.654914	H	-3.470474	-4.785595	0.862352
O	-0.312480	-0.071345	1.723538	O	-1.300987	-3.400935	0.232125

H	-0.024014	-0.274854	2.648845	H	-1.298103	-4.327538	0.520984
N	-5.838270	-0.417398	1.223771	O	4.015732	0.294464	-0.491312
N	-6.351538	-0.215413	0.086358	N	2.893171	0.204979	0.077255
				O	2.260298	1.248896	0.379730
				O	2.420000	-0.930671	0.356653
				N	-6.512574	-1.507077	0.187255
				N	-6.726656	-0.311616	-0.175992

1-Anthracene (-3111.97542) (0)

H	-3.208410	-0.105028	-4.079045
H	-3.425410	4.651915	1.304829
C	0.016916	-0.479613	-2.995038
C	-1.146155	-2.831828	-2.021806
C	-1.318448	-0.765156	-3.308829
C	0.780777	-1.345996	-2.206191
C	0.185174	-2.520994	-1.729470
C	-1.887193	-1.942042	-2.811581
C	-2.146730	0.153812	-4.191673
C	2.226540	-1.005877	-1.905258
C	-1.738937	-4.127175	-1.492830
H	-1.910976	-0.029607	-5.250003
C	-3.972096	2.225216	2.170124
C	-1.948517	1.018022	3.686415
C	-2.744972	2.877772	2.313454
C	-4.216141	0.978437	2.771694
C	-3.197167	0.393147	3.526778
C	-1.741485	2.259306	3.079890
C	-2.478405	4.197060	1.617243
C	-5.536544	0.268550	2.554662
C	-0.843750	0.322608	4.454711
H	-1.998464	4.897833	2.311172
H	-0.060210	1.040553	4.724792
H	2.464906	-0.040246	-2.357261
H	-1.238691	-0.086628	5.392225
H	2.891633	-1.729581	-2.397280
H	-5.679650	-0.502894	3.320360
H	-6.364943	0.979733	2.656545
H	-1.624979	-4.925363	-2.241204
H	-1.152030	-4.453971	-0.623824
H	0.475626	0.435275	-3.362526
H	0.756946	-3.196361	-1.098000
H	-0.788643	2.768630	3.218005
H	-3.379824	-0.561869	4.017338
H	-4.763544	2.701843	1.593925

1-Anthracene...NO₃⁻ (-3392.40903) (0)

H	2.537623	-0.101774	4.676012
H	5.288212	3.415682	-0.782475
C	-0.476758	-0.144840	3.038204
C	0.519697	-2.674839	2.371882
C	0.755900	-0.553194	3.566884
C	-1.221427	-0.969557	2.188603
C	-0.704935	-2.231355	1.861594
C	1.236153	-1.821449	3.224688
C	1.545733	0.338458	4.515495
C	-2.584825	-0.503638	1.705153
C	1.032287	-4.065857	2.024614
H	1.051118	0.349467	5.497717
C	4.624282	1.270030	-2.096069
C	2.174268	1.347742	-3.452303
C	3.825379	2.411348	-1.993198
C	4.229510	0.159530	-2.860899
C	3.005440	0.217621	-3.530260
C	2.599858	2.432313	-2.681489
C	4.281349	3.607297	-1.172209
C	5.115622	-1.070451	-2.966170
C	0.860670	1.391865	-4.215513
H	4.356934	4.488586	-1.825062
H	0.405162	2.383711	-4.107641
H	-2.730772	0.537798	2.011055
H	1.065085	1.254394	-5.286730
H	-3.365131	-1.078239	2.222172
H	4.690779	-1.762079	-3.703437
H	6.106145	-0.775593	-3.340354
H	0.884180	-4.732998	2.886361
H	0.421776	-4.476047	1.210688
H	-0.867346	0.839024	3.288120
H	-1.261777	-2.883185	1.191547
H	1.966234	3.314713	-2.615097
H	2.690309	-0.635195	-4.128546
H	5.576088	1.242750	-1.568726

H	-2.929323	-2.154531	-3.037259	H	2.195264	-2.143997	3.623598
S	1.346276	-2.806087	1.899541	S	-2.831544	-1.011015	-2.904195
C	1.141263	-1.152905	1.605925	C	-1.751454	-0.111191	-1.961320
N	0.436419	-0.360096	2.465216	N	-0.674186	0.546376	-2.472958
N	1.631544	-0.480702	0.522219	N	-1.893559	0.053760	-0.609687
H	0.128314	0.544346	2.125635	H	0.017876	0.840979	-1.784480
H	1.609932	0.529058	0.592913	H	-1.046275	0.343425	-0.119735
N	-3.509464	-3.062490	-0.115917	N	2.795287	-3.371071	0.452289
C	-4.588098	-2.235108	-0.102228	C	4.025176	-3.272862	-0.116373
H	-2.884595	-3.042552	0.682392	H	2.133243	-2.629746	0.223086
S	-5.782984	-2.218383	-1.297878	S	5.336221	-4.245591	0.352652
N	-4.635921	-1.401636	0.982223	N	4.090300	-2.345289	-1.116310
H	-3.775298	-1.257134	1.499625	H	3.303090	-1.700257	-1.150770
N	-2.264867	2.027526	-2.576339	N	2.443067	1.901866	2.835392
C	-1.647275	3.001807	-1.859495	C	2.734725	3.078251	2.219187
H	-3.061555	1.559695	-2.159007	H	2.449586	1.074893	2.238880
S	-0.385346	3.951639	-2.465544	S	2.493599	4.589320	2.956656
N	-2.142276	3.164239	-0.594869	N	3.267592	2.920919	0.972272
H	-2.705059	2.410917	-0.213590	H	3.169199	1.984267	0.582496
C	2.640326	-1.025190	-0.401260	C	-2.905339	-0.633658	0.188647
H	2.695514	-2.067737	-0.105028	H	-2.851253	-1.687990	-0.083927
C	-0.215212	-0.845845	3.673048	C	-0.176936	0.325508	-3.820048
H	-0.982361	-1.592637	3.424922	H	0.256515	-0.681570	-3.913139
H	0.528688	-1.356444	4.291238	H	-1.027219	0.366121	-4.505403
C	-5.653393	-0.375483	1.160750	C	5.340441	-1.831696	-1.647391
H	-6.635485	-0.839732	1.041519	H	6.011418	-2.677222	-1.815722
H	-5.574091	0.395136	0.380001	H	5.834307	-1.175663	-0.913391
C	-3.226936	-4.080006	-1.119937	C	2.515333	-4.165140	1.634656
H	-3.537006	-5.067480	-0.749551	H	2.770036	-5.211716	1.436628
H	-3.857070	-3.856300	-1.981736	H	3.159903	-3.850912	2.467789
C	-1.556068	4.060303	0.391494	C	3.363524	3.995790	0.001094
H	-1.404903	5.035429	-0.077362	H	3.760981	4.879381	0.506196
H	-0.563048	3.703025	0.702627	H	2.365289	4.269680	-0.375555
C	-1.955027	1.657694	-3.951692	C	1.713959	1.805577	4.086983
H	-2.591383	2.221366	-4.648554	H	2.258931	2.350842	4.864736
H	-0.927928	1.972173	-4.142965	H	0.736309	2.300722	3.999777
H	2.116148	1.535608	-1.013581	O	2.749072	-0.016651	0.598881
C	3.087548	1.926586	-0.732911	N	1.649388	-0.034802	-0.017755
C	4.151319	1.042669	-0.335195	O	1.325970	-1.045495	-0.692882
C	3.262691	3.284475	-0.831240	O	0.884610	0.967871	0.033496
C	4.005996	-0.363732	-0.182265	H	-2.682052	2.029653	0.131255
C	5.433975	1.661309	-0.078062	C	-3.732584	2.277052	0.095374
C	4.523190	3.877290	-0.545516	C	-4.696620	1.216879	-0.015578
H	2.425834	3.901171	-1.147923	C	-4.103736	3.596725	0.123770

