

Supporting Information

Quantum chemical study and isothermal titration calorimetry of β -cyclodextrin complexes with mianserin in aqueous solution

Anna Ignaczak^{*a}, Bartłomiej Pałecz^b, Sylwia Belica-Pacha^b

^a Department of Theoretical and Structural Chemistry, Faculty of Chemistry,
University of Lodz, Pomorska 163/165, 90-236 Lodz, Poland.
E-mail: anignacz@uni.lodz.pl

^b Unit of Biophysical Chemistry, Department of Physical Chemistry, Faculty of Chemistry,
University of Lodz, Pomorska 165, 90-236 Lodz, Poland

The optimized structures and corresponding total energies E [hartree] of mianserin, β -CD and their complexes 1:1 and 1:2 in vacuo and in water (PCM) obtained with the B3LYP/6-31G(d,p) method. For the structures presented in the manuscript in Table 2 additionally the zero-point energies ZPE, enthalpies H and free energies G (all in hartree) and total entropies S [cal/mol·K] are given (uncorrected values from Gaussian 09 calculations).

MIA S VACUUM				MIA R VACUUM			
E	-807.48184937			E	-807.48184937		
ZPE	-807.137341			ZPE	-807.137341		
H	-807.120788			H	-807.120788		
G	-807.179489			G	-807.179489		
S	123.546			S	123.546		
Atom	x [Å]	y [Å]	z [Å]	Atom	x [Å]	y [Å]	z [Å]
C	-1.201907	3.909782	-0.102717	C	1.201899	3.909785	-0.102717
C	-0.249819	3.720846	-1.102757	C	0.249812	3.720846	-1.102756
C	0.392566	2.489550	-1.212097	C	-0.392571	2.489549	-1.212096
C	0.113385	1.430295	-0.336768	C	-0.113388	1.430294	-0.336768
C	-0.864127	1.616926	0.658860	C	0.864125	1.616928	0.658860
C	-1.506483	2.857160	0.758034	C	1.506478	2.857163	0.758034
C	-1.306190	0.466723	1.543915	C	1.306192	0.466725	1.543914
C	-1.842448	-0.659142	0.692177	C	1.842449	-0.659139	0.692176
C	-3.198932	-0.975166	0.637037	C	3.198934	-0.975163	0.637036
C	-3.665102	-2.020650	-0.163933	C	3.665105	-2.020646	-0.163934
C	-2.758773	-2.752859	-0.926953	C	2.758777	-2.752855	-0.926954
C	-1.398303	-2.439842	-0.895026	C	1.398306	-2.439840	-0.895026
C	-0.925262	-1.393234	-0.090836	C	0.925265	-1.393233	-0.090836
C	0.979397	0.182645	-0.495343	C	-0.979397	0.182643	-0.495343
N	0.456107	-1.089670	0.049547	N	-0.456105	-1.089671	0.049549
C	2.356537	0.450258	0.151412	C	-2.356537	0.450254	0.151411
C	1.388579	-2.183993	-0.220530	C	-1.388575	-2.183996	-0.220527
C	2.742342	-1.897983	0.421921	C	-2.742339	-1.897987	0.421923
N	3.285832	-0.646845	-0.092013	N	-3.285831	-0.646850	-0.092013
C	4.611299	-0.364135	0.436820	C	-4.611299	-0.364140	0.436818
H	-1.715217	4.861653	-0.002261	H	1.715208	4.861656	-0.002261
H	-0.011400	4.521232	-1.796915	H	0.011390	4.521232	-1.796915
H	1.132370	2.342252	-1.995710	H	-1.132374	2.342250	-1.995710
H	-2.266860	2.991200	1.523320	H	2.266854	2.991205	1.523319
H	-2.072350	0.813412	2.243400	H	2.072354	0.813416	2.243397
H	-0.458287	0.092624	2.131004	H	0.458291	0.092626	2.131007
H	-3.897996	-0.404068	1.243060	H	3.897998	-0.404063	1.243058
H	-4.723860	-2.260566	-0.185935	H	4.723863	-2.260561	-0.185936
H	-3.105581	-3.567527	-1.556405	H	3.105585	-3.567524	-1.556406
H	-0.706247	-3.011638	-1.503830	H	0.706251	-3.011637	-1.503830
H	1.161192	0.052260	-1.577861	H	-1.161190	0.052257	-1.577861
H	2.201198	0.636850	1.232716	H	-2.201199	0.636848	1.232715
H	2.776161	1.363834	-0.281510	H	-2.776163	1.363829	-0.281512
H	1.541061	-2.342112	-1.303254	H	-1.541057	-2.342115	-1.303251
H	0.972872	-3.103003	0.201091	H	-0.972867	-3.103005	0.201094
H	3.436662	-2.711385	0.179846	H	-3.436658	-2.711390	0.179849
H	2.621469	-1.875934	1.523141	H	-2.621467	-1.875935	1.523144
H	4.626745	-0.235062	1.536170	H	-4.626745	-0.235059	1.536166
H	5.002632	0.552675	-0.015841	H	-5.002635	0.552665	-0.015851
H	5.291307	-1.184159	0.183727	H	-5.291304	-1.184169	0.183731

β-CD VACUUM							
β-CD-CCCW				β-CD-EXP			
E	-4275.41135478			E	-4275.37504403		
ZPE	-4274.187102			ZPE	-4274.156320		
H	-4274.114324			H	-4274.080253		
G	-4274.289467			G	-4274.267579		
S	368.620			S	394.261		
Atom	x [Å]	y [Å]	z [Å]	Atom	x [Å]	y [Å]	z [Å]
O	5.781491	-0.331031	1.206985	C	0.201560	-6.133398	-0.115502
C	4.661956	-1.226117	1.007110	C	-0.667052	-6.307538	-1.364310
C	5.105999	-2.269072	-0.030492	O	0.159027	-6.279720	-2.523405
C	5.489238	-1.570881	-1.337731	C	-1.738602	-5.225933	-1.431845
C	6.540211	-0.496929	-1.083744	O	-2.547549	-5.528240	-2.551365
C	6.105130	0.429367	0.059326	C	-2.539562	-5.154814	-0.127112
H	3.815083	-0.664061	0.598423	O	-3.330676	-3.967190	-0.217865
H	5.971634	-2.824844	0.356694	C	-1.588499	-5.075356	1.079211
H	4.582683	-1.082522	-1.728335	O	-0.638474	-6.154705	1.027870
H	7.466965	-0.996963	-0.765355	C	-2.271728	-5.180618	2.428993
H	6.935204	1.078729	0.359291	O	-1.284602	-4.880768	3.413734
C	4.239970	-1.763289	2.387007	C	-4.716378	-4.014766	0.043917
O	4.058107	-3.172916	-0.377458	C	-5.475957	-3.481800	-1.178745
O	6.028332	-2.470638	-2.289057	O	-5.111508	-4.232888	-2.334624
O	6.782264	0.289858	-2.245088	C	-5.199811	-1.997614	-1.383924
O	5.011454	1.194130	-0.377152	O	-6.021799	-1.578787	-2.457584
H	4.250853	-2.854579	2.397886	C	-5.479419	-1.240302	-0.089328
O	2.915498	-1.381418	2.739408	O	-5.092944	0.121912	-0.299006
H	4.967996	-1.402910	3.125817	C	-4.687739	-1.849246	1.072681
H	5.404684	-3.213919	-2.389126	O	-5.044578	-3.247355	1.183580
H	6.882337	-0.337811	-2.976316	C	-4.958102	-1.166861	2.424428
H	2.865262	-0.400923	2.790984	O	-6.272073	-0.664225	2.584509
O	3.863446	4.313829	1.205920	C	-6.072682	1.121164	-0.172632
C	3.865508	2.880419	1.006534	C	-5.976341	2.072599	-1.365068
C	4.957844	2.577086	-0.030909	O	-6.156361	1.328459	-2.567250
C	4.650528	3.311260	-1.338481	C	-4.639820	2.802164	-1.364705
C	4.465991	4.802646	-1.085153	O	-4.674454	3.710325	-2.448699
C	3.470675	5.040506	0.057993	C	-4.418445	3.491770	-0.020524
H	2.898176	2.568379	0.597806	O	-3.064205	3.949303	-0.021255
H	5.932053	2.907866	0.355907	C	-4.629982	2.518436	1.154160
H	3.703457	2.906668	-1.728694	O	-5.907859	1.849679	1.037134
H	5.434761	5.215717	-0.767133	C	-4.584291	3.208272	2.507869
H	3.480609	6.094481	0.357519	O	-5.468600	4.322570	2.495484
C	4.022253	2.215973	2.386658	C	-2.779456	5.265512	0.414659
O	5.689949	3.171380	-2.289897	C	-2.169922	6.057550	-0.749762
O	4.001494	5.481881	-2.246717	O	-3.052363	6.022872	-1.870726
O	2.190780	4.662141	-0.378159	C	-0.803712	5.498672	-1.123878
H	4.882249	1.544097	2.397788	O	-0.282162	6.347322	-2.132999
O	2.897894	1.418556	2.739145	C	0.085833	5.426018	0.114405
H	4.194289	3.010066	3.125267	O	1.312614	4.793892	-0.270577
H	5.882584	2.220350	-2.389226	C	-0.605789	4.623574	1.221878
H	4.554388	5.168366	-2.977947	O	-1.881909	5.247494	1.502832
H	2.100056	1.990674	2.790919	C	0.191685	4.556321	2.532992
O	-0.963685	5.710257	1.205380	O	0.925865	5.732562	2.821472
C	1.058202	4.818000	1.006125	C	2.473805	5.581882	-0.286613
C	1.076162	5.482524	-0.031800	C	3.265092	5.304108	-1.567229
C	0.310216	5.699587	-1.339250	O	2.446248	5.570425	-2.700990
C	-0.970774	6.485312	-1.085929	C	3.772715	3.866791	-1.587674
C	-1.777016	5.855868	0.057642	O	4.566591	3.739855	-2.750317
H	-0.201119	3.867003	0.597902	C	4.540549	3.531457	-0.302915
H	1.425029	6.450533	0.354694	O	4.752884	2.117653	-0.315842
H	0.035866	4.706736	-1.728997	C	3.708292	3.928790	0.927871
H	-0.689634	7.500393	-0.768362	O	3.305255	5.304890	0.827257
H	-2.594718	6.520941	0.357196	C	4.431812	3.802780	2.254078
C	0.775740	4.526962	2.386252	O	3.449290	3.988693	3.273571
O	1.067437	6.424600	-2.291154	C	6.057982	1.596697	-0.177985
O	-1.791652	6.545235	-2.247364	C	6.371248	0.693198	-1.375275
O	-2.279450	4.619206	-0.377918	O	6.244066	1.436086	-2.586607
H	1.837279	4.780257	2.396973	C	5.455848	-0.524263	-1.389239
O	0.698014	3.150969	2.739631	O	5.873189	-1.327931	-2.476890
H	0.262451	5.157109	3.124616	C	5.533012	-1.248777	-0.049532
H	1.931015	5.982128	-2.390560	O	4.509113	-2.247384	-0.064173
H	-1.201959	6.781832	-2.978774	C	5.301408	-0.274996	1.119783
H	-0.246740	2.883917	2.791268	O	6.188711	0.858144	1.016990
O	-5.065211	2.806775	1.206797	C	5.526804	-0.924312	2.475828
C	-3.668242	3.127714	1.006927	O	6.793008	-1.575483	2.483517
C	-3.615777	4.259653	-0.031051	C	4.827706	-3.559523	0.356217

C	-4.263757	3.796348	-1.338207	C	4.582620	-4.532178	-0.805295
C	-5.676692	3.285057	-1.084137	O	5.325124	-4.112397	-1.949095
C	-5.686744	2.261987	0.059214	C	3.097394	-4.625835	-1.129734
H	-3.148804	2.253886	0.598558	O	2.965741	-5.616314	-2.135144
H	-4.154700	5.136133	0.355558	C	2.310651	-4.953237	0.136403
H	-3.658931	2.962772	-1.728367	O	0.918701	-4.931394	-0.206356
H	-6.294591	4.137843	-0.765966	C	2.617881	-3.929199	1.234775
H	-6.716398	2.037273	0.359224	O	4.046238	-3.936897	1.469397
C	-3.055276	3.429073	2.386872	C	1.914600	-4.217409	2.570246
O	-4.358795	4.840565	-2.289931	O	1.754365	-5.596744	2.852171
O	-6.236251	2.681017	-2.245326	H	0.879066	-6.984081	0.004914
O	-5.033303	1.098271	-0.377016	H	-1.165834	-7.284329	-1.282936
H	-2.591743	4.417089	2.397657	H	-0.441137	-6.171853	-3.276806
O	-2.027543	2.510607	2.739698	H	-1.235991	-4.254092	-1.555655
H	-3.867710	3.420283	3.125517	H	-3.328960	-4.940348	-2.543213
H	-3.474351	5.239541	-2.389938	H	-3.184753	-6.041123	-0.049083
H	-6.053775	3.289634	-2.976742	H	-1.058416	-4.116377	1.031116
H	-2.407477	1.605327	2.791103	H	-2.663473	-6.201206	2.551233
O	-5.352606	-2.210290	1.206675	H	-3.111292	-4.474211	2.467896
C	-4.732336	-0.918052	1.007019	H	-1.637972	-5.099575	4.284495
C	-5.585041	-0.170884	-0.030355	H	-5.029462	-5.039543	0.272568
C	-5.627214	-0.965900	-1.337809	H	-6.549908	-3.606951	-0.979701
C	-6.107960	-2.389636	-1.084174	H	-5.468894	-3.734733	-3.086575
C	-5.314142	-3.035597	0.058866	H	-4.134216	-1.870445	-1.630307
H	-3.725522	-1.056964	0.598186	H	-5.912467	-0.615491	-2.580475
H	-6.606137	-0.046051	0.356825	H	-6.546032	-1.297422	0.154399
H	-4.598522	-1.012399	-1.728373	H	-3.613396	-1.782768	0.858537
H	-7.159950	-2.341461	-0.765944	H	-4.211720	-0.373202	2.560076
H	-5.780285	-3.980871	0.358616	H	-4.786908	-1.914050	3.206812
C	-4.584893	-0.251280	2.387061	H	-6.269965	0.253717	2.265396
O	-6.503307	-0.389006	-2.289029	H	-7.072724	0.680224	-0.112447
O	-5.984393	-3.203230	-2.245708	H	-6.778615	2.816839	-1.261765
O	-3.996907	-3.250019	-0.377487	H	-5.876531	1.916614	-3.285327
H	-5.068612	0.726999	2.398511	H	-3.838488	2.058856	-1.498463
O	-3.225800	-0.020190	2.738839	H	-3.985338	4.391033	-2.312744
H	-5.083795	-0.892318	3.125907	H	-5.111972	4.333409	0.075960
H	-6.264143	0.551368	-2.388671	H	-3.829950	1.767651	1.125256
H	-6.346793	-2.680996	-2.976881	H	-3.548050	3.523725	2.687323
H	-2.754965	-0.881693	2.790325	H	-4.866870	2.477154	3.280324
O	-1.609227	-5.562962	1.205462	H	-5.354283	4.802247	3.325072
C	-2.232838	-4.272288	1.006165	H	-3.689277	5.745872	0.787151
C	-3.348573	-4.472801	-0.031356	H	-2.039716	7.096344	-0.414025
C	-2.753092	-5.000833	-1.338940	H	-2.530159	6.371157	-2.611045
C	-1.939736	-6.264485	-1.085742	H	-0.938990	4.475349	-1.505829
C	-0.939936	-6.047139	0.057556	H	0.568063	5.978886	-2.441209
H	-1.496519	-3.571570	0.597532	H	0.285936	6.430598	0.501363
H	-4.082777	-5.193528	0.355455	H	-0.790948	3.598621	0.874488
H	-2.075302	-4.225353	-1.729004	H	0.854911	3.685816	2.495250
H	-2.633370	-7.057048	-0.767942	H	-0.534586	4.381871	3.337732
H	-0.491714	-7.001124	0.357044	H	1.862636	5.518557	2.685907
C	-2.662460	-3.741683	2.386262	H	2.225182	6.644607	-0.209592
O	-3.750186	-5.325690	-2.290486	H	4.134497	5.977720	-1.566899
O	-1.226404	-6.674668	-2.247314	H	2.899071	5.167963	-3.457678
O	0.049199	-5.150957	-0.378347	H	2.900302	3.196152	-1.626544
H	-3.728810	-3.509449	2.397359	H	4.997701	2.861499	-2.745519
O	-1.995363	-2.535480	2.738875	H	5.501644	4.064588	-0.304667
H	-2.473026	-4.531831	3.124850	H	2.820280	3.285453	0.956252
H	-4.336337	-4.552393	-2.389863	H	5.215155	4.572545	2.308121
H	-1.860538	-6.632084	-2.978572	H	4.904140	2.814247	2.321830
H	-1.028328	-2.704922	2.790659	H	3.896757	4.107759	4.120056
O	3.345604	-4.726455	1.206052	H	6.789457	2.409440	-0.107701
C	1.947686	-4.409569	1.006455	H	7.407851	0.345888	-1.262744
C	1.409255	-5.406613	-0.031579	H	6.256935	0.774809	-3.296320
C	2.193942	-5.270060	-1.338826	H	4.419309	-0.179761	-1.529865
C	3.688893	-5.422189	-1.085016	H	5.517947	-2.231170	-2.356580
C	4.141858	-4.504999	0.058466	H	6.519554	-1.711364	0.057618
H	1.858623	-3.396884	0.598189	H	4.262094	0.076958	1.080680
H	1.514729	-6.430146	0.354922	H	4.712539	-1.640962	2.642429
H	2.010513	-4.256572	-1.728824	H	5.471939	-0.142473	3.247616
H	3.875905	-6.458653	-0.767135	H	6.841892	-2.116906	3.280806
H	5.167070	-4.749353	0.358338	H	5.866727	-3.605911	0.695879
C	1.264914	-4.415258	2.386551	H	4.928021	-5.525664	-0.485037
O	1.826500	-6.252013	-2.290622	H	4.983399	-4.648009	-2.682514
O	4.454829	-5.120290	-2.246279	H	2.758259	-3.645595	-1.498766
H	0.418403	-5.104061	2.397306	H	2.022221	-5.697109	-2.372896
O	0.737928	-3.141786	2.739868	H	2.588613	-5.943824	0.511107

H	2.000755	-4.760264	3.124951	H	2.327918	-2.925872	0.895823
H	0.856509	-6.227932	-2.390408	H	0.945883	-3.707472	2.577594
H	4.026310	-5.589353	-2.977737	H	2.531003	-3.765237	3.357744
H	1.473199	-2.491212	2.791554	H	0.817824	-5.803440	2.704722

Complexes 1:1 VACUUM											
[MIA S]-[β-CD-CCCW]				[MIA R]-[β-CD-CCCW]				[MIA S]-[β-CD-EXP]			
CR1				CR1				CR1			
E -5082.91346527				E -5082.90887702				E -5082.87566041			
Atom	x [Å]	y [Å]	z [Å]	Atom	x [Å]	y [Å]	z [Å]	Atom	x [Å]	y [Å]	z [Å]
O	-5.615961	-4.123619	-0.362940	O	3.681184	4.432078	-2.060141	C	6.566693	-1.425433	0.055989
C	-4.216110	-4.024781	-0.717851	C	2.303785	4.008168	-1.935789	C	6.843424	-0.686803	1.367506
C	-3.476810	-5.113134	0.076140	C	1.598547	5.019005	-1.023007	O	6.585846	-1.555354	2.465989
C	-3.679356	-4.890185	1.576914	C	2.288113	5.084106	0.340724	C	5.991134	0.572315	1.462075
C	-5.163996	-4.812914	1.911362	C	3.778351	5.361166	0.170723	O	6.380771	1.232049	2.650544
C	-5.875583	-3.812013	0.991662	C	4.393403	4.383386	-0.837926	C	6.152723	1.451330	0.216825
H	-3.831520	-3.045877	-0.411422	H	2.270160	3.019613	-1.465767	O	5.127751	2.446012	0.298246
H	-3.868784	-6.100951	-0.204580	H	1.636949	6.011168	-1.494168	C	5.970564	0.613928	-1.062002
H	-3.216307	-3.924015	1.831710	H	2.175090	4.098971	0.819451	O	6.830993	-0.540910	-1.024055
H	-5.606998	-5.802375	1.724275	H	3.892543	6.374770	-0.241038	C	6.305403	1.352785	-2.343284
H	-6.961987	-3.891441	1.110758	H	5.420033	4.678957	-1.081739	O	5.854522	0.539609	-3.423173
C	-4.115363	-4.103972	-2.252251	C	1.721641	3.874741	-3.355062	C	5.451875	3.816102	0.218516
O	-2.065754	-5.069290	-0.125429	O	0.243340	4.645704	-0.778670	C	4.909397	4.532818	1.463632
O	-3.126235	-5.936244	2.354664	O	1.752576	6.111675	1.158024	O	5.446529	3.934504	2.640620
O	-5.380783	-4.427595	3.264695	O	4.484810	5.248812	1.401564	C	3.386566	4.494116	1.479446
O	-5.435616	-2.518422	1.315917	O	4.365878	3.099183	-0.272608	O	2.970465	5.252926	2.601677
H	-3.446112	-4.911184	-2.555023	H	0.889219	4.567219	-3.498519	C	2.851287	5.045510	0.162007
O	-3.581479	-2.916823	-2.826491	O	1.201776	2.575528	-3.608373	O	1.426525	4.894328	0.172829
H	-5.117854	-4.320203	-2.644882	H	2.513531	4.134450	-4.070146	C	3.461328	4.300209	-1.029740
H	-2.197419	-6.056921	-2.601631	H	0.773022	6.043140	1.143895	O	4.901577	4.401768	-0.943970
H	-4.776778	-4.968469	3.795182	H	3.978510	5.760245	2.049582	C	3.013052	4.857818	-2.390708
H	-4.176441	-2.162421	-2.619040	H	1.930352	1.921843	-3.528598	O	2.813347	6.258413	-2.422387
O	-7.179410	0.592874	0.402387	O	6.296426	0.199440	-1.453735	C	0.646684	6.064954	0.133478
C	-6.219061	-0.469944	0.194859	C	5.124213	1.045626	-1.391671	C	-0.491533	5.958075	1.149345
C	-6.388574	-1.458073	1.359524	C	5.476657	2.227657	-0.476798	O	0.067522	5.696649	2.436800
C	-6.137630	-0.742652	2.689346	C	5.841606	1.704362	0.915298	C	-1.495419	4.883488	0.756176
C	-7.030517	0.485719	2.814233	C	6.948957	0.659487	0.829015	O	-2.558914	4.962444	1.690175
C	-6.923856	1.363262	1.560242	C	6.600699	-0.411793	-0.213910	C	-1.962019	5.088033	-0.683072
H	-5.205257	-0.056498	0.231655	H	4.301231	0.490488	-0.929561	O	-2.696175	3.912658	-1.025790
H	-7.409228	-1.865903	1.348466	H	6.324304	2.785099	-0.899436	C	-0.765092	5.246572	-1.637662
H	-5.088094	-0.408999	2.690487	H	4.942668	1.221112	1.328226	O	0.120131	6.290803	-1.165768
H	-8.073287	0.142773	2.886659	H	7.867159	1.161604	0.489523	C	-1.175835	5.589565	-3.060033
H	-7.694924	2.141719	1.573926	H	7.464138	-1.059454	-0.403636	O	-2.060205	6.703964	-3.036347
C	-6.440767	-1.031032	-1.221760	C	4.696656	1.380690	-2.831046	C	-3.912900	4.039065	-1.736935
O	-6.404986	-1.573021	3.804780	O	6.298543	2.735257	1.773109	C	-5.063756	3.515259	-0.865702
O	-6.692767	1.269827	3.953514	O	7.171058	0.022819	2.082314	O	-5.051350	4.183644	0.396071
O	-5.642437	1.936633	1.524948	O	5.515085	-1.157909	0.269208	C	-4.966935	2.008360	-0.669052
H	-6.619017	-2.107278	-1.188425	H	4.654766	2.460893	-2.980711	O	-6.162091	1.614040	-0.016589
O	-5.309698	-0.847882	-2.064926	O	3.394374	0.885128	-3.130438	C	-4.771405	1.294811	-2.002890
H	-7.332376	-0.545694	-1.640499	H	5.446729	0.965283	-3.516213	O	-4.515119	-0.082723	-1.698903
H	-5.909585	-2.405173	3.687479	H	5.620024	3.435166	1.785985	C	-3.595641	1.898105	-2.775829
H	-6.600655	0.645406	4.688599	H	7.210083	0.734681	2.738425	O	-3.853854	3.313702	-2.946939
H	-5.132151	0.113938	-2.163438	H	3.428354	-0.098554	-3.145627	C	-3.376963	1.270922	-4.166047

O	-4.711691	4.882456	-0.477705	O	4.448760	-4.442748	-1.014087	O	-4.551228	0.748939	-4.766354
C	-4.858610	3.461576	-0.244770	C	4.481337	-2.996881	-1.006046	C	-5.405722	-1.056408	-2.165566
C	-5.510892	3.303139	1.137618	C	5.486873	-2.570985	0.076835	C	-5.755144	-2.013821	-1.024956
C	-4.623064	3.944199	2.207274	C	5.056608	-3.131398	1.435237	O	-1.293255	0.041947	
C	-4.320397	5.395218	1.853562	C	4.833753	-4.636117	1.364787	C	-4.501080	-2.734423	-0.544341
C	-3.807417	5.507322	0.411977	C	3.937684	-5.007804	0.175352	O	-4.914680	-3.630715	0.471264
H	-3.868863	2.992559	-0.221133	H	3.493797	-2.610272	-0.732338	C	-3.788151	-3.434680	-1.709237
H	-6.495334	3.792034	1.135784	H	6.490024	-2.941351	-0.177750	O	-2.497186	-3.861662	-1.263026
H	-3.673341	3.386788	2.224123	H	4.101817	-2.649717	1.695722	C	-3.588740	-2.456666	-2.881676
H	-5.261221	5.962457	1.911482	H	5.809555	-5.115423	1.195719	O	-4.831701	-1.813146	-3.223536
H	-3.767455	6.557977	0.103401	H	3.954391	-6.091784	0.017727	C	-3.092133	-3.114030	-4.154699
C	-5.624987	2.867836	-1.441051	C	4.770986	-2.530077	-2.443211	O	-2.672370	-2.070604	-5.029941
O	-5.233635	3.940926	3.484888	O	6.026065	-2.893393	2.440399	C	-2.288003	-5.233345	-0.982164
O	-3.352366	5.961524	2.730397	O	4.241275	-5.136853	2.558146	C	-1.702785	-5.387692	0.436490
O	-2.532118	4.923336	0.345003	O	2.624094	-4.573043	0.432501	O	-2.598309	-4.762505	1.341049
H	-6.519231	2.339939	-1.105008	H	5.583089	-1.801669	-2.454526	C	-0.282831	-4.823299	0.497565
O	-4.855348	1.913681	-2.162898	O	3.656638	-1.881326	-3.045110	O	0.278992	-5.146129	1.758869
H	-5.936757	3.699053	-2.087315	H	5.082831	-3.406179	-3.027196	C	0.572724	-5.378585	-0.641251
H	-5.520599	3.029322	3.680384	H	6.228315	-1.939604	2.437348	O	1.789234	-4.623400	-0.612036
H	-3.629654	5.718411	3.626320	H	4.747161	-4.752390	3.289512	C	-0.126895	-5.220063	-1.998247
H	-4.057254	2.353804	-2.531436	H	2.892548	-2.501075	-3.082694	O	-1.434313	-5.817089	-1.941359
O	-0.093177	5.518129	-2.347974	O	-0.309515	-5.986881	-1.297538	C	0.638035	-5.860349	-3.145395
C	-1.175080	4.800153	-1.709236	C	0.745309	-5.011330	-1.125008	O	0.985650	-7.197177	-2.796145
C	-1.520727	5.570533	-0.425414	C	1.543418	-5.452150	0.112837	C	3.017059	-5.295564	-0.833178
C	-0.293209	5.634471	0.486446	C	0.624497	-5.449069	1.336915	C	3.837899	-5.300020	0.463024
C	0.897657	6.224254	-0.250938	C	-0.591285	-6.334623	1.081005	O	3.061534	-5.875370	1.514534
C	1.108147	5.509419	-1.600959	C	-1.263964	-5.979999	-0.252062	C	4.279899	-3.891865	0.837486
H	-0.833905	3.795892	-1.434817	H	0.303874	-4.027136	-0.932025	O	5.123794	-4.023413	1.968302
H	-1.838628	6.590067	-0.685465	H	1.929135	-6.467990	-0.052062	C	4.968117	-3.221723	-0.347473
H	-0.043796	4.601506	0.775999	H	0.276810	-4.415852	1.493565	O	5.237090	-1.867604	0.040767
H	0.670687	7.277452	-0.482216	H	-0.236141	-7.372855	0.998908	C	4.064234	-3.267870	-1.585194
H	1.838340	6.052963	-2.211111	H	-1.996041	-6.749797	-0.520671	O	3.747359	-4.655048	-1.855819
C	-2.305791	4.640151	-2.742270	C	1.516796	-4.924172	-2.455127	C	4.703039	-2.663588	-2.848705
O	-0.513982	6.440204	1.629836	O	1.267837	-5.948425	2.496196	O	6.117266	-2.764453	-2.892820
O	2.095868	6.132166	0.502902	O	-1.554028	-6.228611	2.123302	H	7.260168	-2.261500	-0.074901
O	1.552356	4.201954	-1.347008	O	-1.885632	-4.729119	-0.127452	H	7.903003	-0.392450	1.363616
H	-3.240940	5.052463	-2.359283	H	2.569134	-5.177807	-2.316346	H	6.548411	-0.984380	3.248840
O	-2.574718	3.277541	-3.049794	O	1.500782	-3.614051	-3.008609	H	4.934602	0.266627	1.505255
H	-2.022786	5.203119	-3.641512	H	1.074453	-5.653010	-3.146897	H	5.912057	2.088830	2.702754
H	-1.332751	6.133481	2.062300	H	2.134782	-5.509331	2.577355	H	7.146065	1.921463	0.230044
H	1.866299	6.426206	1.397137	H	-1.061886	-6.315903	2.952905	H	4.924391	0.289207	-1.109721
H	-1.776584	2.876315	-3.461124	H	0.572243	-3.351967	-3.198800	H	7.392946	1.512987	-2.385920
O	3.193449	2.079903	-3.868135	O	-4.460407	-3.389223	-2.394631	H	5.807712	2.331790	-2.335655
C	2.047973	2.584871	-3.146359	C	-3.105995	-3.549488	-1.910466	H	6.210696	0.894883	-4.246510
C	2.578789	3.651134	-2.175405	C	-3.162358	-4.544555	-0.739727	H	6.536027	3.952381	0.138266
C	3.590593	3.028033	-1.201642	C	-4.081787	-4.004038	0.359534	H	5.229067	5.582986	1.404406
C	4.710817	2.323922	-1.971192	C	-5.459346	-3.690944	-0.214393	H	4.912795	4.283088	3.372037
C	4.104639	1.392912	-3.037052	C	-5.324178	-2.789218	-1.447790	H	3.066625	3.445449	1.574673
H	1.598733	1.774510	-2.582257	H	-2.736984	-2.589769	-1.533257	H	1.994889	5.254205	2.633380
H	3.068864	4.452835	-2.745970	H	-3.549414	-5.508202	-1.099897	H	3.116370	6.104602	0.069403

H	3.054575	2.269674	-0.610483	H	-3.641602	-3.070829	0.739870	H	3.186178	3.238511	-0.982358
H	5.294958	3.094853	-2.497098	H	-5.919158	-4.635096	-0.542545	H	2.105853	4.319264	-2.695320
H	4.893832	1.019252	-3.698684	H	-6.290027	-2.677623	-1.953559	H	3.796527	4.616486	-3.116877
C	1.006018	3.032804	-4.186524	C	-2.228789	-3.945510	-3.111534	H	1.894379	6.427564	-2.153594
O	4.155352	4.017487	-0.356156	O	-4.265333	-4.936426	1.412662	H	1.264030	6.942310	0.350818
O	5.548727	1.523040	-1.163232	O	-6.297799	-3.045010	0.737403	H	-1.011363	6.926615	1.157951
O	3.468027	0.330413	-2.371539	O	-4.834204	-1.546406	-1.023708	H	-0.683458	5.497788	3.015529
H	0.710136	4.070106	-4.022988	H	-1.722496	-4.894413	-2.924730	H	-1.003252	3.902188	0.808214
O	-0.193600	2.268245	-4.118219	O	-1.201012	-2.995080	-3.371901	H	-3.339780	4.512220	1.309299
H	1.468490	2.956452	-5.179394	H	-2.885431	-4.070040	-3.982538	H	-2.597644	5.977527	-0.743592
H	3.423256	4.548151	0.010637	H	-3.384585	-5.179202	1.752730	H	-0.216802	4.296098	-1.660641
H	6.028681	2.041275	-0.456968	H	-6.171336	-3.524934	1.569225	H	-1.661174	4.703706	-3.490298
H	0.013801	1.322010	-4.283470	H	-1.608649	-2.130785	-3.600873	H	-0.266742	5.808437	-3.640453
O	2.726802	-2.985174	-3.757151	O	-4.916921	1.614625	-2.901982	H	-2.379684	6.848813	-3.935448
C	2.408874	-1.615391	-3.416636	C	-4.342993	0.347384	-2.502282	H	-4.077068	5.082496	-2.022873
C	3.681052	-1.005734	-2.816078	C	-5.361848	-0.347483	-1.586407	H	-6.004196	3.732482	-1.392506
C	4.104480	-1.787424	-1.569459	C	-5.679198	0.540737	-0.381711	H	-5.611830	3.643367	0.977000
C	4.233308	-3.275139	-1.874165	C	-6.105480	1.933649	-0.823482	H	-4.088207	1.796566	-0.041666
C	2.991968	-3.788948	-2.622140	C	-5.098665	2.513742	-1.826637	H	-6.107026	0.659490	0.178708
H	1.620531	-1.603982	-2.656367	H	-3.428637	0.526268	-1.926363	H	-5.672851	1.384450	-2.617682
H	4.488480	-1.035665	-3.561394	H	-6.284222	-0.560740	-2.145184	H	-2.675688	1.784693	-2.188797
H	3.310043	-1.657812	-0.817807	H	-4.755858	0.632263	0.209093	H	-2.609987	0.492854	-4.088200
H	5.096518	-3.409085	-2.543223	H	-7.073375	1.853410	-1.339854	H	-2.981803	2.062272	-4.814166
H	3.175460	-4.796675	-3.011420	H	-5.489776	3.436098	-2.270839	H	-4.544264	-0.208385	-4.604234
C	1.849921	-0.919582	-4.671671	C	-3.948216	-0.415307	-3.778874	H	-6.306298	-0.599325	-2.586555
O	5.350425	-1.335082	-1.071079	O	-6.726738	0.003472	0.409972	H	-6.461617	-2.757818	-1.421833
O	4.402547	-4.052763	-0.693112	O	-6.213490	2.822627	0.284808	H	-6.298442	-1.880039	0.811626
O	1.904674	-3.792351	-1.734205	O	-3.891098	2.762324	-1.152610	H	-3.808426	-1.979372	-0.145476
H	2.451160	-0.045378	-4.929934	H	-4.350162	-1.429843	-3.757720	H	-4.109034	-4.039584	0.862177
O	0.523634	-0.438726	-4.483717	O	-2.539354	-0.556013	-3.920426	H	-4.385197	-4.298643	-2.034422
H	1.900495	-1.632264	-5.505652	H	-4.384405	0.111738	-4.638022	H	-2.858099	-1.699942	-2.572139
H	5.322825	-0.355546	-1.027929	H	-6.477315	-0.910220	0.644836	H	-3.912600	-3.702203	-4.590269
H	5.015086	-3.571837	-0.114972	H	-6.741238	2.354816	0.948918	H	-2.268316	-3.797059	-3.909204
H	-0.067747	-1.202590	-4.303667	H	-2.137282	0.338801	-3.984640	H	-2.605091	-2.425487	-5.924421
O	-1.210435	-5.695687	-2.199844	O	-1.335835	5.077884	-2.428752	H	-3.232470	-5.782843	-1.054249
C	-0.377875	-4.515917	-2.302280	C	-1.960331	3.779353	-2.318903	H	-1.641721	-6.466448	0.643580
C	1.005930	-4.898894	-1.755199	C	-3.179459	3.974310	-1.407541	H	-2.229626	-4.601795	2.250485
C	0.881385	-5.353706	-0.298926	C	-2.718920	4.436602	-0.018396	H	-0.334013	-3.732295	0.368520
C	-0.140023	-6.477887	-0.175683	C	-1.825819	5.672528	-0.095721	H	1.249811	-5.214712	1.660281
C	-1.455804	-6.095099	-0.865596	C	-0.768475	5.524501	-1.215292	H	0.772784	-6.439666	-0.459949
H	-0.795203	-3.720931	-1.674619	H	-1.267765	3.080006	-1.837114	H	-0.223892	-4.148741	-2.219309
H	1.424511	-5.715337	-2.360504	H	-3.852921	4.722858	-1.848133	H	1.533659	-5.253224	-3.334842
H	0.521149	-4.492519	0.285429	H	-2.116980	3.608619	0.388351	H	-0.000573	-5.833307	-4.040114
H	0.259887	-7.359012	-0.699243	H	-2.466580	6.521633	-0.371321	H	1.505396	-7.567469	-3.520185
H	-2.116818	-6.966384	-0.934602	H	-0.340771	6.507554	-1.440580	H	2.831464	-6.313599	-1.187888
C	-0.429441	-4.029847	-3.762243	C	-2.217505	3.252350	-3.743435	H	4.735867	-5.909752	0.288919
O	2.105709	-5.839819	0.218953	O	-3.820361	4.716480	0.823587	H	3.567132	-5.703963	2.324840
O	-0.410142	-6.798303	1.184960	O	-1.166258	5.985445	1.123915	H	3.383951	-3.300666	1.083509
H	0.575285	-3.965522	-4.183849	H	-3.271941	3.015004	-3.890901	H	5.462529	-3.140255	2.211339
O	-0.990783	-2.727868	-3.884741	O	-1.508244	2.048929	-4.017073	H	5.904335	-3.736910	-0.586040

H	-1.001443	-4.765904	-4.342692	H	-1.938718	4.045936	-4.449416	H	3.127645	-2.735857	-1.375616
H	2.788853	-5.157943	0.072559	H	-4.470402	3.998121	0.706972	H	4.392003	-1.617723	-2.939827
H	0.453299	-6.846658	1.622162	H	-1.346328	5.319638	1.830553	H	4.288326	-3.209025	-3.704920
H	-1.918295	-2.746392	-3.560318	H	-0.543139	2.212248	-3.930358	H	6.463930	-1.894817	-2.636041
C	2.553551	0.553085	5.207700	C	1.333803	-1.234829	1.285727	C	0.473880	1.394504	1.048719
C	2.302187	1.050576	3.930352	C	1.147409	-0.075786	0.532199	C	0.183154	0.201375	0.389692
C	3.323853	1.052520	2.983840	C	0.335136	0.939222	1.034010	C	-0.680080	-0.717341	0.983616
C	4.608216	0.572622	3.280041	C	-0.301680	0.826144	2.279419	C	-1.256462	-0.476466	2.238610
C	4.853132	0.049005	4.563866	C	-0.106519	-0.340951	3.039660	C	-0.981131	0.739006	2.890884
C	3.817550	0.049641	5.507019	C	0.710040	-1.355723	2.526442	C	-0.117087	1.657716	2.284473
C	6.175861	-0.612045	4.907687	C	-0.877349	-0.566719	4.326391	C	-1.727865	1.110956	4.155477
C	6.441921	-1.756599	3.959447	C	-2.354185	-0.603502	4.014164	C	-3.208069	1.182997	3.858300
C	6.356662	-3.093004	4.350954	C	-3.091594	-1.785772	4.036986	C	-3.890388	2.397033	3.797406
C	6.597461	-4.126905	3.443945	C	-4.450340	-1.797141	3.711325	C	-5.263034	2.443154	3.536740
C	6.921877	-3.817444	2.123779	C	-5.074298	-0.607150	3.343692	C	-5.955936	1.255043	3.314604
C	6.997540	-2.484484	1.711028	C	-4.345453	0.583902	3.300250	C	-5.281558	0.033008	3.344193
C	6.755877	-1.444112	2.621189	C	-2.984107	0.602743	3.636311	C	-3.904599	-0.023147	3.612464
C	5.651260	0.740181	2.173851	C	-1.136595	2.026215	2.717907	C	-2.093302	-1.603850	2.829292
N	6.889698	-0.066765	2.282207	N	-2.221284	1.800097	3.698876	N	-3.201546	-1.245352	3.748056
C	6.039500	2.234652	2.107761	C	-0.210972	3.129767	3.270102	C	-1.181303	-2.610015	3.566235
C	7.802487	0.216620	1.170829	C	-2.978149	3.040097	3.894219	C	-3.986160	-2.442908	4.044394
C	8.172317	1.694986	1.142962	C	-2.065525	4.134477	4.434786	C	-3.108892	-3.485278	4.733946
N	6.964602	2.516681	0.999866	N	-0.940072	4.381476	3.523563	N	-1.925688	-3.828244	3.932014
C	7.279874	3.946180	0.922267	C	-0.043468	5.402032	4.078269	C	-1.070384	-4.773173	4.659870
H	1.770083	0.541075	5.959778	H	1.930983	-2.056754	0.905017	H	1.122910	2.136559	0.594802
H	1.318717	1.429089	3.668130	H	1.610279	0.031598	-0.444963	H	0.613844	-0.011348	-0.584290
H	3.124656	1.438551	1.986760	H	0.182011	1.839660	0.442928	H	-0.929343	-1.635324	0.457922
H	4.011222	-0.363954	6.493541	H	0.842879	-2.265696	3.106749	H	0.074314	2.608618	2.775057
H	6.148716	-0.970971	5.940580	H	-0.560424	-1.505523	4.789399	H	-1.368762	2.072947	4.531698
H	6.994616	0.112855	4.823426	H	-0.682085	0.244475	5.038324	H	-1.558945	0.360409	4.937973
H	6.112269	-3.325189	5.384556	H	-2.596743	-2.709784	4.325484	H	-3.339873	3.320174	3.956136
H	6.537637	-5.161591	3.767518	H	-5.004908	-2.729970	3.745409	H	-5.784089	3.396636	3.528525
H	7.117547	-4.612022	1.408513	H	-6.123994	-0.593770	3.068743	H	-7.020951	1.272717	3.104689
H	7.226695	-2.256292	0.676674	H	-4.839918	1.496837	2.986581	H	-5.834804	-0.881092	3.158340
H	5.151828	0.492478	1.223223	H	-1.591872	2.427489	1.797449	H	-2.524465	-2.149319	1.974029
H	6.482381	2.528041	3.076024	H	0.273172	2.753806	4.189377	H	-0.758887	-2.115906	4.459000
H	5.139149	2.831731	1.946629	H	0.575249	3.336926	2.538639	H	-0.354778	-2.910741	2.917932
H	7.375185	-0.058967	0.193950	H	-3.443577	3.400551	2.962146	H	-4.435245	-2.876171	3.133695
H	8.709445	-0.377037	1.316455	H	-3.770937	2.849947	4.622420	H	-4.797690	-2.173451	4.725023
H	8.832719	1.889809	0.290756	H	-2.634698	5.064014	4.542883	H	-3.689776	-4.398873	4.903935
H	8.718947	1.958329	2.065702	H	-1.698763	3.840141	5.434642	H	-2.804145	-3.091037	5.719762
H	7.746523	4.321567	1.848517	H	0.374307	5.101169	5.054424	H	-0.689864	-4.344615	5.602773
H	6.361809	4.502853	0.724520	H	0.781037	5.587809	3.385824	H	-0.234314	-5.060459	4.022192
H	7.974903	4.118131	0.094590	H	-0.596549	6.336230	4.212045	H	-1.649038	-5.670303	4.901123
NR1				NR1				NR1			
E	-5082.91059654			E	-5082.91354642			E	-5082.87810585		
ZPE	-5081.339502			ZPE	-5081.342372						
H	-5081.249673			H	-5081.252671						
G	-5081.461603			G	-5081.463606						
S	446.043			S	443.949						

O	5.785365	3.565024	-0.548862	O	-6.327587	2.606637	-0.457554	C	-5.235286	-0.482332	-2.511554
C	4.357226	3.619105	-0.776628	C	-5.769952	1.277980	-0.324450	C	-5.709073	-1.462012	-1.435392
C	3.800763	4.732098	0.124617	C	-6.338106	0.681288	0.972617	O	-6.175826	-0.729262	-0.307532
C	4.118133	4.426250	1.590665	C	-5.957377	1.564664	2.163777	C	-4.586928	-2.412708	-1.038638
C	5.612426	4.196041	1.779522	C	-6.390603	3.006242	1.926534	O	-5.156584	-3.344142	-0.142853
C	6.127084	3.166924	0.764860	C	-5.901856	3.495422	0.557071	C	-3.954319	-3.083526	-2.263798
H	3.904904	2.668136	-0.475352	H	-4.681229	1.348295	-0.226372	O	-2.757932	-3.711405	-1.793726
H	4.253731	5.693100	-0.157024	H	-7.432645	0.614191	0.898589	C	-3.610140	-2.039789	-3.342373
H	3.590298	3.496673	1.854402	H	-4.859717	1.544547	2.248864	O	-4.766046	-1.225241	-3.626865
H	6.133894	5.144199	1.581529	H	-7.490161	3.036307	1.914076	C	-3.167838	-2.638493	-4.663426
H	7.221684	3.121103	0.786514	H	-6.352544	4.463843	0.312555	O	-2.667694	-1.571258	-5.464171
C	4.127883	3.781675	-2.290629	C	-6.067789	0.510507	-1.625322	C	-2.516707	-5.076820	-2.052880
O	2.378845	4.818643	0.053465	O	-5.784338	-0.601037	1.261579	C	-2.348419	-5.827593	-0.723549
O	3.740043	5.483360	2.454126	O	-6.564786	1.133451	3.368046	O	-3.505980	-5.648532	0.087989
O	5.913022	3.736095	3.092866	O	-5.887272	3.879490	2.932069	C	-1.096022	-5.358549	0.005429
O	5.570522	1.918784	1.084819	O	-4.502296	3.594750	0.598590	O	-0.971218	-6.178010	1.156869
H	3.537327	4.675881	-2.498587	H	-6.598158	-0.419458	-1.412040	C	0.103230	-5.468879	-0.928972
O	3.403388	2.692471	-2.850736	O	-4.883594	0.135870	-2.320054	O	1.243306	-4.925445	-0.250840
H	5.109091	3.896373	-2.770037	H	-6.713913	1.141343	-2.249914	C	-0.152185	-4.711798	-2.235992
H	2.798291	5.680789	2.294187	H	-6.349748	0.190226	3.493596	O	-1.355223	-5.240731	-2.840773
H	5.415772	4.309318	3.695354	H	-6.063346	3.440246	3.777602	C	0.999259	-4.840888	-3.246122
H	3.924996	1.867401	-2.735558	H	-4.395659	0.944595	-2.592350	O	1.654324	-6.095586	-3.245669
O	6.813053	-1.340164	-0.089193	O	-2.428881	5.505346	-1.769395	C	2.286594	-5.810370	0.069052
C	5.991562	-0.152077	-0.175419	C	-3.120466	4.322650	-1.304564	C	2.757111	-5.549456	1.500355
C	6.386356	0.751710	1.003098	C	-3.864819	4.712270	-0.017519	O	1.646160	-5.684589	2.385545
C	6.158903	0.013884	2.325075	C	-2.868512	5.223274	1.025333	C	3.400143	-4.175750	1.628392
C	6.880830	-1.327595	2.327861	C	-2.020975	6.352959	0.455567	O	3.885112	-4.080763	2.953309
C	6.547245	-2.122385	1.058665	C	-1.411784	5.946135	-0.892863	C	4.501168	-4.012173	0.582862
H	4.937830	-0.429388	-0.062329	H	-2.388476	3.544611	-1.061458	O	4.893674	-2.639051	0.625788
H	7.444973	1.033804	0.914604	H	-4.603036	5.495958	-0.238908	C	3.990195	-4.359439	-0.826617
H	5.077744	-0.177161	2.410631	H	-2.200241	4.384406	1.276004	O	3.376963	-5.669678	-0.832158
H	7.963646	-1.133668	2.318835	H	-2.677961	7.215925	0.272386	C	5.090987	-4.356537	-1.874928
H	7.197396	-3.000595	0.976678	H	-0.954601	6.814101	-1.381015	O	6.171563	-5.161229	-1.418544
C	6.165705	0.438759	-1.586289	C	-3.985801	3.800473	-2.465158	C	6.270727	-2.313169	0.642843
O	6.630882	0.750642	3.438492	O	-3.511585	5.719595	2.185227	C	6.585189	-1.547941	1.934991
O	6.531921	-2.110580	3.464378	O	-0.968813	6.717423	1.342483	O	6.182889	-2.325586	3.062001
O	5.198226	-2.508223	1.116277	O	-0.452193	4.944234	-0.667641	C	5.892894	-0.191364	1.941116
H	6.462971	1.487513	-1.531450	H	-5.018076	3.657060	-2.141457	O	6.328092	0.479982	3.110721
O	4.960410	0.412987	-2.342108	O	-3.548007	2.536062	-2.948057	C	6.222060	0.571628	0.661051
H	6.964383	-0.120929	-2.090908	H	-3.974913	4.556614	-3.261414	O	5.440031	1.773047	0.680097
H	6.235910	1.641646	3.399290	H	-4.129131	5.034780	2.503371	C	5.886030	-0.274735	-0.572018
H	6.590292	-1.514745	4.226201	H	-1.374452	6.797896	2.218736	O	6.612669	-1.523587	-0.475469
H	4.673761	-0.519386	-2.465727	H	-2.630327	2.625263	-3.289734	C	6.256608	0.392526	-1.908741
O	3.732031	-5.222632	-0.894242	O	2.210349	4.211159	-3.094251	O	7.368138	1.269163	-1.832556
C	4.095004	-3.845087	-0.640283	C	0.901849	4.004341	-2.518396	C	6.106510	3.006067	0.664974
C	4.838908	-3.825618	0.704442	C	0.792801	5.011945	-1.365802	C	5.489754	3.927548	1.719910
C	3.921813	-4.355322	1.809328	C	1.856605	4.704509	-0.301630	O	5.582245	3.308302	2.998839
C	3.384455	-5.733601	1.445092	C	3.255716	4.665961	-0.920422	C	4.040486	4.244426	1.371754
C	2.794187	-5.738713	0.028652	C	3.254144	3.829860	-2.220193	O	3.586182	5.173354	2.336283
H	3.186089	-3.240138	-0.548454	H	0.840374	2.989616	-2.109912	C	3.911789	4.771649	-0.061612

H	5.735541	-4.457669	0.635656	H	0.947237	6.027043	-1.757508	O	2.511018	4.782326	-0.348341
H	3.070553	-3.660909	1.891162	H	1.620547	3.705836	0.099378	C	4.649945	3.847321	-1.045973
H	4.230778	-6.436499	1.447273	H	3.509754	5.699118	-1.201253	O	6.004380	3.636637	-0.603482
H	2.599860	-6.767630	-0.293988	H	4.181659	4.012712	-2.773870	C	4.742392	4.388069	-2.459866
C	4.871842	-3.332944	-1.866899	C	-0.138152	4.099741	-3.650476	O	5.248191	3.334409	-3.275390
O	4.592463	-4.480985	3.049797	O	1.836801	5.676713	0.731072	C	1.901279	5.940835	-0.876182
O	2.384386	-6.169213	2.359482	O	4.264138	4.147254	-0.069130	C	0.760363	6.374359	0.054356
O	1.604154	-4.991057	0.028739	O	3.143804	2.471605	-1.877809	O	1.269003	6.576359	1.371778
H	5.841204	-2.928693	-1.570726	H	-0.859651	4.895652	-3.460083	C	-0.364188	5.345712	0.051880
O	4.197368	-2.276199	-2.539355	O	-0.901491	2.905160	-3.785810	O	-1.405711	5.872251	0.855502
H	5.042984	-4.185824	-2.537041	H	0.398955	4.333889	-4.578939	C	-0.798788	5.074717	-1.385448
H	5.039211	-3.634838	3.239077	H	0.904230	5.843875	0.966718	O	-1.783633	4.037924	-1.354506
H	2.737359	-5.996451	3.245029	H	3.971707	4.063995	0.878933	C	0.403699	4.653050	-2.237365
H	3.330035	-2.603460	-2.866572	H	-0.301489	2.162170	-4.017673	O	1.397814	5.703648	-2.173428
O	-0.986211	-5.318614	-2.571256	O	4.099903	-0.450315	-3.877040	C	0.050084	4.403047	-3.712706
C	0.179091	-4.704267	-1.972790	C	3.169044	0.512698	-3.332629	O	-0.979236	5.230010	-4.222896
C	0.485787	-5.503283	-0.695275	C	3.991014	1.532919	-2.536985	C	-3.067888	4.329094	-1.855091
C	-0.707427	-5.407670	0.258602	C	4.796455	0.843039	-1.432772	C	-4.126553	3.880781	-0.830416
C	-1.971828	-5.901351	-0.436201	C	5.623924	-0.308657	-1.994142	O	-3.808439	4.492751	0.409088
C	-2.154206	-5.183345	-1.781311	C	4.746761	-1.212840	-2.874196	C	-4.207259	2.358548	-0.763930
H	-0.058569	-3.672490	-1.691920	H	2.480328	0.006605	-2.648227	O	-5.338733	2.012897	0.015342
H	0.662500	-6.555112	-0.960912	H	4.679130	2.053554	-3.217696	C	-4.298971	1.753974	-2.168251
H	-0.848781	-4.347603	0.516381	H	4.076540	0.424296	-0.712765	O	-4.222798	0.334793	-1.983304
H	-1.849968	-6.974400	-0.646830	H	6.412732	0.114318	-2.633795	C	-3.162964	2.257152	-3.062948
H	-2.958668	-5.651225	-2.359568	H	5.364339	-1.944532	-3.407023	O	-3.268078	3.704839	-3.115040
C	1.282999	-4.644080	-3.044520	C	2.334338	1.083968	-4.493062	C	-3.186072	1.706733	-4.500132
O	-0.531621	-6.186850	0.440225	O	5.679847	1.751705	-0.794518	O	-4.478028	1.364758	-4.973178
O	-3.132602	-5.688154	0.358251	O	6.198085	-1.114226	-0.970457	H	-6.066691	0.120688	-2.888131
O	-2.441145	-3.836066	-1.524765	O	3.815972	-1.853174	-2.044186	H	-6.530875	-2.053124	-1.864585
H	2.172245	-5.188408	-2.722021	H	2.453657	2.167922	-4.556082	H	-6.195040	-1.348689	0.440044
O	1.711874	-3.311637	-3.304678	O	0.939868	0.851151	-4.326941	H	-3.794688	-1.823651	-0.551282
H	0.895433	-5.121630	-3.953940	H	2.703810	0.641177	-5.427475	H	-4.489845	-4.027853	0.067474
H	0.357059	-6.001946	1.788474	H	5.165530	2.546668	-0.529196	H	-4.650575	-3.833249	-2.664922
H	-2.895160	-5.948831	1.260393	H	6.559884	-0.518667	-0.297179	H	-2.802867	-1.405131	-2.959045
H	0.956576	-2.792655	-3.659435	H	0.776829	-0.117550	-4.316085	H	-4.030973	-3.128153	-5.138720
O	-3.925981	-1.407207	-3.850540	O	1.848170	-4.848897	-2.862562	H	-2.396784	-3.396629	-4.470330
C	-2.829531	-2.090847	-3.199654	C	2.092337	-3.423688	-2.802992	H	-2.508986	-1.905070	-6.355532
C	-3.439710	-3.177340	-2.301293	C	3.514175	-3.230287	-2.254387	H	-3.337786	-5.509378	-2.635394
C	-4.394563	-2.548954	-1.282011	C	3.633791	-3.874946	-0.871371	H	-2.228371	-6.893885	-0.963683
C	-5.437667	-1.686333	-1.980476	C	3.186047	-5.329513	-0.904979	H	-3.247761	-5.955356	0.971728
C	-4.755381	-0.705963	-2.945472	C	1.821246	-5.465304	-1.592064	H	-1.224249	-4.303737	0.289307
H	-2.286442	-1.383062	-2.564481	H	1.386177	-2.963588	-2.103256	H	-0.179051	-5.901240	1.654270
H	-3.985467	-3.905657	-2.917457	H	4.244381	-3.681322	-2.941058	H	0.281740	-6.520643	-1.179392
H	-3.792653	-1.902113	-3.625573	H	2.965269	-3.321609	-0.195152	H	-0.309229	-3.646745	-2.022228
H	-6.088368	-2.343245	-2.576136	H	3.912323	-5.898026	-1.504709	H	1.706633	-4.021613	-3.059727
H	-5.499746	-0.187416	-3.560317	H	1.593317	-6.520730	-1.779000	H	0.577384	-4.688353	-4.245049
C	-1.857995	-2.571417	-4.291636	C	1.810202	-2.837303	-4.197387	H	2.346831	-6.065581	-2.564157
O	-5.088199	-3.525693	-0.528652	O	4.964067	-3.858343	-0.385986	H	1.958524	-6.849195	-0.037572
O	-6.215979	-0.941044	-1.049475	O	3.097774	-5.880054	0.406167	H	3.516678	-6.307200	1.739037
O	-4.013886	0.209787	-2.181690	O	0.839553	-4.891085	-0.763099	H	1.944402	-5.339787	3.241038

H	-1.671001	-3.642779	-4.195987	H	2.656602	-2.239657	-4.540481	H	2.633495	-3.409478	1.432775
O	-0.583775	-1.941876	-4.204211	O	0.685488	-1.964616	-4.207335	H	4.532131	-3.348911	3.000717
H	-2.326431	-2.388108	-5.267708	H	1.671497	-3.673467	-4.895690	H	5.343807	-4.664520	0.834034
H	-4.426314	-4.088150	-0.084850	H	5.273386	-2.932998	-0.391687	H	3.240135	-3.611433	-1.114822
H	-6.403963	-1.530786	-0.302361	H	3.883990	-5.565381	0.877891	H	5.406194	-3.316105	-2.027100
H	-0.695450	-0.972501	-4.318882	H	-0.114087	-2.470541	-3.942033	H	4.672026	-4.738556	-2.818084
O	-2.896506	3.507767	-3.337384	O	-2.742308	-5.705579	-1.023047	H	6.898136	-5.067182	-2.046709
C	-2.740067	2.084480	-3.140231	C	-1.564564	-4.922887	-1.332016	H	6.875984	-3.221046	0.562568
C	-4.047864	1.598270	-2.506610	C	-0.394001	-5.581943	-0.585495	H	7.671481	-1.382275	1.968099
C	-4.278825	2.293890	-1.159256	C	-0.666476	-5.551545	0.920349	H	6.238538	-1.722008	3.819634
C	-4.189132	3.812865	-1.277985	C	-2.001947	-6.220809	1.226090	H	4.804776	-0.357333	1.966462
C	-2.960408	4.221914	-2.119785	C	-3.115749	-5.644246	0.339717	H	5.921535	1.367468	3.130783
H	-1.919088	1.902634	-2.438205	H	-1.696047	-3.903771	-0.951970	H	7.288472	0.817624	0.629053
H	-4.887320	1.811152	-3.183237	H	-0.292945	-6.624404	-0.919667	H	4.812033	-0.501226	-0.577324
H	-3.471095	1.951418	-0.492209	H	-0.732835	-4.495968	1.226633	H	5.380307	0.919405	-2.299697
H	-5.083089	4.152398	-1.822182	H	-1.908958	-7.289343	0.981289	H	6.497446	-0.415659	-2.610276
H	-3.042819	5.277406	-2.401994	H	-4.020782	-6.255988	0.424881	H	7.007739	2.170390	-1.818520
C	-2.340035	1.448374	-4.484112	C	-1.446992	-4.831691	-2.865332	H	7.178422	2.875087	0.840824
O	-5.548038	1.949025	-0.629985	O	0.333753	-6.226548	1.664360	H	6.063062	4.865905	1.715045
O	-4.103299	4.483616	-0.030245	O	-2.376928	-6.062418	2.590024	H	4.996536	3.814754	3.581998
O	-1.799621	4.008371	-1.353318	O	-3.371800	-4.324104	0.743971	H	3.465894	3.306684	1.422333
H	-3.035560	0.654113	-4.761243	H	-0.489849	-5.227532	-3.208639	H	2.707101	5.504186	2.064183
O	-1.053915	0.839489	-4.437149	O	-1.506460	-3.490786	-3.336507	H	4.322139	5.790082	-0.110794
H	-2.382245	2.229809	-5.254462	H	-2.249781	-5.441828	-3.300192	H	4.120290	2.887688	-1.073518
H	-5.648891	0.979757	-0.714008	H	1.206604	-5.963628	1.313108	H	5.415220	5.258582	-2.464439
H	-4.405939	3.924543	0.728596	H	-1.591433	-6.278620	3.113843	H	3.745630	4.712222	-2.787414
H	-0.380181	1.528109	-4.244182	H	-2.378956	-3.107055	-3.096786	H	5.456935	3.691636	-4.147082
O	1.426731	5.687421	-1.887501	O	-6.413109	-2.411891	-0.061716	H	2.635877	6.746916	-0.981995
C	0.492293	4.590023	-2.017562	C	-5.044278	-2.830887	-0.274597	H	0.359208	7.320880	-0.334890
C	-0.807386	5.028913	-1.327409	C	-4.726306	-3.879469	0.802783	H	0.487600	6.680126	1.936552
C	-0.537047	5.324297	0.149681	C	-4.899446	-3.264297	2.193923	H	0.020019	4.404708	0.475579
C	0.574716	6.360214	0.278181	C	-6.293005	-2.664834	2.341430	H	-2.218172	5.336769	0.708730
C	1.800276	5.947401	-0.548485	C	-6.608216	-1.733397	1.163815	H	-1.222646	5.984822	-1.824694
H	0.889611	3.711500	-1.497757	H	-4.376322	-1.973464	-0.137904	H	0.843493	3.735846	-1.825037
H	-1.185662	5.936758	-1.818705	H	-5.409191	-4.733530	0.692147	H	-0.202796	3.340943	-3.825911
H	-0.194805	4.387912	0.617470	H	-4.161084	-2.453232	2.291456	H	0.955033	4.588914	-4.301355
H	0.203300	7.309041	-0.136390	H	-7.022413	-3.487923	2.313548	H	-1.819286	4.761183	-4.083224
H	2.520715	6.771586	-0.597490	H	-7.665350	-1.445390	1.177525	H	-3.169799	5.402549	-2.044251
C	0.381995	4.234243	-3.511792	C	-4.918584	-3.288702	-1.739285	H	-5.100948	4.244971	-1.188489
O	-1.680416	5.831463	0.816822	O	-4.741011	-4.218986	3.227587	H	-4.066457	3.947757	1.195101
O	0.978778	6.543864	1.631500	O	-6.427430	-1.932747	3.554851	H	-3.281205	1.976717	-0.304575
H	-0.647985	4.334402	-3.859763	H	-4.568636	-4.321222	-1.794318	H	-5.488691	1.049402	-0.070226
O	0.757376	2.888265	-3.779755	O	-3.976264	-2.514734	-2.472313	H	-5.252596	2.024071	-2.633705
H	1.006962	4.941136	-4.073621	H	-5.916402	-3.237493	-2.194767	H	-2.198526	2.003852	-2.605334
H	-2.460608	5.305185	0.534884	H	-3.881726	-4.662730	3.100309	H	-2.518563	0.840875	-4.556935
H	0.163149	6.647302	2.143314	H	-6.046908	-2.493196	4.247602	H	-2.771612	2.487112	-5.150868
H	1.696396	2.763194	-3.519851	H	-4.270961	-1.577346	-2.490188	H	-4.544419	0.398482	-4.902169
C	-7.955434	-1.795030	3.433823	C	8.104244	-0.960702	3.588161	C	-6.862389	-1.937889	4.414869
C	-8.033530	-0.919695	2.351222	C	8.092069	-0.075269	2.511409	C	-7.191857	-1.052614	3.389175
C	-6.984135	-0.035400	2.107209	C	6.926100	0.629383	2.214608	C	-6.255635	-0.108022	2.972394

C	-5.844030	0.000664	2.926494	C	5.758151	0.473857	2.979634	C	-4.983062	-0.019668	3.560216
C	-5.761243	-0.894344	4.008537	C	5.765529	-0.437619	4.051970	C	-4.648559	-0.923393	4.585260
C	-6.822144	-1.778936	4.243273	C	6.943641	-1.140142	4.337366	C	-5.597902	-1.869480	4.994483
C	-4.502715	-0.991206	4.850311	C	4.497474	-0.754398	4.824391	C	-3.251717	-0.959372	5.177872
C	-3.324623	-1.338370	3.971941	C	3.441992	-1.282733	3.881710	C	-2.236722	-1.222594	4.091491
C	-2.730705	-2.599839	3.982359	C	3.047770	-2.620443	3.867429	C	-1.566397	-2.438976	3.970596
C	-1.647778	-2.897311	3.150579	C	2.081669	-3.080501	2.968141	C	-0.641306	-2.656088	2.945670
C	-1.156772	-1.912327	2.296068	C	1.510710	-2.184786	2.065880	C	-0.393607	-1.640294	2.024938
C	-1.751286	-0.648567	2.259765	C	1.899350	-0.843248	2.061238	C	-1.064454	-0.419078	2.125179
C	-2.842887	-0.349124	3.087663	C	2.865223	-0.378464	2.964469	C	-1.991254	-0.196852	3.153541
C	-4.819593	1.083574	2.586178	C	4.592006	1.387866	2.605561	C	-4.101109	1.123191	3.056192
N	-3.450426	0.938856	3.140053	N	3.239722	0.992153	3.062719	N	-2.649396	1.051287	3.352078
C	-5.387365	2.446335	3.034068	C	4.886630	2.808499	3.135817	C	-4.653782	2.447581	3.623159
C	-2.604129	2.049308	2.699237	C	2.245116	1.953012	2.585605	C	-1.953974	2.217298	2.804078
C	-3.181056	3.389787	3.139898	C	2.544536	3.350067	3.118101	C	-2.517851	3.511995	3.377112
N	-4.537564	3.562997	2.604338	N	3.880130	3.781254	2.687723	N	-3.951348	3.613156	3.075116
C	-5.108388	4.849766	3.011199	C	4.187616	5.133681	3.164980	C	-4.518371	4.864144	3.583893
H	-8.762440	-2.492027	3.639527	H	9.002937	-1.518670	3.833953	H	-7.577654	-2.681792	4.752980
H	-8.903551	-0.920679	1.701117	H	8.981597	0.067830	1.904787	H	-8.169192	-1.092441	2.917140
H	-7.047726	0.650048	1.266370	H	6.909582	1.311401	1.367746	H	-6.514971	0.584807	2.176089
H	-6.746646	-2.473791	5.075877	H	6.940832	-1.849081	5.161469	H	-5.329125	-2.570259	5.780896
H	-4.636289	-1.750527	5.626158	H	4.715820	-1.490265	5.603567	H	-3.198235	-1.736742	5.945443
H	-4.304253	-0.033407	5.346491	H	4.114780	0.150167	5.312764	H	-3.018979	0.000965	5.653852
H	-3.114310	-3.356006	4.662996	H	3.495005	-3.308562	4.580640	H	-1.761433	-3.222292	4.698962
H	-1.199603	-3.886626	3.164305	H	1.769606	-4.120565	2.973699	H	-0.113607	-3.601461	2.868749
H	-0.310015	-2.122890	1.648817	H	0.768648	-2.528854	1.351655	H	0.320275	-1.797066	1.221119
H	-1.362132	0.099239	1.577823	H	1.448310	-0.163212	1.346993	H	-0.863774	0.357951	1.395798
H	-4.756040	1.121407	1.488110	H	4.588999	1.457635	1.505235	H	-4.240895	1.174045	1.965528
H	-5.507009	2.436935	4.132703	H	4.939586	2.770872	4.238423	H	-4.580753	2.420964	4.725640
H	-6.376533	2.579569	2.589308	H	5.863821	3.130412	2.765206	H	-5.710761	2.529940	3.358652
H	-2.478998	2.071201	1.602036	H	2.211108	1.993685	1.482316	H	-2.024900	2.271469	1.703396
H	-1.612579	1.922951	3.142626	H	1.260226	1.636511	2.939222	H	-0.894942	2.138396	3.065088
H	-2.549581	4.199693	2.758870	H	1.815199	4.063421	2.724151	H	-2.001867	4.363333	2.920971
H	-3.185328	3.442666	4.243418	H	2.469969	3.343929	4.219957	H	-2.342157	3.541537	4.467383
H	-5.198178	4.941959	4.107005	H	4.175033	5.201854	4.265693	H	-4.428748	4.952308	4.680074
H	-6.102927	4.964788	2.571176	H	5.180601	5.425593	2.811177	H	-5.577749	4.920848	3.318142
H	-4.474818	5.661721	2.643977	H	3.454276	5.828110	2.749237	H	-4.003148	5.711415	3.123100
M1				M1				M1			
E	-5082.90247642			E	-5082.89931164			E	-5082.86441528		
O	5.437453	1.260871	-2.364448	O	1.159170	5.954449	-1.426599	C	0.674040	5.866203	-0.532406
C	4.280781	2.009516	-1.925511	C	-0.008764	5.148518	-1.142672	C	0.074692	5.891874	0.879186
C	4.750268	2.952103	-0.806256	C	-0.700389	5.781105	0.074681	O	1.083132	5.533546	1.815587
C	5.349641	2.134459	0.339766	C	0.258236	5.774886	1.268465	C	-1.126501	4.953874	0.959597
C	6.456128	1.219156	-0.172014	C	1.568217	6.465791	0.903450	O	-1.672768	5.083526	2.257092
C	5.950455	0.397186	-1.365665	C	2.138553	5.905403	-0.406829	C	-2.140694	5.250783	-0.154161
H	3.540247	1.319434	-1.507554	H	0.305787	4.133731	-0.876619	O	-3.102620	4.190772	-0.102741
H	5.504186	3.647473	-1.201262	H	-0.982625	6.816243	-0.164047	C	-1.414538	5.265505	-1.510261
H	4.549065	1.504721	0.752953	H	0.475169	4.723042	1.512987	O	-0.336187	6.210183	-1.464719
H	7.286520	1.845821	-0.530675	H	1.351533	7.531309	0.735359	C	-2.261139	5.644826	-2.708826
H	6.777116	-0.145872	-1.837207	H	2.964068	6.533058	-0.760838	O	-1.476553	5.345978	-3.867041

C	3.647713	2.669861	-3.162424	C	-0.838513	5.052038	-2.435534	C	-4.486024	4.486158	-0.140849
O	3.665790	3.680426	-0.227943	O	-1.848105	5.045310	0.495650	C	-5.149889	3.991153	1.149484
O	5.907314	2.957945	1.352155	O	-0.275794	6.454326	2.390054	O	-4.500533	4.577395	2.275855
O	6.914877	0.326530	0.836210	O	2.546619	6.320740	1.926912	C	-5.114764	2.471275	1.238213
O	4.967685	-0.491067	-0.904907	O	2.579604	6.529602	-0.176823	O	-5.856259	2.125617	2.393557
H	3.563855	3.749425	-3.025454	H	-1.850660	5.427987	-2.276770	C	-5.680094	1.857008	-0.039663
O	2.325077	2.201545	-3.409126	O	-0.983311	3.709574	-2.887160	O	-5.446587	0.445630	0.033379
H	4.302674	2.479381	-4.022484	H	-0.352476	5.676644	-3.196402	C	-4.984557	2.434927	-1.278098
H	5.227306	3.603749	1.620980	H	-1.158011	6.082347	2.576038	O	-5.103176	3.877958	-1.254513
H	6.987646	0.852137	1.646382	H	2.095776	6.528063	2.758989	C	-5.566138	1.917147	-2.609125
H	2.353758	1.239145	-3.611166	H	-0.096341	3.350065	-3.112964	O	-6.923166	1.512739	-2.552753
O	3.797826	-3.488885	-2.691653	O	4.868655	2.673760	-2.327264	C	-6.541713	-0.433320	-0.011423
C	3.766320	-2.084005	-2.345546	C	3.569864	3.122300	-1.878005	C	-6.456587	-1.411683	1.159988
C	4.946160	-1.830637	-1.393379	C	3.805040	4.159744	-0.769708	O	-6.477052	-0.683211	2.385226
C	4.796663	-2.705386	-0.146091	C	4.601255	3.525508	0.373170	C	-5.198994	-2.263353	1.055188
C	4.626629	-4.170777	-0.524272	C	5.877086	2.865933	-0.138592	O	-5.244613	-3.178954	2.133594
C	3.543593	-4.346676	-1.596749	C	5.578675	1.952491	-1.337083	C	-5.145162	-2.952626	-0.305953
H	2.836010	-1.861397	-1.811653	H	3.026485	2.275800	-1.446624	O	-3.838923	-3.526918	-0.420661
H	5.891682	-2.065304	-1.902369	H	4.356402	5.019599	-1.175083	C	-5.366470	-1.954176	-1.459720
H	3.889465	-2.371882	0.379914	H	3.966575	2.743275	0.812940	O	-6.554498	-1.160240	-1.233703
H	5.574246	-4.519195	-0.961604	H	6.550250	3.659427	-0.496944	C	-5.508458	-2.640713	-2.808669
H	3.580033	-5.362713	-2.005386	H	6.512374	1.634037	-1.813337	O	-6.493858	-3.662182	-2.713696
C	3.754084	-1.277992	-3.656698	C	2.773969	3.594218	-3.107317	C	-3.707309	-4.866959	-0.862893
O	5.925610	-2.624792	0.705352	O	4.974857	4.472294	1.359127	C	-3.091323	-5.711566	0.261579
O	4.289381	-4.966689	0.607782	O	6.513707	2.098090	0.874518	O	-3.891694	-5.612633	1.438644
O	2.285345	-4.094317	-1.023161	O	4.848306	0.838351	-0.890889	C	-1.667254	-5.254947	0.543144
H	4.551265	-0.532745	-3.658302	H	2.421321	4.617947	-2.970457	O	-1.142027	-6.122548	1.538328
O	2.543585	-0.552590	-3.846453	O	1.611260	2.803180	-3.331625	C	-0.851063	-5.261637	-0.746992
H	3.931959	-1.976342	-4.485156	H	3.443900	3.571445	-3.976659	O	0.438866	-4.708338	-0.459653
H	6.068041	-1.685192	0.923320	H	4.166156	4.931484	1.652915	C	-1.546375	-4.429504	-1.830313
H	4.898864	-4.694759	1.310142	H	6.517247	2.651717	1.669282	O	-2.890667	-4.934552	-2.009659
H	1.789666	-1.180632	-3.901664	H	1.884449	1.882463	-3.547969	C	-4.472839	-4.472839	-3.190497
O	-0.882624	-5.268226	-2.494928	O	4.503139	-2.323568	-2.756760	O	-0.319604	-5.746238	-3.521540
C	0.165019	-4.293523	-2.276841	C	4.097901	-0.987304	-2.376370	C	1.493871	-5.627707	-0.316980
C	1.202127	-4.960817	-1.359896	C	5.166252	-0.456962	-1.405906	C	2.367012	-5.241560	0.881084
C	0.542189	-5.333850	-0.029985	C	5.235117	-1.370606	-0.179715	O	1.545784	-5.133314	2.041664
C	-0.680161	-6.212530	-0.273573	C	5.456130	-2.822015	-0.589652	C	3.136234	-3.948659	0.628833
C	-1.607579	-5.582279	-1.321905	C	4.471463	-3.249619	-1.687500	O	4.037430	-3.813471	1.706730
H	-0.251030	-3.423014	-1.759103	H	3.141603	-1.037902	-1.844845	C	3.843085	-3.952316	-0.735279
H	1.585546	-5.868750	-1.846653	H	6.143410	-0.432253	-1.907817	O	4.252814	-2.601480	-0.965425
H	0.211041	-4.400106	0.450945	H	4.266239	-1.300074	0.337019	C	2.866219	-4.403266	-1.832208
H	-0.329149	-7.171938	-0.682082	H	6.468031	-2.901105	-1.014569	O	2.299850	-5.673431	-1.479072
H	-2.373974	-6.301383	-1.631950	H	4.781301	-4.207189	-2.120917	C	3.477120	-4.576647	-3.208189
C	0.658460	-3.817196	-3.654483	C	3.868547	-0.181785	-3.667627	O	2.390036	-4.743574	-4.123729
O	1.415105	-6.055943	0.820337	O	6.297599	-1.025552	0.689572	C	5.585664	-2.301618	-1.320560
O	-1.422656	-6.432274	0.920570	O	5.324134	-3.701520	0.522516	C	6.196136	-1.376095	-0.263100
O	-2.200573	-4.438275	-0.764276	O	3.184283	-3.355522	-1.134065	O	6.165531	-2.019436	1.009746
H	1.731038	-3.984749	-3.764353	H	4.457502	0.736888	-3.661087	C	5.442211	-0.053940	-0.216230
O	0.459098	-2.420258	-3.849750	O	2.513639	0.225676	-3.826322	O	6.105602	0.761138	0.735080
H	0.135596	-4.402449	-4.422049	H	4.198718	-0.798369	-4.513958	C	5.380131	0.574710	-1.604663

H	2.258488	-5.569189	0.874053	H	6.184087	-0.094351	0.951273	O	4.452566	1.660077	-1.514900
H	-0.772907	-6.639945	1.608606	H	5.766900	-3.260198	1.263833	C	4.881662	-0.439303	-2.651895
H	-0.504311	-2.225938	-3.831400	H	1.933448	-0.566167	-3.883960	O	5.636759	-1.666629	-2.579833
O	-5.214414	-2.722928	-1.995752	O	0.379286	-5.215647	-2.628827	C	4.981135	0.092638	-4.072361
C	-3.788788	-2.954404	-1.904205	C	1.168588	-4.029477	-2.377358	O	6.297729	0.584041	-4.302021
C	-3.583001	-4.188106	-1.011545	C	2.364264	-4.461156	-1.514408	C	4.797236	2.916789	-2.065604
C	-4.207013	-3.952715	0.366229	C	1.858731	-5.071012	-0.204548	C	4.877574	3.952900	-0.936848
C	-5.667486	-3.540617	0.234444	C	0.875337	-6.203548	-0.477050	O	5.813523	3.528063	0.054184
C	-5.810008	-2.381248	-0.759772	C	-0.213104	-5.752815	-1.461418	C	3.505314	4.165309	-0.312708
H	-3.310844	-2.094924	-1.423898	H	0.571838	-3.309489	-1.807539	O	3.657188	5.180712	0.666967
H	-4.049861	-5.065598	-1.480737	H	2.961808	-5.204320	-2.061034	C	2.492027	4.521712	-1.397896
H	-3.658869	-3.122028	0.836632	H	1.324995	-4.279396	0.343317	O	1.194708	4.589101	-0.796762
H	-6.230624	-4.393734	-0.171985	H	1.427274	-7.027103	-0.954236	C	2.491608	3.453394	-2.496685
H	-6.866882	-2.195505	-0.980990	H	-0.801231	-6.613892	-1.797973	O	3.836558	3.324354	-3.015370
C	-3.234854	-3.049916	-3.337517	C	1.497664	-3.386625	-3.736100	C	1.554244	3.774144	-3.669385
O	-4.165117	-5.109595	1.180316	O	2.910355	-5.603929	0.582025	O	1.511084	5.147003	-4.010824
O	-6.215826	-3.142896	1.486648	O	0.252153	-6.659160	0.718567	H	1.447103	6.632855	-0.636784
O	-5.214944	-1.238218	-0.197912	O	-1.035717	-4.811249	-0.822651	H	-0.272491	6.917193	1.074186
H	-2.692446	-3.986474	-3.479824	H	2.575908	-3.266895	-3.856505	H	0.652267	5.198794	2.616770
O	-2.307390	-2.012405	-3.637210	O	0.942434	-2.082636	-3.870745	H	-0.760228	3.930398	0.789371
H	-4.086416	-3.034819	-4.030704	H	1.133835	-4.057376	-4.525445	H	4.725558	2.257659	2.257659
H	-3.238192	-5.410460	1.231557	H	3.596493	-4.916643	0.676261	H	-2.626650	6.217640	0.036013
H	-5.940913	-3.819622	2.123542	H	0.956552	-6.725460	1.380387	H	-1.017255	4.258385	-1.686805
H	-2.753952	-1.141845	-3.549760	H	-0.037520	-2.139691	-3.834435	H	-2.504696	6.715455	-2.657582
O	-5.835368	2.224979	-1.276270	O	-4.418609	-3.852451	-1.920140	H	-3.192939	5.064819	-2.701183
C	-5.127706	0.963525	-1.290519	C	-2.978117	-3.721202	-1.868979	H	-1.903421	5.729580	-4.642732
C	-5.872548	0.021177	-0.332999	C	-2.447920	-4.884267	-1.016052	H	-4.641223	5.563911	-0.262010
C	-5.896243	0.621744	1.074776	C	-3.055038	-4.814465	0.387373	H	-6.201670	4.309661	1.120878
C	-6.471116	2.033393	1.048980	C	-4.576613	-4.764638	0.314081	H	-4.846283	4.098106	3.045663
C	-5.776897	2.882739	-0.024019	C	-5.043868	-3.678345	-0.664253	H	-4.067508	2.146189	1.333395
H	-4.112229	1.115942	-0.909565	H	-2.717672	-2.781997	-1.371475	H	-5.906354	1.151116	2.455720
H	-6.902299	-0.125926	-0.687740	H	-2.716787	-5.840474	-1.486639	H	-6.753833	2.061141	-0.111203
H	-4.853495	0.682640	1.424489	H	-2.699423	-3.882574	0.853891	H	-3.919873	2.180789	-1.243422
H	-7.534094	1.963400	0.774226	H	-4.928972	-5.730076	-0.078560	H	-4.929146	1.098079	-2.967139
H	-6.308497	3.830765	-0.162781	H	-6.118840	-3.775217	-0.852965	H	-5.489071	2.733244	-3.335283
C	-5.011022	0.500100	-2.753967	C	-2.461747	-3.640977	-3.316335	H	-6.932286	0.565144	-2.339920
O	-6.685758	-0.139347	1.970337	O	-2.710347	-5.937104	1.177960	H	-7.486647	0.118391	0.011885
O	-6.330894	2.682066	2.307837	O	-5.156160	-4.515295	1.590420	H	-7.332947	-2.072741	1.105337
O	-4.451227	3.111541	0.377118	O	-4.752568	-2.418617	-0.113016	H	-6.197014	-1.313152	3.067358
H	-5.431400	-0.499449	-2.877818	H	-1.697712	-4.398984	-3.497067	H	-4.323860	-1.600419	1.138525
O	-3.659290	0.412752	-3.193183	O	-1.847290	-2.389831	-3.610564	H	-4.636521	-3.921516	1.945654
H	-5.586641	1.197028	-3.376989	H	-3.307513	-3.834486	-3.989098	H	-5.913594	-3.731110	-0.348942
H	-6.385939	-1.066582	1.925584	H	-1.738371	-6.019260	1.176954	H	-4.496035	-1.287648	-1.508069
H	-6.629971	2.043297	2.972046	H	-4.696113	-5.101607	2.209832	H	-4.527653	-3.056184	-3.076157
H	-3.256936	1.310128	-3.180150	H	-2.512186	-1.673545	-3.507946	H	-5.783284	-1.882871	-3.557664
O	-2.302830	5.769739	-0.995658	O	-6.312388	0.762693	-1.118833	H	-6.505400	-4.143561	-3.550060
C	-2.830140	4.422398	-0.945403	C	-5.301279	-0.270739	-1.179572	H	-4.681996	-5.261112	-1.166130
C	-3.882331	4.404464	0.174668	C	-5.729008	-1.381130	-0.207236	H	-3.066476	-6.755583	-0.081999
C	-3.218684	4.768827	1.505182	C	-5.857633	-0.813816	-1.208668	H	-3.345141	-5.996234	2.143426
C	-2.495550	6.106266	1.392946	C	-6.783726	0.396935	1.223180	H	-1.707354	-4.222754	0.918085

