

A Combined Experimental and Theoretical Study on Structures, Interactions and Volumetric Properties of Guanidinium–Based Ionic Liquid Mixtures

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Electronic Supplementary Information

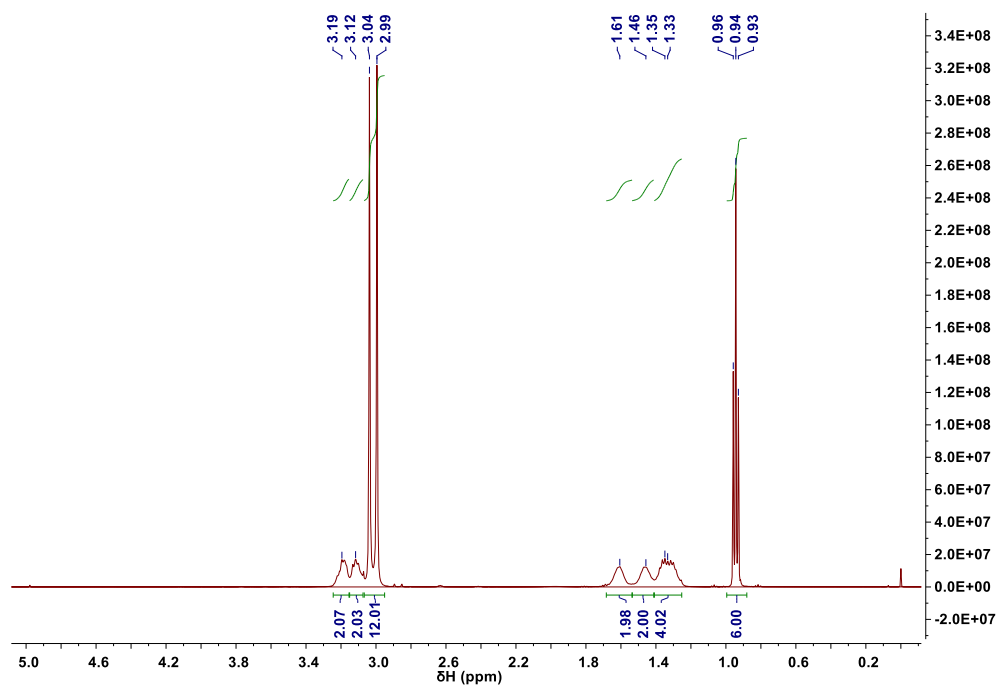


Fig. S1 ^1H NMR spectrum of 2,2-dibutyl-1,1,3,3-tetramethylguanidinium bis(trifluoromethylsulfonyl)amide at 298 K. Solvent is CDCl_3 .

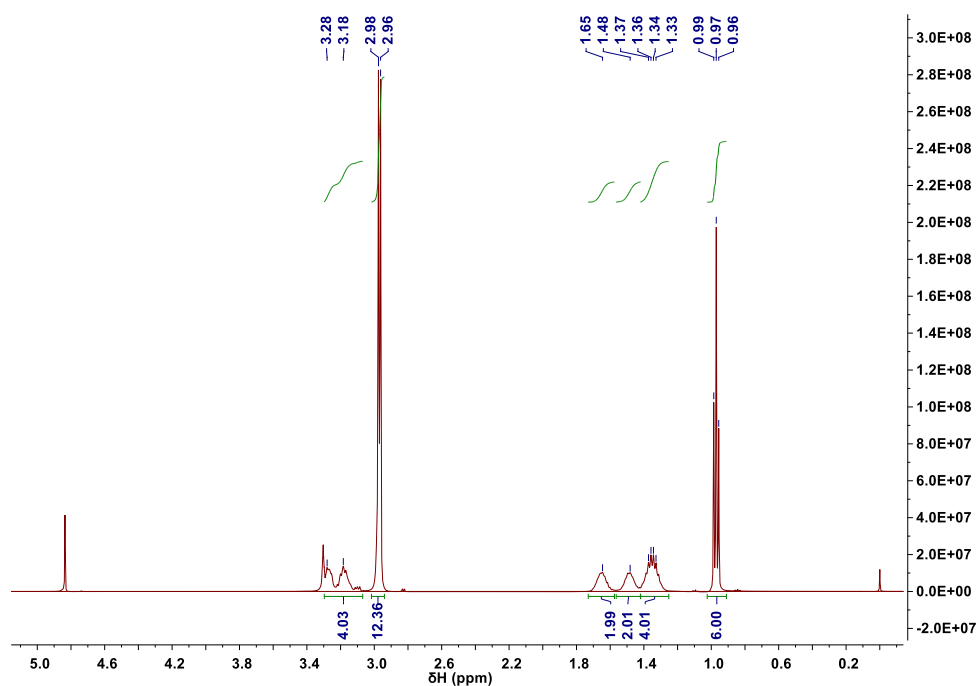


Fig. S2 ^1H NMR spectrum of 2,2-dibutyl-1,1,3,3-tetramethylguanidinium dicyanamide at 298 K. Solvent is CD_3OD .

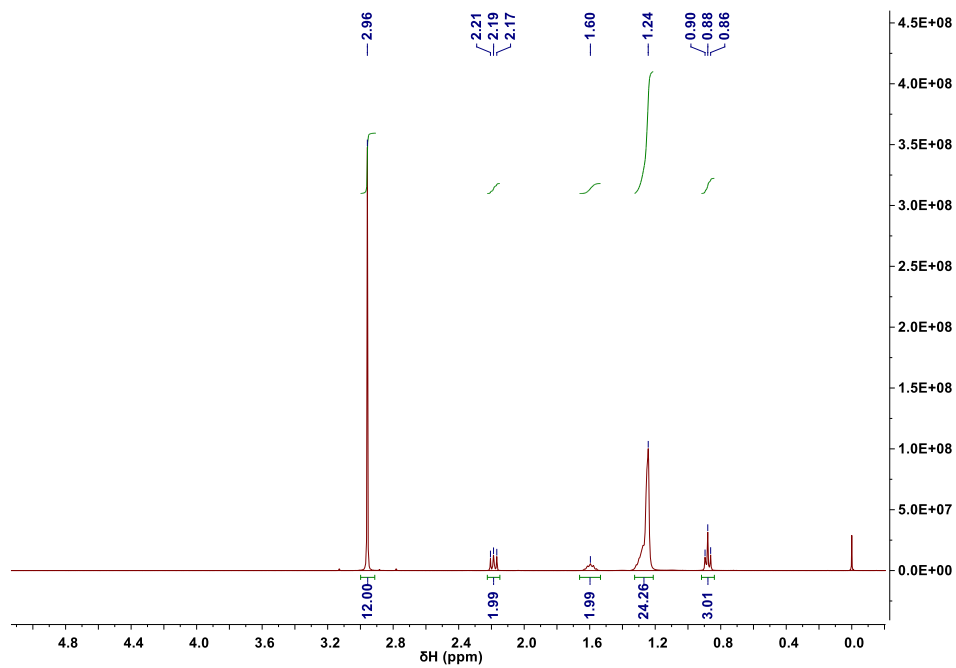


Fig. S3 ^1H NMR spectrum of 1,1,3,3-tetramethylguanidinium palmitate at 298 K. Solvent is CDCl_3 .

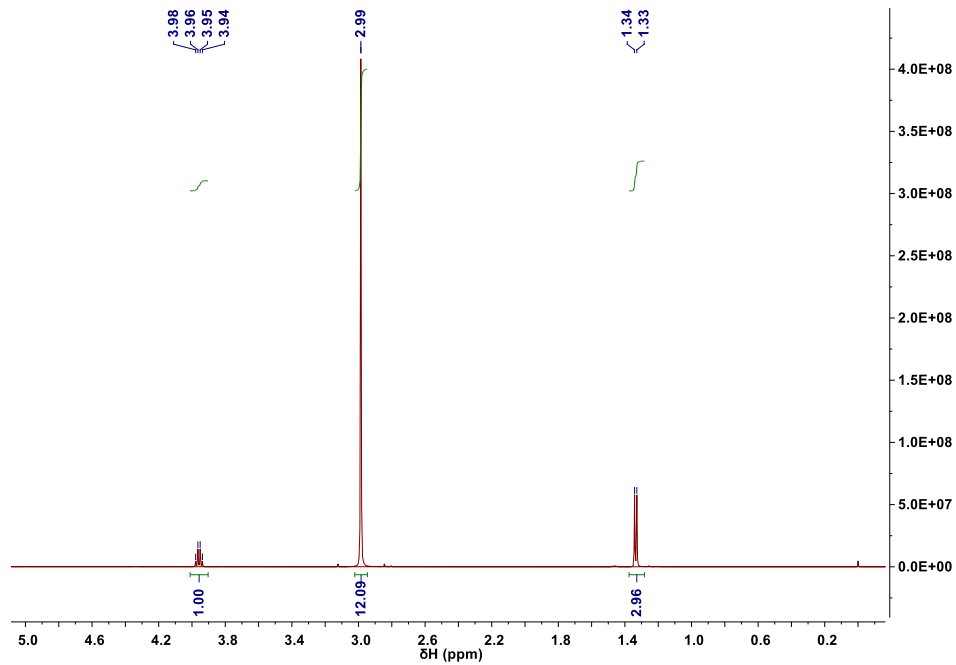


Fig. S4 ^1H NMR spectrum of 1,1,3,3-tetramethylguanidinium L-lactate at 298 K. Solvent is CDCl_3 .