C	5.127744	-1.156973	0.176881	C	-4.355533	-0.163171	-0.030496
C	6.525519	0.863348	0.271122	C	-6.086587	1.616695	-0.096842
C	5.576758	3.080225	-0.188444	C	-5.472608	3.974059	0.035318
H	4.646324	4.953584	-0.626912	H	-3.339246	4.364585	0.207997
C	5.080548	-2.583052	0.344271	C	-5.390704	-1.137197	-0.101244
C	6.412908	-0.522138	0.390895	C	-7.083445	0.643993	-0.171257
H	7.489519	1.334556	0.451992	C	-6.431463	3.005254	-0.075340
H	6.553858	3.511206	0.017522	H	-5.748101	5.025580	0.053856
C	6.196561	-3.308550	0.671775	C	-5.158128	-2.554472	-0.112370
H	4.143592	-3.114249	0.234079	C	-6.774499	-0.716635	-0.168783
C	7.552545	-1.316415	0.732950	H	-8.126131	0.952964	-0.220354
C	7.455246	-2.673755	0.866147	H	-7.484701	3.269619	-0.144356
H	6.116601	-4.385416	0.792664	C	-6.184270	-3.462494	-0.162906
H	8.502259	-0.808760	0.884297	H	-4.146415	-2.936693	-0.102622
H	8.327189	-3.268014	1.125065	C	-7.817634	-1.694189	-0.223208
				C	-7.539085	-3.033073	-0.214223
				H	-5.957515	-4.525486	-0.177153
				H	-8.845263	-1.339858	-0.271517
				H	-8.340611	-3.766355	-0.255593

1-Anthraquinone (-3261.22897) (0)

H	-3.341707	-3.920660	3.083924
H	-6.257130	1.772032	-0.129185
C	-0.393591	-3.081925	1.572640
C	-0.663196	-0.898660	3.306303
C	-1.563232	-2.959095	2.342632
C	0.633651	-2.140237	1.652477
C	0.483938	-1.047206	2.524208
C	-1.679639	-1.865410	3.203434
C	-2.673993	-3.982200	2.216553
C	1.902671	-2.290871	0.841890
C	-0.823006	0.280832	4.244631
H	-2.249356	-4.993469	2.211227
C	-4.108570	2.574530	-1.355808
C	-3.029815	0.767186	-3.200603
C	-4.829548	1.422669	-1.688932
C	-2.859770	2.842634	-1.929555
C	-2.334892	1.930911	-2.850715
C	-4.275015	0.525305	-2.610659
C	-6.191914	1.188581	-1.057712
C	-2.068691	4.091318	-1.582133
C	-2.486389	-0.209726	-4.228662
H	-6.981857	1.588495	-1.710408
H	-2.996676	-1.175317	-4.111353

1-Anthraquinone^{•••}NO₃⁻ (-3541.66614) (0)

H	-2.903079	1.289955	4.546647
H	-6.564803	-2.385246	-0.202114
C	-0.004282	0.249978	3.032990
C	-0.344638	2.762823	1.846763
C	-1.087823	1.048273	3.426442
C	0.911869	0.680977	2.068177
C	0.728088	1.942116	1.483177
C	-1.242191	2.299355	2.820848
C	-2.057321	0.592234	4.508368
C	2.108496	-0.191660	1.731009
C	-0.501617	4.138048	1.212855
H	-1.561724	0.655518	5.488160
C	-5.356433	-0.851505	-1.918998
C	-3.030140	-1.880725	-3.091564
C	-4.898332	-2.112398	-1.529205
C	-4.679898	-0.086595	-2.883925
C	-3.522716	-0.617236	-3.457933
C	-3.729281	-2.612060	-2.128432
C	-5.659980	-2.929806	-0.497361
C	-5.198733	1.279252	-3.301500
C	-1.784139	-2.445685	-3.754008
H	-5.993438	-3.872046	-0.955342
H	-1.608130	-3.466452	-3.393358

H	1.970920	-3.306593	0.430292	H	1.984071	-1.168610	2.214936
H	-2.746028	0.137244	-5.240278	H	-1.957123	-2.520915	-4.836966
H	2.769583	-2.152134	1.492687	H	3.010259	0.258945	2.160182
H	-1.040763	3.972818	-1.949488	H	-4.595289	1.657621	-4.135196
H	-2.476772	4.961200	-2.117365	H	-6.228128	1.179437	-3.673775
H	-1.154359	-0.072179	5.229071	H	-0.198296	4.908755	1.936507
H	0.144857	0.774056	4.392063	H	0.192658	4.220942	0.367731
H	-0.273923	-3.951955	0.927529	H	0.131094	-0.730457	3.484317
H	1.295560	-0.327661	2.607298	H	1.434458	2.291456	0.733910
H	-4.806097	-0.388421	-2.866045	H	-3.358702	-3.593395	-1.838169
H	-1.355686	2.128397	-3.277178	H	-2.991690	-0.034525	-4.208198
H	-4.524614	3.259349	-0.620595	H	-6.260141	-0.453800	-1.460941
H	-2.564917	-1.775507	3.831482	H	-2.087084	2.920410	3.110274
S	1.424989	0.817132	-2.526737	S	2.423822	-0.836386	-2.852166
C	0.602848	-0.635054	-2.267944	C	1.155055	-1.173772	-1.780696
N	-0.477920	-1.041258	-2.989777	N	-0.062426	-1.627242	-2.179901
N	0.987540	-1.527496	-1.299834	N	1.277003	-1.060517	-0.419197
H	-0.855756	-1.959527	-2.784684	H	-0.800054	-1.559230	-1.477838
H	0.315643	-2.239920	-1.037009	H	0.394330	-1.032670	0.091996
N	-1.423268	1.929267	2.514259	N	-2.380781	3.585829	-0.284021
C	-2.072703	2.978059	1.928653	C	-3.592107	3.683541	-0.891236
H	-0.792725	1.377469	1.942522	H	-1.930805	2.671708	-0.325262
S	-3.407226	3.720819	2.658700	S	-4.613155	5.027208	-0.698999
N	-1.549066	3.364828	0.734969	N	-3.888794	2.616603	-1.690205
H	-0.721670	2.885722	0.396894	H	-3.293361	1.801915	-1.551910
N	-4.189682	-2.542754	0.916247	N	-3.353392	-0.997344	3.145893
C	-5.105988	-2.189002	-0.036166	C	-3.961936	-2.154107	2.772867
H	-3.711243	-1.792233	1.403648	H	-3.150038	-0.339884	2.393287
S	-5.606724	-3.258642	-1.245726	S	-4.111706	-3.493819	3.806227
N	-5.569829	-0.917495	0.092045	N	-4.465730	-2.117367	1.504653
H	-5.270232	-0.383369	0.899749	H	-4.132267	-1.339156	0.937264
C	2.044956	-1.270264	-0.319134	C	2.420906	-0.426185	0.228506
H	1.919589	-0.264068	0.076206	H	2.627427	0.529109	-0.253188
C	-0.967122	-0.428759	-4.221449	C	-0.496034	-1.624556	-3.566798
H	-0.420881	0.506807	-4.343075	H	-0.644846	-0.594375	-3.922579
H	-0.697180	-1.071907	-5.071319	H	0.305751	-2.052408	-4.174104
C	-2.043445	4.457667	-0.090879	C	-5.225000	2.340442	-2.187067
H	-1.418664	5.350957	0.051565	H	-5.645154	3.272872	-2.571370
H	-3.038101	4.706448	0.281892	H	-5.884040	2.009675	-1.369020
C	-1.851542	1.318446	3.764358	C	-1.915566	4.507276	0.737499
H	-1.968123	2.107398	4.512104	H	-1.908720	5.523264	0.329205
H	-2.839743	0.850191	3.649245	H	-2.618373	4.526343	1.582780
C	-6.551972	-0.275687	-0.770356	C	-4.871165	-3.302291	0.770605
H	-7.547718	-0.319007	-0.306681	H	-5.492599	-3.916357	1.427015

H	-6.606376	-0.869308	-1.683912	H	-3.994819	-3.913983	0.504180
C	-3.504764	-3.826949	0.930049	C	-2.599524	-0.840370	4.376232
H	-4.256094	-4.618247	0.868088	H	-3.250316	-1.063441	5.228172
H	-2.860024	-3.936015	0.045686	H	-1.780769	-1.572977	4.421189
C	3.444264	-1.389500	-0.931985	O	-3.181542	0.433884	0.558018
C	4.570079	-0.671858	-0.450841	N	-2.134100	0.034843	-0.018591
C	3.627851	-2.284063	-1.993090	O	-1.575749	0.762358	-0.879338
C	4.486409	0.254583	0.716621	O	-1.657399	-1.100714	0.259439
C	5.822122	-0.842387	-1.095321	C	3.680400	-1.299446	0.144172
C	4.870844	-2.475012	-2.591274	C	5.004166	-0.791188	0.132539
H	2.764296	-2.824512	-2.366371	C	3.504384	-2.691417	0.144299
C	5.660562	1.124898	1.022654	C	5.293985	0.668161	0.194429
C	7.036211	-0.059737	-0.706534	C	6.095288	-1.699878	0.057258
C	5.968463	-1.745569	-2.149564	C	4.579578	-3.572785	0.117635
H	4.975742	-3.181144	-3.410296	H	2.488823	-3.072848	0.144552
C	5.539984	2.094326	2.026767	C	6.697447	1.126416	-0.061502
C	6.885064	0.971819	0.350837	C	7.511334	-1.244280	-0.052112
H	6.946928	-1.848982	-2.605450	C	5.878723	-3.078364	0.062068
C	6.623421	2.908778	2.345877	H	4.401174	-4.644892	0.123032
C	7.974718	1.784841	0.683825	C	6.950494	2.500397	-0.160942
C	7.842907	2.753846	1.674754	C	7.761198	0.217000	-0.166359
H	6.521737	3.664896	3.119391	H	6.740958	-3.734417	0.014004
H	8.909150	1.637524	0.152547	C	8.247444	2.958509	-0.376408
H	8.687266	3.388578	1.928657	H	6.114679	3.185317	-0.066613
O	8.115621	-0.250668	-1.257145	C	9.066092	0.683134	-0.369251
O	3.494275	0.312868	1.445094	C	9.308186	2.049107	-0.479227
H	4.590276	2.191566	2.541384	H	8.436472	4.025330	-0.462935
				H	9.866955	-0.045849	-0.437799
				H	10.320108	2.410259	-0.643515
				O	8.445087	-2.043534	-0.069545
				O	4.440907	1.511791	0.466139

