Electronic Supplementary Information (ESI)

Can Phthalocyanines and their Substituted α-*para* (Methoxy)Phenyl Derivatives act as Photosensitizers in Photodynamic Therapy? A TD-DFT Study

*Angelo Domenico Quartarolo, Ida Lanzo, Emilia Sicilia and Nino Russo**

Dipartimento di Chimica and Centro di Calcolo ad Alte Prestazioni per Elaborazioni Parallele e Distribuite-Centro di Eccellenza MURST, Università della Calabria, I-87030 Arcavacata di Rende, Italy

*Address correspondence to this author: Tel. +39-0984-492048, Fax. +39-0984-492044, e-mail: nrusso@unical.it

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1. Cartesian Coordinates (Å) for the optimized molecules 1a-1d and 2a-2d in Molden Format

Molecule 1a

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FINAL HEAT OF FORMATION = -3514.307280

C	-5.119986	0.240877	-2.570859	C	-5.551361	-1.264944	2.113871	H	5.827164	3.897552	2.646053
C	-5.485712	1.506642	-2.053348	C	-6.219198	-0.589934	1.068936	H	4.136865	5.689498	2.530695
C	-6.864542	1.813447	-1.963450	C	-7.218208	0.353948	1.358069	H	-3.840172	5.819460	-2.602424
C	-7.841109	0.888582	-2.367318	C	-7.554936	0.658462	2.687654	H	-5.596011	4.099565	-2.726175
C	-7.460733	-0.365734	-2.874053	C	-6.888296	0.004721	3.737231	H	-5.968521	-0.813979	0.022155
C	-6.094381	-0.683504	-2.975417	C	-5.903448	-0.952361	3.450753	H	-7.735754	0.855221	0.525530
C	-4.455146	2.533373	-1.739626	C	-1.502021	-5.520215	2.120627	H	-8.335882	1.406199	2.905315
C	-3.212835	2.285619	-1.105500	C	-1.215511	-5.894726	3.457255	H	-7.133855	0.240259	4.786252
C	-2.181985	3.275153	-1.067250	C	-0.305757	-6.923431	3.743712	H	-5.376019	-1.455636	4.278096
C	-2.361701	4.564631	-1.623111	C	0.326240	-7.611043	2.694226	H	-1.700009	-5.350416	4.284817
C	-3.651283	4.833517	-2.147458	C	0.046672	-7.252580	1.364912	H	-0.088878	-7.185870	4.792624
C	-4.652140	3.856021	-2.211948	C	-0.850216	-6.211184	1.076016	H	1.038049	-8.424762	2.911882
C	-2.645897	1.107514	-0.407918	C	1.207645	-5.566433	-2.093068	H	0.531141	-7.786117	0.532374
N	-1.333734	1.322019	-0.092329	C	-0.054150	-5.137554	-2.570064	H	-0.252715	-4.059953	-2.676124
C	-1.042852	2.625748	-0.380573	C	-1.038080	-6.065131	-2.943138	H	-2.009845	-5.706090	-3.320673
N	0.069497	3.264630	0.011324	C	-0.785513	-7.445449	-2.848146	H	-1.558962	-8.174140	-3.141910
C	1.165402	2.635135	0.409751	C	0.463932	-7.887855	-2.381511	H	0.673539	-8.967658	-2.301653
N	1.443277	1.304250	0.189549	C	1.449293	-6.958300	-2.010866	H	2.421390	-7.316124	-1.633344
C	2.757761	0.967313	0.450089	C	5.462255	-1.558257	-2.024242	H	7.124340	-2.869606	-1.511080
C	3.364120	2.157092	1.068320	C	6.834781	-1.877614	-1.895739	H	8.892537	-1.212926	-2.113826
C	2.367407	3.199159	1.033197	C	7.829368	-0.944815	-2.232034	H	8.252166	1.058977	-2.978791
C	2.604032	4.487724	1.576755	C	7.472567	0.326347	-2.712302	H	5.820725	1.646042	-3.239740
C	3.899270	4.704501	2.097127	C	6.112424	0.655358	-2.853514	H	4.058307	-0.016292	-2.651753
C	4.855752	3.681425	2.172720	C	5.119393	-0.274855	-2.512946	H	5.845452	0.439800	0.071634
C	4.617144	2.366620	1.707077	C	5.623896	1.320179	2.051744	H	7.572822	-1.200498	0.770648
N	3.329919	-0.159080	0.045825	C	6.174922	0.414776	1.118761	H	8.350773	-1.300764	3.160024
C	2.622181	-1.224992	-0.368958	C	7.151570	-0.511689	1.519856	H	7.367276	0.289874	4.848042
N	1.314130	-1.454171	-0.050092	C	7.588562	-0.564815	2.853694	H	5.639971	1.941824	4.142002
C	1.016446	-2.741159	-0.396099	C	7.043787	0.325190	3.794307	H	2.887213	7.127250	0.953100
C	2.140261	-3.352901	-1.141146	C	6.077245	1.259531	3.394384	H	1.281056	8.981272	1.412202
C	3.180509	-2.371068	-1.123667	C	1.586339	5.563768	1.732694	H	-0.949015	8.487175	2.465163
C	4.416441	-2.589235	-1.780237	C	1.913404	6.903351	1.419264	H	-1.551825	6.114122	3.036719
C	4.596152	-3.874506	-2.350604	C	1.008343	7.945459	1.673977	H	0.056566	4.267497	2.586206
C	3.577254	-4.835111	-2.367797	C	-0.239220	7.669158	2.257315	H	0.183207	4.220417	-2.588838
C	2.295422	-4.588979	-1.815279	C	-0.577135	6.341679	2.574115	H	1.878319	5.988920	-3.050431
N	-0.088375	-3.393433	0.006672	C	0.322993	5.299557	2.311011	H	1.367649	8.396048	-2.534822
C	-1.185034	-2.761812	0.398437	C	-1.300994	5.596137	-1.786103	H	-0.854523	9.003686	-1.525749
N	-1.485540	-1.453321	0.079590	C	-0.040736	5.268761	-2.338279	H	-2.544272	7.229204	-1.056350
C	-2.778699	-1.089165	0.391636	C	0.907307	6.266062	-2.607345	H	-7.175749	2.788124	-1.552800
C	-3.349460	-2.228415	1.124387	C	0.621203	7.612698	-2.321852	H	-8.909260	1.149199	-2.281010
C	-2.353480	-3.274518	1.127610	C	-0.622094	7.952210	-1.763208	H	-8.226143	-1.092045	-3.193612
C	-2.523710	-4.457991	1.893536	C	-1.574510	6.954535	-1.503288	H	-5.782878	-1.659274	-3.383726
C	-3.750213	-4.571226	2.587495	H	-5.642838	-3.698987	3.164142	H	-4.053535	-0.007466	-2.684385
C	-4.715961	-3.555872	2.585366	H	-3.941071	-5.488764	3.167183	H	-1.055915	-5.944609	0.029531
C	-4.540829	-2.338112	1.888700	H	3.746844	-5.777728	-2.912996	H	0.734402	0.616172	-0.098132
N	-3.354312	0.038541	-0.001878	H	5.537007	-4.090449	-2.882604	H	-0.798356	-0.792206	-0.300941

Molecule 1b

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FINAL HEAT OF FORMATION = -5292.617510

Zn	-0.019670	-0.055376	0.035846	C	-3.643807	4.933699	-2.083813	C	5.788404	-0.043653	2.019089
N	-1.764959	-1.047207	0.036504	H	-4.508302	5.403477	-2.580107	C	6.120936	-1.065801	1.103404
N	0.971502	-1.791586	-0.017696	C	-3.756840	3.591067	-1.649637	H	5.830958	-0.969371	0.048723
N	1.721435	0.931592	0.088311	C	-5.723323	0.077312	2.053751	C	6.831805	-2.199630	1.530699
N	-1.007103	1.678374	-0.061873	C	-6.195077	0.931009	1.033081	H	7.087612	-2.977635	0.794512
N	-0.908421	-3.282543	-0.005153	H	-6.003541	0.682875	-0.020660	C	7.212861	-2.345676	2.874805
N	3.217177	-0.936349	0.027746	C	-6.926136	2.086326	1.355485	H	7.764218	-3.242896	3.202418
N	0.872454	3.175850	-0.015682	H	-7.297148	2.727910	0.541346	C	6.882793	-1.340081	3.798710
N	-3.252731	0.830756	-0.016785	C	-7.183131	2.424134	2.694706	H	7.165265	-1.443053	4.859850
C	-2.947664	-0.420147	0.347379	H	-7.752405	3.336891	2.937935	C	6.184113	-0.200871	3.372060
C	-3.819529	-1.384943	1.049056	C	-6.707402	1.591323	3.721073	H	5.913417	0.576339	4.105878
C	-3.107521	-2.638169	1.051739	H	-6.891269	1.847864	4.777844	C	2.916347	5.048931	1.666010
C	-1.830344	-2.383900	0.354567	C	-5.993393	0.426936	3.400886	C	3.550591	6.270399	1.340588
C	0.343814	-2.966001	-0.357115	H	-5.615109	-0.219359	4.210377	H	4.538187	6.252655	0.850797
C	1.311589	-3.824377	-1.065761	C	-2.832456	-5.023729	2.053360	C	2.932232	7.500320	1.616075
C	2.561396	-3.115491	-1.048601	C	-2.680719	-5.444327	3.398859	H	3.441765	8.440008	1.345580
C	2.307494	-1.849530	-0.334301	H	-3.046473	-4.793364	4.210312	C	1.670487	7.533682	2.232458
C	2.918411	0.318093	0.381441	C	-2.049708	-6.656689	3.714901	H	1.187404	8.499118	2.457382
C	3.818697	1.317103	0.996228	H	-1.931985	-6.953935	4.770437	C	1.027331	6.326962	2.559835
C	3.105591	2.566209	0.955352	C	-1.569869	-7.484264	2.686155	H	0.038971	6.341196	3.048618
C	1.798959	2.279048	0.337151	H	-1.078981	-8.442201	2.926550	C	1.640899	5.098365	2.275853
C	-0.383884	2.869736	-0.348521	C	-1.717139	-7.080636	1.348644	H	1.140129	4.160197	2.560721
C	-1.362281	3.765450	-0.992886	H	-1.348905	-7.721455	0.532692	C	0.029059	5.824856	-1.715251
C	-2.602989	3.043727	-1.030595	C	-2.332333	-5.858651	1.030568	C	1.153580	5.218908	-2.322869
C	-2.344716	1.748036	-0.370466	C	-0.107196	-5.757797	-2.036033	H	1.115039	4.151671	-2.589571
C	-5.012143	-1.208899	1.797503	C	-1.206772	-5.036617	-2.560023	C	2.297878	5.970223	-2.626108
C	-5.496689	-2.359639	2.465641	H	-1.134414	-3.943634	-2.669099	H	3.157374	5.480493	-3.113521
H	-6.441849	-2.281108	3.026875	C	-2.371489	-5.699320	-2.974200	C	2.348655	7.341392	-2.319200
C	-4.806408	-3.577098	2.465843	H	-3.211828	-5.116651	-3.386936	H	3.249597	7.930729	-2.558053
H	-5.224486	-4.429108	3.025874	C	-2.466756	-7.099082	-2.874717	C	1.244463	7.954220	-1.704422
C	-3.569582	-3.752070	1.799255	H	-3.383378	-7.618314	-3.199960	H	1.276553	9.026431	-1.449212
C	1.178037	-5.074424	-1.724407	C	-1.382045	-7.830026	-2.361358	C	0.094993	7.204288	-1.410342
C	2.372539	-5.632190	-2.238946	H	-1.445484	-8.927673	-2.275981	H	-0.764343	7.690824	-0.920083
H	2.321949	-6.598916	-2.765391	C	-0.215055	-7.166197	-1.949582	C	-4.991074	2.836469	-1.998319
C	3.592470	-4.941477	-2.220131	H	0.625346	-7.747565	-1.535540	C	-6.263399	3.450491	-1.910922
H	4.460658	-5.387425	-2.731885	C	4.970085	-2.882674	-1.962743	H	-6.348142	4.457119	-1.469306
C	3.715547	-3.635905	-1.688980	C	6.231919	-3.508347	-1.826210	C	-7.419654	2.790119	-2.356514
C	5.076483	1.215016	1.648740	H	6.286840	-4.526289	-1.405996	H	-8.400502	3.286851	-2.270291
C	5.629727	2.434883	2.110685	C	7.412550	-2.844773	-2.197906	C	-7.329335	1.498397	-2.902380
H	6.621239	2.409488	2.590874	H	8.385529	-3.348210	-2.071881	H	-8.235986	0.978307	-3.253232
C	4.952194	3.658496	2.025245	C	7.355586	-1.542450	-2.722203	C	-6.071262	0.877689	-3.003477
H	5.419316	4.559226	2.455849	H	8.281496	-1.020669	-3.015271	H	-5.986745	-0.130548	-3.441692
C	3.642212	3.758232	1.501286	C	6.107838	-0.910906	-2.872339	C	-4.916947	1.538093	-2.558071
C	-1.242484	5.072661	-1.529017	H	6.050877	0.107002	-3.292038	H	-3.935603	1.052525	-2.669065
C	-2.439913	5.648887	-2.016460	C	4.929348	-1.572004	-2.496448	H	-2.437863	-5.558957	-0.021761
H	-2.400085	6.661617	-2.449285	H	3.956961	-1.076974	-2.640728				