Table S1 Densities ($\rho/\text{g}\cdot\text{cm}^{-3}$) of IL–IL mixtures at different temperatures (T) and pressure (p) of 101 kPa.

mole fraction (x)	T / K						
	293.15	298.15	303.15	308.15	313.15	318.15	323.15
x_{1a}	[TMG(C ₂)] _x [C ₂ OSO ₃] _{1-x} (1a+1b)						
0.0000	1.41489	1.41003	1.40519	1.40038	1.39559	1.39080	1.38603
0.1001	1.39458	1.38983	1.38508	1.38036	1.37566	1.37098	1.36632
0.1993	1.37347	1.36884	1.36423	1.35964	1.35507	1.35050	1.34594
0.2993	1.35149	1.34697	1.34248	1.33800	1.33353	1.32908	1.32464
0.4009	1.32807	1.32366	1.31928	1.31492	1.31057	1.30623	1.30191
0.5005	1.30439	1.30011	1.29586	1.29162	1.28738	1.28314	1.27892
0.6008	1.28009	1.27597	1.27188	1.26779	1.26372	1.25965	1.25559
0.6991	1.25524	1.25126	1.24730	1.24335	1.23941	1.23548	1.23156
0.7996	1.22855	1.22472	1.22093	1.21714	1.21335	1.20958	1.20583
0.9001	1.20045	1.19683	1.19322	1.18961	1.18600	1.18239	1.17879
1.0000	1.17076	1.16724	1.16376	1.16028	1.15680	1.15333	1.14987
x_{1a}	[TMG(C ₂)] _x [TMG(C ₂) ₂] _{1-x} [C ₂ OSO ₃] (1a+2a)						
0.0000	1.14134	1.13777	1.13421	1.13065	1.12711	1.12357	1.12003
0.0999	1.14412	1.14056	1.13700	1.13345	1.12991	1.12638	1.12285
0.1997	1.14692	1.14336	1.13981	1.13627	1.13274	1.12921	1.12568
0.2995	1.14989	1.14633	1.14279	1.13925	1.13572	1.13220	1.12868
0.3998	1.15300	1.14945	1.14593	1.14240	1.13888	1.13537	1.13186
0.5001	1.15625	1.15272	1.14920	1.14569	1.14220	1.13871	1.13523
0.5994	1.15936	1.15584	1.15234	1.14884	1.14535	1.14187	1.13839
0.7006	1.16252	1.15900	1.15551	1.15202	1.14854	1.14507	1.14160
0.7995	1.16523	1.16171	1.15823	1.15473	1.15124	1.14776	1.14429
0.8978	1.16784	1.16433	1.16085	1.15737	1.15390	1.15043	1.14697

1.0000	1.17076	1.16724	1.16376	1.16028	1.15680	1.15333	1.14987
x_{2b}	[TMG(C ₂) ₂] _x [TMG(C ₂)] _{1-x} [NTf ₂] (2b+1b)						
0.0000	1.41489	1.41003	1.40519	1.40038	1.39559	1.39080	1.38603
0.1001	1.41070	1.40586	1.40105	1.39626	1.39149	1.38672	1.38197
0.2003	1.40662	1.40180	1.39700	1.39223	1.38748	1.38274	1.37801
0.3002	1.40268	1.39788	1.39310	1.38836	1.38363	1.37891	1.37420
0.3996	1.39881	1.39403	1.38927	1.38454	1.37984	1.37515	1.37047
0.4980	1.39509	1.39033	1.38560	1.38089	1.37621	1.37154	1.36689
0.5975	1.39156	1.38681	1.38208	1.37739	1.37273	1.36808	1.36344
0.6992	1.38796	1.38323	1.37853	1.37385	1.36921	1.36458	1.35997
0.8006	1.38446	1.37974	1.37506	1.37041	1.36578	1.36118	1.35658
0.9000	1.38116	1.37645	1.37179	1.36715	1.36255	1.35797	1.35340
1.0000	1.37786	1.37316	1.36851	1.36390	1.35932	1.35476	1.35021
x_{2b}	[TMG(C ₂) ₂] ₂ [NTf ₂] _x [C ₂ OSO ₃] _{1-x} (2b+2a)						
0.0000	1.14134	1.13777	1.13421	1.13065	1.12711	1.12357	1.12003
0.1001	1.16906	1.16535	1.16166	1.15797	1.15430	1.15063	1.14696
0.1995	1.19575	1.19192	1.18810	1.18429	1.18051	1.17672	1.17294
0.3004	1.22179	1.21783	1.21389	1.20996	1.20605	1.20215	1.19825
0.3991	1.24627	1.24218	1.23812	1.23406	1.23003	1.22601	1.22199
0.5005	1.27050	1.26629	1.26211	1.25795	1.25381	1.24968	1.24556
0.5990	1.29317	1.28887	1.28460	1.28033	1.27609	1.27186	1.26764
0.7000	1.31549	1.31107	1.30669	1.30232	1.29799	1.29367	1.28935
0.8001	1.33693	1.33243	1.32797	1.32354	1.31912	1.31471	1.31031
0.9001	1.35740	1.35280	1.34825	1.34373	1.33923	1.33474	1.33026
1.0000	1.37786	1.37316	1.36851	1.36390	1.35932	1.35476	1.35021

Uncertainties are $u(T) = 0.01$ K, $u(p) = 1000$ Pa, $u(x) = 0.0001$, and $u(\rho) = 0.0003$ g·cm⁻³.

Table S2 Cartesian coordinates for all of the calculated IL-IL clusters

1a				H	-1.907113	2.866970	-0.866547	
H	-0.835144	0.964358	1.185461	H	-3.106272	3.711748	0.140689	
C	-1.732873	-0.588397	0.308160	H	-1.484833	3.364936	0.774011	
N	-2.469003	-0.917673	-0.789963	S	1.559330	1.075749	-0.119087	
N	-0.983744	-1.537945	0.913626	O	0.647774	0.461919	-1.126168	
C	-2.541308	-0.023239	-1.947277	O	2.348015	2.218457	-0.600885	
H	-2.287821	-0.595616	-2.847596	O	0.894803	1.269735	1.209804	
H	-3.547163	0.397769	-2.074914	O	2.654781	-0.134163	0.272622	
H	-1.800394	0.768398	-1.839253	C	3.663953	-0.402672	-0.722697	
C	-3.072125	-2.235110	-0.956140	H	4.217980	0.520047	-0.925530	
H	-3.056821	-2.774889	-0.008041	H	3.178937	-0.728887	-1.652357	
H	-4.115094	-2.112164	-1.273755	C	4.576012	-1.484935	-0.167784	
H	-2.551061	-2.832729	-1.716192	H	4.019281	-2.407825	0.032492	
C	-0.549167	-1.393463	2.307884	H	5.368194	-1.711415	-0.892119	
H	-0.437787	-2.396621	2.732421	H	5.044193	-1.155273	0.766030	
H	0.403185	-0.856241	2.369392					
H	-1.306831	-0.849295	2.875125	1b				
C	-0.203052	-2.500702	0.128850	C	2.843629	-0.492999	0.182562	
H	0.858978	-2.334352	0.336466	N	2.870636	-0.492453	1.535559	
H	-0.474533	-3.529405	0.395915	N	3.723461	0.283922	-0.503335	
H	-0.360002	-2.334339	-0.935439	C	2.332442	-1.612766	2.314511	
N	-1.755800	0.640829	0.828295	H	2.894517	-1.672565	3.251961	
C	-2.815161	1.644801	0.703900	H	1.268670	-1.476541	2.535701	
H	-3.618488	1.238927	0.084357	H	2.462846	-2.546266	1.763967	
H	-3.237134	1.808154	1.705328	C	3.043879	0.753041	2.292111	
C	-2.295729	2.974004	0.150564	H	3.134139	1.598845	1.612893	

H	2.151933	0.916916	2.905296	O	0.435498	1.407295	0.675430
H	3.925729	0.694057	2.941351	O	0.037405	1.727741	-1.800583
C	3.357907	0.981439	-1.741599	C	-1.658733	2.877909	-0.110606
H	3.627026	2.038813	-1.635614	F	-2.271299	2.714841	1.066262
H	3.897040	0.569623	-2.603803	F	-0.940524	4.014060	-0.071599
H	2.282795	0.933067	-1.910269	F	-2.583256	2.987763	-1.072445
C	5.062618	0.568699	0.006495	H	1.109011	-1.523309	0.029680
H	5.786504	0.411250	-0.802021				
H	5.155834	1.606056	0.352818	2a			
H	5.303616	-0.106133	0.829015	C	1.592683	0.267354	0.444791
N	1.986479	-1.295752	-0.456171	N	1.771100	-0.613507	1.458008
S	-1.677175	-0.879568	0.660743	N	0.899440	1.401880	0.657393
O	-2.235586	-0.346893	1.905755	C	2.966872	-1.442220	1.566939
O	-0.544190	-1.838023	0.788282	H	3.265961	-1.479886	2.620814
C	2.121174	-1.825188	-1.819015	H	2.781478	-2.469455	1.227849
H	3.167218	-1.721921	-2.120049	H	3.779457	-1.010699	0.982150
H	1.510607	-1.228569	-2.507294	C	0.706226	-0.943646	2.415392
C	1.686607	-3.290242	-1.870901	H	-0.231090	-0.462615	2.134943
H	1.755193	-3.658257	-2.900594	H	0.544680	-2.027325	2.387354
H	2.323512	-3.916933	-1.236499	H	1.001663	-0.656969	3.432689
H	0.649014	-3.404041	-1.540071	C	0.034382	1.996018	-0.368829
C	-3.043906	-1.898317	-0.141877	H	-0.943153	2.175260	0.085216
F	-2.623811	-2.459331	-1.284589	H	0.455907	2.941997	-0.734705
F	-3.385336	-2.874644	0.713398	H	-0.120776	1.289242	-1.181224
F	-4.118807	-1.146259	-0.390855	C	0.780991	2.019698	1.978500
N	-1.475240	0.155834	-0.566543	H	0.902620	3.102952	1.860948
S	-0.501198	1.431241	-0.466727	H	-0.203663	1.819913	2.414191

H	1.564516	1.649427	2.641115	H	3.993458	-2.168281	-1.023104
N	2.196984	0.035170	-0.754851				
C	2.693529	1.140171	-1.598358	2b			
H	1.867966	1.710890	-2.037704	C	-3.049133	0.038291	0.065733
H	3.212997	0.663812	-2.432680	N	-3.064342	0.726640	-1.095330
C	3.669206	2.074196	-0.880055	N	-3.475890	0.654154	1.200823
H	4.047248	2.820455	-1.588267	C	-3.225999	0.083685	-2.398897
H	3.194012	2.610854	-0.052970	H	-3.912270	0.691872	-2.998748
H	4.525572	1.517065	-0.483474	H	-2.269032	0.013895	-2.928051
S	-2.165129	-0.784869	0.063335	H	-3.650578	-0.912247	-2.275562
O	-0.817705	-1.059743	-0.506198	C	-2.756719	2.162629	-1.156113
O	-2.105447	0.161534	1.217963	H	-2.353499	2.497206	-0.202452
O	-3.022603	-1.964322	0.278300	H	-1.978194	2.311118	-1.909331
O	-2.864565	0.087628	-1.193451	H	-3.648384	2.741002	-1.427455
C	-4.303954	0.176979	-1.221318	C	-2.769592	0.508128	2.476595
H	-4.534208	0.383815	-2.272504	H	-2.445661	1.498507	2.814159
H	-4.725067	-0.799696	-0.960202	H	-3.424956	0.067446	3.239024
C	-4.852508	1.278153	-0.319966	H	-1.874522	-0.097080	2.344617
H	-4.627720	1.075453	0.731173	C	-4.558168	1.635342	1.198291
H	-5.942271	1.343967	-0.439426	H	-5.241681	1.403406	2.023890
H	-4.418201	2.249664	-0.584957	H	-4.185038	2.657601	1.337532
C	2.027149	-1.280231	-1.425338	H	-5.113384	1.581099	0.260751
H	1.375534	-1.115111	-2.292426	N	-2.658897	-1.257006	0.103509
H	1.450273	-1.917290	-0.755886	S	2.456417	-0.980566	-0.598730
C	3.328885	-1.952831	-1.865614	O	3.399751	-0.293255	-1.484283
H	3.085164	-2.903633	-2.353564	O	1.639585	-2.078617	-1.143166
H	3.888842	-1.353332	-2.592331	C	-3.289208	-2.219749	1.031444