C	-1.578362	6.134832	0.162735	C	-6.372498	1.404664	0.141753	H	-0.303186	-5.743594	1.863284
H	-2.026856	3.725237	-0.682793	H	-1.522125	0.815681	-1.145869	H	-0.745794	-6.282221	-1.129850
H	-4.673475	5.132283	-0.054652	H	-6.694983	-1.798044	-0.525182	H	-1.607818	-3.381249	-1.510084
H	-2.475043	3.987461	1.727479	H	-4.855429	-0.482020	1.522409	H	-0.046463	-3.715822	-3.188985
H	-3.255808	6.888709	1.250230	H	-7.800498	0.053151	0.982164	H	-1.579407	-4.172030	-3.944185
H	-1.224235	7.155469	-0.020992	H	-7.131638	2.188160	0.039893	H	0.648593	-5.663867	-3.532433
C	-3.319636	4.060469	-2.358910	C	-5.122633	-0.681082	-2.652812	H	1.104855	-6.642027	-0.189727
O	-4.158157	4.888122	2.558399	O	-6.384681	-1.759556	2.121087	H	3.102177	-6.048060	1.016413
O	-1.716866	6.385953	2.550951	O	-6.773782	1.050646	2.487667	H	2.067812	-4.684259	2.726759
O	-0.495606	5.269853	0.387332	O	-5.132333	1.958229	0.500262	H	2.415351	-3.116324	0.603546
H	-4.366017	3.751599	-2.340170	H	-5.288571	-1.752269	-2.780866	H	4.624363	-3.051223	1.537597
O	-2.599375	2.969680	-2.924065	O	-3.805361	-0.430565	-3.132581	H	4.714610	-4.620018	-0.694262
H	-3.235040	4.957648	-2.985959	H	-5.871002	-0.141341	-3.247940	H	2.071743	-3.650323	-1.904870
H	-4.701747	4.078740	2.570244	H	-5.850421	-2.573417	2.055865	H	4.131986	-5.459376	-3.204000
H	-2.288747	6.197579	3.309908	H	-6.863520	0.349648	3.150477	H	4.073530	-3.690203	-3.459206
H	-1.653457	3.221924	-3.019957	H	-3.627546	0.535363	-3.094506	H	2.739960	-5.021974	-4.978823
O	2.672184	5.370528	-1.489202	O	-3.747813	5.089053	-0.856343	H	6.175642	-3.219619	-1.419745
C	1.328373	4.898962	-1.230754	C	-3.922327	3.652775	-0.818069	H	7.237302	-1.179430	-0.554914
C	0.807316	5.685599	-0.017744	C	-4.915912	3.356535	0.316111	H	6.402748	-1.333007	1.652214
C	1.712047	5.427679	1.189745	C	-4.341457	3.861399	1.642383	H	4.409374	-0.259410	0.101595
C	3.162253	5.751287	0.849974	C	-3.979011	5.338954	1.539433	H	5.863649	1.696048	0.572745
C	3.586790	5.063745	-0.454803	C	-3.118311	5.611072	0.298122	H	6.373239	0.936108	-1.890866
H	1.360268	3.835950	-0.969118	H	-2.965080	3.178017	-0.577089	H	3.825661	-0.655483	-2.445450
H	0.805206	6.759419	-0.252629	H	-5.869758	3.862242	0.109717	H	4.234647	0.890400	-4.182967
H	1.641605	4.354950	1.429895	H	-3.421375	3.289928	1.841783	H	4.729093	-0.723346	-4.765381
H	3.236544	6.836621	0.686112	H	-4.913594	5.906658	1.417137	H	6.304557	1.021891	-5.161944
H	4.553455	5.454612	-0.791592	H	-3.035874	6.689950	0.124988	H	5.743827	2.845754	-2.610303
C	0.526365	5.036317	-2.537735	C	-4.333634	3.192020	-2.227753	H	5.214310	4.902328	-1.377219
O	1.355650	6.220079	2.307477	O	-5.260919	3.729926	2.711547	H	5.638985	4.106451	0.814933
O	4.050086	5.351333	1.888417	O	-3.277857	5.793173	2.691481	H	3.185539	3.223113	0.155661
H	-0.365251	5.646098	-2.382849	H	-5.273459	2.638077	-2.195313	H	2.843039	5.205941	1.207550
O	0.062564	3.784182	-3.030976	O	-3.380997	2.312411	-2.816681	H	2.742853	5.481762	-1.861410
H	1.166298	5.540101	-3.274047	H	-4.481447	4.086916	-2.846379	H	2.190586	2.487594	-2.069281
H	0.402320	6.097004	2.473140	H	-5.577893	2.807669	2.725750	H	0.553967	3.402414	-3.421046
H	3.657724	5.672069	2.714122	H	-3.770336	5.455581	3.454424	H	1.914663	3.196761	-4.531675
H	0.832390	3.210070	-3.241049	H	-2.525009	2.785462	-2.921893	H	0.624970	5.471269	-3.780676
C	4.966344	-0.637088	3.792875	C	-0.065977	-4.227559	5.217391	C	2.691403	3.683044	4.638051
C	4.375984	0.596279	3.522551	C	-0.980218	-3.177254	5.158443	C	1.299134	3.689283	4.728325
C	3.045692	0.640561	3.107804	C	-0.717815	-2.086975	4.332004	C	0.573435	2.613440	4.216866
C	2.279967	-0.523439	2.951813	C	0.442295	-2.016098	3.547253	C	1.208568	1.518653	3.613095
C	2.873755	-1.766599	3.244998	C	1.375521	-3.067234	3.626712	C	2.613830	1.506004	3.541161
C	4.210892	-1.801025	3.660271	C	1.103058	-4.157764	4.462350	C	3.333567	2.591974	4.055189
C	2.052444	-3.042139	3.236125	C	2.708906	-2.986214	2.908965	C	3.346859	0.294280	3.000834
C	0.927621	-2.923558	4.237219	C	3.472086	-1.768743	3.370695	C	3.017530	-0.924634	3.829307
C	0.917056	-3.637024	5.434616	C	4.610911	-1.854850	4.170526	C	3.941030	-1.518580	4.688391
C	-0.130834	-3.501368	6.348684	C	5.300455	-0.707952	4.572728	C	3.614715	-2.657417	5.428222
C	-1.177776	-2.629108	6.061285	C	4.834725	0.542610	4.174177	C	2.336868	-3.201136	5.315131
C	-1.176130	-1.895410	4.873271	C	3.687295	0.648271	3.384237	C	1.391334	-2.608198	4.473674
C	-0.129318	-2.031346	3.949939	C	2.993557	-0.499917	2.974894	C	1.717667	-1.467708	3.722876
C	0.873560	-0.334972	2.391462	C	0.538488	-0.822859	2.598794	C	0.297127	0.472625	2.977766

N	-0.128357	-1.383787	2.686271	N	1.880215	-0.458080	2.092026	N	0.831543	-0.892332	2.778529
C	0.948650	-0.167621	0.856573	C	-0.383011	-1.079479	1.384808	C	-0.167617	1.004656	1.606231
C	-1.431952	-0.993533	2.150619	C	1.802627	0.710062	1.212698	C	-0.204234	-1.763845	2.222650
C	-1.348536	-0.813872	0.638073	C	0.879132	0.431296	0.032941	C	-0.661647	-1.231885	0.868331
N	-0.348574	0.189052	0.293595	N	-0.452024	0.081758	0.507274	N	-1.160716	0.133352	0.988672
C	-0.276052	0.406799	-1.147428	C	-1.379869	-0.120138	-0.596025	C	-1.592276	0.657779	-0.297758
H	5.999778	-0.695855	4.122647	H	-0.251367	-5.085366	5.857273	H	3.273022	4.511202	5.032043
H	4.944330	1.516727	3.614116	H	-1.887778	-3.200793	5.754396	H	0.779462	4.515257	5.206231
H	2.586763	1.603931	2.897216	H	-1.430504	-1.266379	4.290659	H	-0.511778	2.627473	4.279888
H	4.661198	-2.761867	3.894819	H	1.833646	-4.960373	4.526280	H	4.419021	2.570652	4.002410
H	2.691454	-3.895461	3.480786	H	3.283637	-3.896665	3.098473	H	4.423488	0.481855	2.984221
H	1.630294	-3.217423	2.239524	H	2.554481	-2.907588	1.827170	H	3.031294	0.103575	1.967524
H	1.735011	-4.321246	5.646678	H	4.968616	-2.835929	4.474313	H	4.937885	-1.091065	4.765910
H	-0.127806	-4.073983	7.271212	H	6.191627	-0.794192	5.186861	H	4.351672	-3.114057	6.081534
H	-1.998545	-2.508941	6.762798	H	5.354422	1.444754	4.485184	H	2.062671	-4.079542	5.892942
H	-1.992328	-1.210719	4.669660	H	3.331637	1.630697	3.093486	H	0.392793	-3.027925	4.413380
H	0.498455	0.624990	2.790584	H	0.117163	0.048809	3.132226	H	-0.604369	0.402758	3.613098
H	1.347851	-1.108321	0.426323	H	-0.020142	-1.984884	0.857757	H	0.727734	1.138901	0.966887
H	1.659547	0.631350	0.622118	H	-1.390662	-1.298292	1.752385	H	-0.618705	1.990687	1.751192
H	-1.799601	-0.053675	2.600973	H	1.434510	1.606641	1.742994	H	-1.080224	-1.840820	2.891795
H	-2.151344	-1.783557	2.381921	H	2.806966	0.916381	0.837566	H	0.214117	-2.763526	2.086158
H	-2.324756	-0.487106	0.261911	H	0.811408	1.322534	-0.601842	H	-1.470863	-1.863192	0.483476
H	-1.126905	-1.796478	0.176929	H	1.313593	-0.379243	-0.584934	H	0.185280	-1.298308	0.156855
H	0.021049	-0.498416	-1.709003	H	-1.044824	-0.888453	-1.317015	H	-0.780566	0.675811	-1.051584
H	0.447876	1.195120	-1.374631	H	-2.350162	-0.433657	-0.202082	H	-1.960571	1.680298	-0.175333
H	-1.252792	0.729149	-1.520856	H	-4.349708	0.144693	-0.836192	H	-2.409029	0.043446	-0.690198
FA1				FA1				FA1			
E	-5082.91365921			E	-5082.91033493			E	-5082.88073010		
ZPE	-5081.342391			ZPE	-5081.339071			ZPE	-5081.314502		
H	-5081.252669			H	-5081.249309			H	-5081.221695		
G	-5081.463601			G	-5081.460270			G	-5081.442998		
S	443.943			S	444.004			S	465.771		
O	-5.298169	3.675275	-0.776232	O	-5.565184	1.849532	-2.332049	C	-1.888865	6.067414	-0.805124
C	-5.011304	2.256589	-0.806630	C	-5.017879	0.586469	-1.885044	C	-2.582452	6.142363	0.556812
C	-5.804360	1.617971	0.344618	C	-5.892097	0.104125	-0.716821	O	-1.619796	6.439014	1.563907
C	-5.371114	2.233840	1.677099	C	-5.888638	1.145297	0.405790	C	-3.302806	4.836193	0.865061
C	-5.501021	3.751056	1.633407	C	-6.298298	2.512752	-0.125943	O	-3.982803	5.035013	2.088606
C	-4.816972	4.321985	0.384441	C	-5.466384	2.874484	-1.362959	C	-4.242266	4.438048	-0.278666
H	-3.942325	2.097839	-0.626827	H	-3.999491	0.742376	-1.513253	O	-4.665216	3.100772	-0.001818
H	-6.878692	1.792269	0.190540	H	-6.921429	-0.058164	-1.066580	C	-3.499234	4.485833	-1.626035
H	-4.309977	1.980244	1.827159	H	-4.857625	1.217650	0.784413	O	-2.862550	5.768032	-1.793519
H	-6.570619	3.998327	1.562479	H	-7.351554	2.460597	-0.438864	C	-4.391892	4.293885	-2.836683
H	-5.074544	5.379990	0.261791	H	-5.861875	3.777399	-1.841832	O	-3.535621	4.125576	-3.963311
C	-5.325830	1.747387	-2.225013	C	-4.927275	-0.344864	-3.107290	C	-6.039358	2.787195	0.060249
O	-5.547668	0.221437	0.476103	O	-5.379435	-1.086816	-0.122995	C	-6.346712	2.139731	1.418161
O	-6.158511	1.776254	2.761501	O	-6.786083	0.810355	1.449600	O	-5.956410	3.013914	2.474478
O	-4.933368	4.362348	2.787346	O	-6.128989	3.530948	0.855437	C	-5.646743	0.792454	1.540005
O	-3.427430	4.165525	0.522352	O	-4.137051	3.068565	-0.955744	O	-6.058323	0.231059	2.773559
H	-6.028177	0.912801	-2.190243	H	-5.443712	-1.286761	-2.913399	C	-6.011651	-0.077634	0.341807
O	-4.172531	1.258381	-2.899407	O	-3.585474	-0.692520	-3.430484	O	-5.252618	-1.287046	0.439503

H	-5.793680	2.569974	-2.782149	H	-5.423335	0.154097	-3.950348	C	-5.694239	0.647658	-0.969985
H	-6.167922	0.801108	2.737437	H	-6.567303	-0.089607	1.755612	O	-6.407697	1.906539	-0.981390
H	-5.261730	3.855817	3.545252	H	-6.497401	3.171028	1.676205	C	-6.094681	-0.150417	-2.222232
H	-3.517080	1.985195	-2.987308	H	-3.086709	0.123131	-3.659391	O	-7.251532	-0.952574	-2.072811
O	-0.957616	6.113895	-1.391755	O	-1.587238	4.882449	-2.893454	C	-5.951221	-2.496519	0.585040
C	-1.788294	4.952804	-1.150830	C	-2.319975	3.698944	-2.496252	C	-5.286172	-3.332539	1.678981
C	-2.578293	5.243100	0.135865	C	-3.391877	4.157004	-1.495508	O	-5.290457	-2.585864	2.892728
C	-1.596157	5.427393	1.295641	C	-2.724707	4.815369	-0.286213	C	-3.871310	-3.728059	1.274775
C	-0.594381	6.529680	0.968349	C	-1.795938	5.938732	-0.728235	O	-3.374548	-4.569559	2.301764
C	0.042323	6.301262	-0.409491	C	-0.847148	5.468922	-1.841318	C	-4.412815	-4.412815	-0.091151
H	-1.150140	4.078701	-0.980859	H	-1.641937	3.003129	-1.989932	O	-2.528761	-4.542534	-0.499692
H	-3.170044	6.159332	-0.000468	H	-4.067164	4.874639	-1.982927	C	-4.656723	-3.573030	-1.130538
H	-1.053432	4.477033	1.413605	H	-2.126153	4.043965	0.221142	O	-5.970699	-3.226168	-0.635380
H	-1.145006	7.480967	0.921684	H	-2.414522	6.744814	-1.149312	C	-4.830393	-4.288490	-2.460258
H	0.600242	7.190720	-0.722366	H	-0.333687	6.328893	-2.285993	O	-5.370426	-5.584465	-2.228061
C	-2.604584	4.682104	-2.428322	C	-2.827249	3.008147	-3.775570	C	-2.090902	-5.767359	-1.059151
O	-2.237839	5.788032	2.505675	O	-3.677155	5.376467	0.604429	C	-1.049652	-6.396717	-0.125318
O	0.442062	6.611467	1.941050	O	-1.017197	6.438632	0.355680	O	-1.610652	-6.551215	1.178487
O	0.893649	5.188801	-0.324748	O	0.083054	4.568748	-1.295839	C	0.208423	-5.540469	-0.074350
H	-3.675692	4.715647	-2.221340	H	-3.905852	2.849255	-3.727303	O	1.136412	-6.235965	0.743543
O	-2.350946	3.390651	-2.969863	O	-2.251771	1.721963	-3.968627	C	0.721493	-5.288263	-1.488315
H	-2.367416	5.471796	-3.153330	H	-2.613316	3.671391	-4.624278	O	1.843631	-4.403669	-1.379112
H	-2.986343	5.177736	2.646531	H	-4.353981	4.696298	0.784781	C	-0.384423	-4.662843	-2.346707
H	0.003437	6.605578	2.804555	H	-1.639813	6.630415	1.072208	O	-1.524811	-5.556656	-2.333994
H	-1.408375	3.330938	-3.240836	H	-1.278496	1.819105	-4.070529	C	0.025438	-4.423575	-3.810708
O	3.545279	4.190854	-2.666404	O	3.275548	3.758972	-2.932336	O	0.979346	-5.348176	-4.307022
C	2.196860	4.204586	-2.144109	C	1.878866	3.525601	-2.644509	C	3.089238	-4.849576	-1.843786
C	2.151461	5.228850	-1.000322	C	1.450251	4.660212	-1.704722	C	4.162433	-4.544635	-0.799207
C	3.195033	4.892582	0.066726	C	2.256077	4.601683	-0.398647	O	3.818423	-5.166881	0.436435
C	4.575656	4.716624	-0.548804	C	3.759857	4.582775	-0.671812	C	4.330935	-3.042468	-0.613407
C	4.502277	3.740195	-1.729397	C	4.104721	3.587609	-1.801771	O	5.402613	-2.878622	0.295104
H	1.955285	3.218449	-1.733778	H	1.768616	2.568465	-2.122713	C	4.568658	-2.334748	-1.953755
H	2.340109	6.237234	-1.394186	H	1.629363	5.624803	-2.199939	O	4.429590	-0.928731	-1.740069
H	2.905482	3.931918	0.516278	H	1.979524	3.657558	0.100548	C	3.514244	-2.775456	-2.985054
H	4.914601	5.687055	-0.940057	H	4.034644	5.584536	-1.030477	O	3.450651	-4.213696	-3.060191
H	5.457512	3.710276	-2.265230	H	5.123992	3.777355	-2.156179	C	3.793878	-2.292075	-4.394553
C	1.241109	4.467763	-3.320845	C	1.135747	3.404223	-3.987767	O	2.616801	-2.531078	-5.161504
O	3.293134	5.899353	1.058653	O	1.961203	5.714086	0.426110	C	5.567735	-0.090432	-1.797167
O	5.507519	4.216654	0.404135	O	4.556298	4.278354	0.463585	C	5.688117	0.708276	-0.484710
O	4.173484	2.468039	-1.229302	O	3.998153	2.279574	-1.295258	O	5.763156	-0.214701	0.585297
H	0.573418	5.300808	-3.092221	H	0.344456	4.151183	-4.067766	C	4.525796	1.691849	-0.346676
O	0.400092	3.355768	-3.602375	O	0.498159	2.141154	-4.144311	O	4.771891	2.515512	0.785828
H	1.847465	4.741369	-4.194679	H	1.863492	3.583351	-4.790155	C	4.382303	2.530260	-1.616919
H	2.414232	6.004371	1.467718	H	0.990985	5.809560	0.459231	O	3.157323	3.259609	-1.475744
H	5.366945	4.737352	1.209562	H	4.016115	4.064435	1.264051	C	4.341790	1.652542	-2.876634
H	0.961391	2.583406	-3.835807	H	1.175607	1.429656	-4.128492	O	5.487274	0.781511	-2.902656
O	4.867557	-0.616588	-3.101095	O	5.539271	-0.773705	-2.631107	C	4.335600	2.460981	-4.164299
C	4.028202	0.497934	-2.724959	C	4.463721	0.174681	-2.441501	O	5.389097	3.419730	-4.127917
C	4.858926	1.320014	-1.731477	C	5.023205	1.344876	-1.621759	C	3.125527	4.620240	-1.862061
C	5.161939	0.479720	-0.483250	C	5.590443	0.851578	-0.288661	C	2.822497	5.483633	-0.629668

C	5.825128	-0.847933	-0.852670	C	6.597218	-0.270682	-0.515347	O	3.776145	5.198275	0.393767
C	5.081761	-1.516848	-2.031500	C	5.989218	-1.350138	-1.419674	C	1.403751	5.240435	-0.131576
H	3.134250	0.123773	-2.214177	H	3.657770	-0.298193	-1.870560	O	1.188735	6.146248	0.939876
H	5.800754	1.624746	-2.208690	H	5.820940	1.839006	-2.194176	C	0.413066	5.419360	-1.277404
H	4.192957	0.258000	-0.007288	H	4.751620	0.443495	0.296433	O	-0.883441	5.090610	-0.762297
H	6.842211	-0.614445	-1.202951	H	7.470053	0.147672	-1.037674	C	0.794296	4.503307	-2.446527
H	5.699063	-2.322192	-2.444672	H	6.746377	-2.090022	-1.702773	O	2.142992	4.839760	-2.852358
C	3.551325	1.199151	-4.010987	C	3.900337	0.538286	-3.827553	C	-0.127773	4.637017	-3.670791
O	6.009050	1.188877	0.405563	O	6.248005	1.885932	0.423829	O	-0.693575	5.927510	-3.834570
O	5.885080	-1.783229	0.210458	O	7.000134	-0.876936	0.708674	H	-1.476761	7.041010	-1.087260
O	3.859065	-2.024180	-1.561054	O	4.936596	-1.954971	-0.716511	H	-3.328028	6.948937	0.504648
H	3.853125	2.247521	-4.025704	H	3.967423	1.614745	-3.999159	H	-2.053332	6.240279	2.408228
O	2.132306	1.200784	-4.131711	O	2.523999	0.203923	-3.960985	H	-2.546989	4.041124	0.955160
H	4.021019	0.691682	-4.863789	H	4.510257	0.029005	-4.585451	H	-4.526711	4.244355	2.278908
H	5.684032	2.107741	0.461679	H	5.660388	2.672291	0.437606	H	-5.105104	5.118787	-0.293351
H	5.770189	-1.361672	1.105968	H	7.220062	-0.148590	1.308003	H	-2.737887	3.696797	-1.624651
H	1.813248	0.273327	-4.196009	H	2.420143	-0.768407	-3.865365	H	-5.033945	5.180407	-2.947460
O	1.822314	-4.691762	-3.050120	O	3.312025	-5.148525	-1.547091	H	-5.032480	3.416474	-2.676434
C	2.179431	-3.315311	-2.780362	C	3.496854	-3.717074	-1.641962	H	-4.070324	4.167016	-4.765415
C	3.470437	-3.337503	-1.951621	C	4.739155	-3.364341	-0.808927	H	-6.646229	3.688377	-0.081523
C	3.254762	-4.118233	-0.654839	C	4.548517	-3.818354	0.640715	H	-7.432077	1.970286	1.462627
C	2.701780	-5.506664	-0.949662	C	4.148906	-5.285195	0.716512	H	-5.969253	2.466872	3.275879
C	1.489591	-5.422198	-1.885700	C	2.991865	-5.589249	-0.244519	H	-4.558868	0.958576	1.526903
H	1.387646	-2.843882	-2.188355	H	2.630720	-3.208289	-1.204685	H	-5.640959	-0.646747	2.872020
H	4.269412	-3.812790	-2.538281	H	5.628331	-3.848234	-1.236973	H	-7.084000	-0.302326	0.357349
H	2.507886	-3.568163	-0.061780	H	3.729989	-3.216242	1.062200	H	-4.618297	0.858255	-1.021068
H	3.480154	-6.081735	-1.472130	H	5.008070	-5.890534	0.391272	H	-5.230637	-0.753220	-2.531827
H	1.206196	-6.421702	-2.234630	H	2.844834	-6.671928	-0.325283	H	-6.292031	0.572561	-3.020842
C	2.263929	-2.573367	-4.126620	C	3.542174	-3.347714	-3.135345	H	-6.964240	-1.815801	-1.730389
O	4.457405	-4.285864	0.075722	O	5.728287	-3.658824	1.408935	H	-7.002103	-2.312593	0.830209
O	2.313914	-6.183787	0.243942	O	3.756507	-5.655408	2.033789	H	-5.879732	-4.249736	1.801104
O	0.430929	-4.824288	-1.183324	O	1.821078	-4.972063	0.236317	H	-4.682250	-3.045321	3.491030
H	3.255598	-2.136428	-4.262788	H	4.416026	-2.730697	-3.351151	H	-3.262911	-2.815264	1.188896
O	1.343068	-1.492764	-4.214582	O	2.413575	-2.584869	-3.545357	H	-2.646404	-5.112266	1.938520
H	2.096830	-3.305591	-4.927879	H	3.625278	-4.278674	-3.711965	H	-4.364740	-5.395961	0.001557
H	4.900763	-3.411327	0.146211	H	6.011709	-2.729524	1.327536	H	-4.087403	-2.652242	-1.310460
H	3.070003	-6.118233	0.845665	H	4.432954	-5.293974	2.625917	H	-3.844741	-4.347246	-2.940725
H	0.430229	-1.846236	-4.130493	H	1.597245	-3.116882	-3.412062	H	-5.494028	-3.682504	-3.095134
O	-3.107677	-4.979491	-2.187028	O	-1.532553	-6.117680	-0.789486	H	-5.415252	-6.044279	-3.075412
C	-1.791853	-4.377627	-2.150327	C	-0.360406	-5.277161	-0.912388	H	-2.941252	-6.437550	-1.216751
C	-0.888160	-5.336671	-1.358951	C	0.602681	-5.715340	0.204731	H	-0.784731	-7.382998	-0.532116
C	-1.443300	-5.520295	0.056262	C	-0.066369	-5.472698	1.559677	H	-0.870252	-6.815098	1.746873
C	-2.894766	-5.982443	0.004374	C	-1.389564	-6.228324	1.625448	H	-0.047532	-4.568502	0.372727
C	-3.717780	-5.069098	-0.914155	C	-2.260599	-5.901781	0.404450	H	1.987547	-5.755994	0.736786
H	-1.842404	-3.423942	-1.613978	H	-0.643931	-4.232171	-0.745156	H	1.029205	-6.228645	-1.957660
H	-0.850878	-6.309283	-1.870002	H	0.824712	-6.785632	0.088605	H	-0.692124	-3.705866	-1.906480
H	-1.404235	-4.543092	0.559962	H	-0.276110	-4.395339	1.642893	H	0.396855	-3.398508	-3.912281
H	-2.916732	-6.992406	-0.431290	H	-1.166457	-7.305113	1.592006	H	-0.886455	-4.507244	-4.414243
H	-4.709884	-5.499879	-1.090090	H	-3.114945	-6.585981	0.354925	H	1.839905	-4.899569	-4.277725
C	-1.375047	-4.071897	-3.601015	C	0.144842	-5.391320	-2.363020	H	3.060401	-5.919317	-2.072515

O	-0.714061	-6.490261	0.794000	O	0.728353	-5.910245	2.649578	H	5.110733	-4.958412	-1.171739
O	-3.497134	-5.992747	1.294273	O	-2.121469	-5.918632	2.805890	H	4.418160	-4.782671	1.094610
O	-3.824093	-3.809581	-0.304830	O	-2.695478	-4.572352	0.509123	H	3.394217	-2.639386	-0.200389
H	-0.426923	-4.555594	-3.842246	H	1.174533	-5.750559	-2.394739	H	5.530791	-1.913000	0.449053
O	-1.176008	-2.681274	-3.828198	O	0.147573	-4.138505	-3.037060	H	5.578923	-2.571649	-2.317315
H	-2.149101	-4.477130	-4.266107	H	-0.491775	-6.119809	-2.882207	H	2.541293	-2.382608	-2.666613
H	0.232925	-6.263679	0.732524	H	1.649700	-5.632235	2.488383	H	4.655276	-2.847626	-4.793141
H	-2.873943	-6.448178	1.879112	H	-1.492687	-5.983769	3.539600	H	4.053182	-1.225637	-4.363107
H	-2.024979	-2.207746	-3.681746	H	-0.772149	-3.793615	-3.076843	H	2.834602	-2.443444	-6.097264
O	-6.306234	-1.234038	-1.176041	O	-5.521534	-3.082670	-1.315343	H	6.472830	-0.687470	-1.954158
C	-5.024128	-1.896558	-1.286565	C	-4.123187	-3.387958	-1.102535	H	6.617113	1.294581	-0.551373
C	-5.070936	-3.118510	-0.355597	C	-4.043460	-4.266497	0.154964	H	5.705819	0.205520	1.489780
C	-5.337159	-2.666422	1.082557	C	-4.631376	-3.518110	1.354065	H	3.598544	1.115486	-0.211044
C	-6.596073	-1.811432	1.154286	C	-6.048472	-3.049495	1.045398	H	4.323947	3.374820	0.650928
C	-6.548670	-0.691219	0.107082	C	-6.082871	-2.289350	-0.286526	H	5.230848	3.218824	-1.689763
H	-4.234351	-1.222934	-0.936496	H	-3.572188	-2.459749	-0.916853	H	3.425167	1.048400	-2.854741
H	-5.869075	-3.800240	-0.681868	H	-4.609824	-5.193496	-0.012022	H	3.357334	2.951461	-4.250536
H	-4.481216	-2.048972	1.396244	H	-4.003703	-2.631446	1.531671	H	4.456788	1.764702	-5.006927
H	-7.457888	-2.450937	0.912241	H	-6.686658	-3.938725	0.934312	H	5.302987	3.982708	-4.907038
H	-7.521531	-0.191530	0.038903	H	-7.117435	-2.096503	-0.591905	H	4.076617	4.905391	-2.321019
C	-4.768909	-2.175328	-2.778824	C	-3.573399	-4.002174	-2.403011	H	2.906811	6.538044	-0.929018
O	-5.519764	-3.760535	1.963362	O	-4.700064	-4.329092	2.513414	H	3.437810	5.632162	1.192525
O	-6.764526	-1.229442	2.442624	O	-6.559878	-2.204972	2.070858	H	1.327224	4.200528	0.220375
H	-4.556023	-3.233019	-2.943362	H	-3.173529	-5.001739	-2.221325	H	0.246191	6.115473	1.198652
O	-3.642658	-1.466977	-3.283108	O	-2.501967	-3.243102	-2.951684	H	0.422721	6.454209	-1.635477
H	-5.681868	-1.916475	-3.331398	H	-4.405915	-4.087527	-3.113847	H	0.785670	3.457886	-2.112459
H	-4.755399	-4.357781	1.862519	H	-3.806720	-4.677976	2.691142	H	-0.915585	3.879406	-3.606624
H	-6.606025	-1.942733	3.078945	H	-6.338879	-2.640773	2.907605	H	0.481046	4.408341	-4.553980
H	-3.801242	-0.500508	-3.197893	H	-2.829487	-2.344746	-3.179110	H	-1.607538	5.870195	-3.512395
C	0.389942	2.590540	3.677725	C	0.875649	-2.174911	3.493351	C	0.128921	3.244855	4.474188
C	1.132180	2.491015	2.502291	C	1.456086	-1.666403	2.332266	C	0.955690	3.430652	3.367110
C	1.979393	1.400090	2.316281	C	1.689421	-0.296372	2.223891	C	1.907946	2.462419	3.056341
C	2.114420	0.393733	3.283885	C	1.349263	0.593763	3.252347	C	2.073029	1.306989	3.836796
C	1.344794	0.484659	4.460604	C	0.715176	0.084801	4.403832	C	1.227105	1.116603	4.944919
C	0.495488	1.584834	4.636171	C	0.498566	-1.295046	4.506271	C	0.264253	2.090619	5.241239
C	1.327890	-0.640436	5.479653	C	0.153160	1.011072	5.468481	C	1.275662	-0.155130	5.770073
C	0.871589	-1.918070	4.816388	C	-0.842137	1.957557	4.838440	C	1.065944	-1.365427	4.893401
C	-0.383255	-2.479489	5.047375	C	-2.218297	1.850851	5.035374	C	-0.116037	-2.105736	4.910616
C	-0.778928	-3.650321	4.395904	C	-3.105521	2.728605	4.406678	C	-0.277152	-3.231063	4.098433
C	0.090349	-4.263048	3.495748	C	-2.609779	3.719794	3.561830	C	0.768232	-3.622582	3.264867
C	1.347643	-3.706563	3.246372	C	-1.234043	3.834257	3.348369	C	1.947821	-2.876028	3.215411
C	1.749281	-2.532511	3.898631	C	-0.341453	2.959332	3.981493	C	2.104644	-1.733246	4.013083
C	3.159681	-0.686875	2.994216	C	1.775736	2.049766	3.055089	C	3.240470	0.399464	3.434165
N	3.043066	-1.956291	3.744425	N	1.072871	3.067747	3.860124	N	3.300677	-0.954137	4.039558
C	4.560199	-0.089636	3.258392	C	3.287646	2.157274	3.349871	C	4.547513	1.149917	3.766538
C	4.106681	-2.888000	3.364261	C	1.583267	4.410427	3.572559	C	4.500367	-1.672165	3.598563
C	5.475979	-2.279911	3.643474	C	3.070772	4.493764	3.888282	C	5.770916	-0.898296	3.930606
N	5.640649	-1.021751	2.904179	N	3.818497	3.505065	3.099942	N	5.731984	0.422855	3.292957
C	6.956087	-0.421575	3.153949	C	5.251430	3.557981	3.413746	C	6.956739	1.188939	3.532188
H	-0.279829	3.431769	3.835015	H	0.705381	-3.242749	3.600213	H	-0.621785	3.985825	4.734282

H	1.047929	3.252722	1.733606	H	1.709535	-2.331485	1.512759	H	0.873824	4.323666	2.754776
H	2.551791	1.327493	1.394363	H	2.142483	0.096810	1.316251	H	2.556026	2.608405	2.195967
H	-0.101727	1.641246	5.542796	H	0.010020	-1.680069	5.397881	H	-0.391259	1.931250	6.093835
H	0.659372	-0.378438	6.304786	H	-0.325645	0.419138	6.253842	H	0.508659	-0.114251	6.549009
H	2.331667	-0.794773	5.893547	H	0.957277	1.597700	5.928772	H	2.250890	-0.244511	6.264359
H	-1.054257	-1.999283	5.755381	H	-2.599120	1.076960	5.697337	H	-0.915651	-1.802941	5.582484
H	-1.757733	-4.077732	4.592807	H	-4.174003	2.635431	4.577464	H	-1.209941	-3.787286	4.107158
H	-0.206541	-5.166672	2.970639	H	-3.280685	4.400535	3.046854	H	0.680679	-4.512149	2.648101
H	2.005041	-4.190357	2.531896	H	-0.862307	4.598858	2.674208	H	2.736582	-3.192232	2.542027
H	3.101548	-0.909379	1.912310	H	1.637034	2.281435	1.982045	H	3.204526	0.294409	2.335376
H	4.620464	0.196755	4.323489	H	3.456737	1.854496	4.398929	H	4.594720	1.311570	4.858124
H	4.688060	0.811656	2.655025	H	3.827689	1.453532	2.709878	H	4.531761	2.118809	3.268619
H	4.057446	-3.180638	2.303369	H	1.438500	4.707672	2.523114	H	4.494822	-1.874593	2.516242
H	3.992392	-3.796814	3.961982	H	1.043015	5.122251	4.202951	H	4.525102	-2.637080	4.113659
H	6.257718	-2.977647	3.323650	H	3.441018	5.492253	3.633300	H	6.638067	-1.450220	3.551475
H	5.590255	-2.113001	4.729219	H	3.229436	4.332221	4.969610	H	5.877991	-0.802179	5.025555
H	7.095900	-0.150880	4.214003	H	5.452152	3.345151	4.477428	H	7.122379	1.397226	4.602546
H	7.064110	0.468389	2.531454	H	5.787379	2.828334	2.801208	H	6.895116	2.138171	2.993440
H	7.735761	-1.136212	2.873896	H	5.637372	4.553260	3.177088	H	7.816406	0.628813	3.152035
FV1				FV1				FV1			
E	-5082.90232165			E	-5082.90183865			E	-5082.86716115		
O	5.675339	-3.818945	0.324228	O	-7.224551	0.683116	0.412074	C	-2.240050	5.003066	-1.769690
C	4.252910	-3.830546	0.590556	C	-6.259124	-0.385178	0.265844	C	-3.147888	4.804453	-0.550247
C	3.633753	-4.883052	-0.342146	C	-6.420388	-1.301837	1.488527	O	-2.427403	5.175117	0.620151
C	3.914045	-4.514280	-1.801228	C	-6.167746	-0.506418	2.771706	C	-3.648664	3.365673	-0.468388
C	5.409631	-4.326216	-2.026231	C	-7.066423	0.723113	2.825637	O	-4.581222	3.315153	0.595875
C	5.998934	-3.373070	-0.978434	C	-6.968335	1.523561	1.520342	C	-4.254619	2.905840	-1.801460
H	3.828878	-2.850927	0.344466	H	-5.247443	0.034949	0.274658	O	-4.448738	1.496701	-1.662030
H	4.070790	-5.867209	-0.122103	H	-7.439531	-1.713114	1.505843	C	-3.284036	3.214583	-2.953413
H	3.410243	-3.555964	-2.002496	H	-5.119921	-0.168269	2.748631	O	-2.943344	4.608784	-2.933565
H	5.899046	-5.302569	-1.894013	H	-8.107185	0.380089	2.922653	C	-3.821149	2.930245	-4.342679
H	7.093440	-3.379727	-1.030050	H	-7.742670	2.298274	1.489496	O	-2.727401	3.100608	-5.245902
C	4.061809	-4.052856	2.102136	C	-6.480531	-1.032000	-1.113821	C	-5.646144	0.890763	-2.102903
O	2.212630	-4.941070	-0.227172	O	-5.463757	-2.359945	1.503840	C	-6.351039	0.248163	-0.901777
O	3.475869	-5.514647	-2.702558	O	-6.427061	-1.268877	3.936420	O	-6.589404	1.248720	0.086692
O	5.687807	-3.810853	-3.323634	O	-6.728521	1.576407	3.913852	C	-5.511780	-0.891668	-0.340120
O	5.499095	-2.083729	-1.219964	O	-5.689491	2.098240	1.445912	O	-6.274180	-1.498722	0.688071
H	3.446140	-4.934451	2.289643	H	-6.661441	-2.103785	-1.014552	C	-5.141814	-1.866212	-1.454293
O	3.394226	-2.966077	2.732456	O	-5.347319	-0.903203	-1.964419	O	-4.227760	-2.818477	-0.898327
H	5.052102	-4.222655	2.545125	H	-7.370294	-0.571393	-1.563178	C	-4.482496	-1.134026	-2.627775
H	2.537236	-5.701316	-2.514162	H	-5.924725	-2.102440	3.870106	O	-5.376921	-0.089827	-3.081118
H	5.153262	-4.334678	-3.938952	H	-6.631811	0.998450	4.685432	C	-4.160497	-2.052260	-3.817956
H	3.935204	-2.151813	2.629611	H	-5.172209	0.050435	-2.126555	O	-5.053954	-3.140047	-3.991715
O	6.950292	1.041822	0.072280	O	-4.761697	4.911266	-0.740346	C	-4.610804	-4.168574	-0.855881
C	6.052093	-0.091816	0.114922	C	-4.911837	3.508596	-0.417671	C	-4.287374	-4.737037	0.526084
C	6.382394	-0.969750	-1.102159	C	-5.562717	3.438072	0.972642	O	-4.981665	-3.980827	1.516517
C	6.195495	-0.165671	-2.391340	C	-4.675200	4.146817	1.998959	C	-2.785580	-4.721731	0.775806
C	7.008602	1.122248	-2.344169	C	-4.370720	5.571768	1.553061	O	-2.579147	-5.325834	2.038063
C	6.734586	1.885818	-1.042045	C	-3.855354	5.588671	0.108025	C	-2.063184	-5.449103	-0.355727
H	5.018566	0.259124	0.021798	H	-3.923260	3.039581	-0.364801	O	-0.667043	-5.208428	-0.167044

H	7.422878	-1.317013	-1.032643	H	-6.548501	3.923231	0.941421	C	-2.495599	-4.915261	-1.734210
H	5.129428	0.101614	-2.460165	H	-3.725868	3.591109	2.051896	O	-3.937911	-4.923725	-1.854958
H	8.075292	0.853275	-2.349300	H	-5.310556	6.143197	1.572813	C	-1.926199	-5.727569	-2.885956
H	7.443292	2.713781	-0.924611	H	-3.809837	6.616895	-0.267959	O	-2.207986	-7.105319	-2.671314
C	6.194594	-0.751585	1.498696	C	-5.680325	2.841490	-1.573041	C	0.235822	-6.295091	-0.252225
O	6.610802	-0.885094	-3.538111	O	-5.286260	4.225351	3.273992	C	0.959718	-6.451205	1.091976
O	6.712360	1.973239	-3.446215	O	-3.402703	6.191571	2.392914	O	0.002985	-6.594528	2.141003
O	5.415053	2.363697	-1.077221	O	-2.583298	4.994936	0.081368	C	1.876628	-5.263844	1.355139
H	6.452568	-1.807519	1.399001	H	-6.569571	2.329223	-1.201536	O	2.567880	-5.548294	2.559967
O	4.985821	-0.712537	2.248376	O	-4.908266	1.850921	-2.241630	C	2.810190	-5.060423	0.164867
H	7.010423	-0.245413	2.031519	H	-6.000333	3.631329	-2.265492	O	3.587164	-3.884016	0.419901
H	6.153484	-1.746727	-3.536232	H	-5.568240	3.327157	3.529349	C	1.998378	-4.906716	-1.126009
H	6.725413	1.405999	-4.231620	H	-3.681349	6.006450	3.302198	O	1.175940	-6.088384	-1.283182
H	4.734593	0.224039	2.410246	H	-4.114852	2.274001	-2.639344	C	2.858745	-4.754942	-2.388905
O	4.092371	5.060410	1.050917	O	-0.132233	5.404972	-2.635928	O	4.059978	-5.505016	-2.360399
C	4.375188	3.678523	0.728740	C	-1.227226	4.741848	-1.961060	C	4.965415	-4.046886	0.624881
C	5.144528	3.681149	-0.601591	C	-1.563505	5.586554	-0.722157	C	5.412622	-3.205719	1.822187
C	4.292255	4.334924	-1.692059	C	-0.337376	5.683847	0.188852	O	4.668589	-3.585018	2.976209
C	3.837855	5.723694	-1.260505	C	0.865057	6.210709	-0.584623	C	5.252329	-1.716638	1.537306
C	3.207323	5.679751	0.137713	C	1.065382	5.419637	-1.884148	O	5.797126	-1.042752	2.657459
H	3.433135	3.137742	0.586250	H	-0.903104	3.748821	-1.630919	C	5.929716	-1.325626	0.217295
H	6.083024	4.240689	-0.482338	H	-1.868108	6.594484	-1.037496	O	5.495596	0.001389	-0.092004
H	3.398153	3.706676	-1.830117	H	-0.105162	4.665362	0.537840	C	5.493788	-2.281598	-0.906028
H	4.727037	6.368475	-1.198343	H	0.657638	7.254027	-0.865318	O	5.713391	-3.646487	-0.511638
H	3.054199	6.696149	0.517324	H	1.807216	5.915998	-2.519704	C	6.240887	-2.097461	-2.212444
C	5.090700	3.051166	1.938944	C	-2.358053	4.544088	-2.987162	O	5.564654	-2.890197	-3.187513
O	4.998939	4.482251	-2.910239	O	-0.549628	6.556892	1.283339	C	6.434559	1.038002	-0.281416
O	2.894806	6.275771	-2.172720	O	2.060346	6.139097	0.184965	C	6.141568	2.171239	0.707514
O	1.985938	4.992241	0.057852	O	1.484459	4.119643	-1.558033	O	6.221365	1.683525	2.046800
H	6.040111	2.604694	1.638174	H	-3.289350	4.985361	-2.627945	C	4.768752	2.772252	0.433899
O	4.336629	2.002161	2.535354	O	-2.642862	3.171155	-3.227950	O	4.589566	3.818259	1.373923
H	5.298571	3.852159	2.660642	H	-2.066332	5.058077	-3.912651	C	4.693897	3.237851	-1.015819
H	5.377043	3.614805	-3.146960	H	-1.375674	6.289062	1.727568	O	3.336144	3.612947	-1.262088
H	3.265626	6.134675	-3.056615	H	1.838269	6.495859	1.057924	C	5.097337	2.098907	-1.971643
H	3.488794	2.366040	2.875165	H	-1.840566	2.736182	-3.593666	O	6.375676	1.543919	-1.597743
O	-0.684684	5.224900	2.584901	O	3.165952	1.829553	-3.898485	C	5.189952	2.558221	-3.417789
C	0.498263	4.635020	1.995981	C	2.008617	2.377774	-3.224462	O	6.008244	3.721255	-3.491514
C	0.864051	5.500346	0.779478	C	2.520915	3.519346	-2.333200	C	3.064239	4.844296	-1.904720
C	-0.294439	5.499330	-0.220408	C	3.523900	2.969293	-1.316082	C	2.297126	5.756029	-0.937015
C	-1.583662	5.947573	0.457005	C	4.643459	2.212644	-2.020691	O	3.052413	5.934459	0.261037
C	-1.823136	5.150721	1.747644	C	4.078400	1.194601	-3.021658	C	0.930120	5.160540	-0.629878
H	0.265282	3.622765	1.648082	H	1.559848	1.607604	-2.587513	O	0.267310	6.073765	0.232541
H	1.064088	6.529363	1.109984	H	3.010942	4.277879	-2.959716	C	0.177777	4.900101	-1.932899
H	-0.430003	4.465315	-0.573952	H	2.980991	2.261880	-0.669559	O	-1.060412	4.259684	-1.602239
H	-1.469182	7.004692	0.739709	H	5.234235	2.941558	-2.594755	C	1.017548	3.999529	-2.847970
H	-2.643340	5.594543	2.322896	H	4.879527	0.808137	-3.661568	O	2.297100	4.639579	-3.069736
C	1.560512	4.510507	3.103309	C	0.970336	2.752479	-4.298733	C	0.378662	3.730818	-4.216614
O	-0.065259	6.376892	-1.309209	O	4.129369	3.994130	-0.550064	O	-0.325085	4.839323	-4.746004
O	-2.710426	5.790016	-0.397898	O	5.479363	1.527776	-1.092115	H	-2.014631	6.064728	-1.908981
O	-2.118550	3.822905	1.405139	O	3.468858	0.152290	-2.308551	H	-4.019122	5.462707	-0.679919

H	2.484354	5.014693	2.814877	H	0.713890	3.811740	-4.239154	H	-2.927813	4.866400	1.389907
O	1.918869	3.158129	3.365414	O	-0.253378	2.043387	-4.143607	H	-2.785352	2.712688	-0.268150
H	1.166562	4.998799	4.004415	H	1.419390	2.560700	-5.282201	H	-5.112928	2.500105	0.510622
H	0.814832	6.176185	-1.678138	H	3.421592	4.547958	-0.170899	H	-5.215751	3.414166	-1.960494
H	-2.425238	6.083391	-1.276084	H	5.693904	2.161397	-0.391168	H	-2.380706	2.610586	-2.804589
H	1.123798	2.669285	3.673329	H	-0.084859	1.081285	-4.257394	H	-4.636054	3.633759	-4.567019
O	-3.831653	1.432608	3.605007	O	2.603322	-3.157872	-3.660591	H	-4.212394	1.905328	-4.380568
C	-2.659320	2.052199	3.028079	C	2.335405	-1.776578	-3.326201	H	-3.058114	3.051008	-6.151042
C	-3.174764	3.149082	2.087087	C	3.641061	-1.188256	-2.771807	H	-6.299383	1.628198	-2.582460
C	-4.027603	2.527851	0.973381	C	4.114841	-1.982413	-1.549691	H	-7.307809	-0.161604	-1.255413
C	-5.133972	1.647937	1.548724	C	4.198640	-3.472285	-1.862428	H	-6.919620	0.773913	0.865366
C	-4.592052	0.715580	2.653541	C	2.903034	-3.954253	-2.532120	H	-4.578853	-0.468787	0.060775
H	-2.110526	1.310927	2.437090	H	1.571570	-1.732245	-2.542434	H	-5.758976	-2.240020	1.060582
H	-3.778094	3.868071	2.658522	H	4.417274	-1.222684	-3.549020	H	-6.039952	-2.373261	-1.823912
H	-3.347659	1.902980	0.374688	H	3.373937	-1.838481	-0.749310	H	-3.550786	-0.665449	-2.287822
H	-5.875339	2.312019	2.014656	H	5.016631	-3.622434	-2.583251	H	-3.127080	-2.408548	-3.705156
H	-5.426064	0.277170	3.213056	H	3.029825	-4.974148	-2.912330	H	-4.199624	-1.442155	-4.724509
C	-1.734316	2.492811	4.177297	C	1.756538	-1.098283	-4.580609	H	-4.719123	-3.880066	-3.458076
O	-4.631133	3.523051	0.167017	O	5.400726	-1.558686	-1.127001	H	-5.677181	-4.278996	-1.077420
O	-5.780856	0.843274	0.564357	O	4.415762	-4.261678	-0.701131	H	-4.632602	-5.780335	0.544850
O	-3.821030	-0.289510	2.049077	O	1.866989	-3.904840	-1.584034	H	-4.253850	2.366794	2.366794
H	-1.541960	3.566381	4.133884	H	2.332415	-0.207589	-4.838022	H	-2.443658	-3.675004	0.778172
O	-0.457426	1.864876	4.117626	O	0.415618	-0.659038	-4.395537	H	-1.640849	-5.593235	2.110983
H	-2.242858	2.270203	5.124578	H	1.830455	-1.810134	-5.413420	H	-2.282314	-6.520320	-0.297940
H	-3.924222	4.115723	-0.152595	H	5.347363	-0.611402	-0.905748	H	-2.134598	-3.883254	-1.830938
H	-5.560970	1.149487	-0.339057	H	5.011266	-3.771447	-0.112349	H	-0.844657	-5.543418	-2.921677
H	-0.566089	0.893643	4.217230	H	-0.154986	-1.434712	-4.197660	H	-2.375408	-5.364743	-3.822856
O	-2.845342	-3.566062	3.380272	O	-1.288155	-5.781479	-1.853828	H	-1.735247	-7.613096	-3.342141
C	-2.668153	-2.157861	3.102897	C	-0.442275	-4.623911	-2.052288	H	-0.300026	-7.210856	-0.519724
C	-3.973486	-1.639880	2.485234	C	0.947552	-4.990328	-1.507306	H	1.579113	-7.357611	1.031764
C	-4.332395	-2.440433	1.231880	C	0.841645	-5.329894	-0.018001	H	0.512855	-6.496412	2.960919
C	-4.325841	-3.938375	1.503087	C	-0.190852	-6.429228	0.203798	H	1.258371	-4.359675	1.463410
C	-3.027662	-4.343453	2.213683	C	-1.514699	-6.084767	-0.491610	H	3.141539	-4.788895	2.777605
H	-1.863895	-2.030157	2.370628	H	-0.834963	-3.782604	-1.470611	H	3.469435	-5.926632	0.045512
H	-4.788118	-1.715919	3.219076	H	1.339137	-5.858180	-2.056799	H	1.338402	-4.032766	-1.046399
H	-3.552564	-2.234915	0.485049	H	0.500096	-4.421512	0.502496	H	3.069767	-3.691949	-2.544748
H	-5.161541	-4.175639	2.177795	H	0.191625	-7.350885	-0.259352	H	2.246537	-5.096247	-3.233867
H	-3.085399	-5.383346	2.554100	H	-2.181159	-6.954557	-0.489556	H	4.782462	-4.870105	-2.232174
C	-2.227305	-1.465815	4.404763	C	-0.520333	-4.233718	-3.539787	H	5.214237	-5.100890	0.781135
O	-5.613216	-2.100470	0.730397	O	2.069300	-5.787210	0.520618	H	6.480846	-3.412481	1.982862
O	-4.437604	-4.688486	0.297629	O	-0.444767	-6.646744	1.587806	H	4.856029	-2.910420	3.646320
O	-1.959600	-4.176696	1.313387	O	-2.108334	-5.006346	0.184596	H	4.179747	-1.497052	1.430087
H	-2.888503	-0.627439	4.634327	H	0.475438	-4.199574	-3.984926	H	5.837902	-0.083939	2.465312
O	-0.916936	-0.918430	4.318613	O	-1.079797	-2.940201	-3.736381	H	7.021315	-1.354222	0.344092
H	-2.301703	-2.197316	5.220599	H	-1.105845	-5.003430	-4.059900	H	4.424954	-2.118698	-1.090640
H	-5.649309	-1.129066	0.620962	H	2.771795	-5.163543	0.251074	H	7.280877	-2.428642	-2.077853
H	-5.096156	-4.231203	-0.247011	H	0.423545	-6.703057	2.013377	H	6.242920	-1.033770	-2.484346
H	-0.280529	-1.644089	4.135958	H	-2.001232	-2.931876	-3.394127	H	6.119743	-2.957753	-3.973759
O	1.293702	-5.854689	1.709265	O	-5.661181	-4.071745	-0.064254	H	7.455559	0.661855	-0.151085
C	0.369772	-4.756295	1.895800	C	-4.266298	-3.996145	-0.442999	H	6.903571	2.948380	0.556169

C	-0.954676	-5.183617	1.241986	C	-3.516737	-5.031438	0.410088	H	5.831789	2.378476	2.600854
C	-0.725139	-5.426054	-0.252539	C	-3.698138	-4.709718	1.895572	H	4.008071	1.991588	0.580124
C	0.380886	-6.456542	-0.452436	C	-5.178399	-4.610557	2.244118	H	3.951037	4.468353	1.015180
C	1.631500	-6.079385	0.354430	C	-5.903972	-3.672739	1.270499	H	5.362861	4.091690	-1.165980
H	0.749027	-3.870927	1.373678	H	-3.878425	-2.999452	-0.205845	H	4.332996	1.313013	-1.913460
H	-1.313164	-6.108449	1.715936	H	-3.915021	-6.034266	0.200671	H	4.170566	2.768012	-3.767491
H	-0.393939	-4.472776	-0.694271	H	-3.232366	-3.728923	2.080000	H	5.605239	1.734711	-4.016860
H	0.018690	-7.419879	-0.063783	H	-5.622396	-5.610411	2.128232	H	5.952791	4.065738	-4.391242
H	2.341807	-6.913614	0.362243	H	-6.988490	-3.746541	1.408524	H	3.995534	5.311978	-2.238456
C	0.330480	-4.419411	3.398549	C	-4.186251	-4.174391	-1.970327	H	2.156567	6.728226	-1.430328
O	-1.882877	-5.909254	-0.911016	O	-3.134549	-5.702488	2.733310	H	2.435299	6.338243	0.891951
O	0.744353	-6.587878	-1.822364	O	-5.377735	-4.137471	3.571879	H	1.078753	4.193736	-0.127457
H	-0.686000	-4.489608	3.788942	H	-3.529179	-5.006341	-2.229823	H	-0.607294	5.705294	0.468123
O	0.761642	-3.090250	3.667738	O	-3.648661	-3.031701	-2.625481	H	-0.014290	5.837679	-2.465109
H	0.954716	-5.154099	3.924151	H	-5.195936	-4.404400	-2.335617	H	1.193681	3.035618	-2.352721
H	-2.645635	-5.369033	-0.627614	H	-2.210252	-5.843697	2.455320	H	-0.279292	2.860054	-4.128238
H	-0.085562	-6.672016	-2.314469	H	-4.769290	-4.644674	4.129772	H	1.195209	3.457575	-4.898884
H	1.700810	-2.998968	3.392470	H	-4.233422	-2.259430	-2.458749	H	-1.264515	4.594781	-4.755871
C	-3.416785	-3.612803	-3.441038	C	4.112592	2.126835	5.704970	C	-1.167305	5.705190	4.885426
C	-4.494896	-3.383689	-4.295089	C	5.462463	2.069411	6.046856	C	-1.874307	5.045461	5.889063
C	-5.184057	-2.175738	-4.220201	C	6.365523	1.474586	5.168996	C	-2.158630	3.688661	5.748726
C	-4.835653	-1.173876	-3.299191	C	5.956998	0.934598	3.940796	C	-1.754324	2.961577	4.619923
C	-3.710568	-1.384999	-2.481841	C	4.589525	0.973327	3.608223	C	-1.009077	3.622631	3.624964
C	-3.025883	-2.605749	-2.562511	C	3.689568	1.570908	4.499580	C	-0.732161	4.988817	3.771635
C	-3.178380	-0.304969	-1.562932	C	4.063064	0.283927	2.362968	C	-0.411813	2.859853	2.458447
C	-2.940520	0.991418	-2.298482	C	4.409437	-1.185453	2.403030	C	0.480071	1.748066	2.956416
C	-1.648962	1.471851	-2.521700	C	3.447774	-2.176145	2.602494	C	1.868945	1.790739	2.836335
C	-1.427013	2.674322	-3.195240	C	3.796737	-3.528713	2.635941	C	2.661434	0.724667	3.270966
C	-2.518696	3.402862	-3.660682	C	5.134729	-3.890832	2.483730	C	2.055727	-0.391404	3.842985
C	-3.817265	2.931720	-3.456940	C	6.112626	-2.910369	2.292524	C	0.669348	-0.435458	4.000266
C	-4.045505	1.727771	-2.775263	C	5.763561	-1.552073	2.246358	C	-0.131504	0.630219	3.564188
C	-5.793359	0.020550	-3.234129	C	7.072738	0.425010	3.030412	C	-2.259559	1.522082	4.531818
N	-5.363710	1.237088	-2.478222	N	6.700575	-0.523902	1.958140	N	-1.551975	0.599331	3.615537
C	-7.133866	-0.464647	-2.638121	C	7.773076	1.637900	2.378995	C	-3.749807	1.561195	4.123819
C	-6.420202	2.267838	-2.576777	C	7.881896	-0.932694	1.192704	C	-2.161464	-0.730796	3.650869
C	-7.748631	1.764493	-2.023209	C	8.558843	0.282895	0.567981	C	-3.626234	-0.654101	3.236397
N	-8.165494	0.560410	-2.732826	N	8.938751	1.236246	1.605330	N	-4.349097	0.230562	4.140282
C	-9.458447	0.074352	-2.273858	C	9.653904	2.381880	1.064845	C	-5.773392	0.278478	3.856290
H	-2.876785	-4.554682	-3.456257	H	3.392100	2.584616	6.376458	H	-0.939883	6.763441	4.974916
H	-4.801349	-4.138089	-5.013623	H	5.811398	2.477903	6.990588	H	-2.201861	5.579346	6.776221
H	-6.025036	-2.006288	-4.888492	H	7.417877	1.426379	5.439640	H	-2.712469	3.177055	6.532685
H	-2.163966	-2.761707	-1.919142	H	2.633972	1.589467	4.240488	H	-0.159373	5.489592	2.995026
H	-2.241833	-0.645899	-1.112417	H	2.978780	0.415517	2.302931	H	0.154020	3.548970	1.827799
H	-3.879202	-0.136744	-0.704654	H	4.503282	0.726455	1.460948	H	-1.208505	2.422209	1.844514
H	-0.805229	0.896668	-2.149213	H	2.406746	-1.883502	2.714910	H	2.343457	2.659419	2.386664
H	-0.415046	3.035236	-3.351670	H	3.032993	-4.290934	2.751816	H	3.738613	0.757763	3.150742
H	-2.366999	4.337668	-4.193013	H	5.424164	-4.937496	2.515235	H	2.660635	-1.232950	4.168625
H	-4.649375	3.513745	-3.833227	H	7.150179	-3.206978	2.184192	H	0.213629	-1.303129	4.464580
H	-6.000036	0.328420	-4.273748	H	7.825242	-0.057247	3.680698	H	-2.221970	1.101386	5.553383
H	-6.952481	-0.799901	-1.598863	H	7.024267	2.180710	1.764514	H	-3.830170	2.042697	3.129191

H	-7.469028	-1.339767	-3.201572	H	8.096009	2.323349	3.168774	H	-4.289370	2.192286	4.836950
H	-6.578728	2.572972	-3.623887	H	8.620464	-1.457897	1.824022	H	-2.105817	-1.187630	4.655060
H	-6.089446	3.133266	-1.997944	H	7.553006	-1.609007	0.400417	H	-1.619282	-1.376261	2.954658
H	-8.503731	2.544903	-2.175500	H	9.462940	-0.042653	0.040080	H	-4.070334	-1.655177	3.277148
H	-7.663279	1.595418	-0.934932	H	7.878565	0.733119	-0.180169	H	-3.682690	-0.307537	2.186227
H	-9.463615	-0.219157	-1.207226	H	9.050814	2.979211	0.353833	H	-6.000662	0.703236	2.860021
H	-9.757834	-0.796589	-2.865979	H	9.966311	3.042677	1.879875	H	-6.280561	0.891586	4.608378
H	-10.213883	0.854532	-2.413622	H	10.552490	2.040941	0.540562	H	-6.195115	-0.730410	3.891546
S				S				S			
E	-5082.90167028			E	-5082.90200725			E	-5082.86776045		
O	-3.469191	-2.238585	0.710077	O	-3.262421	-2.189404	1.088194	C	0.023857	5.802262	-0.113658
C	-2.833369	-0.942635	0.580108	C	-2.637271	-0.898577	0.899064	C	0.817817	6.240011	-1.347344
C	-3.596498	-0.194671	-0.523550	C	-3.468861	-0.153981	-0.156886	O	0.056849	5.970836	-2.520269
C	-3.500687	-0.975831	-1.837139	C	-3.487461	-0.955977	-1.459266	C	2.167423	5.533902	-1.398906
C	-3.972855	-2.414934	-1.655609	C	-3.976683	-2.377497	-1.216211	O	2.863547	6.074418	-2.504429
C	-3.301141	-3.057247	-0.434592	C	-3.201600	-3.017548	-0.057640	C	2.932336	5.699032	-0.080993
H	-1.795030	-1.081381	0.260550	H	-1.621837	-1.038036	0.512124	O	4.045717	4.805444	-0.159860
H	-4.649010	-0.093522	-0.228834	H	-4.495158	-0.025948	0.214471	C	2.031388	5.328116	1.109340
H	-2.439704	-0.994824	-2.131581	H	-2.452869	-1.003234	-1.832146	O	0.799801	6.069471	1.043615
H	-5.057605	-2.414294	-1.478684	H	-6.403632	1.023492	-1.709059	C	2.630021	5.626589	2.470344
H	-3.787394	-4.008228	-0.190907	H	-3.671465	-3.962601	0.236468	O	1.766458	5.033691	3.438071
C	-2.802833	-0.286691	1.973147	C	-2.520501	-0.226982	2.279605	C	5.349111	5.266947	0.121958
O	-3.048327	1.091060	-0.807699	O	-2.908874	1.112432	-0.502799	C	6.250073	4.994769	-1.090459
O	-4.288424	-0.391035	-2.863321	O	-4.336253	-0.368762	-2.436645	O	5.692704	5.608909	-2.250291
O	-3.674876	-3.212855	-2.801488	O	-3.812969	-3.190450	-2.380637	C	6.434936	3.497467	-1.302603
O	-1.941299	-3.255728	-0.722097	O	-1.873890	-3.230791	-0.465128	O	7.358095	3.351505	-2.365783
H	-3.309230	0.679594	1.960959	H	-3.002885	0.752098	2.275956	C	6.913086	2.851573	-0.005730
O	-1.477077	-0.029516	2.422416	O	-1.169380	0.002736	2.662011	O	6.956566	1.437255	-0.222054
H	-3.336700	-0.946066	2.670069	H	-3.037863	-0.864048	3.009079	C	5.960991	3.187340	1.146861
H	-4.076665	0.560801	-2.897519	H	-4.063482	0.561177	-2.550468	O	5.878100	4.627333	1.264922
H	-4.018735	-2.726863	-3.564702	H	-4.132946	-2.657367	-3.123115	C	6.409138	2.610679	2.500656
H	-0.996551	-0.882021	2.512973	H	-0.701321	-0.859331	2.726969	O	7.811595	2.527525	2.676605
O	0.316727	-5.557714	1.050888	O	0.480393	-5.540244	1.172602	C	8.191398	0.779749	-0.090525
C	-0.296568	-4.271884	0.796524	C	-0.140047	-4.250009	0.959248	C	8.394920	-0.150958	-1.285914
C	-1.324755	-4.479205	-0.326269	C	-1.231594	-4.451574	-0.103588	O	8.348431	0.617753	-2.485180
C	-0.625866	-5.012458	-1.579630	C	-0.605702	-4.978806	-1.397167	C	7.342561	-1.251353	-1.296947
C	0.165513	-6.273469	-1.254597	C	0.202897	-6.241567	-1.125785	O	7.657218	-2.100168	-2.383879
C	1.074176	-6.044169	-0.040016	C	1.176054	-6.023588	0.040279	C	7.334482	-1.982186	0.043627
H	0.466318	-3.567936	0.446426	H	0.604956	-3.548617	0.567900	O	6.185551	-2.832619	0.032752
H	-2.087566	-5.198625	0.003458	H	-1.973054	-5.173724	0.266562	C	7.231415	-0.995816	1.221854
H	0.080620	-4.237936	-1.916879	H	0.080077	-4.202454	-1.771326	O	8.246330	0.030257	1.116396
H	-0.549668	-7.064734	-0.984858	H	-0.496994	-7.034951	-0.824091	C	7.388332	-1.672701	2.573762
H	1.504939	-6.993108	0.298612	H	1.618208	-6.977279	0.349651	O	8.570154	-2.464522	2.566382
C	-0.841573	-3.739217	2.134082	C	-0.601991	-3.720325	2.329170	C	6.316701	-4.175626	0.460285
O	-1.541105	-5.343893	-2.607551	O	-1.580727	-5.303646	-2.371385	C	5.981735	-5.108874	-0.710852
O	0.965442	-6.691678	-2.355506	O	0.943020	-6.651009	-2.270884	O	6.814019	-4.798564	-1.827787
O	2.086755	-5.143154	-0.406208	O	2.174358	-5.126526	-0.372682	C	4.510804	-4.994112	-1.087859
H	-1.906481	-3.512545	2.054229	H	-1.668039	-3.486948	2.314595	O	4.277649	-5.956560	-2.102263
O	-0.212832	-2.528688	2.537953	O	0.057421	-2.515105	2.699156	C	3.640008	-5.205739	0.147477
H	-0.711751	-4.526512	2.888599	H	-0.431145	-4.511395	3.071350	O	2.279237	-4.978993	-0.239803

H	-2.106509	-4.565541	-2.772730	H	-2.168111	-4.531998	-2.479228	C	4.049154	-4.237851	1.262984
H	0.390657	-6.643660	-3.134123	H	0.326073	-6.607023	-3.016614	O	5.454883	-4.440915	1.545206
H	0.749618	-2.688048	2.658300	H	1.022910	-2.685059	2.772914	C	3.266366	-4.431301	2.571345
O	5.257467	-4.671476	1.402899	O	5.433498	-4.702892	1.287692	O	2.911181	-5.776426	2.838345
C	3.874077	-4.372250	1.101099	C	4.040488	-4.385705	1.056331	C	1.406011	-6.077312	-0.232809
C	3.419674	-5.386204	0.039764	C	3.526264	-5.381543	0.004898	C	0.572810	-6.078002	-1.516754
C	4.294812	-5.259902	-1.209748	C	4.340647	-5.242695	-1.283800	O	1.438063	-6.114928	-2.646801
C	5.768990	-5.393755	-0.848088	C	5.829346	-5.395289	-0.995938	C	-0.339194	-4.857802	-1.569760
C	6.129736	-4.455246	0.310784	C	6.255974	-4.479851	0.159077	O	-1.126109	-4.998385	-2.735317
H	3.804257	-3.365238	0.675481	H	3.961087	-3.372464	0.647390	C	-1.180144	-4.739895	-0.292610
H	3.503279	-6.404206	0.445745	H	3.623708	-6.405524	0.392350	O	-1.805883	-3.455852	-0.331998
H	4.130911	-4.253502	-1.625766	H	4.166166	-4.228529	-1.676146	C	-0.275850	-4.842974	0.947322
H	5.942825	-6.423590	-0.502434	H	6.008914	-6.432262	-0.675425	O	0.526341	-6.035039	0.878456
H	7.134434	-4.681233	0.685235	H	7.274003	-4.724702	0.482116	C	-1.018164	-4.914786	2.267226
C	3.093815	-4.370042	2.428571	C	3.326170	-4.393306	2.420394	O	-0.039481	-4.769475	3.295777
O	4.004746	-6.257716	-2.171768	O	3.995191	-6.222992	-2.245496	C	-3.212188	-3.349548	-0.238353
O	6.612707	-5.100040	-1.956426	O	6.621828	-5.091752	-2.138845	C	-3.750480	-2.586987	-1.451338
O	6.059441	-3.130897	-0.150332	O	6.182290	-3.147096	-0.276700	O	-3.381390	-3.275048	-2.651736
H	2.256670	-5.069179	2.386896	H	2.480569	-5.083261	2.411284	C	-3.216408	-1.161199	-1.461210
O	2.527871	-3.099164	2.726535	O	2.789634	-3.120855	2.762492	O	-3.804989	-0.511451	-2.577512
H	3.778275	-4.697254	3.222448	H	4.045394	-4.737959	3.175182	C	-3.556194	-0.481310	-0.140274
H	3.044675	-6.241495	-2.344009	H	3.027523	-6.199875	-2.366134	O	-2.882823	0.781078	-0.137756
H	6.240104	-5.582154	-2.709736	H	6.210036	-5.559445	-2.880715	C	-3.100770	-1.330834	1.060654
H	3.250616	-2.439853	2.823100	H	3.522627	-2.469249	2.830663	O	-3.591764	-2.681397	0.945876
O	7.633592	-0.244369	1.506901	O	7.867918	-0.307090	1.351038	C	-3.597056	-0.774257	2.386249
C	6.542318	-1.158570	1.245909	C	6.752956	-1.201209	1.123118	O	-5.007581	-0.576889	2.313511
C	7.068591	-2.206742	0.253162	C	7.221697	-2.243729	0.096096	C	-3.599748	1.931308	0.268315
C	7.524898	-1.517862	-1.035289	C	7.636807	-1.544719	-1.200941	C	-3.640816	2.935628	-0.890639
C	8.540938	-0.424518	-0.728155	C	8.682259	-0.471885	-0.920707	O	-4.189215	2.308805	-2.053229
C	8.020349	0.508076	0.373546	C	8.220308	0.453955	0.212258	C	-2.251676	3.484106	-1.185432
H	5.716276	-0.614266	0.775253	H	5.916812	-0.638321	0.693976	O	-2.412484	4.469392	-2.191612
H	7.915438	-2.744247	0.702686	H	8.077533	-2.799913	0.503924	C	-1.630258	4.033717	0.095847
H	6.638095	-1.048596	-1.489490	H	6.740393	-1.055142	-1.612828	O	-0.292193	4.439535	-0.219056
H	9.452835	-0.906257	-0.345143	H	9.600640	-0.972920	-0.580358	C	-1.630854	2.961834	1.191749
H	8.820774	1.172060	0.718725	H	9.043427	1.102245	0.533039	O	-2.997427	2.529292	1.395764
C	6.037795	-1.685760	2.601880	C	6.296701	-1.739001	2.491880	C	-1.078900	3.449932	2.540658
O	8.137691	-2.420071	-1.938525	O	8.197907	-2.444079	-2.139838	O	-1.346306	4.814182	2.814032
O	8.845024	0.352548	-1.881415	O	8.953111	0.315597	-2.075200	H	-0.882068	6.405768	-0.003062
O	6.947267	1.253291	-0.141141	O	7.138395	1.220069	-0.250289	H	0.995694	7.321437	-1.256275
H	6.061701	-2.776591	2.626799	H	6.307765	-2.830303	2.502639	H	0.673277	6.054971	-3.263536
O	4.688508	-1.317496	2.862523	O	4.963623	-1.357904	2.811003	H	1.984242	4.456435	-1.532806
H	6.711426	-1.307277	3.382099	H	7.005821	-1.378572	3.248834	H	3.785780	5.749571	-2.485561
H	7.534661	-3.176086	-2.065998	H	7.576172	-3.186686	-2.255745	H	3.279013	6.738040	0.009318
H	9.001349	-0.281863	-2.596787	H	9.070083	-0.311578	-2.804347	H	1.817414	4.253999	1.051276
H	4.624926	-0.337072	2.900792	H	4.911414	-0.377483	2.861966	H	2.690954	6.717070	2.601180
O	5.668637	4.375027	1.335131	O	5.949211	4.337461	1.306217	H	3.644038	5.208655	2.521150
C	5.697416	2.939826	1.150885	C	5.957249	2.904317	1.105312	H	2.020968	5.346444	4.314643
C	6.854467	2.639047	0.185359	C	7.076614	2.602494	0.096669	H	5.335638	6.337073	0.356764
C	6.618738	3.355896	-1.146418	C	6.804386	3.338743	-1.217549	H	7.234040	5.435418	-0.875380
C	6.404965	4.847768	-0.920180	C	6.612805	4.829695	-0.967168	H	6.193117	5.244971	-2.997623

C	5.340555	5.087769	0.158525	C	5.586857	5.065284	0.149091	H	5.459911	3.057704	-1.563866
H	4.759829	2.613419	0.687678	H	5.001239	2.592221	0.670845	H	7.542059	2.400391	-2.494567
H	7.798873	2.986793	0.627317	H	8.040431	2.932072	0.509633	H	7.910020	3.225449	0.252483
H	5.701001	2.937308	-1.588543	H	5.868172	2.934594	-1.633523	H	4.959337	2.801069	0.918941
H	7.349028	5.273050	-0.548391	H	7.572491	5.242675	-0.622605	H	5.935733	1.627933	2.625180
H	5.325428	6.144422	0.448305	H	5.587574	6.118883	0.450147	H	6.011371	3.266800	3.282298
C	5.777618	2.291096	2.545159	C	6.077844	2.238476	2.488346	H	8.091483	1.654976	2.352887
O	7.715039	3.217737	-2.032086	O	7.868902	3.200217	-2.141046	H	9.011242	1.501737	-0.021679
O	6.005872	5.511434	-2.114528	O	6.179413	5.510377	-2.139878	H	9.384365	-0.617569	-1.178674
O	4.091589	4.696901	-0.350364	O	4.319696	4.686107	-0.322153	H	8.263687	-0.024525	-3.206408
H	6.645850	1.633868	2.617879	H	6.936610	1.565706	2.520814	H	6.354122	-0.785625	-1.433577
O	4.646126	1.479095	2.835284	O	4.944004	1.441941	2.811167	H	7.206997	-2.958953	-2.255231
H	5.890044	3.095401	3.284263	H	6.231779	3.031684	3.231888	H	8.251859	-2.571407	0.143045
H	7.925546	2.268254	-2.106500	H	8.063013	2.249219	-2.237776	H	6.241184	-0.523654	1.188251
H	6.604684	5.196145	-2.807821	H	6.751893	5.197944	-2.856363	H	6.496267	-2.289727	2.743925
H	3.837659	2.038706	2.825577	H	4.145559	2.014683	2.843318	H	7.429096	-0.893662	3.349970
O	0.843827	5.736889	1.036561	O	1.122812	5.730415	1.176664	H	8.600173	-2.961727	3.392975
C	1.975907	4.845200	0.904779	C	2.251097	4.839806	1.008300	H	7.329204	-4.356598	0.833572
C	2.953840	5.512549	-0.074690	C	3.194953	5.504764	-0.005853	H	6.175400	-6.139645	-0.381120
C	2.268301	5.728162	-1.426511	C	2.463581	5.718464	-1.333456	H	6.426805	-5.286371	-2.572163
C	0.972663	6.511906	-1.250994	C	1.174452	6.501383	-1.115551	H	4.326139	-3.976393	-1.464382
C	0.100129	5.880328	-0.158461	C	0.339805	5.872695	0.007927	H	3.349635	-5.881053	-2.397048
H	1.642523	3.894784	0.473877	H	1.904032	3.887764	0.592037	H	3.757685	-6.226292	0.526472
H	3.274070	6.481801	0.332851	H	3.531798	6.473936	0.388300	H	3.910745	-3.203186	0.922831
H	2.019948	4.735129	-1.832704	H	2.202128	4.724388	-1.728924	H	2.375926	-3.794549	2.546370
H	1.232726	7.527147	-0.916304	H	1.444503	7.518010	-0.793459	H	3.909266	-4.067162	3.383005
H	-0.736016	6.542875	0.091821	H	-0.486646	6.536848	0.284556	H	1.959872	-5.854483	2.663519
C	2.508310	4.550996	2.319509	C	2.832374	4.551337	2.404609	H	1.960029	-7.015419	-0.131510
O	3.080696	6.455070	-2.330461	O	3.244177	6.443883	-2.265968	H	-0.056570	-6.979787	-1.498113
O	0.222926	6.571244	-2.459476	O	0.384237	6.556365	-2.298540	H	0.888311	-5.877631	-3.409263
O	-0.370482	4.643144	-0.624980	O	-0.149009	4.634161	-0.438322	H	0.294246	-3.958742	-1.623272
H	3.562357	4.822123	2.401376	H	3.893289	4.804577	2.442614	H	-1.794040	-4.282674	-2.756305
O	2.431252	3.170310	2.654071	O	2.745265	3.176009	2.758290	H	-1.937166	-5.536744	-0.281906
H	1.937424	5.164881	3.028621	H	2.299932	5.182850	3.128089	H	0.376203	-3.961076	0.964136
H	3.948660	6.012755	-2.379110	H	4.111709	6.004208	-2.340357	H	-1.530397	-5.885534	2.335194
H	0.855266	6.808320	-3.154134	H	0.992198	6.794200	-3.014439	H	-1.771234	-4.116966	2.306506
H	1.488873	2.888957	2.654574	H	1.799302	2.909432	2.784414	H	-0.437661	-5.010607	4.140862
O	-3.197239	2.766893	0.805067	O	-2.982093	2.830170	1.069721	H	-3.666937	-4.344449	-0.176304
C	-1.801875	3.123274	0.681028	C	-1.579025	3.145777	0.909246	H	-4.845816	-2.553377	-1.368836
C	-1.717968	4.267351	-0.341945	C	-1.494529	4.275133	-0.129399	H	-3.561021	-2.650018	-3.370860
C	-2.300101	3.812680	-1.682875	C	-2.102807	3.805916	-1.453038	H	-2.120896	-1.189280	-1.565301
C	-3.713934	3.277523	-1.497946	C	-3.523150	3.298312	-1.239673	H	-3.732849	0.455261	-2.452257
C	-3.753384	2.230627	-0.378290	C	-3.572346	2.280523	-0.091949	H	-4.638724	-0.335474	-0.081247
H	-1.238759	2.267006	0.293425	H	-1.051169	2.269288	0.517639	H	-2.002873	-1.343915	1.084658
H	-2.282644	5.134462	0.028585	H	-2.045179	5.152311	0.238474	H	-3.076684	0.173412	2.570710
H	-1.665813	2.993430	-2.055890	H	-1.487043	2.969304	-1.819162	H	-3.334986	-1.484202	3.183805
H	-4.362190	4.109599	-1.188583	H	-4.152736	4.151084	-0.948761	H	-5.278474	-0.013239	3.048493
H	-4.790145	1.979093	-0.132676	H	-4.611492	2.062805	0.177813	H	-4.611300	1.657687	0.582788
C	-1.274726	3.427736	2.094650	C	-1.002941	3.448545	2.304864	H	-4.286719	3.769883	-0.584127
O	-2.365464	4.868598	-2.625187	O	-2.167924	4.843145	-2.414974	H	-4.021028	2.931608	-2.778598