Molecule 1c

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FINAL HEAT OF FORMATION = -5540.752520

Zn	0.000425	-0.073803	-0.312990	C	-6.088375	3.696900	1.702524	H	5.229541	-4.747924	5.241739
N	-2.003496	-0.071942	0.131485	H	-6.967893	3.197875	1.262749	C	5.075924	-3.198721	3.726583
N	0.004327	-2.072005	0.142866	C	-6.136380	5.071355	1.985217	H	5.143606	-2.380960	4.463094
N	2.005020	-0.064312	0.129164	H	-7.055754	5.641027	1.769824	C	4.913708	2.960440	1.952025
N	-0.002799	1.939643	0.000032	C	-5.019949	5.716472	2.541930	C	6.078316	3.718591	1.691295
N	-2.360351	-2.444933	0.219692	H	-5.059298	6.793628	2.775036	H	6.958914	3.221607	1.251275
N	2.370514	-2.436249	0.220361	C	-3.851005	4.978792	2.800060	C	6.122201	5.093733	1.971267
N	2.360499	2.320528	0.103347	H	-2.970110	5.474101	3.241683	H	7.039089	5.666330	1.753133
N	-2.367812	2.311759	0.104708	C	-3.799341	3.608471	2.507019	C	5.004351	5.736201	2.528270
C	-2.706480	1.063000	0.447696	H	-2.887976	3.034688	2.735949	H	5.040348	6.814036	2.758925
C	-3.930958	0.678793	1.172905	C	-4.911002	-2.900534	2.344765	C	3.838580	4.994859	2.790191
C	-3.933107	-0.756858	1.229954	C	-5.072336	-3.224153	3.716272	H	2.956651	5.487856	3.232259
C	-2.706614	-1.189750	0.525341	H	-5.139648	-2.409325	4.456068	C	3.791366	3.623629	2.500548
C	-1.118178	-2.808363	-0.129751	C	-5.115592	-4.557429	4.150296	H	2.882437	3.047097	2.732485
C	-0.710038	-4.085443	-0.751275	H	-5.226831	-4.780036	5.224813	C	2.922866	5.178019	-1.404356
C	0.727254	-4.082870	-0.750776	C	-5.011043	-5.600918	3.215777	C	3.579982	4.133120	-2.095455
C	1.129482	-2.803985	-0.129176	H	-5.048126	-6.651913	3.548070	H	3.005306	3.245448	-2.401128
C	2.711506	-1.179291	0.524563	C	-4.854982	-5.294137	1.853897	C	4.938760	4.230506	-2.426571
C	3.936491	-0.742375	1.229296	H	-4.775981	-6.102404	1.110044	H	5.426508	3.407831	-2.975994
C	3.929121	0.693307	1.172049	C	-4.796999	-3.959735	1.418423	C	5.676934	5.371885	-2.067325
C	2.704007	1.073112	0.445825	C	-2.908161	-5.148663	-1.610088	H	6.745694	5.447518	-2.328428
C	1.119486	2.692216	-0.225049	C	-3.532176	-4.022500	-2.198104	C	5.041981	6.413199	-1.370753
C	0.710329	4.014638	-0.744064	H	-2.940756	-3.111093	-2.373500	H	5.612421	7.308670	-1.072851
C	-0.724471	4.012188	-0.742981	C	-4.879890	-4.063062	-2.584502	C	3.679874	6.317945	-1.046194
C	-1.128306	2.688123	-0.223630	H	-5.342038	-3.174309	-3.045833	H	3.194852	7.135230	-0.487531
C	-4.932437	1.460680	1.799194	C	-5.639732	-5.230908	-2.392341	C	-2.942059	5.168701	-1.398595
C	-5.979541	0.738095	2.416924	H	-6.699668	-5.260705	-2.694070	C	-3.702491	6.304826	-1.035681
H	-6.791220	1.298212	2.909401	C	-5.034913	-6.359287	-1.813775	H	-3.219314	7.122537	-0.476030
C	-5.965750	-0.660083	2.507957	H	-5.621082	-7.279567	-1.653667	C	-5.064885	6.397412	-1.359925
H	-6.778587	-1.164953	3.055028	C	-3.684580	-6.318491	-1.430057	H	-5.637460	7.290967	-1.060387
C	-4.924538	-1.455863	1.969279	H	-3.223847	-7.205374	-0.964396	C	-5.697937	5.354602	-2.055964
C	-1.447067	-5.155332	-1.322644	C	2.931185	-5.140199	-1.602539	H	-6.767345	5.427265	-2.315239
C	-0.687400	-6.261789	-1.771467	C	3.709752	-6.307979	-1.418415	C	-4.957287	4.215285	-2.416610
H	-1.212861	-7.113305	-2.233446	H	3.249626	-7.195356	-0.953078	H	-5.443747	3.391388	-2.965337
C	0.714201	-6.259533	-1.769917	C	5.061488	-6.346154	-1.797420	C	-3.596940	4.122884	-2.090385
H	1.243487	-7.109520	-2.230359	H	5.649300	-7.264696	-1.633594	H	-3.019897	3.237667	-2.398771
C	1.469255	-5.150379	-1.319979	C	5.665559	-5.217208	-2.375649	N	-0.000567	-0.131591	-2.485356
C	4.927545	-1.437246	1.972923	H	6.726544	-5.244957	-2.673920	C	1.160872	-0.133118	-3.171265
C	5.967430	-0.638363	2.509621	C	4.903510	-4.051579	-2.572517	H	2.079071	-0.121638	-2.558280
H	6.780688	-1.140262	3.058736	H	5.364951	-3.162421	-3.033744	C	1.206999	-0.146101	-4.572889
C	5.979730	0.759398	2.412437	C	3.554534	-4.013533	-2.190328	H	2.178414	-0.147106	-5.092039
H	6.790711	1.322644	2.902593	H	2.961619	-3.103782	-2.369248	C	-0.001977	-0.157134	-5.287029
C	4.930051	1.478445	1.795170	C	4.915286	-2.880543	2.353780	H	-0.002560	-0.167175	-6.389411
C	1.452433	5.143667	-1.175120	C	4.801595	-3.943673	1.431809	C	-1.210241	-0.153763	-4.571613
C	0.689634	6.289831	-1.506673	H	4.677700	-3.728398	0.361701	H	-2.182187	-0.160955	-5.089734
H	1.216689	7.190767	-1.860879	C	4.859401	-5.276229	1.872837	C	-1.162708	-0.140659	-3.170015
C	-0.712652	6.288011	-1.504388	H	4.780756	-6.087449	1.132103	H	-2.080305	-0.134717	-2.556050
H	-1.243430	7.187302	-1.857225	C	5.014230	-5.577582	3.236065	H	-4.672542	-3.739857	0.349297
C	-1.471036	5.139064	-1.172120	H	5.051131	-6.627180	3.572723				
C	-4.920353	2.942596	1.959102	C	5.118213	-4.530158	4.166237				

Molecule 1d

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FINAL HEAT OF FORMATION = -5788.859900