H	-3.457865	-1.762592	2.007387	H	3.818076	-0.179719	1.669646
H	-2.564517	-3.023158	1.187319	C	2.596998	-0.639176	0.153998
C	-4.607081	-2.783519	0.491432	N	1.706411	-0.091490	-0.707712
H	-5.023569	-3.504375	1.205142	N	3.256146	-1.769570	-0.207655
H	-5.346597	-1.986706	0.349033	C	1.557713	1.360459	-0.835845
H	-4.463426	-3.294503	-0.465715	H	1.553597	1.608338	-1.904289
C	3.506561	-1.789316	0.742949	H	0.622307	1.707518	-0.385409
F	2.743836	-2.431907	1.642221	H	2.418539	1.851131	-0.381675
F	4.314664	-2.686104	0.154743	C	0.875460	-0.898315	-1.597826
F	4.260923	-0.887174	1.381334	H	0.961239	-1.952380	-1.327555
N	1.601859	-0.020323	0.415824	H	-0.169203	-0.586757	-1.487604
S	0.760710	1.238063	-0.086567	H	1.177274	-0.775397	-2.647422
O	0.366224	1.227090	-1.509636	C	3.838102	-2.667392	0.793705
O	-0.295755	1.518339	0.906951	H	3.809499	-3.687212	0.393194
C	1.902194	2.734115	0.077865	H	4.872739	-2.391919	1.025216
F	2.934348	2.648925	-0.763167	H	3.245055	-2.629890	1.709752
F	1.203704	3.851913	-0.207072	C	3.791442	-1.931038	-1.561578
F	2.367110	2.834632	1.331791	H	4.882285	-2.005487	-1.499066
C	-1.454544	-1.733637	-0.633542	H	3.387184	-2.835097	-2.035495
H	-0.689783	-1.950235	0.119752	H	3.553566	-1.055912	-2.164268
H	-1.067110	-0.902362	-1.220163	N	2.831810	-0.117189	1.360802
C	-1.664899	-2.966621	-1.509369	C	1.907237	0.662540	2.191294
H	-0.700351	-3.218068	-1.960952	H	0.956301	0.775281	1.667971
H	-1.994465	-3.836982	-0.931080	H	1.702028	0.069749	3.094096
H	-2.388427	-2.796155	-2.314044	C	2.490725	2.015450	2.604829
				H	2.665286	2.663600	1.740648
1a+1a				H	1.793322	2.521870	3.282114

H	3.446800	1.890072	3.124815	H	-4.243705	0.226158	-2.580311
S	6.148754	0.613835	0.428073	H	-5.063539	-1.336354	-2.839438
O	5.097079	0.931333	-0.575617	C	-6.449167	1.194504	-1.060201
O	7.112519	1.693031	0.695533	H	-5.674343	1.927181	-1.308407
O	5.605008	-0.073513	1.640584	H	-7.344320	1.388588	-1.663299
O	7.033818	-0.648830	-0.254774	H	-6.680573	1.301787	-0.001810
C	7.905052	-0.273225	-1.337188	N	-4.676872	-1.832337	-0.345568
H	8.610423	0.486172	-0.981827	C	-4.539489	-3.172577	0.231094
H	7.309172	0.161657	-2.151133	H	-5.485681	-3.452418	0.700089
C	8.631657	-1.527174	-1.798552	H	-4.376019	-3.874843	-0.597915
H	7.924748	-2.284833	-2.156712	C	-3.373638	-3.272817	1.217360
H	9.317413	-1.281060	-2.619096	H	-3.515998	-2.620856	2.084252
H	9.214113	-1.960968	-0.978240	H	-3.276409	-4.306064	1.569463
H	-3.810135	-1.360336	-0.660056	H	-2.431823	-2.986215	0.737873
C	-5.761004	-1.051451	-0.338839	S	-2.634565	0.939831	0.270021
N	-6.718183	-1.166264	0.622086	O	-3.864217	0.806692	1.093023
N	-5.920306	-0.146626	-1.330593	O	-1.395647	1.206471	1.022489
C	-6.361482	-1.346985	2.031241	O	-2.509695	-0.134003	-0.768662
H	-6.905840	-0.604714	2.626728	O	-2.888919	2.272623	-0.707878
H	-6.629330	-2.347340	2.395024	C	-2.878560	3.552670	-0.034099
H	-5.295512	-1.163262	2.162303	H	-1.922735	3.671498	0.487131
C	-8.135884	-0.965316	0.338643	H	-3.685832	3.573829	0.708924
H	-8.304562	-0.961559	-0.739308	C	-3.068222	4.627231	-1.091704
H	-8.707188	-1.790749	0.780669	H	-4.025094	4.507112	-1.612553
H	-8.509188	-0.024048	0.763091	H	-3.055886	5.617164	-0.619857
C	-5.214371	-0.279814	-2.610156	H	-2.263958	4.588573	-1.834067
H	-5.839163	0.167923	-3.389855				

1b+1b				C	-5.008841	3.456551	-2.345370
C	-2.283643	3.192980	0.076627	H	-5.988073	3.935592	-2.456457
N	-1.033420	2.798538	-0.227901	H	-4.287175	3.995821	-2.969160
N	-2.495985	4.030067	1.129131	H	-5.090843	2.430559	-2.719290
C	-0.684082	2.325544	-1.574368	C	-5.148992	-1.672179	-2.379105
H	0.384654	2.492671	-1.723021	F	-6.077429	-0.721557	-2.544113
H	-0.899538	1.257753	-1.690631	F	-4.652717	-2.001193	-3.582068
H	-1.251764	2.884735	-2.321603	F	-5.716612	-2.752379	-1.835694
C	-0.036966	2.513438	0.814880	N	-4.596792	-0.723697	0.000558
H	-0.503463	2.550860	1.798576	S	-3.912221	-0.243827	1.376918
H	0.355193	1.505388	0.659578	O	-2.476101	0.080929	1.272428
H	0.800273	3.214433	0.759488	O	-4.800226	0.703939	2.059531
C	-3.652328	3.890333	2.019982	C	-3.986049	-1.784009	2.464163
H	-3.291858	3.844581	3.054624	F	-3.273085	-2.783585	1.919866
H	-4.331707	4.747277	1.927791	F	-3.467183	-1.499074	3.670230
H	-4.187974	2.963816	1.815646	F	-5.248769	-2.193810	2.623958
C	-1.528003	5.056540	1.511465	H	-3.197042	1.898772	-1.187494
H	-2.066229	5.997765	1.677056	C	2.277362	-3.171080	0.014755
H	-0.998953	4.794469	2.436163	N	1.033247	-2.746404	-0.272241
H	-0.797042	5.208628	0.715661	N	2.486065	-3.999687	1.074138
N	-3.306406	2.788260	-0.691191	C	0.667152	-2.290947	-1.620089
S	-3.721385	-1.052704	-1.317341	H	-0.405681	-2.448912	-1.749707
O	-2.776193	-2.175330	-1.223696	H	0.893801	-1.227871	-1.756341
O	-3.239980	0.165859	-2.016080	H	1.216979	-2.868248	-2.366798
C	-4.591889	3.472655	-0.874168	C	0.065992	-2.417115	0.784925
H	-4.478725	4.499921	-0.517409	H	0.553158	-2.446393	1.758832
H	-5.360032	2.985771	-0.261053	H	-0.305492	-1.402999	0.619267

H	-0.789821	-3.098008	0.761972	O	5.112439	-0.663532	1.987442
C	3.655903	-3.872308	1.948510	C	3.983451	1.698091	2.474262
H	3.309858	-3.804014	2.986760	F	2.943926	2.460909	2.093380
H	4.316956	-4.743727	1.859668	F	3.782854	1.311231	3.743982
H	4.209088	-2.961097	1.724788	F	5.102623	2.425985	2.415930
C	1.496101	-4.992863	1.484324	H	3.211155	-1.907190	-1.259674
H	2.009273	-5.946310	1.658175				
H	0.983270	-4.703473	2.410330	2a+2a			
H	0.754733	-5.133614	0.696653	C	-3.486662	-1.338447	-0.021821
N	3.296240	-2.807406	-0.778734	N	-2.532316	-1.864152	-0.816830
S	3.699552	1.073841	-1.291319	N	-4.453815	-0.562453	-0.559701
O	2.725431	2.163286	-1.119236	C	-1.939744	-3.183059	-0.564690
O	3.218823	-0.140197	-1.997724	H	-1.852383	-3.697885	-1.528732
C	4.558574	-3.528880	-0.972787	H	-0.942542	-3.109322	-0.118418
H	4.421070	-4.549905	-0.606661	H	-2.597691	-3.761111	0.085918
H	5.349967	-3.061197	-0.374120	C	-1.915020	-1.103506	-1.914673
C	4.956202	-3.535062	-2.449471	H	-2.186734	-0.048666	-1.845744
H	5.919401	-4.043222	-2.570825	H	-0.829319	-1.206040	-1.814450
H	4.210250	-4.056388	-3.059696	H	-2.217252	-1.509814	-2.889205
H	5.063484	-2.514255	-2.831773	C	-5.028242	0.592034	0.136906
C	5.045274	1.769677	-2.411004	H	-5.009658	1.442986	-0.548749
F	5.993097	0.856672	-2.655396	H	-6.064442	0.389991	0.441457
F	4.470940	2.114905	-3.574741	H	-4.408625	0.862171	0.989149
F	5.606679	2.853711	-1.868766	C	-4.887886	-0.715276	-1.947348
N	4.654367	0.751806	-0.030883	H	-5.981511	-0.639918	-1.975608
S	4.085775	0.175675	1.361204	H	-4.465143	0.070909	-2.582826
O	2.697039	-0.321781	1.305443	H	-4.593798	-1.694420	-2.327993

N	-3.496899	-1.646292	1.304019	C	3.394935	1.361242	0.143166
C	-4.749803	-1.755301	2.074389	N	2.483048	1.558832	1.113391
H	-5.205298	-0.772102	2.240700	N	3.007380	1.206461	-1.137129
H	-4.459415	-2.127127	3.059027	C	2.765097	2.352166	2.305159
C	-5.767551	-2.721620	1.464944	H	1.891615	2.980200	2.510581
H	-6.636480	-2.801230	2.128505	H	2.945391	1.712822	3.179242
H	-6.124549	-2.383190	0.487266	H	3.633879	2.989226	2.137799
H	-5.335382	-3.721620	1.347090	C	1.167329	0.902219	1.121512
S	-2.064405	2.593563	-0.226602	H	1.092464	0.205212	0.291251
O	-2.079334	1.494764	0.771116	H	1.085236	0.328805	2.052098
O	-2.601177	2.194857	-1.556548	H	0.363809	1.638438	1.070140
O	-0.793971	3.359025	-0.288557	C	3.693753	0.283036	-2.044552
O	-3.197024	3.643166	0.430699	H	2.943023	-0.389384	-2.468744
C	-3.239872	4.989239	-0.088288	H	4.202031	0.830881	-2.849665
H	-3.639092	5.581351	0.742787	H	4.398546	-0.334994	-1.490639
H	-2.217167	5.326351	-0.289468	C	1.783150	1.802239	-1.683804
C	-4.125738	5.122421	-1.322406	H	2.038279	2.297199	-2.629132
H	-3.733135	4.528229	-2.152410	H	1.037192	1.028102	-1.887761
H	-4.171238	6.175023	-1.632537	H	1.350217	2.534550	-1.003709
H	-5.146363	4.785005	-1.105668	N	4.725211	1.374778	0.467566
C	-2.237134	-1.558192	2.089693	C	5.734912	1.930185	-0.452452
H	-2.333766	-0.683411	2.746283	H	5.880005	1.286506	-1.328468
H	-1.432325	-1.329163	1.392573	H	6.678981	1.914360	0.097543
C	-1.891457	-2.803431	2.906462	C	5.440881	3.366286	-0.890428
H	-0.930395	-2.636886	3.404136	H	6.258138	3.730081	-1.524003
H	-2.635084	-3.019466	3.682601	H	4.513615	3.437909	-1.466967
H	-1.776499	-3.688679	2.275667	H	5.358326	4.031749	-0.023791