O	-4.214492	2.690067	-2.697896	O	-4.041242	2.691791	-2.423218	H	-1.618341	2.657901	-1.543840
H	-0.803378	4.411446	2.127583	H	-0.545892	4.439375	2.329184	H	-1.536110	4.842131	-2.407750
O	-0.280522	2.502263	2.519126	O	0.021264	2.535470	2.681423	H	-2.206198	4.890447	0.460771
H	-2.132594	3.432011	2.779907	H	-1.833623	3.433223	3.022699	H	-1.039599	2.097117	0.862943
H	-1.479104	5.270507	-2.687775	H	-1.281948	5.245122	-2.487184	H	-0.002347	3.253936	2.574704
H	-4.003794	3.315853	-3.407331	H	-3.816214	3.293669	-3.148933	H	-1.550594	2.835203	3.317809
H	-0.668728	1.599359	2.540436	H	-0.356165	1.628793	2.727612	H	-0.512811	5.292897	2.680856
C	-8.234730	-0.481727	4.419618	C	-8.832065	3.316671	-2.272658	C	-10.308207	-0.718132	3.670714
C	-7.147165	-1.183345	3.901906	C	-7.569519	2.726369	-2.286880	C	-9.024226	-1.257701	3.614813
C	-6.995399	-1.291148	2.521069	C	-7.384489	1.489757	-1.672828	C	-8.321572	-1.239117	2.411231
C	-7.917173	-0.715545	1.633863	C	-8.437839	0.818078	-1.035170	C	-8.879567	-0.694763	1.244285
C	-9.000372	0.014078	2.157584	C	-9.709349	1.420393	-1.011816	C	-10.165666	-0.126076	1.308491
C	-9.140704	0.117925	3.546863	C	-9.883985	2.663538	-1.633265	C	-10.859395	-0.148289	2.524823
C	-9.939040	0.778269	1.242341	C	-10.857260	0.798527	-0.238926	C	-10.756377	0.606736	0.118298
C	-9.156461	1.785202	0.432421	C	-10.484208	0.668397	1.218028	C	-9.849106	1.744886	-0.285506
C	-9.237759	3.157247	0.665292	C	-11.047786	1.470537	2.209012	C	-10.179569	3.080813	-0.063490
C	-8.496849	4.065236	-0.095663	C	-10.676153	1.332607	3.548649	C	-9.316277	4.110613	-0.445812
C	-7.653649	3.588006	-1.096222	C	-9.719194	0.382882	3.897334	C	-8.101763	3.794266	-1.050090
C	-7.546755	2.215076	-1.334578	C	-9.134357	-0.419307	2.915160	C	-7.745755	2.460791	-1.267108
C	-8.294639	1.300909	-0.576343	C	-9.506077	-0.286523	1.569704	C	-8.612088	1.424886	-0.886261
C	-7.693954	-1.013455	0.154069	C	-8.103949	-0.567341	-0.482719	C	-8.051120	-0.855294	-0.029462
N	-8.298119	-0.096143	-0.835735	N	-9.008044	-1.135712	0.541931	N	-8.346854	0.055183	-1.158089
C	-8.181666	-2.445024	-0.153109	C	-8.011182	-1.560580	-1.661585	C	-8.202592	-2.307769	-0.532193
C	-7.930265	-0.495929	-2.198665	C	-8.525900	-2.445865	0.978843	C	-7.455611	-0.212123	-2.289702
C	-8.400980	-1.919644	-2.478355	C	-8.454195	-3.408765	-0.200653	C	-7.613274	-1.652964	-2.763054
N	-7.817812	-2.844671	-1.509543	N	-7.558864	-2.879782	-1.224232	N	-7.327717	-2.579332	-1.670179
C	-8.183687	-4.227350	-1.785159	C	-7.406823	-3.798515	-2.345114	C	-7.407707	-3.969217	-2.099355
H	-8.368262	-0.385838	5.493198	H	-8.996948	4.281451	-2.743894	H	-10.870017	-0.723876	4.600378
H	-6.417772	-1.638491	4.565340	H	-6.723568	3.214510	-2.760068	H	-8.568541	-1.687766	4.502304
H	-6.140254	-1.828957	2.116278	H	-5.037569	-2.351023	-0.929928	H	-7.311698	-1.640064	2.371827
H	-9.974386	0.689933	3.946375	H	-10.866548	3.127918	-1.602811	H	-11.848849	0.299990	2.569543
H	-10.706157	1.281629	1.837825	H	-11.753231	1.416304	-0.348706	H	-11.750572	0.984296	0.374733
H	-10.444107	0.088331	0.554985	H	-11.084932	-0.198372	-0.636240	H	-10.863716	-0.077200	-0.732662
H	-9.904081	3.520563	1.443821	H	-11.800225	2.203421	1.928364	H	-11.134047	3.317911	0.400261
H	-8.583306	5.131401	0.090998	H	-11.133844	1.958292	4.308947	H	-9.594322	5.146564	-0.276378
H	-7.071365	4.278250	-1.700330	H	-9.417660	0.264216	4.934210	H	-7.420439	4.584859	-1.352842
H	-6.870028	1.866970	-2.107091	H	-8.383068	-1.146889	3.202368	H	-6.788087	2.234856	-1.724720
H	-6.600666	-1.026830	-0.5001273	H	-7.088445	-0.500163	-0.049203	H	-6.994437	-0.730757	0.264895
H	-9.275345	-2.487827	0.016371	H	-9.000486	-1.606182	-2.156915	H	-9.268119	-2.481337	-0.779431
H	-7.711307	-3.136790	0.552362	H	-7.289855	-1.172507	-2.386248	H	-7.936415	-2.990179	0.280578
H	-6.843277	-0.441337	-2.371661	H	-7.523928	-2.386683	1.441489	H	-6.394460	-0.040437	-2.049086
H	-8.419890	0.187973	-2.897513	H	-9.220817	-2.837241	1.726591	H	-7.727111	0.465272	-3.104156
H	-8.080416	-2.213568	-3.484517	H	-8.067572	-4.375313	0.143228	H	-6.905105	-1.840707	-3.578165
H	-9.507728	-1.951386	-2.454850	H	-9.475340	-3.575782	-0.594762	H	-8.636175	-1.799277	-3.161286
H	-9.273805	-4.408007	-1.731138	H	-8.350697	-3.971592	-2.895155	H	-8.406517	-4.249534	-2.483501
H	-7.695014	-4.890580	-1.064459	H	-6.666630	-3.406106	-3.048025	H	-7.172606	-4.629363	-1.258311
H	-7.843250	-4.505268	-2.787647	H	-7.042098	-4.764200	-1.981711	H	-6.672440	-4.151976	-2.889731
CR2				CR2				CR2			
E	-5082.89989015			E	-5082.90003218			E	-5082.87835718		
O	-3.317894	2.533513	3.471733	O	-4.547600	2.145499	3.560494	C	0.885648	5.743256	-1.840856

C	-2.901046	1.189298	3.136070	C	-3.615803	2.644706	2.573249	C	1.399517	5.589245	-3.276826
C	-3.012090	0.355564	4.421720	C	-4.263335	3.884488	1.939075	O	0.316749	5.752632	-4.187569
C	-2.115045	0.949855	5.510015	C	-5.585900	3.488807	1.276839	C	2.081342	4.238972	-3.469696
C	-2.441364	2.423376	5.723449	C	-6.495902	2.780218	2.274377	O	2.631474	4.238510	-4.773414
C	-2.453276	3.177219	4.387522	C	-5.745358	1.650645	2.992953	C	3.136049	3.980915	-2.386230
H	-1.854717	1.202529	2.812197	H	-3.475969	1.889517	1.792039	O	3.513801	2.610714	-2.547264
H	-4.055543	0.357255	4.767235	H	-4.450501	4.639005	2.715920	C	2.520984	4.220720	-1.000816
H	-1.073860	0.872224	5.159529	H	-5.348538	2.784096	0.464360	O	1.965974	5.546582	-0.950779
H	-3.455338	2.488254	6.145211	H	-6.794362	3.512085	3.039708	C	3.457026	4.114856	0.189663
H	-2.863536	4.184172	4.522973	H	-6.338362	1.274329	3.833972	O	2.629781	4.146876	1.341200
C	-3.753397	0.720542	1.942657	C	-2.256466	2.845691	3.265050	C	4.874377	2.249072	-2.580357
O	-2.558941	-0.985714	4.241314	O	-3.465483	4.440596	0.895663	C	5.136481	1.434052	-3.854756
O	-2.279471	0.299592	6.757017	O	-6.295424	4.609467	0.781652	O	4.722753	2.188698	-4.991550
O	-1.507385	3.050335	6.595685	O	-7.647901	2.233822	1.642246	C	4.419468	0.089656	-3.798719
O	-1.138696	3.239687	3.898959	O	-5.489300	0.624992	2.069098	O	4.819231	-0.632929	-4.948712
H	-4.301081	-0.190343	2.189814	H	-1.913507	3.876628	3.163286	C	4.764593	-0.627691	-2.496025
O	-2.967526	0.405400	0.799061	O	-1.239417	2.032227	2.684980	O	3.973503	-1.818899	-2.444158
H	-4.481641	1.510468	1.717989	H	-2.380541	2.623973	4.332538	C	4.461855	0.273599	-1.295949
H	-2.182584	-0.660541	6.614294	H	-5.692687	5.118723	0.208285	O	5.230518	1.489707	-1.442146
H	-1.404649	2.452867	7.351372	H	-7.997332	2.934618	1.071788	C	4.796752	-0.358790	0.061377
H	-2.503614	1.217373	0.495813	H	-1.474392	1.085647	2.817503	O	5.935222	-1.203250	0.063302
O	0.044297	5.587684	1.322672	O	-4.595121	-2.834049	2.965777	C	4.633305	-3.055590	-2.348836
C	-0.482458	4.321248	1.785240	C	-4.294621	-1.458999	2.630792	C	4.019186	-4.024966	-3.358512
C	-0.686682	4.454265	3.302325	C	-5.641153	-0.731635	2.484594	O	4.139224	-3.469868	-4.665754
C	0.647836	4.771533	3.981570	C	-6.469448	-1.396809	1.382094	C	2.563826	-4.309262	-3.012900
C	1.284928	6.007071	3.356993	C	-6.621831	-2.889574	1.647775	O	2.107808	-5.266509	-3.949353
C	1.332488	5.877939	1.828933	C	-5.258300	-3.539355	1.931008	C	2.453310	-4.790980	-1.567950
H	0.252624	3.531398	1.596790	H	-3.775064	-1.424134	1.666690	O	1.057636	-4.825126	-1.256216
H	-1.402790	5.263310	3.504137	H	-6.189304	-0.776879	3.436160	C	3.171936	-3.833447	-0.598928
H	1.316845	3.913467	3.811526	H	-5.920168	-1.268496	0.436128	O	4.531109	-3.595282	-1.038110
H	0.649983	6.873740	3.593567	H	-7.236020	-3.012932	2.552141	C	3.222585	-4.362959	0.824311
H	1.621080	6.832447	1.374649	H	-5.391284	-4.555750	2.303567	O	3.739583	-5.690083	0.811438
C	-1.734230	3.996923	0.948401	C	-3.327419	-0.923031	3.701208	C	0.514229	-5.976665	-0.641314
O	0.498761	5.029287	5.366041	O	-7.772288	-0.850383	1.287598	C	-0.572111	-6.563672	-1.552662
O	2.606488	6.221545	3.840852	O	-7.227146	-3.561549	0.548843	O	-0.027447	-6.837739	-2.842305
O	2.255335	4.872746	1.497454	O	-4.505362	-3.533085	0.746257	C	-1.757093	-5.612247	-1.659367
H	-2.606315	3.864466	1.591268	H	-3.711427	-0.004268	4.147379	O	-2.738202	-6.276656	-2.438112
O	-1.598241	2.785464	0.215225	O	-2.047873	-0.594323	3.166604	C	-2.251010	-5.246849	-0.262795
H	-1.923396	4.847780	0.280823	H	-3.242859	-1.682109	4.489454	O	-3.292565	-4.270966	-0.408482
H	0.013172	4.281811	5.762202	H	-7.687742	0.118026	1.210029	C	-1.104631	-4.683819	0.583797
H	2.556951	6.122233	4.803353	H	-7.993822	-3.025437	0.296943	O	-0.041122	-5.664638	0.618331
H	-0.878453	2.892327	-0.444201	H	-1.646006	-1.397220	2.761064	C	-1.508175	-4.365636	2.032438
O	3.793390	4.431077	-1.818036	O	-1.573874	-5.673469	0.120116	O	-2.489636	-5.238492	2.566533
C	2.783999	4.191946	-0.808609	C	-2.228088	-4.461255	0.563493	C	-4.593812	-4.647898	-0.048191
C	3.135216	5.080774	0.394432	C	-3.740843	-4.692473	0.417091	C	-5.579822	-4.199209	-1.129741
C	4.528926	4.722162	0.916058	C	-4.083437	-5.002303	-1.042199	O	-5.204798	-4.765740	-2.380275
C	5.558191	4.800262	-0.204933	C	-3.250205	-6.172213	-1.550764	C	-5.633774	-2.678647	-1.215089
C	5.086148	4.008522	-1.431543	C	-1.761997	-5.947333	-1.254549	O	-6.628340	-2.367508	-2.169899
H	2.827660	3.144120	-0.491940	H	-1.934117	-3.629815	-0.086600	C	-5.917214	-2.061675	0.158945
H	3.116887	6.136501	0.089057	H	-4.044179	-5.536913	1.051956	O	-5.723960	-0.652395	0.018863

H	4.487607	3.682021	1.275666	H	-3.829548	-4.111066	-1.637281	C	-4.945643	-2.629721	1.209297
H	5.649956	5.853210	-0.510046	H	-3.560867	-7.074357	-1.003132	O	-4.980740	-4.068173	1.189461
H	5.734491	4.215504	-2.290328	H	-1.192738	-6.862165	-1.453636	C	-5.266446	-2.222501	2.634850
C	1.406967	4.423776	-1.457492	C	-1.716174	-4.150406	1.982392	O	-4.169173	-2.638990	3.450786
O	4.958533	5.595449	1.944532	O	-5.445179	-5.351978	-1.210754	C	-6.752199	0.242500	0.390514
O	6.824999	4.297085	0.205730	O	-3.414891	-6.368483	-2.950917	C	-7.094775	1.145675	-0.800028
O	5.107237	2.640204	-1.114541	O	-1.300874	-4.892713	-2.058525	O	-7.488086	0.344416	-1.913116
H	0.835512	5.167426	-0.899481	H	-2.547925	-4.061790	2.683535	C	-5.912624	2.034444	-1.161928
O	0.607397	3.247033	-1.473741	O	-1.011847	-2.916245	2.056647	O	-6.347682	2.889979	-2.202659
H	1.573781	4.806277	-2.473270	H	-1.082456	-4.988077	2.301837	C	-5.434882	2.800256	0.066881
H	4.260787	5.625804	2.625543	H	-5.989871	-4.655012	-0.799821	O	-4.213269	3.434655	-0.316220
H	7.003362	4.697250	1.069895	H	-4.369023	-6.332341	-3.115244	C	-5.195740	1.850857	1.254551
H	1.065412	2.558693	-2.003256	H	-0.222536	-2.952425	1.471173	O	-6.363569	1.036330	1.489708
O	5.098382	-0.092810	-3.583088	O	2.238699	-4.233361	-2.822082	C	-4.871809	2.587943	2.544052
C	4.471385	0.855055	-2.687241	C	1.018479	-4.061489	-2.062951	O	-5.852943	3.594751	2.771740
C	5.593503	1.715649	-2.085635	C	-0.020628	-5.012129	-2.676801	C	-3.987978	4.779873	0.056259
C	6.587218	0.824789	-1.336003	C	-0.242458	-4.657042	-4.149313	C	-3.779787	5.619777	-1.211694
C	7.106809	-0.281178	-2.246525	C	1.081676	-4.653134	-4.904509	O	-4.889099	5.436166	-2.090642
C	5.944958	-1.016447	-2.927100	C	2.126295	-3.806383	-4.165900	C	-2.474382	5.247763	-1.903587
H	3.973365	0.313401	-1.875351	H	0.662007	-3.031884	-2.175543	O	-2.314294	6.151938	-2.983743
H	6.115838	2.251879	-2.890482	H	0.341112	-6.047091	-2.599075	C	-1.311680	5.287982	-0.911500
H	6.045038	0.358130	-0.498595	H	-0.663429	-3.639883	-4.183394	O	-0.150659	4.822596	-1.608880
H	7.707799	0.186713	-3.040357	H	1.458690	-5.686227	-4.933715	C	-1.633821	4.392522	0.290925
H	6.323754	-1.678714	-3.713513	H	3.118178	-3.954184	-4.607553	O	-2.855364	4.884468	0.891819
C	3.388239	1.601630	-3.487183	C	1.353898	-4.272899	-0.574978	C	-0.552758	4.329163	1.373120
O	7.710945	1.548991	-0.869924	O	-1.095678	-5.579204	-4.802421	O	0.108274	5.555409	1.627209
O	7.892378	-1.228649	-1.531564	O	0.934021	-4.147642	-6.227005	H	0.540359	6.766934	-1.665995
O	5.249519	-1.752650	-1.953815	O	1.743857	-2.457870	-4.247689	H	2.148241	6.378442	-3.438858
H	3.547520	2.680419	-3.446811	H	0.745643	-5.073743	-0.150662	H	0.639740	5.448190	-5.048786
O	2.078919	1.381755	-2.970488	O	1.083953	-3.117892	0.210546	H	1.316239	3.453873	-3.364022
H	3.460397	1.278759	-4.533917	H	2.409488	-4.566049	-0.504239	H	3.186432	3.440571	-4.874700
H	7.386890	2.319919	-0.367673	H	-1.911974	-5.662340	-4.274901	H	4.000308	4.639770	-2.548559
H	8.502143	-0.711404	-0.984461	H	0.156315	-4.591513	-6.596891	H	1.721521	3.483536	-0.859450
H	1.884972	0.417770	-2.979937	H	1.681802	-2.390539	-0.069203	H	4.163650	4.959448	0.170693
O	2.969383	-4.548602	-2.679277	O	3.974225	0.407328	-3.633233	H	4.031392	3.181959	0.118992
C	3.282315	-3.161888	-2.411831	C	3.014279	-0.603094	-3.241782	H	3.134787	4.025825	2.182792
C	4.809546	-3.070195	-2.277941	C	2.745946	-1.470084	-4.482038	H	5.511612	3.140013	-2.556958
C	5.275370	-3.956730	-1.119519	C	2.196557	-0.599835	-5.614729	H	6.217883	1.242635	-3.908387
C	4.773040	-5.385241	-1.301086	C	3.132600	0.568931	-5.895887	H	4.738810	1.565287	-5.734295
C	3.266403	-5.403775	-1.592114	C	3.477544	1.312836	-4.598815	H	3.333707	0.273256	-3.806934
H	2.833380	-2.867071	-1.456974	H	2.076960	-0.119585	-2.945164	H	4.430104	-1.528145	-4.906281
H	5.279844	-3.407246	-3.212282	H	3.681108	-1.948747	-4.805381	H	5.830745	-0.880287	-2.477995
H	4.834644	-3.549586	-0.195861	H	1.229104	-0.194891	-5.278565	H	3.396072	0.535779	-1.295649
H	5.279792	-5.812427	-2.179221	H	4.071693	0.163666	-6.300972	H	3.909334	-0.893689	0.420671
H	2.952275	-6.404746	-1.908206	H	4.286891	2.029862	-4.776496	H	4.984658	0.461876	0.761635
C	2.624316	-2.310264	-3.511519	C	3.576517	-1.328421	-2.006680	H	5.617228	-2.105790	-0.106198
O	6.686439	-4.016744	-1.022152	O	2.048906	-1.322184	-6.823662	H	5.706224	-2.938467	-2.531962
O	5.025952	-6.184798	-0.151364	O	2.560669	1.492196	-6.816374	H	4.580886	-4.968033	-3.299056
O	2.580988	-5.013487	-0.430513	O	2.325275	1.971491	-4.140002	H	3.552849	-3.998103	-5.228898
H	3.368258	-1.718993	-4.048318	H	3.594843	-2.407374	-2.168300	H	1.995981	-3.369867	-3.100226

O	1.690913	-1.376458	-2.975510	O	2.785326	-1.122345	-0.841676	H	1.276820	-5.661994	-3.618002
H	2.140774	-2.990136	-4.224486	H	4.607839	-0.985396	-1.853292	H	2.892466	-5.790167	-1.481137
H	7.026849	-3.102978	-0.996881	H	1.527083	-2.124025	-6.633709	H	2.627957	-2.880324	-0.590220
H	5.948244	-6.017329	0.093386	H	2.203064	0.958396	-7.541597	H	2.200564	-4.339754	1.223750
H	0.971734	-1.866697	-2.516936	H	2.766258	-0.164053	-0.629388	H	3.848072	-3.692412	1.430870
O	-1.000001	-5.601760	0.193383	O	2.314200	4.776021	-1.753011	H	3.651276	-6.047434	1.703411
C	0.126342	-4.820379	-0.269495	C	2.267659	3.376695	-2.118301	H	1.302772	-6.709082	-0.443764
C	1.376910	-5.694636	-0.081333	C	2.444096	3.303438	-3.643636	H	-0.920802	-7.499670	-1.093156
C	1.534237	-6.054713	1.398831	C	1.335329	4.096107	-4.339656	H	-0.796299	-7.011621	-3.408411
C	0.264549	-6.705946	1.934406	C	1.288424	5.524670	-3.812087	H	-1.420725	-4.689935	-2.156897
C	-0.968500	-5.862901	1.583352	C	1.243090	5.534687	-2.278916	H	-3.501411	-5.679093	-2.555459
H	0.231331	-3.926165	0.354904	H	1.287071	2.963583	-1.857142	H	-2.640015	-6.135419	0.245292
H	1.275590	-6.613293	-0.676007	H	3.421838	3.723712	-3.918817	H	-0.716823	-3.768064	0.118883
H	1.699124	-5.115124	1.949228	H	0.378593	3.606270	-4.099660	H	-1.843640	-3.324982	2.082487
H	0.146892	-7.680419	1.437557	H	2.216661	6.030619	-4.116281	H	-0.600587	-4.445145	2.642705
H	-1.885992	-6.421076	1.800653	H	1.389256	6.552697	-1.900946	H	-3.335018	-4.763295	2.536986
C	-0.189497	-4.350241	-1.700569	C	3.328842	2.645581	-1.275806	H	-4.658441	-5.729153	0.106420
O	2.598567	-6.962120	1.619061	O	1.527899	4.171537	-5.740248	H	-6.575290	-4.564302	-0.837205
O	0.314652	-6.877667	3.346257	O	0.158943	6.234270	-4.309567	H	-5.703123	-4.277530	-3.053449
O	-0.924194	-4.673300	2.327138	O	0.000767	5.026985	-1.865641	H	-4.645045	-2.316676	-1.537130
H	0.608440	-4.637723	-2.387217	H	4.025535	2.103665	-1.917506	H	-6.772861	-1.399841	-2.175280
O	-0.298990	-2.932636	-1.797914	O	2.767465	1.670331	-0.402198	H	-6.955927	-2.279586	0.444964
H	-1.116584	-4.841775	-2.022088	H	3.891813	3.402431	-0.714565	H	-3.934654	-2.282495	0.962309
H	3.400516	-6.591713	1.205919	H	1.666406	3.266347	-6.076679	H	-6.197237	-2.719291	2.942297
H	1.182077	-7.264373	3.537778	H	0.128461	6.054375	-5.261127	H	-5.415456	-1.136324	2.681432
H	-1.050704	-2.618764	-1.245994	H	2.135857	2.111431	0.208094	H	-4.458486	-2.662073	4.370884
O	-3.801380	-2.449967	2.921631	O	-1.479777	5.519272	1.467515	H	-7.639158	-0.310014	0.719964
C	-2.645321	-2.914980	2.186075	C	-0.707303	4.796763	0.479923	H	-7.931805	1.788481	-0.493429
C	-2.130468	-4.173977	2.903212	C	-0.675464	5.667251	-0.785487	H	-7.499945	0.945871	-2.674000
C	-1.772432	-3.840829	4.353168	C	-2.101754	5.916240	-1.282590	H	-5.085757	1.391406	-1.502073
C	-2.954313	-3.193043	5.062468	C	-2.957499	6.512684	-0.171301	H	-5.729927	3.645175	-2.264330
C	-3.505241	-2.022584	4.237269	C	-2.839549	5.679170	1.111079	H	-6.186002	3.546074	0.347006
H	-1.860905	-2.150319	2.216591	H	-1.212573	3.853816	0.243395	H	-4.345412	1.198806	1.014045
H	-2.907667	-4.951012	2.885948	H	-0.194683	6.628300	-0.554680	H	-3.871949	3.027128	2.436694
H	-0.943575	-3.116110	4.329692	H	-2.528971	4.940782	-1.563491	H	-4.848475	1.855967	3.364612
H	-3.755427	-3.942396	5.145349	H	-2.569784	7.517329	0.053864	H	-5.545167	4.146672	3.501067
H	-4.457296	-1.678241	4.656222	H	-3.304669	6.206016	1.951702	H	-4.829455	5.155798	0.645801
C	-3.075841	-3.096708	0.720366	C	0.654398	4.452635	1.112431	H	-3.718661	6.674136	-0.905502
O	-1.415427	-4.993321	5.094438	O	-2.140823	6.818486	-2.372808	H	-4.615588	5.839346	-2.929639
O	-2.595468	-2.715385	6.354484	O	-4.329148	6.589013	-0.543479	H	-2.561238	4.213723	-2.271628
H	-2.794863	-4.086187	0.356510	H	1.474498	4.874135	0.528406	H	-1.512821	5.900606	-3.481430
O	-2.455269	-2.168861	-0.165122	O	0.891387	3.048845	1.163148	H	-1.149420	6.307279	-0.544716
H	-4.169600	-3.013675	0.677894	H	0.680175	4.895594	2.116573	H	-1.811743	3.366375	-0.057332
H	-0.723005	-5.468463	4.598610	H	-1.524393	6.495296	-3.056472	H	0.173961	3.565333	1.080627
H	-2.097608	-3.432231	6.775261	H	-4.342939	6.967439	-1.435280	H	-1.048473	3.981315	2.290374
H	-2.632348	-1.249051	0.136878	H	0.179730	2.626573	1.691918	H	1.026396	5.427821	1.328823
C	-1.336639	1.199143	-3.917993	C	1.379515	-0.906605	4.142251	C	-1.072981	-0.865557	3.931552
C	-1.636796	-0.134543	-3.643506	C	1.688089	0.363103	3.656287	C	-0.832981	0.032952	2.892535
C	-2.964982	-0.516941	-3.467686	C	3.016787	0.696480	3.401826	C	0.376434	0.722262	2.843720
C	-4.017032	0.404456	-3.566472	C	4.060650	-0.211361	3.628163	C	1.365234	0.543239	3.821188

C	-3.713971	1.744994	-3.870483	C	3.749882	-1.481065	4.150720	C	1.135279	-0.382529	4.856218
C	-2.375582	2.120659	-4.036243	C	2.410928	-1.809272	4.394306	C	-0.083354	-1.072095	4.892313
C	-4.817662	2.752844	-4.131261	C	4.849273	-2.443780	4.558641	C	2.229265	-0.723131	5.851751
C	-5.667363	2.289649	-5.290548	C	5.719254	-1.804321	5.614654	C	3.437076	-1.254309	5.115721
C	-5.632516	2.908141	-6.539100	C	5.697628	-2.207798	6.948528	C	3.799538	-2.600060	5.148337
C	-6.426813	2.452707	-7.594645	C	6.511033	-1.592755	7.903870	C	4.907326	-3.067474	4.435381
C	-7.260839	1.355064	-7.396861	C	7.351106	-0.551700	7.516614	C	5.656059	-2.174923	3.670904
C	-7.296968	0.713908	-6.156817	C	7.374288	-0.124313	6.187396	C	5.302684	-0.824315	3.623002
C	-6.504062	1.168953	-5.093423	C	6.562180	-0.740230	5.224226	C	4.194181	-0.350924	4.338100
C	-5.410792	-0.126237	-3.241441	C	5.452788	0.236983	3.193705	C	2.583879	1.456190	3.711986
N	-6.571614	0.614249	-3.788251	N	6.615562	-0.409600	3.845146	N	3.830081	1.024828	4.382892
C	-5.572405	-0.207981	-1.707862	C	5.589536	0.045354	1.667371	C	2.206339	2.850991	4.252414
C	-7.818985	-0.059022	-3.432786	C	7.862328	0.180004	3.363145	C	4.902825	1.985060	4.129355
C	-7.962474	-0.134898	-1.916074	C	7.984467	-0.012559	1.854808	C	4.520029	3.368444	4.650182
N	-6.831649	-0.849285	-1.337307	N	6.849565	0.596110	1.172202	N	3.280170	3.825579	4.015499
C	-6.965178	-0.996864	0.102646	C	6.963133	0.476879	-0.272009	C	2.883580	5.166610	4.456440
H	-0.305303	1.515202	-4.042237	H	0.346204	-1.183495	4.325640	H	-2.011134	-1.411392	3.974065
H	-0.846667	-0.874021	-3.572056	H	0.902498	1.091406	3.484590	H	-1.579128	0.192239	2.119199
H	-3.190855	-1.554938	-3.236343	H	3.248024	1.683905	3.009680	H	0.563561	1.420946	2.032313
H	-2.149678	3.157871	-4.271082	H	2.179495	-2.791740	4.798468	H	-0.250131	-1.793742	5.688214
H	-4.379927	3.731839	-4.347234	H	4.407337	-3.369564	4.938519	H	-1.465479	-1.465479	6.565411
H	-5.455994	2.856722	-3.244996	H	5.474043	-2.698172	3.693345	H	2.522048	0.170496	6.416609
H	-4.984603	3.769639	-6.681502	H	5.044987	-3.027225	7.239817	H	3.213562	-3.288628	5.752156
H	-6.394942	2.954180	-8.557314	H	6.489141	-1.928098	8.936461	H	5.184648	-4.116411	4.484866
H	-7.882948	0.986734	-8.207871	H	7.988019	-0.061177	8.247460	H	6.512708	-2.518495	3.099392
H	-7.941931	-0.147788	-6.021763	H	8.024067	0.696564	5.903209	H	5.893145	-0.150632	3.012810
H	-5.454349	-1.164907	-3.616555	H	5.512701	1.324873	3.378984	H	2.788314	1.587080	2.633679
H	-5.487760	0.816181	-1.294429	H	5.488376	-1.034809	1.442717	H	1.973036	2.764660	5.328286
H	-4.745131	-0.792448	-1.295676	H	4.763675	0.561964	1.169131	H	1.308620	3.203739	3.739543
H	-7.870579	-1.083903	-3.842894	H	7.926593	1.260149	3.587746	H	5.142812	2.068126	3.053118
H	-8.652647	0.514040	-3.847459	H	8.697868	-0.319594	3.860694	H	5.804186	1.643265	4.644685
H	-8.885774	-0.671546	-1.1665886	H	8.906861	0.464740	1.501738	H	5.319066	4.081381	4.418195
H	-8.052505	0.893530	-1.512703	H	8.064064	-1.096591	1.637929	H	4.410399	3.326641	5.748336
H	-6.992544	-0.029354	0.641522	H	7.007277	-0.573911	-0.621039	H	2.664955	5.206833	5.536598
H	-6.125823	-1.577076	0.498921	H	6.103634	0.952810	-0.753488	H	1.992665	5.478499	3.903593
H	-7.889919	-1.536291	0.334483	H	7.871802	0.982394	-0.616700	H	3.690146	5.874077	4.241915
NR2				NR2				NR2			
E	-5082.90212451			E	-5082.90014023			E	-5082.86536272		
O	5.440968	1.990133	2.065081	O	-3.600556	1.418589	3.752336	C	-1.324349	-6.239363	-0.314768
C	4.901635	0.722633	1.620150	C	-2.999874	0.203554	3.246925	C	-2.270024	-6.386635	-1.509965
C	6.060532	-0.053014	0.974800	C	-2.965043	-0.796403	4.413748	O	-1.520804	-6.749358	-2.664580
C	6.627058	0.745180	-0.202193	C	-2.150253	-0.219766	5.573866	C	-3.043538	-5.095849	-1.747149
C	7.019750	2.149894	0.239265	C	-2.688995	1.147537	5.976374	O	-3.947526	-5.354693	-2.802598
C	5.871017	2.820214	1.004518	C	-2.827929	2.058314	4.749792	C	-3.746802	-4.631218	-0.468321
H	4.134938	0.900833	0.858285	H	-1.972485	0.409691	2.927174	O	-4.232185	-3.314711	-0.738853
H	6.850589	-0.221212	1.720214	H	-3.991316	-0.997173	4.752374	C	-2.755938	-4.599715	0.709202
H	5.828202	0.830601	-0.955545	H	-1.114701	-0.094282	5.220766	O	-2.088386	-5.871197	0.827420
H	7.869093	2.063695	0.933089	H	-3.696215	1.005984	6.395540	C	-3.404174	-4.327293	2.053759
H	6.217236	3.747427	1.474802	H	-3.380496	2.967303	5.012343	O	-2.358403	-4.023842	2.978718
C	4.210766	0.056018	2.823681	C	-3.801797	-0.226336	2.005188	C	-5.588265	-2.997296	-0.507467

O	5.638604	-1.296136	0.416817	O	-2.316851	-2.019094	4.065129	C	-6.201044	-2.438352	-1.798278
O	7.780807	0.139416	-0.756178	O	-2.196653	-1.044607	6.723867	O	-6.033208	-3.378668	-2.857039
O	7.373352	2.971181	-0.868538	O	-1.847509	1.786721	6.930021	C	-5.580109	-1.094195	-2.158395
O	4.827290	3.083335	0.102005	O	-1.543711	2.377023	4.281725	O	-6.283464	-0.617242	-3.290106
H	4.607836	-0.946607	2.990787	H	-4.177978	-1.244447	2.118722	C	-5.665206	-0.151323	-0.961299
O	2.810989	-0.105098	2.626859	O	-3.015852	-0.234225	0.816878	O	-4.964167	1.045426	-1.312914
H	4.420951	0.663610	3.713737	H	-4.659105	0.451852	1.906952	C	-5.037676	-0.798891	0.277261
H	7.566350	-0.790941	-0.955997	H	-1.955102	-1.951131	6.456924	O	-5.719336	-2.051375	0.532306
H	7.972380	2.439474	-1.413695	H	-1.646131	1.116915	7.600429	C	-5.126825	0.068458	1.544232
H	2.394585	0.780512	2.550542	H	-2.677894	0.673816	0.642474	O	-6.260974	0.915133	1.609680
O	2.091277	5.478717	0.690798	O	-0.751597	5.204013	2.062055	C	-5.662164	2.265160	-1.277117
C	2.715478	4.174431	0.747792	C	-1.077160	3.822015	2.342282	C	-5.403990	3.030097	-2.575030
C	4.138256	4.329197	0.186838	C	-1.281570	3.715214	3.861217	O	-5.813034	2.225935	-3.678796
C	4.079043	4.854051	-1.249700	C	-0.001701	4.132245	4.589906	C	-3.936336	3.418026	-2.692770
C	3.267371	6.141597	-1.316837	C	0.436662	5.522440	4.144832	O	-3.818640	4.182293	-3.877207
C	1.909859	5.964470	-0.624450	C	0.485480	5.611057	2.613985	C	-3.496401	4.179094	-1.444288
H	2.162503	3.477179	0.108327	H	-0.234669	3.184273	2.054028	O	-2.077407	4.327825	-1.535321
H	4.705058	5.033673	0.811906	H	-2.107247	4.374249	4.164494	C	-3.853713	3.402592	-0.163214
H	3.568841	4.091054	-1.858386	H	0.785934	3.414832	4.311181	O	-5.259742	3.054170	-0.166103
H	3.816807	6.919596	-0.766352	H	-0.318036	6.243958	4.491381	C	-3.564388	4.190407	1.103200
H	1.411391	6.933972	-0.514353	H	0.623404	6.650752	2.296607	O	-4.172257	5.474472	1.005633
C	2.604165	3.674634	2.199217	C	-2.275949	3.430542	1.457861	C	-1.500091	5.598258	-1.302661
O	5.364892	5.138745	-1.769436	O	-0.172088	4.175392	5.995079	C	-0.759887	6.050060	-2.568358
O	3.046447	6.556544	-2.660527	O	1.716599	5.864424	4.665700	O	-1.655581	6.055406	-3.678923
O	1.124305	5.089492	-1.392685	O	1.543346	4.809071	2.156854	C	0.432937	5.144393	-2.844303
H	3.583775	3.395227	2.590098	H	-3.117303	3.098272	2.068867	O	1.101121	5.690060	-3.969576
O	1.792869	2.509851	2.322031	O	-1.973257	2.349734	0.583863	C	1.319071	5.064716	-1.604850
H	2.209279	4.498225	2.808290	H	-2.586954	4.321450	0.896978	O	2.357696	4.112898	-1.875128
H	5.925879	4.352077	-1.635385	H	-0.538172	3.318105	6.282425	C	0.502568	4.629045	-0.383047
H	3.903929	6.486878	-3.106153	H	1.693396	5.628733	5.605178	O	-0.599400	5.553814	-0.217567
H	0.897270	2.696049	1.963474	H	-1.287377	2.641228	-0.055886	C	1.312617	4.614565	0.924413
O	-2.537843	4.800513	-1.165628	O	3.089597	5.055723	-1.174697	O	2.338149	5.592420	0.984265
C	-1.180264	4.424675	-0.836746	C	2.142493	4.528470	-0.215320	C	3.674582	4.584026	-1.966982
C	-0.255219	5.398364	-1.582859	C	2.367657	5.293222	1.098166	C	4.352420	3.976048	-3.197002
C	-0.499028	5.293818	-3.090632	C	3.806204	5.087175	1.578915	O	3.613707	4.315424	-4.365490
C	-1.974067	5.510810	-3.408496	C	4.797345	5.472057	0.487281	C	4.473508	2.463471	-3.052677
C	-2.857594	4.614085	-2.531566	C	4.436761	4.788849	-0.838485	O	5.182205	2.011468	-4.188633
H	-0.986164	3.409284	-1.199737	H	2.352524	3.467442	-0.042310	C	5.159202	2.089065	-1.733908
H	-0.462142	6.424884	-1.249043	H	2.183743	6.364547	0.935124	O	5.001876	0.676354	-1.573990
H	-0.223782	4.273425	-3.400379	H	3.929871	4.014473	1.795477	C	4.494181	2.823800	-0.556261
H	-2.223147	6.554416	-3.165146	H	4.722886	6.557925	0.327342	O	4.432376	4.237821	-0.816187
H	-3.909663	4.903983	-2.629682	H	5.034772	5.205975	-1.656516	C	5.225923	2.668078	0.762901
C	-1.063503	4.405079	0.698100	C	0.736834	4.625561	-0.836877	O	4.357982	3.168738	1.782514
O	0.233754	6.259727	-3.821604	O	4.109414	5.870660	2.718900	C	6.140661	-0.140091	-1.378369
O	-2.264637	5.244259	-4.776000	O	6.131282	5.118861	0.837534	C	6.197751	-1.211869	-2.472443
O	-2.672285	3.280368	-2.927047	O	4.671678	3.410271	-0.707271	O	6.219172	-0.594134	-3.758166
H	-0.282088	5.085989	1.040261	H	0.066225	5.194495	-0.190600	C	5.023950	-2.174899	-2.355138
O	-0.707960	3.119517	1.201755	O	0.129308	3.350929	-1.008393	O	5.211539	-3.156019	-3.357432
H	-2.022533	4.740876	1.112831	H	0.827297	5.156313	-1.793861	C	4.975524	-2.759088	-0.947500
H	1.170521	6.195026	-3.556918	H	3.425007	5.700168	3.392690	O	3.759980	-3.505530	-0.851443

H	-1.576284	5.694520	-5.287966	H	6.256322	5.422268	1.749155	C	4.993677	-1.641447	0.109679
H	-1.380485	2.460530	0.915703	H	0.658588	2.832742	-1.652365	O	6.115219	-0.757596	-0.111916
O	-4.962524	0.509442	-2.140843	O	5.049270	1.063732	-3.520955	C	5.093374	-2.179657	1.527566
C	-3.800782	1.341171	-1.910496	C	4.294588	1.783782	-2.517509	O	6.177343	-3.099221	1.615631
C	-3.810563	2.422692	-3.001591	C	5.282311	2.707881	-1.788092	C	3.801046	-4.815276	-0.320406
C	-3.734632	1.761958	-4.380670	C	6.399308	1.878293	-1.150222	C	3.274059	-5.797941	-1.374073
C	-4.846343	0.731815	-4.546586	C	7.070606	0.992664	-2.192629	O	4.024480	-5.660525	-2.579911
C	-4.886056	-0.224900	-3.347338	C	6.024915	0.194005	-2.981580	C	1.790002	-5.571762	-1.632195
H	-2.894528	0.737971	-2.031443	H	3.881203	1.072849	-1.793498	O	1.380879	-6.585915	-2.533705
H	-4.734371	3.012937	-2.924814	H	5.716835	3.419438	-2.504434	C	1.025723	-5.603237	-0.312063
H	-2.767417	1.238711	-4.440821	H	5.935185	1.229067	-0.391234	O	-0.342753	-5.283012	-0.605786
H	-5.806209	1.269020	-4.567887	H	7.592394	1.645341	-2.908180	C	1.621535	-4.598241	0.680748
H	-5.792436	-0.839904	-3.379603	H	6.492357	-0.294887	-3.843611	O	3.025099	-4.915154	0.853949
C	-3.836062	1.823396	-0.450837	C	3.114621	2.470031	-3.230139	C	0.952558	-4.626007	2.066204
O	-3.868098	2.698434	-5.434459	O	7.407100	2.689054	-0.574142	O	0.427028	-5.892041	2.435674
O	-4.684555	-0.032038	-5.736523	O	7.990612	0.082730	-1.599264	H	-0.870257	-7.201675	-0.060269
O	-3.737831	-1.032683	-3.385436	O	5.450287	-0.759495	-2.124880	H	-2.988628	-7.182357	-1.264830
H	-3.820048	2.913575	-0.402639	H	3.113232	3.543622	-3.034799	H	-2.113390	-6.608585	-3.418953
O	-2.687912	1.381651	0.277036	O	1.850014	1.992143	-2.783182	H	-2.322801	-4.310969	-2.024202
H	-4.755564	1.469404	0.029299	H	3.238797	2.314075	-4.309887	H	-4.538219	-4.582217	-2.908479
H	-3.211561	3.405992	-5.294318	H	6.975191	3.332171	0.018643	H	-4.581938	-5.310783	-0.247041
H	-4.497915	0.607259	-6.440178	H	8.519862	0.605187	-0.978287	H	-2.014742	-3.816242	0.510265
H	-2.732785	0.404148	0.368982	H	1.803655	1.020186	-2.923731	H	-3.962195	-5.222475	2.361820
O	-3.325551	-4.188685	-1.528461	O	3.604882	-3.739764	-3.245521	H	-4.107262	-3.490328	1.956669
C	-3.239170	-2.753272	-1.689596	C	3.711809	-2.369528	-2.793716	H	-2.684906	-4.167083	3.875135
C	-3.852521	-2.416624	-3.059212	C	5.209273	-2.072677	-2.626660	H	-6.138112	-3.885299	-0.176142
C	-3.089552	-3.148779	-4.165726	C	5.808409	-3.027209	-1.590060	H	-7.272760	-2.280753	-1.610689
C	-3.042593	-4.645445	-3.887222	C	5.523049	-4.476708	-1.968429	H	-6.256006	-2.894574	-3.667715
C	-2.548538	-4.915738	-2.459836	C	4.033754	-4.678762	-2.278295	H	-4.515675	-1.251397	-2.393164
H	-2.186657	-2.448077	-1.692920	H	3.228413	-2.272239	-1.815464	H	-5.973262	0.286538	-3.496335
H	-4.908090	-2.722975	-3.075118	H	5.718999	-2.209014	-3.590738	H	-6.713538	0.075829	-0.738322
H	-2.057636	-2.764029	-4.163729	H	5.317236	-2.817629	-0.626783	H	-3.980287	-1.016028	0.079193
H	-4.067746	-5.038048	-3.959223	H	6.081140	-4.701705	-2.889469	H	-4.198218	0.644103	1.635634
H	-2.692856	-5.971059	-2.202782	H	3.869111	-5.663937	-2.728742	H	-5.170370	-0.616209	2.398138
C	-3.915075	-2.113327	-0.464742	C	2.931627	-1.485044	-3.782505	H	-6.000859	1.769260	1.225562
O	-3.691451	-2.973534	-5.435544	O	7.213310	-2.890250	-1.481191	H	-6.734353	2.093977	-1.138982
O	-2.192393	-5.325844	-4.803983	O	5.900964	-5.377708	-0.933600	H	-6.003255	3.951009	-2.541942
O	-1.190543	-4.569005	-2.380260	O	3.307331	-4.553399	-1.083026	H	-5.438147	2.652088	-4.464945
H	-4.649341	-1.368197	-0.773751	H	3.581234	-0.732437	-4.232981	H	-3.335972	2.496919	-2.756090
O	-2.998609	-1.425270	0.383654	O	1.882171	-0.766731	-3.141477	H	-2.976646	4.679720	-3.851967
H	-4.438515	-2.908746	0.082182	H	2.542252	-2.130113	-4.580660	H	-3.986237	5.158082	-1.420706
H	-3.815324	-2.017114	-5.579797	H	7.414494	-1.947638	-1.330779	H	-3.257567	2.481676	-0.136389
H	-2.427211	-4.993393	-5.683216	H	6.788774	-5.107745	-0.655193	H	-2.474520	4.272946	1.200076
H	-2.290249	-2.043549	0.678447	H	1.246643	-1.407720	-2.751575	H	-3.946221	3.626023	1.966548
O	1.118172	-5.771911	0.223632	O	-0.142961	-5.736385	-0.579904	H	-3.850095	6.009263	1.741367
C	0.176859	-4.832955	-0.347245	C	0.854614	-4.743476	-0.915534	H	-2.272627	6.318849	-1.017594
C	-0.302588	-5.436641	-1.676170	C	2.220145	-5.445357	-0.842942	H	-0.387670	7.069047	-2.389968
C	0.889529	-5.650880	-2.611882	C	2.445093	-5.984242	0.572606	H	-1.086955	6.152162	-4.459507
C	1.961429	-6.490305	-1.926453	C	1.288906	-6.881767	0.997972	H	0.059214	4.132646	-3.063334
C	2.297742	-5.919456	-0.542819	C	-0.057435	-6.185210	0.758673	H	1.855526	5.112678	-4.195588

H	0.687629	-3.886321	-0.554369	H	0.836687	-3.942531	-0.168212	H	1.756788	6.044776	-1.388372
H	-0.793101	-6.400989	-1.482301	H	2.245181	-6.275499	-1.562698	H	0.091182	3.625658	-0.551805
H	1.315541	-4.660505	-2.876757	H	2.477962	-5.118066	1.252025	H	1.722147	3.610730	1.072347
H	1.554209	-7.500781	-1.773568	H	1.307940	-7.782565	0.366688	H	0.604187	4.803574	1.740051
H	2.926796	-6.621728	0.015495	H	-0.881663	-6.895826	0.886319	H	3.173152	5.136015	0.795529
C	-0.906239	-4.553197	0.711210	C	0.460090	-4.121399	-2.266726	H	3.697644	5.676999	-2.012548
O	0.524722	-6.326835	-3.801455	O	3.632098	-6.749544	0.672922	H	5.364926	4.401088	-3.258206
O	3.155514	-6.555437	-2.698574	O	1.379486	-7.243312	2.371557	H	3.935766	3.724210	-5.063213
O	2.958050	-4.692424	-0.714940	O	-0.177289	-5.119638	1.664891	H	3.457554	2.040157	-3.022473
H	-1.897572	-4.805654	0.330484	H	1.278217	-4.201345	-2.984439	H	5.377989	1.058321	-4.083190
O	-0.965967	-3.179702	1.075640	O	0.166705	-2.731304	-2.156711	H	6.224706	2.351720	-1.795131
H	-0.698367	-5.187127	1.582944	H	-0.400606	-4.678130	-2.658882	H	3.476961	2.430235	-0.442246
H	-0.234695	-5.858530	-4.195815	H	4.367774	-6.210846	0.326917	H	6.160519	3.244574	0.719966
H	2.877053	-6.753348	-3.605152	H	2.296457	-7.521689	2.514310	H	5.468968	1.610185	0.924357
H	-0.113550	-2.918727	1.489592	H	-0.609232	-2.607819	-1.564820	H	4.873739	3.331306	2.581645
O	4.986006	-3.009456	1.854730	O	-3.344305	-3.460256	2.551070	H	7.050796	0.469854	-1.393833
C	3.763385	-3.262766	1.122591	C	-2.140491	-3.631501	1.766683	H	7.126176	-1.780890	-2.323070
C	4.071171	-4.389769	0.124476	C	-1.434957	-4.889818	2.298281	H	6.051938	-1.311812	-4.389419
C	5.191149	-3.951402	-0.822535	C	-1.107658	-4.714265	3.783293	H	4.091239	-1.613754	-2.523732
C	6.416004	-3.506166	-0.032341	C	-2.359871	-4.352699	4.572051	H	4.653038	-3.931901	-3.149879
C	6.024765	-2.489486	1.048263	C	-3.095308	-3.177615	3.914488	H	5.840449	-3.412812	-0.793733
H	3.482731	-2.364533	0.561965	H	-1.479575	-2.771095	1.920307	H	4.060701	-1.069154	0.035056
H	4.385061	-5.288283	0.674156	H	-2.090132	-5.762421	2.166397	H	4.139971	-2.666987	1.764038
H	4.818131	-3.089529	-1.397759	H	-0.394089	-3.879439	3.865943	H	5.233063	-1.329151	2.211676
H	6.828143	-4.387697	0.480817	H	-3.038576	-5.218189	4.549042	H	6.064659	-3.610012	2.426413
H	6.866441	-2.312404	1.727199	H	-4.081328	-3.042700	4.372905	H	4.822455	-5.070248	-0.021905
C	2.646842	-3.534138	2.147848	C	-2.553302	-3.647982	0.283995	H	3.402037	-6.813926	-0.973944
O	5.604411	-4.994558	-1.686480	O	-0.574201	-5.893730	4.356930	H	3.526767	-6.159527	-3.246724
O	7.404443	-2.923144	-0.874690	O	-2.053097	-4.006237	5.918078	H	1.661151	-4.573713	-2.078902
H	2.188883	-4.509292	1.972733	H	-2.164525	-4.536270	-0.216423	H	0.421097	-6.498877	-2.690446
O	1.591726	-2.583114	2.064105	O	-2.040455	-2.536153	-0.444511	H	1.086920	-6.600998	0.134722
H	3.099786	-3.539855	3.147861	H	-3.649778	-3.677764	0.240184	H	1.543749	-3.582159	0.274052
H	4.813191	-5.346677	-2.135310	H	0.171070	-6.189125	3.801479	H	0.172632	-3.859561	2.098549
H	7.493581	-3.519751	-1.632873	H	-1.449218	-4.692326	6.239527	H	1.720410	-4.345186	2.796512
H	1.941054	-1.696539	2.302362	H	-2.364149	-1.700741	-0.038764	H	-0.525609	-5.858161	2.253113
C	-3.979999	-3.853432	5.700884	C	-6.822098	3.024992	-7.059828	C	-3.732150	1.741467	4.883445
C	-4.093232	-3.722697	4.318173	C	-7.352456	1.740173	-7.160547	C	-3.019914	2.912912	5.137628
C	-4.102810	-2.451306	3.748016	C	-7.160615	0.837466	-6.116915	C	-1.626387	2.885297	5.120306
C	-4.010738	-1.292165	4.531338	C	-6.451784	1.185985	-4.958338	C	-0.913334	1.707182	4.855496
C	-3.858053	-1.426939	5.925270	C	-5.898194	2.477550	-4.868568	C	-1.634242	0.529787	4.576160
C	-3.848619	-2.709680	6.486420	C	-6.094350	3.376125	-5.924546	C	-3.033595	0.568553	4.600348
C	-3.574775	-0.220154	6.802259	C	-5.006120	2.866295	-3.704523	C	-0.925360	-0.736950	4.133605
C	-2.317339	0.466257	6.321645	C	-3.817369	1.937161	-3.635913	C	-0.131964	-0.455296	2.879622
C	-1.110479	0.401073	7.016470	C	-2.526720	2.346010	-3.967803	C	-0.934064	-0.934064	1.627446
C	0.040514	1.018151	6.519507	C	-1.449092	1.458962	-3.904410	C	0.231249	-0.647200	0.482585
C	-0.017102	1.703773	5.307918	C	-1.673089	0.141492	-3.509238	C	1.377747	0.138205	0.595097
C	-1.217724	1.776477	4.597871	C	-2.960201	-0.285820	-3.175379	C	1.770871	0.639259	1.839763
C	-2.373539	1.157757	5.092891	C	-4.043261	0.602286	-3.237747	C	1.019880	0.352182	2.989720
C	-4.173221	0.032710	3.788515	C	-6.424997	0.138950	-3.846569	C	0.605946	1.797830	4.984843
N	-3.639714	1.244857	4.449290	N	-5.359719	0.249471	-2.828292	N	1.410381	0.767387	4.291363

C	-5.676655	0.259239	3.516711	C	-7.787754	0.160348	-3.118661	C	0.978399	1.770423	6.483451
C	-3.851440	2.423680	3.607456	C	-5.456866	-0.843590	-1.860588	C	2.839808	1.008978	4.488510
C	-5.342442	2.628104	3.358251	C	-6.809930	-0.807671	-1.157733	C	3.180904	0.981407	5.975077
N	-5.910843	1.451859	2.704795	N	-7.888932	-0.910012	-2.133357	N	2.405824	1.991128	6.685009
C	-7.325442	1.626280	2.407911	C	-9.198970	-0.944290	-1.503210	C	2.750934	2.057829	8.097131
H	-3.970691	-4.836075	6.163931	H	-6.958519	3.743005	-7.863395	H	-4.818070	1.740647	4.886275
H	-4.164862	-4.602129	3.684720	H	-7.905871	1.438440	-8.044981	H	-3.542371	3.841305	5.349180
H	-4.163175	-2.344746	2.668178	H	-7.571067	-0.166544	-6.198711	H	-1.072774	3.800308	5.318884
H	-3.723063	-2.807672	7.561947	H	-5.656123	4.368458	-5.852553	H	-3.583257	-0.342860	4.381362
H	-3.462891	-0.539699	7.842648	H	-4.674310	3.901765	-3.825213	H	-1.651573	-1.533013	3.947833
H	-4.408149	0.491154	6.753147	H	-5.563157	2.797587	-2.761883	H	-0.236739	-1.079465	4.915687
H	-1.073990	-0.134468	7.962227	H	-2.361219	3.379081	-4.264136	H	-1.404011	-1.559170	1.558483
H	0.972453	0.958354	7.074141	H	-0.444628	1.797805	-4.137257	H	-0.077664	-1.034847	-0.483553
H	0.870920	2.165636	4.887119	H	-0.850237	-0.564948	-3.468443	H	1.969111	0.370800	-0.286421
H	-1.241176	2.304907	3.650526	H	-3.108669	-1.309941	-2.851017	H	2.651258	1.269477	1.910582
H	-3.687328	-0.084304	2.804860	H	-6.345923	-0.849344	-4.336368	H	0.904447	2.791578	4.604162
H	-6.201484	0.315096	4.490794	H	-7.920753	1.162291	-2.663785	H	0.639336	0.804568	6.908009
H	-6.071641	-0.608911	2.979816	H	-8.584239	0.028406	-3.858071	H	0.427868	2.565067	6.996758
H	-3.338986	2.336289	2.636157	H	-5.339504	-1.832060	-2.340546	H	3.158817	1.977198	4.065573
H	-3.448158	3.294946	4.131415	H	-4.659897	-0.722686	-1.122884	H	3.394125	0.219151	3.973443
H	-5.486938	3.497652	2.705730	H	-6.880502	-1.654383	-0.464081	H	4.248056	1.197679	6.106468
H	-5.845634	2.843106	4.321469	H	-6.881976	0.122926	-0.559767	H	2.994883	-0.037181	6.369768
H	-7.946110	1.772168	3.312779	H	-9.435601	-0.025818	-0.931565	H	2.541179	1.118964	8.644532
H	-7.704132	0.746827	1.877245	H	-9.974075	-1.075190	-2.265455	H	2.186124	2.862625	8.578360
H	-7.462121	2.499047	1.760876	H	-9.254369	-1.793595	-0.814039	H	3.817446	2.280695	8.205533
M2				M2				M2			
E	-5082.90439992			E	-5082.90268715			E	-5082.86646526		
O	4.519641	2.396064	3.454072	O	-5.203568	1.938454	3.425943	C	1.915268	5.948207	-0.573339
C	4.343309	1.125891	2.784253	C	-4.283142	2.492362	2.456515	C	2.832503	5.904858	-1.796366
C	5.745595	0.620649	2.412071	C	-5.046387	3.583051	1.690232	O	2.089630	6.255019	-2.958931
C	6.431989	1.628683	1.486327	C	-6.264072	2.972038	0.991531	C	3.460975	4.524979	-1.950934
C	6.461613	3.004452	2.139879	C	-7.139944	2.244268	2.003716	O	4.352125	4.617142	-3.043534
C	5.057766	3.400844	2.615015	C	-6.299309	1.266440	2.834734	C	4.149011	4.079111	-0.655477
H	3.765982	1.277465	1.865412	H	-3.983633	1.708436	1.752293	O	4.472057	2.694336	-0.820668
H	6.338595	0.500207	3.329391	H	-5.377939	4.355570	2.398123	C	3.204331	4.257337	0.548144
H	5.833975	1.694090	0.564401	H	-5.893215	2.236907	0.260717	O	2.678018	5.597609	0.574369
H	7.106891	2.947375	3.029095	H	-7.555877	2.991527	2.695780	C	3.875109	4.040016	1.891751
H	5.104096	4.305677	3.230947	H	-6.888232	0.870806	3.669625	O	2.844822	3.999422	2.882356
C	3.514453	0.218501	3.711951	C	-3.020620	2.945333	3.212714	C	5.799462	2.245798	-0.619387
O	5.691284	-0.608562	1.695392	O	-4.249523	4.165212	0.663506	C	6.320779	1.591165	-1.905632
O	7.770812	1.270637	1.195222	O	-7.071535	3.948959	0.360017	O	6.241801	2.511395	-2.991920
O	6.945487	4.003393	1.248781	O	-8.192936	1.524225	1.371937	C	5.544468	0.319084	-2.216986
O	4.252107	3.609936	1.484372	O	-5.870951	0.227093	1.993059	O	6.151112	-0.251094	-3.361848
H	4.093112	-0.656954	4.015377	H	-2.882074	4.025315	3.124953	C	5.572194	-0.604243	-1.003896
O	2.341331	-0.285216	3.076303	O	-1.834175	2.351977	2.693036	O	4.721082	-1.718029	-1.294470
H	3.264695	0.794829	4.612376	H	-3.157953	2.701229	4.274437	C	5.074108	0.124678	0.248793
H	7.766959	0.386618	0.781759	H	-6.515218	4.440689	-0.273417	O	5.867315	1.321207	0.443370
H	7.729225	3.622781	0.824495	H	-8.568829	2.127615	0.713411	C	5.161253	-0.731907	1.525519
H	1.768221	0.468828	2.828140	H	-1.895486	1.379573	2.798234	O	6.219967	-1.674616	1.530548
O	1.081216	5.465696	1.430237	O	-4.631812	-3.046206	3.114295	C	5.284479	-3.005568	-1.311753

C	1.880670	4.260848	1.485437	C	-4.468621	-1.685587	2.648793	C	4.840367	-3.732048	-2.581662
C	3.348806	4.712561	1.484418	C	-5.883029	-1.106283	2.496133	O	5.251657	-2.977688	-3.719252
C	3.645993	5.494690	0.202101	C	-6.668829	-1.930592	1.472590	C	3.332799	-3.945702	-2.581042
C	2.669850	6.654746	0.043815	C	-6.672596	-3.404219	1.862610	O	3.029862	-4.683176	-3.749365
C	1.221897	6.176173	0.213800	C	-5.249272	-3.892689	2.162650	C	2.908800	-4.659799	-1.300178
H	1.698230	3.659824	0.587662	H	-3.983674	-1.692443	1.666400	O	1.479462	-4.636630	-1.276169
H	3.532504	5.353074	2.358298	H	-6.395194	-1.139883	3.467902	C	3.460093	-3.945411	-0.051623
H	3.504121	4.804612	-0.644469	H	-6.154868	-1.829515	0.503741	O	4.889485	-3.751963	-0.169156
H	2.871716	7.378819	0.847266	H	-7.255832	-3.507003	2.789891	C	3.195351	-4.714440	1.232227
H	0.543737	7.033262	0.292156	H	-5.276861	-4.885926	2.624640	O	3.642021	-6.056238	1.074676
C	1.414118	3.431985	2.696266	C	-3.523626	-0.957702	3.622990	C	0.778345	-5.827606	-0.969956
O	4.951485	6.041945	0.194862	O	-8.019945	-1.519857	1.373081	C	-0.102076	-6.215811	-2.165245
O	2.798135	7.282130	-1.226783	O	-7.230340	-4.220170	0.838893	O	0.701564	-6.323735	-3.339539
O	0.884465	5.377286	-0.889843	O	-4.527125	-3.926857	0.959273	C	-1.223690	-5.205129	-2.369343
H	2.252867	3.222665	3.362784	H	-4.009444	-0.074887	4.042866	O	-2.033136	-5.710369	-3.416563
O	0.886024	2.161739	2.318719	O	-2.338391	-0.489503	2.984288	C	-1.989359	-5.010847	-1.064077
H	0.673320	4.023834	3.249287	H	-3.288478	-1.646048	4.445269	O	-2.959580	-3.979483	-1.293030
H	5.585758	5.318832	0.359130	H	-8.033640	-0.561471	1.190285	C	-1.029629	-4.623020	0.066940
H	3.748131	7.418648	-1.359975	H	-8.049817	-3.780684	0.566618	O	-0.022947	-5.658786	0.178425
H	0.058300	2.301673	1.813738	H	-1.817481	-1.264030	2.683390	C	-1.712208	-4.471919	1.437117
O	-2.583821	4.615698	-1.856899	O	-1.414463	-5.837056	0.502034	O	-2.842807	-5.309897	1.614204
C	-1.355142	4.365623	-1.133944	C	-2.169555	-4.651661	0.848364	C	-4.315797	-4.293032	-1.120038
C	-0.406747	5.523396	-1.479432	C	-3.652928	-5.026767	0.711399	C	-5.119263	-3.770971	-2.314090
C	-0.150522	5.534785	-2.989315	C	-3.940746	-5.445183	-0.733280	O	-4.597767	-4.325775	-3.516688
C	-1.460233	5.574122	-3.770603	C	-2.996461	-6.556822	-1.179206	C	-5.091486	-2.247620	-2.364678
C	-2.441607	4.509287	-3.260919	C	-1.537437	-6.202784	-0.859348	O	-5.926390	-1.870847	-3.441227
H	-0.903042	3.433819	-1.491616	H	-1.947461	-3.854144	0.130717	C	-5.527752	-1.642058	-1.025140
H	-0.857458	6.477459	-1.172072	H	-3.888223	-5.857577	1.391374	O	-5.237454	-0.241914	-1.080924
H	0.370087	4.596154	-3.237665	H	-3.761249	-4.564345	-1.370016	C	-4.724664	-2.278084	0.121229
H	-1.927159	6.554559	-3.592764	H	-3.244640	-7.460270	-0.602208	O	-4.837750	-3.713646	0.067624
H	-3.441184	4.684899	-3.674883	H	-0.895743	-7.081670	-0.989618	C	-5.161103	-1.859063	1.512869
C	-1.707241	4.157670	0.349126	C	-1.690592	-4.167856	-2.228549	O	-4.120545	-2.256649	2.399104
O	0.613173	6.656846	-3.392881	O	-5.262679	-5.925376	-0.897622	C	-6.285158	0.699983	-0.985081
O	-1.249285	5.371692	-5.162264	O	-3.108103	-6.815656	-2.573482	C	-6.217133	1.658239	-2.179064
O	-1.968634	3.242035	-3.635950	O	-1.129657	-5.163696	-1.710463	O	-6.328464	0.927725	-3.398795
H	-1.062253	4.764729	0.985173	H	-2.538326	-4.012986	2.897024	C	-4.924303	2.463884	-2.147758
O	-1.514361	2.806601	0.764254	O	-1.009253	-2.918135	2.157926	O	-4.977629	3.355681	-3.245310
H	-2.746246	4.475808	0.504292	H	-1.047985	-4.947345	2.658546	C	-4.793340	3.178112	-0.806952
H	1.397903	6.707407	-2.816583	H	-5.870448	-5.267469	-0.512317	O	-3.477667	3.738335	-0.763451
H	-0.530454	5.971044	-5.412272	H	-4.056679	-6.891381	-2.755080	C	-4.983726	2.199198	0.365826
H	-2.177138	2.248125	0.299052	H	-0.173793	-3.048588	1.655282	O	-6.200577	1.442029	0.213335
O	-4.077431	0.204847	-3.574145	O	2.406390	-4.265427	-2.280966	C	-5.038016	2.904436	1.712180
C	-3.270720	1.245165	-2.976502	C	1.160674	-4.250613	-1.546474	O	-5.993810	3.957569	1.655417
C	-2.897579	2.250624	-4.078858	C	0.184730	-5.194066	-2.268600	C	-3.326160	5.077016	-0.326530
C	-2.162906	1.528692	-5.208956	C	-0.005258	-4.730475	-3.714275	C	-2.730654	5.916247	-1.465089
C	-2.974571	0.344186	-5.713351	C	1.336334	-4.590117	-4.421059	O	-3.536504	5.779381	-2.634867
C	-3.399292	-0.560302	-4.546863	C	2.305808	-3.739239	-3.587991	C	-1.289757	5.512500	-1.750028
H	-2.344546	0.808605	-2.585480	H	0.736222	-3.240325	-1.568321	O	-0.807350	6.415772	-2.729297
H	-3.803208	2.731963	-4.474985	H	0.576489	-6.221159	-2.257943	C	-0.481323	5.543799	-0.456426
H	-1.217005	1.146953	-4.794123	H	-0.482066	-3.738363	-3.679672	O	0.838109	5.072836	-0.765121

H	-3.894800	0.729746	-6.176216	H	1.780173	-5.592259	-4.514395	C	-1.143973	4.662145	0.607302
H	-4.123723	-1.304663	-4.894954	H	3.315619	-3.799523	-4.008755	O	-2.494570	5.147608	0.809698
C	-4.075223	1.797444	-1.791989	C	1.495314	-4.589227	-0.084942	C	-0.419634	4.676776	1.962014
O	-1.920148	2.381319	-6.314648	O	-0.788927	-5.640285	-4.466192	O	0.219443	5.905668	2.268959
O	-2.240647	-0.424628	-6.661102	O	1.191037	-3.999796	-5.708733	H	1.563878	6.967489	-0.386898
O	-2.266038	-1.190465	-4.004130	O	1.855982	-2.408501	-3.573408	H	3.637014	6.636267	-1.631467
H	-4.050326	2.886501	-1.771371	H	0.812889	-5.342495	0.308952	H	2.643122	5.999225	-3.712807
O	-3.548706	1.368505	-0.537736	O	1.373265	-3.457248	0.772188	H	2.653871	3.804298	-2.154460
H	-5.116724	1.471422	-1.911826	H	2.515766	-4.994605	-0.060162	H	4.875947	3.792374	-3.098971
H	-1.517271	3.198723	-5.971087	H	-1.597046	-5.826534	-3.954715	H	5.064198	4.670782	-0.512742
H	-1.833957	0.210502	-7.269256	H	0.449208	-4.456624	-6.132563	H	2.377362	3.544285	0.447198
H	-3.394313	0.390577	-0.579215	H	1.894354	-2.713939	0.377133	H	4.570382	4.869943	2.077517
O	-2.147032	-4.325955	-2.064433	O	3.901565	0.577937	-2.861298	H	4.442645	3.101060	1.869826
C	-2.154637	-2.885489	-2.220172	C	3.011560	-0.510637	-2.514267	H	3.220441	4.251468	3.734446
C	-2.338995	-2.588371	-3.719760	C	2.805867	-1.361518	-3.779185	H	6.442682	3.084052	-0.329357
C	-1.238675	-3.258816	-4.542024	C	2.252256	-0.505329	-4.916801	H	7.371571	1.319987	-1.730281
C	-1.199263	-4.749806	-4.240272	C	3.157496	0.695563	-5.153188	H	6.385752	1.975860	-3.788553
C	-1.088971	-4.989553	-2.729546	C	3.392209	1.460482	-3.843236	H	4.496190	0.587868	-2.419713
H	-1.201644	-2.471944	-1.872954	H	2.048796	-0.106729	-2.183717	H	5.713666	-1.102802	-3.559471
H	-3.314208	-2.983972	-4.037242	H	3.771754	-1.787186	-4.086362	H	6.595944	-0.947750	-0.820177
H	-0.276349	-2.814660	-4.244491	H	1.259607	-0.140285	-4.610958	H	4.029645	0.424176	0.099840
H	-2.146717	-5.194273	-4.578217	H	4.134235	0.326888	-5.499022	H	4.193452	-1.225896	1.674901
H	-1.218787	-6.052831	-2.499567	H	4.165660	2.224110	-3.980973	H	5.308784	-0.051883	2.370385
C	-3.271116	-2.339348	-1.304986	C	3.639609	-1.258212	-1.322089	H	5.864748	-2.505285	1.174002
O	-1.446854	-3.135130	-5.937004	O	2.177967	-1.212539	-6.141570	H	6.376571	-2.952393	-1.261371
O	-0.108999	-5.379581	-4.907627	O	2.603626	1.575666	-6.127077	H	5.330266	-4.715947	-2.589728
O	0.164304	-4.534810	-2.282592	O	2.183431	2.047912	-3.352197	H	4.767452	-3.352118	-4.471200
H	-4.139385	-2.039319	-1.902365	H	3.934948	-2.270017	-1.620079	H	2.841119	-2.960388	-2.598178
O	-2.836888	-1.215518	-0.549444	O	2.730818	-1.353870	-0.233038	H	2.143618	-5.084957	-3.649479
H	-3.580386	-3.158289	-0.645658	H	4.544208	-0.712565	-1.030037	H	3.277938	-5.690427	-1.318568
H	-1.526871	-2.187795	-6.160373	H	1.679689	-2.038365	-5.991801	H	2.971844	-2.965619	0.029985
H	-0.122020	-5.026435	-5.810994	H	2.289707	1.005928	-6.846103	H	2.115792	-4.674831	1.427444
H	-2.761451	-1.419655	0.431035	H	3.056022	-0.867266	0.581979	H	3.719137	-4.207949	2.056681
O	2.164722	-5.750788	0.568194	O	1.670249	5.050177	-1.349954	H	3.358625	-6.556380	1.849787
C	1.127214	-4.986365	-0.087094	C	1.875966	3.640952	-1.601895	H	1.483356	-6.627566	-0.724411
C	1.025880	-5.419952	-1.559199	C	2.151669	3.439975	-3.101841	H	-0.556746	-7.190777	-1.938619
C	2.388593	-5.333081	-2.248499	C	1.024905	4.046207	-3.940565	H	0.070636	-6.393436	-4.073345
C	3.450500	-6.070154	-1.443686	C	0.778462	5.495701	-3.544981	H	-0.776453	-4.238644	-2.649985
C	3.452268	-5.597097	0.013181	C	0.574371	5.619342	-2.031301	H	-2.800295	-5.117687	-3.534919
H	1.379905	-3.920123	-0.054261	H	0.973060	3.081436	-1.330298	H	-2.492378	-5.940833	-0.779706
H	0.651868	-6.451569	-1.624387	H	3.104690	3.915427	-3.374070	H	-0.527077	-3.679335	-0.183349
H	2.665578	-4.268122	-2.289865	H	0.111567	3.469472	-3.726469	H	-1.984083	-3.422921	1.588319
H	3.202128	-7.141492	-1.443489	H	1.672615	6.080251	-3.806800	H	-0.963672	-4.733545	2.195115
H	4.112294	-6.229791	0.617357	H	0.558543	6.674644	-1.736151	H	-3.623440	-4.747265	1.489227
C	-0.154884	-5.218754	0.708319	C	3.019861	3.197064	-0.693143	H	-4.454397	-5.371749	-1.001776
O	2.387993	-5.909454	-3.540875	O	1.312024	4.048437	-5.326325	H	-6.161430	-4.093818	-2.174299
O	4.746506	-5.872569	-2.002636	O	-0.361096	6.025024	-4.217106	H	-4.979509	-3.796370	-4.234129
O	3.882089	-4.258915	0.051637	O	-0.636004	4.993707	-1.686230	H	-4.051693	-1.930112	-2.538328
H	-1.017407	-5.055015	0.055841	H	3.504423	2.319989	-1.131719	H	-5.935462	-0.894464	-3.506897
O	-0.315578	-4.343959	1.806983	O	2.604656	2.819808	0.604118	H	-6.604494	-1.806242	-0.879743

H	-0.161000	-6.274650	1.024490	H	3.757210	4.016342	-0.665788	H	-3.673363	-1.993645	-0.005779
H	1.619883	-5.564534	-4.037163	H	1.578240	3.146598	-5.592057	H	-6.112470	-2.354535	1.757917
H	4.639755	-5.995829	-2.958345	H	-0.270083	5.746273	-5.141275	H	-5.321815	-0.773584	1.524050
H	0.544488	-4.138704	2.223947	H	1.905945	3.418328	0.936730	H	-4.278281	-1.900087	3.284011
O	5.401985	-2.556701	2.939049	O	-2.662460	5.751163	1.292886	H	-7.255384	0.192504	-0.951754
C	4.306720	-2.998785	2.104583	C	-1.610082	5.083220	0.558380	H	-7.062770	2.354249	-2.088389
C	4.887333	-3.879391	0.989291	C	-1.562189	5.687651	-0.852247	H	-6.055924	1.543726	-4.096753
C	5.940307	-3.108845	0.188034	C	-2.921322	5.556547	-1.544382	H	-4.077292	1.767340	-2.249220
C	6.991798	-2.519321	1.120958	C	-4.025919	6.128853	-0.664122	H	-4.339937	4.081563	-3.093447
C	6.323411	-1.733309	2.253008	C	-3.947379	5.535264	0.745721	H	-5.549545	3.967294	-0.743755
H	3.826894	-2.127121	1.646912	H	-1.848491	4.017727	0.474038	H	-4.130518	1.508416	0.380780
H	5.352262	-4.772572	1.430537	H	-1.292124	6.751434	-0.788113	H	-4.033902	3.292136	1.927886
H	5.425983	-2.279146	-0.321275	H	-3.116077	4.482482	-1.688474	H	-5.303985	2.162371	2.479934
H	7.547627	-3.350090	1.579938	H	-3.866964	7.213520	-0.575015	H	-5.907503	4.480221	2.462076
H	7.065733	-1.430753	2.999736	H	-4.646254	6.046878	1.416753	H	-4.293078	5.479123	-0.009417
C	3.276798	-3.673491	3.027325	C	-0.321591	5.215273	1.391249	H	-2.731787	6.965858	-1.137649
O	6.621747	-3.931050	-0.740817	O	-2.968301	6.251084	-2.776985	H	-3.019056	6.185295	-3.348181
O	7.887817	-1.655356	0.428801	O	-5.318623	5.867077	-1.202010	H	-1.284374	4.479376	-2.131723
H	3.200475	-4.744421	2.824207	H	0.428421	5.815579	0.870701	H	0.131447	6.215144	-2.907821
O	1.967515	-3.153594	2.852449	O	0.295559	3.963660	1.646531	H	-0.430526	6.566077	-0.067081
H	3.624239	-3.547095	4.061845	H	-0.582664	5.732706	2.324735	H	-1.191378	3.623862	0.256260
H	5.957964	-4.421211	-1.263490	H	-2.181333	6.003268	-3.299578	H	0.296043	3.849213	1.979012
H	8.132012	-2.119313	-0.385887	H	-5.262131	6.073508	-2.146901	H	-1.175566	4.477338	2.731522
H	1.983512	-2.184891	2.988679	H	-0.352044	3.366704	2.074680	H	1.162565	5.781692	2.076887
C	-6.626940	3.307877	3.875670	C	8.182319	3.651603	2.812040	C	3.607202	-0.885919	5.718601
C	-6.069859	3.136240	2.609881	C	7.407850	3.472598	1.667335	C	3.577927	0.396214	5.172281
C	-5.533261	1.900429	2.254633	C	6.650014	2.312484	1.527795	C	2.524115	0.766441	4.338645
C	-5.534509	0.816759	3.145799	C	6.638178	1.315450	2.513621	C	1.486955	-0.126228	4.026834
C	-6.111739	0.985874	4.418827	C	7.435521	1.489666	3.660421	C	1.507552	-1.414277	4.594066
C	-6.650147	2.232751	4.761101	C	8.196335	2.658357	3.788789	C	2.570707	-1.771776	5.433325
C	-6.256948	-0.177723	5.381853	C	7.566378	0.391982	4.699770	C	0.356583	-2.381587	4.391177
C	-7.068808	-1.278127	4.742995	C	8.099873	-0.865375	4.056326	C	-0.934493	-1.778427	4.888604
C	-8.370159	-1.579756	5.141220	C	9.393369	-1.332820	4.283120	C	-1.585947	-2.244336	6.029982
C	-9.093746	-2.604407	4.526048	C	9.858265	-2.498065	3.668299	C	-2.789631	-1.680113	6.458563
C	-8.506798	-3.330720	3.492734	C	9.017099	-3.199025	2.807636	C	-3.341880	-0.622473	5.737838
C	-7.209208	-3.031476	3.072134	C	7.723239	-2.736586	2.558184	C	-2.693282	-0.132658	4.600342
C	-6.479418	-2.004440	3.686708	C	7.251892	-1.568913	3.174367	C	-1.487496	-0.702826	4.161431
C	-4.817460	-0.445279	2.660117	C	5.673410	0.153360	2.278346	C	0.462082	0.374451	3.010179
N	-5.125449	-1.712554	3.359936	N	5.916998	-1.099665	3.026700	N	-0.846702	-0.313487	2.955765
C	-3.294424	-0.197197	2.739570	C	4.242447	0.639683	2.589501	C	1.096581	0.310781	1.602806
C	-4.352151	-2.823282	2.805535	C	4.919508	-2.111362	2.681004	C	-1.710470	0.295911	1.944103
C	-2.858698	-2.550680	2.920493	C	3.513303	-1.619684	3.004252	C	-1.058785	0.225813	0.568148
N	-2.520985	-1.320515	2.185713	N	3.232861	-0.381011	2.264826	N	0.235146	0.899445	0.582922
C	-1.077722	-1.045246	2.232648	C	1.877470	0.120587	2.535576	C	0.867118	0.882538	-0.730753
H	-7.051471	4.263943	4.168439	H	8.781141	4.548824	2.938711	H	4.420767	-1.190247	6.370300
H	-6.054695	3.956903	1.898341	H	7.393897	4.226820	0.886239	H	4.368052	1.106853	5.397437
H	-5.087634	1.772627	1.271148	H	6.044630	2.176476	0.634980	H	2.504674	1.766432	3.910255
H	-7.103169	2.353170	5.742026	H	8.816936	2.781994	4.672737	H	2.575188	-2.764664	5.876049
H	-6.738430	0.165121	6.302255	H	8.233776	0.722048	5.501030	H	0.564755	-3.316859	4.918660
H	-5.269831	-0.576239	5.646661	H	6.588153	0.173226	5.145431	H	0.242691	-2.615634	3.325212

