Supplementary Material (ESI) for New Journal of Chemistry

Electronic Supporting Information

DFT study of the interaction free energy of of π-π complexes of fullerenes with buckybowls and viologen dimers

Girolamo Casella,[a‡] and Giacomo Saielli*[b]

Tables 1 and 2

Figures of molecular orbitals of complexes of C_{60} with viologen dimers.

Cartesian coordinates of all systems investigated

Table 1 Orbital energies, hartrees except where noted. M06-2X/6-31+G**

	HOMO-1	HOMO	LUMO	LUMO+1	Δ(H-L)	Δ(H-L) in eV
C_{60}[a]	-0.27725	-0.27722	-0.11391	-0.11389	-0.16331	-4.44
C_{70}	-0.27176	-0.26915	-0.11642	-0.11632	-0.15723	-4.28
1	-0.23462	-0.22666	-0.05121	-0.04508	-0.17545	-4.77
2	-0.24203	-0.23431	-0.06940	-0.06311	-0.16491	-4.49
C_{60}@**1**	-0.23927	-0.23099	-0.10328	-0.10206	-0.12893	-3.51
C_{60}@**2**	-0.24828	-0.24164	-0.10482	-0.10349	-0.13682	-3.72
C70@**1** A	-0.23945	-0.23162	-0.10667	-0.10600	-0.12495	-3.40
C70@**2** A	-0.25022	-0.24218	-0.10767	-0.10662	-0.13451	-3.66

[a] 5 degenerate homo; 3 degenerate lumo.

Table 2 Orbital energies, hartrees except where noted. M06-2X/6-31+G**

	HOMO-1	HOMO	LUMO	LUMO+1	Δ(H-L)	Δ(H-L) in eV
C_{60}[a]	-0.27725	-0.27722	-0.11391	-0.11389	-0.16331	-4.44
C_{60}[a] PCM (MeOH)	-0.27160	-0.27156	-0.10827	-0.10825	-0.16329	-4.44
$1BP1^{2+}$	-0.62069	-0.61715	-0.34843	-0.285	-0.26872	-7.31
1BP1	-0.28540	-0.1621	0.01123	0.01789	-0.17333	-4.72
$1BP1^{2+}$ PCM (MeOH)	-0.38407	-0.38151	-0.11288	-0.04970	-0.26863	-7.31
1BP1 PCM (MeOH)	-0.29552	-0.17224	0.00437	0.01051	-0.17661	-4.81
C_{60}@$1BP1^{2+}$	-0.42509	-0.42487	-0.32101	-0.27152	-0.10386	-2.83
C_{60}@1BP1	-0.25731	-0.17516	-0.10021	-0.0992	-0.07596	-2.07
C_{60}@$1BP1^{2+}$ PCM (MeOH)	-0.27819	-0.27738	-0.12202	-0.11658	-0.15536	-4.23
C_{60}@1BP1 PCM (MeOH)	-0.25781	-0.17022	-0.10167	-0.10040	-0.0686	-1.87
$1BP6BP1^{4+}$	-0.68445	-0.68338	-0.42109	-0.42028	-0.26229	-7.14
1BP6BP1	-0.16418	-0.16320	0.00851	0.00951	-0.17171	-4.67
C_{60}@$1BP6BP1^{4+}$	-0.53870	-0.53811	-0.41539	-0.4137	-0.12272	-3.34
C_{60}@1BP6BP1	-0.16761	-0.16492	-0.08944	-0.08827	-0.07548	-2.05
$1BP7BP1^{4+}$	-0.67905	-0.67210	-0.41347	-0.41311	-0.25863	-7.04
1BP7BP1	-0.1619	-0.16135	0.00664	0.01239	-0.16799	-4.57
C_{60}@$1BP7BP1^{4+}$[b]	-0.52568	-0.52395	-0.41145	-0.40252	-0.1125	-3.06
C_{60}@1BP7BP1	-0.16763	-0.16446	-0.09063	-0.08929	-0.07383	-2.01
$1BP8BP1^{4+}$	-0.66555	-0.65734	-0.40762	-0.40553	-0.24972	-6.80
1BP8BP1	-0.16231	-0.16196	0.00934	0.00953	-0.17149	-4.67
C_{60}@$1BP8BP1^{4+}$	-0.5417	-0.54135	-0.41174	-0.40976	-0.12961	-3.53
C_{60}@1BP8BP1	-0.16781	-0.16396	-0.09016	-0.08936	-0.0738	-2.01
$1BP9BP1^{4+}$	-0.6447	-0.63286	-0.40298	-0.40282	-0.22988	-6.26
1BP9BP1	-0.1616	-0.16121	0.00885	0.01112	-0.17006	-4.63
C_{60}@$1BP9BP1^{4+}$	-0.54542	-0.54407	-0.41023	-0.41008	-0.13384	-3.64
C_{60}@1BP9BP1	-0.16784	-0.16329	-0.09063	-0.08923	-0.07266	-1.98

[a] 5 degenerate homo; 3 degenerate lumo.[b]Convergence reached with *sleazy* option of Gaussian09.

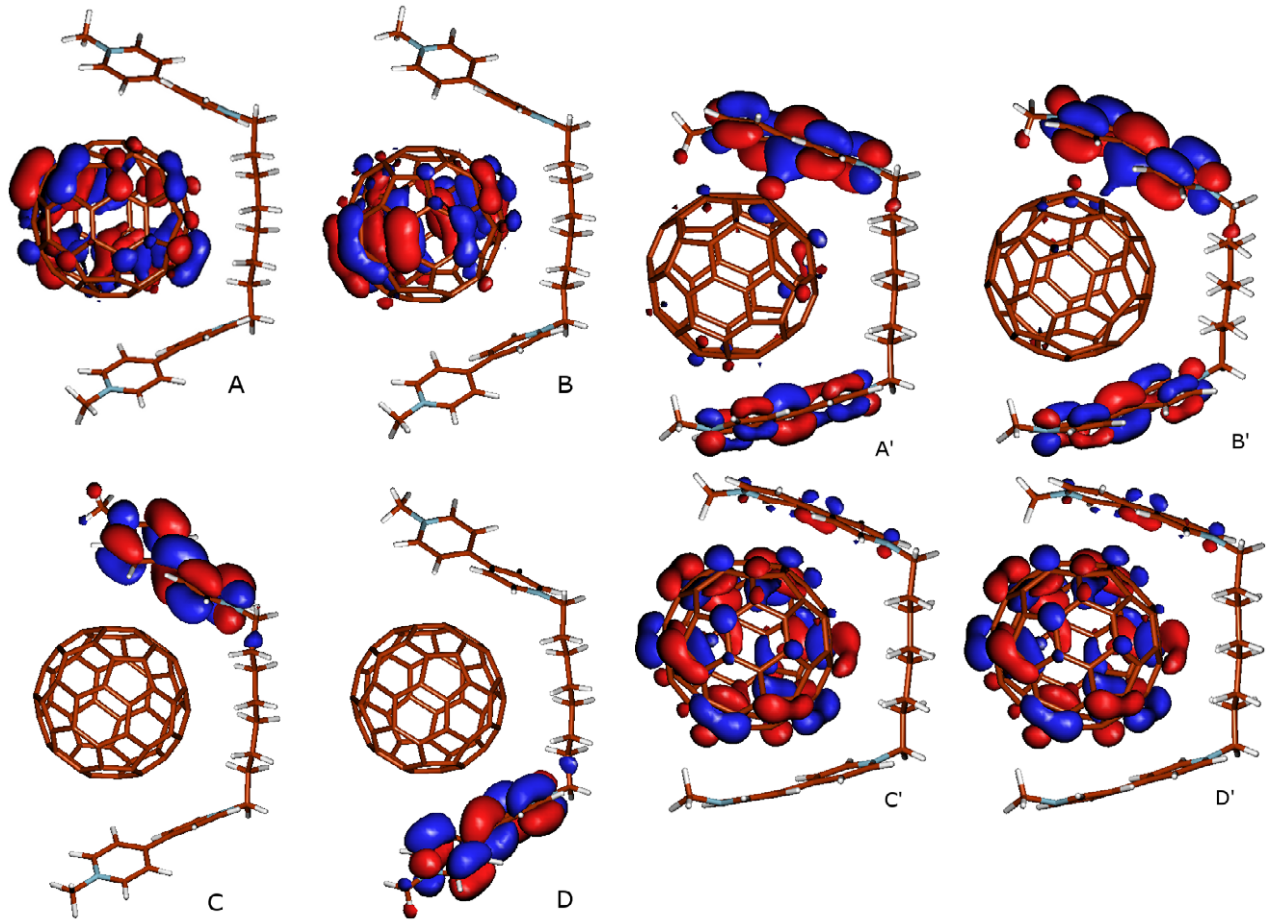

Fig. 1 (Left) Orbitals of the complexes of C_{60} with $1BP8BP1^{2+}$ (cationic form). A: HOMO-1; B: HOMO; C: LUMO; D: LUMO+1. (Right) Orbitals of the complexes of C_{60} with 1BP8BP1 (neutral form). A: HOMO-1; B: HOMO; C: LUMO; D: LUMO+1.