S	2.080089	-2.507244	-0.036336	H	-1.688303	4.966586	-1.216489
O	3.117913	-1.646089	0.572366	C	-1.327816	3.490820	1.825295
O	1.415310	-1.900996	-1.229380	H	-1.859987	2.659465	2.286487
O	1.107885	-3.106615	0.913228	H	-0.295119	3.174897	1.648075
O	3.012056	-3.769353	-0.610890	H	-1.327416	4.364984	2.488821
C	2.326020	-4.905550	-1.173262	C	-5.055755	2.075648	1.090538
H	2.934894	-5.768867	-0.881785	H	-5.053081	1.680431	2.110821
H	1.345321	-5.012664	-0.696087	H	-6.074496	2.397239	0.836671
C	2.210654	-4.810147	-2.690342	H	-4.728441	1.272759	0.431266
H	1.615265	-3.939229	-2.979680	C	-4.260037	4.170499	2.120415
H	1.731856	-5.715664	-3.087187	H	-5.317052	4.447999	2.206673
H	3.202956	-4.719399	-3.147091	H	-3.933602	3.748763	3.078867
C	5.220629	0.489446	1.549255	H	-3.678140	5.067645	1.904779
H	5.810656	-0.306551	1.074606	N	-3.288968	2.884438	-1.149897
H	4.354915	-0.012214	1.982283	S	-3.341447	-1.927135	-0.945170
C	6.061201	1.183958	2.623140	O	-2.625816	-3.183016	-0.682690
H	6.385793	0.436253	3.356254	O	-3.084289	-1.213281	-2.204572
H	6.965855	1.647810	2.213456	C	-4.587915	3.017054	-1.839921
H	5.497853	1.955865	3.156286	H	-5.408585	2.728138	-1.182689
				H	-4.581439	2.291404	-2.657096
2b+2b				C	-4.830612	4.431507	-2.376792
C	-3.111914	3.287311	0.130147	H	-5.797330	4.472035	-2.893078
N	-1.929597	3.812123	0.523109	H	-4.855172	5.163885	-1.561250
N	-4.122471	3.204589	1.031907	H	-4.052056	4.732521	-3.084851
C	-1.100000	4.636567	-0.359872	C	-5.160848	-2.409568	-1.065464
H	-0.774677	5.517818	0.206088	F	-5.929147	-1.329647	-1.294018
H	-0.214911	4.090140	-0.696386	F	-5.321620	-3.268097	-2.083650

F	-5.578451	-2.998984	0.063148	C	2.052333	-2.502181	1.735013
N	-3.435843	-0.866224	0.283943	H	1.096038	-2.083860	2.061153
S	-2.520221	-0.906866	1.609202	H	2.458168	-3.132060	2.538452
O	-1.194555	-1.517123	1.448735	H	2.731374	-1.676619	1.528378
O	-2.630812	0.411573	2.250228	C	0.620425	-4.166399	0.587002
C	-3.417597	-2.041972	2.824910	H	0.672446	-4.733814	1.523975
F	-3.476073	-3.297464	2.361552	H	-0.309782	-3.593416	0.576170
F	-2.761550	-2.046820	3.996764	H	0.631582	-4.868300	-0.248280
F	-4.669840	-1.604471	3.040114	N	3.887339	-3.044269	-0.550742
C	-2.218926	2.139903	-1.871258	S	4.517943	1.149008	1.050088
H	-2.587019	1.116118	-2.003770	O	5.540907	0.883924	0.024963
H	-1.348709	2.084013	-1.217245	O	4.180939	0.048265	1.969049
C	-1.828016	2.725151	-3.228777	C	4.682906	-3.548945	0.591044
H	-1.038812	2.098682	-3.657765	H	4.500369	-2.950187	1.487950
H	-2.664244	2.726784	-3.937019	H	5.725966	-3.373744	0.321237
H	-1.437413	3.744812	-3.150935	C	4.484255	-5.039107	0.871677
C	2.539351	-3.183424	-0.598424	H	5.161475	-5.348115	1.676195
N	1.903142	-3.262217	-1.795099	H	3.463071	-5.268779	1.190769
N	1.800962	-3.293548	0.524517	H	4.712629	-5.641617	-0.015101
C	2.497961	-3.879043	-2.974365	C	5.230450	2.509160	2.143738
H	1.740724	-4.507478	-3.457874	F	4.365758	2.872228	3.098832
H	2.837161	-3.130613	-3.702257	F	6.338998	2.026833	2.729113
H	3.341693	-4.505888	-2.684489	F	5.561806	3.586300	1.421564
C	0.584507	-2.647812	-2.002809	N	3.226652	2.001008	0.538447
H	0.339501	-1.999160	-1.164029	S	2.255964	1.465681	-0.612686
H	0.630085	-2.033270	-2.908535	O	2.289502	0.012939	-0.859560
H	-0.199861	-3.402367	-2.121428	O	0.951543	2.131598	-0.477454

C	2.924441	2.207270	-2.218608	H	6.489279	1.093067	-0.794741
F	4.127759	1.708605	-2.525786	C	8.203282	0.462964	2.068411
F	2.075472	1.914792	-3.226644	H	9.194527	0.303370	1.627627
F	3.020101	3.542773	-2.126329	H	8.175255	1.474909	2.491913
C	4.598078	-2.121340	-1.474751	H	8.054383	-0.264206	2.867754
H	5.011387	-1.310995	-0.865386	N	5.580550	-1.216373	0.215752
H	3.850191	-1.660331	-2.119308	S	1.792892	-0.881445	-0.534060
C	5.717128	-2.765499	-2.296287	O	0.566992	-0.555203	0.206384
H	6.180642	-1.991948	-2.919054	O	2.742218	-1.812976	0.131474
H	6.508668	-3.183675	-1.664670	C	6.288084	-1.681562	-0.984842
H	5.355465	-3.560269	-2.956300	H	7.361521	-1.591213	-0.799640
1a+1b				H	6.036111	-1.034064	-1.833120
C	6.093601	-0.493267	1.217195	C	5.917475	-3.130581	-1.303031
N	5.537520	-0.572190	2.447740	H	6.425197	-3.445870	-2.221220
N	7.193603	0.282195	1.027107	H	6.218183	-3.805117	-0.493501
C	4.676924	-1.697451	2.826474	H	4.839247	-3.236201	-1.460348
H	4.754987	-1.832789	3.909618	C	1.228073	-1.816540	-2.069123
H	3.631254	-1.512065	2.558314	F	2.272520	-2.195824	-2.816987
H	5.015047	-2.610022	2.331939	F	0.572339	-2.915568	-1.661097
C	5.406810	0.613424	3.302984	F	0.402279	-1.072826	-2.809850
H	5.819613	1.488206	2.803587	N	2.519688	0.328218	-1.314821
H	4.343261	0.803386	3.478365	S	3.249773	1.541900	-0.544248
H	5.912917	0.456319	4.262779	O	3.468859	1.311818	0.897210
C	7.400805	1.063981	-0.198161	O	4.375273	2.015793	-1.357541
H	7.640829	2.094665	0.087137	C	1.996350	2.948999	-0.629482
H	8.232939	0.664698	-0.790984	F	0.876810	2.620817	0.029187
				F	2.526567	4.043616	-0.062708

F	1.686966	3.225228	-1.900908	H	-3.093364	2.812931	-0.240524
H	4.580479	-1.444601	0.261117	H	-2.115518	3.046279	-1.705979
H	-4.689146	0.391386	-1.199434	H	-3.854486	2.706334	-1.831858
C	-3.705682	-0.796591	0.076070	S	-6.965044	1.109532	0.165532
N	-2.809989	-0.769511	1.095767	O	-5.977550	0.867981	1.252329
N	-4.580703	-1.828299	-0.005069	O	-7.739869	2.354354	0.280430
C	-2.422755	0.482877	1.745889	O	-6.410541	0.823520	-1.195067
H	-2.511310	0.349791	2.831213	O	-8.075822	-0.152079	0.300493
H	-1.388387	0.755567	1.508263	C	-8.993267	-0.048384	1.405426
H	-3.110720	1.274128	1.449555	H	-9.552283	0.889911	1.319191
C	-2.223478	-1.983155	1.655159	H	-8.428642	-0.029745	2.347535
H	-2.459592	-2.837710	1.019278	C	-9.922225	-1.250985	1.345429
H	-1.135656	-1.860977	1.690621	H	-9.362196	-2.189148	1.436688
H	-2.595100	-2.179241	2.670352	H	-10.648793	-1.202953	2.166272
C	-5.218495	-2.191840	-1.274136	H	-10.471088	-1.269173	0.397434
H	-5.400549	-3.272242	-1.264352				
H	-6.165410	-1.658882	-1.410101	1a+2a			
H	-4.549582	-1.952808	-2.103113	C	-4.591958	-1.467890	-0.345743
C	-5.248393	-2.351766	1.189335	N	-3.521968	-2.256886	-0.599767
H	-6.326530	-2.196385	1.079106	N	-5.042474	-0.629650	-1.300269
H	-5.040976	-3.422344	1.314559	C	-3.371641	-3.586301	-0.014231
H	-4.923197	-1.802068	2.071209	H	-2.993023	-4.264024	-0.787694
N	-3.737714	0.149766	-0.865398	H	-2.655988	-3.584676	0.817342
C	-2.625112	0.979364	-1.337843	H	-4.335480	-3.952937	0.338985
H	-1.726585	0.729681	-0.770463	C	-2.357216	-1.781640	-1.359060
H	-2.426452	0.699267	-2.381777	H	-2.425837	-0.708392	-1.538088
C	-2.942982	2.474654	-1.270394	H	-1.460302	-1.966925	-0.757838