H	-8.816650	-1.014601	5.955648	H	10.040048	-0.784540	4.963719	H	-1.154134	-3.077087	6.579138
H	-10.102400	-2.833851	4.856323	H	10.864979	-2.854092	3.865278	H	-3.288583	-2.064256	7.342839
H	-9.056638	-4.130414	3.004528	H	9.364276	-4.106124	2.321034	H	-4.269729	-0.161792	6.066109
H	-6.768909	-3.600282	2.260272	H	7.083434	-3.287954	1.877577	H	-3.122893	0.705462	4.062069
H	-5.063818	-0.562329	1.588606	H	5.710559	-0.072895	1.195053	H	0.288311	1.443140	3.229240
H	-3.021799	-0.022895	3.794830	H	4.194583	0.903891	3.660631	H	1.333388	-0.749799	1.380112
H	-3.048624	0.709317	2.180572	H	4.015035	1.535892	2.008163	H	2.039223	0.864830	1.622066
H	-4.598215	-3.013637	1.743631	H	4.954665	-2.384523	1.610352	H	-1.931660	1.354285	2.173429
H	-4.598691	-3.727927	3.367701	H	5.127612	-3.014450	3.260676	H	-2.647232	-0.264572	1.926571
H	-2.275702	-3.378621	2.509571	H	2.785072	-2.380993	2.705543	H	-1.706064	0.719928	-0.165543
H	-2.593184	-2.444859	3.986790	H	3.420864	-1.456389	4.091688	H	-0.961699	-0.836802	0.268666
H	-0.725157	-0.847180	3.257585	H	1.746800	0.402635	3.592837	H	1.071908	-0.141531	-1.097148
H	-0.855506	-0.169022	1.617116	H	1.692600	0.991659	1.903964	H	1.816151	1.425908	-0.697463
H	-0.541123	-1.909865	1.837423	H	1.147894	-0.658889	2.297919	H	0.216989	1.379531	-1.457468
FA2				FA2				FA2			
E	-5082.90212458			E	-5082.90406095			E	-5082.87868905		
								ZPE	-5081.312660		
								H	-5081.219726		
								G	-5081.446212		
								S	476.680		
O	2.538861	-4.799931	-1.165955	O	0.044422	-5.774886	-0.080923	C	6.440932	2.419359	1.990630
C	1.181232	-4.424507	-0.836979	C	-0.670296	-4.648809	-0.642435	C	7.465529	1.748582	1.071162
C	0.256401	-5.398469	-1.583005	C	-1.146441	-5.071128	-2.042723	O	7.694198	2.573317	-0.066486
C	0.500096	-5.293906	-3.090803	C	0.053373	-5.459881	-2.909720	C	6.990733	0.361463	0.653930
C	1.975179	-5.510452	-3.408756	C	0.890596	-6.528098	-2.218612	O	8.040356	-0.217233	-0.096545
C	2.858490	-4.613429	-2.531913	C	1.226396	-6.106757	-0.782398	C	6.601854	-0.484094	1.872212
H	0.986755	-3.409174	-1.199950	H	0.011605	-3.797145	-0.744605	O	5.955204	-1.647092	1.348865
H	0.463552	-6.424940	-1.249182	H	-1.828295	-5.928793	-1.954412	C	5.643784	0.305031	2.780479
H	0.224505	-4.273613	-3.400577	H	0.675269	-4.559568	-3.034455	O	6.221457	1.578651	3.110861
H	2.224597	-6.553971	-3.165368	H	0.289252	-7.447320	-2.159081	C	5.323077	-0.363713	4.102986
H	3.910643	-4.902994	-2.630075	H	1.668136	-6.946415	-0.234326	O	4.280654	0.403246	4.705911
C	1.064556	-4.404972	0.697882	C	-1.771198	-4.258055	0.359941	C	6.344512	-2.931860	1.782451
O	-1.123199	-5.089901	-1.392780	O	-1.784890	-4.007099	-2.746361	C	6.755332	-3.769092	0.563442
O	-0.232416	-6.260099	-3.821678	O	-0.340549	-5.980601	-4.166003	O	7.786898	-3.094835	-0.153792
O	2.265595	-5.243865	-4.776279	O	2.104077	-6.781577	-2.918366	C	5.556172	-4.043455	-0.335302
O	2.672732	-3.279755	-2.927371	O	2.118493	-5.023281	-0.829924	O	6.008619	-4.907922	-1.361016
H	0.283246	-5.085997	1.040053	H	-2.744783	-4.220930	-0.131280	C	4.420581	-4.642631	0.488818
O	0.708818	-3.119495	1.201628	O	-1.577493	-2.965000	0.928176	O	3.288052	-4.762648	-0.378437
H	2.023663	-4.740615	1.112558	H	-1.804617	-5.029930	1.139578	C	4.090743	-3.743016	1.684928
H	-1.169205	-6.195597	-3.557016	H	-0.960400	-5.348043	-4.574776	O	5.293079	-3.574910	2.472984
H	1.577496	-5.694536	-5.288222	H	1.860304	-6.870794	-3.851845	C	2.985640	-4.306351	2.594732
H	1.381049	-2.460286	0.915414	H	-0.712784	-2.937722	1.395741	O	2.940370	-5.719716	2.669598
O	4.962319	-0.508251	-2.141327	O	4.275974	-3.966760	1.959193	C	2.727666	-6.035196	-0.579262
C	3.800820	-1.340285	-1.910934	C	3.069190	-3.930951	1.161590	C	2.499081	-6.251331	-2.075387
C	3.810772	-2.421755	-3.002082	C	3.222016	-5.005211	0.073869	O	3.745418	-6.126610	-2.755829
C	3.734491	-1.760998	-4.381118	C	4.453405	-4.707820	-0.785089	C	1.477828	-5.257429	-2.611164
C	4.845958	-0.730579	-4.547094	C	5.692432	-4.566023	0.091320	O	1.263809	-5.585603	-3.970776
C	4.885594	0.226103	-3.347824	C	5.435113	-3.586278	1.243161	C	0.196616	-5.315149	-1.782525
H	2.894390	-0.737320	-2.031776	H	2.981080	-2.951340	0.679109	O	-0.593689	-4.200240	-2.201291
H	4.734759	-3.011742	-2.925446	H	3.337033	-5.989761	0.548821	C	0.491977	-5.201574	-0.275384

H	2.767141	-1.237992	-4.441165	H	4.277217	-3.747711	-1.295119	O	1.495405	-6.167550	0.117705
H	5.805933	-1.267591	-4.568523	H	5.905637	-5.548383	0.538264	C	-0.738722	-5.423210	0.588529
H	5.791866	0.841265	-3.380158	H	6.256027	-3.627419	1.967720	O	-1.375066	-6.634154	0.197279
C	3.836363	-1.822619	-0.451311	C	1.873152	-4.091115	2.118254	C	-1.975526	-2.443802	-2.443802
O	3.868092	-2.697387	-5.434974	O	4.717445	-5.737120	-1.720569	C	-2.267783	-4.068587	-3.918424
O	4.683859	0.033333	-5.736933	O	6.817440	-4.112356	-0.653368	O	-1.437800	-4.874312	-4.754079
O	3.737228	1.033665	-3.385829	O	5.310439	-2.293446	0.709525	C	-2.047771	-2.589594	-4.206469
H	3.820426	-2.912803	-0.403204	H	1.272628	-4.962111	1.850169	O	-2.429316	-2.373201	-5.556091
O	2.688312	-1.381029	0.276781	O	0.985003	-2.978806	2.074578	C	-2.840964	-1.738194	-3.216418
H	4.755934	-1.468644	0.028716	H	2.270514	-4.242149	3.130306	O	-2.521729	-0.367751	-3.471028
H	3.211784	-3.405146	-5.294775	H	3.897421	-5.912580	-2.219133	C	-2.462799	-2.123818	-1.781818
H	4.497450	-0.605946	-6.440661	H	6.841029	-4.652536	-1.457300	O	-2.740529	-3.535003	-1.612947
H	2.733050	-0.403522	0.368699	H	1.468396	-2.170413	2.352274	C	-3.213523	-1.351040	-0.692633
O	3.324545	4.189477	-1.528573	O	5.635149	0.819985	2.644511	O	-4.568747	-1.082062	-1.009355
C	3.238397	2.754061	-1.689766	C	4.893464	-0.268145	2.045395	C	-3.506626	0.412044	-4.103323
C	3.851673	2.417607	-3.059466	C	5.924017	-1.205475	1.398309	C	-2.852146	1.291704	-5.170298
C	3.088439	3.149662	-4.165881	C	6.719545	-0.443301	0.335414	O	-2.160288	0.469199	-6.104970
C	3.041187	4.646310	-3.887268	C	7.344077	0.812839	0.932228	C	-1.911492	2.306678	-4.529967
C	2.547273	4.916423	-2.459808	C	6.294699	1.633591	1.693667	O	-1.453826	3.143528	-5.574187
H	2.185932	2.448700	-1.692976	H	4.240024	0.126506	1.259693	C	-2.604479	3.085298	-3.401736
H	4.907178	2.724175	-3.075478	H	6.609420	-1.584204	2.169496	O	-2.566422	3.796771	-2.720404
H	2.056617	2.764670	-4.163862	H	6.010774	-0.137507	-0.450109	C	-3.303004	2.109204	-2.440856
H	4.066258	5.039111	-3.959396	H	8.106376	0.499618	1.660993	O	-4.179594	1.247017	-3.183665
H	2.691401	5.971760	-2.202711	H	6.778698	2.430166	2.269697	C	-4.160019	2.738521	-1.357216
C	3.914556	2.114200	-0.465004	C	3.991423	-0.877311	3.132661	O	-4.521589	1.713184	-0.439105
O	3.690344	2.974661	-5.435724	O	7.771875	-1.219332	-0.207709	C	-1.673680	5.187768	-2.513708
O	2.190719	5.326597	-4.803849	O	7.931881	1.636944	-0.068350	C	-0.457090	5.885893	-3.131393
O	1.189361	4.569379	-2.380014	O	5.390091	2.172414	0.765271	O	-0.385366	5.586014	-4.524708
H	4.648985	1.369264	-0.774093	H	4.195238	-1.942225	3.256904	C	0.823961	5.465014	-2.422864
O	2.998316	1.425876	0.383409	O	2.608722	-0.778257	2.804962	O	1.872063	6.219503	-3.003056
H	4.437816	2.909726	0.081944	H	4.213296	-0.369199	4.079989	C	0.691697	5.689558	-0.920177
H	3.814667	2.018296	-5.579948	H	7.396341	-2.066091	-0.513419	O	1.834643	5.076206	-0.316172
H	2.425657	4.994506	-5.683182	H	8.455306	1.044811	-0.628755	C	-0.598813	5.051176	-0.375695
H	2.289682	2.043919	0.678011	H	2.358537	0.170843	2.745916	O	-1.740102	5.494956	-1.137579
O	-1.119329	5.771989	0.223948	O	3.099371	4.982421	1.412149	C	-0.849097	5.388830	1.085163
C	-0.178020	4.833129	-0.347058	C	3.459731	3.581737	1.364623	O	-0.757221	6.798336	1.268827
C	0.301317	5.436944	-1.675965	C	4.936684	3.513463	0.942419	C	2.552704	5.788290	0.671553
C	-0.890860	5.651150	-2.611602	C	5.122222	4.183208	-0.421664	C	3.994777	5.998795	0.189994
C	-1.962839	6.490380	-1.926014	C	4.574653	5.604542	-0.401438	O	3.988151	6.650599	-1.079224
C	-2.298988	5.919365	-0.542407	C	3.144240	5.623588	0.152198	C	4.737327	4.671328	0.110818
H	-0.688776	3.886499	-0.554216	H	2.854887	3.075357	0.604129	O	6.076221	4.977297	-0.242466
H	0.791760	6.401314	-1.482025	H	5.556339	4.026700	1.691208	C	4.625161	3.932917	1.442154
H	-1.316774	4.660757	-2.836577	H	4.543956	3.600419	-1.155638	O	5.253618	2.654609	1.280896
H	-1.555721	7.500888	-1.773061	H	5.198837	6.201367	0.280041	C	3.152460	3.769159	1.834690
H	-2.928167	6.621447	0.016005	H	2.820464	6.654399	0.334294	O	2.555761	5.086298	1.896309
C	0.905183	4.553251	0.711253	C	3.108154	2.966578	2.732261	C	2.939020	3.085870	3.192519
O	-0.526217	6.327314	-3.801111	O	6.484713	4.261452	-0.799009	O	3.918497	3.414756	4.161267
O	-3.156975	6.555438	-2.698051	O	4.571894	6.187002	-1.700197	H	6.842567	3.351601	2.398952
O	-2.959032	4.692196	-0.714611	O	2.298346	6.495906	-0.776338	H	8.396282	1.636620	1.646249
H	1.896484	4.805944	0.330587	H	3.975093	2.462966	3.163359	H	8.166386	2.021722	-0.708284

O	0.965023	3.179639	1.075267	O	2.084885	1.978845	2.648022	H	6.083696	0.480903	0.041175
H	0.697262	5.186873	1.583198	H	2.814307	3.784920	3.402632	H	7.831489	-1.159233	-0.254548
H	0.233105	5.859041	-4.195702	H	6.868052	3.366899	-0.734520	H	7.509995	-0.764928	2.423798
H	-2.878606	6.753553	-3.604614	H	5.443437	5.997738	-2.078858	H	4.705841	0.456057	2.232178
H	0.112785	2.918707	1.489603	H	1.276036	2.384057	2.262291	H	6.227259	-0.370940	4.729035
O	-4.986356	3.008378	1.855026	O	-1.359752	5.395437	-0.869353	H	5.009470	-1.400069	3.922794
C	-3.763838	3.262190	1.122914	C	-0.131354	4.747773	-0.463935	H	4.157515	0.102285	5.614371
C	-4.072005	4.389153	0.124853	C	1.023358	5.576081	-1.046650	H	7.173214	-2.862307	2.495853
C	-5.191866	3.950449	-0.822150	C	0.910478	5.620360	-2.572540	H	7.132188	-4.732041	0.936742
C	-6.416577	3.504874	-0.031926	C	-0.463630	6.128766	-2.993624	H	7.867623	-3.571185	-0.995051
C	-6.025018	2.488207	1.048574	C	-1.576837	5.362373	-2.266985	H	5.205727	-3.086605	-0.752548
H	-3.482817	2.364104	0.562230	H	-0.091221	3.742112	-0.896802	H	5.246313	-5.161241	-1.917325
H	-4.386173	5.287550	0.674571	H	0.980254	6.598325	-0.645167	H	4.712553	-5.628013	0.868299
H	-4.818604	3.088669	-1.397357	H	1.026268	4.589121	-2.941686	H	3.774264	-2.756233	1.323713
H	-6.828891	4.386279	0.481313	H	-0.541779	7.183395	-2.690296	H	2.024500	-3.897908	2.256346
H	-6.866613	2.310843	1.727535	H	-2.542707	5.854305	-2.427026	H	3.167250	-3.921290	3.603985
C	-2.647435	3.533950	2.148225	C	-0.165768	4.594028	1.067698	H	2.330115	-6.023451	1.977061
O	-5.605427	4.993470	-1.686114	O	1.873329	6.477929	-3.157422	H	3.378051	-6.815948	-0.172440
O	-7.404909	2.921649	-0.874249	O	-0.664838	6.006375	-4.397228	H	2.099809	-7.266861	-2.207410
O	-5.638578	1.294994	0.417009	O	-1.606302	4.045291	-2.753284	H	3.525941	-6.058927	-3.697617
H	-2.189631	4.509149	1.972944	H	0.698236	5.075108	1.529171	H	1.896593	-4.243941	-2.511648
O	-1.592135	2.583105	2.064824	O	-0.119420	3.230376	1.475603	H	0.424814	-5.177575	-4.263731
H	-3.100490	3.539821	3.148192	H	-1.074821	5.087737	1.435438	H	-0.324614	-6.257214	-1.981271
H	-4.814317	5.345701	-2.135050	H	2.750460	6.228909	-2.810874	H	0.871826	-4.191528	-0.075953
H	-7.494439	3.518395	-1.632273	H	0.136529	6.356634	-4.813989	H	-1.404136	-4.560835	0.450442
H	-1.941328	1.696464	2.303038	H	-0.891947	2.758735	1.091173	H	-0.422430	-5.455649	1.641981
O	-5.440408	-1.991346	2.065108	O	-4.451568	1.739389	-2.373071	H	-2.194759	-6.714201	0.700466
C	-4.901277	-0.723724	1.620265	C	-3.185348	2.317341	-1.979441	H	-2.275177	-5.401880	-2.187322
C	-6.060276	0.051729	0.974852	C	-2.872194	3.430862	-2.991002	H	-3.324747	-4.306229	-4.106843
C	-6.626565	-0.746509	-0.202238	C	-2.781943	2.837689	-4.399430	H	-1.533569	-4.493734	-5.641834
C	-7.019062	-2.151295	0.239195	C	-4.052026	2.064632	-4.736877	H	-0.980215	-2.363612	-4.065224
C	-5.870276	-2.821459	1.004477	C	-4.399934	1.072509	-3.619132	H	-2.180330	-1.462328	-5.804318
H	-4.134481	-0.901762	0.858461	H	-2.401420	1.554814	-2.045513	H	-3.916712	-1.904145	-3.337161
H	-6.850425	0.219680	1.720228	H	-3.670051	4.186115	-2.960634	H	-1.387600	-1.962851	-1.628556
H	-5.827646	-0.831772	-0.955542	H	-1.935322	2.133308	-4.407323	H	-2.675833	-0.416539	-0.500459
H	-7.868437	-2.065180	0.932995	H	-4.880082	2.785886	-4.803171	H	-3.160393	-1.955770	0.222804
H	-6.216393	-3.748744	1.474695	H	-5.402822	0.659806	-3.775174	H	-4.658042	-0.109514	-1.056209
C	-4.210630	-0.057028	2.823894	C	-3.301685	2.737347	-0.503857	H	-4.277539	-0.223962	-4.548896
O	-7.780399	-0.140958	-0.756272	O	-2.619633	3.834000	-5.392383	H	-3.657930	1.841355	-5.678411
O	-7.372476	-2.972672	-0.868588	O	-3.925783	1.349397	-5.960956	H	-1.593058	1.062943	-6.619305
O	-4.826481	-3.084379	0.101995	O	-3.438254	0.049332	-3.615411	H	-1.077315	1.754286	-4.070071
H	-4.608117	0.945402	2.991197	H	-3.092806	3.801749	-0.384005	H	-0.942708	3.881677	-5.185932
O	-2.810936	0.104732	2.627061	O	-2.360380	2.058861	0.325885	H	-3.330575	3.787167	-3.835352
H	-4.420539	-0.664871	3.713847	H	-4.328677	2.544872	-0.170219	H	-2.524549	1.510719	-1.952200
H	-7.566176	0.789496	-0.955899	H	-1.863949	4.395021	-5.136655	H	-5.047576	3.188539	-1.825484
H	-7.971829	-2.441239	-1.413649	H	-3.547051	1.973746	-6.597603	H	-3.590674	3.535825	-0.860614
H	-2.394048	-0.780653	2.550705	H	-2.540839	1.092501	0.297948	H	-5.410753	1.904062	-0.036214
O	-2.089964	-5.479133	0.690800	O	-3.847956	-3.231777	-1.996557	H	-2.602059	5.571730	-2.951078
C	-2.714438	-4.175000	0.747726	C	-3.426284	-1.848329	-2.045158	H	-0.591582	6.967826	-2.992973
C	-4.137217	-4.330104	0.186855	C	-3.866411	-1.296007	-3.409948	H	0.492410	5.887352	-4.807231

C	-4.077969	-4.855041	-1.249653	C	-3.204586	-2.105561	-4.528410	H	0.975887	4.387438	-2.591306
C	-3.266045	-6.142435	-1.316729	C	-3.493547	-3.592733	-4.361814	H	2.644408	6.197608	-2.403737
C	-1.908509	-5.964969	-0.624455	C	-3.176317	-4.052007	-2.932296	H	0.677368	6.764425	-0.712463
H	-2.161666	-3.477644	0.108194	H	-2.333064	-1.800444	-1.991436	H	-0.511767	3.960129	-0.460390
H	-4.703831	-5.034652	0.812017	H	-4.959504	-1.364192	-3.500317	H	-0.094442	4.862555	1.683603
H	-3.567950	-4.091993	-1.858428	H	-2.117093	-1.953822	-4.442842	H	-1.844617	5.011336	1.361167
H	-3.815305	-6.920482	-0.766134	H	-4.569967	-3.750645	-4.524864	H	-0.751405	6.972346	2.217963
H	-1.409834	-6.934356	-0.514265	H	-3.555880	-5.066234	-2.765168	H	2.063129	6.744278	0.880254
C	-2.603238	-3.675065	2.199110	C	-3.979206	-1.142411	-0.795301	H	4.502869	6.634629	0.929296
O	-5.363786	-5.140044	-1.769294	O	-3.667188	-1.727221	-5.811983	H	4.899946	6.578529	-1.403501
O	-3.045127	-6.557457	-2.660390	O	-2.738258	-4.381858	-5.274555	H	4.260916	4.051330	-0.663937
H	-3.582907	-3.395791	2.589945	H	-4.566074	-0.264740	-1.070538	H	6.568853	4.141333	-0.349978
O	-1.792167	-2.510094	2.321854	O	-2.936537	-0.666780	0.054404	H	5.123907	4.498067	2.236359
H	-2.208213	-4.498512	2.808283	H	-4.634047	-1.842883	-0.262594	H	2.627394	3.186125	1.066472
H	-5.924884	-4.353425	-1.635416	H	-3.561904	-0.761345	-5.897474	H	2.896993	2.002903	3.036972
H	-3.902701	-6.488274	-3.105915	H	-2.834423	-3.954915	-6.138971	H	1.952822	3.403951	3.556198
H	-0.896548	-2.696113	1.963255	H	-2.412572	-1.431119	0.382721	H	4.455296	2.617877	4.296977
C	3.979721	3.853815	5.701087	C	-6.889931	-3.138189	3.956213	C	-7.970176	-4.023916	2.481080
C	4.092946	3.723161	4.318364	C	-5.839026	-3.363411	3.068364	C	-7.246343	-3.613701	1.362998
C	4.102649	2.451803	3.748140	C	-4.774367	-2.465715	3.022726	C	-6.732129	-2.319066	1.308593
C	4.010708	1.292612	4.531416	C	-4.727077	-1.336495	3.854439	C	-6.936163	-1.411491	2.359344
C	3.858022	1.427300	5.925355	C	-5.795349	-1.103634	4.740205	C	-7.645647	-1.832737	3.500129
C	3.848466	2.710014	6.486570	C	-6.862131	-2.010649	4.774238	C	-8.151794	-3.137456	3.541011
C	3.574901	0.220439	6.802287	C	-5.854613	0.160537	5.577185	C	-7.768067	-0.941525	4.722636
C	2.317559	-0.466132	6.321668	C	-5.840584	1.375028	4.680490	C	-6.394311	-0.583876	5.238162
C	1.110721	-0.401191	7.016539	C	-6.964836	2.176883	4.489430	C	-5.877961	-1.107312	6.422456
C	-0.040224	-1.018363	6.519560	C	-6.922569	3.292728	3.649782	C	-4.600377	-0.760423	6.869241
C	0.017431	-1.703835	5.307896	C	-5.738171	3.600071	2.983918	C	-3.825713	0.115598	6.112735
C	1.218048	-1.776321	4.597808	C	-4.606342	2.799152	3.151734	C	-4.321320	0.637051	4.915815
C	2.373817	-1.157528	5.092852	C	-4.642405	1.681286	3.998881	C	-5.604194	0.294965	4.466480
C	4.173382	-0.032200	3.788537	C	-3.449809	-0.503418	3.768655	C	-6.430147	0.010518	2.118505
N	3.639971	-1.244428	4.449220	N	-3.498794	0.887141	4.279050	N	-6.194302	0.865090	3.305224
C	5.676865	-0.258510	3.516783	C	-2.327704	-1.250056	4.520189	C	-7.442993	0.733246	1.203772
C	3.851971	-2.423256	3.607457	C	-2.202507	1.543541	4.084885	C	-5.690073	2.176340	2.901741
C	5.343034	-2.627414	3.358378	C	-1.101029	0.788882	4.822030	C	-6.716820	2.882829	2.022117
N	5.911258	-1.451106	2.704897	N	-1.036373	-0.592979	4.360380	N	-6.986838	2.080898	0.820893
C	7.325871	-1.625318	2.408005	C	0.025289	-1.339661	5.020618	C	-7.958323	2.734396	-0.059339
H	3.970322	4.836436	6.164177	H	-7.729520	-3.825799	4.004422	H	-8.376854	-5.029669	2.537800
H	4.164477	4.602641	3.684966	H	-5.847080	-4.229654	2.412922	H	-7.074885	-4.296265	0.535755
H	4.162997	2.345286	2.668294	H	-3.949590	-2.641974	2.336178	H	-6.154906	-2.004765	0.440828
H	3.722909	2.807941	7.562103	H	-7.688446	-1.819050	5.454430	H	-8.690889	-3.461261	4.427890
H	3.462984	0.539916	7.842696	H	-6.758204	0.152279	6.193956	H	-8.342575	-1.456755	5.497820
H	4.408383	-0.490752	6.753165	H	-4.987621	0.208520	6.247701	H	-8.301339	-0.016806	4.468858
H	1.074181	0.134258	7.962347	H	-7.882147	1.932574	5.019814	H	-6.492243	-1.784038	7.011234
H	-0.972136	-0.958712	7.074253	H	-7.804341	3.913711	3.522396	H	-4.219190	-1.168481	7.800467
H	-0.870555	-2.165696	4.887020	H	-5.689656	4.463196	2.325369	H	-2.829617	0.393120	6.445761
H	1.241518	-2.304532	3.650342	H	-3.697690	3.033315	2.609102	H	-3.701636	1.307141	4.329347
H	3.687532	0.084820	2.804857	H	-3.161974	-0.474434	2.704201	H	-5.490062	-0.078635	1.548654
H	6.201684	-0.314267	4.490879	H	-2.623265	-1.338070	5.585354	H	-8.416078	0.781832	1.722891
H	6.071732	0.609700	2.979893	H	-2.249687	-2.263154	4.114220	H	-7.576761	0.145836	0.291393

H	3.339608	-2.336036	2.636102	H	-1.932377	1.615122	3.019611	H	-4.738582	2.109051	2.345725
H	3.448838	-3.294573	4.131446	H	-2.270067	2.560312	4.481559	H	-5.517941	2.774231	3.800425
H	5.487724	-3.496979	2.705921	H	-0.138596	1.273080	4.617235	H	-6.328881	3.859333	1.710395
H	5.846203	-2.842273	4.321643	H	-1.288141	0.849618	5.913105	H	-7.641903	3.051232	2.600253
H	7.946584	-1.771112	3.312861	H	-0.118997	-1.421188	6.115698	H	-8.940919	2.864968	0.423952
H	7.704433	-0.745812	1.877333	H	0.074806	-2.349057	4.601424	H	-8.095634	2.135019	-0.963749
H2	7.462681	-2.498071	1.760973	H2	0.987449	-0.857107	4.829455	H2	-7.585517	3.721020	-0.350605
FV2				FV2				FV2			
E	-5082.90050825			E	-5082.90058173			E	-5082.86908923		
O	5.342962	0.536802	-1.503981	O	-4.882643	3.273028	1.129955	C	5.293376	4.645297	0.924414
C	4.363081	-0.526661	-1.447753	C	-3.573491	3.453928	0.541765	C	6.516722	4.166111	0.138617
C	4.694809	-1.500157	-2.590754	C	-3.712640	4.539780	-0.536886	O	6.479883	4.713661	-1.174936
C	4.639902	-0.764919	-3.932437	C	-4.727270	4.088941	-1.590973	C	6.567163	2.643674	0.093515
C	5.542096	0.462359	-3.913166	C	-6.053813	3.716349	-0.939417	O	7.773879	2.299423	-0.557960
C	5.258131	1.323845	-2.675824	C	-5.834889	2.744163	0.227831	C	6.462901	2.042658	1.499413
H	3.363916	-0.112309	-1.623019	H	-3.260381	2.523061	0.055779	O	6.277454	0.637114	1.312800
H	5.700372	-1.917307	-2.439505	H	-4.050817	5.478184	-0.075289	C	5.264473	2.646321	2.251816
H	3.601737	-0.427878	-4.079132	H	-4.316890	3.189891	-2.077149	O	5.342522	4.083384	2.227228
H	6.584544	0.118332	-3.841093	H	-6.496663	4.632913	-0.522163	C	5.178962	2.253154	3.714072
H	6.025744	2.098329	-2.567982	H	-6.758941	2.630862	0.805608	O	3.918879	2.716825	4.193392
C	4.386843	-1.105471	-0.021827	C	-2.584689	3.735722	1.685032	C	7.090426	-0.284444	2.006260
O	3.738069	-2.552224	-2.705203	O	-2.499121	4.753787	-1.255298	C	7.793013	-1.196787	0.991386
O	5.062174	-1.582378	-5.008781	O	-4.994261	5.100950	-2.544557	O	8.533415	-0.404868	0.065439
O	5.368976	1.261481	-5.078350	O	-6.949234	3.119056	-1.870602	C	6.784651	-2.080530	0.268013
O	3.986975	1.903630	-2.815215	O	-5.419027	1.506506	-0.288208	O	7.532929	-2.951341	-0.560119
H	4.500943	-2.190285	-0.048346	H	-2.018403	4.648133	1.493240	C	5.927513	-2.820441	1.290306
O	3.179951	-0.857282	0.694645	O	-1.617095	2.698070	1.832687	O	4.925484	-3.544045	0.568092
H	5.252807	-0.679336	0.501534	H	-3.162770	3.871944	2.608014	C	5.276780	-1.832238	2.263684
H	4.548706	-2.410974	-4.977364	H	-4.140752	5.411622	-2.899562	O	6.324741	-1.064281	2.901271
H	5.386793	0.647325	-5.827537	H	-6.930349	3.682048	-2.658844	C	4.434934	-2.512512	3.356426
H	3.040510	0.113528	0.767926	H	-2.077234	1.851000	2.034022	O	4.912440	-3.778849	3.772875
O	2.828890	4.854419	-0.938411	O	-5.570306	-1.692775	1.533018	C	4.900871	-4.944021	0.684571
C	3.016177	3.434647	-1.145351	C	-4.930352	-0.467179	1.107163	C	4.768217	-5.562121	-0.707150
C	3.810527	3.272039	-2.451014	C	-5.960529	0.310339	0.271233	O	5.863985	-5.134077	-1.511580
C	3.042898	3.904034	-3.614164	C	-6.401233	-0.531818	-0.928605	C	3.438027	-5.179302	-1.341462
C	2.698996	5.355028	-3.301343	C	-6.910017	-1.892865	-0.470581	O	3.374212	-5.855030	-2.582491
C	2.026893	5.470099	-1.927093	C	-5.897127	-2.562750	0.466622	C	2.287408	-5.544976	-0.406605
H	2.040215	2.951092	-1.264093	H	-4.071635	-0.706697	0.469916	O	1.109995	-4.956418	-0.964575
H	4.788196	3.763896	-2.348115	H	-6.834592	0.546818	0.894255	C	2.515301	-4.988263	1.011091
H	2.102811	3.342882	-3.733518	H	-5.515759	-0.689146	-1.564206	O	3.820648	-5.371071	1.504465
H	3.638997	5.924630	-3.254941	H	-7.834343	-1.734856	0.104642	C	1.477232	-5.473990	2.009460
H	1.949338	6.521967	-1.630191	H	-6.341319	-3.448091	0.934947	O	1.387410	-6.892048	1.938046
C	3.673122	2.865684	0.124977	C	-4.400216	0.235247	2.370380	C	-0.066977	-5.734021	-1.073443
O	3.791590	3.898859	-4.816093	O	-7.446043	0.083383	-1.659918	C	-0.452528	-5.853354	-2.553772
O	1.834953	5.916356	-4.283573	O	-7.160619	-2.759910	-1.571187	O	0.638456	-6.398829	-3.294274
O	0.754338	4.881544	-1.999341	O	-4.760521	-2.914404	-0.278286	C	-0.859766	-4.497537	-3.114886
H	4.591105	2.328751	-0.118816	H	-4.772636	1.259219	2.431466	O	-1.290988	-4.724597	-4.445634
O	2.844330	1.926493	0.802326	O	-2.978443	0.336719	2.389983	C	-1.942171	-3.875194	-2.237288
H	3.929764	3.710246	0.777625	H	-4.767971	-0.320240	3.242576	O	-2.205148	-2.563600	-2.751463
H	4.116822	2.991618	-4.966035	H	-7.169403	0.993356	-1.875913	C	-1.476331	-3.804866	-0.777593

H	2.210668	5.670854	-5.142164	H	-7.658978	-2.236146	-2.216157	O	-1.126414	-5.144543	-0.351058
H	2.001247	2.362869	1.061185	H	-2.581936	-0.561996	2.312930	C	-2.537014	-3.257143	0.193695
O	-1.985294	5.488583	0.383667	O	-2.246408	-5.391525	0.766016	O	-3.877126	-3.525149	-0.198319
C	-0.841809	4.762971	-0.126994	C	-2.778063	-4.051459	0.641885	C	-3.480417	-2.305876	-3.276759
C	-0.338318	5.535840	-1.355844	C	-4.150345	-4.181744	-0.036651	C	-3.350195	-1.566244	-4.610293
C	-1.445928	5.622120	-2.408808	C	-3.989637	-4.831571	-1.413387	O	-2.558697	-2.338105	-5.507390
C	-2.708451	6.225127	-1.804454	C	-3.255179	-6.161915	-1.293204	C	-2.748823	-0.180537	-4.407752
C	-3.085432	5.502457	-0.504998	C	-1.964532	-5.998558	-0.480236	O	-2.760211	0.445440	-5.675011
H	-1.157635	3.762884	-0.443070	H	-2.121197	-3.458401	-0.003533	C	-3.521032	0.607354	-3.342173
H	-0.043762	6.550024	-1.051251	H	-4.807300	-4.803430	0.587735	O	-2.751148	1.779870	-3.065013
H	-1.673575	4.595208	-2.734955	H	-3.379195	-4.153054	-2.029687	C	-3.663152	-0.237426	-2.066465
H	-2.494769	7.273130	-1.547015	H	-3.903719	-6.858750	-0.741751	O	-4.255410	-1.513526	-2.390817
H	-3.879849	6.047324	0.017195	H	-1.537735	-6.979187	-0.241808	C	-4.532423	0.362384	-0.975527
C	0.158812	4.589771	1.031478	C	-2.757736	-3.404017	2.039001	O	-4.320597	-0.415412	0.194349
O	-1.079258	6.433180	-3.510153	O	-5.235285	-5.094771	-2.033173	C	-3.329436	3.058062	-3.223234
O	-3.809702	6.156892	-2.703955	O	-2.928405	-6.702094	-2.568936	C	-2.452142	3.896551	-4.159198
O	-3.506187	4.201979	-0.826992	O	-1.058913	-5.233984	-1.232994	O	-2.321798	3.241655	-5.420053
H	1.121219	5.041951	0.784431	H	-3.761646	-3.100712	2.341946	C	-1.084676	4.147024	-3.536372
O	0.429817	3.222367	1.315354	O	-1.963251	-2.223696	2.073804	O	-0.380179	4.982980	-4.435788
H	-0.250175	5.105164	1.910216	H	-2.391096	-4.150385	2.754991	C	-1.250641	4.767293	-2.153177
H	-0.222393	6.114030	-3.850094	H	-5.754077	-4.268701	-2.034574	O	0.048743	4.789842	-1.555195
H	-3.473753	6.461667	-3.560074	H	-3.732884	-6.628062	-3.103731	C	-2.215866	3.937782	-1.287472
H	-0.397558	2.787875	1.617555	H	-1.023990	-2.463720	1.914900	O	-3.459505	3.720550	-1.984711
O	-5.468316	2.007705	1.380750	O	2.566536	-5.068127	-0.619688	C	-2.536248	4.608077	0.038928
C	-4.239461	2.517238	0.810155	C	1.200554	-4.613078	-0.469870	O	-2.941883	5.952437	-0.198583
C	-4.632225	3.655878	-0.143013	C	0.317673	-5.607900	-1.239179	C	0.486494	5.973873	-0.918507
C	-5.554110	3.115216	-1.239165	C	0.725616	-5.625253	-2.714762	C	1.756685	6.478540	-1.616430
C	-6.756970	2.405698	-0.627892	C	2.215242	-5.914261	-2.858414	O	1.503832	6.648315	-3.010401
C	-6.308757	1.386372	0.428047	C	3.039097	-4.991455	-1.950429	C	2.917980	5.519060	-1.390742
H	-3.755661	1.726914	0.226143	H	1.093805	-3.624554	-0.929606	O	4.058538	6.121287	-1.978544
H	-5.151564	4.443435	0.420869	H	0.438592	-6.612937	-0.811084	C	3.087466	5.253041	0.102350
H	-4.976872	2.378668	-1.819884	H	0.527610	-4.621170	-3.121748	O	4.124253	4.272706	0.245894
H	-7.371709	3.159951	-0.114594	H	2.394484	-6.947003	-2.524298	C	1.771730	4.751103	0.707674
H	-7.172705	1.015357	0.990816	H	4.082265	-5.325093	-1.914601	O	0.751606	5.744770	0.449133
C	-3.289170	2.877174	1.966551	C	0.916868	-4.452169	1.034871	C	1.833355	4.515557	2.225525
O	-6.052050	4.141215	-2.078451	O	0.031597	-6.614762	-3.452557	O	2.698863	5.402037	2.914022
O	-7.530149	1.732172	-1.615304	O	2.657574	-5.749515	-4.201340	H	5.330252	5.728624	1.073480
O	-5.652607	0.329928	-0.224914	O	2.955557	-3.682137	-2.451174	H	7.409643	4.526562	0.669927
H	-2.989617	3.925149	1.911156	H	0.042945	-5.036395	1.327813	H	7.135145	4.217584	-1.688835
O	-2.084737	2.119975	1.923768	O	0.626859	-3.105035	1.390080	H	5.693357	2.289343	-0.475089
H	-3.825243	2.720771	2.911433	H	1.786669	-4.832046	1.586608	H	7.910790	1.334422	-0.478477
H	-5.292071	4.654981	-2.410204	H	-0.923321	-6.493692	-3.295069	H	7.395972	2.237414	2.046585
H	-7.646098	2.365071	-2.339694	H	2.010843	-6.213678	-4.753596	H	4.346494	2.319577	1.748488
H	-2.298913	1.176310	2.083787	H	1.427796	-2.556060	1.244260	H	6.012737	2.721904	4.257510
O	-5.035566	-2.992381	1.240497	O	5.279229	-0.956593	-1.586942	H	5.270621	1.162555	3.802390
C	-4.701185	-1.614535	0.951017	C	4.090622	-1.761513	-1.403236	H	3.903111	2.633189	5.154476
C	-5.898723	-1.008345	0.201961	C	4.129323	-2.871492	-2.466152	H	7.827756	0.241546	2.622829
C	-6.157187	-1.796047	-1.085002	C	4.168931	-2.252302	-3.865079	H	8.478864	-1.847153	1.552903
C	-6.328548	-3.279827	-0.784096	C	5.327177	-1.270172	-3.984929	H	8.786476	-1.013790	-0.646297
C	-5.174373	-3.796069	0.085410	C	5.312808	-0.269296	-2.821854	H	6.122306	-1.437712	-0.332281

H	-3.827469	-1.582630	0.290326	H	3.201609	-1.144529	-1.575565	H	6.919106	-3.569314	-1.003221
H	-6.791468	-1.044455	0.842164	H	5.021802	-3.495082	-2.314738	H	6.549604	-3.512168	1.869004
H	-5.271155	-1.673900	-1.727745	H	3.228398	-1.696867	-4.005791	H	4.630880	-1.140878	1.707503
H	-7.255456	-3.404637	-0.204842	H	6.265694	-1.839849	-3.915476	H	3.399769	-2.578360	2.996568
H	-5.397824	-4.804050	0.452308	H	6.241236	0.312511	-2.811060	H	4.436381	-1.850392	4.228908
C	-4.308728	-0.943520	2.279032	C	4.067824	-2.222279	0.064170	H	4.493605	-4.446489	3.204280
O	-7.328471	-1.362519	-1.751873	O	4.336017	-3.227765	-4.877878	H	5.804875	-5.308926	1.182357
O	-6.386987	-4.056242	-1.975687	O	5.282234	-0.549374	-5.211801	H	4.795080	-6.654646	-0.589027
O	-3.998588	-3.799711	-0.683125	O	4.201252	0.575953	-2.969771	H	5.625965	-5.362230	-2.423292
H	-4.878644	-0.026125	2.432929	H	3.940597	-3.303945	0.127491	H	3.422585	-4.087681	-1.485149
O	-2.936268	-0.559600	2.313253	O	2.987518	-1.662057	0.804390	H	2.445196	-5.868222	-2.888237
H	-4.545734	-1.640928	3.093042	H	5.034128	-1.960585	0.515023	H	2.189646	-6.634325	-0.357235
H	-7.271942	-0.394968	-1.861244	H	3.660425	-3.918495	-4.744945	H	2.458346	-3.893258	0.962851
H	-7.006798	-3.598085	-2.562749	H	5.117030	-1.208045	-5.902869	H	0.520221	-5.000742	1.753652
H	-2.374971	-1.355450	2.178079	H	3.045604	-0.681193	0.779662	H	1.776988	-5.138306	3.013669
O	-0.979865	-5.746353	0.131159	O	3.809631	3.861573	-1.353073	H	0.658181	-7.172450	2.504507
C	-1.815216	-4.565990	0.163701	C	3.649070	2.426021	-1.441447	H	0.087163	-6.719581	-0.623712
C	-3.114405	-4.914628	-0.579199	C	4.363434	1.972102	-2.724564	H	-1.317405	-6.528978	-2.619142
C	-2.794862	-5.318388	-2.020847	C	3.756138	2.674724	-3.941197	H	0.399863	-6.269695	-4.226073
C	-1.770403	-6.446939	-2.045201	C	3.780822	4.186082	-3.750377	H	0.018388	-3.834071	-3.094991
C	-0.557443	-6.102652	-1.171024	C	3.170556	4.570241	-2.396800	H	-1.552801	-3.870285	-4.840158
H	-1.315021	-3.751111	-0.371626	H	2.583986	2.183233	-1.525698	H	-2.852739	-4.482488	-2.274520
H	-3.615984	-5.748279	-0.067827	H	5.431660	2.221524	-2.654558	H	-0.579521	-3.175901	-0.708925
H	-2.355809	-4.440388	-2.520249	H	2.706209	2.351922	-4.020032	H	-2.391594	-2.179993	0.319834
H	-2.241873	-7.341504	-1.611847	H	4.831840	4.510836	-3.740838	H	-2.361999	-3.732802	1.164885
H	0.079595	-6.984729	-1.042437	H	3.350601	5.630222	-2.185718	H	-4.193617	-2.720075	-0.642760
C	-1.957513	-4.144266	1.636639	C	4.168935	1.822161	-0.123214	H	-4.042922	-3.235782	-3.405775
O	-3.940329	-5.775732	-2.715872	O	4.464068	2.391024	-5.134073	H	-4.365081	-1.445336	-5.016849
O	-1.319080	-6.722763	-3.366471	O	3.069959	4.860418	-4.783038	H	-2.314814	-1.735942	-6.227228
O	0.157267	-5.061076	-1.783268	O	1.792903	4.300852	-2.436943	H	-1.720107	-0.304047	-4.034785
H	-3.007619	-4.079577	1.926181	H	4.951155	1.085396	-0.314797	H	-2.447616	1.367629	-5.575786
O	-1.403990	-2.855256	1.892827	O	3.156728	1.132016	0.604051	H	-4.510410	0.881099	-3.734766
H	-1.473219	-4.911228	2.254509	H	4.599031	2.637137	0.473012	H	-2.660427	-0.397591	-1.652397
H	-4.642201	-5.105608	-2.617131	H	4.541780	1.422181	-5.218646	H	-5.582048	0.335657	-1.301802
H	-2.114553	-6.767311	-3.917656	H	3.362423	4.458160	-5.614546	H	-4.248935	1.411788	-0.821706
H	-0.456647	-2.841121	1.623188	H	2.420618	1.751757	0.804440	H	-5.116055	-0.442375	0.763377
O	3.648104	-4.169481	-1.032255	O	-0.699803	5.725626	-0.137304	H	-4.346046	2.971754	-3.622544
C	2.214131	-4.039645	-0.891002	C	0.221726	4.704679	-0.587693	H	-2.952691	4.865094	-4.297693
C	1.583218	-5.119866	-1.782974	C	0.894822	5.245285	-1.857513	H	-1.600509	3.702595	-5.876499
C	2.004767	-4.896955	-3.237975	C	-0.166847	5.518266	-2.926320	H	-0.572873	3.179334	-3.416648
C	3.523856	-4.837699	-3.353447	C	-1.248857	6.444555	-2.381739	H	0.367452	5.397725	-3.961109
C	4.109026	-3.853531	-2.331940	C	-1.774851	5.936477	-1.032663	H	-1.643210	5.784127	-2.256199
H	1.900275	-3.057021	-1.259462	H	-0.339559	3.801370	-0.849938	H	-1.748069	2.967803	-1.073410
H	1.920339	-6.111274	-1.449552	H	1.426878	6.177233	-1.620412	H	-1.631790	4.572144	0.659704
H	1.595797	-3.924424	-3.553814	H	-0.633199	4.553606	-3.181202	H	-3.329128	4.029915	0.535461
H	3.921879	-5.834642	-3.112711	H	-0.792951	7.429998	-2.204445	H	-3.007570	6.396539	0.655565
H	5.199848	-3.948830	-2.291564	H	-2.409571	6.694901	-0.560807	H	-0.303344	6.730529	-0.942661
C	1.879404	-4.092979	0.610253	C	1.147898	4.341549	0.587058	H	2.019534	7.447425	-1.168033
O	1.558548	-5.934071	-4.092489	O	0.374912	6.137615	-4.078458	H	2.376888	6.784141	-3.411293
O	3.938910	-4.445582	-4.657207	O	-2.343634	6.565347	-3.283141	H	2.681673	4.563129	-1.883260

H	1.183886	-4.906268	0.825235	H	2.193414	4.521804	0.331027	H	4.827460	5.535430	-1.841635
O	1.241939	-2.900200	1.057819	O	1.056863	2.960562	0.924852	H	3.369362	6.174508	0.622334
H	2.808710	-4.277749	1.163146	H	0.887018	4.977092	1.442572	H	1.474282	3.814025	0.218955
H	0.595928	-6.033506	-3.970595	H	1.126306	5.597639	-4.387637	H	2.119629	3.475598	2.412720
H	3.417675	-4.979884	-5.274894	H	-1.953713	6.724164	-4.155746	H	0.814339	4.651349	2.609140
H	1.874398	-2.151473	0.993844	H	0.153088	2.781775	1.261484	H	3.501306	4.898286	3.124022
C	1.413328	-3.931328	5.492370	C	1.225372	4.255513	5.225746	C	-7.569788	3.331255	4.893300
C	2.535512	-3.678962	6.279886	C	2.383546	4.146753	5.994043	C	-8.707804	2.536371	4.767890
C	3.114736	-2.412032	6.258956	C	3.069235	2.934526	6.029535	C	-8.628139	1.335179	4.069068
C	2.600777	-1.380336	5.460748	C	2.627953	1.817127	5.306538	C	-7.433703	0.898267	3.474437
C	1.455542	-1.632746	4.683046	C	1.447803	1.924861	4.547920	C	-6.279835	1.688579	3.628030
C	0.878835	-2.908675	4.710686	C	0.762968	3.146417	4.519286	C	-6.371086	2.895026	4.335468
C	0.780311	-0.517950	3.906135	C	0.853370	0.712995	3.854547	C	-4.922578	1.218187	3.142351
C	0.342159	0.572584	4.854802	C	0.532043	-0.352930	4.874931	C	-4.582958	-0.128659	3.736291
C	-0.999334	0.809313	5.151906	C	-0.776735	-0.686733	5.220257	C	-3.588218	-0.264210	4.704906
C	-1.370165	1.818954	6.044598	C	-1.038328	-1.671954	6.176646	C	-3.288018	-1.505192	5.268915
C	-0.384908	2.595238	6.650187	C	0.023967	-2.324002	6.798226	C	-4.002653	-2.627910	4.861525
C	0.963256	2.366726	6.366545	C	1.340576	-1.996860	6.466741	C	-5.009119	-2.509927	3.900924
C	1.341830	1.358364	5.468799	C	1.609763	-1.013352	5.504446	C	-5.310944	-1.266543	3.329828
C	3.402246	-0.083031	5.433418	C	3.537564	0.593081	5.330472	C	-7.544956	-0.391307	2.659458
N	2.685793	1.154839	5.062621	N	2.921352	-0.720079	5.050431	N	-6.289734	-1.107477	2.287346
C	4.595946	-0.253472	4.467175	C	4.688366	0.808142	4.321900	C	-8.326881	-0.102309	1.360063
C	3.577767	2.309135	5.133474	C	3.910347	-1.789371	5.155558	C	-6.646372	-2.364590	1.594525
C	4.748011	2.121409	4.172076	C	5.033104	-1.558169	4.148241	C	-7.458061	-2.084234	0.335297
N	5.483008	0.906033	4.510299	N	5.671408	-0.269710	4.398472	N	-8.663808	-1.331512	0.656237
C	6.654585	0.722865	3.670110	C	6.799784	-0.036497	3.512416	C	-9.486198	-1.082911	-0.517633
H	0.947159	-4.912716	5.497370	H	0.675518	5.191954	5.189214	H	-7.609086	4.271243	5.435734
H	2.955285	-4.457724	6.910090	H	2.749041	4.994398	6.566540	H	-9.648768	2.842897	5.214775
H	3.989174	-2.213877	6.874900	H	3.971460	2.848250	6.631091	H	-9.516553	0.714009	3.981543
H	-0.005467	-3.089128	4.106265	H	-0.148052	3.214579	3.931386	H	-5.473068	3.495479	4.456887
H	-0.081159	-0.919037	3.367751	H	-0.051091	1.007752	3.318046	H	-4.162763	1.949529	3.432926
H	1.477538	-0.093612	3.172956	H	1.567363	0.305114	3.128153	H	-4.894163	1.151274	2.049876
H	-1.760391	0.214434	4.653655	H	-1.597736	-0.188483	4.711337	H	-3.033999	0.618578	5.013450
H	-2.419825	1.997694	6.259128	H	-2.063415	-1.928614	6.427448	H	-2.504340	-1.590288	6.015676
H	-0.658753	3.380588	7.349489	H	-0.164999	-3.088608	7.546857	H	-3.786334	-3.602250	5.290069
H	1.721575	2.973804	6.849980	H	2.159557	-2.507567	6.962535	H	-5.553271	-3.396727	3.600390
H	3.833672	0.050782	6.442648	H	4.002488	0.555751	6.333019	H	-8.164451	-1.087813	3.249883
H	4.199703	-0.442895	3.450601	H	4.252853	0.907118	3.308874	H	-7.724726	0.592950	0.739315
H	5.166854	-1.137522	4.770253	H	5.190097	1.751692	4.561440	H	-9.254947	0.417752	1.613910
H	3.975804	2.467837	6.152344	H	4.348678	-1.855923	6.168060	H	-7.241301	-3.020480	2.250400
H	3.012743	3.199761	4.846359	H	3.416304	-2.739287	4.935707	H	-5.724854	-2.883121	1.318630
H	5.427987	2.978230	4.254594	H	5.785043	-2.350020	4.251847	H	-7.744941	-3.041154	-0.115589
H	4.353002	2.091490	3.138947	H	4.606182	-1.619097	3.128828	H	-6.824280	-1.557214	-0.404096
H	6.411846	0.608413	2.595016	H	6.518655	-0.001572	2.441351	H	-8.978193	-0.468798	-1.286152
H	7.203076	-0.170092	3.987794	H	7.279105	0.915216	3.764856	H	-10.404863	-0.564882	-0.224282
H	7.321863	1.585306	3.773224	H	7.540465	-0.833207	3.640044	H	-9.765941	-2.035458	-0.978851

Complexes 1:2 VACUUM												
[β -CD-CCCW]-[MIA S]-[β -CD-CCCW]				[β -CD-CCCW]-[MIA R]-[β -CD-CCCW]				[β -CD-EXP]-[MIA S]-[β -CD-EXP]				
CAPS A				CAPS A				CAPS A				
E	-9358.41049921			E	-9358.39963617			E	-9358.33648282			
ZPE	-9355.608033							ZPE	-9355.540872			
H	-9355.449270							H	-9355.377594			
G	-9355.788204							G	-9355.735053			
S	713.347							S	752.335			
Atom	x [Å]	y [Å]	z [Å]	Atom	x [Å]	y [Å]	z [Å]	Atom	x [Å]	y [Å]	z [Å]	
O	7.608925	-1.699456	1.316817	O	-2.683142	-4.004146	5.808110	C	1.910512	-3.667889	5.171787	
C	6.792751	-0.795595	2.092189	C	-1.787092	-4.418045	4.753195	C	3.153674	-2.903888	4.671509	
C	5.891598	-1.584491	3.055600	C	-0.370554	-4.049206	5.217430	O	2.984415	-1.527281	4.978961	
C	5.149245	-2.710963	2.330955	C	-0.259470	-2.532876	5.427429	C	3.369514	-3.128219	3.175848	
C	6.061178	-3.544778	1.439947	C	-1.343663	-2.051537	6.392153	O	4.620085	-2.560172	2.805927	
C	6.877185	-2.607615	0.527388	C	-2.722642	-2.605708	5.983063	C	3.313990	-4.616190	2.825959	
H	6.148630	-0.227478	1.414128	H	-2.018942	-3.861633	3.838383	O	3.415317	-4.722064	1.392007	
H	6.481428	-2.001723	3.883850	H	-0.160182	-4.560958	6.167060	C	2.001248	-5.216637	3.335978	
H	4.420870	-2.235024	1.669820	H	-0.415852	-2.046034	4.452462	O	1.965654	-5.018614	4.766620	
H	6.773892	-4.105435	2.062052	H	-1.107379	-2.463857	7.384897	C	1.852727	-6.720102	3.051137	
H	7.616344	-3.184175	-0.039961	H	-3.442990	-2.427722	6.789132	O	3.075952	-7.438320	3.011586	
C	7.746100	0.172009	2.786487	C	-2.054087	-5.907372	4.468981	C	4.439177	-5.499560	0.821137	
O	4.854206	-0.729003	3.568880	O	0.625390	-4.381779	4.252869	C	5.163690	-4.678231	-0.257481	
O	4.489825	-3.562010	3.267613	O	1.019506	-2.198681	5.956479	O	5.619198	-3.510570	0.400762	
O	5.332726	-4.434734	0.604449	O	-1.470591	-0.643585	6.461210	C	4.227492	-4.369856	-1.431355	
O	5.996404	-1.933577	-0.348908	O	-3.134612	-1.954244	4.803570	O	4.926732	-3.913849	-2.589056	
H	7.227579	0.649836	3.622538	H	-1.143053	-6.496775	4.586886	C	3.420241	-5.587067	-1.895262	
O	8.190306	1.213721	1.940399	O	-2.498736	-6.134422	3.136614	O	2.290788	-5.073109	-2.624271	
H	8.586455	-0.414601	3.193384	H	-2.791882	-6.261608	5.200799	C	2.894448	-6.472383	-0.751159	
H	4.019786	-2.985362	3.910584	H	1.696569	-2.716948	5.465983	O	3.916214	-6.692386	0.250966	
H	4.638825	-4.901604	1.108681	H	-0.598602	-0.203569	6.412160	C	2.498936	-7.863103	-1.241073	
H	8.387965	0.842902	1.062214	H	-3.346318	-5.658401	2.995923	O	3.593919	-8.553374	-1.818311	
O	6.602389	-0.605362	-3.737559	O	-6.613246	-1.724478	3.643895	C	2.093900	-5.430576	-3.978977	
C	6.602435	-0.588298	-2.295891	C	-5.287405	-2.299048	3.663317	C	1.995891	-4.150650	-4.836872	
C	6.193794	-1.973858	-1.764061	C	-4.487713	-1.509199	4.706287	O	3.085573	-3.273926	-4.602509	
C	4.869407	-2.444517	-2.378162	C	-4.417564	-0.023583	4.328125	C	0.667222	-3.424525	-4.623665	
C	4.908978	-2.324788	-3.900450	C	-5.822985	0.539286	4.106576	O	0.547714	-2.409262	-5.620921	
C	5.362296	-0.920653	-4.335326	C	-6.628041	-0.390905	3.177787	C	-0.516470	-4.383846	-4.735225	
H	5.877743	0.152945	-1.936822	H	-4.820102	-2.170721	2.681290	O	-1.677309	-3.640882	-4.343222	
H	6.976220	-2.703681	-2.017185	H	-4.984791	-1.604975	5.681869	C	-0.327039	-5.618941	-3.844495	
H	4.061719	-1.805626	-1.996533	H	-3.848275	0.068099	3.391620	O	0.949613	-6.236617	-4.138197	
H	5.660074	-3.034941	-4.278383	H	-6.332087	0.553995	5.082236	C	-1.359281	-6.709192	-4.123289	
H	5.550373	-0.912117	-5.414371	H	-7.681638	-0.089750	3.169237	O	-1.285450	-7.166267	-5.463435	
C	8.018635	-0.141020	-1.882471	C	-5.427270	-3.812231	3.915307	C	-2.810070	-3.621877	-5.192887	
O	4.633174	-3.807630	-2.043218	O	-3.780656	0.704746	5.375850	C	-3.198033	-2.155930	-5.504667	
O	3.652868	-2.569623	-4.501478	O	-5.846538	1.828121	3.518987	O	-2.035565	-1.481038	-5.969160	
O	4.365627	0.025453	-4.006960	O	-6.072883	-0.295477	1.890570	C	-3.842214	-1.470126	-4.300279	
H	8.611430	-0.988435	-1.528676	H	-4.909900	-4.105208	4.830733	O	-4.369396	-0.215697	-4.730594	

O	8.026290	0.799627	-0.817767	O	-4.852327	-4.588611	2.870199	C	-4.950274	-2.361124	-3.731170
H	8.510335	0.264819	-2.775303	H	-6.495517	-4.035408	4.035162	O	-5.485759	-1.687500	-2.585072
H	4.774598	-3.915490	-1.075840	H	-2.979144	0.202556	5.646733	C	-4.372411	-3.737604	-3.379494
H	3.295961	-3.446957	-4.250655	H	-5.099415	2.374939	3.833176	O	-3.894047	-4.312888	-4.615462
H	7.652903	1.635559	-1.128198	H	-5.346042	-4.400813	2.041942	C	-5.358485	-4.717331	-2.728212
O	3.473732	3.272224	-5.490368	O	-7.628255	-1.268308	-1.282257	O	-6.702740	-4.632872	-3.184737
C	4.022708	2.386616	-4.490985	C	-6.840434	-1.493093	-0.092804	C	-6.859731	-1.399408	-2.550148
C	3.909736	0.943951	-5.011760	C	-6.928262	-0.214816	0.751549	C	-7.063027	0.028058	-2.029237
C	2.435979	0.617344	-5.308566	C	-6.423290	1.004372	-0.036367	O	-6.330885	0.880681	-2.898127
C	1.796328	1.671445	-6.213404	C	-7.069221	1.103563	-1.417119	C	-6.608241	0.110734	-0.574907
C	2.094824	3.103323	-5.724891	C	-7.071888	-0.273673	-2.114053	O	-6.901345	1.413427	-0.083833
H	3.440858	2.468997	-3.565333	H	-5.795530	-1.652571	-0.378301	C	-7.234142	-0.979399	0.305117
H	4.506830	0.831131	-5.927263	H	-7.968727	-0.047009	1.063593	O	-6.485465	-0.953263	1.529272
H	1.906364	0.624212	-4.350587	H	-5.345797	0.876243	-0.172451	C	-7.080517	-2.363161	-0.347854
H	2.250618	1.571834	-7.211120	H	-8.118356	1.407152	-1.284568	O	-7.556320	-2.319167	-1.717803
H	1.841882	3.815858	-6.517861	H	-7.707342	-0.236682	-3.005797	C	-7.854957	-3.482501	0.338933
C	5.446158	2.867681	-4.202576	C	-7.329680	-2.792179	0.574774	O	-7.436669	-4.771027	-0.079075
O	2.303604	-0.651550	-5.942352	O	-6.676247	2.202845	0.697977	C	-7.145048	-0.833768	2.768231
O	0.387041	1.550388	-6.301395	O	-6.402100	1.996753	-2.296677	C	-6.569002	0.355300	3.557456
O	1.337581	3.379594	-4.567239	O	-5.745346	-0.592945	-2.466310	O	-6.640122	1.517522	2.739840
H	6.074298	2.006360	-3.960207	H	-7.604976	-2.611706	1.615457	C	-5.148943	0.088484	4.059970
O	5.534749	3.744413	-3.093008	O	-6.325431	-3.800778	0.604846	O	-4.863504	1.107147	5.005931
H	5.841782	3.324019	-5.122605	H	-8.222381	-3.135066	0.035098	C	-4.996082	-1.306164	4.678004
H	2.756931	-1.318409	-5.376256	H	-6.341769	2.056872	1.610314	O	-3.584846	-1.587502	4.769865
H	0.105403	0.618468	-6.386272	H	-6.092406	2.803084	-1.838651	C	-5.667292	-2.405508	3.842826
H	4.929016	4.501500	-3.194588	H	-6.081962	-4.049752	-0.314828	O	-7.023466	-2.023339	5.522960
O	0.268148	6.730254	-3.460775	O	-4.795892	-3.025766	-5.055015	C	-5.794897	-3.722808	4.604680
C	1.156932	5.593210	-3.519621	C	-5.078243	-2.626285	-3.695250	O	-6.605010	-3.581100	5.759854
C	0.565894	4.584622	-4.515438	C	-5.476999	-1.144831	-3.754938	C	-2.994458	-1.718931	6.047067
C	-0.852745	4.172860	-4.098942	C	-4.321652	-0.308734	-4.320820	C	-1.802710	-0.743184	6.181813
C	-1.729924	5.406854	-3.876254	C	-3.859356	-0.859424	-5.669353	O	-2.220018	0.592505	5.955912
C	-1.018294	6.425471	-2.966728	C	-3.660228	-2.386210	-5.594481	C	-0.639380	-1.188567	5.295254
H	1.212374	5.115284	-2.536469	H	-4.171327	-2.725693	-3.088797	O	0.475066	-0.323615	5.509175
H	0.521352	5.043887	-5.513179	H	-6.358120	-1.034033	-4.402676	C	-0.273244	-2.638777	5.616431
H	-0.786615	3.609731	-3.157185	H	-3.484868	-0.365038	-3.609662	O	0.746011	-3.024018	4.686882
H	-1.880331	5.889306	-4.854035	H	-4.662339	-0.669676	-6.397711	C	-1.499577	-3.558224	5.495509
H	-1.569536	7.372456	-2.968247	H	-3.543107	-2.791136	-6.605743	O	-2.584270	-3.046623	6.299280
C	2.556467	6.125744	-3.871920	C	-6.125600	-3.601594	-3.130098	C	-1.242282	-4.959567	6.046349
O	-1.441221	3.375902	-5.122691	O	-4.741531	1.043507	-4.491764	O	-0.904309	-4.920623	7.423622
O	-2.977779	5.118253	-3.271963	O	-2.636895	-0.310661	-6.126706	H	1.898692	-3.693272	6.265771
O	-0.951239	5.894489	-1.666192	O	-2.514507	-2.651547	-4.821494	H	4.023247	-3.309665	5.208596
H	2.968025	5.590882	-4.730109	H	-6.991887	-3.061066	-2.744263	H	3.766973	-1.022822	4.671739
O	3.505385	5.942214	-2.872921	O	-5.626488	-4.367746	-2.039698	H	2.547723	-2.623112	2.650554
H	2.454379	7.185333	-4.141801	H	-6.460381	-4.249267	-3.951006	H	4.863896	-2.885646	1.910615
H	-0.779863	2.704580	-5.404112	H	-5.253533	1.308726	-3.695660	H	4.146623	-5.150277	3.296058
H	-3.416734	4.350778	-3.691215	H	-2.589207	0.655826	-5.980404	H	1.151161	-4.689778	2.885300
H	3.197408	6.402487	-2.024168	H	-4.856980	-4.901174	-2.337045	H	1.295317	-6.837055	2.113266
O	-0.583466	7.583697	1.567755	O	-0.566824	-5.759898	-5.025096	H	1.239909	-7.144880	3.852931
C	-0.127022	6.939750	0.358001	C	-1.557942	-4.888621	-4.433033	H	3.362088	-7.460455	2.085214
C	-1.344326	6.687825	-0.542556	C	-1.579438	-3.618566	-5.293753	H	5.151244	-5.824997	1.585739

C	-2.406177	5.860037	0.195752	C	-0.208258	-2.930795	-5.259568	H	6.007986	-5.279534	-0.624224
C	-2.721475	6.424435	1.580014	C	0.889792	-3.910393	-5.675005	H	6.101991	-2.869287	-0.166352
C	-1.421528	6.751519	2.341684	C	0.744346	-5.248225	-4.919657	H	3.516701	-3.614313	-1.088489
H	0.303214	5.970626	0.618712	H	-1.250711	-4.625549	-3.415330	H	5.356097	-2.037536	-2.463303
H	-1.775997	7.641890	-0.876224	H	-1.816810	-3.896114	-6.330480	H	4.050466	-6.200074	-2.549977
H	-1.982168	4.860504	0.324586	H	-0.018289	-2.602364	-4.226953	H	2.036560	-5.979881	-0.283995
H	-3.276131	7.366249	1.455608	H	0.755626	-4.122692	-6.746365	H	1.738091	-7.764806	-2.020323
H	-1.650780	7.316491	3.251756	H	1.397015	-6.003590	-5.371763	H	2.062434	-8.425718	-0.401933
C	0.994034	7.790477	-0.266464	C	-2.878984	-5.672469	-4.327708	H	4.277662	-8.604843	-1.135295
O	-3.610785	5.785928	-0.564528	O	-0.196900	-1.820343	-6.151542	H	2.932184	-6.045566	-4.324334
O	-3.454740	5.521001	2.395626	O	2.201694	-3.431693	-5.428398	H	2.027407	-4.468271	-5.888313
O	-0.783101	5.535438	2.666156	O	1.093111	-5.030881	-3.575735	H	3.673191	-3.601857	-3.884702
H	0.772241	8.003864	-1.314215	H	-3.671577	-5.182145	-4.896003	H	0.660589	-2.981471	-3.617296
O	2.256014	7.127352	-0.270520	O	-3.351740	-5.757348	-2.987378	H	-0.397575	-2.125815	-5.658079
H	1.043807	8.743347	0.277289	H	-2.713485	-6.670181	-4.754839	H	-0.613643	-4.720635	-5.774576
H	-3.364352	5.483892	-1.467435	H	-1.029133	-1.314325	-6.013962	H	-0.369189	-5.318699	-2.790377
H	-4.208371	5.128938	1.913250	H	2.276909	-2.482612	-5.650960	H	-2.363583	-6.303456	-3.980588
H	2.531645	6.963456	0.655603	H	-2.696515	-6.257745	-2.454718	H	-1.208756	-7.530818	-3.406971
O	1.752636	4.898694	5.256774	O	2.087643	-7.504066	-1.053389	H	-0.376953	-7.474926	-5.592036
C	1.281320	5.259781	3.941575	C	1.141840	-6.673759	-1.766552	H	-2.589045	-4.151971	-6.124874
C	-0.251024	5.319828	3.976824	C	1.915018	-5.976915	-2.893484	H	-3.951574	-2.189446	-6.305147
C	-0.835319	3.981626	4.444265	C	3.054223	-5.142487	-2.300844	H	-2.156724	-0.513447	-5.929191
C	-0.201496	3.545697	5.763769	C	3.950238	-5.961490	-1.376236	H	-3.084245	-1.317722	-3.519184
C	1.337552	3.621410	5.678340	C	3.083223	-6.762255	-0.381235	H	-4.934891	0.137150	-4.010547
H	1.585935	4.482196	3.236838	H	0.749767	-5.905819	-1.091441	H	-5.737231	-2.504105	-4.481482
H	-0.582763	6.117545	4.656257	H	2.310228	-6.722894	-3.597078	H	-3.522125	-3.618617	-2.695075
H	-0.599160	3.222198	3.684999	H	2.571417	-4.361880	-1.705188	H	-5.313348	-4.590056	-1.640272
H	-0.517207	4.256653	6.542335	H	4.509646	-6.685716	-1.987014	H	-5.008846	-5.728703	-2.955820
H	1.763424	3.488753	6.678995	H	3.698815	-7.497520	0.148430	H	-7.103987	-3.859481	-2.751550
C	1.970771	6.574832	3.537983	C	-0.047790	-7.550526	-2.199406	H	-7.306853	-1.507285	-3.544118
O	-2.245822	4.101389	4.610574	O	3.842415	-4.557445	-3.333478	H	-8.137764	0.255572	-2.084603
O	-0.534020	2.223039	6.141522	O	4.841563	-5.167860	-0.607588	H	-6.270394	1.787284	-2.546962
O	1.798595	2.599005	4.815853	O	2.512418	-5.851326	0.529558	H	-5.531054	-0.079058	-0.559718
H	1.237479	7.305352	3.190503	H	-0.198626	-7.488227	-3.279126	H	-6.750631	1.415677	0.889868
O	2.895315	6.411378	2.466050	O	-1.273567	-7.134890	-1.607604	H	-8.292275	-0.752289	0.496850
H	2.467113	6.980167	4.430117	H	0.186694	-8.592248	-1.942755	H	-6.015194	-2.617697	-0.344650
H	-2.604425	4.534671	3.804651	H	3.226331	-4.154135	-3.986433	H	-8.931787	-3.324574	0.171461
H	-1.482182	2.026160	5.994920	H	5.221087	-4.440881	-1.138660	H	-7.667460	-3.429082	1.414689
H	3.503211	5.682535	2.715880	H	-1.198732	-7.219235	-0.631670	H	-7.657406	-4.889778	-1.014967
O	5.149090	1.088831	4.990238	O	1.137558	-6.613488	3.843655	H	-8.220844	-0.692500	2.613932
C	4.138848	1.907842	4.361923	C	1.061780	-6.426044	2.413181	H	-7.207246	0.489391	4.442711
C	2.889231	1.782938	5.244206	C	2.489486	-6.146512	1.926377	H	-5.856560	2.079298	2.904612
C	2.405721	0.325480	5.211356	C	3.056289	-4.895694	2.617734	H	-4.461190	0.144072	3.204560
C	3.536161	-0.638816	5.594639	C	2.938385	-4.992110	4.136962	H	-3.988494	0.923765	5.402341
C	4.880628	-0.295322	4.909215	C	1.515487	-5.439944	4.529695	H	-5.447229	-1.310850	5.677029
H	3.927670	1.506795	3.363535	H	0.441773	-5.550438	2.193146	H	-5.101567	-2.559763	2.915556
H	3.172751	2.047968	6.272197	H	3.132817	-7.010768	2.143065	H	-4.806175	-4.038660	4.947088
H	2.075956	0.104758	4.184663	H	2.456395	-4.036755	2.295214	H	-6.191293	-4.490789	3.924089
H	3.693939	-0.518099	6.677159	H	3.637091	-5.766253	4.487654	H	-7.453174	-3.232312	5.449828
H	5.698621	-0.786359	5.447409	H	1.487327	-5.694067	5.594886	H	-3.733561	-1.495985	6.823411

C	4.721793	3.315666	4.175685	C	0.355316	-7.651396	1.804231	H	-1.468851	-0.797104	7.226074
O	1.335824	0.130955	6.128599	O	4.421556	-4.708110	2.257808	H	-1.982331	0.909213	5.056572
O	3.243754	-1.991527	5.287808	O	3.183745	-3.766666	4.808489	H	-0.950928	-1.142776	4.243137
H	4.598660	3.917917	5.081075	H	0.972782	-8.109431	1.029259	H	1.284626	-0.758189	5.158771
O	4.077464	4.008514	3.120146	O	-0.874561	-7.313766	1.173490	H	0.109554	-2.698701	6.642491
H	5.798238	3.199773	3.987191	H	0.204033	-8.387109	2.605264	H	-1.800637	-3.617022	4.441583
H	0.689914	0.865722	6.010956	H	4.489400	-4.809921	1.282875	H	-0.396629	-5.411750	5.523667
H	2.341637	-2.240623	5.574090	H	3.859200	-3.227607	4.350802	H	-2.135933	-5.575642	5.867375
H	4.132706	3.482976	2.270564	H	-1.490189	-6.934400	1.838969	H	-1.641751	-4.473998	7.864370
O	-3.171505	-4.075817	5.585061	O	7.400257	0.830358	2.140476	C	7.469102	1.450315	1.957565
C	-2.541908	-4.547340	4.373030	C	6.245209	1.578771	2.577993	C	6.799226	0.563703	3.024162
C	-1.044525	-4.675992	4.687397	C	5.455258	0.739586	3.598187	O	6.661225	-0.738892	2.478432
C	-0.466094	-3.305809	5.069812	C	5.102027	-0.639928	3.015848	C	5.463579	1.163846	3.456033
C	-1.265475	-2.689358	6.218180	C	6.341499	-1.326837	2.436272	O	4.963848	0.417352	4.567570
C	-2.779294	-2.767001	5.935445	C	7.102768	-0.384057	1.488862	C	5.579291	2.649797	3.825497
H	-2.675243	-3.804513	3.578999	H	5.593287	1.781760	1.722315	O	4.214919	3.109097	3.844581
H	-0.910777	-5.373425	5.526377	H	6.055206	0.597438	4.507858	C	6.409854	3.446320	2.797057
H	-0.542674	-2.650375	4.189694	H	4.372473	-0.491486	2.207302	O	7.625212	2.757143	2.460532
H	-1.069486	-3.294451	7.116451	H	7.014500	-1.566146	3.273222	C	6.916131	4.813310	3.290981
H	-3.335478	-2.524368	6.847709	H	8.069917	-0.824992	1.221822	O	5.977270	5.582321	4.016623
C	-3.269802	-5.830248	3.933353	C	6.775701	2.906360	3.117236	C	3.758010	3.948310	4.883537
O	-0.284892	-5.112564	3.562305	O	4.209853	1.383154	3.931615	C	2.730738	3.221891	5.752938
O	0.893579	-3.444683	5.475397	O	4.567241	-1.488959	4.025470	O	3.314823	2.013416	6.237078
O	-0.966768	-1.328028	6.466342	O	6.034760	-2.499867	1.701517	C	1.422718	2.934438	5.011361
O	-3.089566	-1.852852	4.911217	O	6.321758	-0.170278	0.340608	O	0.494951	2.406720	5.942670
H	-2.569985	-6.662259	3.836239	H	6.046478	3.329282	3.814617	C	0.887164	4.222700	4.379186
O	-3.893236	-5.693532	2.661167	O	6.981838	3.886689	2.118848	O	-0.261788	3.927284	3.565220
H	-4.002816	-6.084425	4.710185	H	7.698511	2.691347	3.680610	C	1.979477	4.872944	3.511946
H	1.341637	-4.032369	4.828230	H	3.899735	-0.978868	4.536404	O	3.157946	5.102460	4.321645
H	-0.010553	-1.138643	6.379451	H	5.458947	-3.104070	2.210389	C	1.616531	6.248515	2.963590
H	-4.567944	-4.981121	2.705682	H	7.378513	3.491905	1.322571	O	1.275690	7.170443	3.981114
O	-6.426775	-0.452143	4.287705	O	7.075180	0.823319	-3.104309	C	-1.522852	4.204674	4.176376
C	-5.342476	-1.378401	4.047659	C	6.870369	0.992429	-1.685189	C	-2.553112	3.196977	3.623486
C	-4.242505	-1.026269	5.056537	C	6.863836	-0.366023	-0.972349	O	-1.968407	1.886658	3.579432
C	-3.758185	0.414044	4.843989	C	5.925421	-1.362305	-1.656843	C	-3.106829	3.575245	2.246351
C	-4.936386	1.387900	4.886380	C	6.107044	-1.389964	-3.169893	O	-4.344283	2.900359	2.060961
C	-6.084352	0.884283	3.989633	C	6.089252	0.043777	-3.732716	C	-3.291089	5.080750	2.014465
H	-4.956727	-1.233694	3.033045	H	5.894673	1.457966	-1.529918	O	-3.328122	5.225733	0.588027
H	-4.648389	-1.121440	6.073598	H	7.877367	-0.786773	-0.912899	C	-2.127796	5.894428	2.583732
H	-3.286565	0.471531	3.851867	H	4.913551	-1.010629	-1.449497	O	-1.928489	5.532672	3.964615
H	-5.310279	1.412463	5.921042	H	7.090674	-1.820404	-3.408692	C	-2.370847	7.399780	2.578192
H	-6.989563	1.473154	4.176024	H	6.351032	0.028890	-4.796352	O	-3.543438	7.748633	3.298457
C	-5.909867	-2.807694	4.128548	C	7.957353	1.952823	-1.174676	C	-4.318587	5.990910	-0.070383
O	-2.829373	0.765917	5.865044	O	6.103549	-2.676003	-1.130146	C	-5.229876	5.047639	-0.881931
O	-4.615084	2.696153	4.445825	O	5.078567	-2.113061	-3.830327	O	-5.806173	4.115365	0.030101
O	-5.672304	1.016459	2.652285	O	4.787738	0.583574	-3.563006	C	-4.404775	4.356812	-1.962692
H	-5.411109	-3.381607	4.911826	H	8.475241	1.524011	-0.312587	O	-5.281146	3.577697	-2.779875
O	-5.715098	-3.536536	2.921409	O	7.445716	3.201575	-0.730323	C	-3.590422	5.350579	-2.793598
H	-6.975931	-2.732832	4.380270	H	8.692193	2.084977	-1.981303	O	-2.677403	4.547175	-3.565213
H	-2.188109	0.025170	5.958379	H	6.006471	-2.605500	-0.153926	C	-2.793289	6.293127	-1.881358

H	-3.736179	2.976062	4.771639	H	4.946497	-2.995333	-3.431717	O	-3.702358	6.912833	-0.944468
H	-6.206678	-3.081613	2.203571	H	6.803661	3.521490	-1.393748	C	-2.017588	7.405535	-2.623238
O	-7.788052	1.084704	-0.340272	O	3.263948	3.306349	-5.514089	O	-2.473134	7.699126	-3.938376
C	-6.979468	0.444414	0.622168	C	3.802715	2.734742	-4.303286	C	-2.657662	4.636053	-4.960451
C	-6.579183	1.530010	1.679334	C	4.173021	1.282508	-4.646936	C	-2.616645	3.219884	-5.549937
C	-5.807402	2.654690	0.976065	C	2.886672	0.523030	-5.016438	O	-3.760634	2.536159	-5.060923
C	-6.560888	3.192217	-0.238062	C	2.141494	1.241937	-6.145929	C	-1.300361	2.532894	-5.183604
C	-7.060651	2.019510	-1.108509	C	2.015733	2.761399	-5.888068	O	-1.259043	1.281486	-5.854312
H	-6.067962	0.047263	0.213679	H	3.025119	2.745240	-3.529266	C	-0.088560	3.407097	-5.551706
H	-7.476009	1.938221	2.166258	H	4.849602	1.297361	-5.512480	O	1.085989	2.800887	-4.983584
H	-4.869643	2.216247	0.621824	H	2.236169	0.500390	-4.129018	C	-0.249899	4.826499	-4.983831
H	-7.445766	3.740145	0.118823	H	2.751290	1.125485	-7.055062	O	-1.523467	5.373398	-5.408562
H	-7.755512	2.388659	-1.870712	H	1.742328	3.267051	-6.820594	C	0.810441	5.815882	-5.450335
C	-7.762619	-0.756940	1.234376	C	4.933378	3.658338	-3.832731	O	0.764084	7.034838	-4.725533
O	-5.537379	3.720882	1.883008	O	3.185961	-0.798772	-5.451605	C	2.065523	2.287887	-5.861234
O	-5.770502	4.019121	-1.077985	O	0.835896	0.739040	-6.364166	C	2.359655	0.794069	-5.573184
O	-5.940799	1.414952	-1.712684	O	1.036592	2.999969	-4.901561	O	1.128712	0.146218	-5.295460
H	-7.864485	-0.678277	2.318425	H	5.876380	3.414981	-4.331493	C	3.366809	0.543094	-4.442755
O	-7.105280	-1.996191	0.992326	O	5.166818	3.546507	-2.437606	O	3.947455	-0.750100	-4.574476
H	-8.767020	-0.744888	0.790565	H	4.652130	4.682887	-4.109740	C	4.542322	1.514079	-4.477514
H	-5.187481	3.324498	2.712365	H	3.791932	-1.209965	-4.794945	O	5.278151	1.336886	-3.260196
H	-5.196182	4.617665	-0.561590	H	0.815931	-0.238757	-6.324257	C	4.049678	2.958353	-4.618710
H	-7.036912	-2.142215	0.022847	H	4.349111	3.769012	-1.930826	O	3.250817	3.053965	-5.820178
O	-6.000179	-0.720644	-4.700220	O	-1.034274	6.020296	-4.442614	C	5.188577	3.954979	-4.820571
C	-6.024011	-0.477920	-3.276350	C	0.115577	5.170505	-4.220961	O	5.932694	3.665153	-5.991831
C	-5.991411	1.045131	-3.089984	C	-0.006573	3.953188	-5.150951	C	6.636843	0.939718	-3.305498
C	-4.720278	1.637937	-3.715922	C	-1.321845	3.207070	-4.878651	C	6.821557	-0.363748	-2.497043
C	-4.572464	1.201578	-5.172922	C	-2.526536	4.151964	-4.885165	O	6.029847	-1.423768	-3.007063
C	-4.793256	-0.317884	-5.306838	C	-2.255516	5.430525	-4.065671	C	6.520104	-0.097881	-1.024797
H	-5.127359	-0.909049	-2.817859	H	0.100314	4.814129	-3.188333	O	6.862222	-1.253804	-0.264174
H	-6.874428	1.490776	-3.569034	H	0.019123	4.278428	-6.200212	C	7.286420	1.113197	-0.488104
H	-3.858108	1.261178	-3.149420	H	-1.235243	2.751317	-3.882941	O	6.692656	1.441915	0.780395
H	-5.364309	1.699860	-5.752565	H	-2.692269	4.465408	-5.926885	C	7.196433	2.333625	-1.417098
H	-4.888224	-0.583141	-6.365446	H	-3.029019	6.175622	-4.282947	O	7.469342	1.953633	-2.780714
C	-7.242004	-1.216677	-2.693763	C	1.375232	6.028349	-4.391454	C	8.243265	3.395470	-1.085242
O	-4.770592	3.060598	-3.653797	O	-1.532100	2.199762	-5.863984	O	9.560072	2.897323	-1.247112
O	-3.302184	1.478165	-5.735106	O	-3.702671	3.566872	-4.351879	H	8.482246	1.091150	1.749466
O	-3.690601	-0.982563	-4.731758	O	-2.267186	5.105602	-2.692325	H	7.468397	0.539768	3.896308
H	-7.873523	-0.533381	-2.123022	H	2.159583	5.434470	-4.867127	H	5.963850	-1.244824	2.940768
O	-6.872261	-2.252299	-1.790746	O	1.919287	6.473173	-3.162467	H	4.769181	1.092697	2.610211
H	-7.830119	-1.611068	-3.532967	H	1.126158	6.862700	-5.065519	H	4.346946	0.989509	5.074492
H	-5.035691	3.309041	-2.740509	H	-0.697357	1.684298	-5.947357	H	6.026713	2.738614	4.823654
H	-2.932218	2.324620	-5.410398	H	-3.848815	2.658405	-4.685118	H	5.788813	3.564275	1.898800
H	-6.320264	-2.915234	-2.260474	H	1.253136	6.975159	-2.656681	H	7.319450	5.363396	2.428296
O	-2.697240	-4.420106	-5.560427	O	-2.945171	7.256106	0.209766	H	7.750133	4.627006	3.974320
C	-3.357763	-3.421580	-4.749400	C	-2.133728	6.653358	-0.820197	H	5.150775	5.667694	3.519109
C	-3.106695	-2.074020	-5.438620	C	-3.052333	5.873457	-1.772986	H	4.596762	4.314921	5.477091
C	-1.602093	-1.779855	-5.498446	C	-3.914253	4.856607	-1.006173	H	2.494761	3.880226	6.601129
C	-0.853512	-2.937098	-6.159901	C	-4.610458	5.490037	0.197283	H	2.606244	1.539854	6.701509
C	-1.293321	-4.287839	-5.560428	C	-3.593577	6.298858	1.021825	H	1.627884	2.213261	4.207224