C	-1.177443	-0.158989	-3.238823	C	-4.901349	-2.895449	2.246292	H	-2.949663	5.453514	3.131321
N	-0.010847	-0.156528	-2.563898	C	-5.082847	-3.196007	3.620882	H	-2.871878	3.023175	2.588501
C	1.142334	-0.163672	-3.261437	C	-5.109388	-4.520803	4.081088	H	-5.180254	-2.368696	4.343390
C	1.177032	-0.175784	-4.663962	C	-4.967712	-5.580369	3.169811	H	-5.237233	-4.723993	5.157698
C	-0.038052	-0.179792	-5.367568	C	-4.792458	-5.297164	1.805396	H	-4.990723	-6.625238	3.522470
C	-1.239289	-0.170774	-4.640455	C	-4.751263	-3.970991	1.343951	H	-4.683664	-6.117862	1.079124
Zn	0.011850	-0.079908	-0.341009	C	-2.908425	-5.177751	-1.687516	H	-2.950420	-3.149950	-2.476560
N	0.010298	1.936531	-0.158291	C	-3.538907	-4.059820	-2.284424	H	-5.357191	-3.224050	-3.125717
C	1.131196	2.689352	-0.379382	C	-4.890103	-4.106695	-2.657772	H	-6.709911	-5.307051	-2.734663
C	0.716030	4.020442	-0.875905	C	-5.647093	-5.272579	-2.443546	H	-5.619621	-7.311621	-1.678760
C	-0.718833	4.017762	-0.860784	C	-5.035925	-6.392902	-1.856203	H	-3.215988	-7.226519	-1.013493
C	-1.117806	2.685260	-0.355463	C	-3.682127	-6.345874	-1.485605	H	3.243191	-7.223234	-1.008569
C	-1.469500	5.149725	-1.267705	C	2.933596	-5.181624	-1.703581	H	5.644566	-7.315701	-1.682048
C	-0.715017	6.304038	-1.591242	C	3.707711	-6.347780	-1.491939	H	6.730052	-5.324235	-2.766857
C	0.686618	6.307136	-1.605015	C	5.060071	-6.399111	-1.867491	H	5.375572	-3.246422	-3.178199
C	1.452746	5.156029	-1.297415	C	5.668687	-5.285917	-2.470930	H	2.972252	-3.162927	-2.515493
N	2.376664	2.315485	-0.066821	C	4.910866	-4.122636	-2.695932	H	4.634491	-3.772114	0.234170
C	2.732584	1.068506	0.268128	C	3.561553	-4.070805	-2.316106	H	4.710951	-6.106990	1.077015
N	2.032725	-0.071570	-0.028238	C	4.969241	-2.867340	2.186646	H	5.063579	-6.576385	3.521468
C	2.740185	-1.185430	0.360784	C	4.796018	-3.956216	1.304854	H	5.353103	-4.650045	5.120415
C	3.982161	-0.745429	1.036427	C	4.838965	-5.275065	1.787106	H	5.291286	-2.308637	4.268824
C	3.975520	0.691704	0.968252	C	5.039605	-5.537328	3.152339	H	7.006292	3.237608	1.008805
C	4.990606	1.479389	1.565587	C	5.205489	-4.464108	4.043219	H	7.091100	5.672121	1.551383
C	6.059035	0.762913	2.153788	C	5.176501	-3.147060	3.561908	H	5.105687	6.800410	2.605957
C	6.046806	-0.633831	2.262133	C	4.971470	2.960432	1.734022	H	3.028577	5.463879	3.081438
C	4.987842	-1.434791	1.766608	C	6.131080	3.725162	1.469412	H	2.948776	3.034157	2.539758
N	2.386932	-2.444109	0.072692	C	6.177631	5.095247	1.772561	H	2.998863	3.282636	-2.570419
C	1.141541	-2.816856	-0.258293	C	5.067442	5.726772	2.356643	H	5.410755	3.469167	-3.177758
N	0.017660	-2.085435	0.012374	C	3.905511	4.979914	2.619949	H	6.727246	5.506651	-2.517553
C	-1.107505	-2.819756	-0.245327	C	3.855319	3.613934	2.306944	H	5.601951	7.339189	-1.212190
C	-0.703611	-4.105025	-0.856286	C	2.920586	5.198190	-1.541202	H	3.195368	7.140017	-0.593164
C	0.733925	-4.104307	-0.862628	C	3.573259	4.168315	-2.258338	H	-3.205561	7.130203	-0.539078
C	1.471197	-5.180588	-1.420641	C	4.926500	4.279669	-2.607538	H	-5.629127	7.309694	-1.097481
C	0.712067	-6.293332	-1.855474	C	5.663216	5.419799	-2.240911	H	-6.774127	5.462448	-2.363333
C	-0.689289	-6.292993	-1.851563	C	5.033020	6.445023	-1.516748	H	-5.460636	3.431983	-3.049431
C	-1.445038	-5.180136	-1.411106	C	3.676654	6.335681	-1.173536	H	-3.033692	3.262960	-2.499528
N	-2.349408	-2.452092	0.103779	C	-2.942353	5.183879	-1.480968	H	2.066368	-0.156673	-2.656868
C	-2.702267	-1.195660	0.401669	C	-3.696168	6.319290	-1.102085	H	2.143963	-0.181191	-5.191621
N	-2.003855	-0.078473	0.005737	C	-5.061468	6.417928	-1.411575	H	-0.048709	-0.188834	-6.469930
C	-2.701045	1.058292	0.320626	C	-5.702706	5.384386	-2.114035	H	-2.216278	-0.172039	-5.149425
C	-3.929135	0.675867	1.043014	C	-4.967647	4.247849	-2.494595	H	-2.089366	-0.148393	-2.616138
C	-3.933006	-0.761585	1.101737	C	-3.605561	4.146825	-2.177958	H	-4.610094	-3.770251	0.273343
C	-4.924201	-1.457366	1.845936	H	-6.801145	1.298206	2.759980	N	0.030402	0.062261	3.046205
C	-5.971497	-0.660552	2.371713	H	-6.787862	-1.163907	2.915066	C	-1.115606	-0.025354	3.744236
C	-5.986273	0.736940	2.273973	H	-1.218288	-7.148966	-2.301153	C	-1.170947	-0.039452	5.149394
C	-4.932621	1.458676	1.665858	H	1.237801	-7.150266	-2.307029	C	0.032731	0.040157	5.867253
N	-2.355071	2.307056	-0.017070	H	6.874405	-1.132752	2.792210	C	1.235463	0.128542	5.148507
C	-4.915275	2.939098	1.838108	H	6.884062	1.327767	2.617967	C	1.177915	0.134864	3.743361
C	-6.086231	3.697323	1.606335	H	1.210728	7.213110	-1.950685	H	-2.045692	-0.090694	3.150424
C	-6.132241	5.066932	1.911442	H	-1.249486	7.207646	-1.927041	H	-2.142364	-0.113578	5.664807
C	-5.009254	5.704563	2.463798	H	-6.970879	3.204695	1.169513	H	0.033922	0.030907	6.970251
C	-3.836256	4.964299	2.694354	H	-7.054828	5.638876	1.716586	H	2.207557	0.190610	5.664111
C	-3.787274	3.598360	2.380396	H	-5.046535	6.777900	2.714311	H	2.107514	0.198723	3.148093

Molecule 2a

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FINAL HEAT OF FORMATION = -4429.855218

C	-1.841789	6.855741	-1.575534	C	5.585483	1.554493	2.004902	H	4.023364	0.135669	-2.623434
C	-1.517382	5.505820	-1.828596	C	6.145580	0.651949	1.068474	H	5.777749	0.638339	0.034307
C	-0.223944	5.231656	-2.340339	C	7.172811	-0.219999	1.436111	H	7.611546	-0.909145	0.699215
C	0.692265	6.254349	-2.585793	C	7.670309	-0.239043	2.757462	O	8.666902	-1.136695	3.012121
C	0.353458	7.599778	-2.314346	C	7.122006	0.645742	3.709262	H	7.470262	0.653250	4.752650
C	-0.926639	7.896790	-1.803584	C	6.100624	1.528437	3.322454	H	5.669232	2.199230	4.083926
C	-2.536307	4.436387	-1.670210	N	0.050051	-3.409591	0.011052	H	2.620180	7.251357	0.990565
C	-2.306831	3.156194	-1.109103	C	5.506337	-1.346676	-2.045024	H	0.911282	9.033551	1.404167
C	-3.299984	2.127301	-1.135807	C	6.901021	-1.589738	-1.962011	O	-1.444483	8.696934	2.325100
C	-4.557959	2.324013	-1.759529	C	7.836106	-0.609134	-2.304451	H	-1.858000	6.015497	2.854800
C	-4.804484	3.637566	-2.237627	C	7.407068	0.659600	-2.756454	H	-0.167031	4.269279	2.467049
C	-3.839847	4.650745	-2.188464	C	6.022597	0.917847	-2.861797	H	0.054650	4.193745	-2.577928
C	-1.143804	2.558552	-0.415861	C	5.097371	-0.076840	-2.509601	H	1.691823	6.038610	-2.994812
N	-1.382421	1.247206	-0.116214	C	1.439009	-5.541268	-2.072372	O	1.320214	8.527108	-2.577375
C	-2.685515	0.978720	-0.429021	C	0.146402	-5.173404	-2.527804	H	-1.220297	8.929177	-1.564681
C	-5.558750	1.262871	-2.041391	C	-0.797376	-6.132076	-2.898893	H	-2.834034	7.105396	-1.164283
C	-5.173550	-0.010046	-2.517482	C	-0.486958	-7.510356	-2.828316	H	-7.292668	2.505897	-1.580311
C	-6.116520	-0.983984	-2.882062	C	0.793195	-7.901163	-2.381700	H	-8.981136	0.777890	-2.231844
C	-7.496464	-0.701090	-2.779450	C	1.733794	-6.921102	-2.017607	O	-8.495225	-1.569578	-3.104016
C	-7.902566	0.570340	-2.313870	C	-1.286997	-5.588208	2.143384	H	-5.761929	-1.956450	-3.254015
C	-6.949837	1.528547	-1.957850	C	-1.047207	-6.022717	3.474956	H	-4.103918	-0.242144	-2.632376
N	-3.348582	-0.114836	-0.013180	C	-0.092692	-6.997526	3.769812	H	-0.683645	-5.889655	0.073030
C	-2.727472	-1.213783	0.394701	C	0.657030	-7.589316	2.729057	H	0.712301	0.626847	-0.108559
N	-1.421891	-1.528197	0.083783	C	0.427198	-7.180339	1.399132	H	-0.761599	-0.842669	-0.301113
C	-1.071330	-2.823224	0.406490	C	-0.527167	-6.188459	1.118367	C	8.017113	2.852761	-3.488310
C	-2.218630	-3.379437	1.137870	C	-5.468657	-1.466638	2.148299	H	8.964056	3.402578	-3.662664
C	-3.253035	-2.368926	1.134629	C	-6.124905	-0.746554	1.120845	H	7.430823	2.828827	-4.437820
C	-2.343557	-4.567520	1.909907	C	-7.122785	0.183574	1.420485	H	7.424053	3.386008	-2.708072
C	-3.568937	-4.719157	2.602212	C	-7.488859	0.448248	2.758718	C	-1.217829	-9.760969	-3.175026
C	-4.567116	-3.737637	2.603359	C	-6.843526	-0.252590	3.798583	H	-2.144083	-10.254537	3.532624
C	-4.436579	-2.511940	1.908376	C	-5.856026	-1.199591	3.482048	H	-0.371383	-10.046885	3.844111
N	-0.060116	3.245309	-0.022261	H	-5.488732	-3.915613	3.180943	H	-0.995975	-10.111080	2.138649
C	1.059298	2.665119	0.386446	H	-3.734008	-5.645174	3.176478	C	2.379951	-9.125989	2.110428
N	1.391863	1.345607	0.174961	H	3.993441	-5.653898	-2.878001	H	3.050349	-9.834082	2.638935
C	2.719567	1.065454	0.436958	H	5.705739	-3.892667	-2.863074	H	1.773217	-9.689490	1.361675
C	3.276554	2.283048	1.047990	H	5.665267	4.137058	2.610692	H	2.998945	-8.367372	1.574524
C	2.234966	3.281597	1.011391	H	3.896190	5.846699	2.506549	C	9.201421	-1.201527	4.321244
C	2.414460	4.581746	1.552306	H	-4.069194	5.624524	-2.651417	H	9.985893	-1.985262	4.296688
C	3.700367	4.852249	2.073530	H	-5.760476	3.844065	-2.745743	H	9.664542	-0.233507	4.629626
C	4.701707	3.874218	2.144901	H	-5.859529	-0.924420	0.069702	H	8.426709	-1.486217	5.072682
C	4.523724	2.547679	1.680825	H	-7.636696	0.730237	0.616211	C	-8.860231	1.703615	4.262526
N	3.335499	-0.039487	0.039360	O	-8.462496	1.387944	2.941299	H	-9.644705	2.482384	4.171735
C	2.670841	-1.134294	-0.374408	H	-7.091230	-0.068706	4.854475	H	-9.287631	0.818209	4.791751
N	1.374382	-1.415793	-0.050617	H	-5.348160	-1.726803	4.306675	H	-8.013052	2.110362	4.865521
C	1.128596	-2.715149	-0.393498	H	-1.604205	-5.556063	4.304067	C	-2.734333	8.428933	2.846215
C	2.275781	-3.283936	-1.136376	H	0.103046	-7.312141	4.806978	H	-3.254095	9.407025	2.901754
C	3.274260	-2.258529	-1.126475	O	1.568742	-8.532425	3.106858	H	-3.315746	7.744281	2.183797
C	4.518808	-2.425497	-1.783848	H	0.986033	-7.617638	0.559859	H	-2.684407	7.985656	3.869485
C	4.756215	-3.711381	-2.333406	H	-0.109866	-4.107237	-2.619540	C	1.025957	9.894031	-2.354811
C	3.780242	-4.715025	-2.341277	H	-1.794218	-5.838914	-3.263808	H	1.937196	10.457223	-2.642329
C	2.483640	-4.519572	-1.799586	O	-1.472799	-8.368143	-3.215608	H	0.170098	10.241367	-2.981978
C	1.355933	5.615882	1.689866	H	1.070440	-8.963350	-2.311277	H	0.793945	10.099705	-1.282796
C	1.639222	6.976610	1.412108	H	2.725881	-7.247450	-1.663879	C	-8.148528	-2.869050	-3.551255
C	0.691134	7.978520	1.631534	H	7.259609	-2.566628	-1.597486	H	-9.106162	-3.395840	-3.737961
C	-0.582360	7.653037	2.148211	H	8.918222	-0.796633	-2.221598	H	-7.560035	-2.837959	-4.499149
C	-0.880581	6.305746	2.442918	O	8.389321	1.551867	-3.065973	H	-7.567903	-3.430002	-2.781047
C	0.079719	5.310250	2.209490	H	5.650763	1.887324	-3.224375				