H	-2.259328	-2.328065	-2.305235	H	1.656746	-0.849605	0.757983
C	-5.584557	0.697671	-0.989583	C	1.839854	1.978783	2.602234
H	-5.075961	1.423539	-1.628853	H	2.477843	2.858938	2.505791
H	-6.665541	0.733318	-1.179260	H	0.790725	2.290311	2.544227
H	-5.354330	0.964898	0.039644	H	2.021889	1.511764	3.580099
C	-4.866487	-0.894752	-2.728708	C	5.258983	2.346802	0.162621
H	-5.806706	-0.656094	-3.239376	H	5.820681	3.103334	0.721915
H	-4.070466	-0.271005	-3.149317	H	5.954237	1.611249	-0.256414
H	-4.637252	-1.948398	-2.892792	H	4.720665	2.834824	-0.652280
N	-5.244573	-1.585036	0.843509	C	4.876496	1.280233	2.354882
C	-6.703365	-1.380740	0.952260	H	5.796818	0.719965	2.156971
H	-6.969189	-0.325325	0.825508	H	5.098168	2.145069	2.992971
H	-6.960765	-1.637381	1.981983	H	4.184820	0.611397	2.864181
C	-7.522345	-2.259263	0.005160	N	2.991009	0.943207	-0.667911
H	-8.590089	-2.097918	0.192114	C	1.757471	1.000149	-1.459884
H	-7.329749	-2.024698	-1.046301	H	0.927843	1.300303	-0.816934
H	-7.305424	-3.320979	0.167884	H	1.883184	1.800135	-2.203209
S	-2.303879	1.792759	0.002502	C	1.469279	-0.313489	-2.189740
O	-2.917533	0.730082	0.839470	H	1.289681	-1.135043	-1.488599
O	-2.424882	1.521972	-1.458448	H	0.580944	-0.189245	-2.819799
H	3.827818	0.528307	-1.114323	H	2.310686	-0.603905	-2.828434
C	3.123903	1.223165	0.631499	S	5.322663	-1.663884	-0.379175
N	2.106301	1.049306	1.509687	O	4.322921	-1.516062	0.702319
N	4.304942	1.717880	1.078088	O	5.512960	-3.017261	-0.928098
C	1.218044	-0.110880	1.428622	O	5.195912	-0.596207	-1.431299
H	1.154266	-0.560604	2.427970	O	6.747627	-1.279891	0.436676
H	0.214699	0.182826	1.105830	C	7.990575	-1.717006	-0.149630

H	7.854625	-2.723096	-0.559980	C	-7.674816	-1.264771	-2.833006
H	8.678075	-1.780194	0.701569	H	-8.100585	-1.071566	-3.823918
C	8.522336	-0.754142	-1.206069	H	-6.619453	-1.533691	-2.954737
H	8.658179	0.249760	-0.785681	H	-8.212774	-2.092734	-2.372224
H	9.495810	-1.107266	-1.572004	C	-7.377830	1.180647	-2.680909
H	7.834650	-0.683316	-2.053725	H	-7.249660	1.969066	-1.942166
O	-0.950245	2.221546	0.424822	H	-6.399975	0.991222	-3.132918
O	-3.320669	3.083046	0.322143	H	-8.086722	1.489288	-3.458646
C	-2.867687	4.404164	-0.051874	C	-8.640661	1.520967	1.103129
H	-3.389426	5.068106	0.645775	H	-8.349446	2.572284	1.004567
H	-1.792392	4.478341	0.141768	H	-9.534545	1.457104	1.736580
C	-3.203543	4.760748	-1.495339	H	-7.806658	0.995063	1.564664
H	-2.684227	4.100596	-2.195833	C	-9.838847	1.760974	-1.044543
H	-2.899987	5.796245	-1.698214	H	10.753679	1.924629	-0.463033
H	-4.282197	4.679664	-1.674868	H	-9.424412	2.739499	-1.316615
C	-4.477761	-1.553648	2.115621	H	10.096561	1.214398	-1.952861
H	-4.711538	-0.599895	2.605098	N	-7.974563	-1.161036	0.045152
H	-3.420972	-1.491799	1.858581	S	-2.828412	-0.809656	0.996330
C	-4.757489	-2.716515	3.069899	O	-1.550856	-0.560634	0.308764
H	-4.151887	-2.582618	3.973567	O	-3.500792	-2.095635	0.751809
H	-5.805053	-2.757368	3.388644	C	-8.936832	-1.597784	1.079389
H	-4.499242	-3.686334	2.633766	H	-9.375990	-0.735844	1.582732
2b+1b				H	-8.361036	-2.138123	1.835710
C	-8.220576	-0.080780	-0.733157	C	10.050179	-2.484917	0.513981
N	-7.825729	-0.055170	-2.024546	H	10.722320	-2.796936	1.322070
N	-8.906214	0.980264	-0.233403	H	10.647231	-1.941409	-0.227713
				H	-9.647098	-3.384392	0.038779

C	-2.411351	-0.814500	2.834640	H	3.692198	-1.416356	2.041333
F	-3.506193	-1.008338	3.581414	C	3.862296	-2.924561	-0.996636
F	-1.554604	-1.824759	3.059513	H	4.946219	-2.835698	-1.119834
F	-1.827218	0.331439	3.202164	H	3.606953	-3.950290	-0.702933
N	-3.848847	0.456354	1.059744	H	3.393243	-2.694425	-1.953135
S	-4.413894	1.183612	-0.248134	N	2.662595	0.209789	0.326425
O	-4.315076	0.415920	-1.504595	C	1.587106	1.110389	0.773500
O	-5.713758	1.795413	0.082004	H	0.627059	0.700628	0.457082
C	-3.292106	2.678999	-0.512607	H	1.589871	1.099554	1.871932
F	-2.037095	2.295080	-0.778309	C	1.788993	2.543548	0.280532
F	-3.753668	3.391714	-1.555909	H	1.729842	2.610312	-0.811024
F	-3.284897	3.462762	0.572541	H	1.011639	3.188990	0.704762
H	3.611456	0.491732	0.601510	H	2.765742	2.929435	0.589711
C	2.519141	-0.997091	-0.239866	S	6.312492	1.356917	0.012117
N	1.487036	-1.257663	-1.083191	O	6.143643	2.115846	-1.228516
N	3.420881	-1.967091	0.025462	O	5.202869	1.362833	0.997088
C	0.925507	-0.241395	-1.973676	C	8.979814	-1.665536	-0.322256
H	0.864422	-0.661602	-2.985361	C	-6.650585	-1.842421	0.033322
H	-0.078863	0.055007	-1.654455	H	-6.165899	-1.604777	0.986680
H	1.580741	0.629225	-2.001451	H	-6.039681	-1.377366	-0.739045
C	0.822251	-2.559693	-1.124154	C	-6.690710	-3.358884	-0.146292
H	1.188915	-3.191862	-0.314753	H	-5.659641	-3.724573	-0.113472
H	-0.252816	-2.404556	-0.987744	H	-7.241538	-3.858603	0.658096
H	0.995578	-3.066859	-2.082324	H	-7.132097	-3.659410	-1.102576
C	4.213551	-1.975301	1.262329	C	7.689725	2.242022	0.954400
H	4.321535	-3.016395	1.586016	F	7.317971	3.508958	1.201205
H	5.204403	-1.540735	1.096885	F	8.818687	2.255766	0.237224

F	7.928964	1.631902	2.125822	H	-1.701558	3.909814	3.204846
N	6.768328	-0.176182	-0.128302	N	-0.515894	3.803853	-0.400221
S	7.664213	-0.785012	-1.349664	S	-2.952480	-0.783563	-1.451352
O	6.928007	-1.889165	-1.983935	O	-2.303021	-2.097916	-1.591513
O	8.391817	0.175728	-2.179623	O	-2.135481	0.409023	-1.753911
F	8.423724	-2.571844	0.501315	C	-1.341112	4.799180	-1.113628
F	9.824071	-2.305929	-1.146651	H	-2.264139	4.349310	-1.496064
F	9.681801	-0.793397	0.415155	H	-0.758135	5.090338	-1.989127
				C	-1.649641	6.051799	-0.291778
2b+2a				H	-2.196494	6.767841	-0.915786
C	-0.832503	3.355130	0.843257	H	-2.268555	5.834584	0.584338
N	0.155153	3.024398	1.705141	H	-0.726583	6.533613	0.049559
N	-2.120012	3.260946	1.244464	C	-4.329873	-0.763443	-2.737804
C	1.451449	3.711738	1.719928	F	-4.996557	0.399575	-2.717878
H	1.698109	3.945281	2.762794	F	-3.764817	-0.908410	-3.949521
H	2.246547	3.081871	1.312289	F	-5.192958	-1.765632	-2.545950
H	1.380349	4.642941	1.157169	N	-3.916348	-0.598165	-0.162133
C	0.053643	1.877636	2.619301	S	-3.395458	-0.737680	1.350357
H	-0.797839	1.250752	2.353358	O	-1.928370	-0.755204	1.512711
H	0.970209	1.289823	2.510800	O	-4.179992	0.155212	2.213975
H	-0.037808	2.209549	3.661495	C	-3.951709	-2.465355	1.866623
C	-3.220406	2.919432	0.335614	F	-3.332731	-3.400942	1.131728
H	-3.883927	2.223226	0.853875	F	-3.640367	-2.664458	3.160138
H	-3.795406	3.813498	0.058674	F	-5.274312	-2.604169	1.718493
H	-2.839197	2.418705	-0.553808	C	2.704033	-2.736157	-0.693700
C	-2.519507	3.461220	2.640354	N	1.582216	-2.167760	-1.169656
H	-3.378141	4.142987	2.658877	N	3.747423	-2.942637	-1.537454
H	-2.820331	2.515633	3.103555				

C	0.754224	-1.259750	-0.361963	C	7.056153	2.534323	0.161320
H	0.481294	-0.412466	-0.995247	C	0.511680	3.088431	-1.207827
H	-0.165340	-1.741518	-0.025883	H	-0.024227	2.555338	-2.004599
H	1.334429	-0.883129	0.477812	H	0.966507	2.326637	-0.575652
C	1.129814	-2.351709	-2.551376	C	1.603750	3.972120	-1.809327
H	1.622768	-3.218461	-2.995349	H	2.346011	3.312894	-2.269637
H	0.048049	-2.514811	-2.533567	H	1.225842	4.652443	-2.580964
H	1.337728	-1.462134	-3.157441	H	2.116636	4.564773	-1.045261
C	4.640421	-4.088620	-1.414694	C	4.016653	-2.897014	1.397884
H	4.812428	-4.506180	-2.414083	H	4.747953	-2.421886	0.744601
H	5.611317	-3.804357	-0.989269	H	3.776996	-2.138441	2.151642
H	4.183103	-4.855877	-0.789494	C	4.581913	-4.144235	2.081353
C	4.122827	-1.961243	-2.561944	H	5.490949	-3.864560	2.625983
H	5.196397	-1.766711	-2.470322	H	3.885044	-4.571668	2.810783
H	3.909947	-2.341540	-3.569533	H	4.847589	-4.931354	1.367942
H	3.607407	-1.016976	-2.386358	O	3.249188	0.997555	-1.273428
N	2.786165	-3.125452	0.605919	O	4.618152	2.360368	0.347405
C	1.618003	-3.698646	1.310680	C	5.709434	2.762371	-0.511511
H	0.784387	-3.717840	0.607751	H	5.541318	3.828102	-0.705459
H	1.859902	-4.745642	1.540312	H	5.642386	2.232165	-1.467738
C	1.210017	-2.983404	2.601069	H	7.211720	1.468774	0.352555
H	0.981978	-1.928695	2.432108	H	7.106889	3.073012	1.114435
H	0.307202	-3.461705	2.996320	H	7.865139	2.900281	-0.485091
H	1.985884	-3.050935	3.370717				
S	3.933988	0.863475	0.043268	1a+2a+1a+2a			
O	5.050920	-0.113859	0.022780	C	6.588472	-0.648862	-0.723707
O	3.006059	0.739098	1.193017	N	5.788171	-0.861342	-1.784477