1⁺BM (-3244.93754) (0)

H	0.618454	-2.084534	-3.127026
H	0.468170	-0.687673	3.762561
C	-2.811562	-2.029779	-3.218538
C	-2.231643	0.702257	-3.492706
C	-1.475255	-1.608712	-3.222067
C	-3.862706	-1.117307	-3.356459
C	-3.553672	0.245111	-3.483981
C	-1.204430	-0.244379	-3.366061
C	-0.344055	-2.610304	-3.077206
C	-5.302475	-1.606066	-3.378684
C	-1.957691	2.187283	-3.667942

1⁺Nitrophenolate (-3085.16336) (0)

H	1.731013	3.597328	-1.498086
H	1.728115	-3.448272	-1.736856
C	-1.687625	3.599044	-1.194412
C	-0.899942	3.265019	1.478099
C	-0.323015	3.549869	-0.881071
C	-2.665511	3.490035	-0.200101
C	-2.253822	3.317534	1.130103
C	0.049691	3.391704	0.455524
C	0.737031	3.648525	-1.960323
C	-4.139002	3.564197	-0.568842
C	-0.497946	3.087524	2.931811

H	-0.355172	-3.307915	-3.925544	H	0.679189	4.626953	-2.457406
C	-1.341764	1.095228	3.211151	C	0.074052	-3.387098	0.253663
C	-4.007332	0.279641	3.448153	C	-2.648855	-3.495247	-0.367098
C	-1.622221	-0.218704	3.597976	C	-0.316463	-3.468314	-1.084815
C	-2.361905	2.014224	2.925697	C	-0.861728	-3.342135	1.295901
C	-3.687868	1.585956	3.048900	C	-2.219733	-3.399008	0.965196
C	-2.962252	-0.611921	3.711810	C	-1.684992	-3.522858	-1.380506
C	-0.497266	-1.193916	3.892131	C	0.726871	-3.480453	-2.185038
C	-2.075299	3.451024	2.520098	C	-0.441525	-3.247102	2.752384
C	-5.452469	-0.166943	3.603372	C	-4.126572	-3.570251	-0.717308
H	-0.540808	-1.504880	4.944659	H	0.670702	-4.424015	-2.745624
H	-5.476686	-1.243184	3.810559	H	-4.239919	-3.522740	-1.807021
H	-5.323210	-2.676367	-3.142107	H	-4.236546	3.555308	-1.661123
H	-5.899246	0.329085	4.475966	H	-4.534345	-4.541418	-0.403161
H	-5.709518	-1.503380	-4.393991	H	-4.559792	4.520460	-0.226832
H	-2.881087	3.809278	1.869244	H	-1.213801	-2.713944	3.318473
H	-2.099609	4.091128	3.415557	H	-0.386605	-4.259104	3.183992
H	-1.954243	2.429231	-4.742004	H	-0.467018	4.071987	3.425134
H	-2.783621	2.759743	-3.230371	H	-1.268428	2.508573	3.453635
H	-3.041097	-3.087611	-3.108443	H	-1.997556	3.716457	-2.230998
H	-4.358459	0.970902	-3.581517	H	-3.000066	3.215151	1.915643
H	-3.199962	-1.629980	4.013438	H	-2.009641	-3.581259	-2.417727
H	-4.487537	2.290406	2.829578	H	-2.955436	-3.360655	1.766334
H	-0.300976	1.399858	3.133470	H	1.136322	-3.340799	0.476970
H	-0.166016	0.077950	-3.378222	H	1.109424	3.350616	0.691571
S	-8.146940	-0.061331	-0.116720	S	-6.822508	-0.028991	0.421449
C	-6.521908	-0.502015	0.008315	C	-5.226325	-0.015258	-0.142776
N	-5.837571	-0.475155	1.188473	N	-4.536142	-1.155524	-0.425880
N	-5.791147	-0.940377	-1.057397	N	-4.539510	1.138000	-0.376291
H	-4.828299	-0.570275	1.153045	H	-3.538535	-1.079756	-0.596107
H	-4.785152	-1.008004	-0.946080	H	-3.541709	1.073882	-0.549656
N	-0.506392	2.506836	-1.644070	N	0.969302	1.074446	2.608109
C	-0.774928	3.430776	-0.678104	C	0.738264	-0.082812	3.283122
H	-0.253290	1.574783	-1.321236	H	1.275895	0.976471	1.636254
S	-1.288838	5.013211	-1.008842	S	0.211626	-0.138124	4.902351
N	-0.559609	2.955103	0.580260	N	0.982643	-1.190586	2.534531
H	-0.263166	1.983342	0.655309	H	1.289936	-1.025608	1.571547
N	-0.307297	-2.633735	-0.608426	N	0.738276	1.239966	-2.511565
C	-0.483822	-3.114280	0.652536	C	0.486612	0.122553	-3.242116
H	-0.090846	-1.644218	-0.711762	H	1.137698	1.102095	-1.578837
S	-0.811247	-4.744819	0.975884	S	-0.069527	0.174741	-4.849222
N	-0.365074	-2.177754	1.632164	N	0.713567	-1.041048	-2.578340
H	-0.138830	-1.225170	1.351360	H	1.111441	-0.967150	-1.637731
H	-7.254531	-1.312148	-2.485290	H	-6.048028	2.565356	-0.332448

C	-6.259308	-0.864470	-2.434613	C	-5.020124	2.454287	0.021398
H	-6.376094	0.184854	-2.740637	H	-5.060042	2.529167	1.117397
C	-6.360903	0.135187	2.403026	C	-5.007303	-2.488494	-0.075250
H	-6.478009	1.219604	2.265430	H	-5.035823	-2.606049	1.017400
H	-7.362547	-0.261932	2.582925	H	-6.037931	-2.591178	-0.423461
C	-0.737239	3.709807	1.808788	C	0.905357	-2.555212	3.021890
H	-0.675546	4.769687	1.554174	H	1.074560	-2.535519	4.101066
H	0.105294	3.478845	2.472516	H	1.729027	-3.118535	2.567271
C	-0.643449	2.719096	-3.074358	C	0.858274	2.404832	3.177251
H	-0.589449	3.795244	-3.249966	H	1.014411	2.321141	4.255189
H	0.220463	2.258798	-3.569834	H	1.676311	3.011207	2.770224
C	-0.520894	-2.475773	3.046761	C	0.586014	-2.344141	-3.206795
H	0.277194	-3.151721	3.381405	H	1.343272	-2.466415	-3.994263
H	-1.459698	-3.019589	3.196441	H	-0.384570	-2.397872	-3.710814
C	-0.398704	-3.461352	-1.800211	C	0.625858	2.580934	-3.057301
H	0.417046	-4.196595	-1.814408	H	1.402902	2.755733	-3.815479
H	-1.327051	-4.041024	-1.761255	H	-0.331616	2.664379	-3.581242
H	2.058424	2.400706	-0.433642	H	3.589196	-0.008264	2.049795
C	2.643135	1.506220	-0.247165	C	4.084579	-0.010863	1.083504
C	1.933873	0.272913	0.009585	C	3.272198	0.002455	-0.096469
C	4.009660	1.543486	-0.256773	C	5.463996	-0.027088	1.017771
C	2.745407	-0.902846	0.257029	C	3.969090	-0.000874	-1.348101
O	0.658074	0.214271	0.020166	O	1.967825	0.015816	-0.034914
C	4.809687	0.378698	-0.015804	C	6.106101	-0.030754	-0.231057
H	4.518776	2.485262	-0.454002	H	6.069099	-0.037500	1.917108
C	4.109687	-0.846274	0.242649	C	5.348661	-0.017484	-1.413307
H	2.229795	-1.836413	0.456090	H	3.384543	0.009373	-2.263049
C	6.210160	0.490662	-0.044707	H	5.866012	-0.020416	-2.365898
H	4.675317	-1.753934	0.433681	N	7.542177	-0.048329	-0.299251
H	6.580568	1.493974	-0.253081	O	8.186179	-0.060272	0.762532
C	7.156995	-0.513617	0.157166	O	8.082835	-0.050875	-1.417225
H	6.808654	-1.521771	0.365017				
C	8.550681	-0.345348	0.115562				
C	9.233751	0.895212	-0.138918				
C	9.425354	-1.463763	0.340793				
C	10.594207	0.967203	-0.160218				
H	8.678451	1.807987	-0.316526				
C	10.781336	-1.336753	0.308367				
H	9.001572	-2.440941	0.547152				
H	11.120332	1.895202	-0.352395				
N	11.388184	-0.129301	0.065587				
H	11.448520	-2.174477	0.475303				
C	12.844954	-0.035834	-0.050170				
H	13.168754	0.966433	0.237468				