H	-2.904541	-3.403808	-3.752438	H	-1.447563	5.939415	-0.358306	H	0.353672	1.453872	5.763906
H	-3.505855	-2.116982	-6.461714	H	-3.706907	6.567457	-2.318866	H	0.604655	4.937354	5.159605
H	-1.240586	-1.673879	-4.423967	H	-3.245386	4.075059	-0.627218	H	2.228811	4.206756	2.675521
H	-1.131054	-2.944486	-7.224578	H	-5.378055	6.189334	-0.165708	H	0.749839	6.160474	2.307210
H	-0.916952	-5.108639	-6.181138	H	-4.106460	6.863991	1.807628	H	2.461754	6.608667	2.356744
C	-4.828783	-3.844407	-4.578939	C	-1.282169	7.759306	-1.465256	H	2.041872	7.231006	4.569395
O	-1.358264	-0.592249	-6.241479	O	-4.898160	4.294171	-1.871565	H	-1.432149	4.083718	5.257833
O	0.554807	-2.860515	-6.015620	O	-5.182010	4.538013	1.080116	H	-3.390416	3.136646	4.323007
O	-0.774410	-4.378746	-4.255013	O	-2.665855	5.396365	1.579261	H	-1.059942	2.027805	3.265237
H	-5.503058	-3.081945	-4.973258	H	-1.385321	7.739303	-2.552445	H	-2.379904	3.234355	1.494058
O	-5.186969	-4.016486	-3.212480	O	0.110247	7.601451	-1.219701	H	-4.769700	3.276131	1.258490
H	-4.981084	-4.769535	-5.150183	H	-1.649206	8.728428	-1.101490	H	-4.227723	5.420409	2.469512
H	-2.006644	0.089543	-5.953062	H	-4.443003	4.011206	-2.696150	H	-1.226619	5.666954	2.001965
H	0.883027	-1.954200	-6.178034	H	-5.721929	3.875169	0.605670	H	-2.516377	7.738213	1.548249
H	-4.649287	-4.746024	-2.834729	H	0.294201	7.614613	-0.260259	H	-1.479420	7.895146	2.988017
O	-0.306140	-7.451857	-2.302537	O	-0.492280	5.890584	4.504338	H	-3.406852	7.439142	4.205241
C	-1.031588	-6.271195	-2.715024	C	-0.827817	5.916565	3.099631	H	-4.899785	6.580132	0.645938
C	-0.198821	-5.610315	-3.819880	C	-2.296829	5.497385	2.953743	H	-6.018368	5.652932	-1.349711
C	1.192378	-5.237036	-3.295226	C	-2.520487	4.103347	3.549064	H	-6.284214	3.411647	-0.443502
C	1.887260	-6.430320	-2.641014	C	-2.009433	4.048024	4.987183	H	-3.681122	3.707393	-1.460169
C	0.920867	-7.149070	-1.674153	C	-0.578124	4.612309	5.089704	H	-4.757485	3.215671	-3.524427
H	-1.110821	-5.578079	-1.871087	H	-0.206023	5.192014	2.561872	H	-4.238015	5.935071	-3.456284
H	-0.099021	-6.304123	-4.666287	H	-2.943050	6.221217	3.470157	H	-2.075644	5.691338	-1.313301
H	1.052312	-4.457782	-2.536769	H	-1.954120	3.381192	2.942892	H	-0.952739	7.144344	-2.643887
H	2.149733	-7.144561	-3.435687	H	-2.655774	4.697988	5.596689	H	-2.126157	8.320231	-2.033780
H	1.346522	-8.110856	-1.367349	H	-0.318594	4.751622	6.145021	H	-2.121242	7.006277	-4.522186
C	-2.462186	-6.692862	-3.099066	C	-0.503464	7.321429	2.569596	H	-3.529335	5.182252	-5.336408
O	1.999867	-4.744642	-4.362852	O	-3.908916	3.790591	3.536357	H	-2.667977	3.310870	-6.644924
O	3.040469	-6.080737	-1.892442	O	-1.978773	2.740539	5.525372	H	-3.696857	1.573447	-5.218928
O	0.723798	-6.316841	-0.557051	O	0.322957	3.708432	4.483312	H	-1.272148	2.397937	-4.096071
H	-2.685839	-6.409473	-4.129419	H	-1.336022	7.709009	1.979448	H	-0.391080	0.860214	-5.644379
O	-3.448396	-6.058933	-2.292671	O	0.623410	7.338778	1.697519	H	0.003288	3.453028	-6.646050
H	-2.524664	-7.786251	-3.020088	H	-0.351908	7.984300	3.431786	H	-0.225749	4.772922	-3.889739
H	1.458529	-4.098292	-4.869930	H	-4.250109	3.974526	2.632576	H	0.697302	5.980102	-6.532785
H	3.509562	-5.319580	-2.288261	H	-2.816126	2.259180	5.355718	H	1.797380	5.380604	-5.277325
H	-3.321905	-6.342443	-1.360314	H	1.393253	7.003520	2.193295	H	-0.045181	7.505783	-4.968549
O	-0.505138	-7.286560	2.762892	O	3.909367	3.312765	5.220758	H	1.710004	2.379870	-6.893526
C	-0.654130	-6.826104	1.400875	C	2.764742	3.843153	4.519013	H	2.813353	0.392289	-6.490661
C	0.740395	-6.867756	0.760647	C	1.494718	3.310754	5.196526	H	1.156997	-0.829564	-5.459935
C	1.698786	-5.968425	1.551187	C	1.493691	1.782195	5.239715	H	2.856844	0.653245	-3.475156
C	1.711713	-6.313523	3.036556	C	2.775331	1.264265	5.884521	H	3.310102	-1.496687	-4.561288
C	0.263787	-6.408502	3.559391	C	4.022981	1.900565	5.231577	H	5.179761	1.287739	-5.339929
H	-0.998996	-5.786635	1.404156	H	2.780227	3.511986	3.474202	H	3.450182	3.242505	-3.743652
H	1.115939	-7.900260	0.738207	H	1.455981	3.691550	6.227308	H	5.883128	3.885698	-3.979958
H	1.308248	-4.948474	1.460876	H	1.450380	1.407251	4.209588	H	4.771266	4.972487	-4.846179
H	2.181083	-7.299740	3.166312	H	2.771020	1.575669	6.940088	H	5.297045	3.671545	-6.721891
H	0.254710	-6.834698	4.568609	H	4.902736	1.691305	5.849381	H	6.959745	0.797119	-4.341678
C	-1.749540	-7.668451	0.721924	C	2.876430	5.383716	4.553041	H	7.872710	-0.663191	-2.593136
O	3.022823	-6.050100	1.033897	O	0.381572	1.317963	5.994163	H	5.247483	-1.067819	-3.494708
O	2.377047	-5.339247	3.827374	O	2.906622	-0.143502	5.793694	H	5.446977	0.115475	-0.949621

H	-1.373332	-8.124726	-0.195867	H	2.070400	5.817876	5.146854	H	6.772209	-1.032669	0.691309
O	-2.876121	-6.888866	0.336430	O	2.757520	5.995997	3.265345	H	8.342193	0.847913	-0.356011
H	-2.038020	-8.471161	1.413469	H	3.832427	5.642934	5.022067	H	6.189703	2.763280	-1.347706
H	2.968963	-6.001891	0.053920	H	-0.420605	1.806144	5.695866	H	8.140826	3.691829	-0.037667
H	3.200043	-5.033570	3.400036	H	2.064752	-0.595273	6.006074	H	8.064911	4.278913	-1.716281
H	-3.283217	-6.483835	1.134430	H	3.585381	5.866830	2.782989	H	9.615543	2.583707	-2.161524
C	1.510909	-2.869385	-0.250763	C	2.046354	-2.464490	0.151974	C	-3.518294	1.238458	-0.876086
C	2.032565	-2.428983	0.961917	C	2.612186	-1.858490	-0.965287	C	-2.733641	1.235373	-2.024114
C	2.265866	-1.069624	1.156626	C	2.558189	-0.475332	-1.098787	C	-1.463673	0.668848	-1.977441
C	1.976770	-0.126172	0.168323	C	1.933942	0.323876	-0.141184	C	-0.975018	0.100064	-0.799098
C	1.393293	-0.567959	-1.037776	C	1.333226	-0.289329	0.973970	C	-1.806022	0.020897	0.333967
C	1.183698	-1.935916	-1.231450	C	1.410418	-1.678380	1.112083	C	-3.069812	0.606387	0.280160
C	0.779873	0.416106	-2.013942	C	0.373382	0.509425	1.829944	C	-1.398683	-0.790844	1.548488
C	-0.295547	1.135891	-1.244187	C	-0.753033	0.862167	0.889612	C	-1.123702	-2.208977	1.111616
C	-1.645498	0.807355	-1.338461	C	-1.911843	0.094092	0.809663	C	-1.980860	-3.268419	1.407730
C	-2.578758	1.388088	-0.478459	C	-2.854629	0.325975	-0.191586	C	-1.718034	-4.559946	0.941936
C	-2.154263	2.301803	0.484776	C	-2.657344	1.368894	-1.095034	C	-0.589680	-4.784232	0.154379
C	-0.803521	2.645580	0.582151	C	-1.496893	2.145415	-1.027506	C	0.274884	-3.731068	-0.160561
C	0.133065	2.064011	-0.275441	C	-0.516734	1.875841	-0.065308	C	0.022801	-2.440709	0.319957
C	2.336532	1.321074	0.483687	C	1.931937	1.816394	-0.409766	C	0.494547	-0.242548	-0.774084
N	1.531995	2.332899	-0.223381	N	0.724675	2.564951	0.009106	N	0.893518	-1.345676	0.105520
C	3.828598	1.577041	0.186957	C	3.157313	2.515228	0.199832	C	1.255750	1.028077	-0.343725
C	1.922615	3.681668	0.173810	C	0.797378	3.894101	-0.587670	C	2.328145	-1.559587	0.010408
C	3.396075	3.919601	-0.126873	C	2.023128	4.647097	-0.083848	C	3.044043	-0.317529	0.537958
N	4.231634	2.934607	0.582195	N	3.272925	3.895495	-0.296042	N	2.699430	0.834891	-0.294719
C	5.660500	3.182090	0.324492	C	4.387283	4.587179	0.353531	C	3.352677	2.059884	0.143381
H	1.332203	-3.923516	-0.425420	H	2.072708	-3.541758	0.259227	H	-4.488378	1.714296	-0.881035
H	2.266592	-3.126611	1.758101	H	3.090463	-2.441888	-1.741603	H	-3.101006	1.678995	-2.939138
H	2.694638	-0.736565	2.096959	H	3.008248	-0.006321	-1.967399	H	-0.827530	0.673363	-2.859142
H	0.727422	-2.264545	-2.161756	H	0.927792	-2.151940	1.963770	H	-3.709077	0.582358	1.154127
H	0.360844	-0.117039	-2.871809	H	0.015232	-0.085548	2.674935	H	-2.194632	-0.761353	2.295199
H	1.513199	1.144612	-2.368075	H	0.829325	1.427842	2.209305	H	-0.487300	-0.381272	2.002655
H	-1.966973	0.080208	-2.080281	H	-2.061426	-0.714057	1.521486	H	-2.856583	-3.078650	2.022724
H	-3.625333	1.122434	-0.572762	H	-3.724441	-0.315408	-0.261549	H	-2.391427	-5.376226	1.185487
H	-2.863279	2.757848	1.168546	H	-3.395544	1.580079	-1.862136	H	-0.385788	-5.779546	-0.231850
H	-0.487598	3.363822	1.329719	H	-1.356791	2.951176	-1.736876	H	1.127387	-3.908745	-0.804373
H	2.200230	1.456732	1.573670	H	2.028617	1.925068	-1.505057	H	0.808125	-0.476897	-1.808714
H	4.007548	1.407698	-0.888921	H	3.075265	2.477933	1.300239	H	0.856053	1.345799	0.640955
H	4.429302	0.855898	0.746553	H	4.063145	1.970610	-0.082197	H	1.033081	1.828295	-1.057528
H	1.747929	3.868689	1.245572	H	0.842162	3.838128	-1.686825	H	2.650131	-1.724997	-1.033921
H	1.323211	4.396583	-0.391186	H	-0.095551	4.456652	-0.313295	H	2.605438	-2.434359	0.595194
H	3.673574	4.919188	0.215835	H	2.096690	5.592998	-0.626759	H	4.125362	-0.472905	0.512962
H	3.575474	3.876004	-1.209165	H	1.889652	4.866609	0.986932	H	2.754223	-0.166617	1.596215
H	5.885546	3.163201	-0.752781	H	4.250058	4.655979	1.445295	H	3.014048	2.388998	1.145397
H	6.275476	2.452336	0.858744	H	5.320279	4.049861	0.197314	H	3.135874	2.865573	-0.566543
H	5.916107	4.176388	0.703648	H	4.483837	5.596420	-0.057290	H	4.432793	1.916374	0.189356
CAPS B				CAPS B							
E	-9358.38780141			E	-9358.39131373						
O	4.976482	-5.511075	-2.563585	O	2.536932	-7.429975	-0.488201				
C	4.730640	-5.046486	-1.215761	C	1.684427	-6.673317	-1.376901				

C	3.617427	-5.926153	-0.631480	C	2.594682	-5.986769	-2.404322
C	2.364008	-5.810936	-1.504855	C	3.599436	-5.083319	-1.680956
C	2.642866	-6.086919	-2.977130	C	4.368208	-5.826987	-0.594465
C	3.883269	-5.285238	-3.429976	C	3.379998	-6.608648	0.294265
H	4.364484	-4.015048	-1.248786	H	1.167029	-5.893898	-0.807735
H	3.951667	-6.970503	-0.557458	H	3.115523	-6.737178	-3.015355
H	2.052889	-4.766561	-1.418693	H	2.999719	-4.309602	-1.191769
H	2.870040	-7.155388	-3.104343	H	5.041321	-6.554702	-1.070860
H	4.211413	-5.622093	-4.419690	H	3.924477	-7.286780	0.960636
C	6.066017	-5.030748	-0.449449	C	0.607456	-7.617537	-1.940879
O	3.202832	-5.438242	0.644207	O	1.840954	-5.100919	-3.232530
O	1.328095	-6.676973	-1.046692	O	4.524091	-4.498818	-2.594615
O	1.562164	-5.709721	-3.823724	O	5.102246	-4.961148	0.261148
O	3.533581	-3.921871	-3.461173	O	2.634159	-5.674257	1.036104
H	5.989236	-5.618684	0.467495	H	0.613141	-7.599123	-3.032801
O	6.446552	-3.720691	-0.042243	O	-0.708200	-7.238547	-1.550491
H	6.832366	-5.487873	-1.089666	H	0.842864	-8.638353	-1.611653
H	1.263432	-6.574941	-0.071884	H	4.015199	-4.151244	-3.359511
H	0.702820	-5.912830	-3.407492	H	5.539999	-4.247018	-0.241052
H	6.579157	-3.156705	-0.836195	H	-0.781364	-7.275661	-0.571223
O	5.297430	-1.294559	-5.330796	O	0.824005	-6.388553	4.149552
C	5.019704	-2.086905	-4.154654	C	0.932906	-6.239096	2.716160
C	3.943688	-3.106488	-4.557087	C	2.400528	-5.898604	2.424279
C	2.674910	-2.370010	-5.008547	C	2.791564	-4.588098	3.122801
C	2.988670	-1.364768	-6.115480	C	2.470398	-4.650063	4.615807
C	4.206046	-0.498308	-5.735080	C	1.043278	-5.183044	4.847026
H	4.615095	-1.442410	-3.366424	H	0.304425	-5.404539	2.386922
H	4.320740	-3.733493	-5.377463	H	3.042696	-6.711940	2.790877
H	2.290034	-1.822556	-4.136087	H	2.204001	-3.778047	2.665981
H	3.261046	-1.935882	-7.015896	H	3.167047	-5.367876	5.074490
H	4.552398	0.054753	-6.615039	H	0.907707	-5.423198	5.907360
C	6.355416	-2.656705	-3.646187	C	0.381820	-7.519527	2.063652
O	1.702991	-3.295692	-5.487256	O	4.186760	-4.347178	2.965500
O	1.925215	-0.473844	-6.398812	O	2.546110	-3.397548	5.273617
O	3.820664	0.393696	-4.714948	O	0.128563	-4.190236	4.446166
H	6.300348	-3.742253	-3.544662	H	1.119861	-7.961696	1.391892
O	6.705802	-2.162855	-2.358495	O	-0.772016	-7.272955	1.267874
H	7.128465	-2.418046	-4.388566	H	0.167123	-8.240405	2.863582
H	1.675934	-4.060310	-4.871781	H	4.416067	-4.496971	2.022345
H	1.053249	-0.917924	-6.376827	H	3.342025	-2.890863	5.015534
H	6.790249	-1.184971	-2.390736	H	-1.484178	-6.909489	1.838242
O	5.510524	3.553584	-3.912705	O	-3.339419	-3.980947	5.634403
C	5.226405	2.148511	-3.728881	C	-2.314726	-4.355063	4.685370
C	4.216197	1.761032	-4.815584	C	-0.981283	-3.899925	5.291619
C	2.930536	2.586667	-4.676898	C	-0.974221	-2.377611	5.486833
C	3.248550	4.082163	-4.661077	C	-2.181694	-1.940868	6.316944
C	4.392106	4.379700	-3.671994	C	-3.473815	-2.582718	5.772358
H	4.771375	1.994222	-2.744767	H	-2.478894	-3.822435	3.742660
H	4.661166	1.953281	-5.801992	H	-0.849052	-4.387364	6.267915
H	2.460594	2.318654	-3.719733	H	-1.038864	-1.908716	4.493650

H	3.603580	4.356224	-5.666164	H	-2.033061	-2.317720	7.340135
H	4.745521	5.407230	-3.812306	H	-4.292572	-2.430566	6.484522
C	6.564060	1.385606	-3.745384	C	-2.459042	-5.860784	4.394927
O	2.053126	2.308486	-5.762731	O	0.218661	-1.977920	6.155026
O	2.154718	4.899038	-4.283562	O	-2.390850	-0.539180	6.333797
O	3.898059	4.203189	-2.365403	O	-3.772063	-1.978756	4.537937
H	6.578951	0.642577	-4.545108	H	-1.549232	-6.400456	4.663821
O	6.793125	0.667870	-2.538174	O	-2.680066	-6.126308	3.014178
H	7.364213	2.113305	-3.934435	H	-3.283366	-6.244241	5.010529
H	2.012836	1.331816	-5.878053	H	0.972145	-2.453965	5.738012
H	1.314684	4.562944	-4.654625	H	-1.542286	-0.054459	6.367388
H	6.842420	1.313410	-1.800446	H	-3.529047	-5.710338	2.748978
O	5.357268	5.596353	0.699232	O	-7.017917	-1.949169	2.824850
C	5.156457	4.569088	-0.298267	C	-5.695777	-2.462738	3.105835
C	4.223543	5.162879	-1.360636	C	-5.118521	-1.611843	4.245128
C	2.882117	5.573750	-0.738504	C	-5.048817	-0.138870	3.823849
C	3.083098	6.464127	0.491000	C	-6.402572	0.358840	3.318994
C	4.181455	5.896332	1.419785	C	-7.000112	-0.638468	2.303308
H	4.663497	3.706233	0.161929	H	-5.061376	-2.337458	2.221932
H	4.701071	6.042433	-1.814600	H	-5.747587	-1.716262	5.140252
H	2.370992	4.655132	-0.428369	H	-4.326591	-0.083973	3.001508
H	3.437937	7.443406	0.135261	H	-7.089329	0.401648	4.177656
H	4.468089	6.652214	2.159587	H	-8.045969	-0.382472	2.100335
C	6.537587	4.095626	-0.792185	C	-5.814151	-3.974778	3.373857
O	2.085306	6.268492	-1.696595	O	-4.621606	0.676117	4.912669
O	1.914266	6.617542	1.280307	O	-6.340383	1.621308	2.673279
O	3.673898	4.749980	2.060758	O	-6.239226	-0.572086	1.119263
H	6.636515	4.243449	-1.869091	H	-5.410459	-4.226074	4.356555
O	6.747119	2.706693	-0.563777	O	-5.077762	-4.752098	2.436325
H	7.301786	4.702064	-0.288301	H	-6.880095	-4.238137	3.360476
H	2.096519	5.738294	-2.524178	H	-3.835798	0.242774	5.314534
H	1.117297	6.700375	0.720565	H	-5.740313	2.228260	3.147151
H	6.757518	2.547863	0.406210	H	-5.444832	-4.604141	1.536977
O	4.972081	3.121939	5.087282	O	-7.242109	-1.721069	-2.220607
C	4.876879	3.334338	3.661036	C	-6.629094	-1.875326	-0.921361
C	3.926672	4.522250	3.448705	C	-6.892400	-0.574802	-0.151030
C	2.552495	4.203282	4.058826	C	-6.304196	0.626318	-0.907136
C	2.660887	3.767541	5.517549	C	-6.774883	0.669923	-2.358905
C	3.757199	2.690235	5.662759	C	-6.624090	-0.723578	-3.004284
H	4.432713	2.450931	3.189793	H	-5.547261	-1.997247	-1.040344
H	4.344500	5.426489	3.913089	H	-7.974700	-0.433277	-0.022772
H	2.142734	3.355824	3.498868	H	-5.213021	0.510675	-0.919108
H	2.966057	4.635531	6.120507	H	-7.845651	0.922915	-2.365687
H	3.973396	2.518544	6.723002	H	-7.137252	-0.742005	-3.971960
C	6.304624	3.480936	3.105295	C	-7.169760	-3.170828	-0.289866
O	1.685855	5.332332	3.959545	O	-6.666991	1.837214	-0.249461
O	1.460436	3.208761	6.031073	O	-6.046259	1.578243	-3.167950
O	3.299707	1.506081	5.053156	O	-5.250152	-0.989671	-3.169437
H	6.401872	4.404126	2.530890	H	-7.594794	-2.971917	0.695837
O	6.655255	2.428613	2.213694	O	-6.151765	-4.144115	-0.086992

H	6.996401	3.529104	3.956654	H	-7.967214	-3.556547	-0.938622
H	1.767461	5.689211	3.048558	H	-6.494618	1.718255	0.710214
H	0.669929	3.649263	5.663992	H	-5.797615	2.388940	-2.678559
H	6.622386	1.564118	2.680541	H	-5.761092	-4.397987	-0.952131
O	4.588463	-1.863444	5.761414	O	-3.863053	-3.414142	-5.555833
C	4.528550	-0.629845	5.012080	C	-4.337518	-3.005270	-4.253454
C	3.493851	0.258142	5.717927	C	-4.792239	-1.547300	-4.400515
C	2.120148	-0.426600	5.718890	C	-3.614377	-0.664724	-4.832997
C	2.215146	-1.829792	6.318610	C	-2.943070	-1.217063	-6.089886
C	3.392405	-2.607888	5.699985	C	-2.694198	-2.732837	-5.954329
H	4.183779	-0.837151	3.993107	H	-3.512661	-3.050670	-3.534172
H	3.813234	0.429303	6.755580	H	-5.585758	-1.491304	-5.158741
H	1.784938	-0.509898	4.674336	H	-2.879765	-0.667816	-4.014485
H	2.424430	-1.715528	7.393007	H	-3.640787	-1.071882	-6.928240
H	3.577686	-3.517019	6.282565	H	-2.424758	-3.149984	-6.930809
C	5.959371	-0.072820	4.915200	C	-5.403943	-4.016990	-3.796598
O	1.195682	0.341002	6.484481	O	-4.067578	0.658964	-5.095971
O	1.060003	-2.623850	6.122178	O	-1.689886	-0.623231	-6.381125
O	3.062222	-2.932723	4.370942	O	-1.651821	-2.931263	-5.029193
H	6.004255	0.951231	5.290680	H	-6.343428	-3.513102	-3.562233
O	6.433149	-0.018084	3.574515	O	-5.024532	-4.707988	-2.611822
H	6.607873	-0.699108	5.541794	H	-5.583210	-4.715010	-4.624867
H	1.296172	1.283855	6.224057	H	-4.673560	0.924055	-4.367576
H	0.232377	-2.117983	6.248909	H	-1.687002	0.341831	-6.220389
H	6.439940	-0.924492	3.196985	H	-4.206648	-5.221646	-2.790555
O	4.569740	-5.710072	2.501198	O	0.450239	-5.940019	-4.891346
C	4.440142	-4.319303	2.876983	C	-0.656928	-5.111691	-4.467958
C	3.307501	-4.259605	3.909390	C	-0.616393	-3.857778	-5.351563
C	1.992573	-4.743334	3.283772	C	0.700025	-3.103870	-5.126450
C	2.170128	-6.135047	2.674401	C	1.896661	-4.026580	-5.358904
C	3.441582	-6.194109	1.802222	C	1.706387	-5.360752	-4.605661
H	4.154994	-3.730120	1.999164	H	-0.510357	-4.814687	-3.424111
H	3.563928	-4.910770	4.756985	H	-0.693171	-4.157554	-6.406114
H	1.718349	-4.040026	2.483452	H	0.706546	-2.770745	-4.078957
H	2.305675	-6.845813	3.503407	H	1.938175	-4.255529	-6.434193
H	3.672336	-7.234771	1.547334	H	2.453897	-6.089423	-4.939042
C	5.819395	-3.813888	3.340894	C	-1.943083	-5.957198	-4.524902
O	0.969701	-4.802784	4.273650	O	0.797678	-1.989272	-6.006582
O	1.083764	-6.533048	1.853451	O	3.130426	-3.476258	-4.924874
H	5.788770	-3.488883	4.382495	H	-2.665622	-5.526180	-5.220468
O	6.260860	-2.687738	2.589604	O	-2.601023	-6.022224	-3.263920
H	6.528225	-4.648313	3.259528	H	-1.672180	-6.958636	-4.884217
H	1.014256	-3.976364	4.804889	H	-0.073884	-1.533208	-6.020220
H	0.229564	-6.344188	2.289436	H	3.193279	-2.522201	-5.132848
H	6.383749	-2.972664	1.658138	H	-2.007498	-6.473566	-2.624510
O	-5.181676	-4.409626	3.567893	O	4.033775	3.293900	-5.119922
C	-4.972712	-4.284077	2.143970	C	4.444290	2.803142	-3.825303
C	-3.913567	-5.309229	1.715397	C	4.848603	1.332165	-4.015646
C	-2.624289	-5.093062	2.518383	C	3.627538	0.538504	-4.497774
C	-2.880043	-5.059731	4.021378	C	3.049344	1.165221	-5.767427

C	-4.043312	-4.093258	4.337856	C	2.854135	2.691554	-5.617714
H	-4.562324	-3.296847	1.920968	H	3.597578	2.864271	-3.128919
H	-4.280389	-6.335325	1.859794	H	5.640098	1.288144	-4.777546
H	-2.240746	-4.106038	2.233219	H	2.871292	0.574313	-3.702823
H	-3.190054	-6.063701	4.347680	H	3.783537	1.013631	-6.573148
H	-4.347102	-4.211508	5.383640	H	2.690785	3.140838	-6.603616
C	-6.339915	-4.381995	1.451229	C	5.549599	3.744409	-3.323561
O	-3.522891	-5.099861	0.357925	O	5.300622	0.722180	-2.807739
O	-1.672127	-6.104402	2.204957	O	3.982249	-0.809719	-4.790329
O	-1.756568	-4.624074	4.769885	O	1.799305	0.606577	-6.140010
O	-3.618970	-2.766687	4.099527	O	1.758808	2.949282	-4.773064
H	-6.263314	-5.002299	0.556375	H	6.541658	3.377893	-3.598446
O	-6.827061	-3.122717	0.997141	O	5.559843	3.857897	-1.902333
H	-7.043113	-4.860781	2.146699	H	5.397693	4.721982	-3.797790
H	-1.656526	-6.200113	1.226582	H	4.523576	-1.154121	-4.044165
H	-0.919947	-4.971680	4.399968	H	1.809099	-0.368769	-6.069100
H	-6.918852	-2.507477	1.750173	H	4.723684	4.247058	-1.602967
O	-4.965972	0.308939	5.621148	O	-0.575887	5.804824	-4.642732
C	-4.880298	-0.725274	4.615232	C	0.631584	5.067756	-4.344720
C	-3.847237	-1.758792	5.090937	C	0.683749	3.796534	-5.205701
C	-2.486933	-1.097263	5.347895	C	-0.593264	2.972826	-4.988828
C	-2.634007	0.106547	6.278906	C	-1.860642	3.811230	-5.146329
C	-3.769258	1.031011	5.802008	C	-1.778566	5.133462	-4.359473
H	-4.538046	-0.284276	3.673480	H	0.621893	4.747163	-3.301133
H	-4.198984	-2.222390	6.023393	H	0.795336	4.046435	-6.269981
H	-2.092424	-0.745900	4.383243	H	-0.542314	2.597020	-3.958896
H	-2.915182	-0.272761	7.272836	H	-1.955426	4.076089	-6.210212
H	-3.986531	1.774112	6.577158	H	-2.576477	5.804461	-4.696135
C	-6.300891	-1.281188	4.408348	C	1.792384	6.043109	-4.526715
O	-1.596902	-2.031466	5.948526	O	-0.660411	1.890723	-5.911355
O	-1.468569	0.904983	6.366301	O	-3.022921	3.136124	-4.698876
O	-3.362058	1.668889	4.611719	O	-1.925350	4.877155	-2.976011
H	-6.306572	-2.369379	4.499809	H	2.708808	5.477777	-4.718514
O	-6.829937	-1.007455	3.116035	O	2.046261	6.834348	-3.380616
H	-6.940493	-0.865152	5.198526	H	1.581019	6.659313	-5.415745
H	-1.649103	-2.874944	5.444026	H	0.209750	1.429121	-5.898223
H	-0.655326	0.375174	6.492967	H	-3.125453	2.250728	-5.102285
H	-6.773084	-0.046241	2.949641	H	1.217788	7.194265	-3.018615
O	-4.580713	4.873442	3.293410	O	-3.271617	7.074893	-0.351207
C	-4.526473	3.431672	3.379697	C	-2.255217	6.502631	-1.201379
C	-3.524718	3.082169	4.490365	C	-2.929574	5.582625	-2.230009
C	-2.139562	3.667011	4.174471	C	-3.833777	4.529276	-1.565196
C	-2.238483	5.166119	3.883190	C	-4.757858	5.168453	-0.524549
C	-3.367967	5.466618	2.878337	C	-3.967526	6.106833	0.399369
H	-4.168648	3.018707	2.429532	H	-1.575280	5.903770	-0.588400
H	-3.884567	3.504124	5.439474	H	-3.545202	6.187369	-2.910650
H	-1.761648	3.153687	3.279821	H	-3.203448	3.784813	-1.062537
H	-2.498615	5.670008	4.825895	H	-5.503010	5.778277	-1.056705
H	-3.561347	6.544590	2.848386	H	-4.651759	6.661589	1.051125
C	-5.964628	2.922938	3.607113	C	-1.450236	7.668065	-1.805447

O	-1.248783	3.484139	5.269244	O	-4.645790	3.893020	-2.552691
O	-1.046162	5.717198	3.344308	O	-5.400161	4.224710	0.317782
O	-2.973852	5.003999	1.608896	O	-3.087303	5.314886	1.164353
H	-6.065914	2.462086	4.592020	H	-1.498465	7.650411	-2.897007
O	-6.351431	1.914765	2.677394	O	-0.068849	7.610978	-1.482875
H	-6.637230	3.788522	3.557724	H	-1.907613	8.604751	-1.459099
H	-1.307021	2.544410	5.555359	H	-4.045022	3.575363	-3.263080
H	-0.263130	5.462604	3.870563	H	-5.808051	3.500794	-0.198431
H	-6.363243	2.297542	1.784501	H	0.026372	7.625626	-0.509532
O	-4.214588	6.039518	-1.697107	O	-1.315776	6.020498	4.298193
C	-4.212740	5.266937	-0.475763	C	-1.501657	5.999364	2.865762
C	-3.130762	5.836522	0.452734	C	-2.932719	5.535278	2.567236
C	-1.757451	5.849234	-0.236095	C	-3.223878	4.185358	3.229559
C	-1.827680	6.495165	-1.618328	C	-2.872474	4.198002	4.711844
C	-3.018234	5.945295	-2.433275	C	-1.447855	4.760013	4.912563
H	-3.952419	4.227989	-0.695419	H	-0.799377	5.286331	2.423183
H	-3.392754	6.859815	0.756504	H	-3.656502	6.283643	2.920122
H	-1.415199	4.814612	-0.363734	H	-2.579432	3.439050	2.749306
H	-2.005500	7.572725	-1.482727	H	-3.565951	4.873692	5.234036
H	-3.165550	6.565052	-3.324627	H	-1.269545	4.931767	5.979808
C	-5.643961	5.282807	0.082901	C	-1.169073	7.401745	2.320777
O	-0.819411	6.574995	0.563542	O	-4.597169	3.834682	3.064668
O	-0.656422	6.283638	-2.390691	O	-2.908743	2.906081	5.298511
O	-2.758163	4.608818	-2.811025	O	-0.511962	3.826309	4.407736
H	-5.619350	5.403901	1.167835	H	-1.990789	7.781294	1.709707
O	-6.352756	4.074012	-0.147343	O	-0.023621	7.414515	1.475314
H	-6.162797	6.152137	-0.347241	H	-1.038519	8.073608	3.180099
H	-0.885811	6.228714	1.478351	H	-4.829570	3.967713	2.118223
H	0.151117	6.427249	-1.858224	H	-3.701323	2.409080	5.015661
H	-6.375361	3.881749	-1.102980	H	0.713232	7.034851	1.990494
O	-4.143947	2.784379	-5.703094	O	2.978885	3.558040	5.556187
C	-4.122716	3.250121	-4.335752	C	1.956070	3.935257	4.609486
C	-2.933134	4.211584	-4.176222	C	0.617432	3.482753	5.210516
C	-1.625612	3.518806	-4.575538	C	0.620096	1.955197	5.357847
C	-1.735481	2.901983	-5.967699	C	1.831056	1.501268	6.179580
C	-3.001607	2.028709	-6.049067	C	3.146272	2.162584	5.705940
H	-3.963908	2.390498	-3.678965	H	2.129903	3.412707	3.661496
H	-3.083965	5.096910	-4.809799	H	0.519274	3.937737	6.206207
H	-1.449639	2.702429	-3.861906	H	0.685108	1.513071	4.351676
H	-1.842359	3.714027	-6.702279	H	1.659523	1.846148	7.210860
H	-3.163225	1.694883	-7.079919	H	3.910060	2.044358	6.482105
C	-5.504631	3.850507	-4.023265	C	2.110636	5.442790	4.350595
O	-0.548443	4.448040	-4.553326	O	-0.557635	1.518262	6.024447
O	-0.634649	2.076172	-6.302554	O	2.028189	0.099896	6.158799
O	-2.834317	0.926194	-5.188039	O	3.583337	1.563138	4.505806
H	-5.405417	4.858938	-3.615716	H	1.493442	6.032492	5.032784
O	-6.224702	3.115076	-3.039416	O	1.698977	5.800661	3.034628
H	-6.064924	3.913019	-4.965975	H	3.163000	5.702160	4.521291
H	-0.609815	4.971705	-3.722295	H	-1.329197	1.986536	5.632449
H	0.216400	2.491101	-6.053506	H	1.185891	-0.385713	6.278574

H	-6.287167	2.178669	-3.315378	H	2.274301	5.351849	2.394025
O	-4.498177	-2.344330	-5.394993	O	7.008303	1.197077	3.196504
C	-4.308616	-1.009502	-4.873362	C	5.734888	1.850959	3.381687
C	-3.135548	-0.391174	-5.648833	C	4.922256	1.046252	4.407722
C	-1.869487	-1.230857	-5.432270	C	4.774989	-0.413079	3.945055
C	-2.123359	-2.688618	-5.814899	C	6.106521	-1.034279	3.510494
C	-3.409319	-3.210856	-5.145367	C	6.892998	-0.075448	2.595954
H	-4.044982	-1.064302	-3.811132	H	5.189763	1.827734	2.433522
H	-3.383023	-0.368420	-6.719715	H	5.413144	1.074519	5.390057
H	-1.615729	-1.183069	-4.364531	H	4.111324	-0.397282	3.071041
H	-2.281927	-2.724665	-6.903559	H	6.711204	-1.200492	4.414477
H	-3.692573	-4.172565	-5.587615	H	7.917269	-0.441222	2.462395
C	-5.651792	-0.265584	-4.992825	C	6.003680	3.318826	3.738458
O	-0.797924	-0.734623	-6.229353	O	4.214245	-1.215081	4.978403
O	-1.073954	-3.565086	-5.442147	O	5.948908	-2.242343	2.785166
O	-3.170727	-3.351572	-3.767567	O	6.225928	-0.001236	1.361266
H	-5.558138	0.607557	-5.642723	H	5.261555	3.659830	4.465053
O	-6.119225	0.237103	-3.744463	O	5.889647	4.192000	2.630104
H	-6.378449	-0.954756	-5.442649	H	6.995141	3.374556	4.213336
H	-0.763475	0.243711	-6.126325	H	3.422118	-0.744645	5.325625
H	-0.198255	-3.195838	-5.668326	H	5.299736	-2.842848	3.201228
H	-6.237642	-0.510317	-3.128656	H	6.505809	3.927935	1.915699
O	-4.972556	-5.515924	-1.412377	O	7.434056	1.102820	-1.933292
C	-4.674510	-4.261794	-2.072945	C	6.975536	1.260429	-0.572693
C	-3.575021	-4.549830	-3.105345	C	6.942800	-0.106680	0.125144
C	-2.326895	-5.092378	-2.396775	C	6.160227	-1.133387	-0.695497
C	-2.668023	-6.302168	-1.528602	C	6.627155	-1.172599	-2.144627
C	-3.899296	-6.015164	-0.643490	C	6.631928	0.256874	-2.724183
H	-4.286466	-3.543785	-1.342016	H	5.957500	1.662384	-0.579191
H	-3.941908	-5.283670	-3.837183	H	7.962825	-0.474925	0.306187
H	-1.952599	-4.293659	-1.746941	H	5.111657	-0.819389	-0.694484
H	-2.932256	-7.137698	-2.194001	H	7.662351	-1.543689	-2.180707
H	-4.262718	-6.946406	-0.193961	H	7.095856	0.251811	-3.716992
C	-5.989840	-3.690860	-2.636049	C	7.909569	2.277343	0.100686
O	-1.324983	-5.477850	-3.335580	O	6.289240	-2.431847	-0.113523
O	-1.604029	-6.684872	-0.663367	O	5.793430	-1.967427	-2.975065
H	-5.903091	-3.519090	-3.710759	H	8.177160	1.942788	1.105394
O	-6.333207	-2.426428	-2.075877	O	7.323602	3.561927	0.271173
H	-6.781189	-4.433490	-2.467349	H	8.828601	2.335629	-0.499286
H	-1.216733	-4.736850	-3.971345	H	6.103241	-2.338499	0.845972
H	-0.759155	-6.686999	-1.149658	H	5.576288	-2.817528	-2.547072
H	-6.502984	-2.540955	-1.123370	H	6.847165	3.797394	-0.548805
C	-5.672021	-0.090235	0.232659	C	3.336579	4.801079	0.414842
C	-5.551717	0.970188	-0.654227	C	2.378928	5.340048	-0.445779
C	-4.283287	1.464280	-0.959173	C	1.248464	4.583310	-0.764086
C	-3.128571	0.915375	-0.400148	C	1.057797	3.289667	-0.267133
C	-3.251977	-0.158100	0.500616	C	2.005877	2.762850	0.628206
C	-4.524483	-0.642305	0.801679	C	3.134173	3.523730	0.951671
C	-2.032036	-0.820616	1.098152	C	1.826854	1.381138	1.209616
C	-1.089229	-1.388610	0.053140	C	1.843786	0.283812	0.164391

C	-0.667172	-2.706192	0.261492	C	2.675892	-0.809799	0.429294
C	0.097783	-3.415664	-0.649980	C	2.865892	-1.854658	-0.461901
C	0.433266	-2.800120	-1.855713	C	2.246429	-1.780315	-1.707978
C	0.058976	-1.485319	-2.076996	C	1.401210	-0.718610	-1.991013
C	-0.656070	-0.725092	-1.124281	C	1.122743	0.306213	-1.056833
C	-1.787493	1.529364	-0.739923	C	-0.163489	2.501977	-0.713593
N	-0.869395	0.633037	-1.466132	N	0.154245	1.261762	-1.456081
C	-1.128413	2.193103	0.483456	C	-1.202840	2.280729	0.407791
C	0.345267	1.390372	-1.816735	C	-1.110426	0.688982	-1.956472
C	1.044397	1.909549	-0.565323	C	-2.031117	0.329930	-0.798629
N	0.159301	2.816488	0.167845	N	-2.380731	1.540799	-0.058010
C	0.775968	3.237201	1.413531	C	-3.241282	1.232093	1.071118
H	-6.646797	-0.492464	0.484053	H	4.229047	5.354103	0.695735
H	-6.429543	1.419224	-1.102250	H	2.503781	6.318473	-0.895827
H	-4.198258	2.295366	-1.645699	H	0.497484	5.024560	-1.406121
H	-4.626810	-1.453403	1.508547	H	3.879829	3.134962	1.633123
H	-2.363860	-1.643614	1.735899	H	2.632432	1.191844	1.921453
H	-1.507442	-0.135131	1.773585	H	0.906780	1.339626	1.804197
H	-0.964466	-3.195898	1.181075	H	3.212130	-0.827179	1.371554
H	0.351594	-4.444669	-0.439097	H	3.535423	-2.663685	-0.199929
H	0.956758	-3.343426	-2.632566	H	2.431856	-2.526447	-2.470989
H	0.301622	-1.021657	-3.027196	H	0.953446	-0.658810	-2.976821
H	-1.982579	2.343910	-1.447218	H	-0.672764	3.125140	-1.456702
H	-0.992796	1.462261	1.293355	H	-0.751324	1.767108	1.270870
H	-1.801205	2.966970	0.864716	H	-1.536982	3.262464	0.757388
H	0.059347	2.240431	-2.446105	H	-1.608668	1.431470	-2.588990
H	1.028297	0.767416	-2.391841	H	-0.915414	-0.189482	-2.567695
H	1.952373	2.456374	-0.845031	H	-2.954256	-0.120049	-1.182820
H	1.356384	1.046255	0.055088	H	-1.534607	-0.427407	-0.160730
H	0.897309	2.385314	2.112435	H	-2.684172	0.750433	1.898364
H	0.159242	3.992391	1.904100	H	-3.711997	2.135516	1.456468
H	1.761029	3.663001	1.233089	H	-4.033461	0.549170	0.766784

[β -CD]-[β -CD] DIMER VACUUM							
[β -CD-CCCW]-[β -CD-CCCW]				[β -CD-EXP]-[β -CD-EXP]			
E	-8550.94253914			E	-8550.87246983		
Atom	x [Å]	y [Å]	z [Å]	Atom	x [Å]	y [Å]	z [Å]
O	-4.812899	-5.087230	2.797491	C	-5.221245	-4.959359	-0.307770
C	-4.627504	-4.597541	1.450491	C	-5.741969	-3.823597	0.584871
C	-3.576702	-5.504930	0.798204	O	-6.056140	-2.739688	-0.267533
C	-2.253882	-5.445783	1.574584	C	-4.708563	-3.470981	1.652256
C	-2.480243	-5.758447	3.052924	O	-5.294385	-2.548590	2.559830
C	-3.661179	-4.931958	3.597492	C	-4.231191	-4.726675	2.399830
H	-4.238218	-3.574505	1.484770	O	-3.107898	-4.319039	3.184523
H	-3.945800	-6.540228	0.792265	C	-3.820106	-5.838514	1.420513
H	-1.860975	-4.421760	1.489044	O	-4.888628	-6.082156	0.486023
H	-2.754347	-6.821147	3.132758	C	-3.520647	-7.172064	2.078140
H	-3.937967	-5.291136	4.594868	O	-2.938076	-8.005266	1.078774
C	-6.007363	-4.543183	0.769447	C	-3.075538	-4.594910	4.570882
O	-3.257106	-5.089147	-0.526638	C	-2.853828	-3.275677	5.337242
O	-1.331553	-6.385262	1.031659	O	-3.865592	-2.368255	4.932388
O	-1.366056	-5.471359	3.879403	C	-1.439643	-2.743642	5.111402
O	-3.259318	-3.584312	3.649209	O	-1.220869	-1.665613	6.012134
H	-6.014045	-5.139354	-0.144874	C	-0.417145	-3.855474	5.356796
O	-6.368657	-3.222898	0.379641	O	0.873370	-3.332262	5.022565
H	-6.743341	-4.968200	1.464628	C	-0.738495	-5.093067	4.517161
H	-1.347349	-6.291407	0.052568	O	-2.067460	-5.533025	4.875824
H	-0.523703	-5.730477	3.454032	C	0.241091	-6.257192	4.736320
H	-6.425152	-2.657127	1.181052	O	0.756168	-6.357431	6.051372
O	-4.815549	-0.983804	5.719353	C	1.872558	-3.309077	6.017720
C	-4.629532	-1.731680	4.496794	C	2.493892	-1.906917	6.063143
C	-3.579199	-2.807678	4.800159	O	1.441953	-1.002752	6.343765
C	-2.256452	-2.164128	5.238720	C	3.217293	-1.609680	4.754092
C	-2.483280	-1.203100	6.404665	O	3.909932	-0.375170	4.886170
C	-3.663865	-0.261783	6.097320	C	4.203246	-2.736536	4.434863
H	-4.239534	-1.067177	3.718538	O	4.682193	-2.498197	3.108932
H	-3.948847	-3.457729	5.605705	C	3.547806	-4.126193	4.504721
H	-1.862826	-1.592739	4.384974	O	2.862045	-4.291244	5.765961
H	-2.758038	-1.803173	7.285155	C	4.556895	-5.256215	4.372640
H	-3.940956	0.294159	6.999835	O	5.615281	-5.051858	5.299258
C	-6.009222	-2.229753	4.028634	C	6.077007	-2.487469	2.868549
O	-1.334612	-3.174527	5.635464	C	6.453408	-1.144158	2.212884
O	-1.369103	-0.378155	6.696122	O	5.981199	-0.104953	3.057764
O	-3.261319	0.618750	5.076068	C	5.898916	-1.060585	0.792570
H	-6.016385	-3.316331	3.924924	O	6.451471	0.091125	0.164294
O	-6.369098	-1.711378	2.752922	C	6.265073	-2.322501	0.007032
H	-6.745717	-1.950650	4.793647	O	5.620375	-2.223076	-1.268966
H	-1.350310	-3.881828	4.951967	C	5.819573	-3.582233	0.753176
H	-0.526808	-0.872428	6.633852	O	6.458083	-3.570760	2.050494
H	-6.425490	-0.732064	2.810184	C	6.190698	-4.895018	0.042158
O	-4.816692	3.858946	4.332955	O	7.380391	-4.823247	-0.725417
C	-4.630882	2.436808	4.155269	C	6.412216	-2.253647	-2.431678
C	-3.581100	2.002866	5.186134	C	5.993781	-1.094977	-3.348276
C	-2.258068	2.746745	4.957049	O	6.158164	0.096509	-2.604228
C	-2.484613	4.257579	4.932532	C	4.565917	-1.306748	-3.845057
C	-3.664791	4.604483	4.004616	O	4.274106	-0.325047	-4.829890
H	-4.240501	2.242849	3.150635	C	4.382950	-2.712108	-4.438250
H	-3.951269	2.227536	6.196387	O	2.976640	-2.871440	-4.636536
H	-1.864020	2.435368	3.978233	C	4.918774	-3.797062	-3.490363
H	-2.759611	4.571876	5.950583	O	6.273791	-3.484914	-3.115911
H	-3.941768	5.656747	4.132724	C	4.955527	-5.187750	-4.094878
C	-6.010745	1.760509	4.252184	O	5.245244	-6.095082	-3.034645
O	-1.336854	2.426735	5.994845	C	2.476913	-3.262554	-5.899727
O	-1.370173	4.999631	4.469597	C	1.409760	-2.243973	-6.349052
O	-3.261756	4.355206	2.679569	O	2.004775	-0.957276	-6.312057
H	-6.018288	1.001783	5.036863	C	0.152454	-2.352235	-5.487162
O	-6.370426	1.086672	3.051253	O	-0.871145	-1.562625	-6.081600
H	-6.747169	2.532719	4.510940	C	-0.290744	-3.814380	-5.387726
H	-1.352972	1.451375	6.121692	O	-1.395350	-3.852244	-4.478974
H	-0.528042	4.642568	4.817386	C	0.857452	-4.702957	-4.903410
H	-6.426578	1.742256	2.321464	O	1.942435	-4.566188	-5.848416
O	-4.815766	5.794668	-0.317523	C	0.492846	-6.191064	-4.785808
C	-4.630550	4.769195	0.683822	O	-0.451419	-6.645839	-5.738401
C	-3.580974	5.304436	1.666095	C	-2.599982	-4.450148	-4.900975

C	-2.257629	5.588792	0.942132	C	-3.758471	-3.485515	-4.607375
C	-2.483542	6.511696	-0.254384	O	-3.453053	-2.265450	-5.260117
C	-3.663479	6.002620	-1.104600	C	-3.963254	-3.338745	-3.102743
H	-4.240170	3.862580	0.209522	O	-5.165287	-2.611049	-2.883722
H	-3.951007	6.234445	2.120267	C	-4.051408	-4.718846	-2.442798
H	-1.863707	4.629298	0.575382	O	-4.103346	-4.498562	-1.028730
H	-2.758528	7.503630	0.134577	C	-2.848542	-5.595075	-2.806443
H	-3.940049	6.758833	-1.847594	O	-2.800662	-5.696414	-4.254374
C	-6.010717	4.423739	1.272547	C	-2.906949	-7.015047	-2.215252
O	-1.336560	6.200345	1.839776	O	-4.220193	-7.510779	-2.024142
O	-1.368716	6.612239	-1.122711	H	-6.008575	-5.299120	-0.987099
O	-3.260334	4.811127	-1.735599	H	-6.647968	-4.188419	1.091270
H	-6.018520	4.563933	2.355014	H	-6.202571	-1.907059	0.228235
O	-6.370896	3.064873	1.050249	H	-3.833148	-3.029872	1.153651
H	-6.746737	5.107898	0.830073	H	-4.699476	-2.464214	3.341142
H	-1.353050	5.691251	2.681344	H	-5.044004	-5.079995	3.049930
H	-0.526781	6.661300	-0.626365	H	-2.926492	-5.507911	0.878128
H	-6.426448	2.903018	0.082647	H	-4.460958	-7.597440	2.458971
O	-4.812926	3.365348	-4.730322	H	-2.840086	-7.014461	2.924760
C	-4.628349	3.508921	-3.304194	H	-2.893514	-8.907455	1.418112
C	-3.578800	4.610539	-3.109777	H	-4.017662	-5.054260	4.889609
C	-2.255136	4.221689	-3.782758	H	-2.955419	-3.500081	6.409169
C	-2.480371	3.861234	-5.250356	H	-3.639496	-1.446983	5.175252
C	-3.660410	2.879346	-5.383039	H	-1.347628	-2.407310	4.067772
H	-4.238276	2.572804	-2.890867	H	-0.258410	-1.449952	6.017246
H	-3.948496	5.545476	-3.553996	H	-0.442099	-4.148448	6.412199
H	-1.861446	3.336858	-3.260854	H	-0.733720	-4.832276	3.450959
H	-2.754874	4.783708	-5.783791	H	1.050156	-6.163171	4.000523
H	-3.936416	2.770054	-6.437672	H	-0.298854	-7.183850	4.512457
C	-6.008791	3.753923	-2.667675	H	1.596101	-5.869649	6.067422
O	-1.334098	5.304803	-3.701127	H	1.449717	-3.561557	6.995028
O	-1.365370	3.244578	-5.869494	H	3.234446	-1.896590	6.876137
O	-3.257892	1.643012	-4.844718	H	1.707849	-0.073484	6.181038
H	-6.016782	4.687653	-2.102395	H	2.473929	-1.556196	3.945534
O	-6.369443	2.732990	-1.743946	H	4.565837	-0.308390	4.153662
H	-6.744428	3.834573	-3.478790	H	5.029005	-2.700846	5.153017
H	-1.350958	5.645573	-2.778483	H	2.820967	-4.213788	3.686858
H	-0.523608	3.664460	-5.599807	H	4.926935	-5.253763	3.340323
H	-6.425110	1.875549	-2.220628	H	4.037709	-6.209126	4.557254
O	-4.811031	-1.599250	-5.582649	H	6.345346	-5.631012	5.048987
C	-4.626462	-0.394943	-4.805431	H	6.623360	-2.618248	3.807518
C	-3.576338	0.443707	-5.544916	H	7.550382	-1.105588	2.146290
C	-2.252837	-0.325281	-5.660050	H	5.978918	0.756733	2.596003
C	-2.478238	-1.697105	-6.293939	H	4.802290	-0.987806	0.843589
C	-3.658655	-2.412824	-5.609365	H	6.248489	0.047904	-0.798976
H	-4.236947	-0.655742	-3.815698	H	7.350948	-2.374217	-0.124949
H	-3.945597	0.679485	-6.552972	H	4.732041	-3.558979	0.901385
H	-1.859715	-0.469482	-4.642718	H	5.349936	-5.211874	-0.583201
H	-2.752443	-1.538512	-7.347741	H	6.325875	-5.652570	0.824179
H	-3.934734	-3.305460	-6.181524	H	7.103040	-4.743642	-1.652446
C	-6.006803	0.255863	-4.600600	H	7.474072	-2.173483	-2.180986
O	-1.331136	0.413891	-6.455138	H	6.665768	-1.099978	-4.219371
O	-1.363472	-2.566022	-6.198071	H	5.721749	0.863197	-3.030509
O	-3.256492	-2.762864	-4.307045	H	3.884572	-1.217159	-2.986650
H	-6.014361	1.280020	-4.978068	H	3.421967	-0.566409	-5.263079
O	-6.367961	0.341435	-3.226572	H	4.912788	-2.759787	-5.400145
H	-6.742400	-0.327749	-5.169693	H	4.286186	-3.819489	-2.595166
H	-1.347988	1.347616	-6.146008	H	5.734335	-5.213739	-4.871488
H	-0.521373	-2.093006	-6.355454	H	3.987451	-5.404662	-4.564451
H	-6.424190	-0.565937	-2.853665	H	5.436965	-6.960907	-3.415004
O	-4.810539	-5.361272	-2.232684	H	3.287490	-3.298519	-6.635907
C	-4.625890	-4.002771	-2.689781	H	1.127893	-2.501011	-7.380657
C	-3.575220	-4.058038	-3.806039	H	1.329098	-0.250002	-6.359250
C	-2.251971	-4.627324	-3.275862	H	0.384809	-1.990138	-4.474331
C	-2.477457	-5.978005	-2.598213	H	-1.732671	-1.815054	-5.676380
C	-3.658471	-5.889189	-1.612516	H	-0.603003	-4.170703	-6.375590
H	-4.236811	-3.391395	-1.868698	H	1.205711	-4.355930	-3.922189
H	-3.943927	-4.699209	-4.619100	H	0.139057	-6.374215	-3.763604
H	-1.859270	-3.921615	-2.528832	H	1.417912	-6.763135	-4.919841
H	-2.750951	-6.703438	-3.379103	H	-1.319637	-6.620179	-5.304146
H	-3.934562	-6.893113	-1.271506	H	-2.563606	-4.674547	-5.971337
C	-6.006115	-3.437039	-3.071584	H	-4.673235	-3.925982	-5.030329

O	-1.329702	-4.788386	-4.348982	H	-4.013651	-1.531111	-4.937342
O	-1.362942	-6.444017	-1.858212	H	-3.099855	-2.805481	-2.678224
H	-6.013102	-3.093566	-4.107645	H	-5.383107	-2.649616	-1.922902
O	-6.367843	-2.309478	-2.282011	H	-4.959041	-5.231591	-2.778043
H	-6.741655	-4.245958	-2.970546	H	-1.924764	-5.109137	-2.469231
H	-1.346527	-3.964852	-4.886743	H	-2.351686	-7.028062	-1.271924
H	-0.520851	-6.273960	-2.326791	H	-2.382400	-7.677248	-2.915752
H	-6.424254	-2.583519	-1.340058	H	-4.412161	-7.420280	-1.076537
O	4.817167	-4.449616	-3.723537	C	5.221615	4.958222	-0.328283
C	4.631004	-4.228708	-2.307550	C	5.743395	3.824630	0.566512
C	3.581363	-5.246022	-1.842488	O	6.056010	2.738472	-0.283594
C	2.258400	-5.040519	-2.593352	C	4.711477	3.475070	1.636337
C	2.485318	-5.061813	-4.104195	O	5.298412	2.554957	2.545503
C	3.665286	-4.144503	-4.478913	C	4.235402	4.732807	2.381299
H	4.240451	-3.218704	-2.144221	O	3.113046	4.327427	3.168517
H	3.951836	-6.262638	-2.035792	C	3.823313	5.842278	1.399707
H	1.863623	-4.052944	-2.312005	O	4.890586	6.083172	0.463111
H	2.760707	-6.088867	-4.387324	C	3.525176	7.177604	2.054341
H	3.942464	-4.304527	-5.526741	O	2.941552	8.008451	1.053626
C	6.010690	-4.304730	-1.628189	C	3.082474	4.607025	4.554156
C	3.261326	-5.093232	-0.462533	C	2.861786	3.289854	5.324372
O	1.337799	-6.068766	-2.242087	O	3.872997	2.381343	4.920552
O	1.370890	-4.621982	-4.860197	C	1.447305	2.757215	5.101889
O	3.261884	-2.812559	-4.270238	O	1.229744	1.681604	6.005792
H	6.017919	-5.065473	-0.845464	C	0.425138	3.869725	5.345647
O	6.370312	-3.083569	-0.991737	O	-0.865846	3.345632	5.014598
H	6.747289	-4.587387	-2.391805	O	0.745364	5.104888	4.502081
H	1.353389	-6.165390	-1.263258	O	2.074745	5.545949	4.857777
H	0.528775	-4.959140	-4.493094	C	-0.234031	6.269587	4.719062
H	6.426613	-2.374296	-1.669451	O	-0.747218	6.373808	6.034537
O	4.815862	0.139028	-5.801091	C	-1.863618	3.324994	6.011214
C	4.630627	-0.830286	-4.745320	C	-2.484793	1.922910	6.061224
C	3.580987	-1.828525	-5.250042	O	-1.432394	1.019546	6.342696
C	2.257643	-1.113550	-5.556299	C	-3.210094	1.622205	4.754007
C	2.483614	0.053852	-6.515792	O	-3.902243	0.387886	4.890247
C	3.663592	0.919349	-6.033262	C	-4.196712	2.748088	4.433451
H	4.240382	-0.328336	-3.853636	O	-4.677839	2.506189	3.108943
H	3.950853	-2.310957	-6.165775	C	-3.541287	4.137989	4.498601
H	1.863961	-0.717332	-4.608501	O	-2.853534	4.306466	5.758309
H	2.758645	-0.365622	-7.495199	C	-4.550697	5.267561	4.365170
H	3.940188	1.638569	-6.812106	O	-5.607499	5.065594	5.294112
C	6.010776	-1.408204	-4.381994	C	-6.073059	2.494613	2.870903
O	1.336312	-2.029476	-6.139686	C	-6.450350	1.149555	2.219423
O	1.368923	0.918786	-6.643286	O	-5.976614	0.112635	3.066266
O	3.260484	1.586874	-4.861859	C	-5.898149	1.062297	0.798395
H	6.018302	-2.494498	-4.488489	O	-6.451570	-0.091113	0.174052
O	6.371223	-1.144017	-3.030716	C	-6.265636	2.322162	0.010156
H	6.746743	-0.987284	-5.079672	O	-5.622832	2.219570	-1.266538
H	1.353314	-2.855221	-5.605337	C	-5.819185	3.583898	0.752369
H	0.526912	0.421286	-6.677222	O	-6.455729	3.575649	2.050638
H	6.426819	-0.171895	-2.898770	C	-6.191502	4.894760	0.038452
O	4.813453	4.624665	-3.508997	O	-7.382397	4.820916	-0.727048
C	4.628829	3.194753	-3.608697	C	-6.416394	2.246989	-2.428159
C	3.579242	2.966562	-4.703819	C	-5.999093	1.086010	-3.342332
C	2.255687	3.651486	-4.336080	O	-6.162207	-0.103550	-2.594920
C	2.481031	5.129472	-4.021054	C	-4.571951	1.296685	-3.841608
C	3.660888	5.292061	-3.043449	O	-4.281357	0.312589	-4.824384
H	4.238764	2.810348	-2.660328	C	-4.389936	2.700561	-4.438633
H	3.949041	3.381565	-5.652049	O	-2.983875	2.859458	-4.639162
H	1.861716	3.157246	-3.435633	C	-4.924632	3.787869	-3.492839
H	2.755855	5.634173	-4.959449	O	-6.279117	3.476494	-3.115789
H	3.936994	6.349518	-2.966436	C	-4.962315	5.176994	-4.100868
C	6.009259	2.550963	-3.834019	O	-5.250627	6.087047	-3.042591
O	1.334793	3.536539	-5.416355	C	-2.485771	3.247405	-5.903898
O	1.365934	5.767615	-3.424141	C	-1.419242	2.227639	-6.352107
O	3.258080	4.791941	-1.791280	O	-2.014101	0.941004	-6.310891
H	6.017187	1.957233	-4.749909	C	-0.160667	2.338187	-5.492359
O	6.369862	1.659074	-2.785134	O	0.862029	1.547200	-6.086433
H	6.744939	3.359180	-3.939560	C	0.282615	3.800573	-5.397108
H	1.351425	2.603710	-5.728197	O	1.388706	3.840580	-4.490338
H	0.524102	5.483435	-3.834239	C	-0.864958	4.690169	-4.913168
H	6.425277	2.161905	-1.942749	O	-1.951078	4.551168	-5.856552

O	4.810768	5.629226	1.427172	C	-0.500132	6.178423	-4.799237
C	4.626520	4.815414	0.247178	O	0.442059	6.631275	-5.754766
C	3.576432	5.528668	-0.613968	C	2.592592	4.437550	-4.915737
C	2.252869	5.667296	0.150967	C	3.751614	3.473699	-4.621608
C	2.477980	6.342964	1.502717	O	3.445278	2.252015	-5.270895
C	3.658302	5.680844	2.239365	C	3.958766	3.330616	-3.116949
H	4.237103	3.834068	0.538101	O	5.161051	2.603379	-2.897999
H	3.945660	6.528995	-0.880650	C	4.048121	4.712404	-2.460731
H	1.859756	4.654841	0.326195	O	4.102380	4.495878	-1.046183
H	2.752262	7.391389	1.311876	C	2.844669	5.587767	-2.824536
H	3.934179	6.280247	3.113998	O	2.794207	5.685481	-4.272627
C	6.006969	4.591084	-0.396869	C	2.904154	7.009250	-2.237102
O	1.331246	6.439407	-0.612297	O	4.217760	7.505439	-2.049710
O	1.363076	6.273782	2.373956	H	6.007940	5.295978	-1.009774
O	3.256209	4.389864	2.629286	H	6.650253	4.190523	1.070602
H	6.014535	4.937133	-1.432071	H	6.203192	1.907107	0.214092
O	6.368336	3.215148	-0.440522	H	3.835266	3.032806	1.140160
H	6.742400	5.177836	0.169201	H	4.704691	2.472831	3.327961
H	1.348237	6.101961	-1.536150	H	5.049164	5.087567	3.029429
H	0.521114	6.416914	1.896195	H	2.928835	5.510596	0.859409
H	6.424183	2.870007	0.477778	H	4.466132	7.603649	2.432824
O	4.810329	2.395985	5.289917	H	2.845686	7.022386	2.902260
C	4.625618	2.811391	3.918091	H	2.897696	8.911509	1.390736
C	3.575041	3.928893	3.939209	H	4.024977	5.067272	4.870461
C	2.251816	3.416564	4.524712	H	2.964874	3.517122	6.395552
C	2.477492	2.780814	5.895619	H	3.647237	1.460724	5.166198
C	3.658251	1.792606	5.836834	H	1.353865	2.418135	4.059272
H	4.236351	1.972137	3.332061	H	0.267295	1.465887	6.012654
H	3.943879	4.761242	4.555059	H	0.451514	4.165626	6.400197
H	1.858878	2.648254	3.842358	H	0.739244	4.840982	3.436643
H	2.751489	3.583691	6.596444	H	-1.044149	6.173184	3.984737
H	3.934503	1.482575	6.850719	H	0.305480	7.195615	4.491581
C	6.005878	3.175485	3.340934	H	-1.587070	5.885989	6.053287
O	1.329793	4.494333	4.652792	H	-1.439412	3.580114	6.987246
O	1.362966	2.055919	6.384749	H	-3.224188	1.914630	6.875297
O	3.256537	0.682671	5.070694	H	-1.698381	0.089804	6.182829
H	6.013191	4.200630	2.966138	H	-2.467940	1.566860	3.944465
O	6.367259	2.351821	2.237902	H	-4.559262	0.318993	4.158932
H	6.741457	3.098875	4.152490	H	-5.021285	2.714203	5.153056
H	1.346341	5.006309	3.812979	H	-2.815783	4.223485	3.679340
H	0.520756	2.518239	6.198830	H	-4.922466	5.262249	3.333491
H	6.423563	1.418722	2.540680	H	-4.031297	6.221020	4.546328
O	4.812377	-2.639786	5.170912	H	-6.338064	5.643948	5.043454
C	4.626866	-1.308476	4.640130	H	-6.617854	2.627761	3.810441
C	3.576040	-0.628690	5.527059	H	-7.547426	1.110668	2.154723
C	2.253173	-1.406541	5.491962	H	-5.974933	-0.750237	2.606734
C	2.479728	-2.874621	5.849615	H	-4.801428	0.989762	0.847862
C	3.660721	-3.444203	5.040278	H	-6.250024	-0.050472	-0.789630
H	4.237557	-1.374097	3.618638	H	-7.351714	2.373418	-0.120340
H	3.945096	-0.590959	6.561708	H	-4.731435	3.561208	0.899048
H	1.859923	-1.352312	4.465935	H	-5.351743	5.209980	-0.589076
H	2.753895	-2.921831	6.914251	H	-6.325469	5.654377	0.818679
H	3.937496	-4.430036	5.430053	H	-7.106522	4.739142	-1.654321
C	6.006651	-0.629293	4.564790	H	-7.477873	2.167323	-2.175715
O	1.331095	-0.835182	6.414689	H	-6.672314	1.088652	-4.212483
O	1.365615	-3.709606	5.588000	H	-5.726586	-0.871368	-3.019970
O	3.259010	-3.537471	3.694819	H	-3.889448	1.209327	-2.983895
H	6.013298	0.303012	5.132435	H	-3.429847	0.553025	-5.259352
O	6.367870	-0.280423	3.233079	H	-4.920998	2.745661	-5.399975
H	6.742694	-1.310959	5.011054	H	-4.290892	3.812654	-2.598521
H	1.347101	0.140626	6.291311	H	-5.742188	5.200943	-4.876477
H	0.523219	-3.276507	5.833831	H	-3.994886	5.392736	-4.572322
H	6.424372	-1.098902	2.692322	H	-5.442943	6.951875	-3.424913
O	4.815411	-5.686520	1.159417	H	-3.297275	3.281696	-6.639135
C	4.629350	-4.441620	1.869419	H	-1.138883	2.481988	-7.384790
C	3.578900	-4.711782	2.954079	H	-1.338488	0.233518	-6.356484
C	2.256143	-5.169974	2.324253	H	-0.391434	1.978548	-4.478274
C	2.483153	-6.364885	1.399437	H	1.724130	1.800494	-5.683012
C	3.663815	-6.086648	0.449274	H	0.593167	4.154620	-6.386338
H	4.239554	-3.684018	1.181382	H	-1.212048	4.345334	-3.930756
H	3.948496	-5.496987	3.628582	H	-0.144065	6.363414	-3.778152
H	1.862414	-4.334153	1.727020	H	-1.425461	6.750327	-4.932198

H	2.757859	-7.226489	2.026353	H	1.311179	6.606485	-5.322265
H	3.941079	-7.005919	-0.078415	H	2.554486	4.659229	-5.986614
C	6.008994	-3.958557	2.353229	H	4.665691	3.913212	-5.047049
O	1.334403	-5.535641	3.346424	H	4.006359	1.518497	-4.947108
O	1.369090	-6.681625	0.583677	H	3.095980	2.798528	-2.689713
H	6.015782	-3.821227	3.436069	H	5.380498	2.644530	-1.937647
O	6.369349	-2.699580	1.795775	H	4.955231	5.224187	-2.798870
H	6.745399	-4.732032	2.098226	H	1.921494	5.102671	-2.484481
H	1.350167	-4.830787	4.032449	H	2.350629	7.024729	-1.292796
H	0.526741	-6.603995	1.075648	H	2.378312	7.669631	-2.938351
H	6.425942	-2.786983	0.818698	H	4.411428	7.417496	-1.102211

MIA S WATER			
E	-807.48797877		
ZPE	-807.143659		
H	-807.127101		
G	-807.185831		
S	123.609		
Atom	x [Å]	y [Å]	z [Å]
C	-1.217403	3.907627	-0.107994
C	-0.259666	3.721000	-1.104646
C	0.389088	2.491685	-1.210131
C	0.110086	1.431676	-0.334004
C	-0.872074	1.616337	0.658245
C	-1.521265	2.854480	0.753867
C	-1.312635	0.466500	1.544650
C	-1.841387	-0.662730	0.691957
C	-3.198144	-0.982240	0.635361
C	-3.660966	-2.031592	-0.164550
C	-2.750337	-2.764438	-0.923919
C	-1.389680	-2.448077	-0.890535
C	-0.919642	-1.396559	-0.088672
C	0.979778	0.185765	-0.490831
N	0.459977	-1.090304	0.052913
C	2.357445	0.456142	0.153660
C	1.397122	-2.181377	-0.227230
C	2.751523	-1.892674	0.411969
N	3.292079	-0.636363	-0.099135
C	4.613380	-0.350120	0.446711
H	-1.734618	4.857615	-0.010677
H	-0.020869	4.521686	-1.798181
H	1.133694	2.348325	-1.989606
H	-2.284340	2.986507	1.516594
H	-2.082514	0.811194	2.240189
H	-0.464589	0.098535	2.135334
H	-3.899127	-0.412143	1.239997
H	-4.719097	-2.274260	-0.187477
H	-3.093342	-3.582421	-1.551111
H	-0.695863	-3.022284	-1.494744
H	1.159009	0.055461	-1.573476
H	2.205537	0.633137	1.236789
H	2.772299	1.374171	-0.273945
H	1.541717	-2.333278	-1.311257
H	0.989413	-3.105133	0.190897
H	3.446443	-2.704131	0.168015
H	2.634664	-1.871715	1.513095
H	4.612185	-0.229619	1.546160
H	5.004389	0.572544	0.006242
H	5.299277	-1.165956	0.197284

β-CD WATER							
β-CD-CCCW				β-CD-EXP			
E	-4275.44518493			E	-4275.42677403		
ZPE	-4274.226515			ZPE	-4274.212074		
H	-4274.152344			H	-4274.135256		
G	-4274.330395			G	-4274.322392		
S	374.741			S	393.862		
Atom	x [Å]	y [Å]	z [Å]	Atom	x [Å]	y [Å]	z [Å]
O	1.970660	-5.446896	1.204542	C	-0.111387	-6.047638	-0.275500
C	0.706586	-4.772415	1.006590	C	-0.944218	-6.093753	-1.559652
C	-0.076459	-5.587552	-0.033635	O	-0.067020	-5.982068	-2.677342
C	0.714998	-5.658629	-1.343198	C	-1.996658	-4.990191	-1.559516
C	2.117649	-6.201973	-1.093608	O	-2.808777	-5.185738	-2.703934
C	2.797151	-5.443102	0.055606	C	-2.817482	-4.989428	-0.261232
H	0.888284	-3.771024	0.600367	O	-3.559784	-3.765545	-0.286563
H	-0.247994	-6.602285	0.349302	C	-1.883106	-5.031141	0.959685
H	0.804694	-4.632745	-1.732537	O	-0.977518	-6.141236	0.837602

H	2.028622	-7.253417	-0.784949	C	-2.575856	-5.198142	2.297500
H	3.719894	-5.951167	0.353230	O	-1.578740	-5.008629	3.307238
C	0.045665	-4.604171	2.385766	C	-4.942420	-3.761570	-0.006491
O	-1.319382	-4.973459	-0.375106	C	-5.693876	-3.170821	-1.209604
O	0.084433	-6.501385	-2.294413	O	-5.368696	-3.922281	-2.378281
O	2.946511	-6.098198	-2.248095	C	-5.354165	-1.695611	-1.389269
O	3.067324	-4.132157	-0.374171	O	-6.181205	-1.200317	-2.429700
H	-0.959669	-5.027341	2.387995	C	-5.564362	-0.949853	-0.073309
O	-0.105609	-3.235382	2.759466	O	-5.120833	0.397137	-0.273883
H	0.651256	-5.149487	3.121089	C	-4.775740	-1.620201	1.056925
H	-0.840582	-6.202619	-2.385664	O	-5.218060	-2.995893	1.151353
H	2.432913	-6.443986	-2.993205	C	-4.957164	-0.950061	2.425608
H	0.778150	-2.805304	2.781604	O	-6.252241	-0.408658	2.655337
O	5.489756	-1.856269	1.205619	C	-6.045291	1.440242	-0.091870
C	4.173833	-2.422840	1.007177	C	-5.935144	2.414789	-1.265879
C	4.322504	-3.543547	-0.032813	O	-6.195557	1.700483	-2.472270
C	4.871823	-2.969310	-1.342418	C	-4.560815	3.069509	-1.287326
C	6.171535	-2.212061	-1.092700	O	-4.568652	4.023836	-2.335619
C	6.002407	-1.207790	0.056733	C	-4.250648	3.702913	0.068668
H	3.505358	-1.655737	0.600382	O	-2.867208	4.067580	0.022153
H	5.008767	-4.310443	0.350180	C	-4.488056	2.719934	1.230834
H	4.126106	-2.259103	-1.731792	O	-5.807850	2.128114	1.129804
H	6.937759	-2.937592	-0.784208	C	-4.379773	3.377258	2.596501
H	6.975265	-0.803739	0.354331	O	-5.242397	4.510066	2.642445
C	3.628835	-2.833849	2.386068	C	-2.464777	5.342172	0.483309
O	5.137117	-3.987829	-2.293666	C	-1.838778	6.122951	-0.683140
O	6.607499	-1.499076	-2.246935	O	-2.768933	6.184081	-1.764254
O	5.146068	-0.179033	-0.372834	C	-0.532304	5.473386	-1.121766
H	3.333214	-3.883755	2.388716	O	0.033925	6.304749	-2.125457
O	2.463549	-2.098995	2.757890	C	0.392529	5.291685	0.081875
H	4.431883	-2.699497	3.122184	O	1.562691	4.602130	-0.368059
H	4.326817	-4.524885	-2.384373	C	-0.324854	4.491300	1.174717
H	6.557283	-2.115769	-2.992375	O	-1.526729	5.217579	1.532795
H	2.678063	-1.139868	2.780624	C	0.495638	4.263527	2.445293
O	4.874003	3.134368	1.205455	O	1.244336	5.397858	2.855328
C	4.498055	1.751703	1.008090	C	2.746823	5.356302	-0.473313
C	5.467866	1.169389	-0.031258	C	3.477542	4.977294	-1.764245
C	5.361495	1.956118	-1.341287	O	2.600531	5.191428	-2.866903
C	5.577982	3.444812	-1.092649	C	3.962714	3.532821	-1.705756
C	4.686222	3.938540	0.055996	O	4.735632	3.306953	-2.871142
H	3.481726	1.705664	0.600976	C	4.755123	3.256656	-0.418771
H	6.495161	1.228464	0.352109	O	4.923388	1.835979	-0.364340
H	4.341727	1.814419	-1.731200	C	3.964882	3.749038	0.805224
H	6.622658	3.592868	-0.783808	O	3.605716	5.129929	0.625889
H	4.975599	4.951583	0.353044	C	4.704785	3.676001	2.125848
C	4.479550	1.070987	2.387825	O	3.746437	3.955532	3.152321
O	6.324265	1.528750	-2.291573	C	6.205847	1.276901	-0.178720
O	5.292148	4.228689	-2.247845	C	6.504812	0.313771	-1.334442
O	3.348160	3.909010	-0.374034	O	6.430891	1.026509	-2.569458
H	5.116180	0.185278	2.392013	C	5.533837	-0.860098	-1.319261
O	3.178413	0.618627	2.760071	O	5.942482	-1.752728	-2.343478
H	4.875040	1.783594	3.123069	C	5.514753	-1.525407	0.055153
H	6.238921	0.560413	-2.382503	O	4.418141	-2.446577	0.030632
H	5.743940	3.804459	-2.992463	C	5.316939	-0.491810	1.178411
H	2.562149	1.384281	2.781787	O	6.281656	0.575260	1.045400
O	0.588278	5.762768	1.203977	C	5.470483	-1.085533	2.568412
C	1.434452	4.606468	1.006816	O	6.716176	-1.773870	2.654490
C	2.493920	5.001019	-0.033163	C	4.599003	-3.752769	0.538332
C	1.811720	5.406948	-1.343263	C	4.361827	-4.768276	-0.590934
C	0.783088	6.504796	-1.095109	O	5.219431	-4.460503	-1.689866
C	-0.158038	6.116925	0.054747	C	2.899658	-4.763717	-1.019221
H	0.836347	3.783147	0.600405	O	2.740925	-5.796724	-1.981771
H	3.088147	5.841444	0.349475	C	1.995345	-4.951880	0.199133
H	1.286203	4.520874	-1.731593	O	0.639554	-4.857293	-0.248886
H	1.318949	7.414215	-0.787872	C	2.304653	-3.875559	1.246061
H	-0.768859	6.975358	0.351735	O	3.702944	-4.003627	1.602545
C	1.956085	4.168298	2.386368	C	1.473433	-3.964101	2.526304
O	2.745523	5.891871	-2.294796	O	1.288465	-5.290133	2.998306
O	-0.009101	6.768787	-2.249848	H	0.544454	-6.921100	-0.215747
O	-0.970195	5.052552	-0.373851	H	-1.458862	-7.064751	-1.579583
H	3.045415	4.113065	2.389134	H	-0.618028	-5.841103	-3.461339
O	1.498092	2.869608	2.760271	H	-1.474737	-4.022236	-1.609953