Molecule 2b

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FINAL HEAT OF FORMATION = -6208.160530

C	-5.114228	0.004531	-2.285817	C	0.328890	-7.224561	1.444480	H	5.669449	1.693660	-3.434077
C	-5.565053	1.272141	-1.852680	C	-0.615439	-6.224046	1.158023	H	4.005640	0.020053	-2.724977
C	-6.965507	1.494080	-1.857233	C	1.293931	-5.578882	-2.007542	H	5.816624	0.560197	-0.147537
C	-7.864867	0.504499	-2.256755	C	0.009233	-5.173617	-2.454213	H	7.604687	-1.038585	0.526042
C	-7.394811	-0.760610	-2.673899	C	-0.965437	-6.105578	-2.812690	O	8.655550	-1.283624	2.838606
C	-6.003643	-1.003206	-2.689241	C	-0.696045	-7.492254	-2.736532	H	7.515910	0.553463	4.568968
C	-4.614371	2.367637	-1.535402	C	0.576970	-7.919229	-2.302650	H	5.761894	2.149461	3.891033
C	-3.351299	2.203555	-0.906517	C	1.549581	-6.966203	-1.952311	H	2.860411	7.254351	0.773950
C	-2.364065	3.248226	-0.904040	C	5.457241	-1.489155	-2.134051	H	1.258488	9.117947	1.242971
C	-2.636474	4.527692	-1.454980	C	6.845802	-1.772122	-2.075570	O	-1.060417	8.903841	2.289463
C	-3.953796	4.713095	-1.946215	C	7.801201	-0.835153	-2.477752	H	-1.563465	6.251954	2.888630
C	-4.894309	3.677048	-2.000235	C	7.399397	0.428144	-2.968080	H	0.026106	4.424317	2.443827
C	-2.739843	1.059897	-0.205612	C	6.021068	0.726244	-3.046688	H	-0.055108	4.406476	-2.443160
N	-1.428559	1.365940	0.067163	C	5.074791	-0.224385	-2.633496	H	1.473554	6.331371	-2.900510
C	-1.160338	2.672071	-0.271318	C	5.654833	1.493141	1.816976	O	1.000825	8.795333	-2.441856
Zn	-0.014264	-0.047254	0.106214	C	6.185963	0.568163	0.886049	H	-1.514190	9.066971	-1.329231
N	1.399654	1.367770	0.060013	C	7.187288	-0.331912	1.258624	H	-3.025695	7.164229	-0.895153
C	2.726562	1.089882	0.302418	C	7.685727	-0.357796	2.579400	H	-7.360539	2.461925	-1.510012
C	3.356067	2.291318	0.888462	C	7.165604	0.548844	3.526150	H	-8.952130	0.677891	-2.237812
C	2.341409	3.313951	0.878528	C	6.170888	1.459741	3.134096	O	-8.346285	-1.665077	-3.041919
C	1.130582	2.690214	0.311652	C	1.563682	5.688702	1.565835	H	-5.597812	-1.968751	-3.025370
C	2.575710	4.611663	1.401817	C	1.891157	7.030832	1.249158	H	-4.034202	-0.197036	-2.340525
C	3.885530	4.849471	1.883908	C	1.001858	8.078164	1.499706	H	-0.773115	-5.930337	0.111498
C	4.856805	3.843000	1.940824	C	-0.255288	7.818608	2.087717	C	-7.934292	-2.958936	-3.446931
C	4.622857	2.518203	1.492791	C	-0.597101	6.490946	2.421172	H	-8.862616	-3.519009	-3.679794
N	3.329777	-0.043252	-0.072058	C	0.304556	5.449217	2.155857	H	-7.293011	-2.923417	-4.359852
C	2.680104	-1.168293	-0.398404	C	-1.661087	5.635620	-1.625883	H	-7.381598	-3.489884	-2.635967
N	1.393310	-1.463299	-0.015157	C	-0.375826	5.427020	-2.186511	C	0.642714	10.146029	-2.211999
C	1.081279	-2.763640	-0.333297	C	0.480305	6.495516	-2.454011	H	1.512731	10.754973	-2.532012
C	2.205286	-3.340407	-1.092821	C	0.089250	7.820837	-2.155647	H	-0.250943	10.444744	-2.810994
C	3.225028	-2.327284	-1.131354	C	-1.183129	8.052439	-1.594374	H	0.436311	10.343759	-1.133375
C	4.449769	-2.535491	-1.819493	C	-2.038020	6.966784	-1.344572	C	-2.326441	8.703696	2.892100
C	4.647253	-3.835456	-2.345899	H	-5.520675	-3.904299	3.301407	H	-2.797913	9.705280	2.960375
C	3.648501	-4.818057	-2.318208	H	-3.819714	-5.686570	3.172955	H	-2.977021	8.035226	2.279111
C	2.371122	-4.586935	-1.752575	H	3.827944	-5.766756	-2.849650	H	-2.234052	8.275120	3.918711
N	-0.025565	-3.400267	0.073211	H	5.579911	-4.046694	-2.893837	C	-8.781626	1.928889	1.537722
C	-1.131925	-2.776975	0.490415	H	5.839305	4.077849	2.381790	H	-9.242107	2.329281	0.611546
N	-1.428216	-1.465547	0.197855	H	4.122968	5.842422	2.299295	H	-9.576888	1.452399	2.160201
C	-2.717902	-1.169308	0.565997	H	-4.212381	5.685047	-2.397293	H	-8.330350	2.773318	2.112335
C	-3.278049	-2.329626	1.285829	H	-5.853236	3.865059	-2.509427	C	2.256837	-9.192745	2.162053
C	-2.272007	-3.361784	1.226647	H	-6.044228	-0.742065	0.499452	H	2.910935	-9.915455	2.691187
C	-2.410881	-4.573515	1.954485	O	-7.807968	0.993082	1.119783	H	1.632214	-9.744504	1.419228
C	-3.640712	-4.738842	2.639515	H	-7.970309	1.259839	3.845726	H	2.893197	-8.453955	1.618439
C	-4.608707	-3.730763	2.707503	H	-6.597205	-0.076881	5.436956	C	-1.505346	-9.721996	-3.040714
C	-4.440116	-2.469891	2.084770	H	-4.966163	-1.771221	4.592923	H	-2.453609	-10.189318	-3.375044
N	-3.358962	-0.051885	0.210944	H	-1.664027	-5.545009	4.342574	H	-0.679621	-10.050017	-3.716301
N	-0.015891	3.305941	-0.000561	H	0.028191	-7.314661	4.855534	H	-1.280007	-10.058761	-2.000735
C	-5.395682	-1.390533	2.485081	O	1.466733	-8.572367	3.158634	C	9.187476	-1.357818	4.148169
C	-6.153125	-0.620420	1.586178	H	0.877608	-7.677787	0.607288	H	9.946808	-2.166107	4.128468
C	-7.090693	0.322620	2.069646	H	-0.217617	-4.100834	-2.545682	H	9.681018	-0.403232	4.451480
C	-7.253251	0.522578	3.456315	H	-1.957085	-5.784439	-3.167969	H	8.404135	-1.613448	4.901176
C	-6.480491	-0.236204	4.351950	O	-1.712404	-8.321970	-3.104798	C	8.059628	2.567705	-3.809002
C	-5.571213	-1.187761	3.881117	H	0.823767	-8.988828	-2.230717	H	9.019331	3.077242	-4.029880
C	-1.360438	-5.604586	2.181429	H	2.535307	-7.320082	-1.607568	H	7.449472	2.521082	-4.742406
C	-1.115201	-6.026008	3.516119	H	7.183998	-2.745742	-1.683748	H	7.503355	3.153526	-3.039552
C	-0.169990	-7.008361	3.816304	H	8.878725	-1.053244	-2.413391				
C	0.564048	-7.621456	2.777099	O	8.400608	1.274869	-3.338164				

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FINAL HEAT OF FORMATION = -6456.299030