C60

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C	1.549117	0.705595	-3.121730
C	1.033177	-0.639225	-3.341537
C	1.599526	-1.722549	-2.668419
C	2.706939	-1.508388	-1.745316
C	3.200755	-0.220188	-1.534432
C	2.609614	0.910926	-2.237982
C	3.545861	0.218098	-0.188085
C	3.381206	-0.651689	0.891552
C	2.865360	-1.996930	0.672154
C	2.535411	-2.415601	-0.617944
C	3.165861	1.619337	-0.058960
C	2.638914	2.091694	1.143918
C	2.468061	1.183727	2.271294
C	2.830746	-0.158289	2.147251
C	1.510135	3.013157	1.132448
C	0.956808	3.425030	-0.081072
C	1.506725	2.930442	-1.336765
C	2.587702	2.047518	-1.326182
C	0.641602	2.675700	2.252241
C	1.233088	1.544952	2.955986
C	0.413727	0.548476	3.488017
C	0.792293	-0.852270	3.359710
C	1.974466	-1.198240	2.703342
C	1.995913	-2.334864	1.791952
C	-0.744560	2.763094	2.111623
C	-1.599603	1.722685	2.668533
C	-1.033092	0.639131	3.341292
C	-1.549046	-0.705552	3.121530
C	-0.420822	-1.627860	3.133356
C	-0.400143	-2.716242	2.260053
C	0.834475	-3.077659	1.575016
C	1.322922	-3.191395	-0.844639
C	0.490408	-3.514931	0.228040
C	-0.956681	-3.424564	0.081094
C	-1.506673	-2.930100	1.336694
C	-2.588052	-2.047698	1.326381
C	-2.609912	-0.910933	2.238149
C	0.744661	-2.763146	-2.111622
C	-0.641647	-2.675749	-2.252178
C	-1.510345	-3.013521	-1.132625
C	-3.165910	-1.619342	0.059011
C	-2.639052	-2.091821	-1.143917
C	-2.467852	-1.183670	-2.271072
C	-1.232994	-1.544933	-2.955762
C	-0.413701	-0.548582	-3.488016
C	0.420825	1.627760	-3.133267
C	-0.792240	0.852151	-3.359339
C	-1.974700	1.198336	-2.703630
C	-2.831052	0.158292	-2.147546
C	-3.200694	0.220214	1.534410
C	-3.545615	-0.218066	0.188004
C	-3.381204	0.651666	-0.891636
C	-2.706808	1.508431	1.745277
C	-2.865056	1.996760	-0.672104
C	-2.535363	2.415626	0.617935
C	-1.322874	3.191326	0.844611
C	-0.490437	3.515174	-0.228097
C	-1.995935	2.334774	-1.791935
C	-0.834435	3.077669	-1.575020
C	0.400199	2.716257	-2.260046

C70

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C	0.000112	0.558710	-3.523298
C	-0.000141	-2.522267	2.521320
C	-0.000119	-3.325206	1.287678
C	-0.000017	-3.177818	-1.620417
C	0.000032	-2.252998	-2.765897
C	-1.207588	-1.579362	-3.093785
C	-1.207582	-0.188367	-3.468459
C	-1.207488	2.453327	-2.457652
C	-1.207717	3.240362	-1.251363
C	-1.207449	3.096453	1.573712
C	-1.207428	2.191555	2.694778
C	-1.207538	-0.540255	3.431107
C	-1.207587	-1.886025	2.916742
C	-1.207480	-3.430010	0.545963
C	-1.207359	-3.356128	-0.892665
C	-2.445884	-2.726376	-1.308888
C	-2.445821	-1.853251	-2.389697
C	-2.445934	0.401935	-2.996911
C	-2.446213	1.699957	-2.501028
C	-2.446331	2.975569	-0.544348
C	-2.445768	2.904175	0.843468
C	-2.445957	1.436963	2.661484
C	-2.446007	0.095163	3.023027
C	-2.445809	-2.087543	2.188665
C	-2.446237	-2.846681	1.024643
C	-3.227193	-2.417912	-0.123344
C	-3.227345	-0.629688	-2.336739
C	-3.227977	2.028567	-1.321274
C	-3.226952	1.883272	1.520440
C	-3.226832	-0.864484	2.260982
C	-3.972441	-1.237779	-0.062719
C	-3.972092	-0.322497	-1.195596
C	-3.972871	1.038133	-0.676091
C	-3.972258	0.964017	0.778468
C	-3.972125	-0.442787	1.157539
C	1.207286	-3.430050	0.546007
C	2.446034	-2.846752	1.024736
C	3.227122	-2.418000	-0.123222
C	3.972392	-1.237890	-0.062547
C	3.972060	-0.442939	1.157717
C	3.972293	0.963891	0.778651
C	3.972954	1.038025	-0.675903
C	3.972106	-0.322583	-1.195419
C	3.226666	-0.864616	2.261102
C	3.226955	1.883122	1.520613
C	3.228120	2.028428	-1.321109
C	3.227496	-0.629768	-2.336632
C	2.445932	-1.853337	-2.389628
C	2.445861	-2.726439	-1.308813
C	2.445565	-2.087640	2.188747
C	2.445831	0.095044	3.023125
C	2.445880	1.436840	2.661617
C	2.445882	2.904095	0.843595
C	2.446492	2.975527	-0.544221
C	2.446311	1.699867	-2.500873
C	2.446120	0.401882	-2.996847
C	1.207719	-1.579411	-3.093770
C	1.207764	-0.188431	-3.468406
C	1.207714	2.453353	-2.457591
C	1.207957	3.240449	-1.251334
C	0.000080	3.522868	-0.557710
C	0.000053	3.448358	0.912215
C	1.207504	3.096391	1.573787
C	1.207374	2.191508	2.694823
C	-0.000057	1.619141	3.177874
C	1.207292	-3.356161	-0.892615
C	1.207314	-1.886083	2.916817
C	1.207313	-0.540333	3.431176
C	-0.000097	0.197382	3.560947
C	0.000108	1.933533	-2.996757

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C	-3.452156	-3.320259	1.555112
C	-2.833199	-2.233043	0.886307
C	-3.487956	-0.959308	0.906819
C	-4.720572	-0.844613	1.599185
C	-5.312248	-1.931938	2.216837
C	-4.672185	-3.182620	2.193017
C	-2.814734	0.190537	0.346854
C	-1.419186	0.121588	0.170112
C	-0.759430	-1.154559	0.157281
C	-1.509814	-2.337223	0.314604
C	0.661486	-1.220902	-0.024084
C	1.427028	-0.017668	-0.197063
C	0.766143	1.257338	-0.185927
C	-0.654813	1.322955	-0.002579
C	2.820867	-0.085102	-0.378818
C	3.493485	1.063494	-0.938075
C	2.836432	2.336523	-0.921563
C	1.514271	2.440242	-0.349533
C	4.731197	0.950416	-1.621306
C	5.322656	2.037857	-2.237919
C	4.678219	3.286693	-2.222639
C	3.455295	3.423752	-1.590749
C	-1.303084	2.573892	0.007630
C	-0.504408	3.750865	0.239752
C	0.913714	3.686843	0.066948
C	1.307567	-2.472047	-0.038879
C	2.734184	-2.503309	0.178168
C	3.500397	-1.302448	0.007724
C	-3.491702	1.406156	-0.041110
C	-2.727568	2.603267	-0.210356
C	1.703205	4.809193	0.422126
C	1.121416	5.973859	0.908798
C	-0.278638	6.034739	1.087840
C	-1.059075	4.945181	0.772567
C	-0.910179	-3.582840	-0.102862
C	0.508735	-3.647306	-0.273807
C	4.868966	-1.318324	0.339937
C	5.499701	-2.469683	0.803308
C	4.747491	-3.649145	0.986974
C	3.395037	-3.644838	0.688951
C	-3.391510	3.751921	-0.719595
C	-4.737771	3.748434	-1.007596
C	-5.494951	2.569280	-0.825591
C	-4.870632	1.414515	-0.370447
C	-1.699259	-4.705724	-0.459043
C	-1.117057	-5.870207	-0.944698
C	0.283448	-5.931406	-1.122205
C	1.063618	-4.842294	-0.805844
H	-2.122687	4.971789	1.007790
H	-0.704380	6.937000	1.526325
O	1.805610	7.101649	1.291682
H	2.784691	4.713052	0.385239
H	-2.780820	-4.609604	-0.423721
O	-1.800578	-6.998402	-1.328509
H	0.709062	-6.833545	-1.561118
H	2.127515	-4.868346	-1.039895
H	-2.802205	4.637540	-0.955375
H	-5.237254	4.622176	-1.425777
O	-6.820731	2.669794	-1.171511
H	-5.415729	0.475553	-0.337658
H	2.805399	-4.530397	0.925523
H	5.200753	-4.545526	1.405848
O	6.837818	-2.336040	1.093227
H	5.458342	-0.404092	0.314598
H	-5.168221	0.142821	1.708914
H	-6.247314	-1.805373	2.765344
H	-5.108682	-4.031281	2.722843
H	-2.911978	-4.263890	1.632408
H	5.186218	-0.034098	-1.722225
H	6.263752	1.913053	-2.775963
H	5.115546	4.134753	-2.752731
H	2.913313	4.366017	-1.672073
C	7.472576	-3.516241	1.614004
H	8.519708	-3.226880	1.774123
H	7.025028	-3.830213	2.575087
H	7.426491	-4.354802	0.894843
C	-3.228651	-6.925950	-1.173203
H	-3.599578	-7.908127	-1.494238