H	1.646917	4.922679	3.121309	H	-3.577440	-4.583282	-2.640567
H	3.449700	5.221570	-2.384679	H	-3.496294	-5.852204	-0.256438
H	0.603476	6.857822	-2.995064	H	-1.315071	-4.093409	0.979375
H	0.515235	2.865490	2.781948	H	-3.015962	-6.202187	2.359568
O	-4.140796	4.054053	1.205486	H	-3.376272	-4.454476	2.391401
C	-2.709241	3.993703	1.008001	H	-1.957853	-5.242627	4.164674
C	-2.356486	5.067114	-0.032735	H	-5.298190	-4.773824	0.209717
C	-3.099930	4.786949	-1.342420	H	-6.769669	-3.255944	-1.002028
C	-4.599565	4.669019	-1.093360	H	-5.718911	-3.417233	-3.128733
C	-4.883336	3.691392	0.056422	H	-4.291565	-1.612189	-1.662969
H	-2.439138	3.012302	0.602206	H	-6.008294	-0.243114	-2.528682
H	-2.642324	6.056212	0.349089	H	-6.627169	-0.959711	0.192693
H	-2.736046	3.823149	-1.730659	H	-3.706144	-1.614750	0.815623
H	-4.975122	5.655365	-0.785569	H	-4.186421	-0.178754	2.534659
H	-5.935299	3.748997	0.353569	H	-4.769248	-1.709356	3.191945
C	-2.041164	4.128381	2.387444	H	-6.231353	0.511300	2.341703
O	-2.896411	5.818759	-2.294539	H	-7.064497	1.050043	-0.013879
O	-5.301005	4.215459	-2.247874	H	-6.694249	3.196070	-1.121766
O	-4.557569	2.392872	-0.372210	H	-5.914474	2.274312	-3.201062
H	-1.320161	4.946839	2.390895	H	-3.808111	2.288714	-1.474387
O	-1.309407	2.961391	2.760033	H	-3.806715	4.625430	-2.210251
H	-2.823948	4.354961	3.122783	H	-4.878101	4.589382	0.206947
H	-1.933219	5.950224	-2.385357	H	-3.733887	1.926131	1.170997
H	-4.987310	4.748828	-2.993295	H	-3.332132	3.665567	2.748800
H	-1.918094	2.189729	2.782213	H	-4.647111	2.637916	3.364684
O	-5.750695	-0.709242	1.207621	H	-5.078290	4.969607	3.476241
C	-4.811846	0.372925	1.009175	H	-3.316919	5.881966	0.906650
C	-5.432995	1.318114	-0.030281	H	-1.621173	7.139058	-0.324879
C	-5.679564	0.562670	-1.339840	H	-2.263372	6.507943	-2.526854
C	-6.521434	-0.683792	-1.090014	H	-0.758258	4.477713	-1.530562
C	-5.931679	-1.515358	0.058445	H	0.803846	5.838579	-2.505102
H	-3.876526	-0.027138	0.601855	H	0.668470	6.265002	0.501264
H	-6.383643	1.711640	0.353468	H	-0.615672	3.507467	0.785566
H	-4.699639	0.246626	-1.729610	H	1.154167	3.406031	2.276154
H	-7.526529	-0.363164	-0.780692	H	-0.211863	3.978333	3.236560
H	-6.631748	-2.302398	0.356220	H	2.182366	5.136015	2.825850
C	-4.499021	0.979539	2.388092	H	2.526034	6.427588	-0.461997
O	-6.360899	1.365414	-2.290612	H	4.354727	5.634623	-1.846897
O	-6.605221	-1.514736	-2.244651	H	3.011727	4.781816	-3.642465
O	-4.713759	-2.069485	-0.372760	H	3.079468	2.876040	-1.687375
H	-4.687304	2.053922	2.390574	H	5.150593	2.423184	-2.799539
O	-3.130607	0.821844	2.760474	H	5.730134	3.758076	-0.473844
H	-5.164930	0.510759	3.124045	H	3.056360	3.140044	0.885304
H	-5.862606	2.199976	-2.382889	H	5.517474	4.414308	2.131571
H	-6.828820	-0.937031	-2.989496	H	5.136315	2.675820	2.250979
H	-2.908616	-0.135596	2.782733	H	4.213827	4.059927	3.991511
O	-3.031197	-4.937870	1.203559	H	6.966476	2.062224	-0.123532
C	-3.292001	-3.528847	1.006927	H	7.523808	-0.070631	-1.189805
C	-4.417971	-3.424234	-0.032770	H	6.442858	0.356902	-3.270819
C	-3.980077	-4.085645	-1.343192	H	4.522776	-0.473864	-1.519392
C	-3.529533	-5.521124	-1.095406	H	5.505245	-2.614975	-2.191424
C	-2.512679	-5.580303	0.053897	H	6.458072	-2.057927	0.214091
H	-2.395931	-3.046473	0.600516	H	4.305158	-0.075641	1.098837
H	-5.317952	-3.923866	0.349559	H	4.627602	-1.766702	2.739602
H	-3.122437	-3.515325	-1.732091	H	5.410886	-0.270788	3.303392
H	-4.406772	-6.108005	-0.787630	H	6.740676	-2.227549	3.507074
H	-2.334479	-6.618813	0.350414	H	5.601645	-3.862425	0.961771
C	-3.571315	-2.907926	2.386752	H	4.606876	-5.765430	-0.198634
O	-5.032361	-4.117401	-2.294158	H	4.898565	-4.997588	-2.431758
O	-2.930875	-6.102516	-2.250504	H	2.670279	-3.784606	-1.464947
H	-4.529367	-2.386529	2.390616	H	1.836925	-5.734133	-2.346563
O	-2.595770	-1.935584	2.759561	H	2.171517	-5.930817	0.657295
H	-3.618308	-3.721767	3.121779	H	2.144674	-2.879535	0.814193
H	-5.376585	-3.208122	-2.383540	H	0.508811	-3.481818	2.341051
H	-3.521500	-5.916545	-2.995545	H	1.994148	-3.366056	3.287543
H	-1.708395	-2.358159	2.781826	H	0.327865	-5.452805	2.991567

Complexes 1:1 WATER							
[MIA S]-[β -CD-CCCW]				[MIA S]-[β -CD-EXP]			
CR1				CR1			
E	-5082.95164526			E	-5082.92868737		
Atom	x [Å]	y [Å]	z [Å]	Atom	x [Å]	y [Å]	z [Å]
O	6.644907	2.185138	0.057069	C	-6.124933	2.554255	0.192631
C	5.320884	2.666426	-0.270494	C	-6.439330	1.874098	1.527910
C	5.007830	3.812555	0.703230	O	-5.898690	2.658102	2.588839
C	5.062999	3.300909	2.146084	C	-5.881514	0.455800	1.546672
C	6.402485	2.628969	2.427095	O	-6.313704	-0.143380	2.755314
C	6.727305	1.593793	1.340363	C	-6.316425	-0.344999	0.310045
H	4.591950	1.864216	-0.109810	O	-5.499958	-1.521638	0.312778
H	5.741016	4.618980	0.569204	C	-6.064830	0.469274	-0.970763
H	4.267356	2.548843	2.261582	O	-6.666451	1.770612	-0.852589
H	7.187251	3.398207	2.393054	C	-6.628743	-0.136088	-2.240794
H	7.760905	1.247842	1.441265	O	-6.141306	0.658930	-3.325177
C	5.307884	3.015764	-1.768767	C	-6.078202	-2.802417	0.197088
O	3.683189	4.316746	0.531719	C	-5.679790	-3.641921	1.421050
O	4.897160	4.352266	3.084091	O	-6.106809	-2.979309	2.610209
O	6.416724	1.968973	3.689982	C	-4.174515	-3.881961	1.435550
O	5.828406	0.520412	1.465660	O	-3.899991	-4.750421	2.523694
H	4.971853	4.041798	-1.924152	C	-3.735889	-4.470226	0.096774
O	4.413374	2.193898	-2.517391	O	-2.306238	-4.577396	0.111526
H	6.334720	2.927949	-2.146663	C	-4.197132	-3.585463	-1.066523
H	4.079006	4.830370	2.848969	O	-5.635564	-3.447999	-0.982788
H	6.058458	2.595086	4.336649	C	-3.837246	-4.149001	-2.447763
H	4.676254	1.251812	-2.417761	O	-3.907615	-5.565679	-2.548437
O	6.335773	-2.834010	0.039922	C	-1.749398	-5.867948	0.046663
C	5.845315	-1.473459	0.024152	C	-0.622026	-5.992162	1.075309
C	6.324067	-0.810991	1.324758	O	-1.150512	-5.658817	2.357814
C	5.775524	-1.576535	2.532860	C	0.563735	-5.108906	0.710947
C	6.143486	-3.053532	2.445749	O	1.600351	-5.401181	1.636116
C	5.771796	-3.624478	1.069513	O	0.996272	-5.353448	-0.733672
H	4.749540	-1.481422	0.019488	O	1.943134	-4.322195	-1.030828
H	7.421752	-0.811925	1.354184	C	-0.197982	-5.266627	-1.700510
H	4.678165	-1.491080	2.508756	O	-1.258060	-6.150822	-1.256795
H	7.233837	-3.143060	2.554481	C	0.154674	-5.647304	-3.128389
H	6.200725	-4.623704	0.943896	O	0.793052	-6.920894	-3.132087
C	6.313671	-0.823514	-1.289267	C	3.120217	-4.645852	-1.744381
O	6.290016	-1.070437	3.754238	C	4.343102	-4.370352	-0.854574
O	5.485451	-3.829710	3.443369	O	4.195747	-5.073772	0.379944
O	4.370233	-3.668687	0.968725	C	4.517164	-2.877487	-0.606193
H	6.853638	0.103340	-1.091420	O	5.758019	-2.713280	0.063509
O	5.228719	-0.467785	-2.145136	C	4.466503	-2.097952	-1.917208
H	6.997756	-1.521894	-1.788427	O	4.484503	-0.707852	-1.574620
H	6.128182	-0.107659	3.765789	C	3.200965	-2.446826	-2.705471
H	5.604051	-3.363035	4.284047	O	3.206940	-3.878663	-2.929275
H	4.705947	-1.271833	-2.360836	C	3.093904	-1.739888	-4.065693
O	2.511531	-5.735124	-1.443264	O	4.342584	-1.486554	-4.698830
C	3.155440	-4.519385	-0.996516	C	5.561828	0.078145	-2.013787
C	3.761953	-4.819414	0.382547	C	6.053603	0.947143	-0.854485
C	2.655550	-5.235334	1.356962	O	6.466655	0.104435	0.218079
C	1.855632	-6.404323	0.792477	C	4.948700	1.899110	-0.415462
C	1.404892	-6.112167	-0.646216	O	5.480954	2.716021	0.613618
H	2.403870	-3.729975	-0.883342	C	4.425009	2.719686	-1.601508
H	4.496499	-5.630447	0.290796	O	3.227484	3.381800	-1.177785
H	1.977905	-4.375766	1.475854	C	4.077957	1.806704	-2.791609
H	2.513684	-7.284334	0.757512	O	5.177770	0.918913	-3.090364
H	1.002221	-7.018634	-1.109201	C	3.784865	2.561027	-4.073847
C	4.134237	-4.077085	-2.098187	O	3.248294	1.624311	-5.003978
O	3.182214	-5.634750	2.612147	C	3.255764	4.777208	-0.955428
O	0.697431	-6.688783	1.572542	C	2.674919	5.088852	0.439884
O	0.431973	-5.097363	-0.611539	O	3.428531	4.359773	1.398667
H	5.139947	-3.949911	-1.695554	C	1.175799	4.790295	0.480561
O	3.782361	-2.819460	-2.673373	O	0.646709	5.301673	1.694992
H	4.164987	-4.865482	-2.861231	C	0.448993	5.402444	-0.719101
H	3.768957	-4.920546	2.926619	O	-0.869213	4.840660	-0.681769
H	0.983023	-6.717367	2.497821	C	1.148122	5.068366	-2.043247
H	2.884431	-2.881944	-3.068165	O	2.531909	5.462122	-1.957735
O	-1.938247	-4.377755	-3.335573	C	0.531962	5.760430	-3.247482
C	-0.700225	-4.205085	-2.608029	O	0.424116	7.159207	-2.991006

C	-0.713914	-5.220027	-1.453637	C	-1.978033	5.660930	-1.003950
C	-1.917672	-4.948559	-0.545459	C	-2.820180	5.903188	0.258389
C	-3.208189	-4.968795	-1.357303	O	-1.978502	6.439599	1.279999
C	-3.086585	-4.045739	-2.578946	C	-3.485510	4.615233	0.726416
H	-0.666426	-3.195802	-2.182810	O	-4.343226	4.956241	1.805223
H	-0.777326	-6.237994	-1.860557	C	-4.230700	3.945744	-0.428059
H	-1.791087	-3.942401	-0.118793	O	-4.731825	2.697777	0.061239
H	-3.372494	-5.990883	-1.725767	C	-3.274935	3.733375	-1.607815
H	-3.938008	-4.188372	-3.251929	O	-2.768453	5.035865	-1.993623
C	0.454398	-4.323646	-3.617520	C	-3.900157	3.071402	-2.838632
O	-2.031820	-5.915032	0.488712	O	-5.235691	3.478169	-3.102392
O	-4.332524	-4.537052	-0.594288	H	-6.624892	3.525188	0.127288
O	-3.028870	-2.719893	-2.117937	H	-7.533368	1.822538	1.619628
H	1.172444	-5.080269	-3.298830	H	-5.906822	2.101684	3.382276
O	1.195624	-3.111013	-3.747737	H	-4.783471	0.522559	1.513302
H	0.031561	-4.633205	-4.581966	H	-6.054034	-1.087284	2.740198
H	-1.163245	-5.978959	0.931142	H	-7.377718	-0.611282	0.398330
H	-4.360750	-5.073627	0.211129	H	-4.980271	0.577020	-1.090268
H	0.591520	-2.391292	-4.035981	H	-7.726096	-0.119981	-2.198529
O	-3.728713	0.268828	-4.132852	H	-6.295362	-1.177403	-2.329179
C	-2.866671	-0.742807	-3.566773	H	-6.591399	0.384566	-4.134954
C	-3.776216	-1.709381	-2.799070	H	-7.167262	-2.732422	0.113316
C	-4.534910	-0.967215	-1.691203	H	-6.187951	-4.612624	1.336848
C	-5.270199	0.258665	-2.234371	H	-5.664978	-3.435535	3.343743
C	-4.340830	1.080658	-3.148353	H	-3.669308	-2.914799	1.573426
H	-2.174584	-0.275706	-2.857584	H	-2.935369	-4.900992	2.558359
H	-4.491735	-2.169931	-3.493218	H	-4.183401	-5.462016	-0.030868
H	-3.787428	-0.620965	-0.961273	H	-3.747806	-2.588926	-0.978974
H	-6.103255	-0.100693	-2.857792	H	-2.839056	-3.784796	-2.716869
H	-4.923061	1.826548	-3.698606	H	-4.543737	-3.728597	-3.170791
C	-2.025561	-1.344411	-4.705841	H	-3.045258	-5.915295	-2.265505
O	-5.478790	-1.830421	-1.070592	H	-2.514010	-6.626751	0.237148
O	-5.738436	1.133076	-1.223969	H	-0.288182	-7.039101	1.067943
O	-3.367930	1.703549	-2.344768	H	-0.401656	-5.612604	2.970435
H	-2.142686	-2.428242	-4.745419	H	0.256232	-4.056797	0.792169
O	-0.627300	-1.109351	-4.538807	H	2.442535	-5.066509	1.267898
H	-2.385698	-0.923534	-5.653509	H	1.462461	-6.340560	-0.816671
H	-5.020975	-2.663822	-0.846983	H	-0.568689	-4.234466	-1.703591
H	-6.272401	0.660636	-0.521596	H	0.813569	-4.868351	-3.531714
H	-0.462887	-0.141035	-4.505428	H	-0.768209	-5.659441	-3.725493
O	-1.412936	4.681810	-3.239615	H	1.091332	-7.096364	-4.034176
C	-1.638661	3.258812	-3.115685	H	3.095077	-5.690648	-2.067186
C	-3.062605	3.076737	-2.572534	H	5.230712	-4.738003	-1.388588
C	-3.196988	3.763629	-1.210134	H	4.863650	-4.701727	0.978406
C	-2.777107	5.226696	-1.308918	H	3.685276	-2.531527	0.025213
C	-1.409565	5.358025	-1.995828	H	5.860463	-1.768016	0.287633
H	-0.931201	2.840880	-2.390772	H	5.336721	-2.345292	-2.534244
H	-3.780898	3.514603	-3.278685	H	2.312868	-2.191830	-2.114931
H	-2.514801	3.252703	-0.513232	H	2.537075	-0.806594	-3.937481
H	-3.510797	5.751108	-1.937714	H	2.501296	-2.388780	-4.720932
H	-1.202428	6.406990	-2.230406	H	4.577834	-0.567587	-4.485391
C	-1.346868	2.610528	-4.480203	H	6.371719	-0.546416	-2.402068
O	-4.531356	3.718273	-0.729985	H	6.908427	1.534081	-1.219318
O	-2.692648	5.851021	-0.030255	H	6.522229	0.674260	1.000649
O	-0.427264	4.837975	-1.134853	H	4.110993	1.294741	-0.039522
H	-2.208625	2.039103	-4.828601	H	4.750490	3.279693	0.957940
O	-0.260441	1.686708	-4.429345	H	5.183948	3.455465	-1.898984
H	-1.149660	3.412737	-5.203124	H	3.197113	1.213005	-2.520536
H	-4.855929	2.797114	-0.829744	H	4.717369	3.008637	-4.445777
H	-3.515947	5.646344	0.437084	H	3.077943	3.371590	-3.857204
H	0.547050	2.157206	-4.125184	H	3.165157	2.064670	-5.859987
O	3.178298	5.527847	-1.392109	H	4.281161	5.153888	-1.022775
C	1.977354	4.764764	-1.652562	H	2.802096	6.169315	0.602808
C	0.812705	5.534545	-1.011827	H	2.964522	4.201216	2.266521
C	1.050236	5.678971	0.494648	H	1.034314	3.700914	0.427079
C	2.406742	6.320615	0.764729	H	-0.307079	5.476374	1.565423
C	3.513105	5.598890	-0.018651	H	0.406285	6.489470	-0.596806
H	2.056703	3.785067	-1.168261	H	1.086567	3.986386	-2.213856
H	0.735318	6.529270	-1.470543	H	-0.453104	5.311431	-3.429136
H	1.052624	4.667176	0.928557	H	1.165360	5.562800	-4.123131
H	2.373279	7.358959	0.404941	H	-0.028189	7.560810	-3.744563
H	4.446410	6.168900	0.029381	H	-1.638727	6.605335	-1.439109

C	1.892729	4.529153	-3.170760	H	-3.605134	6.629006	0.003247
O	0.057040	6.484385	1.109227	H	-2.509403	6.430180	2.092218
O	2.748489	6.291756	2.147906	H	-2.699567	3.922324	1.062843
H	0.940974	4.886718	-3.565889	H	-4.721766	4.130082	2.165291
O	1.965972	3.146643	-3.516670	H	-5.059044	4.576911	-0.766826
H	2.700674	5.098761	-3.647883	H	-2.427691	3.112489	-1.291805
H	-0.813486	6.116525	0.864326	H	-3.850208	1.986377	-2.708818
H	1.972040	6.605968	2.634689	H	-3.261414	3.325963	-3.695469
H	2.817307	2.776969	-3.192793	H	-5.789993	2.687327	-2.983588
C	-3.579044	-3.590246	4.389916	C	-0.752240	-1.266588	0.948812
C	-3.554778	-3.461543	3.000895	C	-0.228953	-0.149717	0.297674
C	-4.119253	-2.331778	2.409937	C	0.760333	0.607713	0.924063
C	-4.718082	-1.316493	3.173077	C	1.237681	0.280211	2.201765
C	-4.728239	-1.443992	4.575407	C	0.723752	-0.860216	2.846565
C	-4.155503	-2.581887	5.160559	C	-0.266705	-1.617711	2.209265
C	-5.251867	-0.330931	5.464356	C	-1.341028	-1.347001	4.141582
C	-4.478014	0.940094	5.207377	C	2.793223	-1.689958	3.898258
C	-3.565692	1.458544	6.126700	C	3.242780	-3.010145	3.864549
C	-2.858719	2.634369	5.857377	C	4.591887	-3.311366	3.651827
C	-3.063825	3.293297	4.646346	C	5.498997	-2.271175	3.455806
C	-3.963937	2.780212	3.708549	C	5.061170	-0.944741	3.457844
C	-4.677233	1.601537	3.975439	C	3.708021	-0.633421	3.672483
C	-5.380795	-0.187010	2.380982	C	2.242979	1.242894	2.821734
N	-5.667960	1.078633	3.097838	N	3.238328	0.697760	3.777188
C	-6.700587	-0.719782	1.784732	C	1.505381	2.403289	3.526451
C	-6.282543	2.055318	2.192660	C	4.220490	1.737640	4.090743
C	-7.579960	1.508899	1.606666	C	3.527361	2.928588	4.746723
N	-7.322140	0.257986	0.880955	N	2.444806	3.472180	3.909856
C	-8.543433	-0.283212	0.276327	C	1.749137	4.549263	4.627484
H	-3.143100	-4.460812	4.871249	H	-1.506127	-1.883938	0.470935
H	-3.096727	-4.229131	2.382758	H	-0.577049	0.125567	-0.693288
H	-4.110343	-2.240679	1.327613	H	1.185648	1.462871	0.405126
H	-4.158749	-2.668385	6.244072	H	-0.645516	-2.511116	2.699160
H	-5.162282	-0.625711	6.513338	H	0.799034	-2.222821	4.507723
H	-6.313078	-0.149065	5.254648	H	1.281858	-0.568135	4.912086
H	-3.419764	0.943004	7.072643	H	2.526781	-3.814239	4.011537
H	-2.160726	3.030562	6.588750	H	4.927936	-4.344288	3.656679
H	-2.521061	4.207001	4.421399	H	6.550660	-2.484957	3.290316
H	-4.103187	3.300895	2.767365	H	5.781176	-0.150909	3.294661
H	-4.715540	0.037891	1.528525	H	2.795035	1.694743	1.981096
H	-7.382720	-0.982331	2.612346	H	0.973354	2.002232	4.406562
H	-6.488803	-1.618931	1.205607	H	0.764322	2.839056	2.851330
H	-5.608681	2.339252	1.368207	H	4.766914	2.067330	3.191216
H	-6.505091	2.960571	2.763664	H	4.949701	1.335879	4.797937
H	-8.000463	2.240966	0.909415	H	4.258477	3.723511	4.927944
H	-8.313364	1.348930	2.415733	H	3.128787	2.608775	5.725189
H	-9.305636	-0.540432	1.029512	H	1.288912	4.189463	5.562488
H	-8.293502	-1.181847	-0.293167	H	0.980892	4.971356	3.979863
H	-8.969022	0.456785	-0.407507	H	2.467085	5.335554	4.879288
NR1				NR1			
E	-5082.94773970			E	-5082.93235230		
ZPE	-5081.382122						
H	-5081.290965						
G	-5081.506278						
S	453.163						
O	5.712257	3.584666	-0.569615	C	1.615721	-5.869485	-1.313942
C	4.285901	3.646550	-0.801115	C	2.281673	-6.055475	0.052766
C	3.733391	4.763906	0.096429	O	1.276913	-6.335023	1.025006
C	4.039874	4.454799	1.565233	C	3.084828	-4.814271	0.423389
C	5.531927	4.211975	1.763875	O	3.756464	-5.100400	1.637251
C	6.049285	3.185157	0.746109	C	4.053311	-4.410525	-0.698476
H	3.827314	2.698818	-0.497830	O	4.527032	-3.106406	-0.344789
H	4.192545	5.721409	-0.183198	C	3.314330	-4.357558	-2.046795
H	3.501340	3.531560	1.828343	O	2.616697	-5.595336	-2.273152
H	6.063421	5.156326	1.578790	C	4.196994	-4.151616	-3.261641
H	7.142644	3.138462	0.771795	O	3.320712	-3.941508	-4.372593
C	4.062253	3.808558	-2.314740	C	5.909352	-2.833763	-0.296326
O	2.311000	4.856945	0.017657	C	6.261125	-2.291685	1.098458
O	3.652905	5.519476	2.419456	O	5.868863	-3.241191	2.088369
O	5.826933	3.730794	3.072446	C	5.592021	-0.941986	1.330653
O	5.488543	1.934859	1.057801	O	6.049669	-0.455575	2.583141
H	3.450252	4.687097	-2.523383	C	5.930877	0.004960	0.181852

O	3.367692	2.701522	-2.887940	O	5.193604	1.214524	0.395394
H	5.041627	3.949493	-2.789920	C	5.562235	-0.625693	-1.165676
H	2.712699	5.712858	2.241258	O	6.271594	-1.882348	-1.280211
H	5.350179	4.301507	3.693469	C	5.916374	0.246154	-2.377709
H	3.888713	1.880781	-2.741755	O	7.115979	0.997143	-2.240431
O	6.755463	-1.316322	-0.109090	C	5.916033	2.405858	0.577185
C	5.930218	-0.131917	-0.198591	C	5.288320	3.195551	1.727633
C	6.310855	0.770308	0.985096	O	5.307598	2.369524	2.890500
C	6.071550	0.029688	2.304517	C	3.874969	3.640074	1.368304
C	6.799224	-1.309685	2.313424	O	3.388092	4.439000	2.436288
C	6.486858	-2.103024	1.036260	C	3.883637	4.391564	0.037267
H	4.876424	-0.414059	-0.095212	O	2.509958	4.577228	-0.314528
H	7.368117	1.056095	0.906177	C	4.599412	3.583657	-1.060589
H	4.990699	-0.164479	2.381671	O	5.919628	3.191504	-0.609049
H	7.881156	-1.114891	2.322914	C	4.761223	4.348206	-2.363427
H	7.145057	-2.974157	0.959199	O	5.368844	5.609548	-2.099630
C	6.118364	0.464633	-1.603802	C	2.095731	5.818512	-0.857282
O	6.525056	0.781009	3.419259	C	1.165113	6.520516	0.143206
O	6.434341	-2.109071	3.435379	O	1.838061	6.643571	1.397398
O	5.138630	-2.499631	1.076467	C	-0.137494	5.746976	0.299695
H	6.391712	1.518786	-1.542140	O	-0.986690	6.518184	1.136852
O	4.926926	0.415884	-2.387808	C	-0.760116	5.462138	-1.067206
H	6.937228	-0.075844	-2.095943	O	-1.903885	4.632345	-0.848113
H	6.115124	1.665390	3.364063	C	0.255708	4.752680	-1.968942
H	6.489623	-1.537198	4.215470	O	1.418336	5.611717	-2.078687
H	4.633614	-0.517926	-2.480374	C	-0.247943	4.431878	-3.379075
O	3.713000	-5.227252	-0.942291	O	-1.079542	5.436966	-3.941409
C	4.060671	-3.847750	-0.681413	C	-3.173964	5.204052	-1.045522
C	4.799730	-3.823695	0.665155	C	-4.099945	4.775479	0.093891
C	3.885605	-4.366720	1.767561	O	-3.536175	5.189841	1.336639
C	3.365864	-5.751667	1.399073	C	-4.316193	3.267245	0.064110
C	2.780691	-5.758658	-0.020932	O	-5.267748	2.968021	1.069276
H	3.144888	-3.252921	-0.588919	C	-4.753710	2.775056	-1.325375
H	5.704489	-4.442180	0.597285	O	-4.616149	1.349253	-1.323786
H	3.026219	-3.683369	1.851807	C	-3.835231	3.360658	-2.411554
H	4.216732	-6.447836	1.404760	O	-3.743609	4.789055	-2.270854
H	2.596401	-6.786954	-0.347545	C	-4.283301	3.112330	-3.837555
C	4.836953	-3.323650	-1.901820	O	-3.200099	3.513007	-4.682580
O	4.563539	-4.473278	3.008939	C	-5.756179	0.525105	-1.445020
O	2.357046	-6.203394	2.298448	C	-5.811205	-0.454063	-0.254800
O	1.584309	-5.017879	-0.020218	O	-5.837284	0.308520	0.939900
H	5.795506	-2.900435	-1.599312	C	-4.647642	-1.444302	-0.316072
O	4.147429	-2.277614	-2.584832	O	-4.845842	-2.433022	0.688657
H	5.029776	-4.171964	-2.571132	C	-4.555725	-2.084190	-1.702706
H	4.985040	-3.611351	3.189896	O	-3.325417	-2.819758	-1.707130
H	2.692107	-6.053479	3.194963	C	-4.570258	-1.029841	-2.820351
H	3.271874	-2.607948	-2.885284	O	-5.729603	-0.187236	-2.665164
O	-1.022537	-5.320559	-2.602941	C	-4.610235	-1.626834	-4.217046
C	0.149836	-4.721040	-2.003974	O	-5.681002	-2.565518	-4.303634
C	0.466746	-5.537517	-0.741226	C	-3.287901	-4.081581	-2.348373
C	-0.719563	-5.463926	0.224590	C	-3.044100	-5.178579	-1.299547
C	-1.992389	-5.940550	-0.467263	O	-4.028656	-5.052445	-0.272056
C	-2.183775	-5.202476	-1.801080	C	-1.634923	-5.089930	-0.725937
H	-0.081142	-3.692395	-1.705422	O	-1.447753	-6.226269	0.108585
H	0.652543	-6.582906	-1.021083	C	-0.599122	-5.016290	-1.848344
H	-0.856467	-4.410512	0.509482	O	0.677534	-4.823871	-1.231310
H	-1.883840	-7.010963	-0.693074	C	-0.939352	-3.855424	-2.789387
H	-2.991591	-5.661370	-2.379833	O	-2.263465	-4.108326	-3.320702
C	1.246075	-4.654289	-3.081794	C	0.027404	-3.665360	-3.960944
O	-0.519050	-6.266747	1.378192	O	0.507430	-4.879940	-4.520474
O	-3.152102	-5.724137	0.332380	H	1.137193	-6.797770	-1.640073
O	-2.470739	-3.856521	-1.520440	H	2.969873	-6.908349	-0.029976
H	2.146093	-5.177459	-2.756277	H	1.673510	-6.180463	1.895651
O	1.652636	-3.315486	-3.364348	H	2.379552	-3.979651	0.554067
H	0.865419	-5.149771	-3.984109	H	4.341176	-4.344126	1.848897
H	0.365253	-6.057432	1.736506	H	4.885758	-5.124934	-0.740639
H	-2.941522	-6.038112	1.224276	H	2.592096	-3.533857	-2.000043
H	0.878532	-2.802130	-3.684708	H	4.823995	-5.040410	-3.413439
O	-3.986836	-1.412698	-3.812072	H	4.849448	-3.285230	-3.098578
C	-2.882560	-2.101624	-3.181538	H	3.844862	-3.949986	-5.184185
C	-3.480494	-3.191127	-2.278493	H	6.491520	-3.733554	-0.518925
C	-4.414242	-2.561295	-1.240029	H	7.350533	-2.151538	1.133217

C	-5.471322	-1.699505	-1.919327	H	5.916629	-2.777921	2.939349
C	-4.806904	-0.714992	-2.894024	H	4.502050	-1.088845	1.345995
H	-2.327860	-1.397525	-2.551698	H	5.626348	0.408908	2.746528
H	-4.038076	-3.913978	-2.888669	H	7.006128	0.215857	0.181801
H	-3.800894	-1.913265	-0.595628	H	4.485014	-0.828780	-1.196255
H	-6.132636	-2.353578	-2.504899	H	5.064506	0.902531	-2.589471
H	-5.561922	-0.200710	-3.497267	H	6.036103	-0.419278	-3.238864
C	-1.933005	-2.581367	-4.292015	H	6.876019	1.838058	-1.814728
O	-5.082151	-3.544589	-0.465851	H	6.968491	2.196562	0.790539
O	-6.235103	-0.949347	-0.977338	H	5.906131	4.088779	1.892064
O	-4.055708	0.203514	-2.140354	H	4.901051	2.876973	3.607785
H	-1.735502	-3.650093	-4.196142	H	3.249926	2.743239	1.246527
O	-0.658449	-1.941060	-4.239466	H	2.729857	5.069250	2.078880
H	-2.423326	-2.407051	-5.258548	H	4.383108	5.357517	0.165254
H	-4.399957	-4.119937	-0.069177	H	4.008047	2.683188	-1.265497
H	-6.436953	-1.539865	-0.235355	H	3.765902	4.468281	-2.809597
H	-0.782313	-0.969093	-4.315082	H	5.372276	3.744231	-3.049017
O	-2.966256	3.503525	-3.320239	H	5.386662	6.105454	-2.928831
C	-2.802608	2.083130	-3.113996	H	2.964356	6.439534	-1.094482
C	-4.103599	1.592224	-2.469249	H	0.936116	7.519146	-0.254365
C	-4.327079	2.294795	-1.123715	H	1.162804	6.933723	2.031251
C	-4.256095	3.813286	-1.259106	H	0.089690	4.778642	0.769811
C	-3.033526	4.230504	-2.107607	H	-1.778080	5.982077	1.340881
H	-1.976498	1.909553	-2.415347	H	-1.058729	6.396027	-1.555069
H	-4.947592	1.795645	-3.141404	H	0.566625	3.808596	-1.505355
H	-3.511847	1.965178	-0.460278	H	-0.775112	3.473846	-3.344236
H	-5.150869	4.136499	-1.810484	H	0.640267	4.291018	-4.010303
H	-3.130937	5.280522	-2.401172	H	-1.955610	5.031317	-4.066330
C	-2.412322	1.442165	-4.457580	H	-3.106458	6.294496	-1.101186
O	-5.588437	1.936624	-0.577855	H	-5.067178	5.273225	-0.063693
O	-4.198736	4.504324	-0.017852	H	-4.009347	4.707346	2.031474
O	-1.867559	4.038312	-1.343519	H	-3.351910	2.783338	0.281055
H	-3.103768	0.641222	-4.722630	H	-5.433974	1.996465	1.047061
O	-1.117400	0.842656	-4.423716	H	-5.798104	3.061914	-1.506114
H	-2.468144	2.217051	-5.233021	H	-2.841595	2.915793	-2.281206
H	-5.668819	0.964079	-0.645185	H	-5.186911	3.700620	-4.045210
H	-4.334510	3.910619	0.765813	H	-4.519866	2.049639	-3.968159
H	-0.448899	1.530570	-4.209269	H	-3.507332	3.515079	-5.598628
O	1.359081	5.698282	-1.934100	H	-6.667193	1.131780	-1.473560
C	0.418074	4.605285	-2.039229	H	-6.744037	-1.028759	-0.355551
C	-0.876126	5.064395	-1.353690	H	-5.550643	-0.192567	1.755468
C	-0.602234	5.398490	0.115202	H	-3.712464	-0.893837	-0.133713
C	0.522976	6.423099	0.224955	H	-4.428542	-3.264682	0.387066
C	1.741025	5.982796	-0.601033	H	-5.404742	-2.762217	-1.839905
H	0.811152	3.734462	-1.502907	H	-3.662400	-0.418611	-2.744128
H	-1.259808	5.955850	-1.867801	H	-3.643024	-2.107697	-4.410085
H	-0.278800	4.471721	0.613246	H	-4.737702	-0.808616	-4.939128
H	0.164264	7.372094	-0.198434	H	-5.633753	-2.982905	-5.173814
H	2.468374	6.797951	-0.669886	H	-4.220420	-4.258821	-2.891434
C	0.300609	4.225759	-3.525867	H	-3.153272	-6.150285	-1.801159
O	-1.753099	5.932621	0.754189	H	-3.777761	-5.678647	0.424402
O	0.949200	6.616965	1.571128	H	-1.554734	-4.164706	-0.136718
H	-0.734606	4.296166	-3.863240	H	-0.557539	-6.163846	0.509953
O	0.706814	2.882388	-3.782452	H	-0.599303	-5.942526	-2.432493
H	0.901773	4.937500	-4.106305	H	-0.966406	-2.914763	-2.225635
H	-2.521406	5.377342	0.500215	H	0.861864	-3.045176	-3.620949
H	0.152757	6.765385	2.101781	H	-0.511467	-3.092904	-4.728395
H	1.642290	2.771361	-3.502425	H	1.466955	-4.893771	-4.359138
C	-7.723858	-1.798974	3.686300	C	-0.502633	-4.610406	4.288348
C	-7.850174	-0.938813	2.595033	C	-1.367649	-4.535279	3.196265
C	-6.809988	-0.062192	2.289210	C	-2.071796	-3.355505	2.960861
C	-5.632286	-0.017006	3.053516	C	-1.941533	-2.237146	3.798430
C	-5.501973	-0.896356	4.144412	C	-1.054811	-2.309707	4.889203
C	-6.553087	-1.775164	4.442047	C	-0.347332	-3.498623	5.114999
C	-4.207435	-0.983889	4.930670	C	-0.776906	-1.096424	5.755795
C	-3.070845	-1.346368	4.004629	C	-0.257220	0.037974	4.905048
C	-2.477429	-2.609032	4.012579	C	1.076971	0.444644	4.942228
C	-1.430259	-2.921923	3.140189	C	1.531334	1.502626	4.149646
C	-0.974948	-1.952437	2.247520	C	0.635148	2.161108	3.309788
C	-1.570872	-0.688344	2.213190	C	-0.700047	1.752688	3.244168
C	-2.627436	-0.373013	3.081345	C	-1.159048	0.682432	4.028587
C	-4.622688	1.059453	2.651556	C	-2.862866	-1.059164	3.478929

N	-3.227967	0.916518	3.138037	N	-2.519392	0.263895	4.054643
C	-5.163432	2.428831	3.113144	C	-4.290580	-1.436613	3.929309
C	-2.400268	2.019917	2.641261	C	-3.499120	1.266074	3.627588
C	-2.951301	3.364461	3.100164	C	-4.900248	0.884212	4.089912
N	-4.333413	3.540341	2.630742	N	-5.280631	-0.424670	3.539437
C	-4.879390	4.828426	3.075522	C	-6.628795	-0.813895	3.966583
H	-8.522589	-2.489477	3.940203	H	0.054897	-5.520637	4.489748
H	-8.749098	-0.946907	1.985908	H	-1.494074	-5.377540	2.523855
H	-6.911756	0.611657	1.442964	H	-2.750202	-3.296353	2.114133
H	-6.440612	-2.457176	5.280812	H	0.341960	-3.543850	5.954266
H	-4.307145	-1.731609	5.721936	H	-0.048887	-1.355825	6.529125
H	-3.987184	-0.019179	5.403680	H	-1.697751	-0.771528	6.255629
H	-2.831057	-3.352321	4.722701	H	1.763733	-0.063752	5.614440
H	-0.982888	-3.911403	3.153769	H	2.572487	1.807869	4.183542
H	-0.155853	-2.175095	1.569439	H	0.979367	2.995079	2.705160
H	-1.209450	0.047340	1.503589	H	-1.379276	2.272050	2.577052
H	-4.611592	1.082694	1.550576	H	-2.891116	-0.965730	2.379310
H	-5.225469	2.431139	4.215972	H	-4.286804	-1.584441	5.023657
H	-6.174813	2.562205	2.721427	H	-4.569645	-2.379155	3.455209
H	-2.331231	2.025577	1.539582	H	-3.513270	1.393010	2.532810
H	-1.387768	1.896949	3.034169	H	-3.229416	2.228216	4.070436
H	-2.337887	4.171058	2.685936	H	-5.612443	1.636216	3.735622
H	-2.901945	3.425426	4.201298	H	-4.936082	0.871349	5.192792
H	-4.915212	4.909223	4.174060	H	-6.710785	-0.907362	5.061426
H	-5.893180	4.951726	2.685012	H	-6.890662	-1.774708	3.515080
H	-4.257454	5.640058	2.688704	H	-7.347702	-0.063310	3.626754
M1				M1			
E	-5082.94072289			E	-5082.92006341		
O	5.509708	0.893844	-2.374631	C	0.463060	5.823395	-0.655353
C	4.408516	1.726180	-1.944042	C	-0.143717	5.915187	0.748806
C	4.941010	2.644775	-0.833855	O	0.870478	5.610741	1.702238
C	5.485211	1.800120	0.321425	C	-1.338002	4.975001	0.875253
C	6.521327	0.798636	-0.176818	O	-1.907907	5.187243	2.154120
C	5.963398	0.005853	-1.368257	C	-2.345835	5.186244	-0.264444
H	3.621353	1.093414	-1.520048	O	-3.280320	4.106011	-0.152520
H	5.736028	3.287648	-1.234073	C	-1.611558	5.136638	-1.615440
H	4.642122	1.237578	0.746232	O	-0.541157	6.096738	-1.612264
H	7.401400	1.353556	-0.532682	C	-2.456751	5.448063	-2.834253
H	6.751994	-0.594037	-1.833596	O	-1.659080	5.129277	-3.980053
C	3.826620	2.419640	-3.186793	C	-4.670601	4.356097	-0.215604
O	3.901710	3.442085	-0.262578	C	-5.327744	3.895107	1.093695
O	6.095178	2.603870	1.321687	O	-4.697859	4.556284	2.190382
O	6.901958	-0.127178	0.837748	C	-5.242511	2.381072	1.244590
O	4.919705	-0.812455	-0.904587	O	-5.993198	2.036910	2.397904
H	3.795887	3.501201	-3.047783	C	-5.762674	1.692143	-0.015713
O	2.482196	2.020847	-3.456346	O	-5.501484	0.291208	0.134497
H	4.481176	2.199589	-4.039734	C	-5.060175	2.236590	-1.265050
H	5.443366	3.278132	1.593307	O	-5.255229	3.671294	-1.305783
H	7.034974	0.386549	1.648180	C	-5.573076	1.632028	-2.582109
H	2.454690	1.051216	-3.618585	O	-6.945264	1.256332	-2.572430
O	3.578411	-3.746414	-2.674192	C	-6.582049	-0.607803	0.105392
C	3.631191	-2.340666	-2.338145	C	-6.470812	-1.564640	1.293915
C	4.819263	-2.153924	-1.382428	O	-6.490074	-0.800939	2.498387
C	4.613217	-3.007531	-0.127335	C	-5.203360	-2.400971	1.185161
C	4.351231	-4.464066	-0.491782	O	-5.219337	-3.322747	2.262172
C	3.267769	-4.580336	-1.574508	C	-5.138526	-3.099195	-0.172937
H	2.713410	-2.057857	-1.810749	O	-3.815965	-3.640380	-0.275605
H	5.749325	-2.449268	-1.885903	C	-5.389520	-2.123653	-1.339790
H	3.728554	-2.614598	0.396063	O	-6.593727	-1.350671	-1.106574
H	5.276848	-4.881650	-0.913343	C	-5.544083	-2.828786	-2.676854
H	3.244899	-5.598590	-1.975412	O	-6.549627	-3.831854	-2.566369
C	3.677929	-1.545897	-3.654253	C	-3.639661	-4.974296	-0.712436
O	5.748119	-2.973263	0.723658	C	-2.977147	-5.789208	0.409963
C	3.937885	-5.229897	0.637465	O	-3.768380	-5.697875	1.594247
O	2.022352	-4.243633	-1.011898	C	-1.560046	-5.290411	0.661433
H	4.513814	-0.845300	-3.652577	O	-0.978134	-6.142469	1.640569
O	2.508405	-0.755135	-3.865511	C	-0.769794	-5.271906	-0.646878
H	3.825914	-2.257666	-4.476580	O	0.517134	-4.703326	-0.381580
H	5.941780	-2.036176	0.915120	C	-1.511812	-4.444240	-1.702268
H	4.558579	-5.029157	1.353670	O	-2.831740	-5.016448	-1.870707
H	1.717067	-1.337655	-3.887327	C	-0.829692	-4.407076	-3.070519
O	-1.208311	-5.233332	-2.477884	O	-0.322928	-5.665141	-3.488549

C	-0.102932	-4.325437	-2.262698	C	1.590181	-5.610447	-0.282433
C	0.891080	-5.050661	-1.342997	C	2.504914	-5.206683	0.878364
C	0.210095	-5.377076	-0.010359	O	1.716539	-5.101137	2.063654
C	-1.064763	-6.180998	-0.249904	C	3.247079	-3.907340	0.583849
C	-1.951614	-5.499901	-1.303387	O	4.196717	-3.735763	1.620401
H	-0.465476	-3.429423	-1.747705	C	3.900749	-3.914577	-0.806943
H	1.221004	-5.980259	-1.825481	O	4.290138	-2.558490	-1.050844
H	-0.063573	-4.423306	0.467051	C	2.884830	-4.377968	-1.863019
H	-0.777297	-7.163891	-0.650100	O	2.344448	-5.653185	-1.476842
H	-2.759280	-6.171721	-1.610626	C	3.440365	-4.553965	-3.261889
C	0.421595	-3.887445	-3.640523	O	2.320593	-4.742531	-4.134491
O	1.051170	-6.138158	0.841906	C	5.602409	-2.248304	-1.469058
O	-1.832097	-6.342087	0.939819	C	6.248410	-1.307900	-0.444364
O	-2.472123	-4.317162	-0.750080	O	6.272194	-1.949589	0.831279
H	1.483898	-4.111812	-3.743054	C	5.484493	0.007774	-0.377393
O	0.296993	-2.480413	-3.849991	O	6.195043	0.858527	0.509528
H	-0.126191	-4.448979	-4.407847	C	5.322841	0.620813	-1.767156
H	1.917531	-5.689650	0.882683	O	4.372711	1.683529	-1.618691
H	-1.221378	-6.636610	1.631599	C	4.796569	-0.410257	-2.783064
H	-0.652381	-2.228929	-3.806303	O	5.589340	-1.616658	-2.732446
O	-5.372624	-2.425705	-1.994211	C	4.821429	0.100224	-4.213743
C	-3.965339	-2.744948	-1.898646	O	6.133704	0.558432	-4.529781
C	-3.838574	-3.983963	-0.999184	C	4.643338	2.949791	-2.182554
C	-4.445815	-3.700582	0.378367	C	4.710204	3.996658	-1.058881
C	-5.878219	-3.196841	0.245483	O	5.686364	3.602618	-0.094476
C	-5.948076	-2.038901	-0.760422	C	3.342911	4.169508	-0.409465
H	-3.436498	-1.914158	-1.420347	O	3.464498	5.207998	0.552730
H	-4.358252	-4.832573	-1.463411	C	2.294250	4.473572	-1.479303
H	-3.846037	-2.906149	0.847282	O	1.015950	4.541946	-0.841098
H	-6.498347	-4.014100	-0.149572	C	2.302754	3.372026	-2.545224
H	-6.990159	-1.789785	-0.984052	O	3.636360	3.310396	-3.107832
C	-3.417749	-2.882906	-3.329791	C	1.307000	3.584686	-3.687023
O	-4.462859	-4.859733	1.195634	O	1.231695	4.928584	-4.139009
O	-6.401389	-2.740743	1.490167	H	1.223375	6.597323	-0.793408
O	-5.279076	-0.931071	-0.208873	H	-0.495818	6.947052	0.888806
H	-2.917698	-3.843506	-3.461311	H	0.440840	5.399103	2.544575
O	-2.443313	-1.888942	-3.646063	H	-0.963667	3.944790	0.781424
H	-4.266611	-2.838206	-4.024292	H	-2.790613	4.764526	2.175719
H	-3.550012	-5.203636	1.237724	H	-2.855562	6.149809	-0.136435
H	-6.189952	-3.420774	2.147207	H	-1.199748	4.127423	-1.735759
H	-2.839548	-0.996301	-3.538331	H	-2.735323	6.510007	-2.828558
O	-5.682705	2.559312	-1.298074	H	-3.370439	4.842085	-2.812197
C	-5.060999	1.253922	-1.309981	H	-2.113419	5.447027	-4.771401
C	-5.860716	0.366176	-0.345253	H	-4.862614	5.419653	-0.388115
C	-5.838847	0.971609	1.061817	H	-6.387920	4.180481	1.048035
C	-6.318501	2.419127	1.035396	H	-5.024440	4.117335	2.991527
C	-5.577547	3.216450	-0.048080	H	-4.186290	2.101708	1.372846
H	-4.036035	1.341007	-0.933764	H	-5.979420	1.063576	2.493002
H	-6.898055	0.281644	-0.695196	H	-6.839565	1.865766	-0.115859
H	-4.794663	0.962356	1.410773	H	-3.985375	2.037829	-1.198185
H	-7.386264	2.423786	0.773693	H	-4.938512	0.776791	-2.839468
H	-6.045897	4.195811	-0.187754	H	-5.436203	2.386412	-3.363913
C	-4.982658	0.778379	-2.770962	H	-6.980157	0.328933	-2.283863
O	-6.670887	0.252089	1.957457	H	-7.536230	-0.073179	0.131477
O	-6.116096	3.072456	2.285453	H	-7.340352	-2.235614	1.263344
O	-4.234412	3.358162	0.343464	H	-6.201787	-1.395849	3.207442
H	-5.447812	-0.201640	-2.884669	H	-4.337601	-1.726024	1.261457
O	-3.638773	0.627502	-3.228871	H	-4.555361	-4.019137	2.082176
H	-5.532561	1.495725	-3.393318	H	-5.883765	-3.905529	-0.202811
H	-6.411322	-0.687995	1.910475	H	-4.534390	-1.441212	-1.410786
H	-6.458037	2.478383	2.970092	H	-4.571912	-3.263888	-2.941002
H	-3.181895	1.497387	-3.188649	H	-5.804517	-2.082243	-3.440192
O	-1.931075	5.883025	-1.024077	H	-6.557628	-4.330956	-3.393561
C	-2.543917	4.573709	-0.975725	H	-4.600074	-5.410970	-1.001774
C	-3.590114	4.617267	0.148274	H	-2.929129	-6.835602	0.077056
C	-2.900995	4.932561	1.479529	H	-3.212597	-6.050529	2.307738
C	-2.092590	6.221696	1.371438	H	-1.619947	-4.261238	1.041421
C	-1.182141	6.199095	0.134246	H	-0.149208	-5.727315	1.945686
H	-1.784999	3.826123	-0.718952	H	-0.656828	-6.288897	-1.037249
H	-4.335144	5.392197	-0.075441	H	-1.620946	-3.408669	-1.356635
H	-2.209291	4.104438	1.699520	H	-0.030826	-3.659871	-3.031654
H	-2.797952	7.055019	1.241276	H	-1.576782	-4.047833	-3.792192

H	-0.766894	7.195613	-0.046453	H	0.641517	-5.559458	-3.583901
C	-3.063389	4.247734	-2.386440	H	1.219840	-6.628095	-0.130744
O	-3.838228	5.094764	2.532077	H	3.250200	-6.006155	0.992849
O	-1.277866	6.443667	2.519013	H	2.277692	-4.721193	2.756944
O	-0.153009	5.264953	0.348344	H	2.514148	-3.085695	0.581568
H	-4.124274	3.996246	-2.361245	H	4.770473	-2.976315	1.392181
O	-2.407603	3.119890	-2.966002	H	4.778005	-4.574184	-0.799910
H	-2.934832	5.140981	-3.010971	H	2.079847	-3.634323	-1.905101
H	-4.422374	4.312644	2.529338	H	4.110385	-5.423419	-3.284728
H	-1.843721	6.315174	3.294684	H	4.010093	-3.660767	-3.544567
H	-1.444115	3.304708	-3.033927	H	2.647902	-4.982069	-5.011486
O	3.014699	5.186625	-1.525980	H	6.197861	-3.158796	-1.590346
C	1.647678	4.793331	-1.264194	H	7.275949	-1.107827	-0.777365
C	1.173612	5.610038	-0.052855	H	6.522416	-1.267809	1.474034
C	2.062033	5.303127	1.156662	H	4.477396	-0.202765	0.010854
C	3.530148	5.540477	0.816419	H	5.853098	1.769873	0.401039
C	3.911259	4.828892	-0.490538	H	6.286436	1.012240	-2.109321
H	1.621257	3.730794	-0.999214	H	3.757446	-0.651151	-2.528313
H	1.230291	6.680801	-0.289581	H	4.085962	0.910583	-4.295479
H	1.929595	4.238328	1.404063	H	4.510151	-0.716308	-4.880112
H	3.672847	6.618671	0.655397	H	6.095024	0.978526	-5.398869
H	4.898807	5.159014	-0.828307	H	5.576563	2.923726	-2.753124
C	0.851391	4.971452	-2.568578	H	5.006327	4.953231	-1.512273
O	1.736640	6.119317	2.270251	H	5.530745	4.168882	0.678673
O	4.401267	5.078472	1.845043	H	3.066777	3.224842	0.081118
H	-0.003557	5.630940	-2.414859	H	2.641512	5.228175	1.079722
O	0.315183	3.741935	-3.056404	H	2.518064	5.424869	-1.973711
H	1.514894	5.433402	-3.310718	H	2.075174	2.404136	-2.080666
H	0.776997	6.033824	2.427834	H	0.325979	3.233580	-3.352205
H	4.057500	5.425791	2.681451	H	1.621455	2.931643	-4.513147
H	1.050458	3.116803	-3.243385	H	0.318787	5.226960	-3.974344
C	4.892834	-0.834961	3.836071	C	2.866882	4.005946	4.498225
C	4.375338	0.425283	3.537357	C	1.488562	3.946380	4.709787
C	3.050528	0.539334	3.116494	C	0.778246	2.818953	4.295867
C	2.218610	-0.582254	2.982431	C	1.415686	1.737017	3.670100
C	2.738022	-1.851405	3.305629	C	2.809622	1.789895	3.479592
C	4.070432	-1.956066	3.727323	C	3.514293	2.927354	3.896074
C	1.844819	-3.077811	3.324080	C	3.556839	0.593409	2.924648
C	0.723335	-2.867425	4.314406	C	3.353380	-0.603619	3.823281
C	0.667052	-3.548014	5.530776	C	4.371892	-1.115557	4.627781
C	-0.377000	-3.329293	6.434841	C	4.161636	-2.236942	5.436214
C	-1.373070	-2.407481	6.117315	C	2.907755	-2.846533	5.445646
C	-1.324453	-1.705921	4.909854	C	1.869624	-2.335810	4.660819
C	-0.280612	-1.923780	3.997382	C	2.076858	-1.212031	3.844128
C	0.827110	-0.323883	2.411353	C	0.508693	0.627617	3.144968
N	-0.235247	-1.309740	2.718126	N	1.092224	-0.719422	2.953193
C	0.920299	-0.186983	0.874630	C	-0.088271	1.082808	1.796520
C	-1.512339	-0.852241	2.167344	C	0.056460	-1.658728	2.518049
C	-1.409098	-0.708218	0.652497	C	-0.526544	-1.202755	1.184147
N	-0.352481	0.233554	0.294308	N	-1.084916	0.142101	1.293242
C	-0.254714	0.404064	-1.152675	C	-1.631933	0.592055	0.018682
H	5.921512	-0.945096	4.166607	H	3.435716	4.875257	4.814321
H	4.997307	1.311687	3.610951	H	0.970309	4.763392	5.203638
H	2.650691	1.523309	2.882736	H	-0.296117	2.777486	4.458153
H	4.462005	-2.937023	3.982708	H	4.591031	2.957717	3.751446
H	2.433021	-3.958722	3.594770	H	4.619124	0.825252	2.817891
H	1.417437	-3.253494	2.329551	H	3.170982	0.347492	1.927506
H	1.443469	-4.272029	5.765143	H	5.349468	-0.640298	4.604576
H	-0.410951	-3.876992	7.371798	H	4.969795	-2.629554	6.045768
H	-2.190346	-2.223987	6.809056	H	2.725859	-3.715388	6.071849
H	-2.101938	-0.984660	4.682936	H	0.894413	-2.809654	4.693998
H	0.505185	0.661324	2.794120	H	-0.334595	0.540904	3.853287
H	1.264396	-1.155922	0.461517	H	0.744803	1.230335	1.080878
H	1.677471	0.564942	0.631237	H	-0.573789	2.052924	1.940604
H	-1.825832	0.114612	2.599121	H	-0.757673	-1.745747	3.258819
H	-2.280188	-1.591950	2.407360	H	0.505896	-2.646013	2.390150
H	-2.363971	-0.339363	0.262289	H	-1.327389	-1.886998	0.881360
H	-1.234041	-1.708409	0.210693	H	0.266143	-1.254218	0.412119
H	-0.004444	-0.533296	-1.683084	H	-0.875248	0.617642	-0.788202
H	0.515801	1.142163	-1.395260	H	-2.041975	1.600322	0.126402
H	-1.208418	0.768434	-1.546809	H	-2.440266	-0.076232	-0.293637
FA1				FA1			

E	-5082.95082036			E	-5082.93428442		
ZPE	-5081.384820			ZPE	-5081.372338		
H	-5081.293854			H	-5081.278580		
G	-5081.507487			G	-5081.502429		
S	449.629			S	471.130		
O	-5.677011	3.065430	-0.811105	C	-2.187587	5.967891	-0.724855
C	-5.221624	1.692768	-0.836268	C	-2.876834	5.995940	0.641267
C	-5.937585	0.964197	0.311047	O	-1.908313	6.309105	1.639855
C	-5.587471	1.627376	1.646408	C	-3.551957	4.661117	0.925895
C	-5.899401	3.118970	1.602300	O	-4.242051	4.802955	2.154054
C	-5.285961	3.768137	0.352797	C	-4.480450	4.251191	-0.223872
H	-4.142351	1.664188	-0.648709	O	-4.847669	2.892409	0.036932
H	-7.023207	1.006176	0.151336	C	-3.747728	4.345120	-1.574843
H	-4.504961	1.503182	1.804409	O	-3.143553	5.649464	-1.722273
H	-6.989957	3.238719	1.531723	C	-4.647069	4.153266	-2.780618
H	-5.670457	4.785248	0.227217	O	-3.804499	4.065918	-3.926987
C	-5.464870	1.146507	-2.253668	C	-6.206233	2.514195	0.080689
O	-5.510632	-0.391804	0.440492	C	-6.496150	1.846783	1.434598
O	-6.318372	1.061896	2.722767	O	-6.162362	2.746217	2.490243
O	-5.404426	3.804423	2.749529	C	-5.727237	0.536954	1.560175
O	-3.886671	3.780140	0.495041	O	-6.125565	-0.067870	2.780290
H	-6.050964	0.227330	-2.219589	C	-6.022408	-0.345462	0.349895
O	-4.253862	0.811769	-2.929988	O	-5.206082	-1.516938	0.459080
H	-6.034802	1.898964	-2.813913	C	-5.719996	0.403912	-0.952135
H	-6.192767	0.094218	2.688290	O	-6.514906	1.613722	-0.967007
H	-5.674511	3.286979	3.522756	C	-6.035433	-0.404277	-2.218011
H	-3.682659	1.609578	-2.987414	O	-7.176365	-1.246984	-2.116781
O	-1.634515	5.989053	-1.400623	C	-5.850228	-2.758879	0.593304
C	-2.337230	4.747675	-1.159871	C	-5.150144	-3.568214	1.686962
C	-3.172492	4.955269	0.112990	O	-5.199252	-2.818649	2.898403
C	-2.239417	5.267047	1.287248	C	-3.718350	-3.894963	1.280819
C	-1.358547	6.469593	0.962384	O	-3.172892	-4.723984	2.295598
C	-0.677861	6.295910	-0.403627	C	-3.703571	-4.570798	-0.090794
H	-1.610230	3.948982	-0.974535	O	-2.330307	-4.634472	-0.487004
H	-3.870335	5.788959	-0.040916	C	-4.503788	-3.766823	-1.132090
H	-1.595672	4.386633	1.433797	O	-5.833659	-3.479913	-0.632446
H	-2.004800	7.356564	0.896849	C	-4.655094	-4.491749	-2.458931
H	-0.213919	7.235735	-0.719029	O	-5.182069	-5.794696	-2.225911
C	-3.105457	4.384575	-2.442846	C	-1.829148	-5.828190	-1.058637
O	-2.955039	5.560345	2.476418	C	-0.753087	-6.410605	-0.130404
O	-0.343017	6.673759	1.940824	O	-1.315094	-6.592738	1.169464
O	0.285911	5.279089	-0.292438	C	0.465625	-5.496534	-0.082708
H	-4.171502	4.273687	-2.240228	O	1.448227	-6.150164	0.707637
O	-2.682003	3.140566	-2.999860	C	0.948983	-5.201082	-1.500594
H	-2.973653	5.203984	-3.160973	O	2.041716	-4.282127	-1.392950
H	-3.606594	4.845926	2.614400	C	-0.195150	-4.609616	-2.331986
H	-0.776211	6.649996	2.806769	O	-1.277559	-5.573425	-2.334287
H	-1.728643	3.194454	-3.231679	C	0.180211	-4.295145	-3.786766
O	3.073464	4.591413	-2.588768	O	1.130352	-5.188888	-4.354677
C	1.723775	4.450592	-2.089883	C	3.290271	-4.676208	-1.905327
C	1.548545	5.452428	-0.939112	C	4.381260	-4.342351	-0.888760
C	2.597674	5.206366	0.148447	O	4.082804	-4.994314	0.344739
C	4.003023	5.190513	-0.437897	C	4.499061	-2.836868	-0.694335
C	4.061765	4.238040	-1.640550	O	5.597027	-2.629961	0.176151
H	1.587272	3.439841	-1.690177	C	4.661327	-2.105555	-2.034357
H	1.643953	6.477786	-1.319647	O	4.455433	-0.708207	-1.798368
H	2.402115	4.213004	0.576792	C	3.602630	-2.577423	-3.047889
H	4.247043	6.199043	-0.800588	O	3.580873	-4.019982	-3.128289
H	5.021453	4.331390	-2.158672	C	3.850339	-2.077321	-4.457834
C	0.765892	4.617947	-3.280838	O	2.690629	-2.379316	-5.228466
O	2.552494	6.200296	1.160201	C	5.555269	0.179705	-1.835588
O	4.969319	4.763829	0.518869	C	5.625381	0.971369	-0.514865
O	3.872346	2.924083	-1.173244	O	5.712665	0.039961	0.547956
H	-0.001060	5.360150	-3.054820	C	4.423909	1.908239	-0.383017
O	0.067201	3.415434	-3.599156	O	4.631045	2.739779	0.752646
H	1.348926	4.976195	-4.139278	C	4.242090	2.745054	-1.650601
H	1.646309	6.209020	1.523038	O	2.976690	3.405330	-1.507129
H	4.781560	5.247811	1.337268	C	4.254195	1.873888	-2.915767
H	0.720190	2.707906	-3.797328	O	5.446383	1.064135	-2.931800
O	4.930928	-0.039737	-3.067875	C	4.221530	2.681426	-4.202522
C	3.972204	0.970491	-2.683198	O	5.263183	3.655617	-4.178286
C	4.699639	1.877411	-1.683112	C	2.864740	4.765263	-1.880204

C	5.108587	1.070008	-0.443084	C	2.542926	5.605511	-0.634085
C	5.924994	-0.164266	-0.826651	O	3.539817	5.360463	0.358274
C	5.259862	-0.914382	-2.004166	C	1.149007	5.282949	-0.108130
H	3.125389	0.494487	-2.176237	O	0.889582	6.172163	0.969059
H	5.593826	2.301429	-2.158794	C	0.127415	5.409288	-1.235604
H	4.177645	0.732340	0.039656	O	-1.142915	5.027223	-0.696657
H	6.901484	0.191250	-1.187790	C	0.532969	4.509772	-2.409005
H	5.966737	-1.635554	-2.426685	O	1.847211	4.934341	-2.847225
C	3.427378	1.627967	-3.964011	C	-0.422708	4.566362	-3.608663
O	5.869905	1.874431	0.444529	O	-1.027878	5.836944	-3.818080
O	6.121851	-1.087447	0.235071	H	-1.810689	6.960942	-0.986524
O	4.110012	-1.569054	-1.529060	H	-3.645944	6.780165	0.607852
H	3.588737	2.706328	-3.951657	H	-2.306506	6.078428	2.493298
O	2.018978	1.447932	-4.114702	H	-2.769807	3.890633	1.001708
H	3.971500	1.206339	-4.818888	H	-4.755098	3.984552	2.315877
H	5.405506	2.728601	0.542117	H	-5.368538	4.896544	-0.224757
H	5.864437	-0.718705	1.126474	H	-2.963602	3.579093	-1.593179
H	1.817048	0.487028	-4.159438	H	-5.337092	5.006037	-2.853646
O	2.390376	-4.431617	-3.056199	H	-5.239331	3.239848	-2.641611
C	2.591801	-3.027757	-2.773117	H	-4.367397	4.030311	-4.711455
C	3.875328	-2.914705	-1.941524	H	-6.855810	3.382465	-0.068103
C	3.750591	-3.728886	-0.652491	H	-7.571713	1.623635	1.467732
C	3.345259	-5.167253	-0.952842	H	-6.157494	2.216480	3.303013
C	2.137119	-5.207622	-1.899774	H	-4.650249	0.760885	1.570283
H	1.752028	-2.652732	-2.177708	H	-5.643256	-0.912882	2.873503
H	4.723936	-3.285793	-2.531394	H	-7.081783	-0.625408	0.347671
H	2.955492	-3.266386	-0.047854	H	-4.659814	0.682781	-0.981529
H	4.181318	-5.662204	-1.466452	H	-5.143487	-0.981236	-2.487949
H	1.969853	-6.227962	-2.259194	H	-6.219268	0.308958	-3.028063
C	2.596712	-2.270504	-4.112276	H	-6.872916	-2.094274	-1.748098
O	4.974759	-3.756519	0.065433	H	-6.908263	-2.625649	0.837804
O	3.003523	-5.885793	0.231676	H	-5.702076	-4.510911	1.806257
O	1.011768	-4.735404	-1.201504	H	-4.591852	-3.247168	3.519851
H	3.521672	-1.703016	-4.228855	H	-3.154190	-2.953669	1.201744
O	1.537848	-1.320057	-4.211656	H	-2.400579	-5.198272	1.926116
H	2.541928	-3.009783	-4.921953	H	-4.125982	-5.577035	-0.003429
H	5.296557	-2.831778	0.146291	H	-3.977973	-2.822187	-1.316119
H	3.753870	-5.805327	0.838498	H	-3.666600	-4.538658	-2.932553
H	0.678261	-1.786072	-4.112193	H	-5.318014	-3.900893	-3.106786
O	-2.482434	-5.281636	-2.219377	H	-5.178376	-6.267211	-3.068682
C	-1.239960	-4.542673	-2.175812	H	-2.640346	-6.543714	-1.220768
C	-0.238947	-5.399320	-1.385227	H	-0.445430	-7.382752	-0.539732
C	-0.774048	-5.652823	0.028033	H	-0.582615	-6.854372	1.748427
C	-2.170518	-6.263558	-0.025637	H	0.170963	-4.544221	0.382306
C	-3.083895	-5.443543	-0.948645	H	2.270412	-5.621096	0.680453
H	-1.395051	-3.601837	-1.636071	H	1.283629	-6.124727	-1.984916
H	-0.087428	-6.356817	-1.901097	H	-0.555353	-3.685319	-1.864350
H	-0.837794	-4.681532	0.540667	H	0.546337	-3.265617	-3.842908
H	-2.089153	-7.272232	-0.454942	H	-0.742019	-4.349011	-4.377077
H	-4.021110	-5.979234	-1.129844	H	1.994656	-4.749140	-4.281876
C	-0.853869	-4.191383	-3.623378	H	3.294732	-5.744883	-2.139176
O	0.064642	-6.541211	0.754804	H	5.331675	-4.721031	-1.290080
O	-2.782525	-6.324445	1.259728	H	4.682314	-4.611991	1.004238
O	-3.329072	-4.201283	-0.338794	H	3.564419	-2.474991	-0.241311
H	0.151990	-4.544991	-3.853162	H	5.651008	-1.664237	0.367558
O	-0.838921	-2.784326	-3.860830	H	5.670536	-2.284481	-2.428686
H	-1.559446	-4.697537	-4.294766	H	2.622719	-2.219585	-2.710471
H	0.976474	-6.196564	0.700232	H	4.742786	-2.576450	-4.861307
H	-2.146445	-6.744677	1.856932	H	4.047101	-0.998398	-4.421717
H	-1.734582	-2.417206	-3.688631	H	2.879709	-2.166799	-6.151846
O	-6.091337	-1.930000	-1.208252	H	6.487695	-0.372500	-1.990597
C	-4.742423	-2.440597	-1.316515	H	6.533486	1.590686	-0.560795
C	-4.649022	-3.659025	-0.385343	H	5.709525	0.449604	1.461902
C	-4.962858	-3.239556	1.054169	H	3.521251	1.293296	-0.250917
C	-6.312050	-2.533495	1.127994	H	4.119720	3.565512	0.629891
C	-6.398380	-1.418779	0.075290	H	5.050051	3.481556	-1.713706
H	-4.036167	-1.679748	-0.965713	H	3.370945	1.222928	-2.905766
H	-5.363221	-4.426915	-0.710830	H	3.235356	3.155910	-4.281168
H	-4.182759	-2.529483	1.369034	H	4.340358	1.990535	-5.048640
H	-7.097419	-3.266684	0.895075	H	5.164355	4.208160	-4.964722
H	-7.422740	-1.039296	0.005609	H	3.787820	5.106336	-2.357461
C	-4.456381	-2.691526	-2.806984	H	2.566626	6.664230	-0.927468

O	-5.006612	-4.354906	1.929944	H	3.222496	5.780327	1.172857
O	-6.544588	-1.955881	2.409886	H	1.137744	4.240584	0.243614
H	-4.108107	-3.712612	-2.967291	H	-0.044694	6.066523	1.241704
O	-3.430124	-1.843982	-3.321531	H	0.085585	6.443596	-1.593514
H	-5.394614	-2.555880	-3.360351	H	0.599344	3.467670	-2.073455
H	-4.173173	-4.850471	1.817222	H	-1.190272	3.796350	-3.486970
H	-6.326354	-2.634599	3.065912	H	0.162794	4.309764	-4.499412
H	-3.693294	-0.903875	-3.204678	H	-1.915125	5.783455	-3.423796
C	0.006255	2.551476	3.654645	C	0.073557	3.185422	4.538074
C	0.756366	2.529685	2.479225	C	0.872670	3.412948	3.417312
C	1.723794	1.541665	2.299988	C	1.869287	2.495241	3.089822
C	1.971559	0.563163	3.274602	C	2.105876	1.348818	3.866290
C	1.193093	0.571180	4.449569	C	1.289443	1.116214	4.989077
C	0.223176	1.568763	4.619505	C	0.281626	2.039330	5.303083
C	1.301964	-0.545183	5.472448	C	1.417789	-0.151862	5.811422
C	0.993436	-1.867062	4.809389	C	1.245301	-1.368561	4.934669
C	-0.192536	-2.564068	5.041880	C	0.099762	-2.164625	4.982129
C	-0.456098	-3.774328	4.393175	C	-0.029728	-3.295085	4.169633
C	0.478278	-4.289381	3.495460	C	1.009346	-3.634133	3.304423
C	1.667185	-3.597754	3.244670	C	2.152116	-2.833151	3.226923
C	1.935770	-2.382685	3.892471	C	2.278158	-1.685600	4.025369
C	3.136448	-0.389326	2.995000	C	3.308843	0.500644	3.440385
N	3.157397	-1.669643	3.737161	N	3.439265	-0.858067	4.026059
C	4.457802	0.360157	3.277794	C	4.587319	1.304100	3.761988
C	4.318463	-2.474200	3.346580	C	4.658415	-1.516714	3.540003
C	5.610353	-1.722245	3.641361	C	5.901200	-0.693954	3.857928
N	5.639815	-0.439749	2.922707	N	5.792798	0.639611	3.250669
C	6.875297	0.299164	3.215090	C	6.990084	1.449344	3.498125
H	-0.752184	3.313817	3.809557	H	-0.710120	3.886824	4.809469
H	0.588318	3.271763	1.705049	H	0.733319	4.299938	2.806474
H	2.303142	1.531121	1.379900	H	2.496442	2.675245	2.220639
H	-0.377763	1.562246	5.525090	H	-0.350316	1.846601	6.166276
H	0.606909	-0.359092	6.295525	H	0.668384	-0.148910	6.607545
H	2.316337	-0.582619	5.887503	H	2.407674	-0.193728	6.282255
H	-0.912311	-2.159622	5.749196	H	-0.694076	-1.902996	5.677440
H	-1.381400	-4.307607	4.590046	H	-0.932436	-3.897793	4.206970
H	0.285223	-5.221774	2.972388	H	0.944379	-4.522940	2.683623
H	2.376030	-4.010566	2.535029	H	2.937856	-3.112213	2.534376
H	3.115040	-0.612518	1.912168	H	3.262217	0.405254	2.341535
H	4.477798	0.639436	4.345851	H	4.650108	1.449362	4.854834
H	4.486559	1.278549	2.686720	H	4.517155	2.280916	3.283476
H	4.300995	-2.751729	2.280906	H	4.629204	-1.698027	2.454639
H	4.306889	-3.399767	3.928308	H	4.740662	-2.489017	4.033662
H	6.465814	-2.324199	3.317567	H	6.781930	-1.199927	3.449247
H	5.701801	-1.560294	4.729254	H	6.030928	-0.615152	4.951073
H	6.964034	0.552059	4.283951	H	7.160955	1.627608	4.572021
H	6.889644	1.215279	2.622299	H	6.882671	2.414058	2.995579
H	7.736000	-0.313917	2.932559	H	7.865753	0.938102	3.088371
FV1				FV1			
E	-5082.94064844			E	-5082.92409006		
O	6.619483	-2.732162	0.005380	C	1.060547	-4.987055	-2.452766
C	5.251505	-3.076631	0.324627	C	1.958965	-5.246760	-1.240108
C	4.852637	-4.232649	-0.605225	O	1.132759	-5.596372	-0.131260
C	4.979654	-3.793160	-2.067212	C	2.828343	-4.032839	-0.931167
C	6.379455	-3.258234	-2.347925	O	3.734580	-4.415744	0.090977
C	6.778014	-2.208774	-1.300102	C	3.556551	-3.516626	-2.181584
H	4.601862	-2.219859	0.113398	O	4.088646	-2.241632	-1.806039
H	5.507181	-5.094805	-0.420468	C	2.567595	-3.365503	-3.349227
H	4.257879	-2.978342	-2.231875	O	1.865357	-4.603994	-3.549285
H	7.089889	-4.093004	-2.263612	C	3.198643	-3.018243	-4.683106
H	7.840462	-1.962308	-1.393208	O	2.127884	-2.732985	-5.588658
C	5.180386	-3.354793	1.836151	C	5.434870	-1.912393	-2.072993
O	3.484806	-4.607497	-0.441470	C	6.141111	-1.594067	-0.746279
O	4.735456	-4.865915	-2.962858	O	6.032944	-2.722104	0.121155
O	6.476044	-2.660152	-3.637797	C	5.542056	-0.344211	-0.111113
O	5.982527	-1.065576	-1.490753	O	6.299579	-0.056864	1.054102
H	4.751175	-4.338762	2.029385	C	5.560859	0.801558	-1.121000
O	4.349713	-2.423491	2.528117	O	4.897224	1.914446	-0.511721
H	6.203904	-3.340999	2.232393	C	4.850088	0.386337	-2.414983
H	3.873792	-5.258403	-2.724669	O	5.513882	-0.792057	-2.932950
H	6.071544	-3.279170	-4.263739	C	4.853502	1.468690	-3.503470
H	4.697595	-1.513960	2.393499	O	6.021308	2.280182	-3.531930

O	6.775268	2.290145	-0.205013	C	5.611961	3.114497	-0.351814
C	6.158259	0.983577	-0.139597	C	5.388626	3.640631	1.067146
C	6.594928	0.220738	-1.399417	O	5.830594	2.648114	1.990962
C	6.137055	0.976947	-2.650376	C	3.922530	3.991668	1.279773
C	6.639433	2.416189	-2.621560	O	3.811786	4.561084	2.573263
C	6.303451	3.081960	-1.279070	C	3.437721	4.943073	0.186247
H	5.068300	1.094707	-0.159722	O	2.015844	5.014324	0.333308
H	7.688397	0.121477	-1.407716	C	3.787771	4.427467	-1.222383
H	5.036246	0.993627	-2.643083	O	5.195734	4.089145	-1.299514
H	7.734734	2.399108	-2.714379	C	3.495216	5.440911	-2.315903
H	6.822911	4.041428	-1.190260	O	4.136817	6.672776	-1.998959
C	6.538071	0.354332	1.212053	C	1.371308	6.271808	0.286624
O	6.620279	0.370576	-3.838343	C	0.673635	6.527050	1.631967
O	6.070894	3.203776	-3.664260	O	1.629441	6.423087	2.687065
O	4.910974	3.261185	-1.206481	C	-0.473774	5.545320	1.835133
H	6.995791	-0.625307	1.068879	O	-1.129803	5.913232	3.041683
O	5.406844	0.137257	2.054441	C	-1.407796	5.572767	0.625162
H	7.271830	1.010489	1.697676	O	-2.413277	4.573174	0.822333
H	6.371867	-0.573231	-3.809747	C	-0.613998	5.296168	-0.656229
H	6.160314	2.691992	-4.481960	O	0.420998	6.304962	-0.758596
H	4.959673	0.995568	2.226506	C	-1.444180	5.330372	-1.939748
O	3.214999	5.600853	1.072333	O	-2.382221	6.394955	-1.983808
C	3.750059	4.311587	0.693458	C	-3.695782	5.031934	1.178023
C	4.404168	4.489690	-0.684968	C	-4.278479	4.128624	2.267802
C	3.357140	4.960160	-1.699152	O	-3.355606	4.080001	3.356015
C	2.659227	6.222069	-1.204013	C	-4.577533	2.732531	1.731329
C	2.160417	6.040129	0.237155	O	-5.269329	2.036686	2.755723
H	2.930054	3.590615	0.600860	C	-5.370730	2.773362	0.415609
H	5.210204	5.232042	-0.614253	O	-5.307105	1.444259	-0.115023
H	2.604894	4.161676	-1.793023	C	-4.718241	3.761465	-0.564791
H	3.394677	7.039202	-1.195195	O	-4.571075	5.043529	0.068343
H	1.836735	7.000825	0.649984	C	-5.495294	4.004494	-1.843061
C	4.666518	3.832108	1.832407	O	-4.638886	4.748549	-2.716385
O	3.938179	5.251091	-2.960177	C	-6.482576	0.748164	-0.470667
O	1.545280	6.573821	-2.020214	C	-6.558672	-0.553107	0.338149
O	1.098245	5.118988	0.230257	O	-6.577484	-0.241248	1.732215
H	5.661457	3.593050	1.454796	C	-5.381607	-1.457403	-0.004164
O	4.189229	2.641365	2.457399	O	-5.554011	-2.664500	0.724674
H	4.760317	4.649185	2.559318	C	-5.308136	-1.686974	-1.511610
H	4.460364	4.471896	-3.231240	O	-4.058725	-2.344850	-1.751526
H	1.848595	6.534836	-2.939465	C	-5.357286	-0.354279	-2.282615
H	3.294603	2.807270	2.829390	O	-6.485867	0.436245	-1.848210
O	-1.378380	4.758227	2.930262	C	-5.474773	-0.542817	-3.785534
C	-0.149156	4.434409	2.240268	O	-6.584180	-1.391602	-4.070322
C	-0.045763	5.389196	1.040649	C	-4.019908	-3.475126	-2.598723
C	-1.253208	5.192923	0.118128	C	-3.545472	-4.693205	-1.790296
C	-2.552147	5.367194	0.897074	O	-4.395155	-4.869468	-0.656653
C	-2.537275	4.492541	2.161027	C	-2.092775	-4.519538	-1.364537
H	-0.204426	3.407292	1.862995	O	-1.708048	-5.716124	-0.701235
H	-0.018542	6.426632	1.399688	C	-1.227989	-4.210664	-2.587028
H	-1.214701	4.161947	-0.265467	O	0.112162	-3.997204	-2.131008
H	-2.623340	6.415828	1.219697	C	-1.776065	-2.968467	-3.300803
H	-3.385909	4.738354	2.807252	O	-3.143764	-3.253820	-3.685019
C	0.993601	4.490110	3.268742	C	-1.005127	-2.552101	-4.552932
O	-1.258107	6.122462	-0.954002	O	-0.613861	-3.643630	-5.371974
O	-3.695875	5.015914	0.122587	H	0.564062	-5.912175	-2.759751
O	-2.581871	3.146260	1.765378	H	2.616822	-6.088081	-1.498255
H	1.780553	5.170238	2.940217	H	1.707654	-5.691401	0.641837
O	1.624428	3.223379	3.455860	H	2.170200	-3.221422	-0.585913
H	0.581924	4.868779	4.213167	H	4.420463	-3.721752	0.172387
H	-0.384345	6.077599	-1.387676	H	4.365040	-4.209240	-2.449615
H	-3.550457	5.350850	-0.774916	H	1.853839	-2.575523	-3.086482
H	0.954507	2.568212	3.752035	H	3.799946	-3.866600	-5.036001
O	-3.596277	0.301069	3.847315	H	3.853566	-2.146966	-4.561928
C	-2.633800	1.210480	3.266792	H	2.492873	-2.634391	-6.477885
C	-3.435669	2.241733	2.465696	H	5.941244	-2.731452	-2.593255
C	-4.260899	1.552925	1.373510	H	7.199413	-1.401092	-0.969824
C	-5.097128	0.406767	1.931473	H	6.353543	-2.428866	0.987943
C	-4.269519	-0.482367	2.879735	H	4.494243	-0.551987	0.150193
H	-1.981930	0.659761	2.579715	H	5.974656	0.784825	1.431872
H	-4.104220	2.791970	3.140590	H	6.595792	1.067975	-1.362623
H	-3.547844	1.141762	0.642868	H	3.807290	0.128564	-2.195483