C	-1.129676	-0.383075	-3.230133	C	-2.577065	-4.719564	-2.262140	H	5.954785	-1.847822	-3.086616
N	0.004446	-0.109410	-2.553803	C	-3.884626	-5.057738	-2.613185	H	3.620552	-2.339977	-2.457229
C	1.124187	0.180054	-3.247348	C	-4.359653	-6.377286	-2.428394	H	5.333983	-2.640069	0.235840
C	1.155348	0.205991	-4.649294	C	-3.488832	-7.348694	-1.891611	H	5.962717	-4.927046	1.000007
C	-0.024176	-0.080692	-5.355052	C	-2.172418	-6.991553	-1.549867	O	6.466158	-5.664842	3.390487
C	-1.189391	-0.381030	-4.631354	C	4.011299	-4.355369	-1.741418	H	6.235215	-3.493381	5.093347
Zn	0.015821	-0.085350	-0.376864	C	5.030905	-5.328744	-1.583294	H	5.637788	-1.225935	4.327799
N	-0.440465	1.871343	-0.047051	C	6.356241	-5.068009	-1.940256	H	6.157487	4.640232	1.218299
C	0.480790	2.861026	-0.269656	C	6.714823	-3.813375	-2.482707	H	5.713402	7.059989	1.692833
C	-0.221498	4.063515	-0.764464	C	5.714472	-2.832371	-2.658980	O	3.547256	8.059326	2.599959
C	-1.620106	3.739931	-0.747376	C	4.388482	-3.110741	-2.291605	H	1.705136	6.041516	3.024788
C	-1.708804	2.350384	-0.248020	C	5.449369	-1.745372	2.222123	H	2.151765	3.661445	2.564550
C	-2.607151	4.682473	-1.138644	C	5.535023	-2.816962	1.300846	H	2.203011	3.843794	-2.415698
C	-2.124762	5.977533	-1.454072	C	5.885154	-4.101815	1.723223	H	4.533054	4.565233	-2.976523
C	-0.759163	6.290841	-1.475315	C	6.143855	-4.373198	3.084349	O	5.608214	6.808046	-2.418752
C	0.246536	5.337699	-1.178580	C	6.055280	-3.323306	4.021439	H	3.801998	8.383788	-1.038015
N	1.778006	2.775914	0.044242	C	5.719951	-2.032658	3.580501	H	1.503521	7.671761	-0.500978
C	2.401025	1.635984	0.368221	C	4.182217	3.962528	1.846571	H	-4.722242	6.262293	-0.408485
N	1.971481	0.373721	0.044638	C	5.177468	4.945612	1.621137	H	-7.147298	5.882124	-0.880560
C	2.914083	-0.557765	0.421305	C	4.939448	6.298367	1.877587	O	-8.166528	3.869435	-2.075542
C	4.015324	0.134220	1.123567	C	3.689400	6.716948	2.382481	H	-6.164146	2.104124	-2.788880
C	3.690069	1.534159	1.078794	C	2.687883	5.753278	2.623730	H	-3.772915	2.485007	-2.316918
C	4.504174	2.517526	1.697188	C	2.938945	4.399843	2.350308	H	2.019695	0.397845	-2.639855
C	5.691782	2.037847	2.299912	C	1.667728	5.702715	-1.411916	H	2.092452	0.448351	-5.174548
C	5.986117	0.671669	2.387238	C	2.554327	4.838370	-2.103136	H	-0.035415	-0.069361	-6.457420
C	5.141753	-0.334712	1.853503	C	3.851500	5.235011	-2.428737	H	-2.137383	-0.611600	-5.142249
N	2.863136	-1.855552	0.100100	C	4.323743	6.515659	-2.060252	H	-2.014256	-0.607484	-2.609203
C	1.735407	-2.491253	-0.248929	C	3.464241	7.389804	-1.364028	H	-3.523089	-4.716897	0.309579
N	0.476871	-2.035672	0.042074	C	2.156297	6.978745	-1.057145	C	8.454864	-2.399425	-3.314895
C	-0.452454	-3.002616	-0.236771	C	-4.053554	4.398321	-1.324570	H	9.547592	-2.489436	-3.479690
C	0.226959	-4.146319	-0.880319	C	-5.033305	5.350490	-0.944543	H	7.960378	-2.159327	-4.286850
C	1.627337	-3.819643	-0.887400	C	-6.390699	5.149862	-1.202383	H	8.261793	-1.569916	-2.594109
C	2.588701	-4.689207	-1.468050	C	-6.821752	3.981245	-1.867859	C	-6.189293	-7.904826	-2.613757
C	2.096115	-5.936443	-1.924295	C	-5.864275	3.023113	-2.264260	H	-7.238643	-7.856951	-2.968599
C	0.731591	-6.253241	-1.919790	C	-4.505523	3.236012	-1.985824	H	-5.638305	-8.670875	-3.210149
C	-0.256812	-5.351218	-1.455527	H	-6.924537	-0.343435	2.828754	H	-6.182278	-8.206348	-1.539296
N	-1.741681	-2.934615	0.124964	H	-6.349118	-2.735391	2.949288	C	6.729066	-5.994012	4.741424
C	-2.361833	-1.795673	0.456169	H	0.407837	-7.197020	-2.388300	H	6.965042	-7.077638	4.755714
N	-1.932254	-0.542641	0.077868	H	2.799790	-6.642976	-2.393373	H	7.601989	-5.427271	5.145978
C	-2.873781	0.398635	0.409531	H	6.896378	0.357314	2.923164	H	5.843603	-5.806686	5.394931
C	-3.978342	-0.264363	1.127325	H	6.366743	2.760726	2.786818	C	-2.844337	-8.893628	2.783520
C	-3.652219	-1.664751	1.167415	H	-0.451543	7.291637	-1.820418	H	-2.705340	-9.801602	3.405314
C	-4.459864	-2.583457	1.895033	H	-2.847315	6.742976	-1.781073	H	-3.566389	-9.122514	1.963060
C	-5.664452	-2.051364	2.422156	H	-7.544728	1.469246	1.269252	H	-1.864709	-8.607881	2.330980
C	-5.999308	-0.694483	2.342910	H	-8.185730	3.841799	1.750213	C	2.327360	8.530287	3.142341
C	-5.139155	0.260462	1.750187	O	-6.671397	5.661230	2.707748	H	2.436101	9.629729	3.240286
N	-2.827012	1.696478	0.082726	H	-4.143460	4.629440	3.137898	H	1.460900	8.308590	2.474329
C	-5.474590	1.700329	1.914475	H	-3.516714	2.294791	2.651917	H	2.125447	8.094339	4.150320
C	-6.794665	2.162368	1.685118	H	-4.612231	-3.621191	4.365386	C	-5.777193	6.606571	3.263788
C	-7.164430	3.483229	1.951112	H	-4.135179	-5.956107	5.120157	H	-6.351689	7.549167	3.372239
C	-6.220351	4.391878	2.477188	O	-3.334477	-7.890856	3.652674	H	-5.408172	6.288209	4.268170
C	-4.902741	3.950480	2.723263	H	-3.062366	-7.014136	1.042765	H	-4.898785	6.790310	2.599881
C	-4.543965	2.624358	2.435492	H	-2.225110	-3.691432	-2.432258	C	6.127644	8.083735	-2.092096
C	-4.118883	-3.984921	2.269350	H	-4.571958	-4.311961	-3.042103	H	7.166599	8.103364	-2.479607
C	-4.289015	-4.372962	3.626622	O	-5.651314	-6.607641	-2.797609	H	5.544276	8.904996	-2.573679
C	-4.019352	-5.671676	4.062433	H	-3.822885	-8.383839	-1.729247	H	6.147447	8.254010	-0.989303
C	-3.573287	-6.646007	3.142649	H	-1.509859	-7.762352	-1.122373	C	-8.657314	2.715245	-2.731980
C	-3.404098	-6.284915	1.790395	H	4.779320	-6.309082	-1.145620	H	-9.758770	2.833514	-2.783544
C	-3.668172	-4.970456	1.367744	H	7.145525	-5.822765	-1.798218	H	-8.253670	2.623895	-3.769130
C	-1.684041	-5.677034	-1.715382	O	8.029618	-3.649932	-2.802280	H	-8.417447	1.782571	-2.167540

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FINAL HEAT OF FORMATION = -6704.410680