	H	-3.512982	-6.744491	-0.119691
	H	-3.667146	-6.136480	-1.810925
	C	3.233747	7.029040	1.134768
	H	3.604969	8.011113	1.455726
5	H	3.672800	6.239370	1.771767
	H	3.516840	6.847981	0.080916
	C	-7.583448	1.460984	-1.008832
	H	-8.609385	1.731171	-1.290373
	H	-7.215869	0.656223	-1.671634
10	H	-7.563082	1.108125	0.039190

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15	C	1.627967	-4.665630	0.112236
	C	1.314593	-3.448564	-0.570884
	C	2.456169	-2.634843	-0.747839
	C	3.742823	-2.782444	-0.123526
	C	3.962694	-3.958294	0.582600
20	C	2.894867	-4.909464	0.634311
	C	2.390899	-1.355433	-1.333116
	C	1.192012	-0.729516	-1.600219
	C	0.000855	-1.506834	-1.445439
	C	0.001687	-2.870615	-0.935348
25	C	1.191182	0.730927	-1.600157
	C	-0.000876	1.506846	-1.445405
	C	-1.192036	0.729528	-1.600143
	C	-1.191206	-0.730911	-1.600110
	C	3.598265	-0.681521	-1.052634
30	C	3.597465	0.685672	-1.052523
	C	2.389344	1.358210	-1.332972
	C	4.451118	1.466378	-0.237017
	C	5.418084	0.724011	0.470927
	C	5.418948	-0.718056	0.470773
35	C	4.452871	-1.461407	-0.237342
	C	2.453063	2.637585	-0.747392
	C	3.739489	2.786514	-0.122912
	C	1.310496	3.449882	-0.570269
	C	1.622222	4.666864	0.113732
40	C	2.888789	4.912061	0.635982
	C	3.957863	3.962348	0.583712
	C	-0.001700	2.870613	-0.935276
	C	-2.390909	1.355429	-1.332954
	C	-2.456174	2.634846	-0.747711
45	C	-1.314606	3.448600	-0.570859
	C	-2.389351	-1.358191	-1.332850
	C	-3.597455	-0.685668	-1.052328
	C	-3.598257	0.681518	-1.052423
	C	-4.452858	1.461406	-0.237131
50	C	-3.742824	2.782470	-0.123394
	C	-3.962708	3.958394	0.582608
	C	-2.894921	4.909622	0.634138
	C	-1.628027	4.665773	0.112051
	C	-2.453059	-2.637595	-0.747352
55	C	-1.310498	-3.449929	-0.570386
	C	-5.418917	0.718034	0.470988
	C	-5.418049	-0.724039	0.471125
	C	-4.451095	-1.466405	-0.236840
	C	-3.739467	-2.786563	-0.122837
60	C	-3.957830	-3.962495	0.583630
	C	-2.888795	-4.912275	0.635647
	C	-1.622245	-4.667045	0.113373
	O	5.169302	4.112505	1.204746
	C	5.342614	5.332593	1.951401
65	O	-5.174311	4.107348	1.203605
	C	-5.349051	5.327592	1.949677
	O	-5.169248	-4.112741	1.204680
	C	-5.342400	-5.332796	1.951431
	O	5.174343	-4.107247	1.203510
70	C	5.348857	-5.327141	1.950215
	H	0.877457	5.443519	0.257300
	H	3.049904	5.861420	1.143732
	H	-3.049949	-5.861751	1.143168
	H	-0.877535	-5.443809	0.256652
75	H	-0.884439	5.443772	0.254530
	H	-3.057378	5.859229	1.140999
	H	0.884319	-5.443527	0.254941
	H	3.057301	-5.858999	1.141314
	H	-6.115194	1.225168	1.142984
80	H	-6.113731	-1.231883	1.143208
	H	6.115222	-1.225209	1.142756
	H	6.113763	1.231854	1.143012
	H	6.357547	-5.253803	2.376517
	H	4.606327	-5.414336	2.763739
85	H	5.288652	-6.214275	1.294776
	H	6.351599	5.260493	2.377266
	H	5.280991	6.219669	1.296009
	H	4.600357	5.418843	2.765281
	H	-6.357842	5.254415	2.375780
90	H	-4.606728	5.415210	2.763352
	H	-5.288713	6.214416	1.293829
	H	-6.351269	-5.260646	2.377557
	H	-5.280990	-6.219899	1.296057
	H	-4.599920	-5.419035	2.765104
95				