H	13.310317	-0.758001	0.623939
H	13.172066	-0.238701	-1.076164

BM (-671.23225) (0)

H	-4.896827	-2.114933	0.005849
C	-4.244829	-1.246007	0.005494
C	-4.900182	0.067666	0.012880
C	-2.892510	-1.367654	-0.001404
C	-3.989255	1.222963	0.012090
O	-6.131690	0.198754	0.019263
C	-2.011263	-0.222194	-0.002014
H	-2.434192	-2.356123	-0.006760
C	-2.639442	1.080290	0.005140
H	-4.456840	2.203786	0.017459
C	-0.634679	-0.421523	-0.008894
H	-2.008861	1.965921	0.005004
H	-0.322204	-1.465711	-0.012813
C	0.386046	0.550711	-0.010868
H	0.096728	1.598844	-0.008495
C	1.754377	0.296401	-0.015989
C	2.365237	-1.015686	-0.022740
C	2.710217	1.380637	-0.018874
C	3.714200	-1.175841	-0.028300
H	1.751579	-1.908563	-0.028851
C	4.050984	1.164268	-0.024574
H	2.350916	2.404895	-0.021126
H	4.179265	-2.155481	-0.031596
N	4.585006	-0.107689	-0.039537
H	4.771875	1.974223	-0.024858
C	6.024564	-0.312817	0.076002
H	6.296450	-1.262779	-0.390494
H	6.551758	0.489889	-0.445996
H	6.348076	-0.327002	1.124656

Nitrophenolate (-511.42113) (0)

C	-0.952525	-0.523143	-1.201567
C	-0.825352	-1.362992	-0.013970
C	-1.380029	-0.771538	1.200289
C	-1.969367	0.466884	1.219940
C	-2.064403	1.237490	0.034430
C	-1.543068	0.714579	-1.175146
H	-0.551098	-0.927716	-2.128748
H	-1.305351	-1.365965	2.108897
H	-2.375425	0.887608	2.134193
H	-1.627081	1.322424	-2.070252
O	-0.286038	-2.494425	-0.034988
N	-2.671475	2.511511	0.058135
O	-3.126054	2.953172	1.140815
O	-2.744279	3.174998	-1.004120

1ⁱⁱⁱAI1 (-3163.70800) (0)

H	-0.152127	-3.797069	-3.135562
H	-1.996922	3.469642	-3.753565
C	0.398587	-3.285805	0.211880
C	-2.393026	-3.512992	0.145608
C	-0.250554	-3.401287	-1.031680
C	-0.320721	-3.250815	1.414859
C	-1.717818	-3.368468	1.359256
C	-1.641498	-3.526967	-1.038299
C	0.504699	-3.398933	-2.352565

1ⁱⁱⁱAI1 out of cavity (-3163.73293) (0)

H	-1.664809	-3.453030	-2.520681
H	-1.943611	1.522327	-3.922743
C	-0.697241	-3.251432	0.727956
C	-3.469052	-3.364934	1.080443
C	-1.512430	-3.522129	-0.380423
C	-1.233262	-3.024284	1.998610
C	-2.624146	-3.084059	2.159085
C	-2.896278	-3.574812	-0.182837
C	-0.942082	-3.781474	-1.765047

C	0.381054	-3.099640	2.759910	C	-0.323537	-2.721829	3.174822
C	-3.903268	-3.652271	0.107359	C	-4.973009	-3.447103	1.288836
H	1.360181	-4.084198	-2.281990	H	-0.819577	-4.866576	-1.908952
C	-2.982814	3.498670	-1.399066	C	-3.154601	2.855104	-1.978535
C	-1.218876	3.727241	0.761435	C	-1.422271	3.668762	0.061988
C	-1.614539	3.620891	-1.653500	C	-1.773572	2.776824	-2.188793
C	-3.491185	3.474413	-0.093956	C	-3.690793	3.335641	-0.774749
C	-2.596624	3.585272	0.971600	C	-2.810778	3.732955	0.237433
C	-0.745620	3.754474	-0.557269	C	-0.924061	3.196068	-1.155493
C	-1.130774	3.618812	-3.097710	C	-1.246295	2.266056	-3.519791
C	-4.971516	3.267628	0.167468	C	-5.193437	3.434465	-0.561689
C	-0.270498	3.885657	1.944117	C	-0.473230	4.095459	1.166499
H	-0.724916	4.610350	-3.346128	H	-1.230224	3.094936	-4.244968
H	0.766106	3.770772	1.601327	H	0.561949	3.971752	0.823439
H	1.456290	-2.944663	2.594812	H	0.721889	-2.744618	2.841555
H	-0.345858	4.913911	2.326325	H	-0.601077	5.166563	1.375686
H	0.303236	-4.042898	3.318667	H	-0.421206	-3.511357	3.932671
H	-5.123376	3.089839	1.238203	H	-5.391157	3.687043	0.487008
H	-5.536448	4.176237	-0.086784	H	-5.599875	4.260391	-1.162295
H	-4.170242	-4.688989	-0.147359	H	-5.306273	-4.488191	1.175232
H	-4.314151	-3.456087	1.104243	H	-5.209780	-3.154849	2.318868
H	1.484108	-3.204958	0.237316	H	0.381970	-3.205858	0.608008
H	-2.296037	-3.343140	2.280330	H	-3.059783	-2.910011	3.141052
H	0.323301	3.862581	-0.731102	H	0.153665	3.147715	-1.286696
H	-2.986809	3.545467	1.985649	H	-3.217218	4.094554	1.180001
H	-3.663691	3.393673	-2.240997	H	-3.823360	2.528638	-2.772486
H	-2.149364	-3.635180	-1.994086	H	-3.538729	-3.783350	-1.036211
S	-1.348768	0.592450	5.049179	S	-1.317166	1.455346	4.843735
C	-0.460385	0.501531	3.615657	C	-0.697375	1.021354	3.322690
N	-0.169869	1.576354	2.832815	N	-0.441470	1.926789	2.342896
N	0.042408	-0.673136	3.124667	N	-0.415745	-0.263374	2.981203
H	0.162331	1.395092	1.888228	H	-0.048572	1.568866	1.469788
H	0.785642	-0.588620	2.446154	H	-0.037329	-0.424352	2.046901
N	-4.351852	-1.330105	-0.654156	N	-5.437966	-1.195608	0.399520
C	-5.310671	-0.364684	-0.647700	C	-6.132145	-0.195816	-0.214273
H	-3.379314	-1.013034	-0.659501	H	-4.468993	-1.020935	0.645400
S	-6.973537	-0.677303	-0.830584	S	-7.648990	-0.436167	-0.923563
N	-4.811592	0.887106	-0.460658	N	-5.517515	1.020172	-0.186377
H	-3.797079	0.983674	-0.476700	H	-4.543355	1.055322	0.095042
N	0.062112	-1.030139	-3.085046	N	0.404650	-1.671902	-1.970440
C	0.414621	0.194224	-3.604596	C	0.192025	-0.806095	-2.997398
H	-0.680302	-0.989974	-2.391445	H	0.568171	-1.252866	-1.053489
S	1.794405	0.413825	-4.561181	S	-0.144208	-1.301684	-4.590122
N	-0.440005	1.215975	-3.291867	N	0.289255	0.496810	-2.618904