C	-5.433807	0.596846	-2.144568	N	-0.141336	-3.412729	-0.002792	H	0.500612	-9.068839	-2.140667
C	-5.614531	1.856614	-1.534528	C	5.501409	-1.807021	-2.061105	H	2.278033	-7.459231	-1.540862
C	-6.942753	2.242283	-1.222397	C	6.867507	-2.177073	-1.969945	H	7.132618	-3.174341	-1.581442
C	-8.031918	1.412366	-1.496440	C	7.891103	-1.298571	-2.335275	H	8.950626	-1.585362	-2.245512
C	-7.829697	0.157237	-2.111067	C	7.582560	-0.007343	-2.819142	H	5.950586	1.372238	-3.309186
C	-6.517260	-0.244656	-2.438762	C	6.228527	0.378575	-2.928359	H	4.163993	-0.203213	-2.665281
C	-4.485389	2.803292	-1.342027	C	5.213203	-0.515071	-2.552798	H	5.905554	0.219477	-0.047158
C	-3.188655	2.469280	-0.870495	C	1.123002	-5.678257	-2.016271	H	7.606055	-1.462696	0.648369
C	-2.112862	3.421635	-0.891742	C	-0.133842	-5.229693	-2.498607	H	7.551818	0.142145	4.686979
C	-2.289980	4.738305	-1.389698	C	-1.143703	-6.127712	-2.846202	H	5.883763	1.818908	3.986579
C	-3.614114	5.078611	-1.762551	C	-0.938967	-7.521810	-2.721946	H	3.296338	7.073937	0.861917
C	-4.665092	4.152888	-1.737650	C	0.305075	-7.992030	-2.251970	H	1.782694	9.012962	1.331964
C	-2.627555	1.231578	-0.282609	C	1.314310	-7.073065	-1.912921	H	-1.213423	6.273957	2.878779
N	-1.301569	1.444596	-0.008029	C	-1.763136	-5.575315	2.016453	H	0.289057	4.370227	2.428307
C	-0.941705	2.731828	-0.309023	C	-1.755342	-6.059292	3.352963	H	0.181364	4.306001	-2.526960
Zn	0.051833	-0.064299	0.094585	C	-0.882573	-7.067424	3.767695	H	1.898614	6.027607	-3.117464
N	-1.465822	-1.420827	0.041270	C	0.019591	-7.642819	2.846029	H	-0.630530	9.118187	-1.405634
C	-1.243872	-2.738385	0.352893	C	0.021368	-7.185157	1.512742	H	-2.323337	7.417063	-0.835754
C	-2.461904	-3.282373	0.996834	C	-0.855349	-6.162611	1.111845	H	-7.121785	3.212893	-0.730626
C	-3.429421	-2.214617	0.967082	C	-5.748706	-1.290179	1.662793	H	-9.057852	1.708314	-1.228005
C	-2.751631	-1.061050	0.335621	C	-7.107898	-1.555840	1.361254	H	-6.324400	-1.213695	-2.922020
C	-2.741394	-4.508265	1.661254	C	-8.107300	-0.605593	1.583293	H	-4.419970	0.272771	-2.423206
C	-4.067841	-4.655889	2.141144	C	-7.779574	0.651493	2.135628	H	1.606921	1.269894	-2.556549
C	-5.024054	-3.637240	2.059903	C	-6.434923	0.933034	2.456357	H	1.619434	1.380310	-5.089898
C	-4.725544	-2.360936	1.523853	C	-5.441682	-0.027911	2.212574	H	-0.086495	0.002718	-6.369761
N	0.242805	3.288503	-0.022940	O	-8.819900	1.519265	2.314677	H	-1.720405	-1.421097	-5.047112
C	1.356754	2.608486	0.285844	C	-8.551979	2.789045	2.878734	H	-1.567849	-1.400475	-2.516155
N	1.571920	1.288308	0.003480	O	0.839860	-8.620036	3.335539	H	-0.829017	-5.822808	0.068543
C	2.861687	0.928753	0.303537	C	1.780921	-9.211705	2.459993	H	9.391626	2.550202	-3.797520
C	3.541203	2.089207	0.925707	O	-1.986780	-8.316434	-3.081864	H	7.808856	2.104802	-4.557314
C	2.581376	3.163854	0.901131	C	-1.846390	-9.720724	-2.963980	H	7.859036	2.705922	-2.843229
C	2.866240	4.439867	1.450487	O	8.644737	0.779424	-3.152229	H	-2.809564	-10.156326	-3.298764
C	4.173748	4.607346	1.967766	C	8.397012	2.097741	-3.608566	H	-1.025680	-10.111820	-3.611879
C	5.089134	3.551241	2.039969	O	8.623418	-1.750374	2.972698	H	-1.654366	-10.029623	-1.908750
C	4.797946	2.244434	1.572088	C	9.143385	-1.839794	4.285423	H	9.866845	-2.680561	4.275600
N	-3.308636	0.119565	0.025635	O	-0.559317	8.905018	2.341421	H	9.676382	-0.905911	4.586913
C	-1.207516	5.727017	-1.631870	C	-1.844828	8.761642	2.916512	H	8.345432	-2.056559	5.035675
C	0.004974	5.361045	-2.269317	O	1.750574	8.536995	-2.686584	H	2.339642	-9.956157	3.063117
C	0.963671	6.314985	-2.611268	C	1.578472	9.921141	-2.445101	H	1.284338	-9.733639	1.606870
C	0.753050	7.681170	-2.315290	O	-8.951428	-0.586840	-2.341770	H	2.498920	-8.460233	2.052199
C	-0.440878	8.068586	-1.673374	C	-8.808415	-1.856784	-2.951163	H	-2.263934	9.785524	2.996304
C	-1.401007	7.095896	-1.347705	N	0.024888	-0.070294	-2.455750	H	-2.519050	8.140825	2.279145
N	3.408420	-0.245562	-0.042462	C	-0.878747	-0.798902	-3.136083	H	-1.795818	8.309445	3.936167
C	2.705272	-1.340743	-0.373827	C	-0.959899	-0.806607	-4.538889	H	-9.526916	3.315067	2.933813
N	1.410550	-1.578291	0.005491	C	-0.055132	-0.017888	-5.267538	H	-8.126322	2.705291	3.907759
C	1.020698	-2.840551	-0.355867	C	0.889670	0.744984	-4.562579	H	-7.851713	3.386025	2.246577
C	2.124284	-3.475121	-1.106375	C	0.888242	0.685055	-3.158667	H	2.489599	10.418699	-2.835634
C	3.200158	-2.520526	-1.116507	H	-6.021318	-3.805707	2.498426	H	0.685179	10.327352	-2.977854
C	4.423508	-2.792856	-1.784607	H	-4.346208	-5.606618	2.624359	H	1.480482	10.144127	-1.355986
C	4.557948	-4.096154	-2.322727	H	3.645461	-5.982342	-2.842273	H	-9.831807	-2.275904	-3.035511
C	3.508917	-5.024691	-2.313817	H	5.486862	-4.353650	-2.857255	H	-8.362511	-1.780063	-3.971878
C	2.238690	-4.728542	-1.763043	H	6.071870	3.731630	2.505495	H	-8.182485	-2.545309	-2.334684
C	1.906547	5.566639	1.605416	H	4.451065	5.582938	2.399779	N	0.068733	-0.062090	2.456786
C	2.307580	6.894813	1.315560	H	-3.804208	6.085424	-2.169309	C	-0.696433	0.796079	3.158210
C	1.469237	7.983731	1.567793	H	-5.649988	4.461281	-2.125038	C	-0.718961	0.826068	4.561403
C	0.190818	7.781403	2.131346	H	-7.383032	-2.528607	0.920649	C	0.090989	-0.079800	5.265646
C	-0.226142	6.468191	2.434612	H	-9.157715	-0.808944	1.323074	C	0.888659	-0.976209	4.537243
C	0.624910	5.384729	2.166659	H	-6.145001	1.900178	2.892435	C	0.844752	-0.929405	3.134736
C	5.770189	1.166860	1.911943	H	-4.400711	0.204186	2.482597	H	-1.315151	1.484186	2.555449
C	6.265431	0.213501	0.989652	H	-2.434773	-5.606690	4.094067	H	-1.362386	1.548163	5.089030
C	7.216697	-0.734486	1.375293	H	-0.871528	-7.422451	4.810426	H	0.099326	-0.087004	6.368475
C	7.700063	-0.780317	2.701019	H	0.702770	-7.610776	0.762547	H	1.540015	-1.706222	5.043248
C	7.212803	0.151752	3.640408	H	-0.308378	-4.150362	-2.621969	H	1.452391	-1.610885	2.514344
C	6.267437	1.108694	3.235432	H	-2.115134	-5.774445	-3.226053				

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FINAL HEAT OF FORMATION = -4384.345420

C	-2.443212	-2.734483	-9.644914	C	-7.016887	-1.003620	-12.643982	H	-6.906544	-1.432959	-13.652347
N	-2.654820	-4.027550	-9.324851	C	-7.576852	0.268521	-12.439999	H	-5.537682	-4.911769	-15.190274
C	-1.590916	-4.807835	-9.044272	C	-7.713046	0.806447	-11.136971	H	-4.946894	-6.861283	-16.688955
C	-0.273938	-4.327485	-9.071905	C	-7.297914	0.085370	-10.004162	H	-4.076356	-8.989254	-15.722707
C	-0.054052	-2.980809	-9.402606	N	-6.204825	-2.063404	-7.952663	H	-3.768659	-9.238593	-13.224415
C	-1.161331	-2.168790	-9.694724	C	-5.800348	-2.986631	-7.073041	H	-3.133455	-10.618397	-9.479106
Zn	-4.687063	-4.834449	-9.246427	N	-5.296588	-4.229943	-7.367751	H	-2.609985	-12.031892	-7.446952
N	-4.352095	-6.689577	-8.465408	C	-5.018853	-4.904562	-6.204211	H	-2.842612	-11.086685	-5.149763
C	-4.019795	-7.812947	-9.191834	C	-5.340990	-4.037517	-5.052126	H	-3.616061	-8.705364	-4.805423
C	-3.650083	-8.887107	-8.259136	C	-5.833727	-2.812764	-5.606255	H	-6.142837	-6.780405	-3.913895
C	-3.789297	-8.349926	-6.950812	C	-6.153967	-1.698564	-4.787627	H	-5.441203	-8.800202	-2.610450
C	-4.249344	-6.961111	-7.118135	C	-5.915823	-1.866276	-3.402626	O	-3.579681	-8.920681	-0.870880
C	-3.504446	-9.128014	-5.816807	C	-5.438970	-3.068062	-2.859384	H	-2.437310	-6.420315	-0.559358
C	-3.077606	-10.451595	-6.020209	C	-5.155079	-4.203701	-3.654841	H	-3.156353	-4.425879	-1.828676
C	-2.943937	-10.987990	-7.323992	N	-4.530347	-6.145863	-6.099289	H	-5.174518	0.776568	-4.229019
C	-3.231043	-10.212148	-8.459608	C	-4.698600	-5.445616	-2.973205	H	-6.141700	2.998852	-4.871405
N	-4.028175	-7.956352	-10.520521	C	-5.324833	-6.699175	-3.182516	O	-8.249514	3.393331	-6.252401
C	-4.419759	-7.011880	-11.382625	C	-4.940037	-7.830620	-2.460231	H	-9.356012	0.963508	-6.972691
N	-4.851005	-5.739291	-11.090100	C	-3.894102	-7.756160	-1.510085	H	-8.375709	-1.221244	-6.366458
C	-5.203265	-5.094965	-12.253161	C	-3.256147	-6.518400	-1.287397	H	-1.813714	-5.857290	-8.786562
C	-4.968408	-5.999453	-13.389322	C	-3.670018	-5.384956	-2.009108	H	0.561759	-5.004470	-8.834668
C	-4.473001	-7.211402	-12.838822	C	-6.700933	-0.394763	-5.254495	H	0.968277	-2.568890	-9.432278
C	-4.148970	-8.301458	-13.661677	C	-6.096564	0.816003	-4.832558	H	-1.040789	-1.106421	-9.959136
C	-4.325265	-8.152802	-15.048159	C	-6.624858	2.060496	-5.186562	H	-3.342722	-2.137058	-9.869607
C	-4.819640	-6.944818	-15.596675	C	-7.801777	2.136621	-5.963685	C	-2.539099	-8.907032	0.089214
C	-5.149531	-5.854425	-14.773333	C	-8.428659	0.941530	-6.381246	H	-2.451054	-9.946812	0.464640
N	-5.705097	-3.862656	-12.379132	C	-7.871897	-0.300939	-6.034439	H	-1.564009	-8.598956	-0.358828
C	-5.974793	-3.045956	-11.357040	H	-5.320528	-3.150113	-1.766645	H	-2.772959	-8.229652	0.945182
N	-5.754067	-3.274083	-10.016314	H	-6.158464	-1.032599	-2.723024	C	-9.427351	3.534895	-7.025469
C	-6.206818	-2.200641	-9.280427	H	-7.402872	0.493342	-8.986098	H	-9.595607	4.625554	-7.134880
C	-6.736801	-1.185986	-10.206464	H	-8.152637	1.810587	-11.013575	H	-9.316494	3.080700	-8.039288
C	-6.594101	-1.722461	-11.514345	H	-7.916176	0.860982	-13.306307	H	-10.312745	3.079251	-6.521194

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FINAL HEAT OF FORMATION = -5075.008150