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	C	-1.521984	0.653386	5.936988
100	C	-1.658411	0.128649	4.628551
	C	-1.702406	-1.290564	4.460925
	C	-1.609144	-2.112461	5.611040
	C	-1.454679	-1.570518	6.876183
	C	-1.410087	-0.175385	7.040393
105	C	-1.948434	-1.834133	3.145244
	C	-2.536784	-0.997973	2.177683
	C	-2.479963	0.430244	2.341275
	C	-1.855002	0.978570	3.476661
	C	-2.943711	1.285611	1.289481
110	C	-3.486338	0.725483	0.083694
	C	-3.555077	-0.699199	-0.072010
	C	-3.075358	-1.556015	0.974622
	C	-3.880755	1.570526	-0.971627
	C	-3.968929	1.010012	-2.297956
115	C	-4.025013	-0.413140	-2.454721
	C	-4.007634	-1.255048	-1.283604
	C	-3.846210	1.812726	-3.462342
	C	-3.796570	1.254458	-4.726392
	C	-3.839565	-0.142724	-4.879113
120	C	-3.937721	-0.954095	-3.764090
	C	-3.039831	-2.949388	0.769453
	C	-3.882380	-3.504816	-0.260036
	C	-4.379006	-2.652107	-1.292859
	C	-2.800131	2.682358	1.408141
125	C	-3.579363	3.520556	0.531816
	C	-4.133650	2.963099	-0.666773
	C	-1.550201	-3.160536	2.739955
	C	-2.115140	-3.724277	1.553874
	C	-5.292286	-3.174226	-2.240105
130	C	-5.690699	-4.506288	-2.193659
	C	-5.203088	-5.349013	-1.169558
	C	-4.330871	-4.850637	-0.226591
	C	-1.352313	2.327744	3.387101
	C	-1.840108	3.187805	2.354895
135	C	-4.989238	3.758742	-1.450965
	C	-5.296590	5.072090	-1.098798
	C	-4.757636	5.621743	0.083966
	C	-3.925266	4.847021	0.874664
	C	-1.591247	-4.960764	1.086508
140	C	-0.564157	-5.607215	1.736179
	C	0.009826	-5.036992	2.896285
	C	-0.484018	-3.834448	3.388348
	C	-0.248039	2.745579	4.171222
	C	0.355472	3.979526	3.961253
145	C	-0.141745	4.842209	2.956677
	C	-1.203673	4.446498	2.174878
	H	-4.028983	-5.484296	0.607689
	H	-5.570091	-6.374073	-1.126974
	O	-6.578445	-5.096849	-3.058118
150	H	-5.734679	-2.494045	-2.963007
	H	0.185932	2.036502	4.870978
	O	1.469521	4.435503	4.618782
	H	0.380204	5.782434	2.780423
	H	-1.501674	5.070268	1.331899
155	H	-1.952282	-5.363101	0.140469
	H	-0.131974	-6.528796	1.347179
	O	1.073058	-5.730442	3.417073
	H	0.004630	-3.340087	4.223879
	H	-3.583200	5.248989	1.828932
160	H	-5.021077	6.627020	0.406787
	O	-6.161749	5.724649	-1.943605
	H	-5.498136	3.340606	-2.317919
	H	-1.728172	-3.190584	5.495408
	H	-1.412068	-2.225701	7.747648
165	H	-1.332039	0.255586	8.039894
	H	-1.574128	1.734088	6.074474
	H	-3.709180	2.887468	-3.347463
	H	-3.673611	1.897780	-5.599478
	H	-3.743537	-0.588167	-5.870536
170	H	-3.868368	-2.035929	-3.878346
	C	-6.513031	7.062671	-1.548744
	H	-7.197347	7.417133	-2.330568
	H	-7.028750	7.076117	-0.570945
	H	-5.626609	7.721325	-1.505694
175	C	2.014058	3.526527	5.594260
	H	2.873427	4.056375	6.025616
	H	1.278314	3.297632	6.387534
	H	2.352095	2.585395	5.123257
	C	-7.089998	-4.233806	-4.090106
180	H	-7.744658	-4.873346	-4.695951
	H	-7.675545	-3.397905	-3.665675
	H	-6.275530	-3.828234	-4.719376
	C	1.729742	-5.090634	4.526882
	H	2.547595	-5.769744	4.801583
185	H	2.141092	-4.107156	4.234156
	H	1.045328	-4.963763	5.386251
	C	3.597401	3.477631	-1.871701
	C	2.636527	3.169015	-2.835175
	C	1.249295	2.953952	-2.443169
190	C	0.882963	3.053378	-1.098232
	C	1.888722	3.375958	-0.090121
	C	3.216222	3.584577	-0.469537
	C	-0.036745	2.083105	-0.521524
	C	-0.551380	1.055218	-1.313246
195	C	-0.172631	0.950951	-2.714557
	C	0.709836	1.881134	-3.269359
	C	-0.649690	-0.295633	-0.775253
	C	-0.219857	-0.558539	0.521618
	C	0.312866	0.512426	1.347342
200	C	0.403996	1.805264	0.839545
	C	-0.344610	-1.235749	-1.842237
	C	0.371911	-2.401461	-1.557095
	C	0.807799	-2.678065	-0.193642
	C	0.514401	-1.772980	0.825247
205	C	2.128435	-3.290956	-0.255483
	C	2.509685	-3.395134	-1.657174
	C	1.424496	-2.845157	-2.461339
	C	3.089140	-2.985171	0.710464
	C	4.473661	-2.763410	0.314603
210	C	4.840864	-2.862565	-1.029235
	C	3.837043	-3.185470	-2.036189
	C	5.013291	-1.689026	1.139682
	C	5.896027	-0.759843	0.584792
	C	6.279301	-0.864132	-0.817434
215	C	5.761504	-1.892001	-1.607086
	C	5.327182	-1.616352	-2.970608
	C	5.430005	-0.324001	-3.487405
	C	5.969771	0.749829	-2.662961
	C	6.385245	0.486151	-1.357087

	C	6.069488	1.423500	-0.287172
	C	5.766469	0.654444	0.912686
	C	4.137608	-2.414130	-3.234933
	C	2.774406	-2.045262	1.782877
5	C	3.962834	-1.243453	2.046145
	C	3.838513	0.112990	2.361363
	C	4.758966	1.081927	1.779213
	C	3.100177	-1.886745	-4.005154
	C	1.714335	-2.107329	-3.611853
10	C	1.511984	-1.452912	1.837879
	C	0.964625	-0.892631	-3.907492
	C	-0.045260	-0.465679	-3.043824
	C	2.519324	0.730126	2.427210
	C	1.381080	-0.037831	2.166328
15	C	1.763293	1.432787	-4.171771
	C	1.887426	0.077485	-4.486006
	C	3.206909	-0.536830	-4.545093
	C	4.347562	0.227598	-4.292667
	C	2.625351	2.081687	1.885750
20	C	1.588578	2.604498	1.108943
	C	2.953115	2.230106	-3.905097
	C	4.300065	3.034562	0.334808
	C	4.009417	2.297312	1.485731
	C	4.217628	1.641269	-3.965785
25	C	4.916303	2.861334	-1.934237
	C	5.219758	1.963293	-2.958714
	C	5.349082	2.585395	-0.570492

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	C	4.885992	-2.356231	1.338703
	C	3.807314	-2.980495	1.994787
	C	2.983887	-3.787110	1.173946
35	C	3.123656	-3.846666	-0.182334
	C	4.108721	-3.117999	-0.892734
	C	5.036850	-2.427058	-0.088329
	C	3.562146	-3.020521	-2.278828
	C	2.233557	-3.573981	-2.260160
40	C	1.976514	-4.082747	-0.970238
	C	3.943623	-2.335529	-3.424113
	C	3.024958	-2.320339	-4.522007
	C	1.725176	-2.800460	-4.426694
	C	1.215408	-3.363180	-3.209982
45	C	0.696371	-4.223793	-0.465346
	C	-0.387047	-3.979372	-1.375191
	C	-0.175727	-3.539646	-2.755889
	C	-1.666858	-3.912415	-0.727572
	C	-2.734275	-3.474325	-1.493173
50	C	-2.563732	-2.928361	-2.785566
	C	-1.334261	-2.971862	-3.473259
	C	-1.819107	-3.852467	0.730601
	C	-0.701863	-3.851015	1.633893
	C	0.545709	-4.161183	0.992567
55	C	1.699273	-3.970008	1.735223
	C	-3.928392	-2.939694	-0.956522
	C	-4.067311	-2.877767	0.401026
	C	-3.017691	-3.357754	1.217049
	C	-3.118743	-2.709155	2.467431
60	C	-2.059411	-2.683875	3.395537
	C	-0.776088	-3.279818	2.978282
	C	0.497452	-3.014872	3.676559
	C	1.690465	-3.334944	2.997495
	C	-4.252536	-1.823704	2.432304
65	C	-4.816451	-1.867072	1.052697
	C	-5.546814	-1.015628	0.202851
	C	-5.400481	-1.079674	-1.225200
	C	-4.519361	-1.995535	-1.830081
	C	-3.663795	-2.038925	-3.049249
70	C	-1.362391	-2.207230	-4.684621
	C	-2.433969	-1.384563	-5.012745
	C	-3.574251	-1.223085	-4.167212
	C	-4.411703	-0.950402	3.497661
	C	-3.489092	-1.060115	4.584011
75	C	-2.364847	-1.873710	4.539163
	C	2.988026	-2.751017	3.220051
	C	3.119853	-1.876960	4.287819
	C	1.989823	-1.706628	5.146188
	C	0.740761	-2.241265	4.859691
80	H	1.116009	-2.738158	-5.322559
	H	3.340365	-1.887328	-5.470281
	O	5.157984	-1.707924	-3.407363
	O	-5.407434	-0.017827	3.408490
	H	-3.642446	-0.453506	5.475484
85	H	-1.726619	-1.859846	5.414805
	H	-0.527990	-2.204851	-5.376071
	H	-2.366256	-0.802454	-5.930769
	O	-4.554864	-0.285243	-4.338115
	H	-0.048292	-2.021719	5.568484
90	H	2.090141	-1.095782	6.042378
	O	4.299694	-1.193363	4.397418
	H	-5.878671	-0.304698	-1.828104
	H	-6.136428	-0.197622	0.622849
	H	5.551960	-1.692978	1.895238
95	H	5.812526	-1.815621	-0.554970
	C	4.299532	-0.098013	5.338052
	H	5.266934	0.398344	5.189711
	H	3.476782	0.608452	5.121746
	H	4.226202	-0.456403	6.380074
100	C	5.456990	-0.886577	-4.555734
	H	6.418290	-0.412666	-4.317940
	H	5.563836	-1.495074	-5.471158
	H	4.685300	-0.110860	-4.704867
	C	-4.334124	0.663734	-5.402874
105	H	-5.167850	1.373231	-5.323583
	H	-3.374987	1.196754	-5.269853
	H	-4.359039	0.174104	-6.392729
	C	-5.418274	0.982511	4.449316
	H	-6.203884	1.688805	4.152147
110	H	-5.670379	0.542844	5.430788
	H	-4.447073	1.506162	4.508923
	C	-0.691456	5.531411	0.996221
	C	0.619160	5.777517	0.582542
	C	0.961532	5.707539	-0.831532
115	C	-0.020498	5.396152	-1.772589
	C	-1.388654	5.138954	-1.341920
	C	-1.717684	5.204976	0.013042
	C	0.284882	4.487441	-2.870563
	C	1.560272	3.928567	-2.979189
120	C	2.585546	4.253624	-1.996099
	C	2.291794	5.124024	-0.945133
	C	1.713260	2.525324	-3.339393
	C	0.581756	1.740052	-3.571345
	C	-0.750421	2.321980	-3.461938
125	C	-0.895216	3.668273	-3.118003
	C	2.833332	1.983443	-2.579226
	C	2.775466	0.677685	-2.084310
	C	1.593264	-0.136700	-2.325457
	C	0.521296	0.379895	-3.053595
130	C	1.346079	-0.937047	-1.135169
	C	2.371324	-0.614632	-0.153916
	C	3.256003	0.385197	-0.738972
	C	0.035431	-1.172861	-0.721362
	C	-0.305885	-1.100753	0.689167
135	C	0.676260	-0.791632	1.626282
	C	2.042860	-0.544832	1.199440
	C	-1.638188	-0.526953	0.805067
	C	-1.934727	0.338676	1.858007
	C	-0.908181	0.662694	2.838961
140	C	0.368922	0.108854	2.726536
	C	1.549223	0.923855	2.979125
	C	1.403113	2.270514	3.325172
	C	0.071052	2.851988	3.435657
	C	-1.059615	2.065769	3.199249
145	C	-2.180710	2.607663	2.438415
	C	-2.723677	1.536071	1.609454
	C	2.586877	0.518934	2.033953
	C	-1.085625	-0.637414	-1.479672
	C	-2.120903	-0.239325	-0.536802
150	C	-2.877470	0.908380	-0.778488
	C	-3.182102	1.816464	0.319026
	C	3.432781	1.477219	1.474379
	C	3.775524	1.408556	0.056441
	C	-0.845725	0.123146	-2.622263
155	C	3.830378	2.770866	-0.458520
	C	3.371653	3.052203	-1.747410
	C	-2.629164	1.704979	-1.973463
	C	-1.633707	1.318923	-2.876049
	C	2.771360	4.831273	0.399007
160	C	3.523900	3.680209	0.638783
	C	3.276378	2.882150	1.832984
	C	2.285620	3.271352	2.737372
	C	-2.775520	3.110414	-1.612252
	C	-1.929430	4.070514	-2.172566
165	C	1.738543	5.237351	1.342917
	C	-2.600555	4.203838	0.598802
	C	-3.117953	3.178456	-0.195529
	C	1.499888	4.473250	2.486843
	C	-0.940172	4.731479	2.188210
170	C	0.131401	4.213116	2.917515
	C	-2.119934	3.912056	1.943040