H	-5.911775	0.843844	2.525880	H	3.954435	2.082763	-3.380075
H	-4.932677	-1.143513	3.446629	H	4.772076	0.962125	-4.470875
C	-1.753335	1.765819	4.400080	H	5.848982	3.039518	-2.949776
O	-5.141891	2.474054	0.751553	H	6.679090	2.961686	-0.539068
O	-5.636826	-0.429204	0.908291	H	5.989323	4.553463	1.182303
O	-3.359308	-1.231990	2.114366	H	5.487117	2.904610	2.860253
H	-1.777054	2.856707	4.408451	H	3.331116	3.066359	1.207492
O	-0.379871	1.406566	4.256003	H	2.949663	5.020611	2.634602
H	-2.158271	1.404922	5.354426	H	3.890290	5.928578	0.336128
H	-4.601688	3.197224	0.378915	H	3.191941	3.528292	-1.419397
H	-5.855519	0.099128	0.113891	H	2.406586	5.561414	-2.380018
H	-0.299194	0.426925	4.267948	H	3.852493	5.037397	-3.273863
O	-1.692881	-4.319825	3.216851	H	3.853134	7.327020	-2.650787
C	-1.785532	-2.891004	3.013393	H	2.092303	7.062809	0.060171
C	-3.177735	-2.612669	2.428804	H	0.261638	7.545696	1.605478
C	-3.349828	-3.362531	1.104567	H	1.111921	6.400153	3.507857
C	-3.065446	-4.849428	1.290073	H	-0.055087	4.532153	1.919875
C	-1.726937	-5.062411	2.012335	H	-1.771380	5.211624	3.263831
H	-1.030424	-2.577574	2.283808	H	-1.874091	6.558655	0.525556
H	-3.945297	-2.943113	3.141347	H	-0.136295	4.310307	-0.594009
H	-2.613942	-2.954616	0.394575	H	-1.948195	4.364586	-2.044573
H	-3.853504	-5.271588	1.929934	H	-0.737522	5.420708	-2.776819
H	-1.618059	-6.110687	2.308149	H	-3.264067	5.985282	-2.050423
C	-1.458115	-2.204103	4.350576	H	-3.651424	6.066200	1.530631
O	-4.666632	-3.228821	0.591983	H	-5.223229	4.584007	2.594818
O	-3.016031	-5.546668	0.048103	H	-3.745606	3.520301	4.042780
O	-0.687035	-4.679047	1.147421	H	-3.618448	2.241916	1.507276
H	-2.263055	-1.529710	4.645973	H	-5.629763	1.205549	2.382137
O	-0.280125	-1.401874	4.283236	H	-6.411007	3.060599	0.617102
H	-1.361910	-2.983149	5.117865	H	-3.730491	3.366625	-0.831393
H	-4.901551	-2.280082	0.618698	H	-6.410923	4.565334	-1.613975
H	-3.802002	-5.283516	-0.453235	H	-5.773144	3.042901	-2.290984
H	0.482035	-1.967392	4.026668	H	-5.154541	5.042849	-3.478732
O	2.835471	-5.679187	1.521065	H	-7.368704	1.367119	-0.297431
C	1.703756	-4.800517	1.719823	H	-7.492269	-1.062542	0.063883
C	0.486317	-5.490279	1.085733	H	-6.444410	-1.078498	2.203209
C	0.739151	-5.725438	-0.406625	H	-4.454656	-0.953046	0.304022
C	2.036920	-6.498045	-0.615670	H	-4.995633	-3.357070	0.314168
C	3.188832	-5.842896	0.160356	H	-6.142193	-2.321959	-1.827788
H	1.881210	-3.854722	1.195707	H	-4.431407	0.198595	-2.082487
H	0.308568	-6.451668	1.585657	H	-4.535572	-0.981948	-4.144896
H	0.841615	-4.739291	-0.885152	H	-5.594823	0.444882	-4.251970
H	1.902622	-7.511126	-0.210358	H	-6.571690	-1.580387	-5.017690
H	4.067537	-6.495591	0.158832	H	-5.004088	-3.655251	-3.041165
C	1.611502	-4.490667	3.224060	H	-3.615112	-5.574855	-2.442747
O	-0.310741	-6.466311	-1.008041	H	-3.947457	-5.516758	-0.088867
O	2.406261	-6.564704	-1.990381	H	-2.029273	-3.663489	-0.676965
H	0.621568	-4.736548	3.610368	H	-0.800366	-5.599347	-0.360145
O	1.811826	-3.107879	3.513790	H	-1.253325	-5.046016	-3.294717
H	2.349940	-5.113970	3.744654	H	-1.778277	-2.114182	-2.612108
H	-1.149330	-6.012978	-0.797399	H	-0.132065	-1.972241	-4.239037
H	1.614673	-6.833639	-2.479895	H	-1.658456	-1.873980	-5.120098
H	2.699144	-2.833458	3.191504	H	0.359124	-3.618894	-5.413651
C	-4.123734	-2.864477	-5.084645	C	-1.462712	-6.266932	5.415019
C	-5.463645	-2.736946	-5.451031	C	-0.515132	-5.841809	6.346003
C	-6.296832	-1.895939	-4.716958	C	0.344589	-4.794614	6.018760
C	-5.830892	-1.173460	-3.605953	C	0.290068	-4.154822	4.770845
C	-4.472264	-1.284218	-3.255557	C	-0.683474	-4.570574	3.841502
C	-3.641001	-2.131271	-4.002596	C	-1.544794	-5.622796	4.181215
C	-3.867276	-0.436082	-2.153502	C	-0.888711	-3.827457	2.534147
C	-4.088970	1.031744	-2.438638	C	-1.209377	-2.378707	2.819808
C	-3.033627	1.869082	-2.806294	C	-2.487675	-1.846224	2.645664
C	-3.245524	3.218660	-3.102332	C	-2.752792	-0.502580	2.930548
C	-4.540220	3.731733	-3.045759	C	-1.724918	0.318417	3.391882
C	-5.609039	2.906722	-2.684790	C	-0.443453	-0.203471	3.585821
C	-5.398258	1.557099	-2.370086	C	-0.173312	-1.553600	3.313601
C	-6.895270	-0.371494	-2.854894	C	1.370622	-3.105442	4.510813
N	-6.447338	0.693143	-1.908369	N	1.125147	-2.121431	3.430571
C	-7.815148	-1.339347	-2.080955	C	2.700565	-3.832234	4.211818
C	-7.639147	1.399730	-1.393666	C	2.246430	-1.181756	3.330276
C	-8.577878	0.439427	-0.669113	C	3.540604	-1.930289	3.032262
N	-8.987572	-0.645679	-1.556709	N	3.813182	-2.894373	4.095995

C	-9.910478	-1.564001	-0.900472	C	5.079230	-3.588683	3.892914
H	-3.457014	-3.513640	-5.644447	H	-2.142284	-7.080513	5.651140
H	-5.858149	-3.281386	-6.303655	H	-0.446371	-6.315791	7.320555
H	-7.338627	-1.795216	-5.011559	H	1.080443	-4.463711	6.747854
H	-2.591791	-2.204874	-3.728751	H	-2.298702	-5.932580	3.462075
H	-2.795690	-0.642093	-2.084583	H	-1.698056	-4.296873	1.967987
H	-4.308530	-0.699370	-1.187100	H	0.018186	-3.880799	1.919743
H	-2.028940	1.456863	-2.852090	H	-3.285500	-2.480599	2.266770
H	-2.409896	3.857679	-3.371146	H	-3.750304	-0.099299	2.795659
H	-4.729627	4.773726	-3.288557	H	-1.917970	1.366754	3.603231
H	-6.606131	3.328350	-2.646044	H	0.343535	0.443845	3.956842
H	-7.524351	0.110401	-3.623046	H	1.518213	-2.555240	5.458048
H	-7.219845	-1.827991	-1.284929	H	2.568601	-4.434438	3.291639
H	-8.155131	-2.124890	-2.761726	H	2.913453	-4.526112	5.030755
H	-8.197937	1.885312	-2.209951	H	2.381897	-0.599459	4.258471
H	-7.296345	2.168050	-0.697693	H	2.036685	-0.479267	2.519450
H	-9.468176	0.994295	-0.351889	H	4.370146	-1.216835	2.969578
H	-8.086886	0.055388	0.243588	H	3.453411	-2.428935	2.048749
H	-9.470096	-2.067907	-0.020047	H	5.104930	-4.178711	2.957979
H	-10.229993	-2.336085	-1.607493	H	5.265726	-4.272410	4.727205
H	-10.798026	-1.016920	-0.566978	H	5.896852	-2.861128	3.860755
S				S			
E	-5082.93870703			E	-5082.92246450		
O	-3.384239	-2.359146	0.734545	C	0.104051	5.698390	-0.287328
C	-2.775689	-1.053328	0.596557	C	0.888440	6.056993	-1.552637
C	-3.550790	-0.325710	-0.511729	O	0.123191	5.668589	-2.690523
C	-3.437580	-1.109125	-1.823507	C	2.258914	5.388410	-1.543114
C	-3.892557	-2.553304	-1.631380	O	2.969696	5.873802	-2.668448
C	-3.208606	-3.180174	-0.407743	C	3.008558	5.650531	-0.228115
H	-1.733990	-1.171621	0.278494	O	4.131217	4.762237	-0.249766
H	-4.605167	-0.245009	-0.219465	C	2.099553	5.342851	0.973679
H	-2.376028	-1.114418	-2.115694	O	0.864762	6.068329	0.845067
H	-4.976433	-2.557461	-1.449863	C	2.668908	5.718715	2.327128
H	-3.677443	-4.137081	-0.158017	O	1.786956	5.172612	3.313674
C	-2.765107	-0.389413	1.984860	C	5.426154	5.239818	0.041081
O	-3.024441	0.970605	-0.793264	C	6.348632	4.935289	-1.149589
O	-4.229195	-0.533126	-2.852368	O	5.797279	5.518439	-2.329427
O	-3.589680	-3.364628	-2.766308	C	6.541419	3.431928	-1.313642
O	-1.844840	-3.354173	-0.700316	O	7.498737	3.242833	-2.343123
H	-3.280127	0.571609	1.961747	C	6.984477	2.817756	0.012550
O	-1.444318	-0.113784	2.449421	O	7.038404	1.399062	-0.176091
H	-3.297508	-1.049856	2.681317	C	6.001395	3.183426	1.130050
H	-4.030830	0.422579	-2.881324	O	5.938170	4.627876	1.210215
H	-3.943322	-2.906938	-3.542899	C	6.390197	2.631951	2.508619
H	-0.942102	-0.956343	2.513878	O	7.790305	2.573629	2.752529
O	0.467127	-5.595995	1.077557	C	8.261980	0.741085	0.037234
C	-0.178071	-4.327923	0.818241	C	8.518478	-0.222846	-1.122675
C	-1.203638	-4.565299	-0.300405	O	8.535206	0.525988	-2.336135
C	-0.495258	-5.086829	-1.554744	C	7.459350	-1.316472	-1.153117
C	0.329773	-6.326779	-1.228646	O	7.821738	-2.219712	-2.183858
C	1.233303	-6.070624	-0.013874	C	7.359683	-2.002387	0.209310
H	0.566365	-3.607890	0.460292	O	6.191889	-2.828016	0.147232
H	-1.950155	-5.297942	0.033868	C	7.213190	-0.983012	1.354639
H	0.188940	-4.296841	-1.900780	O	8.251479	0.025019	1.265934
H	-0.360656	-7.138973	-0.959734	C	7.300591	-1.617732	2.732201
H	1.687507	-7.006272	0.327343	O	8.498112	-2.384063	2.822508
C	-0.731157	-3.802145	2.154026	C	6.249628	-4.156557	0.628487
O	-1.416296	-5.433602	-2.576113	C	5.975340	-5.123843	-0.533969
O	1.152734	-6.724970	-2.321898	O	6.901530	-4.868640	-1.589875
O	2.222221	-5.142718	-0.384100	C	4.538848	-4.980602	-1.020651
H	-1.796549	-3.581853	2.072295	O	4.332373	-5.970462	-2.019170
O	-0.110393	-2.584811	2.565404	C	3.571035	-5.120079	0.154399
H	-0.598728	-4.587653	2.909211	O	2.248637	-4.889854	-0.340632
H	-1.988352	-4.657933	-2.734402	C	3.926293	-4.105232	1.246862
H	0.590395	-6.717998	-3.110893	O	5.295162	-4.355853	1.651305
H	0.857688	-2.728232	2.658000	C	3.038838	-4.166645	2.491234
O	5.389724	-4.595228	1.406390	O	2.724873	-5.487336	2.906984
C	3.998078	-4.333316	1.112076	C	1.409353	-6.013376	-0.465571
C	3.564585	-5.356954	0.051968	C	0.634464	-5.924020	-1.782822
C	4.427832	-5.204902	-1.204234	O	1.565887	-5.825617	-2.857059
C	5.908417	-5.300729	-0.853304	C	-0.325995	-4.739723	-1.763587
C	6.251593	-4.357755	0.309050	O	-1.089945	-4.805757	-2.954477

H	3.899464	-3.328142	0.687031	C	-1.206468	-4.746842	-0.503958
H	3.674982	-6.372355	0.455224	O	-1.854815	-3.471319	-0.474187
H	4.234325	-4.203987	-1.619881	C	-0.334899	-4.927453	0.750184
H	6.116257	-6.326388	-0.516444	O	0.490238	-6.096112	0.604593
H	7.262352	-4.559888	0.677426	C	-1.097248	-5.110498	2.047065
C	3.225653	-4.355367	2.442673	O	-0.137288	-5.027800	3.106370
O	4.141761	-6.209137	-2.164485	C	-3.260229	-3.385702	-0.365388
O	6.743955	-4.968516	-1.958891	C	-3.810487	-2.573507	-1.541911
O	6.143845	-3.032251	-0.146731	O	-3.446799	-3.221429	-2.765377
H	2.393110	-5.058667	2.396000	C	-3.277614	-1.146968	-1.495583
O	2.650342	-3.090065	2.765415	O	-3.890737	-0.432172	-2.559968
H	3.914605	-4.688185	3.229745	C	-3.571118	-0.520487	-0.135123
H	3.178242	-6.200317	-2.322483	O	-2.858133	0.721543	-0.106240
H	6.408194	-5.462862	-2.721447	C	-3.111919	-1.429768	1.019990
H	3.363559	-2.416383	2.827616	O	-3.636679	-2.763326	0.846632
O	7.669401	-0.114687	1.497393	C	-3.567838	-0.932672	2.381745
C	6.598600	-1.053261	1.242997	O	-4.978915	-0.716477	2.357022
C	7.140398	-2.088383	0.245948	C	-3.504735	1.873199	0.398486
C	7.570479	-1.390034	-1.047656	C	-3.621618	2.919642	-0.721065
C	8.564755	-0.273174	-0.749509	O	-4.284529	2.332078	-1.843088
C	8.034058	0.645752	0.360725	C	-2.247025	3.445768	-1.114534
H	5.757150	-0.527637	0.777756	O	-2.449132	4.484186	-2.062680
H	8.000687	-2.607914	0.688322	C	-1.491413	3.923124	0.126720
H	6.670927	-0.942704	-1.497986	O	-0.181856	4.320015	-0.291679
H	9.493581	-0.730842	-0.380090	C	-1.419364	2.792069	1.158894
H	8.822376	1.325294	0.700053	O	-2.779610	2.413837	1.483927
C	6.117684	-1.593859	2.601076	C	-0.697095	3.149039	2.458358
O	8.187489	-2.291844	-1.952490	O	-0.996821	4.449802	2.941785
O	8.834646	0.526094	-1.897983	H	-0.817386	6.285238	-0.230963
O	6.937874	1.367530	-0.143436	H	1.032441	7.146680	-1.549191
H	6.152741	-2.683938	2.619687	H	0.703747	5.737001	-3.462877
O	4.764379	-1.241368	2.884460	O	2.107093	4.300486	-1.614853
H	6.795174	-1.213671	3.376520	H	3.894903	5.561061	-2.604187
H	7.584914	-3.051143	-2.069236	H	3.344742	6.695181	-0.199630
H	9.020667	-0.084506	-2.626728	H	1.894806	4.265612	0.971997
H	4.680356	-0.261854	2.892075	H	2.726461	6.812150	2.409817
O	5.603380	4.462821	1.334058	H	3.678437	5.302971	2.428640
C	5.663578	3.029564	1.149183	H	2.052806	5.501701	4.182371
C	6.822988	2.753359	0.180191	H	5.406439	6.314577	0.247507
C	6.567832	3.463362	-1.153033	H	7.326386	5.388633	-0.934851
C	6.322191	4.951584	-0.928683	H	6.304420	5.154810	-3.071966
C	5.258264	5.169255	0.157232	H	5.575868	2.983484	-1.592252
H	4.732208	2.682953	0.687501	H	7.672696	2.284422	-2.426565
H	7.761148	3.118635	0.618524	H	7.975217	3.198442	0.284102
H	5.659957	3.024334	-1.594806	H	5.002464	2.805087	0.882350
H	7.257255	5.402389	-0.566521	H	5.932552	1.643074	2.624494
H	5.221139	6.224404	0.446235	H	5.944008	3.288087	3.263308
C	5.763701	2.382995	2.541892	H	8.089649	1.697115	2.456924
O	7.668716	3.332285	-2.038177	H	9.082439	1.459623	0.125186
O	5.888095	5.609565	-2.115756	H	9.499530	-0.689084	-0.956647
O	4.014991	4.747347	-0.345640	H	8.491695	-0.116988	-3.060044
H	6.635722	1.730922	2.605391	H	6.485750	-0.849566	-1.366257
O	4.638005	1.561656	2.848664	H	7.322796	-3.051889	-2.054376
H	5.878898	3.186403	3.280877	H	8.253755	-2.611919	0.375843
H	7.879543	2.381548	-2.107806	H	6.234177	-0.497709	1.262382
H	6.490067	5.336256	-2.823834	H	6.411803	-2.246240	2.869454
H	3.820465	2.106691	2.814396	H	7.276504	-0.820247	3.488394
O	0.745551	5.716504	1.036858	H	8.477753	-2.861170	3.662410
C	1.900545	4.855610	0.907397	H	7.223457	-4.355183	1.085599
C	2.861125	5.543301	-0.074303	H	6.117444	-6.146502	-0.157010
C	2.171367	5.737151	-1.428468	H	6.567113	-5.361586	-2.356209
C	0.854891	6.488107	-1.257978	H	4.414102	-3.974380	-1.446604
C	-0.000761	5.840188	-0.159713	H	3.462253	-5.806328	-2.431766
H	1.592184	3.895399	0.478818	H	3.640103	-6.123051	0.588645
H	3.161121	6.519300	0.329743	H	3.863393	-3.086842	0.843228
H	1.950297	4.737936	-1.834283	H	2.126374	-3.598068	2.287066
H	1.083977	7.513227	-0.933369	H	3.575854	-3.641339	3.293545
H	-0.852042	6.482169	0.088042	H	1.756012	-5.573281	2.849513
C	2.441780	4.582802	2.321732	H	1.992186	-6.938239	-0.428776
O	2.980358	6.475461	-2.330185	H	0.045845	-6.847524	-1.877800
O	0.091121	6.513086	-2.460634	H	1.062711	-5.585289	-3.649220
O	-0.438750	4.586627	-0.620323	H	0.272212	-3.816164	-1.731758

H	3.495081	4.856934	2.393197	H	-1.780906	-4.112488	-2.917624
O	2.371418	3.203371	2.679837	H	-1.946688	-5.554404	-0.577709
H	1.875014	5.203424	3.027654	H	0.300157	-4.038659	0.846869
H	3.852005	6.037478	-2.370363	H	-1.598313	-6.087502	2.042588
H	0.694860	6.778468	-3.170249	H	-1.856954	-4.325386	2.140774
H	1.434460	2.906651	2.652053	H	-0.566212	-5.285290	3.933044
O	-3.231416	2.656262	0.800418	H	-3.707435	-4.384642	-0.341539
C	-1.844337	3.047184	0.682937	H	-4.904881	-2.544949	-1.449193
C	-1.781458	4.183849	-0.348898	H	-3.658203	-2.597615	-3.476662
C	-2.338583	3.704809	-1.693905	H	-2.185865	-1.173362	-1.630839
C	-3.740027	3.131217	-1.518780	H	-3.822720	0.525080	-2.370030
C	-3.762498	2.097307	-0.384975	H	-4.647138	-0.342787	-0.045874
H	-1.258413	2.201750	0.305138	H	-2.015556	-1.468601	1.022698
H	-2.369278	5.039482	0.009120	H	-3.030709	-0.002289	2.602530
H	-1.679131	2.902482	-2.058856	H	-3.292009	-1.680397	3.137669
H	-4.416499	3.948090	-1.231338	H	-5.229457	-2.283320	3.183328
H	-4.794519	1.821217	-0.147549	H	-4.489774	1.614054	0.797072
C	-1.334872	3.377041	2.096049	H	-4.220429	3.756021	-0.335357
O	-2.410703	4.761578	-2.637655	H	-4.194748	2.969195	-2.569602
O	-4.215264	2.496567	-2.704518	H	-1.674083	2.620995	-1.563460
H	-0.871879	4.364246	2.119059	H	-1.575327	4.754913	-2.405398
O	-0.334486	2.465411	2.548187	H	-2.010863	4.769879	0.587645
H	-2.197682	3.384660	2.774591	H	-0.910516	1.922677	0.723943
H	-1.526789	5.173106	-2.685302	H	0.378736	3.036920	2.293116
H	-4.075854	3.119471	-3.433365	H	-0.990754	2.396459	3.203807
H	-0.698091	1.552094	2.538630	H	-0.153281	4.936873	2.959716
C	-8.456741	-0.643403	4.374099	C	-10.412224	-0.708572	3.727960
C	-7.335389	-1.296464	3.862085	C	-9.123604	-1.237200	3.653874
C	-7.139895	-1.344554	2.482637	C	-8.428048	-1.186891	2.446339
C	-8.049737	-0.756940	1.590140	C	-8.996049	-0.621286	1.293975
C	-9.168227	-0.078181	2.109651	C	-10.286739	-0.063453	1.377587
C	-9.353296	-0.032570	3.497806	C	-10.974757	-0.117304	2.597141
C	-10.101383	0.694885	1.196286	C	-10.888100	0.694224	0.207831
C	-9.323289	1.756323	0.453712	C	-9.990086	1.851247	-0.163986
C	-9.455589	3.114829	0.741915	C	-10.334677	3.178036	0.094901
C	-8.719687	4.077632	0.044279	C	-9.477905	4.227145	-0.252535
C	-7.830930	3.669403	-0.948744	C	-8.254657	3.939314	-0.856160
C	-7.673478	2.311293	-1.241439	C	-7.885623	2.615190	-1.110294
C	-8.414224	1.341173	-0.546463	C	-8.746216	1.560004	-0.768623
C	-7.775031	-0.988532	0.107148	C	-8.174004	-0.745823	0.012544
N	-8.366262	-0.041414	-0.864935	N	-8.469344	0.203329	-1.084655
C	-8.224916	-2.414970	-0.273896	C	-8.329059	-2.180320	-0.538706
C	-7.934372	-0.378016	-2.226852	C	-7.572349	-0.025430	-2.221717
C	-8.371775	-1.795260	-2.583808	C	-7.734175	-1.449035	-2.744539
N	-7.812657	-2.754757	-1.633237	N	-7.452910	-2.414431	-1.683997
C	-8.166976	-4.127825	-1.975790	C	-7.544447	-3.789397	-2.163079
H	-8.624757	-0.594754	5.445951	H	-10.968538	-0.738632	4.660291
H	-6.614715	-1.760486	4.528737	H	-6.658490	-1.680763	4.529321
H	-6.260912	-1.846666	2.084073	H	-7.416262	-1.581543	2.394168
H	-10.214117	0.500321	3.893465	H	-11.967121	0.322283	2.657208
H	-10.901261	1.151056	1.785647	H	-11.884660	1.055631	0.475729
H	-10.563129	0.017686	0.467120	H	-10.990564	0.031365	-0.660190
H	-10.158328	3.423532	1.511903	H	-11.294054	3.392750	0.559269
H	-8.845056	5.131643	0.273058	H	-9.766794	5.255151	-0.055028
H	-7.252009	4.404306	-1.501192	H	-7.576377	4.743742	-1.127087
H	-6.963401	2.016124	-2.006304	H	-6.919523	2.409677	-1.559886
H	-6.678003	-0.969634	-0.015032	H	-7.115089	-0.631884	0.304483
H	-9.322595	-2.483010	-0.142264	H	-9.394751	-2.342198	-0.793356
H	-7.764909	-3.127672	0.417136	H	-8.066896	-2.891878	0.250117
H	-6.841242	-0.303133	-2.345811	H	-6.513514	0.136371	-1.964487
H	-8.401361	0.326418	-2.920206	H	-7.835964	0.680222	-3.014227
H	-8.011491	-2.041248	-3.588877	H	-7.028915	-1.612328	-3.566831
H	-9.477803	-1.841755	-2.603836	H	-8.757123	-1.576822	-3.148296
H	-9.257559	-4.309090	-1.960013	H	-8.548465	-4.407204	-2.547471
H	-7.698280	-4.818547	-1.268122	H	-7.305034	-4.480802	-1.349318
H	-7.799234	-4.362801	-2.979414	H	-6.819752	-3.945141	-2.968415
CR2				CR2			
E	-5082.93931568			E	-5082.93085002		
O	3.228585	-2.599957	3.535712	C	0.149309	5.739724	-1.932110
C	2.831845	-1.249169	3.204944	C	0.663080	5.614961	-3.370365
C	2.927984	-0.426273	4.498048	O	-0.452618	5.607552	-4.257558
C	2.002876	-1.018571	5.565468	C	1.520537	4.364245	-3.534842

C	2.307827	-2.498006	5.775403	O	2.070237	4.402109	-4.840530
C	2.341825	-3.242194	4.432763	C	2.605253	4.272526	-2.450584
H	1.790009	-1.248957	2.865529	O	3.156529	2.957168	-2.583656
H	3.963961	-0.438688	4.861942	C	1.972105	4.464058	-1.064627
H	0.969098	-0.925545	5.198344	O	1.249565	5.709806	-1.047547
H	3.308996	-2.581281	6.221912	C	2.922548	4.514724	0.119319
H	2.739282	-4.252934	4.568786	O	2.112215	4.530579	1.285359
C	3.706967	-0.779331	2.029927	C	4.552567	2.773467	-2.637511
O	2.487673	0.919428	4.313309	C	4.902046	1.995690	-3.916647
O	2.151919	-0.363242	6.814636	O	4.385946	2.699863	-5.045058
O	1.343718	-3.131852	6.611677	C	4.356998	0.572810	-3.852511
O	1.035664	-3.286233	3.915234	O	4.831619	-0.111703	-5.000857
H	4.238611	0.138534	2.283333	C	4.802379	-0.094459	-2.552855
O	2.943016	-0.477298	0.862998	O	4.174472	-1.380224	-2.499660
H	4.448331	-1.561833	1.824317	C	4.399194	0.761556	-1.348240
H	2.054225	0.595938	6.659587	O	5.014952	2.061852	-1.504308
H	1.229176	-2.563848	7.388032	C	4.820123	0.179496	0.005413
H	2.458438	-1.283032	0.576942	O	6.072529	-0.494826	0.000797
O	-0.132222	-5.603373	1.306665	C	4.992457	-2.520233	-2.416520
C	0.406109	-4.350391	1.788944	C	4.482582	-3.568349	-3.407456
C	0.579625	-4.495381	3.308241	O	4.510711	-3.001417	-4.715576
C	-0.773564	-4.794182	3.961022	C	3.082147	-4.025328	-3.022544
C	-1.420900	-6.015687	3.317792	O	2.716708	-5.061091	-3.919033
C	-1.434468	-5.878721	1.788276	C	3.051491	-4.487304	-1.565665
H	-0.313092	-3.546969	1.594306	O	1.667569	-4.655503	-1.241308
H	1.280629	-5.313752	3.519866	C	3.683506	-3.450268	-0.617975
H	-1.425150	-3.924193	3.786390	O	4.993355	-3.058172	-1.100267
H	-0.811308	-6.896999	3.563504	C	3.849089	-3.964704	0.802001
H	-1.727797	-6.825531	1.323783	O	4.562662	-5.197803	0.774346
C	1.678412	-4.043452	0.979537	C	1.245860	-5.813437	-0.549306
O	-0.643697	-5.050830	5.350228	C	0.243643	-6.581401	-1.425500
O	-2.761828	-6.207815	3.760169	O	0.843134	-6.865813	-2.689413
O	-2.333270	-4.854636	1.442558	C	-1.042691	-5.782311	-1.597213
H	2.531656	-3.891279	1.641832	O	-1.950557	-6.601597	-2.320458
O	1.562895	-2.848705	0.207774	C	-1.587041	-5.364304	-0.231131
H	1.889839	-4.908872	0.338341	O	-2.738908	-4.543824	-0.451755
H	-0.158335	-4.301134	5.744735	C	-0.512370	-4.596172	0.545799
H	-2.750517	-6.134870	4.726145	O	0.638413	-5.466685	0.679083
H	0.818724	-2.947420	-0.426493	C	-0.936950	-4.137884	1.941363
O	-3.815511	-4.385620	-1.892977	O	-1.701721	-5.099203	2.654442
C	-2.819128	-4.165313	-0.867852	C	-3.992723	-5.107002	-0.148804
C	-3.203072	-5.050076	0.327512	C	-4.990612	-4.755379	-1.255397
C	-4.598567	-4.668920	0.831238	O	-4.474999	-5.212850	-2.502560
C	-5.614161	-4.726668	-0.304557	C	-5.265931	-3.255846	-1.280067
C	-5.108702	-3.943569	-1.525152	O	-6.285208	-3.040216	-2.239410
H	-2.851296	-3.117384	-0.549174	C	-5.653985	-2.734329	0.111812
H	-3.196347	-6.104673	0.021660	O	-5.650205	-1.306177	0.009874
H	-4.546629	-3.631950	1.197344	C	-4.625758	-3.204579	1.155658
H	-5.726545	-5.776227	-0.611943	O	-4.490313	-4.634830	1.087321
H	-5.746716	-4.139506	-2.392722	C	-4.977287	-2.887500	2.595987
C	-1.437717	-4.420928	-1.495483	O	-3.827938	-3.213621	3.388659
O	-5.043342	-5.540324	1.858627	C	-6.779671	-0.563138	0.417005
O	-6.877533	-4.189358	0.077611	C	-7.259045	0.309197	-0.751138
O	-5.108193	-2.574088	-1.206934	O	-7.569911	-0.528110	-1.864770
H	-0.880528	-5.161206	-0.920147	C	-6.201240	1.341832	-1.116650
O	-0.621660	-3.250333	-1.521348	O	-6.754539	2.176377	-2.122301
H	-1.593239	-4.815517	-2.507842	C	-5.775554	2.135239	0.116075
H	-4.348345	-5.566515	2.543851	O	-4.639293	2.901905	-0.296100
H	-7.103858	-4.586707	0.931683	C	-5.405662	1.205005	1.285200
H	-1.084408	-2.548104	-2.029612	O	-6.473641	0.261712	1.521994
O	-5.025118	0.165859	-3.663668	C	-5.152991	1.949230	2.585397
C	-4.427985	-0.792963	-2.760619	O	-6.269450	2.787840	2.873936
C	-5.571272	-1.641299	-2.183558	C	-4.539399	4.258616	0.081836
C	-6.566830	-0.741061	-1.445508	C	-4.445330	5.123753	-1.185408
C	-7.056998	0.377360	-2.358606	O	-5.557328	4.832513	-2.031999
C	-5.872686	1.098179	-3.018876	C	-3.125135	4.884234	-1.909761
H	-3.939357	-0.260570	-1.936730	O	-3.062418	5.808890	-2.986157
H	-6.084290	-2.168953	-2.998600	C	-1.948582	5.028150	-0.941832
H	-6.035706	-0.287017	-0.594697	O	-0.760059	4.697497	-1.667576
H	-7.655848	-0.073702	-3.162674	C	-2.155017	4.088542	0.252121
H	-6.228309	1.768135	-3.808049	O	-3.398509	4.469677	0.889856
C	-3.341043	-1.551338	-3.541826	C	-1.047513	4.094982	1.302655

O	-7.700685	-1.466572	-0.998025	O	-0.543224	5.383244	1.621579
O	-7.830787	1.344852	-1.654561	H	-0.326543	6.713598	-1.782501
O	-5.180882	1.818692	-2.029273	H	1.293869	6.493721	-3.566163
H	-3.507379	-2.628217	-3.496180	H	-0.119955	5.356031	-5.131849
O	-2.032840	-1.336253	-3.009477	H	0.868894	3.485416	-3.410615
H	-3.394791	-1.236122	-4.591423	H	2.719920	3.674593	-4.918837
H	-7.377388	-2.233580	-0.487641	H	3.376257	5.032506	-2.632619
H	-8.476334	0.854832	-1.123858	H	1.273940	3.635674	-0.896855
H	-1.840173	-0.372071	-2.998179	H	3.549175	5.416995	0.048292
O	-2.860252	4.594733	-2.692422	H	3.580194	3.637266	0.091906
C	-3.194714	3.210558	-2.442073	H	2.627675	4.388363	2.122520
C	-4.724625	3.136069	-2.336962	H	5.072069	3.736728	-2.620088
C	-5.202861	4.018239	-1.178847	H	5.997818	1.943085	-3.982120
C	-4.681165	5.443389	-1.337072	H	4.466607	2.097086	-5.800476
C	-3.168588	5.446363	-1.604214	H	3.257457	0.618914	-3.853472
H	-2.767158	2.903026	-1.481176	H	4.532288	-1.040688	-4.947091
H	-5.174246	3.483026	-3.276642	H	5.892139	-0.208356	-2.548942
H	-4.787949	3.598351	-0.249450	H	3.310288	0.891114	-1.334991
H	-5.168667	5.889671	-2.215699	H	4.021522	-0.480967	0.360525
H	-2.837665	6.445091	-1.906203	H	4.889334	1.012122	0.712592
C	-2.528970	2.360864	-3.537312	H	5.886659	-1.428194	-0.198317
O	-6.618518	4.078602	-1.111887	H	6.035911	-2.268732	-2.629079
O	-4.929716	6.237632	-0.180732	H	5.160596	-4.431694	-3.357792
O	-2.507548	5.035313	-0.433975	H	3.994639	-3.591501	-5.285466
H	-3.267912	1.768500	-4.078459	H	2.400260	-3.166806	-3.117555
O	-1.593747	1.425269	-2.997073	H	1.938363	-5.525882	-3.550000
H	-2.041200	3.039777	-4.247705	H	3.586492	-5.438238	-1.475037
H	-6.952266	3.161265	-1.094368	H	3.032939	-2.568013	-0.589923
H	-5.860584	6.107697	0.053838	H	2.847577	-4.092052	1.231709
H	-0.893557	1.912632	-2.507310	H	4.381743	-3.207120	1.393847
O	1.062092	5.587942	0.272103	H	4.568560	-5.551973	1.673170
C	-0.061579	4.823663	-0.223250	H	2.105152	-6.439620	-0.291805
C	-1.307107	5.707335	-0.051738	H	0.003641	-7.522063	-0.910018
C	-1.495001	6.052509	1.429527	H	0.119918	-7.171035	-3.260092
C	-0.231604	6.685754	2.002402	H	-0.812487	-4.869152	-2.165491
C	1.002722	5.836747	1.664422	H	-2.736682	-6.063731	-2.537775
H	-0.188413	3.923433	0.388654	H	-1.862614	-6.247270	0.355183
H	-1.186710	6.629534	-0.635378	H	-0.210257	-3.705150	-0.018619
H	-1.683909	5.110141	1.966456	H	-1.492568	-3.201478	1.837038
H	-0.094233	7.667774	1.527698	H	-0.018562	-3.907015	2.498458
H	1.919365	6.383670	1.907020	H	-2.575100	-4.697883	2.809924
O	0.278167	4.370163	-1.653056	H	-3.913224	-6.192488	-0.039734
C	-2.565924	6.962186	1.625139	H	-5.930777	-5.275469	-1.023023
O	-0.298290	6.829535	3.418419	H	-5.023023	-4.819998	-3.198188
O	0.931036	4.636467	2.392028	H	-4.337344	-2.741013	-1.571118
H	-0.511733	4.657454	-2.348059	H	-6.560426	-2.101760	-2.193935
O	0.401245	2.950824	-1.765387	H	-6.656368	-3.098062	0.373002
H	1.205680	4.870234	-1.958554	H	-3.664162	-2.731945	0.920838
H	-3.354083	6.586001	1.189187	H	-5.844528	-3.487414	2.899918
H	-1.155241	7.234522	3.618705	H	-5.232809	-1.825614	2.688721
H	1.121552	2.631855	-1.176549	H	-4.088372	-3.223449	4.319087
O	3.771883	2.383650	3.036541	H	-7.580012	-1.230226	0.752410
C	2.638377	2.867980	2.279856	H	-8.164942	0.835095	-0.419723
C	2.119362	4.124978	2.995882	H	-7.687473	0.061617	-2.625525
C	1.721669	3.782748	4.434522	H	-5.315913	0.809322	-1.496224
C	2.879669	3.116765	5.167727	H	-6.191370	2.972471	-2.200297
C	3.443253	1.950260	4.342980	H	-6.592371	2.796505	0.423452
H	1.844938	2.111711	2.284812	H	-4.490926	0.658050	1.024345
H	2.902598	4.894550	3.002705	H	-4.234723	2.537284	2.466258
H	0.885117	3.068738	4.386473	H	-4.989710	1.210653	3.382617
H	3.684991	3.855995	5.284031	H	-6.034814	3.334772	3.634914
H	4.381823	1.595541	4.780534	H	-5.397920	4.549979	0.694006
C	3.105303	3.061433	0.828243	H	-4.482678	6.176768	-0.872001
O	1.349927	4.940407	5.165502	H	-5.361559	5.256907	-2.882140
O	2.488242	2.614204	6.442521	H	-3.121302	3.851630	-2.289801
H	2.826150	4.050013	0.462429	H	-2.262295	5.608457	-3.509576
O	2.515157	2.131756	-0.082162	H	-1.885705	6.054461	-0.564327
H	4.199933	2.986888	0.812664	H	-2.252266	3.055843	-0.105721
H	0.670043	5.410495	4.646121	H	-0.237757	3.455697	0.939596
H	1.995962	3.322704	6.883351	H	-1.462137	3.619344	2.202838
H	2.660125	1.212482	0.236306	H	0.405490	5.354093	1.386969
C	1.391743	-1.225214	-3.900666	C	-0.982460	-0.941081	4.188542

C	1.689448	0.109151	-3.622612	C	-0.872098	-0.075436	3.100046
C	3.017826	0.494604	-3.449841	C	0.251780	0.740338	2.982035
C	4.072585	-0.424828	-3.551201	C	1.278927	0.722709	3.936865
C	3.771805	-1.765884	-3.859089	C	1.177303	-0.166340	5.023828
C	2.433035	-2.144731	-4.025281	C	0.045627	-0.986284	5.130668
C	4.876984	-2.771307	-4.123413	C	2.325416	-0.328478	6.002457
C	5.726682	-2.298668	-5.279653	C	3.563451	-0.773318	5.258823
C	5.691227	-2.912548	-6.531742	C	4.067219	-2.069964	5.363872
C	6.485091	-2.450921	-7.586343	C	5.206389	-2.463666	4.654889
C	7.319558	-1.353055	-7.383138	C	5.844037	-1.544574	3.822888
C	7.356286	-0.716885	-6.139494	C	5.345869	-0.244743	3.696668
C	6.562562	-1.176704	-5.077224	C	4.202784	0.154945	4.405427
C	5.465015	0.109478	-3.224780	C	2.389196	1.753275	3.745921
N	6.629260	-0.627406	-3.770136	N	3.701670	1.484154	4.376379
C	5.625108	0.193157	-1.690585	C	1.890369	3.123284	4.251175
C	7.874068	0.057181	-3.414731	C	4.656232	2.534754	4.016669
C	8.014900	0.137647	-1.898304	C	4.159465	3.894527	4.498927
N	6.877607	0.847824	-1.319845	N	2.842033	4.194947	3.924868
C	7.008042	0.982174	0.125594	C	2.336156	5.499127	4.368762
H	0.360090	-1.542350	-4.019785	H	-1.849175	-1.588534	4.283445
H	0.896617	0.845079	-3.542731	H	-1.650407	-0.038739	2.343494
H	3.242119	1.533093	-3.219481	H	0.337670	1.409367	2.130086
H	2.210044	-3.181373	-4.265111	H	-0.020751	-1.677864	5.966637
H	4.441370	-3.749247	-4.345455	H	2.057805	-1.060772	6.768718
H	5.512713	-2.878251	-3.235703	H	2.533651	0.624320	6.504729
H	5.045508	-3.775081	-6.677064	H	3.568562	-2.776350	6.022763
H	6.453581	-2.948304	-8.551078	H	5.591350	-3.473648	4.758150
H	7.942124	-0.981148	-8.192015	H	6.728727	-1.832289	3.262360
H	8.003772	0.142109	-6.000970	H	5.850840	0.451211	3.036662
H	5.505067	1.147513	-3.601680	H	2.540140	1.857731	2.656167
H	5.554418	-0.832697	-1.278238	H	1.715957	3.059497	5.339189
H	4.791687	0.768272	-1.276138	H	0.937072	3.358477	3.771069
H	7.917526	1.078826	-3.831543	H	4.827288	2.583085	2.926418
H	8.713228	-0.509808	-3.825444	H	5.613963	2.317152	4.495293
H	8.935082	0.678091	-1.648685	H	4.864154	4.672728	4.188516
H	8.108421	-0.887799	-1.490330	H	4.115572	3.895757	5.601710
H	7.033425	0.009055	0.651211	H	2.186209	5.540815	5.459522
H	6.166996	1.557890	0.524315	H	1.381609	5.701409	3.874785
H	7.932302	1.518227	0.364128	H	3.047379	6.280358	4.086550
NR2				NR2			
E	-5082.94134197			E	-5082.91964695		
O	-5.643198	-1.238765	2.057471	C	0.264440	-6.334210	-0.291880
C	-4.948273	-0.078572	1.544225	C	-0.621718	-6.714314	-1.481297
C	-5.990445	0.778264	0.809852	O	0.200719	-6.881945	-2.633200
C	-6.621047	-0.029893	-0.328461	C	-1.692866	-5.656561	-1.712461
C	-7.191821	-1.342827	0.196049	O	-2.522034	-6.128436	-2.758905
C	-6.150079	-2.086927	1.044221	C	-2.479405	-5.379957	-0.426329
H	-4.189591	-0.398943	0.821314	O	-3.284820	-4.229421	-0.702951
H	-6.770592	1.093326	1.515465	C	-1.520919	-5.090118	0.743464
H	-5.823265	-0.262750	-1.050550	O	-0.547500	-6.152040	0.858362
H	-8.042883	-1.109644	0.851837	C	-2.210558	-4.988759	2.090648
H	-6.616356	-2.927471	1.567849	O	-1.258303	-4.479086	3.024392
C	-4.218427	0.589048	2.722784	C	-4.673015	-4.257652	-0.450338
O	-5.403705	1.918425	0.182156	C	-5.425727	-3.888873	-1.738373
O	-7.673783	0.682321	-0.958650	O	-5.034588	-4.778683	-2.782435
O	-7.606839	-2.206669	-0.858566	C	-5.170297	-2.435208	-2.121874
O	-5.123967	-2.537284	0.195073	O	-5.997189	-2.147273	-3.237563
H	-4.486546	1.643582	2.797228	C	-5.465395	-1.528685	-0.928645
O	-2.798669	0.556042	2.580915	O	-5.116574	-0.193836	-1.312345
H	-4.534535	0.086573	3.646026	C	-4.660546	-1.978300	0.295191
H	-7.324923	1.557365	-1.215196	O	-5.020121	-3.351842	0.579881
H	-8.142348	-1.672016	-1.463494	C	-4.910631	-1.138247	1.554351
H	-2.503955	-0.379323	2.519582	O	-6.239241	-0.650035	1.691568
O	-2.722432	-5.199683	1.029927	C	-6.114132	0.795718	-1.264603
C	-3.178605	-3.828687	0.968518	C	-6.074406	1.609309	-2.559428
C	-4.599875	-3.851413	0.386341	O	-6.266071	0.719861	-3.657331
C	-4.582521	-4.486083	-1.007368	C	-4.759606	2.368342	-2.675624
C	-3.933733	-5.865065	-0.961067	O	-4.844123	3.170991	-3.840800
C	-2.578285	-5.803943	-0.241461	C	-4.508212	3.198496	-1.416635
H	-2.533761	-3.260574	0.288460	O	-3.163039	3.675120	-1.523726
H	-5.258828	-4.430136	1.047157	C	-4.659494	2.354207	-0.137302
H	-3.975320	-3.838928	-1.658935	O	-5.930794	1.656624	-0.147548

H	-4.584799	-6.531641	-0.377659	C	-4.594143	3.181857	1.134785
H	-2.205555	-6.814729	-0.047788	O	-5.551054	4.234642	1.060838
C	-3.025946	-3.226501	2.375152	C	-2.877196	5.034190	-1.259426
O	-5.891715	-4.637321	-1.532387	C	-2.288941	5.676470	-2.524766
O	-3.722824	-6.402631	-2.263844	O	-3.199154	5.504797	-3.611091
O	-1.676246	-5.086847	-1.047010	C	-0.929986	5.068976	-2.850229
H	-3.968424	-2.801327	2.721663	O	-0.408714	5.784385	-3.960989
O	-2.079668	-2.157146	2.415459	C	-0.015843	5.135502	-1.626720
H	-2.736686	-4.033056	3.060424	O	1.200391	4.456058	-1.956313
H	-6.335342	-3.769766	-1.471453	C	-0.695533	4.472411	-0.423544
H	-4.552114	-6.289457	-2.751684	O	-1.954566	5.152951	-0.195343
H	-1.210189	-2.476573	2.086153	C	0.118080	4.515552	0.873016
O	1.989521	-5.200949	-0.746210	O	0.845476	5.721765	1.064224
C	0.677640	-4.653833	-0.479877	C	2.354899	5.241136	-2.129861
C	-0.339514	-5.571555	-1.175041	C	3.114284	4.765110	-3.371115
C	-0.060325	-5.612821	-2.680744	O	2.248833	4.836545	-4.501043
C	1.385080	-6.019542	-2.946006	C	3.649864	3.351144	-3.170342
C	2.350774	-5.162959	-2.114491	O	4.429097	3.045427	-4.312304
H	0.604541	-3.653614	-0.921752	C	4.448908	3.237125	-1.863838
H	-0.262384	-6.584291	-0.757990	O	4.686058	1.839160	-1.656932
H	-0.213016	-4.596339	-3.075056	C	3.632185	3.815674	-0.695847
H	1.511984	-7.063287	-2.624725	O	3.213546	5.156242	-1.008816
H	3.363501	-5.575391	-2.163143	C	4.373174	3.906119	0.623101
C	0.537787	-4.507393	1.045543	O	3.400449	4.247625	1.618502
O	-0.901452	-6.540100	-3.347597	C	6.005125	1.371671	-1.456352
O	1.737194	-5.882988	-4.319938	C	6.346725	0.325853	-2.524777
O	2.323748	-3.849266	-2.614035	O	6.201122	0.903361	-3.821791
H	-0.340472	-5.042055	1.409843	C	5.467488	-0.908856	-2.374578
O	0.364170	-3.148384	1.452937	O	5.910016	-1.846044	-3.342158
H	1.428638	-4.946189	1.511684	C	5.555702	-1.450930	-0.949696
H	-1.824305	-6.326770	-3.110304	O	4.552624	-2.467828	-0.837739
H	1.026312	-6.295418	-4.832926	C	5.297456	-0.339352	0.083648
H	1.120180	-2.611084	1.126209	O	6.153749	0.794956	-0.176458
O	4.922208	-1.318805	-2.003051	C	5.551407	-0.787674	1.512826
C	3.670801	-1.990085	-1.729657	O	6.865034	-1.331871	1.611630
C	3.556394	-3.139913	-2.740981	C	4.899377	-3.726531	-0.296662
C	3.559568	-2.575058	-4.165246	C	4.628393	-4.818125	-1.343428
C	4.785387	-1.695742	-4.393338	O	5.344239	-4.516004	-2.540808
C	4.939044	-0.669231	-3.261178	C	3.134206	-4.948871	-1.614237
H	2.841965	-1.294495	-1.901370	O	2.967382	-6.045435	-2.499419
H	4.403613	-3.826474	-2.613054	C	2.386412	-5.143098	-0.297333
H	2.659992	-1.949878	-4.275037	O	0.985763	-5.168288	-0.600231
H	5.676483	-2.339456	-4.374588	C	2.718805	-4.011564	0.681735
H	5.912448	-0.172814	-3.326438	O	4.155183	-3.998473	0.874185
C	3.648493	-2.371417	-0.240559	C	2.051167	-4.159698	2.056798
O	3.574889	-3.604554	-5.141122	O	1.872479	-5.506305	2.482417
O	4.715796	-0.988339	-5.628212	H	0.941508	-7.156282	-0.042182
O	3.894591	0.265781	-3.364963	H	-1.116351	-7.663927	-1.232992
H	3.496067	-3.444104	-0.115440	H	-0.394007	-6.890803	-3.398760
O	2.572593	-1.738203	0.457136	H	-1.194546	-4.717955	-1.999249
H	4.611579	-2.103604	0.209678	H	-3.280359	-5.516120	-2.851192
H	2.836360	-4.211017	-4.941120	H	-3.113459	-6.245544	-0.193524
H	4.473661	-1.634992	-6.307676	H	-1.002524	-4.146437	0.536612
H	2.714699	-0.765500	0.444861	H	-2.563742	-5.986220	2.386357
O	3.865406	3.578441	-1.756271	H	-3.079016	-4.325142	1.999602
C	3.599350	2.158169	-1.816580	H	-1.635911	-4.554781	3.910603
C	4.180011	1.647200	-3.144836	H	-4.981218	-5.246511	-0.096706
C	3.523285	2.381696	-4.317554	H	-6.499331	-4.007027	-1.535438
C	3.657737	3.890815	-4.150707	H	-5.380841	-4.400171	-3.605516
C	3.193424	4.325139	-2.752674	H	-4.107485	-2.321873	-2.384506
H	2.516393	1.989380	-1.822032	H	-5.899798	-1.199031	-3.454744
H	5.264611	1.817606	-3.162298	H	-6.531070	-1.580724	-0.679687
H	2.452402	2.126465	-4.310340	H	-3.588186	-1.939299	0.068467
H	4.721598	4.153464	-4.239274	H	-4.187632	-0.315511	1.569880
H	3.464349	5.370003	-2.571427	H	-4.696060	-1.774705	2.418925
C	4.171126	1.528606	-0.536246	H	-6.263621	0.221175	1.260079
O	4.114133	2.024060	-5.556875	H	-7.102271	0.346586	-1.127055
O	2.893596	4.607367	-5.116763	H	-6.896595	2.337280	-2.518994
O	1.801087	4.150376	-2.667849	H	-6.033142	1.213960	-4.458009
H	4.810444	0.678454	-0.775180	H	-3.943047	1.635494	-2.763186
O	3.158277	1.019634	0.335144	H	-4.126942	3.836681	-3.809983
H	4.780619	2.286876	-0.028585	H	-5.211988	4.036636	-1.385342

H	4.103278	1.049879	-5.616431	H	-3.847045	1.618181	-0.108999
H	3.090979	4.212595	-5.979162	H	-3.573900	3.574688	1.226265
H	2.520093	1.735111	0.558272	H	-4.784607	2.524970	1.995358
O	-0.377008	5.798296	-0.200347	H	-5.408924	4.812751	1.821808
C	0.455291	4.720653	-0.687730	H	-3.779975	5.558835	-0.933095
C	1.020228	5.170213	-2.043720	H	-2.153828	6.748185	-2.321965
C	-0.126152	5.459252	-3.017676	H	-2.702310	5.744254	-4.409758
C	-1.101057	6.464865	-2.414808	H	-1.075467	4.009652	-3.108117
C	-1.519627	6.034790	-1.001468	H	0.412447	5.340053	-4.249854
H	-0.160482	3.827778	-0.843934	H	0.195379	6.178163	-1.366814
H	1.623430	6.077314	-1.905526	H	-0.906931	3.420072	-0.650031
H	-0.663928	4.513690	-3.187482	H	0.790826	3.654316	0.883595
H	-0.585114	7.431434	-2.324243	H	-0.591594	4.381979	1.700712
H	-2.066601	6.842513	-0.504937	H	1.787524	5.485785	1.013161
C	1.483954	4.394693	0.409377	H	2.094310	6.299364	-2.223571
O	0.346587	5.993817	-4.243695	H	3.968845	5.442420	-3.509901
O	-2.278556	6.610084	-3.204164	H	2.675561	4.339726	-5.215241
O	-2.318458	4.882591	-1.104066	H	2.791080	2.667442	-3.086027
H	2.501164	4.461399	0.021175	H	4.880870	2.189702	-4.161071
O	1.346683	3.067504	0.915155	H	5.399516	3.776060	-1.968555
H	1.371141	5.135719	1.210995	H	2.747973	3.182369	-0.555319
H	1.038509	5.393119	-4.581110	H	5.150808	4.677535	0.553249
H	-1.988478	6.726296	-4.121163	H	4.848299	2.943830	0.846193
H	0.444153	2.951326	1.286263	H	3.863194	4.490848	2.431340
O	-4.589982	3.647353	1.513262	H	6.715424	2.203770	-1.492979
C	-3.330918	3.705356	0.803748	H	7.393612	0.030202	-2.369960
C	-3.481422	4.781270	-0.282126	H	6.230976	0.164720	-4.450027
C	-4.622956	4.405414	-1.231926	H	4.422615	-0.617517	-2.562102
C	-5.910981	4.162913	-0.452410	H	5.521520	-2.719006	-3.128557
C	-5.665707	3.193335	0.712902	H	6.550499	-1.877169	-0.783193
H	-3.143306	2.741764	0.316989	H	4.248418	-0.027715	0.011031
H	-3.697111	5.749161	0.189360	H	4.790915	-1.534334	1.772134
H	-4.340477	3.468049	-1.735531	H	5.425971	0.079137	2.177093
H	-6.236000	5.120192	-0.020359	H	6.952305	-1.726672	2.488978
H	-6.536675	3.166354	1.375435	H	5.949062	-3.732741	0.011590
C	-2.216570	3.927300	1.841378	H	4.989597	-5.770033	-0.929502
O	-4.876165	5.427345	-2.182717	H	4.995866	-5.116695	-3.218400
O	-6.941121	3.620787	-1.274338	H	2.778334	-4.016713	-2.078480
H	-1.628558	4.812534	1.595361	H	2.010596	-6.168148	-2.658362
O	-1.290152	2.842877	1.890791	H	2.685054	-6.091397	0.161901
H	-2.689382	4.087996	2.818753	H	2.416240	-3.047280	0.255623
H	-4.030346	5.637170	-2.623141	H	1.092778	-3.633940	2.043079
H	-6.970564	4.160805	-2.078151	H	2.694772	-3.651303	2.784143
H	-1.768627	2.021771	2.140603	H	0.955647	-5.741874	2.260300
C	4.130785	4.086395	5.323137	C	-3.952439	0.883622	5.026011
C	4.344346	3.757710	3.984628	C	-3.524842	2.194553	5.237945
C	4.251733	2.425988	3.582245	C	-2.163717	2.490206	5.173992
C	3.956741	1.399051	4.491779	C	-1.204554	1.502581	4.902370
C	3.709373	1.737528	5.836974	C	-1.641353	0.184868	4.662601
C	3.802695	3.079243	6.230312	C	-3.010716	-0.102786	4.733535
C	3.222793	0.696172	6.828848	C	-0.670840	-0.891969	4.214653
C	1.934672	0.087050	6.325427	C	0.006707	-0.458867	2.935809
C	0.696369	0.370712	6.902051	C	-0.291376	-1.039589	1.702177
C	-0.480943	-0.186263	6.392634	C	0.348691	-0.619615	0.531559
C	-0.415514	-1.034146	5.287670	C	1.295072	0.402706	0.600448
C	0.816618	-1.325219	4.695182	C	1.593083	1.007785	1.825640
C	1.999944	-0.766888	5.201386	C	0.949327	0.590826	3.001658
C	4.015535	-0.023192	3.936695	C	0.255274	1.946852	4.981016
N	3.287603	-1.074951	4.685057	N	1.264120	1.116822	4.282383
C	5.495809	-0.450622	3.827365	C	0.663673	2.051270	6.466873
C	3.415394	-2.367398	4.002780	C	2.599412	1.704002	4.426737
C	4.884383	-2.766573	3.907798	C	2.977519	1.806341	5.900500
N	5.637344	-1.750493	3.175052	N	1.999537	2.620087	6.616782
C	7.040011	-2.120534	3.023223	C	2.356548	2.790408	8.020141
H	4.198591	5.118036	5.655931	H	-5.007864	0.632071	5.071990
H	4.575266	4.529681	3.256541	H	-4.241659	2.981934	5.450626
H	4.397953	2.169687	2.536433	H	-1.833620	3.512749	5.341354
H	3.603214	3.334420	7.267977	H	-3.339408	-1.121642	4.547308
H	3.069400	1.161490	7.806413	H	-1.200419	-1.835610	4.059185
H	3.970948	-0.097375	6.944311	H	0.095055	-1.054639	4.982911
H	0.655526	1.028124	7.767167	H	-1.016134	-1.848134	1.667644
H	-1.436205	0.042184	6.856199	H	0.111257	-1.088104	-0.418754

H	-1.316963	-1.459881	4.857808	H	1.800374	0.741554	-0.299789
H	0.845726	-1.980411	3.830636	H	2.314691	1.816858	1.860272
H	3.621023	0.017514	2.906882	H	0.301152	2.971302	4.569117
H	5.934780	-0.449340	4.844734	H	0.585846	1.043460	6.920670
H	6.035764	0.295372	3.235965	H	-0.050434	2.699866	6.983605
H	2.987829	-2.342156	2.987896	H	2.661162	2.706283	3.969446
H	2.873453	-3.118463	4.583962	H	3.317205	1.058205	3.914105
H	4.967037	-3.721017	3.375799	H	3.963620	2.276254	5.987906
H	5.288422	-2.915717	4.928188	H	3.053935	0.787005	6.326808
H	7.567054	-2.223900	3.990146	H	2.392800	1.835926	8.577761
H	7.562193	-1.360805	2.433237	H	1.626704	3.441421	8.511697
H	7.113720	-3.075890	2.494292	H	3.341329	3.262507	8.094658
M2				M2			
E	-5082.94460038			E	-5082.92045830		
O	-4.873173	1.353033	-3.618664	C	1.227718	6.101450	-0.621565
C	-4.465587	0.192519	-2.858699	C	2.121732	6.151515	-1.861825
C	-5.748725	-0.550900	-2.457413	O	1.312157	6.409283	-3.006094
C	-6.632016	0.366325	-1.605375	C	2.900393	4.851035	-2.017550
C	-6.913996	1.668184	-2.347224	O	3.765723	5.026605	-3.124095
C	-5.607669	2.294023	-2.857205	C	3.655978	4.497721	-0.729809
H	-3.949619	0.517742	-1.948089	O	4.129544	3.155553	-0.900703
H	-6.292439	-0.851346	-3.362648	C	2.717213	4.572194	0.489676
H	-6.076304	0.603329	-0.685210	O	2.032098	5.842001	0.517385
H	-7.531959	1.435607	-3.226373	C	3.430015	4.449079	1.823112
H	-5.823634	3.121582	-3.540144	O	2.426088	4.349842	2.835653
C	-3.455521	-0.594313	-3.711768	C	5.497371	2.853134	-0.707057
O	-5.470301	-1.692256	-1.647615	C	6.080410	2.263489	-2.000838
O	-7.878350	-0.235747	-1.295674	O	5.894234	3.184197	-3.074455
O	-7.575792	2.623294	-1.522650	C	5.442884	0.915997	-2.315736
O	-4.866481	2.742372	-1.749989	O	6.107113	0.399292	-3.457321
H	-3.805104	-1.613683	-3.884345	C	5.563781	-0.003695	-1.103927
O	-2.182509	-0.718930	-3.074575	O	4.846826	-1.206689	-1.404374
H	-3.364818	-0.092216	-4.683183	C	4.982113	0.666872	0.145088
H	-7.695287	-1.087526	-0.854464	O	5.665381	1.927086	0.348875
H	-8.298820	2.155176	-1.078913	C	5.122369	-0.179332	1.419496
H	-1.807660	0.173091	-2.918882	O	6.296842	-0.980418	1.473224
O	-2.145336	5.210159	-1.887592	C	5.556064	-2.420587	-1.420812
C	-2.680618	3.866922	-1.853896	C	5.187324	-3.199323	-2.684781
C	-4.209967	4.006835	-1.837254	O	5.504207	-2.398482	-3.821231
C	-4.641831	4.784453	-0.589652	C	3.714489	-3.585499	-2.665504
C	-3.922284	6.127461	-0.516994	O	3.479188	-4.374655	-3.818840
C	-2.408785	5.948369	-0.707784	C	3.379914	-4.328519	-1.372351
H	-2.364800	3.371587	-0.928773	O	1.953563	-4.450932	-1.339767
H	-4.536967	4.541705	-2.738612	C	3.862564	-3.555231	-0.130158
H	-4.352204	4.187638	0.289079	O	5.261750	-3.201233	-0.269721
H	-4.284643	6.754142	-1.344554	C	3.713096	-4.348067	1.157324
H	-1.926062	6.920104	-0.852388	O	4.350513	-5.613062	1.006311
C	-2.070904	3.082730	-3.028519	C	1.370077	-5.701263	-1.028905
O	-6.036959	5.040262	-0.582845	C	0.529112	-6.177718	-2.223430
O	-4.139378	6.784547	0.728405	O	1.349444	-6.219158	-3.390776
O	-1.890571	5.298330	0.424882	C	-0.680113	-5.273493	-2.433062
H	-2.855493	2.640751	-3.644198	O	-1.457323	-5.853897	-3.468383
O	-1.253320	1.993247	-2.595107	C	-1.457182	-5.138920	-1.125794
H	-1.499951	3.784175	-3.649846	O	-2.526685	-4.213584	-1.356275
H	-6.495555	4.186425	-0.702309	C	-0.535030	-4.650905	-0.003081
H	-5.093313	6.756056	0.895297	O	0.552012	-5.601130	0.119473
H	-0.482143	2.346022	-2.103317	C	-1.224320	-4.527842	1.363224
O	1.669758	5.322240	1.354774	O	-2.244790	-5.492074	1.594377
C	0.509066	4.787455	0.676268	C	-3.844086	-4.674191	-1.189134
C	-0.651075	5.749436	0.972348	C	-4.697781	-4.220669	-2.376239
C	-0.889896	5.814826	2.484589	O	-4.108613	-4.702275	-3.581080
C	0.392691	6.173930	3.228852	C	-4.834079	-2.703423	-2.395164
C	1.560940	5.290072	2.766201	O	-5.702246	-2.385412	-3.467226
H	0.259215	3.806602	1.096152	C	-5.345983	-2.184197	-1.046210
H	-0.409533	6.750098	0.590327	O	-5.225470	-0.757693	-1.079164
H	-1.207561	4.811906	2.809789	C	-4.484665	-2.741651	0.100722
H	0.651791	7.213205	2.980271	O	-4.415095	-4.183141	0.014697
H	2.509238	5.682606	3.147311	C	-5.012075	-2.412539	1.484015
C	0.880106	4.573389	-0.800213	O	-3.986151	-2.742032	2.418582
O	-1.872841	6.782346	2.818019	C	-6.375292	0.049548	-0.934929
O	0.253148	6.022892	4.638319	C	-6.451281	1.035112	-2.107439
O	1.341368	3.982330	3.230113	O	-6.503270	0.312384	-3.336682

H	0.113326	4.992698	-1.451931	C	-5.264726	1.990745	-2.081211
O	0.976238	3.190331	-1.146830	O	-5.453983	2.913979	-3.141059
H	1.824382	5.097259	-0.996796	C	-5.170249	2.677296	-0.720550
H	-2.654887	6.607931	2.260805	O	-3.921625	3.379599	-0.707785
H	-0.559019	6.487542	4.889028	C	-5.212956	1.654096	0.428809
H	1.711397	2.786682	-0.632768	O	-6.347146	0.773846	0.278466
O	3.950926	1.375031	3.389861	C	-5.313659	2.304377	1.798669
C	2.964928	2.198619	2.726891	O	-6.422090	3.200568	1.814747
C	2.441332	3.227224	3.742057	C	-3.891736	4.718262	-0.252826
C	1.870132	2.512588	4.968486	C	-3.408709	5.629446	-1.392011
C	2.891095	1.548208	5.556096	O	-4.237970	5.432228	-2.537053
C	3.441312	0.615286	4.465856	C	-1.944048	5.363986	-1.720704
H	2.122419	1.574137	2.408247	O	-1.556310	6.326804	-2.688288
H	3.252768	3.899899	4.050560	C	-1.106510	5.444155	-0.446054
H	0.997148	1.930645	4.635519	O	0.243197	5.112781	-0.794153
H	3.737988	2.131703	5.944132	C	-1.657845	4.482629	0.611820
H	4.291675	0.045875	4.853778	O	-3.036119	4.853484	0.863668
C	3.638030	2.773904	1.472998	C	-0.897769	4.511399	1.943333
O	1.498406	3.434303	5.982073	O	-0.401398	5.793381	2.309474
O	2.332018	0.751193	6.597273	H	0.770321	7.078223	-0.439028
O	2.417869	-0.252559	4.039029	H	2.838172	6.972347	-1.717339
H	3.409361	3.832941	1.358382	H	1.857763	6.208355	-3.781834
O	3.188895	2.142345	0.271892	H	2.179889	4.040773	-2.206667
H	4.723567	2.662652	1.590636	H	4.369237	4.256691	-3.173514
H	0.932706	4.109494	5.563564	H	4.499963	5.188287	-0.603415
H	1.836859	1.349029	7.176939	H	1.978687	3.766252	0.405155
H	3.200806	1.162562	0.407434	H	4.058896	5.335672	1.977030
O	2.811319	-3.530821	2.396605	H	4.073394	3.560868	1.808887
C	2.583935	-2.101274	2.432406	H	2.838901	4.530631	3.690372
C	2.723379	-1.640888	3.892971	H	6.050682	3.749735	-0.410952
C	1.750377	-2.401390	4.792244	H	7.155342	2.108339	-1.833247
C	1.965047	-3.899585	4.629331	H	6.089421	2.690490	-3.886744
C	1.893245	-4.301067	3.148119	H	4.373863	1.072441	-2.524147
H	1.572646	-1.881912	2.071957	H	5.735947	-0.483674	-3.654920
H	3.750626	-1.836285	4.228773	H	6.618815	-0.231694	-0.916895
H	0.726107	-2.154656	4.473565	H	3.917094	0.871585	-0.013737
H	2.974372	-4.145363	4.988319	H	4.224630	-0.798811	1.521572
H	2.208753	-5.341232	3.020984	H	5.141684	0.505527	2.273231
C	3.588214	-1.452318	1.458141	H	6.070128	-1.838642	1.076904
O	1.937650	-2.098465	6.164915	H	6.634873	-2.242278	-1.384129
O	0.999720	-4.646473	5.367340	H	5.789741	-4.118242	-2.696046
O	0.575248	-4.122426	2.678067	H	5.068806	-2.812429	-4.581944
H	4.357708	-0.906582	2.012472	H	3.112393	-2.664396	-2.691500
O	2.951572	-0.537840	0.570433	H	2.623900	-4.838116	-3.708605
H	4.079731	-2.258391	0.902328	H	3.849310	-5.317430	-1.389447
H	1.869664	-1.129667	6.276334	H	3.267821	-2.638106	-0.039534
H	0.948054	-4.229267	6.241572	H	2.640661	-4.462449	1.358539
H	2.897103	-0.902480	-0.360918	H	4.157347	-3.770491	1.980244
O	-1.165876	-6.118117	0.105339	H	4.148734	-6.138348	1.791598
C	-0.291745	-5.079792	0.591793	H	2.144969	-6.431830	-0.779111
C	-0.126623	-5.238054	2.114832	H	0.167895	-7.189302	-1.991029
C	-1.493262	-5.268591	2.810096	H	0.744924	-6.356472	-4.137082
C	-2.422224	-6.282788	2.151091	H	-0.324720	-4.274035	-2.726536
C	-2.474133	-6.056745	0.638104	H	-2.260804	-5.310313	-3.590394
H	-0.746988	-4.102623	0.388045	H	-1.863594	-6.113263	-0.834131
H	0.408798	-6.171589	2.333568	H	-0.112885	-3.672809	-0.265312
H	-1.940312	-4.268967	2.698212	H	-1.626760	-3.516274	1.469183
H	-2.015368	-7.289224	2.322661	H	-0.450072	-4.657080	2.128459
H	-3.034631	-6.857838	0.145680	H	-3.085341	-5.058022	1.369881
C	1.018835	-5.185586	-0.179140	H	-3.865824	-5.763930	-1.097407
O	-1.394696	-5.627157	4.177386	H	-5.697627	-4.659087	-2.247852
O	-3.747170	-6.197114	2.672283	H	-4.518380	-4.201914	-4.303774
O	-3.075837	-4.806946	0.400755	H	-3.836044	-2.268288	-2.555895
H	1.723496	-4.461447	0.251110	H	-5.822704	-1.413609	-3.489882
O	0.867956	-5.001315	-1.579775	H	-6.395470	-2.477777	-0.913387
H	1.441628	-6.187408	-0.036950	H	-3.474787	-2.326472	0.002803
H	-0.676865	-5.100752	4.584217	H	-5.925452	-2.995222	1.671607
H	-3.663268	-6.146299	3.636426	H	-5.267976	-1.347555	1.520342
H	0.257162	-4.257579	-1.750650	H	-4.238807	-2.408190	3.290231
O	-4.645094	-3.603438	-2.693717	H	-7.277017	-0.569372	-0.891388
C	-3.570326	-3.746096	-1.738354	H	-7.373908	1.619022	-1.984838
C	-4.055769	-4.688510	-0.629416	H	-6.322175	0.954909	-4.040135

C	-5.309087	-4.110431	0.036300	H	-4.344055	1.406774	-2.232520
C	-6.375547	-3.806950	-1.011185	H	-4.857562	3.676518	-2.996093
C	-5.787271	-2.966243	-2.152899	H	-6.003648	3.379046	-0.611482
H	-3.352973	-2.769289	-1.292364	H	-4.290444	1.061019	0.402633
H	-4.284182	-5.674521	-1.055300	H	-4.372105	2.833211	1.992083
H	-5.020322	-3.164786	0.520027	H	-5.427115	1.513080	2.552914
H	-6.713591	-4.758902	-1.445181	H	-6.393252	3.685894	2.649581
H	-6.502477	-2.889637	-2.977842	H	-4.882889	5.022291	0.096214
C	-2.316285	-4.197556	-2.502920	H	-3.500103	6.668523	-1.045507
O	-5.872654	-5.004763	0.981660	H	-3.792736	5.886737	-3.269465
O	-7.482949	-3.099918	-0.459348	H	-1.853892	4.345258	-2.127642
H	-1.956446	-5.162083	-2.139748	H	-0.611867	6.187435	-2.898882
O	-1.225184	-3.294762	-2.332026	H	-1.146763	6.459409	-0.037184
H	-2.582491	-4.304801	-3.562515	H	-1.634510	3.453171	0.234452
H	-5.176433	-5.233451	1.628342	H	-0.085184	3.781375	1.893562
H	-7.720250	-3.551144	0.364577	H	-1.594508	4.173576	2.720094
H	-1.486673	-2.402384	-2.642738	H	0.541386	5.800288	2.073181
C	6.642616	3.500347	-4.123866	C	3.894354	-0.349872	5.720422
C	6.037474	3.426185	-2.869408	C	3.642938	0.907196	5.170077
C	5.530323	2.207655	-2.420601	C	2.515969	1.095739	4.370598
C	5.608218	1.045599	-3.204748	C	1.624118	0.046150	4.098280
C	6.227335	1.119712	-4.467339	C	1.871051	-1.217838	4.667322
C	6.737656	2.349653	-4.904888	C	3.004874	-1.394279	5.472241
C	6.440042	-0.120551	-5.315099	C	0.882633	-2.356998	4.505286
C	7.265348	-1.129925	-4.553964	C	-0.466183	-1.959782	5.056104
C	8.588742	-1.417311	-4.889190	C	-0.981654	-2.509724	6.230439
C	9.330126	-2.355001	-4.164121	C	-2.238118	-2.134882	6.714920
C	8.737866	-3.006914	-3.083863	C	-2.984051	-1.186957	6.015562
C	7.417840	-2.720121	-2.725988	C	-2.475552	-0.613261	4.846589
C	6.669704	-1.780164	-3.450751	C	-1.214778	-0.988797	4.354110
C	4.922334	-0.193680	-2.626058	C	0.495927	0.367299	3.119015
N	5.297125	-1.512903	-3.186398	N	-0.696546	-0.510444	3.121743
C	3.395950	-0.016584	-2.774744	C	1.075815	0.383189	1.687298
C	4.559132	-2.587784	-2.517952	C	-1.685456	-0.027906	2.153906
C	3.057167	-2.392205	-2.681367	C	-1.091314	-0.014495	0.750150
N	2.653968	-1.098649	-2.108885	N	0.095854	0.834263	0.702927
C	1.205893	-0.884597	-2.214077	C	0.668574	0.880176	-0.638297
H	7.045734	4.440717	-4.488251	H	4.765883	-0.513991	6.347279
H	5.961375	4.308552	-2.240863	H	4.314173	1.738495	5.364548
H	5.041948	2.159739	-1.449859	H	2.328169	2.075655	3.937286
H	7.223500	2.397052	-5.876036	H	3.183741	-2.370451	5.915555
H	6.939527	0.153111	-6.248292	H	1.256665	-3.245073	5.021622
H	5.473574	-0.572114	-5.570709	H	0.770076	-2.608184	3.443000
H	9.038182	-0.912069	-5.740389	H	-0.397631	-3.257226	6.761524
H	10.355376	-2.575308	-4.445817	H	-2.628722	-2.582658	7.623629
H	9.299989	-3.738218	-2.510121	H	-3.960395	-0.880314	6.380027
H	6.975864	-3.231110	-1.877786	H	-3.062182	0.134514	4.324228
H	5.135373	-0.199011	-1.541757	H	0.167670	1.399086	3.338560
H	3.146030	0.028370	-3.848507	H	1.452518	-0.633512	1.456783
H	3.101183	0.933352	-2.321739	H	1.928943	1.067048	1.664369
H	4.796339	-2.646167	-1.440680	H	-2.037716	0.989505	2.400073
H	4.847304	-3.539448	-2.971357	H	-2.540521	-0.706770	2.175282
H	2.516589	-3.197758	-2.175046	H	-1.833116	0.374969	0.043856
H	2.799089	-2.434875	-3.753483	H	-0.856601	-1.053934	0.446704
H	0.856216	-0.882723	-3.258189	H	0.998030	-0.112554	-0.998443
H	0.947123	0.076394	-1.761683	H	1.534493	1.548839	-0.653044
H	0.679919	-1.674509	-1.673866	H	-0.074031	1.267031	-1.342866
FA2				FA2			
E	-5082.94134191			E	-5082.93271690		
				ZPE	-5081.371176		
				H	-5081.277347		
				G	-5081.504693		
				S	478.490		
O	1.990859	-5.200739	-0.746230	C	5.854599	3.332457	1.735230
C	0.678915	-4.653711	-0.480013	C	6.945971	2.788244	0.809067
C	-0.338081	-5.571515	-1.175273	O	6.969036	3.572614	-0.380582
C	-0.058791	-5.612677	-2.680958	C	6.708937	1.313061	0.504217
C	1.386686	-6.019206	-2.946132	O	7.825732	0.853974	-0.236913
C	2.352207	-5.162554	-2.114496	C	6.491223	0.497370	1.787419
C	0.605810	-3.653507	-0.921912	O	6.029157	-0.783481	1.345166
H	-0.260827	-6.584266	-0.758279	C	5.437092	1.178255	2.676707
H	-0.211598	-4.596201	-3.075243	O	5.813580	2.546479	2.909232

H	1.513699	-7.062948	-2.624881	C	5.245919	0.556767	4.045991
H	3.365001	-5.574831	-2.163131	O	4.100079	1.185404	4.630260
C	0.538890	-4.507176	1.045390	C	6.607002	-1.966026	1.852613
O	-1.674892	-5.087014	-1.047251	C	7.156173	-2.795949	0.681664
O	-0.899739	-6.540039	-3.347923	O	8.081189	-2.001625	-0.059677
O	1.738888	-5.882543	-4.320034	C	6.022619	-3.297897	-0.205588
O	2.324985	-3.848833	-2.613920	O	6.599308	-4.157629	-1.175335
H	-0.339050	-5.042326	1.409745	C	4.969230	-4.004810	0.644752
O	0.364415	-3.148199	1.452529	O	3.884631	-4.344236	-0.226770
H	1.430000	-4.945326	1.511634	C	4.493385	-3.092125	1.780401
H	-1.822638	-6.326934	-3.110602	O	5.651374	-2.725393	2.568915
H	1.027996	-6.294869	-4.833097	C	3.452964	-3.736952	2.706436
H	1.120437	-2.610666	1.126221	O	3.620777	-5.135138	2.907025
O	4.922706	-1.317707	-2.002543	C	3.519067	-5.695860	-0.348243
C	3.671437	-1.989331	-1.729332	C	3.341779	-6.032810	-1.830053
C	3.557490	-3.139195	-2.740669	O	4.570620	-5.766473	-2.503021
C	3.560767	-2.574371	-4.164942	C	2.191535	-5.231646	-2.424666
C	4.786399	-1.694757	-4.392847	O	2.020940	-5.671531	-3.761640
C	4.939597	-0.668175	-3.260690	C	0.923132	-5.414017	-1.591213
H	2.842434	-1.293969	-1.901159	O	-0.006078	-4.441886	-2.081330
H	4.404845	-3.825560	-2.612582	C	1.181256	-5.175731	-0.091535
H	2.661051	-1.949426	-4.274901	O	2.312545	-5.965358	0.354851
H	5.677654	-2.338246	-4.373920	C	-0.008769	-5.533322	0.782486
H	5.912888	-0.171515	-3.325809	O	-0.424400	-6.864646	0.492039
C	3.649029	-2.370694	-0.240244	C	-1.347155	-4.817043	-2.324804
O	3.576494	-3.603894	-5.140785	C	-1.657281	-4.622849	-3.818070
O	4.716844	-0.987396	-5.627751	O	-0.712272	-5.357893	-4.595613
O	3.894929	0.266567	-3.364702	C	-1.631866	-3.143392	-4.180705
H	3.496700	-3.443402	-0.115183	O	-2.025857	-3.035162	-5.542279
O	2.573015	-1.737602	0.457398	C	-2.544881	-2.356188	-3.240002
H	4.612056	-2.102812	0.210071	O	-2.420031	-0.970931	-3.571366
H	2.837983	-4.210441	-4.940981	C	-2.129952	-2.609556	-1.786125
H	4.475263	-1.634174	-6.307293	O	-2.230422	-4.035252	-1.546152
H	2.714993	-0.764881	0.445070	C	-2.969219	-1.881979	-0.736287
O	3.864786	3.579297	-1.756165	O	-4.363124	-1.890904	-1.008678
C	3.599088	2.158952	-1.816430	C	-3.497801	-0.384963	-4.264509
C	4.179970	1.648072	-3.144615	C	-2.952801	0.547495	-5.348888
C	3.523131	2.382345	-4.317408	O	-2.093163	-0.202208	-6.203762
C	3.657199	3.891503	-4.150632	C	-2.229782	1.736400	-4.724564
C	3.192698	4.325791	-2.752648	O	-1.885793	2.616458	-5.780600
H	2.516175	1.989895	-1.821950	C	-3.089077	2.423080	-3.650683
H	5.264529	1.818757	-3.162028	O	-2.206982	3.329030	-2.976785
H	2.452314	2.126838	-4.310257	C	-3.642889	1.380065	-2.666172
H	4.721004	4.154407	-4.239131	O	-4.333571	0.352369	-3.398819
H	3.463380	5.370728	-2.571449	C	-4.628994	1.898213	-1.635630
C	4.170920	1.529604	-0.536004	O	-4.838712	0.864913	-0.678398
O	4.114145	2.024799	-5.556675	C	-2.566478	4.682479	-2.809996
O	2.892946	4.607818	-5.116777	C	-1.474312	5.570339	-3.419653
O	1.800394	4.150746	-2.667934	O	-1.326666	5.247817	-4.802717
H	4.810559	0.679661	-0.774826	C	-0.159480	5.391974	-2.670863
O	3.158125	1.020338	0.335260	O	0.763187	6.320459	-3.218591
H	4.780085	2.288117	-0.028312	C	-0.360506	5.593857	-1.170402
H	4.103613	1.050612	-5.616155	O	0.861082	5.172905	-0.551810
H	3.090451	4.213016	-5.979136	C	-1.541141	4.759346	-0.641910
H	2.519738	1.735647	0.558351	O	-2.717692	5.004547	-1.442169
O	-0.378115	5.798215	-0.200465	C	-1.891913	5.069884	0.803354
C	0.454397	4.720713	-0.687809	O	-2.095660	6.473396	0.949735
C	1.019296	5.170386	-2.043775	C	1.437049	5.971900	0.460884
C	-0.127125	5.459185	-3.017758	C	2.831638	6.431245	0.005873
C	-1.102235	6.464618	-2.414938	O	2.721261	7.097598	-1.251762
C	-1.520778	6.034457	-1.001622	C	3.785318	5.246122	-0.083693
H	-0.161218	3.827735	-0.844036	O	5.070181	5.764119	-0.400046
H	1.622297	6.077620	-1.905563	C	3.774668	4.463085	1.229454
H	-0.664701	4.513512	-3.187574	O	4.619355	3.320264	1.060175
H	-0.586465	7.431279	-2.324327	C	2.341052	4.041118	1.571251
H	-2.067932	6.842072	-0.505111	O	1.543720	5.246594	1.669680
C	1.483044	4.394923	0.409363	C	2.194441	3.261136	2.877996
O	0.345533	5.993818	-4.243781	O	2.988522	3.769051	3.939630
O	-2.279719	6.609639	-3.204359	H	6.105774	4.344909	2.064615
O	-2.319342	4.882092	-1.104236	H	7.902455	2.883061	1.342340
H	2.500271	4.461828	0.021241	H	7.539030	3.113769	-1.015191
O	1.345961	3.067695	0.915098	H	5.784902	1.231774	-0.088590