C	-2.376920	-2.714143	-9.643717	C	-4.623048	-8.188732	-14.998590	N	-4.516304	-6.138035	-6.057544
N	-2.600637	-3.984922	-9.250918	C	-5.150687	-6.998856	-15.523939	C	-4.764268	-5.488307	-2.922936
C	-1.546962	-4.747125	-8.892717	C	-5.324151	-5.834214	-14.739350	C	-5.422069	-6.711212	-3.171046
C	-0.228186	-4.271114	-8.914390	N	-5.682059	-3.820220	-12.313426	C	-5.109220	-7.875999	-2.451748
C	0.004506	-2.948429	-9.323776	C	-5.947186	-3.011127	-11.287101	C	-4.100282	-7.844519	-1.463819
C	-1.092256	-2.154472	-9.694758	N	-5.709914	-3.239162	-9.948683	C	-3.424673	-6.630478	-1.208651
Zn	-4.632259	-4.794613	-9.202468	C	-6.168027	-2.170557	-9.207938	C	-3.761858	-5.476180	-1.921179
N	-4.314557	-6.649151	-8.430579	C	-6.714227	-1.159246	-10.126841	C	-6.687399	-0.394932	-5.169210
C	-3.986861	-7.767350	-9.167611	C	-6.581232	-1.692551	-11.436628	C	-6.105506	0.819735	-4.728310
C	-3.640114	-8.857106	-8.242474	C	-7.021246	-0.975369	-12.561166	C	-6.650865	2.060244	-5.071337
C	-3.786235	-8.333087	-6.930311	C	-7.587342	0.292788	-12.347527	C	-7.822671	2.127419	-5.857043
C	-4.229899	-6.938678	-7.085226	C	-7.715336	0.826978	-11.042212	C	-8.424919	0.927993	-6.297477
C	-3.521740	-9.124269	-5.800589	C	-7.283882	0.106792	-9.915187	C	-7.851202	-0.309335	-5.960970
C	-3.107611	-10.450319	-6.013066	N	-6.165412	-2.036342	-7.880569	H	-5.336909	-3.186560	-1.698366
C	-2.968229	-10.974615	-7.321296	C	-5.762275	-2.965452	-7.006923	H	-6.142753	-1.051518	-2.640642
C	-3.235064	-10.185277	-8.452846	N	-5.257604	-4.205719	-7.311158	H	-7.381696	0.511396	-8.895152
N	-3.982017	-7.899950	-10.495358	C	-4.996801	-4.893470	-6.151635	H	-8.162308	1.827090	-10.911741
C	-4.354308	-6.959933	-11.371158	C	-5.329239	-4.038608	-4.993470	H	-7.937275	0.884698	-13.209828
N	-4.766753	-5.685172	-11.071007	C	-5.807928	-2.804995	-5.539075	H	-6.915145	-1.400095	-13.572298
C	-5.160634	-5.048125	-12.221148	C	-6.132270	-1.698520	-4.711823	C	-5.835178	-4.597172	-15.390182
C	-4.978957	-5.958293	-13.368855	C	-5.902060	-1.880015	-3.327062	H	-5.395024	-6.950387	-16.597942
C	-4.454206	-7.174392	-12.829405	C	-5.442233	-3.092100	-2.791577	H	-4.459150	-9.043312	-15.675571
C	-4.234295	-8.317060	-13.643372	C	-5.167576	-4.223938	-3.595880	C	-3.622626	-9.595472	-13.192048

H	-3.127451	-10.582043	-9.475169	C	-9.471071	3.510596	-6.903644	C	-3.613445	-12.059405	-13.200506
H	-2.642107	-12.020185	-7.452032	H	-9.661015	4.599287	-6.996014	C	-2.400548	-12.070907	-12.481293
H	-2.884597	-11.096620	-5.147369	H	-9.350579	3.075448	-7.924768	C	-1.800026	-10.840878	-12.123228
H	-3.637758	-8.707122	-4.787539	H	-10.347643	3.028880	-6.408046	C	-2.405908	-9.631054	-12.466050
H	-6.215958	-6.753553	-3.931911	C	-4.359893	-10.159389	-0.918178	H	-5.155524	-10.840097	-14.104165
H	-5.665211	-8.800588	-2.666946	H	-3.887883	-10.872696	-0.212373	H	-4.113890	-12.995096	-13.490840
O	-3.713969	-8.916636	-0.712568	H	-5.452946	-10.101084	-0.699798	O	-1.737705	-13.198225	-12.089976
H	-2.635010	-6.619754	-0.441020	H	-4.220614	-10.533530	-1.960871	H	-0.846398	-10.865621	-11.572469
H	-3.219717	-4.538983	-1.711569	C	-5.149461	-3.361124	-15.294824	H	-1.918754	-8.685838	-12.182985
H	-5.188264	0.787656	-4.116937	C	-5.601993	-2.226722	-15.970901	C	-8.319306	-1.103516	-18.156635
H	-6.186209	3.001937	-4.738959	C	-6.778008	-2.280544	-16.755888	H	-8.423140	-0.068198	-18.540569
O	-8.291189	3.380230	-6.131621	C	-7.477471	-3.500306	-16.862585	H	-8.239635	-1.805570	-19.021061
H	-9.345801	0.942332	-6.899231	C	-6.994773	-4.638828	-16.192085	H	-9.228000	-1.364050	-17.562595
H	-8.335529	-1.233424	-6.310247	H	-4.233624	-3.298145	-14.687937	C	-2.292979	-14.458837	-12.417724
H	-1.780838	-5.777718	-8.575771	H	-5.059298	-1.270147	-15.908184	H	-1.599877	-15.219266	-12.003927
H	0.598872	-4.932569	-8.612127	O	-7.148894	-1.113158	-17.359798	H	-3.301814	-14.599594	-11.960271
H	1.028439	-2.540240	-9.352682	H	-8.399208	-3.578987	-17.457647	H	-2.373730	-14.602829	-13.521732
H	-0.961397	-1.110675	-10.021066	H	-7.558011	-5.583322	-16.276196				
H	-3.269108	-2.130701	-9.927492	C	-4.200949	-10.831343	-13.552002				

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FINAL HEAT OF FORMATION = -5074.998650

C	3.138788	-3.627264	5.851873	C	3.455131	1.564951	7.369269	H	-2.342490	-6.773056	10.451165
N	3.518498	-2.443082	6.372827	C	3.524017	2.793948	6.534689	H	-0.680744	-6.522684	12.294368
C	4.784423	-2.021902	6.176809	C	2.805648	2.482466	5.334830	H	1.173442	-4.808540	12.135516
C	5.723613	-2.768461	5.450432	C	2.737533	3.364595	4.226821	H	6.267330	-1.301422	13.894407
C	5.327977	-4.001149	4.906025	C	3.357656	4.621080	4.414364	H	7.266696	0.682801	12.840636
C	4.009839	-4.439485	5.111573	C	3.976630	4.971226	5.621250	H	3.208143	3.717181	9.331531
Zn	2.088079	-1.196094	7.452366	C	4.084906	4.087265	6.726958	H	4.026986	4.905999	11.370476
N	3.144695	-0.743313	9.153603	N	4.168836	1.343974	8.482295	O	5.943829	6.592878	11.487466
C	3.248603	-1.601754	10.219433	C	4.655712	4.637063	7.983464	H	7.052614	6.907889	8.980433
C	4.360741	-1.171468	11.080970	C	4.058882	4.409155	9.249495	H	6.240777	5.736053	6.972223
C	4.907665	0.008241	10.477164	C	4.503068	5.076733	10.392305	H	1.032215	4.928703	2.761497
C	4.076475	0.263468	9.272638	C	5.576252	5.993574	10.318086	H	0.087594	4.449513	0.490215
C	5.999871	0.693805	11.079432	C	6.196456	6.224899	9.073447	O	0.478654	2.346248	-0.905083
C	6.413612	0.196996	12.341887	C	5.732758	5.550890	7.933476	H	2.139224	0.618309	0.467921
C	5.852374	-0.938226	12.939887	C	2.120181	3.044368	2.912669	H	3.058548	1.093343	2.707872
C	4.836659	-1.693163	12.310773	C	1.286346	3.982488	2.254613	H	6.995066	2.880082	12.376828
N	2.450389	-2.636374	10.500280	C	0.748670	3.723743	0.990202	H	8.606182	4.568805	11.503964
C	1.423937	-3.056901	9.760646	C	1.043009	2.512065	0.326895	O	9.502925	4.730129	9.119271
N	1.035152	-2.589327	8.526701	C	1.882526	1.568681	0.959092	H	8.428683	2.690497	7.588639
C	-0.085110	-3.272496	8.107493	C	2.401408	1.839211	2.234241	H	6.852615	1.006547	8.466342
C	-0.443812	-4.268084	9.127495	C	4.399813	-2.965737	12.946006	H	4.068370	-2.072097	14.906411
C	0.506918	-4.130624	10.173773	C	4.081080	-3.009209	14.325334	H	3.492964	-4.237911	16.032536
C	0.436581	-4.929909	11.325708	C	3.755296	-4.210284	14.963323	O	3.440356	-6.547118	14.944676
C	-0.597598	-5.878402	11.402689	C	3.757919	-5.422759	14.238643	H	4.100264	-6.328313	12.270340
C	-1.541856	-6.019956	10.357045	C	4.082214	-5.402137	12.864525	H	4.647371	-4.189142	11.166815
C	-1.478903	-5.213101	9.208753	C	4.389447	-4.185203	12.236490	H	5.046023	-1.045898	6.619903
N	-0.781783	-3.078616	6.982982	C	6.805452	1.795300	10.491317	H	6.747005	-2.383962	5.315732
C	-0.511291	-2.120346	6.090873	C	7.322298	2.819156	11.326375	H	6.039594	-4.613035	4.327348
N	0.522569	-1.211918	6.129200	C	8.218140	3.774368	10.847612	H	3.653798	-5.398521	4.703669
C	0.425108	-0.358890	5.056498	C	8.634028	3.745348	9.498968	H	2.094119	-3.928480	6.038750
C	-0.740583	-0.742099	4.246063	C	8.129029	2.741245	8.646048	C	3.442832	-7.793100	14.271897
C	-1.335147	-1.853234	4.901987	C	7.223872	1.789935	9.143860	H	3.158060	-8.552579	15.027851
C	-2.505281	-2.446632	4.400615	H	4.368662	5.994884	5.730012	H	2.702458	-7.816195	13.436069
C	-3.064663	-1.908106	3.228537	H	3.348739	5.348302	3.585382	H	4.452160	-8.044536	13.866744
C	-2.471327	-0.799158	2.576529	H	-0.836373	0.666193	2.585706	C	9.960962	4.749400	7.779899
C	-1.302425	-0.201258	3.078759	H	-2.940842	-0.393178	1.664792	H	10.648570	5.616050	7.700769
N	1.199165	0.690727	4.781315	H	-3.984316	-2.351147	2.810788	H	10.518962	3.818230	7.519187
C	2.156930	1.183543	5.570223	H	-2.966581	-3.301464	4.920353	H	9.121468	4.882298	7.056307
N	2.603278	0.667774	6.762469	H	-2.214467	-5.308022	8.393974	C	6.984717	7.553691	11.454508

H	7.107530	7.912289	12.496977	C	0.733247	1.145915	-1.612699	H	0.369690	0.249415	-1.055278
H	7.947495	7.112140	11.103661	H	0.176364	1.226914	-2.568322	H	1.819706	1.017242	-1.835534
H	6.725721	8.419988	10.799510	H	1.819706	1.017242	-1.835534				