H	-1.056865	1.040305	-2.488880	H	0.475034	0.667113	-1.629819
H	0.356992	-2.076732	4.669691	H	0.051041	-1.288899	4.753803
C	-0.152893	-1.994714	3.699128	C	-0.606875	-1.387636	3.879955
H	-1.219421	-2.129757	3.900724	H	-1.631164	-1.367911	4.269750
C	-0.508909	2.955762	3.149889	C	-0.664229	3.353004	2.497013
H	-1.546594	3.006026	3.495536	H	-1.674545	3.516018	2.888202
H	0.108441	3.299445	3.990576	H	0.021815	3.767617	3.248550
C	-5.585372	2.105385	-0.627704	C	-5.991621	2.177045	-0.933927
H	-6.602993	1.907943	-0.286118	H	-7.050044	2.325251	-0.705548
H	-5.659603	2.370068	-1.694181	H	-5.932318	1.981441	-2.013943
C	-4.604101	-2.735614	-0.907597	C	-5.813948	-2.600735	0.322117
H	-5.684557	-2.881633	-0.856894	H	-6.873662	-2.687053	0.574062
H	-4.292625	-2.994740	-1.930544	H	-5.708912	-2.966961	-0.709128
C	-0.037755	2.607320	-3.485307	C	0.157568	1.638578	-3.504222
H	0.219280	2.750321	-4.538077	H	0.399692	1.303853	-4.515306
H	0.886327	2.814254	-2.923343	H	0.910806	2.380332	-3.211571
C	1.081729	-2.050903	-2.830538	C	0.408658	-3.118476	-2.082639
H	1.627588	-2.213823	-3.762017	H	0.687010	-3.372523	-3.107987
H	1.811011	-1.676809	-2.097487	H	1.194814	-3.502011	-1.421308
O	10.106851	-0.102729	1.767278	O	12.966800	-0.198607	-0.469344
N	8.941858	-0.527070	1.895617	N	11.912343	0.024615	0.157466
C	7.925767	0.174022	1.197176	C	10.696645	-0.189512	-0.539945
O	8.646028	-1.514410	2.594513	O	11.888911	0.416935	1.339316
C	6.616551	-0.203149	1.270178	C	9.484595	0.023535	0.050281
H	8.307195	1.008596	0.625327	H	10.848261	-0.528985	-1.555263
H	6.399132	-1.069559	1.891962	H	9.504961	0.366354	1.083034
C	5.540469	0.437047	0.611312	C	8.226879	-0.165101	-0.569229
H	5.754009	1.303995	-0.013092	H	8.203582	-0.508438	-1.603315
C	4.233852	0.005822	0.726438	C	7.031160	0.066338	0.081901
H	4.055959	-0.869783	1.356159	H	7.087400	0.409592	1.117632
C	3.103312	0.587292	0.116019	C	5.738993	-0.097922	-0.459600
H	3.251768	1.459717	-0.519490	H	5.653112	-0.439678	-1.491077
C	1.819157	0.088488	0.272953	C	4.582031	0.153250	0.257034
H	1.736633	-0.824181	0.866870	H	4.705655	0.494823	1.288314
C	0.636861	0.591377	-0.303114	C	3.258467	0.014303	-0.199962
C	-0.628408	-0.010469	-0.148707	C	2.173079	0.297718	0.623716
H	0.730236	1.424268	-0.990742	H	3.071651	-0.322725	-1.218008
H	-0.717091	-0.782864	0.625751	H	2.414467	0.640703	1.647732
O	-1.667274	0.236129	-0.842960	O	0.928261	0.202484	0.322651

1stAI2 (-3241.11446) (0)

H	-0.065959	-0.718626	-4.957407
H	-2.598532	4.718516	-0.425831
C	0.916535	-2.464735	-2.172277

1stAI3 (-3088.98335) (0)

H	1.396248	2.520378	-4.404213
H	1.968655	-4.433644	-2.508413
C	-0.311686	3.074161	-1.461344

C	-1.825485	-3.036345	-2.236166	C	2.324924	3.628588	-0.693008
C	0.106811	-1.833291	-3.134998	C	0.721400	2.924879	-2.403467
C	0.378445	-3.348726	-1.226475	C	-0.058181	3.496385	-0.147914
C	-0.996776	-3.622690	-1.277406	C	1.268782	3.775872	0.212489
C	-1.254544	-2.144527	-3.155676	C	2.031331	3.201737	-1.996538
C	0.660983	-0.839434	-4.145038	C	0.445409	2.555024	-3.858129
C	1.251925	-4.014020	-0.168703	C	-1.208471	3.672997	0.840439
C	-3.307747	-3.356265	-2.283540	C	3.753179	3.920013	-0.263956
H	1.571959	-1.253235	-4.598131	H	-0.133368	3.368402	-4.316772
C	-3.229185	3.029490	1.381129	C	2.504495	-3.578384	-0.136729
C	-1.195316	2.057621	3.039244	C	0.336311	-2.924351	1.522009
C	-1.928208	3.507770	1.206364	C	1.202733	-3.736663	-0.627272
C	-3.538062	2.069377	2.353316	C	2.751352	-3.102578	1.158573
C	-2.510440	1.592469	3.168559	C	1.656477	-2.779423	1.970834
C	-0.923389	3.023303	2.060824	C	0.131440	-3.410382	0.220177
C	-1.662395	4.537203	0.115785	C	0.990328	-4.294165	-2.032076
C	-4.941748	1.507599	2.482409	C	4.170417	-2.926668	1.671848
C	-0.101744	1.547916	3.970599	C	-0.867163	-2.603994	2.406347
H	-1.386267	5.495108	0.580208	H	0.548462	-5.297090	-1.955250
H	0.879680	1.858701	3.589089	H	-1.701702	-2.289678	1.768378
H	2.275461	-3.620630	-0.240980	H	-2.068000	3.087188	0.493658
H	-0.209691	2.037874	4.949018	H	-1.198044	-3.531341	2.897882
H	1.334355	-5.087783	-0.388324	H	-1.536809	4.723031	0.826394
H	-4.920401	0.646044	3.159451	H	4.138846	-2.575030	2.709491
H	-5.612068	2.251718	2.936533	H	4.680342	-3.899447	1.682942
H	-3.518870	-3.989938	-3.158028	H	4.132117	4.793728	-0.811592
H	-3.584914	-3.938271	-1.397255	H	3.761932	4.187999	0.798939
H	1.983383	-2.247839	-2.152872	H	-1.338314	2.867201	-1.757977
H	-1.435687	-4.305061	-0.552794	H	1.494842	4.116046	1.220907
H	0.095407	3.390257	1.951730	H	-0.889442	-3.535788	-0.136564
H	-2.743844	0.832027	3.909767	H	1.850305	-2.414246	2.976790
H	-4.014081	3.398160	0.724258	H	3.345308	-3.830609	-0.779890
H	-1.884085	-1.675127	-3.908337	H	2.840149	3.091807	-2.716060
S	-0.438792	-3.090139	4.090335	S	-2.516584	1.044073	3.923803
C	0.242948	-2.069069	2.930967	C	-1.015169	0.922665	3.143517
N	0.328304	-0.717354	3.065386	N	-0.302269	-0.236500	3.044731
N	0.768769	-2.527107	1.752764	N	-0.410003	1.971947	2.511234
H	0.543344	-0.173639	2.232794	H	0.535223	-0.207453	2.472668
H	1.399003	-1.899871	1.273918	H	0.436478	1.763405	1.993987
N	-4.059648	-1.225005	-1.252039	N	4.314018	1.554402	0.167483
C	-5.086906	-0.672055	-0.551358	C	5.120700	0.469606	0.357761
H	-3.128386	-0.835484	-1.087844	H	3.312753	1.382549	0.171478
S	-6.725913	-1.042174	-0.818938	S	6.793529	0.507883	0.130983
N	-4.674640	0.200781	0.407406	N	4.444409	-0.641652	0.780734