N	7.933795	-0.792895	-0.859181	H	4.980062	0.817326	2.689795
C	4.461672	-0.253056	-1.897218	C	3.196151	-2.337825	3.618344
H	4.290125	-0.008592	-2.950181	F	4.335848	-1.759515	4.020821
H	3.682972	-0.943496	-1.555407	F	2.164309	-1.593407	4.058385
H	4.427630	0.677482	-1.333673	F	3.106542	-3.555290	4.160242
C	6.126451	-1.833429	-2.824244	N	4.426717	-3.291068	1.507050
H	6.960339	-2.455787	-2.501075	S	4.739128	-4.094388	0.143401
H	5.261006	-2.484883	-2.980013	O	3.817478	-3.804410	-0.969619
H	6.376156	-1.330396	-3.766979	O	6.184240	-4.071144	-0.103319
C	8.745123	-1.448775	0.163708	C	4.381566	-5.885751	0.612591
H	9.403175	-2.176182	-0.326444	F	3.091021	-6.033877	0.950240
H	9.367747	-0.732019	0.715383	F	4.642790	-6.680243	-0.437901
H	8.102382	-1.993007	0.856180	F	5.143338	-6.269835	1.643627
C	8.637500	-0.298960	-2.040764	H	5.088990	-0.533292	0.643072
H	9.516204	0.266958	-1.709575	H	-3.297900	-2.544669	-0.199059
H	8.974947	-1.118024	-2.690444	C	-1.724492	-3.316583	-1.191208
H	7.990420	0.382191	-2.593756	N	-0.667652	-4.155588	-1.064197
N	6.066586	-0.304473	0.459776	N	-2.219096	-3.055220	-2.424694
S	3.091818	-2.422033	1.739028	C	-0.540009	-5.073586	0.070714
O	1.800641	-3.064276	1.452004	H	-0.291819	-6.067925	-0.319639
O	3.249611	-1.014791	1.297396	H	0.252111	-4.757781	0.755941
C	6.766327	0.470070	1.494112	H	-1.494657	-5.139906	0.592717
H	7.536912	1.062816	0.994998	C	0.411524	-4.213521	-2.050554
H	7.254053	-0.211477	2.203182	H	0.317554	-3.382632	-2.751544
C	5.800514	1.387819	2.240976	H	1.372566	-4.131884	-1.532814
H	6.342107	1.895355	3.047689	H	0.393159	-5.158383	-2.610158
H	5.397474	2.153709	1.572873	C	-2.965106	-1.825846	-2.715142

H	-2.729883	-1.518915	-3.740299	C	-7.313553	0.298421	1.152659
H	-4.044748	-1.985802	-2.626778	N	-7.045017	-0.163134	2.399493
H	-2.663092	-1.028567	-2.035168	N	-7.831556	-0.525668	0.219731
C	-2.331237	-4.104938	-3.437210	C	-7.018742	0.731586	3.558527
H	-3.383219	-4.199184	-3.727892	H	-7.377880	0.173335	4.429576
H	-1.733361	-3.863189	-4.325026	H	-6.007096	1.101498	3.763369
H	-2.008144	-5.060723	-3.025896	H	-7.678998	1.584154	3.389096
N	-2.288278	-2.734369	-0.127586	C	-6.495931	-1.506693	2.626021
C	-1.613814	-2.300170	1.101609	H	-6.218902	-1.975056	1.681201
H	-0.560086	-2.577600	1.047119	H	-5.592884	-1.407274	3.239637
H	-1.656478	-1.202607	1.123748	H	-7.211074	-2.143254	3.160038
C	-2.270529	-2.858372	2.365548	C	-7.463483	-0.429782	-1.200840
H	-2.198430	-3.949260	2.414387	H	-7.116852	-1.412398	-1.531302
H	-1.775105	-2.442169	3.250242	H	-8.327696	-0.125254	-1.804638
H	-3.331641	-2.590043	2.406888	H	-6.651210	0.283190	-1.339417
S	-5.619066	-4.061769	-0.581749	C	-8.691644	-1.661867	0.569434
O	-4.526971	-5.027116	-0.827564	H	-9.535226	-1.672036	-0.130839
O	-6.716582	-4.528578	0.291432	H	-8.158890	-2.616025	0.496504
O	-5.141839	-2.680349	-0.252049	H	-9.082634	-1.532735	1.580262
O	-6.322599	-3.774569	-2.082636	N	-7.088245	1.596374	0.885676
C	-6.946898	-4.921166	-2.700288	S	-3.679837	3.259211	1.263280
H	-7.717773	-5.314233	-2.027098	O	-2.255634	2.939637	1.427560
H	-6.190130	-5.700107	-2.854112	O	-4.632555	2.748325	2.273003
C	-7.545962	-4.464621	-4.020546	C	-7.781233	2.414476	-0.117526
H	-6.773892	-4.059099	-4.683941	H	-8.661173	1.857735	-0.448758
H	-8.022704	-5.313908	-4.525137	H	-7.126242	2.564982	-0.981715
H	-8.304149	-3.689828	-3.861093	C	-8.198501	3.762510	0.471411

H	-8.693099	4.363067	-0.300628	H	1.050978	3.879475	4.022240
H	-8.895357	3.634951	1.307981	C	3.022880	5.819474	0.171691
H	-7.328888	4.325580	0.824396	H	2.926115	6.829850	0.587032
C	-3.777247	5.129531	1.491198	H	4.044897	5.668230	-0.186290
F	-5.040157	5.566454	1.382997	H	2.320831	5.710981	-0.655925
F	-3.320365	5.441680	2.716150	C	3.458466	5.034168	2.470320
F	-3.022468	5.760764	0.581999	H	4.520928	5.112408	2.214547
N	-4.343765	3.090902	-0.191346	H	3.144001	5.942721	2.999454
S	-3.705003	2.334509	-1.470169	H	3.319323	4.172225	3.123224
O	-2.534917	1.491373	-1.194263	N	1.947000	3.213682	-0.227057
O	-4.813659	1.792351	-2.262325	C	0.794362	2.602306	-0.910742
C	-3.045824	3.746351	-2.533819	H	-0.037963	2.523781	-0.210904
F	-2.072316	4.410928	-1.887152	H	0.478230	3.297901	-1.698432
F	-2.537188	3.247024	-3.670831	C	1.128492	1.248925	-1.533594
F	-4.021986	4.610181	-2.840154	H	1.425863	0.515712	-0.776654
H	-6.323640	2.046481	1.392385	H	0.243268	0.869648	-2.054723
H	2.800550	3.347274	-0.790882	H	1.943794	1.346033	-2.258564
C	1.948021	3.754823	0.996901	S	5.754559	3.471827	-1.311037
N	1.220420	3.221630	2.009616	O	5.846446	4.122314	0.022026
N	2.697818	4.858923	1.232071	O	6.689366	2.335844	-1.495047
C	0.936506	1.787044	2.105686	O	4.355643	3.185235	-1.739217
H	1.123670	1.468293	3.137910	O	6.193882	4.628328	-2.421293
H	-0.108402	1.573911	1.857187	C	7.546597	5.121505	-2.317423
H	1.601327	1.224527	1.450759	H	8.242426	4.283485	-2.443603
C	0.593720	4.051066	3.039056	H	7.695173	5.554838	-1.320829
H	0.689614	5.105913	2.778962	C	7.733088	6.163863	-3.407602
H	-0.469705	3.796539	3.090771	H	7.029751	6.993737	-3.278682

H	8.753490	6.564755	-3.368078	C	-0.886971	-3.462085	1.433809
H	7.570753	5.724634	-4.397827	H	-1.965747	-3.279830	1.368945
				H	-0.486094	-3.451169	0.415501
1a+1b+1a+1b				H	-0.735341	-4.462302	1.854734
C	2.075079	-2.694662	1.496376	S	4.342227	0.587704	1.805860
N	3.152102	-3.506311	1.590627	O	3.751216	-0.522179	2.597501
N	1.831604	-2.048068	0.336460	O	4.481506	0.252803	0.361257
C	3.170655	-4.694991	2.438450	H	10.337002	-0.836066	0.601528
H	3.679130	-5.499085	1.894910	C	9.704989	0.136923	2.237389
H	3.715602	-4.516600	3.373740	N	8.734051	0.113542	3.181986
H	2.152372	-5.009801	2.666851	N	10.902012	0.700452	2.535132
C	4.443570	-3.165393	0.979492	C	7.856442	-1.044997	3.352159
H	4.432952	-2.142175	0.608068	H	7.880156	-1.338596	4.409748
H	5.214429	-3.230282	1.754325	H	6.826348	-0.800617	3.076643
H	4.693356	-3.869861	0.176706	H	8.244924	-1.878474	2.767623
C	1.306991	-0.678558	0.293819	C	8.517921	1.213958	4.116956
H	1.978240	-0.083680	-0.331892	H	9.134911	2.068286	3.833552
H	0.293591	-0.661002	-0.129219	H	7.462534	1.503432	4.069777
H	1.322595	-0.235094	1.287529	H	8.765965	0.919968	5.146282
C	2.241627	-2.582416	-0.962289	C	11.804089	1.173118	1.483345
H	1.415052	-2.439360	-1.668126	H	12.384323	2.012321	1.882970
H	3.123187	-2.058693	-1.347853	H	12.484731	0.379558	1.156281
H	2.452801	-3.649601	-0.882522	H	11.222211	1.520112	0.627143
N	1.204889	-2.598313	2.538183	C	11.536944	0.482629	3.838120
C	-0.241788	-2.392060	2.316323	H	12.461451	-0.086071	3.690404
H	-0.445853	-1.391661	1.919717	H	11.764750	1.441338	4.321277
H	-0.700085	-2.426192	3.306797	H	10.883914	-0.109333	4.477083