Molecule 3d

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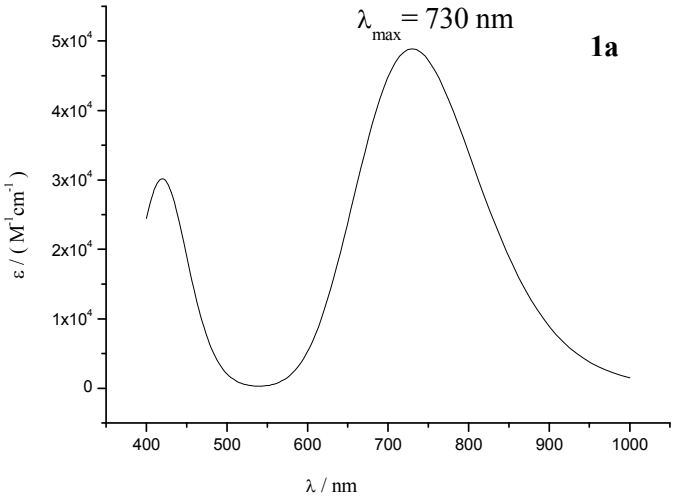
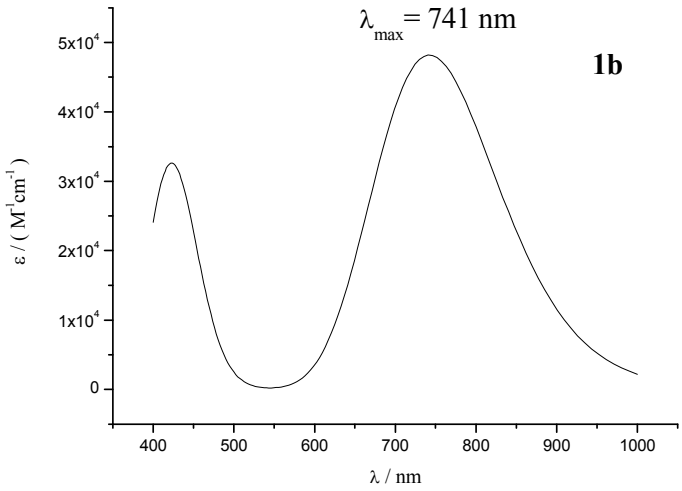
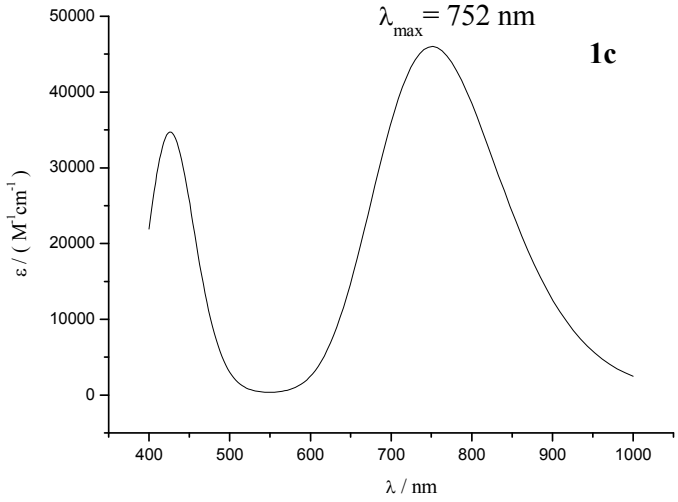
FINAL HEAT OF FORMATION = -5765.656110

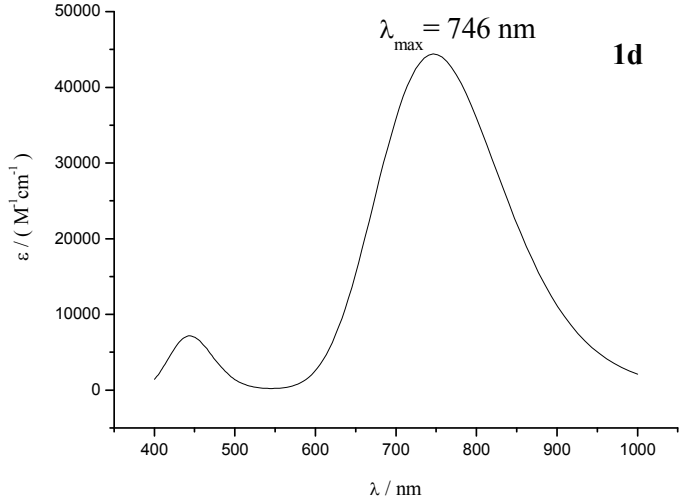
C	-0.202197	0.131130	-0.000893	C	-5.069077	-9.491958	-0.871297	H	-10.702617	-1.335534	4.327999
C	0.039060	0.075372	1.387862	C	-8.241132	-0.341789	4.069844	H	-1.960477	1.682737	5.276435
C	1.386320	0.154915	1.820486	C	-8.734456	0.307008	5.229775	H	-0.234448	1.681478	3.513281
C	2.441421	0.272968	0.911428	C	-8.476378	1.657338	5.477609	H	-4.512023	-8.044480	-3.162735
C	2.180577	0.335162	-0.475479	C	-7.715417	2.415867	4.561566	H	-2.809158	-8.593297	-4.918138
C	0.844084	0.267697	-0.927528	C	-7.219948	1.792174	3.397016	H	-1.541398	-12.041222	-2.595435
C	-1.067941	0.028115	2.380864	C	-7.478881	0.431989	3.168047	H	-3.252903	-11.514814	-0.887420
C	-2.165803	-0.869260	2.351595	C	-10.435436	-5.414840	2.136856	H	-9.294083	-5.300511	0.282367
C	-3.227158	-0.791649	3.310699	C	-10.125262	-5.794882	0.806045	H	-10.644945	-7.031586	-0.910636
C	-3.176856	0.105510	4.408363	C	-10.879852	-6.752845	0.128536	H	-13.133853	-7.506242	2.619015
C	-2.063416	0.981305	4.431905	C	-11.976290	-7.380312	0.762312	H	-11.787096	-5.805905	3.797649
C	-1.062988	0.956524	3.449760	C	-12.295944	-7.029285	2.089651	H	-9.320308	-0.269346	5.964560
C	-2.470435	-2.040540	1.503587	C	-11.529856	-6.057404	2.755568	H	-8.855181	2.154489	6.384627
N	-3.683361	-2.560155	1.879393	N	-3.436181	-6.748711	-0.893660	H	-6.631954	2.354668	2.657169
C	-4.216140	-1.809253	2.896378	C	-8.180578	-9.183493	2.231134	H	-7.100862	-0.030151	2.243994
Zn	-4.256456	-4.510830	1.558573	C	-7.885544	-8.599799	3.489227	H	-4.211334	-2.059453	5.758377
N	-2.853411	-4.594620	0.081954	C	-8.762506	-8.712435	4.568145	H	-5.637143	-2.023835	7.815679
C	-2.693981	-5.640218	-0.802107	C	-9.982932	-9.411048	4.428334	H	-5.647902	2.319319	7.714165
C	-1.521400	-5.368202	-1.647033	C	-10.301932	-9.993521	3.184929	H	-4.241767	2.277155	5.690670
C	-1.000644	-4.116294	-1.219087	C	-9.405196	-9.874978	2.109946	H	1.610832	0.099246	2.898579
C	-1.866718	-3.654810	-0.125239	C	-4.010744	-9.740527	-1.888880	H	3.487942	0.318924	1.251437
C	-0.907415	-6.090111	-2.684562	C	-3.859668	-8.921404	-3.035444	H	0.603138	0.325387	-1.999503
C	0.235624	-5.533839	-3.284044	C	-2.912314	-9.218757	-4.017349	H	-1.237071	0.085101	-0.371878
C	0.754703	-4.287152	-2.855839	C	-2.059214	-10.338973	-3.876976	H	-6.929830	-8.072850	3.628971
C	0.143161	-3.563366	-1.818222	C	-2.190154	-11.165030	-2.741588	H	-9.682877	-10.318962	1.140126
N	-5.476296	-1.888850	3.340304	C	-3.165537	-10.864349	-1.773620	H	-8.523412	-8.268015	5.547015
C	-6.358697	-2.828323	2.986855	O	-1.153225	-10.531942	-4.880269	H	-11.247822	-10.535088	3.036014
N	-6.057459	-4.040064	2.410915	C	-0.274907	-11.638824	-4.796984	H	-1.590817	-5.992725	1.980638
C	-7.201782	-4.790765	2.277755	O	-10.774353	-9.466535	5.540382	H	-0.249068	-7.041076	3.847021
C	-8.354533	-3.996810	2.747256	C	-11.993118	-10.181242	5.468788	H	-1.225588	-7.044933	6.192084
C	-7.817221	-2.750328	3.207612	O	-12.655716	-8.300964	0.014827	H	-3.516459	-6.008894	6.546125
C	-8.647365	-1.735885	3.752867	C	-13.803921	-8.910501	0.571743	H	4.080465	0.633915	-3.137511
C	-10.011082	-2.086510	3.912472	O	-7.513100	3.727063	4.889111	H	2.581141	-0.381624	-3.087804
C	-10.537223	-3.300263	3.452450	C	-6.793986	4.547929	3.986278	H	2.459762	1.426507	-2.971080
C	-9.745604	-4.276674	2.798027	O	-6.499485	0.042774	9.033404	H	-7.520708	0.924422	10.546272
N	-1.669942	-2.516750	0.545800	C	-6.922869	1.236586	9.665864	H	-6.058218	1.852048	10.012392
C	-4.116705	0.108958	5.559039	O	3.271475	0.460302	-1.286826	H	-7.561436	1.858187	8.994289
C	-4.536322	-1.095512	6.178436	C	3.071932	0.537164	-2.686513	H	-6.766012	5.558423	4.442716
C	-5.320895	-1.086398	7.331718	N	-3.193585	-5.473933	3.206351	H	-5.748302	4.187007	3.836744
C	-5.729527	0.137142	7.909855	C	-3.719898	-5.479629	4.448403	H	-7.298505	4.611809	2.992519
C	-5.330112	1.348047	7.308677	C	-3.048808	-6.031340	5.549175	H	-14.208067	-9.584030	-0.211398
C	-4.531414	1.319536	6.153901	C	-1.782267	-6.603644	5.348758	H	-13.557287	-9.516062	1.477484
N	-7.266487	-6.055002	1.851604	C	-1.238093	-6.603022	4.054671	H	-14.583388	-8.158621	0.842680
C	-6.303467	-6.693982	1.178883	C	-1.978109	-6.025088	3.013186	H	-12.459411	-10.102021	6.472119
N	-5.179302	-6.108519	0.653411	H	0.539051	-2.594653	-1.473409	H	-12.687608	-9.744636	4.710961
C	-4.547145	-6.988676	-0.188889	H	1.656504	-3.881477	-3.344849	H	-11.829720	-11.259074	5.227119
C	-5.289224	-8.265960	-0.194006	H	0.740697	-6.076865	-4.100349	H	0.360086	-11.598530	-5.705374
C	-6.355703	-8.107031	0.749555	H	-1.315159	-7.061466	-3.008120	H	0.378823	-11.583025	-3.893718
C	-7.187951	-9.193661	1.124748	H	-5.819888	-11.521067	-1.034177	H	-0.828241	-12.608404	-4.782598
C	-6.950355	-10.410647	0.439538	H	-7.554416	-11.292834	0.707267	H	-4.718515	-5.020355	4.549635
C	-5.944127	-10.549879	-0.527163	H	-11.625746	-3.460708	3.517819				

2. Simulated Electronic Spectra of molecules 1a, 1b, 1c and 1d









3. Simulated Electronic Spectra of molecules 2a, 2b, 2c and 2d