H	-3.684851	0.443318	0.412366	H	3.441784	-0.631462	0.624021
N	-0.079884	1.311185	-3.065459	N	0.424505	0.057060	-3.836496
C	0.088611	2.608285	-2.638599	C	-0.122836	-1.194449	-3.897650
H	-0.717729	0.763183	-2.494077	H	1.216706	0.178092	-3.212463
S	1.297192	3.620000	-3.256836	S	-1.630105	-1.497222	-4.598611
N	-0.799662	3.015442	-1.680833	N	0.618175	-2.177427	-3.297789
H	-1.280641	2.258437	-1.179682	H	1.392875	-1.870056	-2.717446
H	1.418305	-4.528006	1.929517	H	-1.853272	3.399118	2.895420
C	0.769024	-3.907512	1.295305	C	-0.928865	3.319581	2.320524
H	-0.242292	-4.308744	1.407141	H	-0.214798	4.032764	2.751793
C	-0.079585	0.031515	4.245009	C	-0.688131	-1.556313	3.526388
H	-1.056209	-0.328386	4.584485	H	0.057148	-1.899728	4.255755
H	0.621142	-0.170308	5.066189	H	-1.632181	-1.438497	4.061314
C	-5.564851	1.081144	1.144552	C	5.042706	-1.965924	0.845764
H	-6.501581	0.547695	1.315489	H	6.029190	-1.871465	1.303924
H	-5.815720	1.967238	0.540490	H	5.205006	-2.369271	-0.165568
C	-4.224325	-2.126263	-2.376261	C	4.747870	2.771801	-0.499815
H	-5.269465	-2.440728	-2.384707	H	5.730489	3.044525	-0.109163
H	-4.043054	-1.588718	-3.319016	H	4.880808	2.594155	-1.577986
C	-0.552926	4.228917	-0.904984	C	0.077217	-3.501602	-2.986162
H	-0.465001	5.070511	-1.596987	H	-0.046953	-4.068771	-3.914547
H	0.421376	4.159797	-0.396605	H	-0.929444	-3.394724	-2.561722
C	1.048173	0.556902	-3.617168	C	-0.342546	1.264349	-4.145629
H	1.466223	1.139762	-4.440375	H	-0.614742	1.242273	-5.205124
H	1.841105	0.462848	-2.861106	H	-1.288415	1.256531	-3.587772
C	8.207969	0.710571	0.472791	H	-9.693298	0.071171	1.069814
C	6.949465	0.156600	0.352807	C	-8.657611	0.285549	1.314026
H	8.297720	1.791927	0.574139	C	-7.649949	-0.065571	0.493455
H	6.889639	-0.929358	0.251404	H	-8.471494	0.797090	2.255359
C	5.727344	0.862169	0.349407	C	-6.261436	0.201103	0.783746
H	5.761066	1.947017	0.449664	H	-7.870668	-0.578475	-0.442013
C	4.494685	0.247221	0.221747	C	-5.224973	-0.151356	-0.027857
H	4.492220	-0.840941	0.116027	H	-6.040179	0.714973	1.719388
C	3.240063	0.886668	0.219428	C	-3.863425	0.131370	0.300787
H	3.213980	1.971104	0.321627	H	-5.429058	-0.671562	-0.963463
C	2.040199	0.204177	0.072380	C	-2.789999	-0.240581	-0.468116
H	2.125867	-0.871588	-0.094179	H	-3.673243	0.652666	1.240990
C	0.748482	0.760557	0.046491	C	-1.456526	0.062757	-0.074531
C	-0.425670	0.010583	-0.176033	H	-2.945144	-0.788332	-1.397131
H	0.667464	1.840551	0.092928	C	-0.373600	-0.376584	-0.774232
H	-0.333777	-1.081291	-0.115645	H	-1.310667	0.676773	0.802674
O	-1.570942	0.481460	-0.469492	H	-0.459377	-0.983943	-1.655543
C	9.391559	-0.066144	0.469600	N	0.955702	-0.091824	-0.432757
C	10.657534	0.427746	0.586004	O	1.857109	-0.433641	-1.231456

N	11.793235	-0.423478	0.574882	O	1.258538	0.479731	0.640891
O	12.906170	0.125161	0.689650				
O	11.643951	-1.653478	0.454847				
H	10.916077	1.472043	0.694351				
H	9.301128	-1.145786	0.367491				

I^{III}AI3 out of cavity (-3088.99345) (0)

H	-0.496765	5.329136	0.704180
H	1.298694	-0.323119	4.403437
C	-1.387246	3.445902	-2.018528
C	-3.715176	3.233140	-0.479931
C	-1.433900	4.058150	-0.755573
C	-2.472524	2.728383	-2.522754
C	-3.632845	2.628310	-1.736002
C	-2.600802	3.943790	-0.001083
C	-0.243499	4.845616	-0.248427
C	-2.400780	2.067676	-3.885911
C	-4.985503	3.134427	0.346276
H	-0.017315	5.659496	-0.950741
C	-0.334223	-1.906069	3.113080
C	0.563226	-2.815382	0.621705
C	0.950982	-1.566106	2.684514
C	-1.185288	-2.694866	2.322029
C	-0.724384	-3.135613	1.077214
C	1.383541	-2.033878	1.436338
C	1.872309	-0.746558	3.568570
C	-2.571027	-3.095171	2.805968
C	1.091866	-3.313289	-0.711886
H	2.625777	-1.407150	4.023460
H	2.039190	-2.804036	-0.931043
H	-1.467219	2.353235	-4.385324
H	1.336214	-4.382522	-0.638987
H	-3.220541	2.430935	-4.519127
H	-3.119147	-3.565376	1.980365
H	-2.483748	-3.860420	3.589593
H	-5.408272	4.137093	0.495393
H	-5.736604	2.554110	-0.201940
H	-0.489157	3.541631	-2.626018
H	-4.493048	2.082710	-2.119591
H	2.374574	-1.772126	1.077510
H	-1.380795	-3.742313	0.457161
H	-0.676259	-1.550321	4.083085
H	-2.646182	4.418730	0.976440
S	-2.221739	-2.509671	-3.761854

AI1 (-590.00679) (0)

C	-0.374179	-0.515343	0.000205
C	0.994846	-0.344088	0.000032
H	-1.095282	0.290680	0.000492
H	1.584141	-1.259752	-0.000298
C	1.673028	0.880034	0.000149
H	1.089430	1.801627	0.000413
C	3.068892	0.981300	-0.000077
H	3.623021	0.038431	-0.000337
C	3.824787	2.149296	0.000024
H	3.302087	3.106713	0.000123
C	5.233040	2.162479	0.000002
H	5.721518	1.182790	-0.000108
N	-0.966476	-1.783354	0.000006
O	-2.221591	-1.834563	0.000195
O	-0.252776	-2.814862	-0.000439
C	6.067845	3.261856	0.000082
C	7.494611	3.123400	-0.000002
H	5.660413	4.271929	0.000209
H	7.840409	2.057078	-0.000136
O	8.330744	4.032297	0.000055

AI2 (-667.41594) (0)

C	-0.323870	-0.567458	0.000125
C	1.037900	-0.363801	-0.000018
H	-1.065900	0.219227	0.000335
H	1.651373	-1.263198	-0.000225
C	1.683393	0.881062	0.000079
H	1.072996	1.784962	0.000273
C	3.072315	1.021259	-0.000064
H	3.656420	0.097145	-0.000259
C	3.790805	2.216980	0.000015
H	3.233249	3.154704	0.000057
C	5.192265	2.282305	0.000040
H	5.723597	1.326478	-0.000005
N	-0.885135	-1.853056	0.000009
O	-2.137015	-1.933533	0.000192
O	-0.144924	-2.863601	-0.000205

C	-1.242696	-1.393670	-2.951627	C	5.972450	3.430748	0.000113
N	-0.238807	-1.768107	-2.112189	C	7.383098	3.413286	0.000078
N	-1.406152	-0.046388	-3.090543	H	5.472038	4.399780	0.000202
H	0.395712	-1.058041	-1.758942	H	7.851383	2.424122	-0.000014
H	-0.935290	0.564588	-2.431280	C	8.235926	4.495810	0.000147
N	-4.264143	1.161150	1.638503	C	9.662246	4.330592	-0.000016
C	-4.302354	0.245826	2.642743	H	7.848074	5.513326	0.000328
H	-3.611380	1.007146	0.876960	H	9.989910	3.259232	-0.000198
S	-5.195526	0.483870	4.069761	O	10.510855	5.225919	0.000031
N	-3.591804	-0.887662	2.414581				
H	-2.970228	-0.916900	1.613599	AI3 (-515.30021) (0)			
N	0.945810	3.062618	0.999872	C	-0.345984	-0.449753	0.000170
C	1.745281	1.966362	1.126804	C	1.000771	-0.394689	-0.000019
H	0.416591	3.350632	1.819573	H	-1.021561	0.394899	0.000449
S	2.607278	1.304441	-0.184249	H	1.539274	-1.339607	-0.000292
N	1.767694	1.451070	2.384726	C	1.754908	0.826959	0.000130
H	1.317704	1.993137	3.119924	H	1.204165	1.766781	0.000377
H	-2.489036	0.131070	-4.859771	C	3.115524	0.851987	-0.000030
C	-2.508899	0.536526	-3.844187	H	3.653032	-0.096859	-0.000286
H	-3.470288	0.232235	-3.408294	C	3.909438	2.049457	0.000101
C	0.139105	-3.159774	-1.901882	H	3.377932	3.001276	0.000395
H	-0.777220	-3.737011	-1.753582	C	5.267419	2.052080	-0.000116
H	0.612770	-3.568882	-2.804947	H	5.795807	1.098022	-0.000405
C	-3.418700	-1.957334	3.390969	N	-1.041162	-1.714924	0.000011
H	-4.402765	-2.337334	3.681613	O	-2.275589	-1.654327	0.000213
H	-2.960401	-1.554836	4.303177	O	-0.386165	-2.762231	-0.000321
C	-4.792317	2.516489	1.739011	C	6.081330	3.247901	0.000013
H	-5.746713	2.467771	2.266777	C	7.426020	3.240202	0.000031
H	-4.117075	3.138713	2.343033	H	5.551614	4.200395	0.000092
C	2.635890	0.384785	2.859185	H	7.989743	2.310143	-0.000046
H	3.364075	0.809672	3.564727	H	8.001990	4.160234	0.000122
H	3.197240	0.018352	1.998961				
C	1.044184	4.024480	-0.088598				
H	1.886994	4.710266	0.088544				
H	1.274292	3.471776	-1.001432				
O	-1.218554	3.110732	3.286136				
N	-0.894639	2.603701	4.375307				
C	-1.937115	2.059049	5.172084				
O	0.287411	2.543314	4.767037				
C	-1.677581	1.524838	6.391756				
H	-2.911023	2.087783	4.700811				
H	-0.654714	1.556958	6.760274				
C	-2.686330	0.921434	7.204316				
H	-3.692847	0.855472	6.795347				