N	9.514943	-0.357997	1.010740	H	3.580951	4.454853	-0.101927
C	8.247031	-0.466218	0.282619	H	2.373565	3.167077	-0.304784
H	7.431300	-0.101384	0.908423	C	1.704753	-2.342262	3.914042
H	8.302218	0.211150	-0.581046	H	1.396104	-1.323081	4.178582
C	7.987199	-1.889340	-0.217072	H	2.792314	-2.306732	3.868169
H	7.884506	-2.596999	0.612205	C	1.211660	-3.327806	4.975299
H	7.064377	-1.901018	-0.808095	H	1.617391	-3.027929	5.948351
H	8.809457	-2.242236	-0.849050	H	0.119960	-3.332554	5.069765
S	11.875132	-2.880940	1.609420	H	1.537881	-4.353525	4.778348
O	10.927453	-2.553330	2.698372	C	20.133009	-6.168529	1.141949
O	12.020377	-4.304694	1.260564	N	21.210032	-6.980178	1.236200
O	11.713754	-1.978386	0.416325	N	19.889534	-5.521935	-0.017966
O	13.340834	-2.409608	2.293744	C	21.228585	-8.168858	2.084023
C	14.548470	-2.973437	1.743575	H	21.737060	-8.972952	1.540483
H	14.380052	-4.034380	1.531076	H	21.773532	-7.990467	3.019313
H	15.273363	-2.894341	2.561726	H	20.210302	-8.483668	2.312424
C	15.045129	-2.232045	0.506764	C	22.501500	-6.639260	0.625065
H	15.204283	-1.169650	0.727566	H	22.490882	-5.616042	0.253641
H	16.000989	-2.661459	0.177682	H	23.272359	-6.704149	1.399898
H	14.326451	-2.309413	-0.314263	H	22.751286	-7.343728	-0.177720
O	5.544883	1.216525	2.398164	C	19.364921	-4.152425	-0.060607
O	3.122219	1.736193	1.904820	H	20.036170	-3.557547	-0.686319
C	3.461746	3.101821	1.573089	H	18.351521	-4.134869	-0.483646
H	2.728872	3.696975	2.128684	H	19.380525	-3.708961	0.933102
H	4.457834	3.324803	1.969255	C	20.299557	-6.056283	-1.316716
C	3.376040	3.391443	0.078822	H	19.472982	-5.913227	-2.022553
H	4.102351	2.795449	-0.481049	H	21.181117	-5.532560	-1.702280

H	20.510731	-7.123468	-1.236949	H	29.280141	-1.953754	0.272716
N	19.262819	-6.072180	2.183756	C	29.594874	-2.991237	3.483693
C	17.816141	-5.865927	1.961896	H	30.519381	-3.559938	3.335977
H	17.612076	-4.865528	1.565290	H	29.822680	-2.032528	3.966850
H	17.357844	-5.900059	2.952370	H	28.941844	-3.583200	4.122656
C	17.170958	-6.935952	1.079382	N	27.572873	-3.831864	0.656313
H	16.092182	-6.753697	1.014518	C	26.304961	-3.940085	-0.071807
H	17.571835	-6.925036	0.061074	H	25.489230	-3.575251	0.553996
H	17.322588	-7.936169	1.500307	H	26.360148	-3.262716	-0.935473
S	22.400157	-2.886162	1.451433	C	26.045129	-5.363207	-0.571499
O	21.809146	-3.996046	2.243074	H	25.942436	-6.070866	0.257778
O	22.539436	-3.221063	0.006830	H	25.122307	-5.374885	-1.162522
H	28.394932	-4.309933	0.247101	H	26.867387	-5.716103	-1.203477
C	27.762919	-3.336943	1.882962	S	29.933062	-6.354807	1.254993
N	26.791981	-3.360324	2.827559	O	28.985383	-6.027197	2.343945
N	28.959942	-2.773414	2.180705	O	30.078307	-7.778561	0.906137
C	25.914372	-4.518864	2.997732	O	29.771684	-5.452253	0.061898
H	25.938086	-4.812463	4.055321	O	31.398764	-5.883475	1.939317
H	24.884278	-4.274484	2.722216	C	32.606400	-6.447304	1.389148
H	26.302854	-5.352341	2.413196	H	32.437982	-7.508247	1.176649
C	26.575851	-2.259908	3.762529	H	33.331293	-6.368208	2.207299
H	27.192841	-1.405580	3.479125	C	33.103059	-5.705912	0.152337
H	25.520464	-1.970434	3.715350	H	33.262213	-4.643517	0.373139
H	26.823895	-2.553898	4.791855	H	34.058919	-6.135326	-0.176744
C	29.862019	-2.300748	1.128918	H	32.384381	-5.783280	-0.668690
H	30.442253	-1.461545	1.528543	O	23.602813	-2.257341	2.043737
H	30.542661	-3.094308	0.801854	O	21.180149	-1.737673	1.550393

C	21.519676	-0.372045	1.218662	C	16.250800	-0.100300	2.322300
H	20.786802	0.223108	1.774257	H	15.812800	-0.379600	3.286800
H	22.515764	-0.149063	1.614828	H	17.285200	0.216700	2.486000
C	21.433970	-0.082423	-0.275604	H	15.646500	0.703500	1.904300
H	22.160281	-0.678417	-0.835476	C	16.500700	-2.585400	2.033000
H	21.638881	0.980986	-0.456354	H	17.486100	-2.517800	2.504900
H	20.431495	-0.306789	-0.659211	H	15.762400	-2.868300	2.791000
C	19.762683	-5.816129	3.559615	H	16.529300	-3.346800	1.253000
H	19.454034	-4.796948	3.824155	N	16.035500	-0.163800	-0.645900
H	20.850244	-5.780599	3.513742	S	11.407500	2.366200	-1.456100
C	19.269590	-6.801673	4.620872	O	10.371400	1.699900	-2.468400
H	19.675321	-6.501796	5.593924	O	12.918600	2.501000	-1.957000
H	18.177890	-6.806421	4.715338	C	17.390200	0.453400	-0.514500
H	19.595811	-7.827392	4.423921	H	17.529700	0.890900	0.474900
2b+1b+2b+1b				H	17.414600	1.265200	-1.242300
C	15.659100	-1.176400	0.167500	C	18.507600	-0.556800	-0.828400
N	14.818600	-2.144600	-0.257700	H	19.481500	-0.060300	-0.772300
N	16.176300	-1.277500	1.424700	H	18.501200	-1.379600	-0.109700
C	14.627800	-2.469100	-1.688300	H	18.379600	-0.957100	-1.838200
H	14.595200	-3.558500	-1.794800	C	10.754100	4.165800	-1.052400
H	13.685200	-2.039100	-2.037400	F	11.732900	4.820300	-0.391400
H	15.460900	-2.070400	-2.267300	F	10.474500	4.771900	-2.232100
C	13.798100	-2.727200	0.652200	F	9.633800	4.082300	-0.288800
H	13.780300	-2.158200	1.578500	N	11.240100	1.858500	0.256200
H	12.829500	-2.596000	0.166900	S	12.099400	0.348400	0.480700
H	13.995400	-3.786300	0.842300	O	12.017400	-0.631300	-0.805100
				O	13.521500	0.389400	1.218500

C	10.888100	-0.419000	1.807200	H	7.936800	2.558900	-0.190100
F	9.756800	-0.807900	1.160600	C	7.723700	1.313100	1.572900
F	11.515600	-1.501200	2.351100	H	7.637900	0.249800	1.817600
F	10.610900	0.500800	2.756700	H	8.612200	1.713200	2.064700
H	5.776100	1.019100	-0.077200	H	6.826500	1.817400	1.936200
C	6.614000	0.489600	-1.885400	S	3.615000	0.413200	1.694800
N	7.696200	-0.056300	-2.502800	O	4.354100	-0.712900	2.535600
N	5.464000	0.629300	-2.600400	O	4.547900	1.535500	1.009500
C	8.681200	-0.912300	-1.803300	C	1.449400	-1.333500	-1.583500
H	8.760700	-1.859000	-2.351800	C	15.023900	0.586200	-1.470200
H	9.667500	-0.437200	-1.778900	H	14.862200	1.554400	-0.994000
H	8.335900	-1.125600	-0.792300	H	14.078900	0.053900	-1.406700
C	8.046600	0.305100	-3.897300	C	15.414800	0.788300	-2.938000
H	7.266800	0.949700	-4.305700	H	14.601800	1.364400	-3.391200
H	8.995900	0.846000	-3.869800	H	16.340400	1.363600	-3.048300
H	8.137900	-0.592700	-4.517900	H	15.525200	-0.161200	-3.468800
C	4.385300	1.527600	-2.127000	C	2.487700	1.502700	2.863600
H	3.784100	1.817700	-2.990200	F	3.279600	2.373100	3.533500
H	3.763600	1.015400	-1.394200	F	1.852900	0.679900	3.745000
H	4.822700	2.412700	-1.662900	F	1.561500	2.168500	2.125600
C	5.018500	-0.435600	-3.538600	N	2.257700	-0.142300	0.710300
H	4.137600	-0.905100	-3.104200	S	2.745500	-1.637400	-0.136700
H	4.781400	-0.007800	-4.516500	O	4.209900	-1.496900	-0.771900
H	5.810400	-1.174700	-3.641000	O	2.341400	-3.022500	0.530400
N	6.658600	0.921200	-0.620900	F	1.986800	-0.411100	-2.433700
C	7.857500	1.495500	0.053300	F	1.253700	-2.506800	-2.237500
H	8.761000	1.020700	-0.310000	F	0.269700	-0.873800	-1.082100

C	-2.405800	-0.782600	2.649300	H	1.260600	-2.584400	2.571100
N	-3.462500	-0.650400	3.491600	H	0.495100	-1.091700	3.104100
N	-1.635000	0.308100	2.419600	H	-0.028000	-2.651800	3.802000
C	-4.024800	-1.786300	4.248500	C	-6.530300	-3.006200	-2.990000
H	-4.254400	-1.450100	5.265300	F	-5.290200	-2.921700	-3.520900
H	-4.942400	-2.137200	3.765500	F	-7.080600	-4.220900	-3.246500
H	-3.291000	-2.591100	4.288000	F	-7.331100	-2.021500	-3.478800
C	-4.319800	0.561400	3.460800	N	-6.104900	-1.068700	-1.199200
H	-4.031700	1.178900	2.612200	S	-5.500000	-0.445000	0.325300
H	-5.344000	0.227500	3.289600	O	-6.048800	-1.251600	1.611800
H	-4.251200	1.120500	4.399800	O	-3.957000	-0.007800	0.369200
C	-1.103600	0.620700	1.068400	C	-6.489400	1.244200	0.332900
H	-1.321200	1.675400	0.867500	F	-7.763800	0.991500	0.727300
H	-0.024900	0.457900	1.010600	F	-5.887000	2.067200	1.238700
H	-1.637200	0.022700	0.333900	F	-6.475500	1.803500	-0.897500
C	-1.387700	1.326900	3.463000	H	-11.698500	-0.207600	-2.090900
H	-0.322000	1.557700	3.459200	C	-11.563500	-1.714500	-0.698300
H	-1.956800	2.242800	3.272000	N	-10.737900	-2.140300	0.301400
H	-1.668000	0.922900	4.437000	N	-12.870400	-2.056100	-0.656800
N	-2.105100	-1.984600	2.100900	C	-9.783400	-1.195100	0.932300
S	-6.367300	-2.830900	-1.044700	H	-9.903100	-1.280200	2.029900
O	-7.768800	-3.271700	-0.413900	H	-8.738500	-1.455600	0.703200
O	-5.085900	-3.677900	-0.608500	H	-10.061500	-0.193900	0.642800
C	-0.697200	-2.362500	1.757200	C	-10.689300	-3.544200	0.745100
H	-0.382100	-1.877400	0.831900	H	-11.488400	-4.112300	0.239200
H	-0.726100	-3.435200	1.553800	H	-9.718600	-3.960200	0.469600
C	0.313500	-2.143900	2.894500	H	-10.836100	-3.605100	1.823200