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175	C	2.023709	4.837696	3.659742
	C	2.075396	3.990083	2.526188
	C	2.039533	4.582797	1.224961
	C	1.939230	5.992384	1.124175
	C	1.863843	6.793541	2.250951
180	C	1.909742	6.211321	3.530032
	C	2.216453	3.741236	0.065730
	C	2.809192	2.475541	0.242216
	C	2.822190	1.872631	1.547377
	C	2.263174	2.562572	2.641113
185	C	3.302434	0.531690	1.705438
	C	3.758548	-0.215888	0.565212
	C	3.759156	0.393589	-0.734241
	C	3.281651	1.738788	-0.890229
	C	4.139448	-1.563044	0.709536
190	C	4.134072	-2.401749	-0.464311
	C	4.131351	-1.793669	-1.761175
	C	4.135759	-0.354541	-1.866019
	C	3.929031	-3.802803	-0.373950
	C	3.742267	-4.582595	-1.500122
195	C	3.748977	-3.987518	-2.774868
	C	3.932408	-2.622514	-2.896790
	C	3.168263	2.288166	-2.183174
	C	3.936441	1.688901	-3.244569
	C	4.433687	0.359946	-3.086713
200	C	3.224723	-0.094942	2.964445
	C	3.991547	-1.299286	3.171742
	C	4.455935	-2.043219	2.037361
	C	1.734558	4.082132	-1.250698
	C	2.231353	3.361659	-2.381554
205	C	5.273928	-0.189195	-4.085598
	C	5.603342	0.540015	-5.224028
	C	5.118117	1.858968	-5.375857
	C	4.315353	2.413670	-4.404038
	C	1.833573	1.791041	3.782499
210	C	2.326629	0.457629	3.943594
	C	5.286570	-3.159038	2.249391
	C	5.651370	-3.567802	3.530652
	C	5.208260	-2.829859	4.649355
	C	4.405470	-1.718333	4.456091
215	C	1.625540	3.601729	-3.645603
	C	0.579495	4.482684	-3.794253
	C	0.066365	5.167949	-2.668112
	C	0.646880	4.974888	-1.419585
	C	0.800079	2.256583	4.635963

	C	0.258838	1.438312	5.618527
	C	0.756522	0.125021	5.789820
	C	1.755525	-0.344945	4.969397
	H	4.019754	3.459945	-4.490365
5	H	5.434896	2.427044	-6.250035
	O	6.417515	0.101773	-6.238056
	H	5.714812	-1.167480	-3.910133
	H	0.356458	3.226340	4.425206
	O	-0.796372	1.767618	6.430573
10	H	0.279235	-0.513427	6.533114
	H	2.049673	-1.392006	5.042663
	H	1.934104	2.999444	-4.499756
	H	0.079039	4.619699	-4.752480
	O	-1.038889	5.939909	-2.916899
15	H	0.213400	5.433876	-0.534623
	H	4.140528	-1.106010	5.318320
	H	5.523584	-3.093261	5.656982
	O	6.473584	-4.666903	3.589627
	H	5.724604	-3.693800	1.407829
20	H	1.993437	6.451783	0.136065
	H	1.814621	7.878597	2.146075
	H	1.899303	6.843516	4.418984
	H	2.142611	4.395713	4.649468
	H	3.828529	-4.255588	0.612069
25	H	3.542280	-5.650239	-1.394953
	H	3.552582	-4.592338	-3.661836
	H	3.830419	-2.155289	-3.876222
	C	6.876384	-5.065971	4.911596
	H	7.507301	-5.951388	4.757722
30	H	7.465310	-4.277107	5.414183
	H	6.007541	-5.334875	5.539363
	C	-1.384660	3.056859	6.173422
	H	-2.206712	3.141355	6.896163
	H	-0.657552	3.873631	6.336850
35	H	-1.783515	3.118250	5.143257
	C	6.928301	-1.234119	-6.076376
	H	7.527686	-1.418931	-6.977381
	H	7.569440	-1.318026	-5.180341
	H	6.109532	-1.974663	-6.012702
40	C	-1.642079	6.532966	-1.751194
	H	-2.510856	7.085517	-2.131847
	H	-1.972131	5.756575	-1.035304
	H	-0.949005	7.230362	-1.245441
	C	-1.393461	-1.387758	2.940834
45	C	-1.933101	0.482541	-3.568871
	C	-0.706829	0.791454	-2.818345
	C	0.560218	0.521085	-0.224829
	C	0.407351	0.008581	1.140101
	C	-0.420232	0.720321	2.043910
50	C	-1.313708	0.031510	2.935891
	C	-3.865553	-1.173452	3.111814
	C	-5.065327	-1.475747	2.373611
	C	-6.327651	-1.227714	-0.146528
	C	-6.170752	-0.721210	-1.486266
55	C	-4.397643	0.641280	-3.220579
	C	-3.098217	1.257344	-3.312279
	C	-0.746294	1.849905	-1.868967
	C	-0.116412	1.711737	-0.585847
	C	-0.878936	2.471971	0.383459
60	C	-1.030847	1.983001	1.675600
	C	-2.489384	0.862546	3.117688
	C	-3.744919	0.268903	3.201199
	C	-5.690828	-0.221035	2.001839
	C	-6.311216	-0.098521	0.763142
65	C	-6.053756	0.722988	-1.406915
	C	-5.182702	1.391534	-2.259452
	C	-3.076347	2.393415	-2.410008
	C	-1.917741	2.686450	-1.700708
	C	-2.000157	3.090507	-0.303184
70	C	-2.314233	2.086397	2.347629
	C	-4.881596	0.868195	2.522013
	C	-6.153038	1.118663	-0.013090
	C	-4.372323	2.489774	-1.758789
	C	-3.243548	3.174256	0.330205
75	C	-3.404122	2.661488	1.684417
	C	-4.717498	2.037123	1.774665
	C	-5.368235	2.166480	0.477777
	C	-4.459146	2.869340	-0.415872
	C	0.214231	-0.261505	-2.558602
80	C	0.015199	-1.597587	-3.090577
	C	0.545346	-2.560410	-2.136557
	C	-0.108395	-3.776581	-1.926247
	C	-1.324727	-4.080065	-2.668714
	C	-2.236786	-4.779901	-1.775303
85	C	-1.587272	-4.907961	-0.478677
	C	-0.270260	-4.289790	-0.571482
	C	-1.826614	-3.155753	-3.590227
	C	-3.609527	-4.523713	-1.843818
	C	-2.339514	-4.773439	0.691454
90	C	0.229422	-3.561586	0.511588
	C	0.894745	-2.290335	0.287390
	C	1.049008	-1.803102	-1.004290
	C	-1.145093	-1.889245	-3.799681
	C	-3.253181	-2.884924	-3.646897
95	C	-4.123601	-3.553629	-2.794153
	C	-4.384220	-4.374448	-0.623518
	C	-3.763609	-4.496812	0.614381
	C	-1.817131	-4.009702	1.811134
	C	-0.563326	-3.416617	1.722313
100	C	0.532701	-1.387290	1.359795
	C	-0.361946	-2.080546	2.249063
	C	-2.914091	-3.287082	2.428024
	C	-4.113635	-3.587824	1.689110
	C	-5.145673	-2.623337	1.539603
105	C	-5.803286	-2.493696	0.228768
	C	-5.376566	-3.337824	-0.831252
	C	-5.216550	-2.831789	-2.170640
	C	-5.482073	-1.469951	-2.479618
	C	0.839813	-0.394252	-1.269600
110	C	-2.144808	-0.855983	-3.999543
	C	-3.444794	-1.470906	-3.906198
	C	-4.559312	-0.761685	-3.381538
	C	-2.721437	-2.013770	3.031967