C	-2.417228	0.414004	8.442609
H	-1.398706	0.484015	8.827022
C	-3.390417	-0.212726	9.287900
H	-4.408577	-0.288951	8.907500
C	-3.102346	-0.708799	10.520938
H	-2.081060	-0.629054	10.895323
C	-4.066693	-1.345490	11.388812
C	-3.767598	-1.831200	12.607209
H	-5.086679	-1.425680	11.014297
H	-2.760585	-1.768801	13.013173
H	-4.518015	-2.304000	13.232849

Table S2. Calculated solvation free energies, ΔG_{298} (kJ mol⁻¹), of the various species in cyclohexane, chloroform and acetonitrile.^A

Species	C ₆ H ₁₂	CHCl ₃	CH ₃ CN
F ⁻	-190.0	-301.7	-367.7
Cl ⁻	-152.4	-240.1	-291.3
Br ⁻	-141.6	-222.1	-268.7
NO ₃ ⁻	-129.7	-206.3	-248.9
AcO ⁻	-127.4	-210.7	-258.4
HSO ₄ ⁻	-130.8	-208.3	-253.1
H ₂ PO ₄ ⁻	-139.6	-225.8	-278.3
H ₂ O	-9.4	-19.7	-25.9
1	14.8	-0.4	-8.5
1 ...F ⁻	-43.8	-88.3	-91.8
1 ...Cl ⁻	-51.6	-93.4	-97.1
1 ...Br ⁻	-54.9	-96.5	-100.2
1 ...NO ₃ ⁻	-55.0	-100.0	-105.1
1 ...AcO ⁻	-60.5	-105.1	-111.7
1 ...HSO ₄ ⁻	-60.6	-104.2	-109.8
1 ...H ₂ PO ₄ ⁻	-60.7	-103.6	-111.6
1 ...H ₂ O	0.7	-17.8	-14.4
2	-9.2	-37.0	-42.2
2 ...F ⁻	-41.5	-79.3	-77.1
2 ...Cl ⁻	-48.9	-81.2	-77.5
2 ...Br ⁻	-53.0	-85.2	-82.2
2 ...NO ₃ ⁻	-53.0	-89.0	-89.4
2 ...AcO ⁻	-58.0	-92.0	-88.4
2 ...HSO ₄ ⁻	-56.5	-89.3	-87.0
2 ...H ₂ PO ₄ ⁻	-59.3	-93.3	-91.5
2 ...H ₂ O	-9.3	-27.8	-24.8

^A PCM calculations at B3LYP/6-311+G**// B3LYP/6-31G* level.

Table S3. NBO population analysis of the thiourea groups in the various complexes.

Species	Charge Distribution (q)						Charge Transfer (Δq)						Anion
	H1	N(-H1)	C	S	N(-H2)	H2	H1	N(-H1)	C	S	N(-H2)	H2	
1	0.379	-0.621	0.313	-0.291	-0.644	0.382							
1\cdotsF$^-$	0.442	-0.657	0.333	-0.372	-0.665	0.436	0.063	-0.036	0.020	-0.081	-0.021	0.054	0.147
1\cdotsCl$^-$	0.427	-0.661	0.334	-0.360	-0.661	0.427	0.048	-0.040	0.021	-0.069	-0.017	0.045	0.152
1\cdotsBr$^-$	0.421	-0.666	0.333	-0.354	-0.666	0.421	0.042	-0.045	0.020	-0.063	-0.022	0.039	0.199
1\cdotsNO$_3^-$	0.417	-0.653	0.336	-0.351	-0.653	0.417	0.038	-0.032	0.023	-0.060	-0.009	0.035	0.137
1\cdotsAcO$^-$	0.433	-0.672	0.329	-0.347	-0.668	0.430	0.054	-0.051	0.016	-0.056	-0.024	0.048	0.157
1\cdotsHSO$_4^-$	0.420	-0.658	0.333	-0.345	-0.660	0.415	0.041	-0.037	0.020	-0.054	-0.016	0.033	0.117
1\cdotsH$_2$PO$_4^-$	0.404	-0.658	0.336	-0.350	-0.663	0.434	0.025	-0.037	0.023	-0.059	-0.019	0.052	0.143
	H3	N(-H3)	C	S	N(-H4)	H4	H3	N(-H3)	C	S	N(-H4)	H4	
1	0.380	-0.621	0.313	-0.291	-0.645	0.382							
1\cdotsF$^-$	0.443	-0.657	0.333	-0.373	-0.665	0.436	0.063	-0.036	0.020	-0.082	-0.020	0.054	
1\cdotsCl$^-$	0.427	-0.660	0.334	-0.359	-0.660	0.427	0.047	-0.039	0.021	-0.068	-0.015	0.045	
1\cdotsBr$^-$	0.421	-0.666	0.333	-0.354	-0.666	0.421	0.041	-0.045	0.020	-0.063	-0.021	0.039	
1\cdotsNO$_3^-$	0.417	-0.653	0.336	-0.351	-0.653	0.417	0.037	-0.032	0.023	-0.060	-0.008	0.035	
1\cdotsAcO$^-$	0.427	-0.658	0.340	-0.360	-0.658	0.429	0.047	-0.037	0.027	-0.069	-0.013	0.047	
1\cdotsHSO$_4^-$	0.411	-0.654	0.331	-0.334	-0.660	0.417	0.031	-0.033	0.018	-0.043	-0.015	0.035	
1\cdotsH$_2$PO$_4^-$	0.429	-0.665	0.312	-0.340	-0.656	0.422	0.049	-0.044	-0.001	-0.049	-0.011	0.040	
	H5	N(-H5)	C	S	N(-H6)	H6	H5	N(-H5)	C	S	N(-H6)	H6	
1	0.380	-0.621	0.313	-0.291	-0.645	0.382							
1\cdotsF$^-$	0.443	-0.657	0.333	-0.373	-0.665	0.436	0.063	-0.036	0.020	-0.082	-0.020	0.054	
1\cdotsCl$^-$	0.427	-0.661	0.334	-0.362	-0.661	0.427	0.047	-0.040	0.021	-0.071	-0.016	0.045	
1\cdotsBr$^-$	0.421	-0.666	0.333	-0.354	-0.666	0.421	0.041	-0.045	0.020	-0.063	-0.021	0.039	
1\cdotsNO$_3^-$	0.417	-0.653	0.336	-0.352	-0.653	0.417	0.037	-0.032	0.023	-0.061	-0.008	0.035	
1\cdotsAcO$^-$	0.435	-0.671	0.333	-0.365	-0.667	0.433	0.055	-0.050	0.020	-0.074	-0.022	0.051	
1\cdotsHSO$_4^-$	0.418	-0.645	0.335	-0.358	-0.662	0.423	0.038	-0.024	0.022	-0.067	-0.017	0.041	
1\cdotsH$_2$PO$_4^-$	0.429	-0.679	0.334	-0.353	-0.648	0.427	0.049	-0.058	0.021	-0.062	-0.003	0.045	

Table S4. RESP charges of receptor **1**, acetate and nitrate anions used in AMBER molecular dynamics simulations.