C	-13.732600	-1.974100	-1.860600	C	-13.019700	3.523700	-0.495400
H	-14.473400	-2.778900	-1.805600	F	-12.530800	3.826900	0.722500
H	-14.244800	-1.004600	-1.891200	F	-14.275200	3.996000	-0.670000
H	-13.113100	-2.105800	-2.750300	F	-12.199900	4.001200	-1.468500
C	-13.581800	-2.197600	0.639500	N	-14.751700	1.075200	-0.866500
H	-14.427900	-1.506500	0.686700	S	-15.560600	1.284200	0.714900
H	-13.938500	-3.226400	0.766400	O	-15.998400	-0.087100	1.406100
H	-12.889600	-1.944600	1.441800	O	-14.819700	2.395100	1.590600
N	-11.104500	-0.986500	-1.722500	F	-17.609100	1.274600	-1.048100
C	-9.704500	-1.012600	-2.214100	F	-18.123100	2.142400	0.936100
H	-9.129800	-1.704400	-1.611200	F	-16.875600	3.299700	-0.493100
H	-9.728100	-1.405700	-3.239400				
C	-9.089600	0.395800	-2.213700	2b+2a+2b+2a			
H	-8.962400	0.754000	-1.192800	C	8.132515	3.253406	-0.261173
H	-8.105100	0.357000	-2.685900	N	7.001647	3.541452	-0.946575
H	-9.741700	1.093700	-2.746600	N	9.271234	3.002504	-0.943430
S	-13.063400	1.542900	-0.712600	C	5.997561	4.493406	-0.450472
O	-12.223500	0.911800	0.492900	H	5.756207	5.185469	-1.267201
O	-12.459200	1.320000	-2.194200	H	5.077157	3.980274	-0.139146
C	-17.180600	2.066300	-0.039000	H	6.412235	5.062919	0.382016
C	-3.182800	-2.821600	1.470100	C	6.626861	2.829737	-2.175997
H	-3.052400	-2.757800	0.385900	H	7.258551	1.956211	-2.317330
H	-4.144900	-2.365100	1.695400	H	5.593375	2.494720	-2.064606
C	-3.192800	-4.295000	1.897200	H	6.695703	3.487461	-3.052665
H	-4.008300	-4.768200	1.343500	C	10.300733	2.068823	-0.472331
H	-2.259700	-4.810300	1.651300	H	10.640647	1.478244	-1.328704
H	-3.379400	-4.404400	2.971000	H	11.161993	2.608801	-0.055910

H	9.884926	1.382994	0.268121	F	9.940784	-3.152625	-3.475657
C	9.547269	3.607587	-2.246389	C	2.991240	-1.991847	0.491950
H	10.575010	3.990260	-2.239519	N	4.233928	-1.825502	0.985132
H	9.456351	2.878946	-3.047641	N	1.961507	-2.187416	1.346933
H	8.864864	4.436926	-2.430761	C	5.225290	-0.935355	0.358441
N	8.107012	3.249513	1.096389	H	5.673937	-0.348392	1.150538
S	9.160543	-1.729713	0.551673	H	6.001325	-1.505355	-0.152369
O	8.077339	-2.722626	0.583278	H	4.720619	-0.250022	-0.315504
O	8.976636	-0.478799	1.339211	C	4.665168	-2.443413	2.240565
C	9.278812	3.628493	1.912031	H	3.996596	-3.264466	2.503935
H	10.032277	2.834008	1.919227	H	5.671924	-2.838518	2.098584
H	8.908413	3.706801	2.935497	H	4.688637	-1.712956	3.055132
C	9.902421	4.967490	1.514571	C	0.835990	-3.068031	1.035640
H	10.706237	5.213487	2.217518	H	0.619901	-3.672488	1.925848
H	10.335329	4.945752	0.509593	H	-0.065675	-2.513910	0.766789
H	9.159454	5.771803	1.551714	H	1.106407	-3.740133	0.218568
C	10.645708	-2.574389	1.348429	C	1.852215	-1.447888	2.605542
F	11.720279	-1.772472	1.356085	H	0.835612	-1.039537	2.671546
F	10.322876	-2.863197	2.621253	H	2.008718	-2.108082	3.468028
F	10.953148	-3.711506	0.717050	H	2.554975	-0.609582	2.629666
N	9.854827	-1.483788	-0.893134	N	2.780579	-1.995650	-0.851117
S	9.031416	-0.992529	-2.182108	C	3.754962	-2.602294	-1.790600
O	7.672715	-0.497453	-1.908952	H	4.586973	-2.986436	-1.200105
O	9.912418	-0.188158	-3.035188	H	3.264756	-3.471664	-2.251009
C	8.770744	-2.571521	-3.183728	C	4.268527	-1.677350	-2.897022
F	8.013661	-3.445932	-2.504949	H	4.780237	-0.799555	-2.497686
F	8.142496	-2.270078	-4.335238	H	4.988429	-2.231665	-3.509347

H	3.462154	-1.340605	-3.557903	C	-4.154202	2.395880	-1.279931
S	2.878827	1.992375	0.891188	N	-5.039150	2.138670	-2.269155
O	1.495925	1.520708	0.656349	N	-2.936493	1.810365	-1.312702
O	3.705262	2.132124	-0.333574	C	-5.976550	3.146751	-2.773135
C	0.631552	4.352514	2.328945	H	-5.944270	3.120087	-3.870161
C	6.994851	2.557273	1.810701	H	-7.001396	2.950440	-2.457334
H	7.427275	1.626579	2.226358	H	-5.664240	4.136839	-2.438202
H	6.264092	2.259625	1.059740	C	-5.205993	0.795194	-2.841675
C	6.311546	3.375599	2.901982	H	-4.701459	0.056065	-2.224783
H	5.460791	2.798312	3.267107	H	-6.276861	0.572402	-2.850859
H	6.968441	3.583934	3.752225	H	-4.819287	0.750736	-3.868608
H	5.925313	4.324971	2.516245	C	-2.206316	1.402022	-0.104482
C	1.594867	-1.333956	-1.444288	H	-1.825705	0.388631	-0.264059
H	0.987464	-0.955980	-0.626743	H	-1.349901	2.058775	0.086133
H	1.964639	-0.454106	-1.987126	H	-2.878660	1.376107	0.745181
C	0.771225	-2.219020	-2.381363	C	-2.267653	1.483604	-2.572699
H	-0.104786	-1.659669	-2.720092	H	-1.218900	1.794617	-2.494019
H	1.338789	-2.516110	-3.270393	H	-2.294379	0.412533	-2.776725
H	0.404264	-3.121436	-1.887259	H	-2.737284	2.015103	-3.397830
O	3.569734	1.307944	2.015003	N	-4.484660	3.264855	-0.291800
O	2.737710	3.604111	1.352235	S	-4.246887	-1.068755	2.466358
C	2.044401	3.860953	2.593813	O	-5.188478	-2.028571	3.055372
H	2.637616	4.623118	3.111849	O	-4.792916	0.203701	1.934422
H	2.037079	2.959178	3.212924	C	-3.480255	4.127313	0.363705
H	0.042796	3.595403	1.769195	H	-2.818600	3.550382	1.018332
H	0.649890	5.272897	1.725359	H	-4.048862	4.793606	1.013085
H	0.105681	4.568592	3.276279	C	-2.658831	4.964475	-0.619784

H	-1.978994	5.616773	-0.060645	H	-12.948077	-2.040935	1.783677
H	-2.046218	4.342865	-1.281949	H	-13.055809	-1.554666	0.076970
H	-3.309298	5.593607	-1.236983	H	-12.190544	-3.048481	0.530724
C	-3.097913	-0.526917	3.865694	C	-11.311549	0.029618	1.662161
F	-2.401717	0.550464	3.468103	H	-12.179334	0.530724	1.222459
F	-3.832499	-0.191016	4.935737	H	-11.466978	-0.081012	2.743402
F	-2.246977	-1.497341	4.222473	H	-10.442684	0.654306	1.458079
N	-3.078049	-1.730352	1.540386	N	-9.955345	-2.402160	-0.666177
S	-3.335965	-2.267449	0.051923	C	-9.006328	-3.519547	-0.865481
O	-4.592467	-1.829589	-0.582312	H	-8.422513	-3.626441	0.049919
O	-2.080053	-2.172617	-0.698562	H	-9.605152	-4.435374	-0.964543
C	-3.565806	-4.132255	0.263866	C	-8.078839	-3.395027	-2.077101
F	-4.671896	-4.400411	0.974218	H	-7.462420	-2.494515	-2.035575
F	-3.687282	-4.708150	-0.944725	H	-7.408282	-4.261601	-2.093166
F	-2.511293	-4.678048	0.889580	H	-8.634653	-3.389733	-3.019817
C	-9.983964	-1.696899	0.494767	S	-9.552404	1.685338	-1.301338
N	-8.850079	-1.425458	1.165356	O	-10.959649	1.207786	-1.360895
N	-11.167427	-1.279499	1.013202	O	-8.579652	0.864087	-2.057743
C	-7.583369	-1.132683	0.483828	C	-11.665908	4.150451	-2.699364
H	-7.112937	-0.274082	0.984448	C	-5.820052	3.168026	0.363816
H	-6.885916	-1.974559	0.536435	H	-5.646032	2.760461	1.376692
H	-7.769942	-0.856538	-0.551561	H	-6.401399	2.417638	-0.168321
C	-8.803358	-1.324323	2.626476	C	-6.604413	4.476824	0.437945
H	-9.676277	-1.812399	3.064366	H	-7.583988	4.258903	0.866300
H	-7.893887	-1.820761	2.972430	H	-6.119396	5.226112	1.074220
H	-8.768360	-0.276915	2.949990	H	-6.766165	4.915124	-0.551477
C	-12.408119	-2.022508	0.829010	C	-10.789151	-2.003853	-1.824750

H	-11.389597	-1.148307	-1.521371
H	-10.109649	-1.610644	-2.588295
C	-11.647004	-3.126430	-2.411824
H	-12.235749	-2.719881	-3.241756
H	-11.043014	-3.947312	-2.813720
H	-12.345723	-3.548729	-1.681068
O	-9.115118	2.034277	0.075760
O	-9.501486	3.119539	-2.165784
C	-10.452289	4.141187	-1.780512
H	-9.897774	5.083859	-1.852168
H	-10.740457	4.000554	-0.732973
H	-12.207878	3.203968	-2.623851
H	-11.359797	4.298017	-3.741568
H	-12.341236	4.970022	-2.419311