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150

	C	-1.930604	0.686357	5.047297
	C	-2.673875	1.239701	3.954926
120	C	-3.636712	0.339131	3.453953
	C	-3.750466	-1.062041	3.763391
	C	-2.907891	-1.567046	4.744822
	C	-2.052337	-0.645823	5.421482
	C	-4.381600	0.599149	2.281276
125	C	-4.083916	1.654603	1.437316
	C	-3.113950	2.603754	1.901671
	C	-2.397158	2.456841	3.166604
	C	-4.423459	1.489715	0.019495
	C	-3.803846	2.253883	-1.025407
130	C	-3.029571	3.352693	-0.530681
	C	-2.704849	3.527910	0.885726
	C	-4.953257	-0.622019	1.856393
	C	-5.278774	-0.772773	0.537715
	C	-5.009577	0.293481	-0.348111
135	C	-5.255399	-2.023039	-0.127627
	C	-5.013162	-3.135522	0.701201
	C	-4.658177	-2.977473	2.085881
	C	-4.547473	-1.704227	2.676150
	C	-4.880430	-0.247544	-1.645540
140	C	-5.082173	-1.668575	-1.569594
	C	-4.308641	0.470854	-2.714725
	C	-4.216609	-0.320071	-3.907067
	C	-4.466265	-1.686358	-3.901093
	C	-4.821754	-2.407578	-2.717742
145	C	-3.711010	1.784598	-2.405763
	C	-2.248124	4.034535	-1.443391
	C	-2.030435	3.561360	-2.754455
	C	-2.745155	2.469961	-3.291874
	C	-1.650435	4.365700	1.189036
150	C	-0.856052	5.023066	0.226126
	C	-1.155040	4.856644	-1.095162
	C	-0.177608	4.897550	-2.117929
	C	-0.785293	4.103326	-3.230381
	C	-0.295469	3.605384	-4.431257
155	C	-1.082454	2.625857	-5.111092
	C	-2.235020	2.067390	-4.568179
	C	-0.880236	4.228932	2.361476
	C	-1.228103	3.332747	3.392394
	C	1.104426	5.300066	-1.695310
160	C	1.415929	5.488253	-0.301080
	C	0.453520	5.269815	0.704056
	C	0.407846	4.829302	2.133089
	C	1.371631	4.645542	3.115383
	C	0.984676	3.944663	4.300270
165	C	-0.241698	3.304220	4.433341
	O	-4.890914	-3.768233	-2.618583
	C	-4.469252	-4.503674	-3.788065
	O	0.930282	4.051333	-4.840848
	C	1.461104	3.425626	-6.028133
170	O	2.631786	5.108051	2.852591
	C	3.644133	4.748098	3.816922
	O	-2.909853	-2.920792	4.936905
	C	-1.884858	-3.428378	5.818852
	H	-3.952896	0.122542	-4.862473
175	H	-4.355955	-2.229496	-4.838450
	H	1.691365	3.869234	5.125517
	H	-0.420831	2.792385	5.373409
	H	-2.708827	1.285126	-5.150453
	H	-0.742452	2.246423	-6.073280
180	H	-1.210534	1.276923	5.601932
	H	-1.428411	-1.002827	6.239388
	H	1.927429	5.342656	-2.412454
	H	2.459047	5.668817	-0.032543
	H	-4.345168	-3.865194	2.639091
185	H	-4.950199	-4.135988	0.267423
	H	-1.986794	-4.519570	5.766971
	H	-0.879047	-3.130256	5.472073
	H	-2.043467	-3.092132	6.858887
	H	-4.503101	-5.557203	-3.483434
190	H	-5.158902	-4.342946	-4.635563
	H	-3.439737	-4.231662	-4.082133
	H	2.453896	3.873208	-6.160014
	H	1.558520	2.333018	-5.898173
	H	0.836555	3.644203	-6.912199
195	H	4.583984	5.114844	3.384952
	H	3.467950	5.240034	4.789740
	H	3.697447	3.652288	3.948988
	C	2.202217	-0.343245	-3.648974
	C	2.607564	-3.847963	2.148311
200	C	3.147237	-4.420042	0.903814
	C	3.531494	-3.934163	-1.941857
	C	3.307750	-2.963376	-3.025673
	C	1.994099	-2.826479	-3.551487
	C	1.446597	-1.530052	-3.860934
205	C	0.145200	0.725330	-2.755993
	C	-0.381409	1.287635	-1.540194
	C	-0.746942	0.806384	1.217871
	C	-0.530912	-0.142698	2.276418
	C	0.530635	-2.684032	2.897479
210	C	1.197798	-3.831130	2.332147
	C	2.235518	-4.929984	-0.059744
	C	2.425845	-4.690761	-1.467725
	C	1.117517	-4.595886	-2.086859
	C	0.905645	-3.677976	-3.110928
215	C	0.016843	-1.576649	-3.615657
	C	-0.618125	-0.469144	-3.065558
	C	-1.461392	0.433727	-1.090867
	C	-1.649922	0.202567	0.261825
	C	-1.301710	-1.332568	1.983103

C	-0.784703	-2.586581	2.290713
C	0.299387	-4.441530	1.371150
C	0.809526	-4.984120	0.196225
C	0.107807	-4.789958	-1.060723
C	-0.329780	-2.913117	-3.159566
C	-1.629211	-0.647656	-2.041281
C	-2.016669	-1.120601	0.735884
C	-0.938866	-3.681175	1.347769
C	-1.076018	-4.045615	-1.092273
C	-1.300034	-3.086663	-2.165487
C	-1.971045	-1.925771	-1.597493
C	-2.160001	-2.168460	-0.173610
C	-1.611464	-3.479475	0.138005
C	4.378564	-3.918023	0.403914
C	5.149173	-2.929977	1.135039
C	5.834024	-2.078708	0.177899
C	5.973962	-0.710651	0.429417
C	5.438246	-0.143199	1.659042
C	4.886321	1.168621	1.347276
C	5.080427	1.410762	-0.075823
C	5.751528	0.248846	-0.643452
C	4.788480	-0.968786	2.580595
C	3.710515	1.595606	1.971353
C	4.087354	2.067186	-0.808232
C	5.398218	-0.201632	-1.917857
C	5.245540	-1.624472	-2.169622
C	5.457656	-2.541666	-1.146633
C	4.638431	-2.388528	2.309621
C	3.560976	-0.525721	3.218846
C	3.033381	0.726514	2.922920
C	2.677449	2.268960	1.202089
C	2.862140	2.498128	-0.156795
C	3.718091	1.588640	-2.130789
C	4.358454	0.479873	-2.671770
C	4.138151	-1.812292	-3.086579
C	3.589230	-0.515472	-3.393137
C	2.285777	1.748194	-2.297467
C	1.757915	2.303277	-1.077714
C	0.456292	1.971255	-0.617379
C	0.264518	1.719573	0.819461
C	1.383716	1.828438	1.687083
C	1.601863	0.880005	2.748275
C	0.707856	-0.203146	2.964190
C	4.568294	-3.678049	-1.004292
C	3.341226	-2.817080	2.795265
C	2.676159	-1.668189	3.357021
C	1.263705	-1.527222	3.284939
C	1.524080	0.832045	-3.075743