receptor 1		AcO⁻	
S1	-0.447766	C1	-0.314234
C19	0.329510	H1	0.031991
N2	-0.449680	H2	0.031991
H20	0.311514	H3	0.031991
C22	0.101252	C2	0.904432
C8	-0.039723	O2	-0.843085
H6	0.049087	O1	-0.843085
H8	0.049087		
H25	0.039192	NO₃⁻	
H26	0.039192	O1	-0.660577
N1	-0.449680	N1	0.981730
H19	0.311514	O3	-0.660577
C23	0.101252	O2	-0.660577
H27	0.039192		
H28	0.039192		
C18	-0.039723		
H5	0.049087		
H7	0.049087		
C11	0.026502		
C15	-0.220955		
H15	0.153660		
C14	-0.220955		
H16	0.153660		
C13	0.026502		
C10	-0.220955		
H17	0.153660		
C12	0.026502		
C16	-0.039723		
H2	0.049087		
H4	0.049087		
C26	0.101252		
H33	0.039192		
H34	0.039192		
N6	-0.449680		
H24	0.311514		
C21	0.329510		
S3	-0.447766		
N5	-0.449680		
H23	0.311514		
C27	0.101252		
H35	0.039192		

H36	0.039192
C7	-0.039723
H1	0.049087
H3	0.049087
C3	0.026502
C6	-0.220955
H18	0.153660
C1	-0.220955
H13	0.153660
C4	0.026502
C5	-0.220955
H14	0.153660
C2	0.026502
C9	-0.039723
H11	0.049087
H12	0.049087
C25	0.101252
H31	0.039192
H32	0.039192
N3	-0.449680
H21	0.311514
C20	0.329510
S2	-0.447766
N4	-0.449680
H22	0.311514
C24	0.101252
H29	0.039192
H30	0.039192
C17	-0.039723
H9	0.049087
H10	0.049087

Table S5. Calculated gas-phase TD-DFT transition energies (nm) of **BM** and **1^{···}BM**.^{A,B}

level	BM	1^{···}BM
B3LYP/6-31G*	421.2 (1.13), 407.3 (0.36)	457.7 (0.23), 443.5 (1.45)
B3LYP/6-31+G*	439.4 (1.04), 420.6 (0.45)	465.6 (0.57), 454.2 (1.10)
B3LYP/6-311+G**	441.8 (0.94), 422.8 (0.54)	467.6 (0.56), 454.8 (1.15)
B3LYP/6-311+G(2d,p)	444.2 (0.85), 424.5 (0.61)	466.1 (0.64), 454.5 (1.40)
B3LYP/6-311+G(2df,p)	443.8 (0.87), 424.1 (0.59)	467.7 (0.66), 455.7 (1.39)
B3LYP/6-311+G(3df,2p)	444.9 (0.85), 424.9 (0.60)	

^A Based on B3LYP/6-31G* optimized geometry.

^B Oscillator strength in parenthesis.

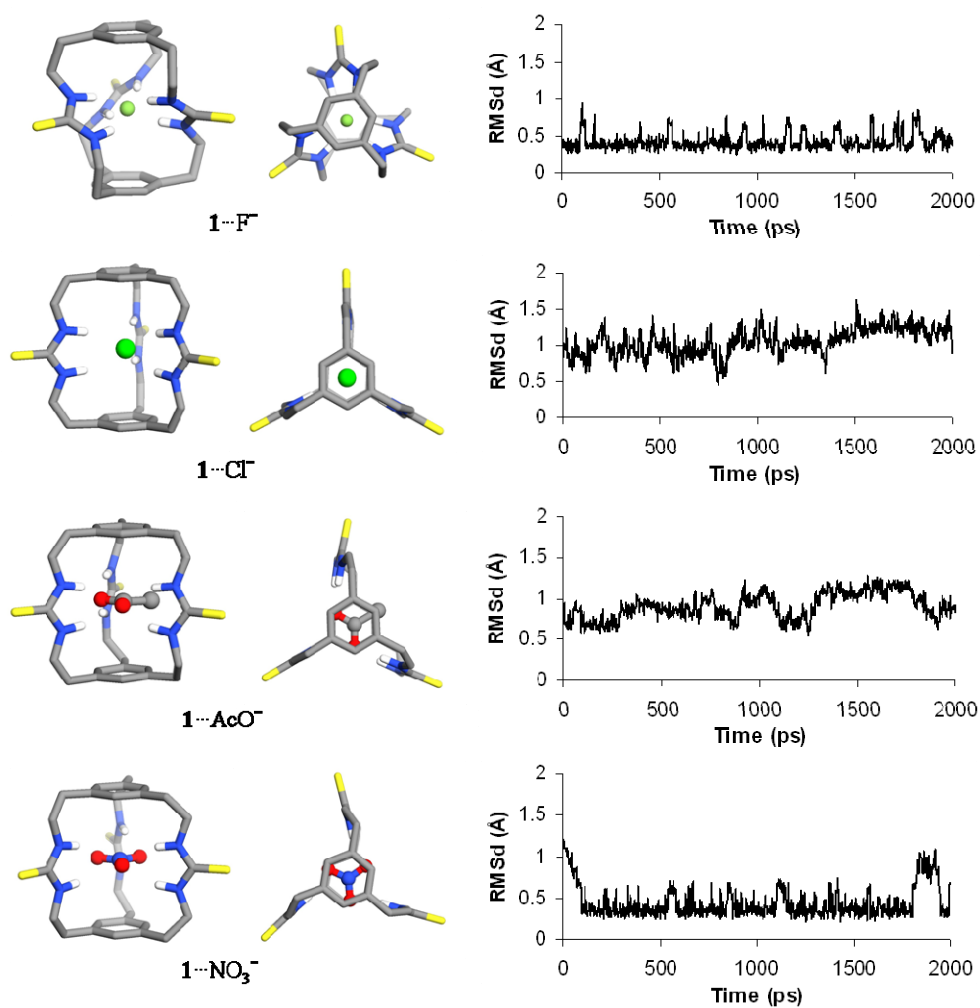


Figure S1. Time-average MD structures (side and top views) and corresponding RMSD plots of $\mathbf{1}\cdots\text{F}^-$, $\mathbf{1}\cdots\text{Cl}^-$, $\mathbf{1}\cdots\text{AcO}^-$ and $\mathbf{1}\cdots\text{NO}_3^-$.

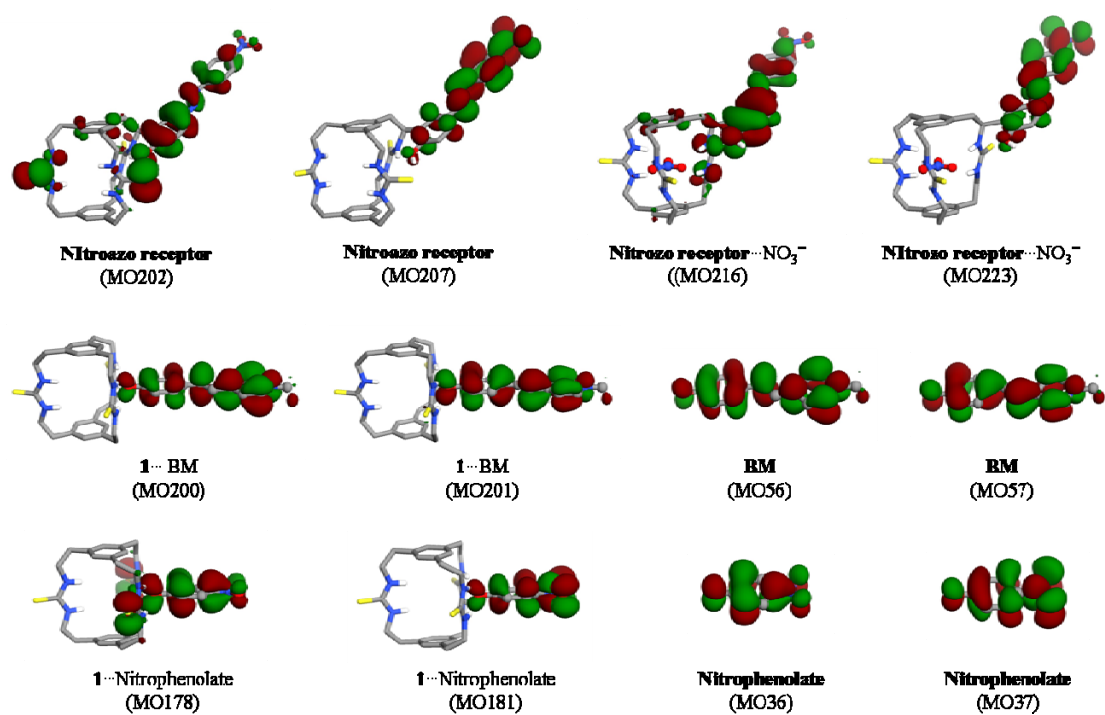


Figure S3. Molecular orbitals (MOs) involved in the main excitations.