H	1.370022	5.135904	1.210991	H	7.761466	-0.119353	-0.316378
H	1.037592	5.393263	-4.581160	H	7.443084	0.398644	2.325262
H	-1.989612	6.725588	-4.121384	H	4.478229	1.145742	2.145635
H	0.443430	2.951338	1.286149	H	6.143845	0.727296	4.654557
O	-4.590733	3.646366	1.512976	H	5.090432	-0.523509	3.940238
C	-3.331658	3.704617	0.803510	H	4.028922	0.903431	5.551684
C	-3.482325	4.780524	-0.282346	H	7.404461	-1.733858	2.565444
C	-4.623749	4.404489	-1.232205	H	7.674136	-3.666485	1.107764
C	-5.911755	4.161712	-0.452742	H	8.265512	-2.493107	-0.875284
C	-5.666342	3.192161	0.712561	H	5.545843	-2.431127	-0.687769
H	-3.143845	2.741068	0.316742	H	5.878618	-4.529325	-1.721440
H	-3.698215	5.748365	0.189155	H	5.395832	-4.912951	1.084822
H	-4.341074	3.467204	-1.735846	H	4.055281	-2.178494	1.361385
H	-6.236977	5.118920	-0.020684	H	2.455772	-3.516780	2.309089
H	-6.537338	3.165009	1.375052	H	3.530940	-3.245082	3.681705
C	-2.217389	3.926763	1.841179	H	3.097706	-5.581084	2.219467
O	-4.877104	5.426416	-2.182958	H	4.273010	-6.346955	0.104126
O	-6.941756	3.619375	-1.274705	H	3.099709	-7.102292	-1.901094
O	-5.404078	1.917322	0.181791	H	4.377290	-5.785123	-3.452562
H	-1.629503	4.812078	1.595149	H	2.462116	-4.165296	-2.395086
O	-1.290801	2.842483	1.890677	H	1.146969	-5.363708	-4.077052
H	-2.690265	4.087423	2.818528	H	0.534070	-6.426752	-1.738225
H	-4.031312	5.636411	-2.623348	H	1.406839	-4.112866	0.055752
H	-6.971518	4.159589	-2.078374	H	-0.807446	-4.810555	0.573962
H	-1.769147	2.021290	2.140438	H	0.284505	-5.425531	1.836367
O	-5.642986	-1.239973	2.057012	H	-1.241857	-7.028881	0.980166
C	-4.948267	-0.079633	1.543818	H	-1.515890	-5.853497	-2.018199
C	-5.990590	0.777017	0.809444	H	-2.669029	-5.011181	-4.001622
C	-6.620966	-0.031236	-0.328926	H	-0.827389	-5.049100	-5.508517
C	-7.191474	-1.344323	0.195494	H	-0.605848	-2.770236	-4.048749
C	-6.149631	-2.088217	1.043721	H	-1.876536	-2.112809	-5.826393
H	-4.189521	-0.399833	0.820902	H	-3.584916	-2.678960	-3.357071
H	-6.770841	1.091898	1.515026	H	-1.085942	-2.305029	-1.639861
H	-5.823102	-0.263878	-1.050993	H	-2.601069	-0.854071	-0.660628
H	-8.042635	-1.111358	0.851233	H	-2.772592	-2.370395	0.228140
H	-6.615770	-2.928875	1.567292	H	-4.641507	-0.952595	-1.066998
C	-4.218539	0.588070	2.722393	H	-4.134000	-1.154856	-4.710838
O	-7.673821	0.680781	-0.959132	H	-3.814913	0.925181	-5.916782
O	-7.606206	-2.208231	-0.859182	H	-1.641930	0.429682	-6.782650
O	-5.123378	-2.538350	0.194621	H	-1.327353	1.358624	-4.219752
H	-4.486730	1.642588	2.796783	H	-1.523450	3.437715	-5.390325
O	-2.798766	0.555148	2.580585	H	-3.908728	2.972426	-4.132081
H	-4.534656	0.085608	3.645638	H	-2.791731	0.940751	-2.132526
H	-7.325135	1.555908	-1.215617	H	-5.565605	2.172160	-2.141901
H	-8.141938	-1.673727	-1.464046	H	-4.217407	2.800378	-1.164360
H	-2.503958	-0.380201	2.519457	H	-5.667484	1.046674	-0.149451
O	-2.721175	-5.200140	1.029625	H	-3.535630	4.886640	-3.276205
C	-3.177795	-3.829291	0.968327	H	-1.800036	6.614462	-3.315827
C	-4.598976	-3.852347	0.385920	H	-0.517440	5.691386	-5.100692
C	-4.581278	-4.486935	-1.007812	H	0.188178	4.359416	-2.826728
C	-3.932204	-5.865768	-0.961461	H	1.520047	6.398936	-2.603267
C	-2.576819	-5.804326	-0.241765	H	-0.546184	6.653875	-0.968393
H	-2.533018	-3.260851	0.288472	H	-1.276148	3.696739	-0.704440
H	-5.257896	-4.431270	1.046600	H	-1.065734	4.720251	1.434904
H	-3.974136	-3.839613	-1.659267	H	-2.794866	4.503457	1.071401
H	-4.583155	-6.532486	-0.378085	H	-2.204280	6.655871	1.892191
H	-2.203870	-6.815031	-0.048088	H	0.794050	6.828404	0.683762
C	-3.025681	-3.227349	2.375120	H	3.215078	7.130419	0.762464
O	-5.890364	-4.638429	-1.533020	H	3.629762	7.192336	-1.579520
O	-3.721110	-6.403299	-2.264228	H	3.434241	4.575902	-0.882061
H	-3.968284	-2.802143	2.721244	H	5.666233	5.009825	-0.572773
O	-2.079317	-2.158086	2.416164	H	4.147780	5.086681	2.048729
H	-2.736848	-4.034072	3.060382	H	1.933452	3.418519	0.764823
H	-6.334223	-3.771001	-1.472012	H	2.439535	2.213377	2.679272
H	-4.550361	-6.290174	-2.752149	H	1.131517	3.298662	3.155624
H	-1.209935	-2.477252	2.086361	H	3.595166	3.051267	4.196679
C	4.129968	4.087256	5.322677	C	-6.708177	-4.671176	3.450981
C	4.343621	3.758259	3.984261	C	-6.206397	-4.307603	2.201299
C	4.251023	2.426443	3.582177	C	-5.972512	-2.962522	1.916096
C	3.955962	1.399723	4.491928	C	-6.239188	-1.959087	2.861060
C	3.708497	1.738515	5.837027	C	-6.724941	-2.328012	4.130114
C	3.801800	3.080317	6.230064	C	-6.951129	-3.683220	4.404717

C	3.221830	0.697379	6.829083	C	-6.894290	-1.298140	5.231644
C	1.933747	0.088146	6.325704	C	-5.568983	-0.629540	5.512806
C	0.695410	0.371927	6.902201	C	-4.842988	-0.872890	6.678892
C	-0.481855	-0.185228	6.392894	C	-3.616127	-0.243632	6.911378
C	-0.416373	-1.033423	5.288161	C	-3.106841	0.634856	5.956486
C	0.815781	-1.324595	4.695787	C	-3.813570	0.878367	4.775853
C	1.999076	-0.766066	5.201880	C	-5.046069	0.251002	4.538971
C	4.014823	-0.022652	3.937201	C	-6.051725	-0.522012	2.378118
N	3.286741	-1.074237	4.685654	N	-5.848596	0.530831	3.400670
C	5.495113	-0.450132	3.828237	C	-7.275914	-0.128008	1.523009
C	3.414598	-2.366808	4.003640	C	-5.630996	1.827763	2.755710
C	4.883591	-2.766056	3.908991	C	-6.847045	2.210688	1.918810
N	5.636740	-1.750138	3.176214	N	-7.098681	1.189289	0.891460
C	7.039427	-2.120259	3.024744	C	-8.254611	1.535873	0.057086
H	4.197758	5.118974	5.655240	H	-6.894418	-5.714444	3.688909
H	4.574596	4.530057	3.256008	H	-5.992010	-5.064790	1.452733
H	4.397299	2.169898	2.536434	H	-5.572835	-2.680836	0.943200
H	3.602244	3.335733	7.267656	H	-7.317346	-3.963266	5.389103
H	3.068371	1.162903	7.806541	H	-7.275395	-1.782603	6.134572
H	3.969971	-0.096151	6.944772	H	-7.620043	-0.533810	4.927304
H	0.654515	1.029563	7.767145	H	-5.253230	-1.551460	7.422625
H	-1.437143	0.043303	6.856364	H	-3.070286	-0.435660	7.830179
H	-1.317834	-1.459339	4.858504	H	-2.154643	1.131069	6.121147
H	0.845066	-1.980047	3.831444	H	-3.398445	1.556628	4.038363
H	3.620502	0.017812	2.907305	H	-5.179190	-0.527634	1.702648
H	5.933897	-0.448649	4.845686	H	-8.175737	-0.143386	2.161705
H	6.035186	0.295732	3.236781	H	-7.412342	-0.870004	0.731594
H	2.987209	-2.341734	2.988672	H	-4.739044	1.823880	2.105614
H	2.872542	-3.117757	4.584863	H	-5.480565	2.583193	3.530437
H	4.966300	-3.720597	3.377170	H	-6.664748	3.169306	1.422358
H	5.287429	-2.915047	4.929483	H	-7.724613	2.328499	2.576863
H	7.566262	-2.223466	3.991796	H	-9.186427	1.596659	0.641642
H	7.561759	-1.360659	2.434723	H	-8.382719	0.780145	-0.722596
H	7.113207	-3.075716	2.496003	H	-8.082216	2.504000	-0.420945
FV2				FV2			
E	-5082.93997849			E	-5082.92243942		
O	-5.075568	3.549339	-1.415610	C	4.053913	5.408813	0.355910
C	-4.747428	2.141158	-1.379727	C	5.261171	5.134410	-0.545265
C	-5.645464	1.501495	-0.309715	O	4.932046	5.514245	-1.878832
C	-5.372969	2.154401	1.049199	C	5.672005	3.668215	-0.464207
C	-5.544752	3.666551	0.959725	O	6.867266	3.526383	-1.211544
C	-4.743952	4.233378	-0.221489	C	5.841835	3.207954	0.991332
H	-3.702298	2.019254	-1.073915	O	5.963259	1.783108	0.924252
H	-6.699902	1.637980	-0.584121	C	4.611089	3.608474	1.822321
H	-4.328397	1.936649	1.318230	O	4.368260	5.018415	1.677531
H	-6.606235	3.881824	0.771269	C	4.724671	3.352517	3.312148
H	-5.011680	5.280386	-0.395677	O	3.429140	3.589719	3.873127
C	-4.880185	1.590246	-2.810170	C	6.997889	1.120259	1.617068
O	-5.359167	0.115354	-0.126532	C	7.830019	0.308193	0.612478
O	-6.253414	1.676277	2.054855	O	8.318885	1.182430	-0.403798
O	-5.114428	4.326129	2.147691	C	7.002809	-0.825074	0.016299
O	-3.374596	4.111601	0.071552	O	7.873958	-1.597297	-0.794179
H	-5.551900	0.731212	-2.834298	C	6.366739	-1.647895	1.134639
O	-3.637288	1.128854	-3.338616	O	5.516040	-2.618675	0.514210
H	-5.308132	2.380594	-3.440298	C	5.566141	-0.745233	2.079727
H	-6.229040	0.700896	2.030683	O	6.468578	0.257397	2.606164
H	-5.518438	3.854928	2.891463	C	4.921165	-1.490785	3.256118
H	-2.995582	1.873192	-3.352882	O	5.681274	-2.584535	3.755212
O	-0.696666	6.017979	-1.580667	C	5.774759	-3.980555	0.746535
C	-1.569189	4.876377	-1.414593	C	5.719516	-4.732863	-0.584319
C	-2.506646	5.200305	-0.241880	O	6.687310	-4.164582	-1.464096
C	-1.686002	5.443789	1.028278	C	4.317760	-4.669017	-1.175445
C	-0.636066	6.523174	0.789704	O	4.320302	-5.468517	-2.346183
C	0.171124	6.227369	-0.482827	C	3.284279	-5.143759	-0.154106
H	-0.971041	3.996866	-1.151056	O	2.007288	-4.815661	-0.711102
H	-3.094235	6.097056	-0.479333	C	3.453808	-4.438976	1.205032
H	-1.168393	4.503217	1.273366	O	4.829449	-4.534063	1.653233
H	-1.156963	7.478490	0.632502	C	2.571084	-5.024356	2.294355
H	0.784792	7.092826	-0.751936	O	2.783768	-6.431089	2.367744
C	-2.238457	4.596263	-2.771376	C	0.964221	-5.769984	-0.678161
O	-2.501762	5.862558	2.110503	C	0.562103	-6.123004	-2.119034
O	0.275271	6.635118	1.879565	O	1.713690	-6.569899	-2.834750

O	0.977798	5.099708	-0.248188	C	-0.076207	-4.922157	-2.805711
H	-3.324454	4.578317	-2.671531	O	-0.513458	-5.353577	-4.087358
O	-1.874799	3.326902	-3.312156	C	-1.217153	-4.371177	-1.949957
H	-1.968455	5.409653	-3.457250	O	-1.716941	-3.197479	-2.597847
H	-3.228098	5.216108	2.200119	C	-0.700847	-4.041041	-0.544573
H	-0.257895	6.669000	2.687757	O	-0.153926	-5.259358	0.018588
H	-0.899739	3.294586	-3.432502	C	-1.756922	-3.497036	0.417804
O	3.940867	4.202390	-2.240477	O	-3.005279	-4.167091	0.336472
C	2.535259	4.149459	-1.902630	C	-2.969436	-3.302668	-3.232655
C	2.323687	5.112097	-0.723295	C	-2.919925	-2.573903	-4.578563
C	3.179988	4.661596	0.464082	O	-1.863872	-3.126611	-5.359873
C	4.644295	4.559340	0.052000	C	-2.741545	-1.072893	-4.374724
C	4.785155	3.707836	-1.218018	O	-2.844555	-0.464591	-5.650165
H	2.278544	3.135795	-1.575003	C	-3.767210	-0.512440	-3.377108
H	2.609401	6.128619	-1.024874	O	-3.333364	0.820821	-3.085698
H	2.832087	3.661073	0.761146	C	-3.776732	-1.365286	-2.098402
H	5.008552	5.569161	-0.184554	O	-4.000020	-2.743463	-2.444648
H	5.803060	3.778479	-1.614273	C	-4.841564	-1.008661	-1.079032
C	1.735263	4.441097	-3.184121	O	-4.574778	-1.783892	0.089291
O	3.094531	5.561903	1.557591	C	-4.230160	1.903572	-3.202975
O	5.450375	3.974990	1.071762	C	-3.633402	2.945735	-4.157450
O	4.467090	2.377657	-0.893393	O	-3.395719	2.335256	-5.426101
H	1.051687	5.277654	-3.033713	C	-2.350483	3.529471	-3.578618
O	0.922230	3.339311	-3.586276	O	-1.922377	4.556970	-4.458482
H	2.447337	4.714658	-3.973374	C	-2.584601	4.044831	-2.160191
H	2.147807	5.716760	1.740572	O	-1.286730	4.347281	-1.635417
H	5.241515	4.439446	1.895665	C	-3.281085	2.987807	-1.285046
H	1.491938	2.553343	-3.739676	O	-4.470393	2.504173	-1.946491
O	5.377128	-0.587382	-2.869768	C	-3.689692	3.515382	0.079366
C	4.503689	0.493060	-2.468199	O	-4.462333	4.702797	-0.081885
C	5.270030	1.326987	-1.430594	C	-1.088213	5.556142	-0.932011
C	5.646079	0.450448	0.232036	C	-0.032968	6.396911	-1.668541
C	6.414273	-0.784852	-0.688144	O	-0.441106	6.580843	-3.024015
C	5.661131	-1.495854	-1.821779	C	1.335549	5.730610	-1.593217
H	3.609838	0.078674	-1.988882	O	2.268292	6.618952	-2.192943
H	6.178939	1.739196	-1.888621	C	1.683490	5.407063	-0.139843
H	4.710501	0.120707	0.244284	O	2.934775	4.712352	-0.138092
H	7.385118	-0.460302	-1.088825	C	0.575266	4.547813	0.479358
H	6.287086	-2.276087	-2.266160	O	-0.658878	5.300735	0.390578
C	4.050656	1.229505	-3.740668	C	0.798536	4.163223	1.941908
O	6.458205	1.151577	0.698628	O	1.316249	5.217983	2.738573
O	6.607657	-1.717842	0.371692	H	3.851547	6.482766	0.404013
O	4.481265	-2.043316	-1.290138	H	6.092489	5.749131	-0.172113
H	4.275317	2.294854	-3.672197	H	5.633640	5.175507	-2.454386
O	2.642539	1.140071	-3.954577	H	4.862668	3.062798	-0.900459
H	4.606809	0.813648	-4.590686	H	7.223383	2.628790	-1.052371
H	6.002673	1.986969	0.919534	H	6.752922	3.652973	1.412133
H	6.935892	-1.214768	1.131759	H	3.751007	3.045920	1.439810
H	2.384895	0.195245	-4.037003	H	5.472854	4.029948	3.744670
O	2.490183	-4.711125	-2.856059	H	5.043986	2.317517	3.483298
C	2.844162	-3.333105	-2.595395	H	3.500215	3.565822	4.836413
C	4.085139	-3.354613	-1.690296	H	7.630793	1.837212	2.149466
C	3.764291	-4.090589	-0.386018	H	8.674979	-0.130778	1.161184
C	3.210162	-5.480896	-0.673385	H	8.678853	0.611065	-1.100077
C	2.070776	-5.411080	-1.700835	H	6.194139	-0.387291	-0.588090
H	2.026881	-2.844286	-2.053312	H	7.369166	-2.355240	-1.149859
H	4.911274	-3.860140	-2.207868	H	7.148067	-2.150168	1.715563
H	2.988935	-3.510267	0.137835	H	4.770404	-0.237861	1.521426
H	4.013871	-6.087134	-1.114938	H	3.921360	-1.817986	2.949109
H	1.806109	-6.416701	-2.042500	H	4.792463	-0.771051	4.071290
C	2.994506	-2.622397	-3.951229	H	5.399095	-3.371685	3.259214
O	4.913891	-4.240574	0.431286	H	6.750728	-4.117514	1.221941
O	2.710865	-6.111122	0.503568	H	5.968004	-5.783990	-0.382284
O	0.964506	-4.783357	-1.099514	H	6.493256	-4.506852	-2.349844
H	3.961033	-2.121692	-4.020324	H	4.092465	-3.619545	-1.418651
O	2.013342	-1.605509	-4.150942	H	3.391705	-5.653169	-2.594737
H	2.942370	-3.382411	-4.741505	H	3.378674	-6.225953	-0.017956
H	5.314539	-3.356966	0.541523	H	3.189902	-3.381888	1.080898
H	3.383893	-5.994558	1.190717	H	1.528846	-4.789599	2.044678
H	1.117485	-2.007187	-4.105166	H	2.814977	-4.531450	3.246183
O	-2.488896	-5.108710	-2.332452	H	2.135153	-6.793496	2.985298
C	-1.199138	-4.460058	-2.241057	H	1.278990	-6.660968	-0.127000

C	-0.333982	-5.332658	-1.317779	H	-0.179251	-6.932956	-2.068992
C	-0.984739	-5.399921	0.067000	H	1.449763	-6.591075	-3.768497
C	-2.414536	-5.918570	-0.044116	H	0.684101	-4.133835	-2.905645
C	-3.195431	-5.127985	-1.106236	H	-0.803644	-4.566533	-4.587820
H	-1.320422	-3.474745	-1.777156	H	-2.015109	-5.114814	-1.851852
H	-0.251064	-6.342137	-1.741857	H	0.102745	-3.296736	-0.609693
H	-1.019564	-4.374029	0.463200	H	-1.879758	-2.428419	0.216588
H	-2.376937	-6.966990	-0.372140	H	-1.345925	-3.590653	1.433125
H	-4.148915	-5.620321	-1.321802	H	-3.663226	-3.490379	0.090696
C	-0.681589	-4.235356	-3.672589	H	-3.242110	-4.351942	-3.378539
O	-0.272438	-6.250373	0.952909	H	-3.885608	-2.743594	-5.075653
O	-3.120117	-5.816665	1.190337	H	-1.738712	-2.544703	-6.124055
O	-3.404168	-3.826404	-0.621006	H	-1.744612	-0.903904	-3.939401
H	0.296686	-4.697210	-3.811100	H	-2.841152	0.506701	-5.528752
O	-0.507323	-2.852547	-3.980475	H	-4.762610	-0.500577	-3.839869
H	-1.388408	-4.707848	-4.366722	H	-2.796573	-1.262424	-1.618325
H	0.676104	-6.024417	0.885925	H	-5.835084	-1.237275	-1.490370
H	-2.553881	-6.201788	1.875225	H	-4.792723	0.065811	-0.866903
H	-1.367343	-2.387432	-3.882639	H	-5.141037	-1.504249	0.841029
O	-5.898172	-1.401811	-1.810745	H	-5.205165	1.561684	-3.564631
C	-4.590915	-2.019243	-1.772984	H	-4.369555	3.753797	-4.267690
C	-4.680256	-3.214600	-0.812994	H	-2.861458	2.963998	-5.935538
C	-5.109063	-2.732201	0.574479	H	-1.600494	2.725766	-3.524109
C	-6.403514	-1.933342	0.497567	H	-1.258525	5.102696	-3.990585
C	-6.290614	-0.838143	-0.572347	H	-3.201475	4.948628	-2.199602
H	-3.864023	-1.305879	-1.369018	H	-2.589268	2.150926	-1.129054
H	-5.401344	-3.948121	-1.197263	H	-2.775280	3.712154	0.652941
H	-4.316766	-2.063394	0.939868	H	-4.260704	2.734362	0.599645
H	-7.216712	-2.608934	0.197575	H	-4.632869	5.060438	0.799333
H	-7.265829	-0.375061	-0.753013	H	-2.031107	6.102661	-0.837842
C	-4.176275	-2.338106	-3.219641	H	0.026810	7.371853	-1.164252
O	-5.312140	-3.807431	1.477263	H	0.331674	6.944773	-3.484446
O	-6.717727	-1.312700	1.743556	H	1.293175	4.783701	-2.151386
H	-3.920069	-3.393644	-3.324022	H	3.129621	6.161553	-2.247881
O	-3.019198	-1.611994	-3.632191	H	1.765378	6.328140	0.446771
H	-5.031395	-2.124990	-3.874121	H	0.459656	3.619414	-0.094067
H	-4.506459	-4.359732	1.471013	H	1.464919	3.295765	1.968918
H	-6.670631	-2.004920	2.419822	H	-0.173627	3.837740	2.339017
H	-3.198511	-0.648673	-3.557971	H	2.176146	4.909124	3.076708
C	1.424076	-4.676500	5.204150	C	-4.847104	3.294474	4.605034
C	1.957809	-3.858161	6.199788	C	-6.182388	2.998782	4.879267
C	1.992768	-2.477778	6.008175	C	-6.728291	1.804718	4.414285
C	1.507925	-1.882791	4.833339	C	-5.975626	0.885197	3.664843
C	0.945649	-2.710636	3.842517	C	-4.620749	1.173185	3.413962
C	0.913852	-4.097813	4.042483	C	-4.080097	2.377210	3.889670
C	0.276452	-2.115511	2.619139	C	-3.705187	0.172669	2.735094
C	-0.839617	-1.189953	3.041297	C	-3.712475	-1.143654	3.477165
C	-2.185354	-1.522476	2.884187	C	-2.598936	-1.571795	4.202843
C	-3.197552	-0.635538	3.264437	C	-2.611911	-2.776673	4.909960
C	-2.853823	0.597887	3.816336	C	-3.763415	-3.560202	4.899388
C	-1.510984	0.934006	4.007962	C	-4.890593	-3.143456	4.186662
C	-0.491210	0.045609	3.631684	C	-4.878686	-1.939232	3.469014
C	1.725652	-0.374237	4.706637	C	-6.754632	-0.327124	3.151128
N	0.889782	0.364347	3.729871	N	-5.984523	-1.508360	2.654595
C	3.210458	-0.120691	4.361001	C	-7.712329	0.121555	2.026887
C	1.218281	1.793086	3.748148	C	-6.941783	-2.583429	2.312776
C	2.688826	2.006979	3.405834	C	-7.913697	-2.128689	1.230196
N	3.530607	1.303029	4.367610	N	-8.642018	-0.942129	1.663294
C	4.951025	1.537436	4.133718	C	-9.607116	-0.500446	0.663301
H	1.389904	-5.753984	5.336129	H	-4.401181	4.218754	4.960001
H	2.341589	-4.287443	7.120443	H	-6.794502	3.686660	5.454585
H	2.409263	-1.843307	6.787014	H	-7.767571	1.576778	4.637932
H	0.474795	-4.728591	3.272773	H	-3.030641	2.586940	3.700125
H	-0.112498	-2.918076	1.987698	H	-2.688758	0.574275	2.708862
H	1.003972	-1.544880	2.028830	H	-4.007741	0.009897	1.695810
H	-2.443491	-2.480946	2.440764	H	-1.705428	-0.953048	4.204691
H	-4.239837	-0.899336	3.115260	H	-1.732152	-3.095671	5.460408
H	-3.630643	1.300490	4.104435	H	-3.794945	-4.498110	5.445884
H	-1.261821	1.890527	4.453810	H	-5.775768	-3.767539	4.196852
H	1.556684	0.059676	5.708851	H	-7.387106	-0.672728	3.985927
H	3.424177	-0.590873	3.380444	H	-7.105271	0.466223	1.166141
H	3.834609	-0.621246	5.107385	H	-8.290977	0.980447	2.377617

H	1.016099	2.250948	4.732158	H	-7.519859	-2.896102	3.196013
H	0.595662	2.300028	3.006321	H	-6.374141	-3.444836	1.952894
H	2.916234	3.078514	3.440050	H	-8.628304	-2.936759	1.038641
H	2.874196	1.659946	2.369943	H	-7.362352	-1.953865	0.286709
H	5.298378	1.180681	3.147051	H	-9.136411	-0.208536	-0.293730
H	5.539982	1.029047	4.903974	H	-10.165680	0.360625	1.043038
H	5.160775	2.610115	4.198267	H	-10.318221	-1.306749	0.458167

Complexes 1:2 WATER							
[β-CD-CCCW]-[MIA S]-[β-CD-CCCW]				[β-CD-EXP]-[MIA S]-[β-CD-EXP]			
CAPS A				CAPS A			
E	-9358.46539934			E	-9358.41721784		
ZPE	-9355.671029			ZPE	-9355.629055		
H	-9355.510461			H	-9355.464636		
G	-9355.853740			G	-9355.823550		
S	722.491			S	755.398		
Atom	x [Å]	y [Å]	z [Å]	Atom	x [Å]	y [Å]	z [Å]
O	-7.680125	1.411234	1.317935	C	1.962593	-4.372807	4.625719
C	-6.825226	0.550646	2.100288	C	3.228475	-3.596040	4.205367
C	-5.954233	1.385639	3.052787	O	3.113100	-2.266573	4.694482
C	-5.258062	2.528606	2.307487	C	3.416411	-3.630110	2.690233
C	-6.204514	3.316429	1.410447	O	4.690732	-3.082492	2.371272
C	-6.988088	2.339266	0.511528	C	3.285940	-5.052202	2.142308
H	-6.159864	0.000514	1.427397	O	3.358697	-4.961425	0.708964
H	-6.558237	1.790182	3.875651	C	1.955893	-5.659670	2.595681
H	-4.513132	2.071510	1.651246	O	1.958092	-5.661720	4.042637
H	-6.934133	3.859816	2.026774	C	1.719984	-7.092665	2.100860
H	-7.751671	2.878005	-0.058425	O	2.899628	-7.880936	1.987222
C	-7.741184	-0.441356	2.805169	C	4.339774	-5.698428	0.012975
O	-4.880507	0.580777	3.573473	C	5.070382	-4.764933	-0.964072
O	-4.624287	3.413895	3.231650	O	5.632312	-3.733211	-0.167003
O	-5.510173	4.222226	0.558583	C	4.099822	-4.243542	-2.027265
O	-6.084847	1.685532	-0.356554	O	4.763344	-3.600358	-3.115284
H	-7.192526	-0.918932	3.621825	C	3.269144	-5.366225	-2.657697
O	-8.195146	-1.477823	1.949146	O	2.153253	-4.719661	-3.296066
H	-8.581625	0.121843	3.241755	C	2.734535	-6.399096	-1.646428
H	-4.125394	2.858763	3.872287	O	3.755005	-6.781285	-0.691827
H	-4.823133	4.710940	1.052230	C	2.304672	-7.699083	-2.320454
H	-8.331092	-1.114599	1.053822	O	3.381088	-8.325180	-3.005514
O	-6.647076	0.264218	-3.716822	C	1.889816	-4.932868	-4.670535
C	-6.670264	0.291483	-2.274223	C	1.785969	-3.562740	-5.371330
C	-6.290156	1.696364	-1.773637	O	2.936189	-2.764895	-5.125758
C	-4.977032	2.183644	-2.393484	C	0.499741	-2.829859	-4.985060
C	-5.010481	2.035962	-3.912237	O	0.364138	-1.690169	-5.830728
C	-5.417253	0.608507	-4.319961	C	-0.715455	-3.743343	-5.158483
H	-5.945629	-0.431411	-1.880695	O	-1.850304	-3.029695	-4.643651
H	-7.087185	2.405124	-2.035533	O	-0.521377	-5.076987	-4.423057
H	-4.155471	1.570065	-1.999639	C	0.715132	-5.688668	-4.860568
H	-5.780174	2.713864	-4.308429	C	-1.601695	-6.104174	-4.745958
H	-5.604760	0.572064	-5.397538	O	-1.647807	-6.405523	-6.135332
C	-8.090922	-0.151175	-1.866696	C	-3.000204	-2.893940	-5.457145
O	-4.769523	3.557497	-2.075157	C	-3.379209	-1.398650	-5.585976
O	-3.756436	2.311625	-4.510146	O	-2.216412	-0.684716	-5.984927
O	-4.386326	-0.298270	-3.973896	C	-4.000211	-0.853710	-4.300223
H	-8.678020	0.697305	-1.508110	O	-4.528365	0.444516	-4.574150
O	-8.108667	-1.105890	-0.810046	C	-5.104316	-1.796134	-3.813437
H	-8.584448	-0.549283	-2.760504	O	-5.606661	-1.258516	-2.583560
H	-4.918717	3.672157	-1.109834	C	-4.533077	-3.208538	-3.637278
H	-3.434438	3.206861	-4.274956	O	-4.085202	-3.639692	-4.942664
H	-7.786802	-1.952683	-1.147222	C	-5.519520	-4.244847	-3.087043
O	-3.344413	-3.531233	-5.397788	O	-6.861778	-4.110064	-3.547395
C	-3.937458	-2.648243	-4.421270	C	-6.981993	-0.979101	-2.477054
C	-3.892971	-1.211254	-4.968354	C	-7.164822	0.385523	-1.799597
C	-2.433727	-0.828140	-5.273590	O	-6.462420	1.331942	-2.598938
C	-1.746595	-1.869261	-6.157882	C	-6.648338	0.307209	-0.367519
C	-1.974938	-3.306183	-5.645489	O	-6.889310	1.552875	0.281853
H	-3.356457	-2.685121	-3.491638	C	-7.256170	-0.860061	0.417432
H	-4.497379	-1.140709	-5.881986	O	-6.453434	-0.961356	1.605164
H	-1.904132	-0.789262	-4.316808	C	-7.147553	-2.171822	-0.380393
H	-2.203641	-1.811766	-7.156720	O	-7.651861	-1.985486	-1.728324
H	-1.697337	-4.018336	-6.428894	C	-7.937675	-3.330457	0.215158
C	-5.334572	-3.191771	-4.137171	O	-7.597823	-4.579519	-0.376052
O	-2.353670	0.433633	-5.933075	C	-7.062004	-0.979692	2.875378
O	-0.342023	-1.676701	-6.252486	C	-6.418872	0.090150	3.779991
O	-1.199870	-3.534622	-4.486408	O	-6.462861	1.351456	3.113322
H	-5.975325	-2.376326	-3.793012	C	-4.997884	-0.279807	4.205774
O	-5.360543	-4.180125	-3.117060	O	-4.648862	0.597669	5.269756
H	-5.749941	-3.570942	-5.083328	C	-4.867451	-1.744280	4.637202
H	-2.823751	1.092312	-5.370551	O	-3.460237	-2.052142	4.658780

H	-0.108830	-0.729240	-6.314878	C	-5.588239	-2.707032	3.684095
H	-4.645904	-4.830638	-3.240082	O	-6.944300	-2.255458	3.475939
O	0.064449	-6.812789	-3.361897	C	-5.718702	-4.117411	4.251128
C	-0.890391	-5.732567	-3.439973	O	-6.478533	-4.134983	5.453246
C	-0.357197	-4.693459	-4.437412	C	-2.856435	-2.414298	5.883161
C	1.032971	-4.199030	-4.015348	C	-1.624595	-1.518946	6.147184
C	1.980438	-5.377899	-3.783377	O	-1.994312	-0.146396	6.139504
C	1.329161	-6.428293	-2.865092	C	-0.481981	-1.861123	5.189211
H	-0.983955	-5.252214	-2.460549	O	0.673103	-1.108808	5.555527
H	-0.285353	-5.148322	-5.434194	C	-0.186532	-3.362843	5.250098
H	0.928399	-3.637490	-3.076146	O	0.813670	-3.630997	4.257823
H	2.163384	-5.859530	-4.754966	C	-1.457246	-4.186746	4.986508
H	1.933837	-7.340672	-2.853525	O	-2.496665	-3.781004	5.903050
C	-2.249290	-6.354895	-3.799584	C	-1.271063	-5.678427	5.247614
O	1.578169	-3.366347	-5.036092	O	-0.894983	-5.934582	6.595550
C	3.208929	-5.008205	-3.177575	H	1.971186	-4.541274	5.706480
O	1.223884	-5.885388	-1.570237	H	4.086588	-4.101132	4.670959
H	-2.686155	-5.858285	-4.667593	H	3.896206	-1.741839	4.426464
O	-3.218142	-6.220889	-2.762515	H	2.615490	-3.021129	2.251086
H	-2.080283	-7.408732	-4.056148	H	4.894893	-3.288252	1.430525
H	0.878412	-2.733157	-5.314726	H	4.103368	-5.677205	2.517529
H	3.600695	-4.217210	-3.601159	H	1.123082	-5.038022	2.246444
H	-2.864495	-6.604431	-1.937108	H	1.189770	-7.042053	1.143897
O	0.919917	-7.539346	1.688912	H	1.053414	-7.583981	2.817511
C	0.441750	-6.936642	0.466807	H	3.206938	-7.795030	1.070305
C	1.649773	-6.648723	-0.435533	H	5.054052	-6.147951	0.708780
C	2.672515	-5.766612	0.294717	H	5.861113	-5.348312	-1.455638
C	3.012522	-6.301607	1.684131	H	5.976502	-2.974812	-0.685423
C	1.724671	-6.662023	2.452048	H	3.412019	-3.550745	-1.536797
H	-0.030504	-5.982130	0.709843	H	5.119391	-2.714008	-2.884602
H	2.119498	-7.587597	-0.756595	H	3.884540	-5.886003	-3.400745
H	2.205246	-4.785846	0.415234	H	1.887839	-5.963598	-1.108674
H	3.599125	-7.224804	1.574206	H	1.534689	-7.478396	-3.064354
H	1.970859	-7.201572	3.371710	H	1.870101	-8.365282	-1.562233
C	-0.637821	-7.845902	-0.145860	H	4.077046	-8.471568	-2.347935
O	3.872023	-5.640626	-0.470840	H	2.694467	-5.522944	-5.120081
O	3.718920	-5.359642	2.484672	H	1.741643	-3.754836	-6.450721
O	1.038489	-5.464162	2.748908	H	3.429562	-3.106160	-4.347228
H	-0.406473	-8.062518	-1.190270	H	0.562192	-2.524435	-3.930428
O	-1.932421	-7.242041	-0.157113	H	-0.558827	-1.356037	-5.743712
H	-0.644836	-8.793293	0.408851	H	-0.856450	-3.952218	-6.225389
H	3.605903	-5.348319	-1.371417	H	-0.493351	-4.900013	-3.341597
H	4.423533	-4.915027	1.974893	H	-2.578989	-5.698977	-4.475220
H	-2.200187	-7.044447	0.764993	H	-1.418729	-7.006687	-4.145915
O	-1.540048	-4.885284	5.313286	H	-0.754435	-6.690219	-6.379102
C	-1.043621	-5.252195	4.008487	H	-2.807598	-3.308973	-6.450981
C	0.489867	-5.248023	4.053584	H	-4.144357	-1.333544	-6.373076
C	1.010271	-3.875139	4.495265	H	-2.317876	0.740665	-5.825041
C	0.357502	-3.448331	5.807908	H	-3.227324	-0.292091	-3.521454
C	-1.177676	-3.585971	5.721745	H	-5.073532	0.715025	-3.804452
H	-1.375458	-4.502087	3.286225	H	-5.908862	-1.841247	-4.556551
H	0.850321	-6.017506	4.749015	H	-3.670303	-3.181903	-2.959748
H	0.741796	-3.141476	3.721967	H	-5.485606	-4.218633	-1.992825
H	0.698258	-4.134180	6.597283	H	-5.167966	-5.232356	-3.400957
H	-1.610631	-3.460766	6.719281	H	-7.276373	-3.415680	-3.006008
C	-1.673350	-6.602662	3.628856	H	-7.458385	-0.979594	-3.462150
O	2.427306	-3.925986	4.658756	H	-8.238986	0.616403	-1.791355
O	0.639669	-2.106502	6.171013	H	-6.353217	2.178728	-2.131117
O	-1.679364	-2.593530	4.845737	H	-5.576207	0.102059	-0.420358
H	-0.909938	-7.299295	3.278724	H	-6.684161	1.437261	1.237579
O	-2.623473	-6.497183	2.568236	H	-8.300814	-0.644271	0.676654
H	-2.135691	-7.024336	4.531447	H	-6.088787	-2.449024	-0.428121
H	2.798780	-4.350939	3.854084	H	-9.012482	-3.118586	0.123716
H	1.568803	-1.863440	5.977704	H	-7.694415	-3.410611	1.277501
H	-3.238182	-5.766374	2.797820	H	-7.904432	-4.576716	-1.294063
O	-5.098459	-1.239408	5.004879	H	-8.137374	-0.795429	2.786783
C	-4.049329	-2.015446	4.384756	H	-7.032577	0.139344	4.690283
C	-2.807886	-1.823486	5.266585	H	-5.618511	1.825022	3.259505
C	-2.393609	-0.345494	5.217693	H	-4.328025	-0.130096	3.347893
C	-3.566571	0.563910	5.604365	H	-3.768152	0.332242	5.601567
C	-4.893288	0.157677	4.917958	H	-5.295473	-1.863876	5.639029
H	-3.858706	-1.614872	3.382275	H	-5.059174	-2.742260	2.724390

H	-3.078477	-2.091428	6.296311	H	-4.725488	-4.501959	4.494890
H	-2.079127	-0.114465	4.189236	H	-6.165793	-4.767010	3.485558
H	-3.720320	0.436281	6.685924	H	-7.324966	-3.713561	5.242186
H	-5.733143	0.613556	5.451213	H	-3.570709	-2.294735	6.703592
O	-4.565088	-3.451254	4.215496	H	-1.285702	-1.748380	7.165009
O	-1.323528	-0.096600	6.125470	H	-1.753475	0.301082	5.298371
O	-3.337545	1.932354	5.300613	H	-0.783651	-1.612974	4.162061
H	-4.403949	-4.038917	5.123941	H	1.453707	-1.477374	5.085131
O	-3.903437	-4.124335	3.156204	H	0.195873	-3.614206	6.246285
H	-5.647942	-3.388948	4.038673	H	-1.782650	-4.032394	3.950020
H	-0.648046	-0.802779	5.999415	H	-0.469609	-6.063860	4.614464
H	-2.427007	2.205144	5.533873	H	-2.204114	-6.197593	4.986727
H	-3.990731	-3.612493	2.301161	H	-1.571815	-5.513980	7.146741
O	2.995790	4.301883	5.513783	C	7.497208	1.040621	1.867578
C	2.340706	4.733019	4.300520	C	6.876667	0.030883	2.850594
C	0.839338	4.799078	4.615784	O	6.668575	-1.187553	2.147158
C	0.325701	3.408344	5.016051	C	5.588490	0.590879	3.445553
C	1.150535	2.848577	6.174575	O	5.130806	-0.297527	4.469655
C	2.660043	2.983354	5.888631	C	5.771541	2.007303	4.011442
H	2.504003	3.988592	3.513161	O	4.426434	2.492506	4.174994
H	0.673501	5.501259	5.443371	C	6.561044	2.924929	3.053592
H	0.431834	2.744096	4.146008	O	7.727957	2.262958	2.528447
H	0.932374	3.460260	7.062165	C	7.151074	4.186342	3.707975
H	3.227010	2.781464	6.802896	O	6.286530	4.867987	4.598525
C	3.008438	6.043226	3.849217	C	4.044043	3.164521	5.356593
O	0.061846	5.183211	3.482381	C	3.010951	2.340076	6.126000
O	-1.042685	3.489310	5.414756	O	3.574915	1.055619	6.393353
O	0.903931	1.478505	6.451726	C	1.685507	2.218558	5.368323
O	3.008576	2.065416	4.877561	O	0.735076	1.573296	6.202206
H	2.269198	6.835780	3.725885	C	1.180033	3.609624	4.977455
O	3.661470	5.918547	2.586604	O	0.022317	3.482089	4.127810
H	3.715199	6.349569	4.630907	C	2.273926	4.394874	4.231675
H	-1.510903	4.042807	4.751665	O	3.483378	4.421278	5.026760
H	-0.036202	1.241648	6.315632	C	1.938924	5.865238	4.005329
H	4.346164	5.216617	2.642027	O	1.689955	6.556475	5.220663
O	6.407265	0.808217	4.271761	C	-1.229952	3.744767	4.746125
C	5.281899	1.680487	4.022113	C	-2.290937	2.812103	4.116064
C	4.199934	1.295614	5.038509	O	-1.749363	1.494134	3.964019
C	3.783284	-0.168411	4.846388	C	-2.841485	3.317380	2.777961
C	5.004219	-1.085939	4.908878	O	-4.092746	2.681487	2.532420
C	6.127002	-0.549626	3.998272	C	-3.007446	4.838599	2.692270
H	4.900223	1.502458	3.010922	O	-3.109405	5.115460	1.288400
H	4.599683	1.427076	6.052632	C	-1.806174	5.572465	3.290737
H	3.316636	-0.264395	3.855288	O	-1.597879	5.101293	4.637243
H	5.382085	-1.072367	5.941447	C	-2.004005	7.079978	3.401961
H	7.058169	-1.091562	4.192407	O	-3.154804	7.415372	4.167775
C	5.785013	3.133915	4.080990	C	-4.093350	5.987514	0.767523
O	2.861979	-0.544004	5.869206	C	-5.064745	5.177772	-0.114466
O	4.739520	-2.420526	4.500092	O	-5.625590	4.147818	0.699589
O	5.716933	-0.721970	2.663833	C	-4.308509	4.610639	-1.310924
H	5.254773	3.700070	4.848201	O	-5.241413	3.965740	-2.180977
O	5.570547	3.833020	2.855852	C	-3.498908	5.681284	-2.044234
H	6.850696	3.112870	4.342680	O	-2.652559	4.971085	-2.964065
H	2.189810	0.171679	5.939678	C	-2.628649	6.470230	-1.057363
H	3.849857	-2.709229	4.787289	O	-3.478673	6.996479	-0.010485
H	6.064703	3.370956	2.143796	C	-1.841285	7.631738	-1.692897
O	7.828773	-0.731124	-0.334865	O	-2.425579	8.192883	-2.865908
C	6.992926	-0.117664	0.671578	C	-2.711659	5.252316	-4.336858
C	6.648807	-1.206047	1.696893	C	-2.738600	3.925977	-5.109633
C	5.929037	-2.372941	1.008267	O	-3.869306	3.199363	-4.641902
C	6.711202	-2.895265	-0.193554	C	-1.419158	3.179035	-4.918701
C	7.151464	-1.716384	-1.088344	O	-1.443384	2.016386	-5.737332
H	6.061235	0.227153	0.210404	C	-0.219543	4.075892	-5.262059
H	7.563669	-1.562513	2.188022	O	0.962606	3.362577	-4.859147
H	4.973955	-1.981888	0.645121	C	-0.305901	5.413705	-4.505022
H	7.622226	-3.390754	0.171195	O	-1.595599	6.032697	-4.746503
H	7.866119	-2.062235	-1.841651	C	0.740987	6.433825	-4.933336
C	7.721178	1.125356	1.213749	O	0.764107	7.571298	-4.077373
O	5.696917	-3.435796	1.932720	C	1.962804	3.099799	-5.824267
O	5.961439	-3.783529	-1.014210	C	2.282546	1.588868	-5.876771
O	6.001711	-1.179860	-1.702902	O	1.043133	0.908191	-5.962575
H	7.814040	1.075765	2.299618	C	3.149830	1.106298	-4.703783

O	7.018834	2.336303	0.936010	O	3.720558	-0.170805	-4.985475
H	8.730050	1.144975	0.781680	C	4.336391	2.047993	-4.490036
H	5.321865	-3.035800	2.749115	O	5.019670	1.632746	-3.299344
H	5.390350	-4.367496	-0.478384	C	3.869492	3.505678	-4.377990
H	6.924538	2.442615	-0.036858	O	3.131039	3.849139	-5.571514
O	5.959368	0.922564	-4.717063	C	5.023291	4.502498	-4.329767
C	5.996859	0.696768	-3.290824	O	5.841483	4.418828	-5.489553
C	6.040984	-0.823593	-3.085722	C	6.393515	1.289133	-3.376064
C	4.800358	-1.481867	-3.706113	C	6.590762	-0.104506	-2.746089
C	4.640702	-1.079333	-5.170529	O	5.778512	-1.078002	-3.387303
C	4.777204	0.448940	-5.325669	C	6.324707	-0.040086	-1.244723
H	5.079933	1.086669	-2.834952	O	6.666297	-1.293224	-0.654686
H	6.945666	-1.230720	-3.556010	C	7.134017	1.077722	-0.581404
H	3.919076	-1.136252	-3.149970	O	6.636135	1.202534	0.760662
H	5.462239	-1.539281	-5.738764	C	6.973835	2.418930	-1.313613
H	4.865520	0.705877	-6.385813	O	7.204079	2.246045	-2.728123
C	7.180128	1.498043	-2.722501	C	7.999117	3.459792	-0.871785
O	4.913890	-2.902120	-3.611773	O	9.329124	3.037027	-1.143391
O	3.390549	-1.443266	-5.738184	H	8.480718	0.691022	1.538141
O	3.637694	1.059903	-4.762417	H	7.601840	-0.122493	3.661844
H	7.832964	0.856723	-2.128868	H	5.962104	-1.719720	2.565107
O	6.765864	2.548050	-1.850105	H	4.842907	0.656391	2.645093
H	7.759546	1.891788	-3.567413	H	4.520176	0.201720	5.057312
H	5.188554	-3.111405	-2.691388	H	6.277919	1.945024	4.982396
H	3.036689	-2.265562	-5.342179	H	5.888739	3.196766	2.230144
H	6.160125	3.154925	-2.330126	H	7.518116	4.847157	2.910151
O	2.488766	4.441025	-5.631041	H	8.015728	3.874662	4.302247
C	3.194564	3.482307	-4.811029	H	5.438038	5.051507	4.167598
C	3.005018	2.116334	-5.484172	H	4.916891	3.383745	5.973355
C	1.514074	1.757200	-5.531715	H	2.815061	2.858319	7.074420
C	0.715520	2.868515	-6.212353	H	2.887214	0.531464	6.832420
C	1.090432	4.247415	-5.631623	H	1.857404	1.639660	4.450907
H	2.742105	3.453533	-3.813681	H	0.632529	0.640192	5.918471
H	3.400739	2.163832	-6.507306	H	0.910755	4.171938	5.877998
H	1.159727	1.649898	-4.496035	H	2.474252	3.916887	3.264847
H	0.993094	2.875921	-7.276229	H	1.037050	5.945808	3.397819
H	0.680835	5.041449	-6.263931	H	2.766182	6.323798	3.445309
C	4.643818	3.974586	-4.649616	H	2.484204	6.447039	5.764258
O	1.321644	0.541927	-6.251967	H	-1.158163	3.544049	5.817021
O	-0.691572	2.725718	-6.072113	H	-3.126319	2.725027	4.814715
O	0.567404	4.333772	-4.326226	H	-0.835942	1.623874	3.657777
H	5.352539	3.231756	-5.017971	H	-2.122839	3.034946	1.994532
O	4.991316	4.205458	-3.285168	H	-4.511387	3.138400	1.770254
H	4.759419	4.888071	-5.246690	H	-3.917789	5.145259	3.218264
H	2.001072	-0.098444	-5.943302	H	-0.921007	5.366909	2.676422
H	-0.963483	1.792324	-6.169618	H	-2.149699	7.499445	2.402943
H	4.401967	4.900724	-2.919156	H	-1.094197	7.520438	3.833112
O	-0.019404	7.415871	-2.416211	H	-3.036323	7.002382	5.035921
C	0.750621	6.259691	-2.816116	H	-4.628744	6.499473	1.572721
C	-0.056134	5.549989	-3.910464	H	-5.856043	5.854563	-0.463105
C	-1.428824	5.129905	-3.373003	H	-6.145485	3.526343	0.158987
C	-2.170851	6.308541	-2.746270	H	-3.586714	3.882409	-0.928277
C	-1.238010	7.079293	-1.785875	H	-4.755445	3.685437	-2.984737
H	0.858668	5.580598	-1.963512	H	-4.159288	6.367952	-2.584805
H	-0.184452	6.224825	-4.766788	H	-1.907644	5.784769	-0.599845
H	-1.257761	4.373445	-2.598281	H	-0.821418	7.295127	-1.906831
H	-2.453684	7.000260	-3.552560	H	-1.776640	8.429237	-0.946584
H	-1.698936	8.029256	-1.497865	H	-2.161237	7.623151	-3.607767
C	2.159555	6.736489	-3.211417	H	-3.594769	5.851101	-4.580583
O	-2.214130	4.574608	-4.429688	H	-2.856526	4.161137	-6.176418
O	-3.322383	5.927671	-2.003079	H	-3.822758	2.258542	-4.901930
O	-1.013194	6.273149	-0.653345	H	-1.320920	2.908546	-3.860340
H	2.401994	6.425971	-4.228852	H	-0.539462	1.622383	-5.731917
O	3.176623	6.183530	-2.377783	H	-0.200393	4.258122	-6.344546
H	2.170014	7.833389	-3.174279	H	-0.195220	5.217661	-3.432512
H	-1.637793	3.943782	-4.917675	H	0.560611	6.721344	-5.978562
H	-3.716573	5.105931	-2.357242	H	1.728300	5.970480	-4.873996
H	3.015882	6.465258	-1.449990	H	-0.031321	8.092044	-4.253331
O	0.196363	7.349740	2.643152	H	1.620134	3.425933	-6.811122
C	0.354125	6.878764	1.286087	H	2.871151	1.428638	-6.791784
C	-1.044304	6.853070	0.653194	H	1.129193	-0.069738	-5.949357
C	-1.960134	5.930200	1.466540	H	2.546266	1.074829	-3.786227

C	-1.982361	6.301937	2.944786	H	3.084704	-0.916829	-4.964340
C	-0.536692	6.458769	3.460403	H	5.010092	1.972440	-5.351310
H	0.742746	5.854570	1.299637	H	3.234931	3.632185	-3.491647
H	-1.460854	7.867798	0.611632	H	5.662134	4.278459	-3.473374
H	-1.531138	4.924744	1.393549	H	4.609724	5.512570	-4.201669
H	-2.486790	7.271246	3.062177	H	5.251223	4.549586	-6.246559
H	-0.538179	6.903378	4.460332	H	6.725199	1.282610	-4.418559
C	1.404947	7.761876	0.591520	H	7.636663	-0.393906	-2.904432
O	-3.287843	5.945600	0.945788	H	5.003388	-0.642146	-3.812298
O	-2.611805	5.315342	3.755398	H	5.257929	0.175770	-1.104800
H	1.014034	8.163881	-0.344399	H	6.625500	-1.191796	0.324239
O	2.585644	7.040198	0.242705	H	8.195543	0.803942	-0.567986
H	1.637644	8.602950	1.257263	H	5.961081	2.804551	-1.147226
H	-3.222670	5.875060	-0.032150	H	7.924146	3.606862	0.208328
H	-3.400415	4.944801	3.314968	H	7.772361	4.413398	-1.368956
H	2.985728	6.650497	1.051625	H	9.356383	2.829366	-2.089385
C	-1.583436	2.797824	-0.264260	C	-3.520908	1.369213	-0.721005
C	-2.105174	2.346483	0.945231	C	-2.712337	1.520810	-1.842271
C	-2.299892	0.980948	1.143312	C	-1.446225	0.944558	-1.849773
C	-1.971685	0.042422	0.161470	C	-0.981234	0.218018	-0.750645
C	-1.396874	0.498226	-1.043610	C	-1.831617	-0.002752	0.349719
C	-1.223831	1.871293	-1.240685	C	-3.095554	0.586195	0.348659
C	-0.753161	-0.470558	-2.014895	C	-1.439669	-0.959328	1.458961
C	0.349640	-1.143522	-1.242006	C	-1.175916	-2.315120	0.850302
C	1.685982	-0.764583	-1.346277	C	-2.051505	-3.390458	1.003634
C	2.645007	-1.301998	-0.485543	C	-1.801459	-4.618235	0.383158
C	2.258901	-2.221105	0.489357	C	-0.667990	-4.759587	-0.416759
C	0.921913	-2.614815	0.597322	C	0.213093	-3.687027	-0.591714
C	-0.040489	-2.078403	-0.262114	C	-0.024805	-2.461508	0.043199
C	-2.277125	-1.415686	0.485232	C	0.483702	-0.144091	-0.753174
N	-1.427038	-2.403658	-0.205681	N	0.861855	-1.361282	-0.026731
C	-3.754416	-1.734783	0.181028	C	1.253288	1.046875	-0.148849
C	-1.763438	-3.761139	0.213681	C	2.294983	-1.578436	-0.154212
C	-3.224706	-4.065544	-0.090135	C	3.025323	-0.429009	0.539805
N	-4.104780	-3.102188	0.593712	N	2.696492	0.834600	-0.123050
C	-5.519586	-3.407209	0.325008	C	3.346160	1.981422	0.502790
H	-1.428889	3.855597	-0.441330	H	-4.489440	1.845947	-0.685979
H	-2.365920	3.039088	1.737681	H	-3.061033	2.088565	-2.693742
H	-2.725838	0.638507	2.081398	H	-0.795874	1.067466	-2.712203
H	-0.768883	2.209672	-2.167652	H	-3.753683	0.438360	1.196558
H	-0.358009	0.067774	-2.879763	H	-2.237948	-1.017857	2.201607
H	-1.464028	-1.227173	-2.354885	H	-0.530150	-0.610674	1.963344
H	1.975682	-0.033503	-2.096676	H	-2.932850	-3.267256	1.627031
H	3.680306	-0.998429	-0.589559	H	-2.486845	-5.449029	0.519206
H	2.987365	-2.642381	1.174814	H	-0.474940	-5.702946	-0.919773
H	0.637655	-3.335503	1.355123	H	1.069026	-3.795651	-1.245931
H	-2.142972	-1.536262	1.576375	H	0.806316	-0.245119	-1.806142
H	-3.934332	-1.586299	-0.897482	H	0.854548	1.229165	0.868874
H	-4.388530	-1.032542	0.727506	H	1.043255	1.941469	-0.744526
H	-1.587423	-3.920887	1.289285	H	2.613007	-1.607231	-1.211712
H	-1.131343	-4.460753	-0.335098	H	2.561172	-2.528593	0.304487
H	-3.463505	-5.068839	0.271037	H	4.104657	-0.592396	0.490898
H	-3.399457	-4.052902	-1.174752	H	2.737209	-0.422337	1.609029
H	-5.737765	-3.410744	-0.753089	H	3.002852	2.148216	1.540979
H	-6.163861	-2.685367	0.833979	H	3.125845	2.886636	-0.072776
H	-5.744679	-4.402332	0.721130	H	4.426297	1.835844	0.525227

[β -CD]-[β -CD] DIMER WATER							
[β -CD-CCCW]-[β -CD-CCCW]				[β -CD-EXP]-[β -CD-EXP]			
E	-8550.99227908			E	-8550.95018374		
Atom	x [Å]	y [Å]	z [Å]	Atom	x [Å]	y [Å]	z [Å]
O	4.815588	3.620518	4.535495	C	0.307051	0.321704	7.121579
C	4.631287	3.689226	3.104087	C	-0.581667	-0.886947	6.796032
C	3.582945	4.779786	2.849135	O	0.272607	-1.909539	6.311090
C	2.260033	4.425934	3.542339	C	-1.668771	-0.485129	5.804713
C	2.485895	4.154931	5.028251	O	-2.570983	-1.575174	5.644995
C	3.661634	3.176453	5.218105	C	-2.425137	0.760809	6.292108
H	4.239281	2.733004	2.740805	O	-3.236452	1.176026	5.188951
H	3.952629	5.737504	3.238796	C	-1.458827	1.888384	6.694351
H	1.865478	3.513429	3.072368	O	-0.478536	1.383732	7.626216
H	2.766189	5.104465	5.506748	C	-2.132473	3.061436	7.381258
H	3.939863	3.127311	6.275582	O	-1.155637	4.090575	7.515776
C	6.012099	3.900987	2.458803	C	-4.619812	1.396960	5.368906
O	3.262724	4.901055	1.464722	C	-5.392664	0.555202	4.333035
O	1.335597	5.502325	3.391601	O	-4.986390	-0.798788	4.483352
O	1.364031	3.584951	5.686496	C	-5.171194	1.095486	2.921712
O	3.254916	1.912221	4.749683	O	-6.075269	0.436016	2.039904
H	6.015290	4.791519	1.828803	C	-5.416751	2.605993	2.891950
O	6.390298	2.818514	1.609404	O	-5.096805	3.060780	1.572613
H	6.744000	4.045435	3.263839	C	-4.567139	3.317850	3.946691
H	1.354868	5.776946	2.447099	O	-4.934990	2.768176	5.233208
H	0.523042	3.953692	5.347049	C	-4.762348	4.839037	3.984269
H	6.415683	1.989317	2.136311	O	-6.087120	5.273037	3.702241
O	4.808198	-1.285989	5.665407	C	-6.094757	3.719277	0.825008
C	4.624175	-0.124316	4.826203	C	-6.151990	3.094828	-0.574992
C	3.574628	0.754479	5.518581	O	-6.447437	1.718540	-0.400328
C	2.251946	-0.008830	5.672631	C	-4.841068	3.345640	-1.310620
C	2.477628	-1.339382	6.387585	O	-4.976797	2.896134	-2.655352
C	3.654632	-2.097251	5.742441	C	-4.497841	4.838842	-1.289208
H	4.233373	-0.436843	3.851735	O	-3.164008	4.949467	-1.797177
H	3.943078	1.047188	6.510657	C	-4.567392	5.440872	0.125795
H	1.858762	-0.210708	4.665731	O	-5.834986	5.109722	0.743964
H	2.756507	-1.121369	7.428670	C	-4.439304	6.954811	0.133608
H	3.932649	-2.954580	6.363544	O	-5.411816	7.511914	-0.744903
C	6.004871	0.512952	4.590756	C	-2.890405	5.861988	-2.841853
O	1.326060	0.779585	6.419033	C	-2.238311	5.096116	-4.012200
O	1.356265	-2.209989	6.350969	O	-3.098319	4.019005	-4.364469
O	3.249725	-2.519437	4.461451	C	-0.828399	4.638880	-3.645130
H	6.007297	1.560611	4.894644	O	-0.198619	4.138857	-4.821758
O	6.384019	0.502904	3.215102	C	-0.027734	5.812537	-3.075337
H	6.736574	-0.026320	5.205910	O	1.252034	5.303497	-2.684005
H	1.345004	1.689221	6.044744	C	-0.767348	6.448881	-1.896313
H	0.514906	-1.715103	6.426017	O	-2.047119	6.904058	-2.396697
H	6.410741	-0.425922	2.895093	C	-0.037784	7.640705	-1.262995
O	4.807521	-5.228277	2.533902	O	0.695060	8.436750	-2.186359
C	4.621981	-3.847977	2.918554	C	2.401509	5.853148	-3.287429
C	3.570980	-3.842142	4.035973	C	3.319842	4.710588	-3.741775
C	2.249375	-4.439322	3.533387	O	2.567093	3.903486	-4.631540
C	2.476764	-5.827712	2.939129	C	3.850818	3.946000	-2.533200
C	3.655163	-5.795068	1.946022	O	4.816210	3.001799	-2.983398
H	4.231844	-3.281343	2.066083	C	4.478168	4.907524	-1.510538
H	3.938759	-4.435033	4.883858	O	4.729924	4.135086	-0.332339
H	1.856913	-3.778166	2.747215	C	3.527886	6.070622	-1.178531
H	2.754850	-6.505594	3.759079	O	3.090431	6.708917	-2.397245
H	3.934257	-6.815004	1.663385	C	4.160586	7.159565	-0.333214
C	6.001698	-3.265388	3.271735	O	3.117648	8.048180	0.059045
O	1.322004	-4.531935	4.613826	C	6.035517	4.076015	0.208602
O	1.356697	-6.342553	2.234043	C	6.442257	2.599728	0.356971
O	3.251405	-5.057024	0.816720	O	6.365575	1.998712	-0.927403
H	6.002138	-2.849222	4.280063	C	5.560937	1.912143	1.395116
O	6.381396	-2.196286	2.406202	O	6.075699	0.606039	1.637231
H	6.734093	-4.082023	3.235288	C	5.548015	2.713295	2.699380
H	1.339792	-3.672154	5.091638	O	4.558715	2.103720	3.537195
H	0.514578	-6.093720	2.666876	C	5.215922	4.194374	2.459950
H	6.410249	-2.525826	1.480766	O	6.102202	4.730425	1.455327
O	4.813984	-5.238392	-2.500786	C	5.369342	5.048614	3.707071
C	4.626535	-4.678773	-1.181959	O	6.672958	4.858318	4.250226
C	3.574577	-5.548918	-0.482268	C	4.898289	1.755312	4.864678

C	2.254104	-5.528405	-1.264367	C	4.604463	0.255436	5.078717
C	2.483731	-5.929655	-2.719913	O	5.289901	-0.474093	4.068080
C	3.662661	-5.132490	-3.311991	C	3.101118	-0.010020	5.089978
H	4.236423	-3.659006	-1.270830	O	2.886180	-1.355601	5.508312
H	3.942096	-6.581555	-0.416771	C	2.404030	0.958181	6.048472
H	1.861490	-4.501567	-1.238334	O	0.997924	0.705843	5.954531
H	2.762325	-6.993259	-2.738082	C	2.745008	2.407337	5.692912
H	3.943127	-5.547383	-4.285281	O	4.182299	2.539888	5.795862
C	6.005307	-4.591744	-0.504320	C	2.092580	3.452723	6.606797
O	1.326058	-6.430928	-0.664270	O	1.954059	3.041222	7.961446
O	1.364832	-5.699937	-3.563738	H	1.008590	0.067422	7.921333
O	3.258641	-3.789505	-3.439518	H	-1.064153	-1.205601	7.731110
H	6.004216	-5.120077	0.450031	H	-0.225887	-2.606054	5.835410
O	6.385172	-3.248494	-0.208226	H	-1.191599	-0.233750	4.846956
H	6.738470	-5.073047	-1.164208	H	-3.354307	-1.246865	5.145153
H	1.342592	-6.268398	0.305870	H	-3.055254	0.482430	7.147273
H	0.522091	-5.883314	-3.100469	H	-0.951264	2.247868	5.791614
H	6.414493	-2.730512	-1.042910	H	-2.507655	2.733653	8.361355
O	4.823311	-1.308012	-5.647354	H	-2.986773	3.388977	6.776102
C	4.634363	-1.990427	-4.387891	H	-1.548249	4.811401	8.025537
C	3.583310	-3.080469	-4.633539	H	-4.925871	1.117490	6.381842
C	2.263245	-2.457046	-5.107381	H	-6.462667	0.652957	4.565260
C	2.494386	-1.569145	-6.328260	H	-5.205149	-1.325626	3.687500
C	3.672270	-0.608448	-6.072154	H	-4.130240	0.903583	2.623704
H	4.242940	-1.285387	-3.646458	H	-6.067793	0.913348	1.177212
H	3.952596	-3.775324	-5.399340	H	-6.471160	2.806944	3.111247
H	1.868807	-1.837394	-4.289064	H	-3.503645	3.116512	3.771225
H	2.774844	-2.217997	-7.170586	H	-4.046403	5.293799	3.290597
H	3.953945	-0.105927	-7.002836	H	-4.501239	5.179539	4.991933
C	6.012775	-2.465308	-3.895608	H	-6.124980	5.450031	2.747225
O	1.336413	-3.489572	-5.440322	H	-7.069061	3.629326	1.314398
O	1.375564	-0.766989	-6.676880	H	-6.962710	3.589737	-1.128317
O	3.266068	0.328430	-5.102412	H	-6.239061	1.199484	-1.205406
H	6.012465	-3.541018	-3.714398	H	-4.038521	2.796901	-0.798092
O	6.390178	-1.859686	-2.659868	H	-4.216593	3.252095	-3.171827
H	6.746926	-2.248213	-4.682063	H	-5.198522	5.374294	-1.938381
H	1.352152	-4.146660	-4.708304	H	-3.752666	5.021430	0.728013
H	0.532886	-1.243810	-6.532092	H	-3.421600	7.209169	-0.184735
H	6.418875	-0.884087	-2.774828	H	-4.577972	7.311523	1.164269
O	4.827831	3.602751	-4.536698	H	-5.212585	8.451987	-0.843704
C	4.639027	2.192613	-4.284753	H	-3.812382	6.348150	-3.174099
C	3.590287	1.704202	-5.292161	H	-2.154072	5.796686	-4.855076
C	2.269450	2.462720	-5.102737	H	-2.625830	3.349723	-4.899240
C	2.499727	3.971023	-5.169346	H	-0.893814	3.852896	-2.878678
C	3.675956	4.370609	-4.256791	H	0.758375	4.007621	-4.625372
H	4.245509	2.052837	-3.272027	H	0.097348	6.579074	-3.847643
H	3.961571	1.869606	-6.312205	H	-0.944453	5.701470	-1.113362
H	1.873368	2.209085	-4.108750	H	0.621477	7.272114	-0.471569
H	2.781559	4.225270	-6.201383	H	-0.799651	8.271374	-0.789649
H	3.957547	5.411632	-4.444037	H	1.621795	8.150908	-2.114624
C	6.017761	1.512100	-4.345971	H	2.128015	6.476861	-4.143379
O	1.344563	2.078839	-6.119203	H	4.173615	5.161773	-4.267529
O	1.379773	4.742918	-4.761157	H	2.979141	3.024626	-4.764926
O	3.267548	4.196661	-2.920372	H	3.008864	3.436762	-2.042896
H	6.019078	0.699799	-5.074043	H	5.264348	2.623290	-2.190449
O	6.392578	0.923559	-3.101225	H	5.419219	5.297790	-1.920087
H	6.752449	2.262477	-4.665010	H	2.658079	5.668018	-0.646113
H	1.360919	1.096850	-6.176583	H	4.925193	7.676055	-0.930904
H	0.537778	4.331912	-5.044983	H	4.652483	6.700966	0.533478
H	6.420172	1.621795	-2.410182	H	3.519881	8.801979	0.510102
O	4.824299	5.795978	-0.005086	H	6.744232	4.597934	-0.442003
C	4.637609	4.720026	-0.951193	H	7.479823	2.579447	0.719286
C	3.589876	5.202727	-1.962413	H	6.339205	1.020916	-0.863370
C	2.267787	5.526376	-1.253067	H	4.533661	1.857491	1.007446
C	2.495815	6.518618	-0.114679	H	5.658453	0.261309	2.461022
C	3.671140	6.054813	0.768209	H	6.535423	2.644289	3.167885
H	4.244059	3.840557	-0.429987	H	4.178328	4.278957	2.113570
H	3.961098	6.103904	-2.468157	H	4.594061	4.748046	4.421427
H	1.871685	4.590679	-0.832615	H	5.198683	6.098948	3.431935
H	2.777602	7.484334	-0.558694	H	6.694024	5.287318	5.115444
H	3.951087	6.850336	1.465926	H	5.955313	1.963993	5.053787
C	6.017437	4.344842	-1.519612	H	4.999519	-0.016656	6.067810

O	1.343976	6.081494	-2.188172	H	4.934498	-1.381907	3.985727
O	1.374573	6.679781	0.741818	H	2.700897	0.148331	4.077892
H	6.019829	4.406526	-2.608719	H	1.923619	-1.471899	5.685180
O	6.393701	3.005497	-1.202024	H	2.748167	0.771611	7.071436
H	6.750789	5.063486	-1.131826	H	2.447084	2.622982	4.659437
H	1.361896	5.514433	-2.991894	H	1.118988	3.728929	6.191377
H	0.533295	6.645423	0.242300	H	2.727358	4.346330	6.579050
H	6.420102	2.901322	-0.225145	H	1.033355	2.744738	8.061670
O	-4.808163	5.541095	-1.745252	C	0.259074	-0.321063	-7.123619
C	-4.624125	4.799818	-0.518777	C	-0.628582	0.886851	-6.792458
C	-3.574590	5.561821	0.300443	O	0.227910	1.910251	-6.313213
C	-2.251939	5.652935	-0.472932	C	-1.708978	0.484205	-5.794140
C	-2.477657	6.256668	-1.857485	O	-2.611265	1.573443	-5.629045
C	-3.654592	5.551603	-2.560046	C	-2.467260	-0.762620	-6.276299
H	-4.233263	3.803067	-0.750555	C	-3.270661	-1.178566	-5.167622
H	-3.943085	6.574493	0.511171	O	-1.502545	-1.889288	-6.684912
H	-1.858746	4.632892	-0.591801	O	-0.528803	-1.383769	-7.623122
H	-2.756554	7.312092	-1.725310	C	-2.179471	-3.063037	-7.367430
H	-3.932631	6.100487	-3.465310	O	-1.202461	-4.091180	-7.508117
C	-6.004792	4.617266	0.135622	C	-4.654930	-1.401162	-5.338226
O	-3.254775	4.890250	1.517233	C	-5.421698	-0.560135	-4.297241
O	-1.326044	6.461262	0.251814	O	-5.017892	0.794256	-4.450520
O	-1.356288	6.148962	-2.722187	C	-5.190157	-1.100088	-2.887409
O	-3.249524	4.240396	-2.875958	O	-6.089243	-0.441787	-1.999533
H	-6.007144	5.005761	1.154933	C	-5.433767	-2.610879	-2.855899
O	-6.383997	3.245416	0.238080	O	-5.104505	-3.064879	-1.538605
H	-6.736502	5.186332	-0.452073	C	-4.590573	-3.321962	-3.916302
H	-1.345246	6.162767	1.189043	O	-4.967643	-2.772726	-5.200329
H	-0.514963	6.264607	-2.235112	C	-4.784566	-4.843324	-3.952536
H	-6.410684	2.850650	-0.661512	O	-6.107280	-5.278468	-3.662669
O	-4.807176	2.097485	-5.417933	C	-6.096294	-3.725492	-0.784694
C	-4.621759	2.594002	-4.073789	C	-6.145427	-3.101651	0.615876
C	-3.570593	3.708018	-4.159411	O	-6.444110	-1.725727	0.443644
C	-2.248984	3.158063	-4.713211	C	-4.829445	-3.350794	1.343111
C	-2.476277	2.452160	-6.048312	O	-4.957457	-2.902172	2.688892
C	-3.654796	1.465162	-5.934604	C	-4.483988	-4.843462	1.318702
H	-4.231791	1.790814	-3.439109	O	-3.146916	-4.952388	1.818444
H	-3.938155	4.504473	-4.819879	C	-4.561320	-5.444582	-0.096274
H	-1.856715	2.428613	-3.989861	O	-5.833557	-5.115477	-0.705934
H	-2.754144	3.213886	-6.791099	C	-4.430284	-6.958226	-0.106098
H	-3.933784	1.100052	-6.928055	O	-5.396341	-7.517932	0.777822
C	-6.001543	2.993938	-3.522349	C	-2.865730	-5.864675	2.861327
O	-1.321411	4.227157	-4.893785	C	-2.206707	-5.098229	4.027394
O	-1.356299	1.707044	-6.503458	O	-3.065400	-4.021966	4.385451
O	-3.251131	0.399992	-5.106611	C	-0.799687	-4.639635	3.651022
H	-6.001947	4.032948	-3.190056	O	-0.162512	-4.138991	4.823427
O	-6.381690	2.218816	-2.386143	C	-0.001662	-5.812543	3.076035
H	-6.733758	2.890927	-4.333442	O	1.274970	-5.302267	2.676134
H	-1.339431	4.773946	-4.076133	C	-0.748342	-6.449838	1.901995
H	-0.514114	2.158618	-6.290717	O	-2.024464	-6.906044	2.410775
H	-6.410147	1.269497	-2.638754	C	-0.021849	-7.641270	1.264342
O	-4.814115	-2.921012	-5.015932	O	0.718045	-8.436081	2.183104
C	-4.626465	-1.560871	-4.566053	C	2.428985	-5.850710	3.271869
C	-3.574518	-0.934829	-5.490570	C	3.349289	-4.707237	3.719909
C	-2.254089	-1.712805	-5.406481	O	2.601791	-3.900756	4.614645
C	-2.483979	-3.196320	-5.687095	C	3.871421	-3.942244	2.507741
C	-3.662922	-3.721017	-4.844120	O	4.839073	-2.997230	2.951332
H	-4.236361	-1.566095	-3.542444	C	4.492631	-4.903257	1.480858
H	-3.942408	-0.953937	-6.524951	O	4.735646	-4.130572	0.300998
H	-1.861133	-1.602704	-4.385367	C	3.541233	-6.067245	1.155387
H	-2.762623	-3.301410	-6.745615	O	3.112724	-6.705908	2.377094
H	-3.943522	-4.724856	-5.178201	C	4.169343	-7.155508	0.305812
C	-6.005151	-0.878206	-4.534742	O	3.124836	-8.045392	-0.079273
O	-1.326261	-1.188812	-6.355432	C	6.037413	-4.070646	-0.249026
O	-1.365184	-4.018690	-5.389228	C	6.442084	-2.594063	-0.400165
O	-3.258870	-3.738585	-3.495224	O	6.373952	-1.993244	0.884783
H	-6.004127	0.029527	-5.139717	C	5.553069	-1.907093	-1.432139
O	-6.384588	-0.472821	-3.220219	O	6.065125	-0.600599	-1.677899
H	-6.738495	-1.575310	-4.960046	C	5.531603	-2.708273	-2.736295
H	-1.342679	-0.208600	-6.272996	O	4.536107	-2.099291	-3.567183
H	-0.522474	-3.572106	-5.610250	C	5.202181	-4.189565	-2.494572
H	-6.413867	-1.262211	-2.635539	O	6.095887	-4.724953	-1.496186

O	-4.823420	-5.736011	-0.841465	C	5.347611	-5.043818	-3.742626
C	-4.634381	-4.536546	-1.624506	O	6.647580	-4.853050	-4.294261
C	-3.583565	-4.870660	-2.690995	C	4.866246	-1.750693	-4.896994
C	-2.263423	-5.291944	-2.031004	C	4.569651	-0.251082	-5.109094
C	-2.494428	-6.435990	-1.046025	O	5.261241	0.478985	-4.103053
C	-3.672344	-6.102227	-0.109543	C	3.066022	0.013121	-5.110369
H	-4.242662	-3.740091	-0.982466	O	2.847162	1.358459	-5.527463
H	-3.952951	-5.690752	-3.320828	C	2.363435	-0.955825	-6.064072
H	-1.868950	-4.425585	-1.480524	O	0.957790	-0.704521	-5.961001
H	-2.774778	-7.328712	-1.623627	C	2.707952	-2.404619	-5.710402
H	-3.954060	-6.988771	0.467315	O	4.144613	-2.536021	-5.823181
C	-6.012731	-4.084334	-2.137810	C	2.050110	-3.450851	-6.619370
O	-1.336644	-5.708358	-3.032826	O	1.902062	-3.040068	-7.973231
O	-1.375583	-6.717467	-0.217943	H	0.955238	-0.066204	-7.927876
O	-3.266186	-5.059097	0.744872	H	-1.117343	1.204926	-7.724477
H	-6.012561	-3.992137	-3.224744	H	-0.268012	2.606100	-5.833907
O	-6.389487	-2.802831	-1.635723	H	-1.225487	0.233640	-4.839347
H	-6.747145	-4.850001	-1.856712	H	-3.391130	1.244509	-5.124241
H	-1.352346	-5.032607	-3.747663	H	-3.103444	-0.484962	-7.127186
H	-0.532902	-6.612520	-0.705092	H	-0.988783	-2.248280	-5.785494
H	-6.418131	-2.837207	-0.653968	H	-2.561234	-2.735701	-8.345132
O	-4.828041	-4.226770	3.961660	H	-3.029531	-3.391404	-6.756781
C	-4.639241	-4.091298	2.535598	H	-1.597633	-4.812500	-8.015187
C	-3.590536	-5.135435	2.131507	H	-4.968181	-1.122090	-6.349064
C	-2.269686	-4.884447	2.871906	H	-6.493138	-0.659084	-4.522202
C	-2.499903	-4.826909	4.380587	H	-5.231282	1.320885	-3.653067
C	-3.676183	-3.884685	4.703940	H	-4.147509	-0.906885	-2.596289
H	-4.245634	-3.093493	2.313204	H	-6.075727	-0.919405	-1.137094
H	-3.961846	-6.138446	2.380084	H	-6.489423	-2.812959	-3.068034
H	-1.873569	-3.914678	2.537482	H	-3.526113	-3.119592	-3.748002
H	-2.781562	-5.834601	4.718839	H	-4.064231	-5.297341	-3.262932
H	-3.957697	-3.985857	5.756802	H	-4.529038	-5.183757	-4.961651
C	-6.018074	-4.207763	1.862464	H	-6.138990	-5.456202	-2.707571
O	-1.344872	-5.929058	2.572780	H	-7.073950	-3.637074	-1.267641
O	-1.379886	-4.356572	5.116175	H	-6.951807	-3.597966	1.174263
O	-3.267983	-2.566956	4.420950	H	-6.230619	-1.206773	1.247360
H	-6.019785	-4.999785	1.112370	H	-4.030974	-2.800555	0.825839
O	-6.392724	-3.015205	1.174180	H	-4.193623	-3.257386	3.200509
H	-6.752715	-4.464197	2.636519	H	-5.179862	-5.380536	1.971706
H	-1.361129	-6.066821	1.598813	H	-3.751345	-5.023035	-0.703420
H	-0.537966	-4.673679	4.730138	H	-3.410157	-7.210792	0.205863
H	-6.420346	-2.269415	1.813617	H	-4.574427	-7.314412	-1.136193
O	-4.824388	0.469393	5.776922	H	-5.194616	-8.457670	0.874738
C	-4.637774	-0.561381	4.781778	H	-3.785116	-6.351613	3.199580
C	-3.590055	-1.529874	5.345372	H	-2.116276	-5.798805	4.869622
C	-2.267963	-0.796396	5.609634	H	-2.589771	-3.351941	4.916509
C	-2.495809	0.419139	6.505707	H	-0.870945	-3.853762	2.884978
C	-3.671183	1.261253	5.971587	H	0.792985	-4.006747	4.620540
H	-4.244169	-0.113648	3.862753	H	0.129324	-6.578827	3.847608
H	-3.961132	-1.960269	6.284948	H	-0.931205	-5.702783	1.120041
H	-1.872269	-0.453595	4.642606	H	0.631590	-7.272470	0.468194
H	-2.777406	0.055462	7.504516	H	-0.786300	-8.272980	0.796587
H	-3.951079	2.021663	6.707473	H	1.643931	-8.149074	2.105279
C	-6.017576	-1.158481	4.454121	H	2.161910	-6.474658	4.129674
O	-1.343802	-1.682928	6.238857	H	4.207021	-5.157570	4.239915
O	-1.374501	1.285866	6.596089	H	3.014068	-3.021589	4.745324
O	-3.262804	1.861093	4.764723	H	3.025738	-3.433724	2.023138
H	-6.020074	-2.238872	4.604724	H	5.281580	-2.618436	2.155371
O	-6.393544	-0.951514	3.093214	H	5.436800	-5.292670	1.883975
H	-6.751033	-0.713089	5.138441	H	2.667415	-5.665563	0.628876
H	-1.361583	-2.530145	5.739106	H	4.938678	-7.671037	0.898265
H	-0.533232	0.785190	6.602850	H	4.654747	-6.696346	-0.564236
H	-6.419778	0.013580	2.909447	H	3.524716	-8.797546	-0.535152
O	-4.815571	4.816782	3.237219	H	6.750976	-4.592087	0.396649
C	-4.631231	3.395815	3.422854	H	7.477096	-2.573063	-0.769685
C	-3.582948	3.230951	4.530636	H	6.346151	-1.015464	0.821102
C	-2.260050	3.892988	4.121401	H	4.528470	-1.853193	-1.037333
C	-2.486007	5.351733	3.729703	H	5.641855	-0.256223	-2.498759
C	-3.661598	5.460717	2.738769	H	6.515658	-2.638612	-3.211689
H	-4.239240	2.955414	2.499593	H	4.167098	-4.274846	-2.140929
H	-3.952679	3.697607	5.453245	H	4.567533	-4.743587	-4.451880
H	-1.865305	3.350053	3.250433	H	5.179157	-6.094200	-3.466301

H	-2.766572	5.906379	4.636795	H	6.663017	-5.281476	-5.159877
H	-3.939818	6.510565	2.602857	H	5.922149	-1.958428	-5.093302
C	-6.012037	2.770079	3.686726	H	4.957836	0.021347	-6.100810
O	-1.335761	3.830973	5.206681	H	4.905705	1.386524	-4.018311
O	-1.364131	5.961314	3.107976	H	2.672627	-0.145426	-4.095643
H	-6.015160	2.215080	4.625845	H	1.883391	1.473839	-5.698181
O	-6.390226	1.834966	2.677361	H	2.700761	-0.769234	-7.089302
H	-6.743910	3.584263	3.764776	H	2.417319	-2.620190	-4.674838
H	-1.354936	2.912138	5.557754	H	1.079575	-3.727562	-6.197191
H	-0.523159	5.653113	3.503225	H	2.685693	-4.344002	-6.595503
H	-6.415782	2.292315	1.807872	H	0.980293	-2.744928	-8.067422