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C	-3.017134	0.628255	5.686960
C	-2.947503	0.108095	4.370812
C	-2.955462	-1.310745	4.192899
C	-3.032163	-2.135418	5.342684
C	-3.074525	-1.597781	6.617926
C	-3.067034	-0.203552	6.792228
C	-2.997019	-1.852032	2.852773
C	-3.428939	-1.010020	1.806927
C	-3.427785	0.416894	1.988067
C	-2.983994	0.965581	3.208842
C	-3.752003	1.278276	0.890860
C	-4.024242	0.722838	-0.406179
C	-4.025098	-0.698650	-0.585951
C	-3.757136	-1.563692	0.527627
C	-4.186787	1.571757	-1.515265
C	-3.935187	1.030105	-2.827091
C	-3.928363	-0.391557	-3.005065
C	-4.186727	-1.244253	-1.872281
C	-3.528232	1.850151	-3.911066
C	-3.128861	1.306769	-5.118351
C	-3.110155	-0.089397	-5.288945
C	-3.500386	-0.916612	-4.251997
C	-3.700620	-2.957916	0.325551
C	-4.321704	-3.496502	-0.859459
C	-4.550529	-2.638603	-1.977822
C	-3.676790	2.677157	1.044392
C	-4.296559	3.502776	0.035434
C	-4.540255	2.952679	-1.264829
C	-2.561149	-3.187154	2.516054
C	-2.943754	-3.749096	1.257489
C	-5.218175	-3.145504	-3.118001
C	-5.644978	-4.468963	-3.166975
C	-5.438752	-5.312846	-2.051802
C	-4.801555	-4.829683	-0.930140
C	-2.523255	2.332584	3.211923
C	-2.902541	3.198760	2.136887
C	-5.208226	3.737447	-2.221424
C	-5.629889	5.035405	-1.936031
C	-5.412195	5.572838	-0.649460
C	-4.764318	4.807303	0.306170
C	-2.384651	-5.004150	0.887256
C	-1.491699	-5.669252	1.693577
C	-1.084589	-5.094607	2.919492
C	-1.622221	-3.877744	3.323055
C	-1.569085	2.782647	4.158322
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C	-1.425800	4.929512	3.039782
C	-2.330657	4.501679	2.096762
H	-4.721981	-5.465471	-0.047542
H	-5.835259	-6.326973	-2.093975
O	-6.310391	-5.047635	-4.218287
H	-5.456364	-2.457529	-3.925568
H	-1.199586	2.071889	4.892628
O	-0.024274	4.540448	4.886193
H	-0.948101	5.906797	2.971921
H	-2.542976	5.144518	1.243289
H	-2.596539	-5.404052	-0.103938
H	-1.023986	-6.603131	1.381493
O	-0.114414	-5.791150	3.593262
H	-1.248378	-3.383344	4.215806
H	-4.671117	5.198565	1.320037
H	-5.781971	6.561378	-0.384352
O	-6.281341	5.684534	-2.956598
H	-5.477380	3.321243	-3.191477
H	-3.128073	-3.213683	5.209825
H	-3.158425	-2.257157	7.483557
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H	-3.453458	2.926653	-3.757438
H	-2.784362	1.961146	-5.920689
H	-2.745582	-0.520846	-6.222516
H	-3.401498	-1.997457	-4.357798
C	-6.748890	7.008671	-2.643688
H	-7.228682	7.363052	-3.565463
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H	-5.914507	7.683588	-2.377864
C	0.530910	3.581242	5.806819
H	1.326524	4.123059	6.333931
H	-0.224245	3.229076	6.533146
H	0.958455	2.714988	5.267996
C	-6.552881	-4.177320	-5.339024
H	-7.059637	-4.807057	-6.081810
H	-7.206691	-3.331060	-5.060732
H	-5.608234	-3.787274	-5.760088
C	0.433007	-5.113316	4.739976
H	1.213620	-5.784578	5.120560
H	0.877990	-4.141616	4.453553
H	-0.332567	-4.951215	5.520508
C	2.054970	-1.063295	-3.775761
C	3.470793	2.982771	1.488109
C	2.983693	3.562626	0.225331
C	2.118276	2.927010	-2.482075
C	1.897726	1.826675	-3.436872
C	3.029576	1.216423	-4.041965
C	3.106920	-0.212414	-4.210251
C	3.778207	-2.637017	-2.914614
C	4.252823	-3.205351	-1.679012
C	5.091325	-2.586095	0.950945
C	5.309308	-1.508941	1.882871
C	5.159841	1.295708	2.214959
C	4.816755	2.530493	1.554917
C	3.881509	3.645187	-0.872566
C	3.453987	3.331168	-2.211601
C	4.581667	2.751317	-2.915594
C	4.373238	1.713514	-3.815770
C	4.498992	-0.602838	-4.088838
C	4.828880	-1.793823	-3.452639
C	5.598702	-2.715071	-1.449589
C	6.010025	-2.411112	-0.157504
C	6.363513	-0.665288	1.352926
C	6.289943	0.713719	1.515317
C	5.734423	2.715074	0.446973
C	5.274181	3.261286	-0.745495
C	5.721725	2.717373	-2.015666
C	5.294218	0.590709	-3.857434
C	5.970172	-1.847702	-2.554788
C	6.813171	-1.227130	0.090868
C	6.660823	1.596260	0.422752
C	6.606020	1.635879	-2.045587
C	6.388251	0.547287	-2.988423
C	6.732490	-0.700347	-2.320231
C	7.164941	-0.382818	-0.965966
C	7.087053	1.061592	-0.796265
C	1.603689	3.432498	-0.094571
C	0.663167	2.831247	0.828944
C	-0.360649	2.145457	0.057462
C	-0.865365	0.926384	0.506056
C	-0.390810	0.353811	1.757708
C	-0.318324	-1.086854	1.589538
C	-0.745030	-1.404355	0.232582
C	-1.081839	-0.158508	-0.434321
C	0.581778	1.023170	2.501847
C	0.727743	-1.804456	2.175200
C	-0.112585	-2.423671	-0.478514
C	-0.790279	0.017639	-1.787759
C	-0.241741	1.279663	-2.249697
C	-0.032042	2.318447	-1.347213
C	1.122521	2.285082	2.023850
C	1.679066	0.278844	3.090541
C	1.751535	-1.102811	2.930586
C	1.397923	-2.853812	1.422218
C	0.987020	-3.155419	0.126939
C	0.217089	-2.228017	-1.879764
C	-0.114099	-1.037991	-2.519747
C	0.750308	1.002581	-3.271104
C	0.827949	-0.428085	-3.439323
C	1.501458	-2.849564	-2.136146
C	1.976247	-3.419776	-0.899576
C	3.364984	-3.474471	-0.602228
C	3.801705	-3.153287	0.766634
C	2.814898	-2.804827	1.729279
C	3.032598	-1.726270	2.661304
C	4.239519	-0.973447	2.649855
C	1.175666	3.116204	-1.435644
C	2.539064	2.318472	2.331448
C	2.882056	1.081771	2.990886
C	4.161843	0.486610	2.822279
C	2.404177	-2.323946	-3.099692

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C	3.355259	-1.145069	-4.391771
C	3.985629	-0.830443	-3.145438
C	4.187750	-1.974967	-2.346853
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	C	2.879407	-2.418702	-4.676555
	C	4.641137	-1.892796	-1.010340
	C	4.745393	-0.690777	-0.332784
	C	4.567354	0.509208	-1.100672
5	C	4.206598	0.489096	-2.517820
	C	4.602806	-0.731314	1.127306
	C	4.260855	0.423270	1.910364
	C	4.324559	1.652785	1.170347
	C	4.473436	1.692698	-0.290007
10	C	4.363496	-3.131597	-0.389726
	C	4.226262	-3.170202	0.968232
	C	4.371697	-1.970299	1.701176
	C	3.375967	-4.090467	1.628949
	C	2.805307	-5.078505	0.804065
15	C	2.956184	-5.042203	-0.624883
	C	3.676065	-4.012928	-1.260034
	C	3.666243	-2.123611	2.913339
	C	3.069419	-3.434129	2.932425
	C	3.326472	-1.030036	3.733055
20	C	2.527389	-1.425930	4.856078
	C	1.970459	-2.693835	4.944806
	C	2.153246	-3.694846	3.941390
	C	3.618007	0.321282	3.217902
	C	3.799496	2.780518	1.781349
25	C	3.062946	2.712210	2.986345
	C	2.976704	1.536107	3.755937
	C	4.070850	2.851517	-0.929627
	C	3.502290	3.967754	-0.276676
	C	3.359340	3.928446	1.080667
30	C	2.299804	4.582620	1.756131
	C	2.159475	3.832577	3.034296
	C	1.193979	3.839025	4.033129
	C	1.209889	2.764237	4.970161
	C	2.043492	1.661575	4.836411
35	C	3.622181	2.866214	-2.268232
	C	3.731746	1.749301	-3.118349
	C	1.488706	5.407666	0.955872
	C	1.647776	5.455921	-0.472213
	C	2.617675	4.676536	-1.127736
40	C	2.766512	4.007860	-2.452415
	C	2.066763	4.090877	-3.648048
	C	2.339530	3.101004	-4.642268
	C	3.131561	1.986070	-4.398715
	O	1.451613	-4.866453	3.873199
45	C	0.302037	-4.949022	4.743255
	O	0.264968	4.841955	4.002344
	C	-0.809755	4.727226	4.959529
	O	1.141865	5.090420	-3.770234
	C	0.308787	5.029968	-4.947887
50	O	2.320947	-4.706708	-3.905869
	C	1.424355	-4.799068	-5.033641
	H	2.330678	-0.752122	5.682408
	H	1.347643	-2.919264	5.809322
	H	1.893050	3.202889	-5.630167
55	H	3.277398	1.305258	-5.229989
	H	1.925626	0.885324	5.581492
	H	0.506306	2.770939	5.800981
	H	3.192988	-0.394918	-5.155747
	H	2.391093	-2.573237	-5.637222
60	H	0.632203	5.922607	1.396616
	H	0.902311	6.002084	-1.054137
	H	2.376934	-5.752228	-1.218910
	H	2.118480	-5.814167	1.227161
	H	0.948706	-5.782569	-4.933526
65	H	0.655595	-4.005508	-4.999054
	H	1.972288	-4.751285	-5.991227
	H	-0.227958	-5.855646	4.423584
	H	0.599115	-5.049685	5.802191
	H	-0.352375	-4.067049	4.617514
70	H	-1.475505	5.570045	4.735131
	H	-1.357655	3.775526	4.834839
	H	-0.438192	4.815664	5.995785
	H	-0.421916	5.838181	-4.816254
	H	0.894914	5.208958	-5.866730
75	H	-0.214830	4.059229	-5.017592
	C	-2.710380	-0.716763	-3.709166
	C	-2.282434	-1.913148	2.955129
	C	-2.439717	-3.036920	2.015505
	C	-2.711049	-3.735149	-0.798624
80	C	-2.775958	-3.183634	-2.162130
	C	-3.975777	-2.544587	-2.579103
	C	-3.942207	-1.323557	-3.343602
	C	-3.715875	1.489855	-3.162037
	C	-3.560408	2.589239	-2.243351
85	C	-3.296841	3.270857	0.490709
	C	-3.233572	2.729755	1.825232
	C	-3.297791	0.333895	3.332644
	C	-3.413669	-1.099800	3.239113
	C	-3.716890	-3.257124	1.432391
90	C	-3.851334	-3.603571	0.040485
	C	-5.091542	-3.029820	-0.444960
	C	-5.152569	-2.509130	-1.732408
	C	-5.099782	-0.531866	-2.975494
	C	-4.987603	0.851132	-2.884287
95	C	-4.736819	2.634209	-1.396211
	C	-4.606823	2.966595	-0.052980
	C	-4.504878	2.091180	2.109017
	C	-4.536582	0.915479	2.850573
	C	-4.723727	-1.407983	2.698733
100	C	-4.872505	-2.467654	1.811699
	C	-5.739772	-2.333198	0.653270
	C	-5.863984	-1.266768	-1.982143
	C	-5.634825	1.564118	-1.796302
	C	-5.369711	2.246420	0.952231
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	C	-6.417656	-1.133442	0.420799
	C	-6.480623	-0.587531	-0.927796
	C	-6.363759	0.861096	-0.833091
	C	-6.227760	1.210415	0.574630
110	C	-6.259631	-0.022364	1.349962
	C	-1.314294	-3.441417	1.246395
	C	-0.007611	-2.842211	1.435251
	C	0.677978	-2.820636	0.156131
	C	1.482764	-1.733197	-0.192088
115	C	1.627477	-0.619835	0.733545
	C	1.653170	0.613098	-0.040814
	C	1.513753	0.261282	-1.441638
	C	1.411105	-1.184562	-1.539245
	C	0.973642	-0.646741	1.964220
120	C	1.043561	1.766912	0.452877
	C	0.776539	1.079668	-2.297044
	C	0.553615	-1.753768	-2.483245
	C	-0.285191	-2.879896	-2.112260
	C	-0.224826	-3.399992	-0.822961
125	C	0.137407	-1.777358	2.319049
	C	0.323350	0.548978	2.469319
	C	0.357191	1.729527	1.733127
	C	0.253359	2.599824	-0.432660
	C	0.127284	2.268961	-1.777251
130	C	-0.122596	0.484843	-3.268164
	C	-0.234745	-0.900506	-3.356117
	C	-1.572377	-2.727312	-2.766476
	C	-1.540073	-1.504799	-3.531894
	C	-1.312546	1.310650	-3.354831
135	C	-1.158178	2.411426	-2.433183
	C	-2.279136	2.972562	-1.761625
	C	-2.142624	3.326145	-0.337494
	C	-0.896231	3.088992	0.303287
	C	-0.832130	2.550397	1.639097
140	C	-2.014713	2.233351	2.361972
	C	-1.448600	-3.786430	-0.147297
	C	-1.012138	-1.281893	3.050752
	C	-0.895817	0.153061	3.145082
	C	-2.047992	0.985950	3.147204
145	C	-2.592258	0.746990	-3.615347

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150	C	0.170165	-0.000984	-0.213310
	C	0.056238	0.160910	1.179161
	C	1.186992	0.159109	1.976632
	N	2.426457	-0.009181	1.430285
	C	2.565799	-0.173248	0.085701
155	C	1.458191	-0.167134	-0.747673
	H	-0.911575	0.322425	1.655577
	H	1.149644	0.292472	3.057854
	C	3.623618	-0.009695	2.322648
	H	3.580812	-0.310104	-0.285308
160	H	1.615356	-0.326167	-1.815216
	C	-1.022468	0.003430	-1.081931
	C	-2.236917	-0.561194	-0.652299
	C	-3.343196	-0.552170	-1.483358
	N	-3.279151	0.011104	-2.724994
165	C	-2.117673	0.569599	-3.164700
	C	-0.984984	0.571296	-2.365745
	H	-2.326722	-1.043177	0.322038
	H	-4.301327	-0.987359	-1.199068
	C	-4.494375	0.005863	-3.592586
170	H	-2.135552	1.008643	-4.161467
	H	-0.083949	1.051220	-2.749756
	H	-4.257460	0.500657	-4.541427
	H	-4.793399	-1.035910	-3.778038
	H	-5.300744	0.548331	-3.078339
175	H	4.522452	-0.159708	1.713671
	H	3.680001	0.958292	2.841215
	H	3.523843	-0.827321	3.050991

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180	C	0.133500	-0.029984	-0.238872
	C	0.082099	-0.274988	1.194382
	C	1.194986	-0.350282	1.964302
185	N	2.487052	-0.247591	1.429007
	C	2.578907	0.070724	0.066405
	C	1.488978	0.153012	-0.735003
	H	-0.881193	-0.408935	1.686878
	H	1.160565	-0.532876	3.039171
190	C	3.604059	0.062356	2.312266
	H	3.596544	0.208200	-0.301553
	H	1.655367	0.362739	-1.791763
	C	-0.992888	0.030905	-1.046709
	C	-2.348339	-0.152080	-0.550556
195	C	-3.438271	-0.070522	-1.352022
	N	-3.346427	0.247117	-2.714827
	C	-2.054402	0.350569	-3.249959
	C	-0.941507	0.275970	-2.479970
	H	-2.514739	-0.361093	0.506353
200	H	-4.455915	-0.207938	-0.984072
	C	-4.463103	-0.063845	-3.598120
	H	-2.019951	0.533234	-4.324823
	H	0.021730	0.410650	-2.972369
	H	-4.367649	0.531136	-4.520220
205	H	-4.508969	-1.137291	-3.870999
	H	-5.404332	0.213845	-3.097796
	H	4.544974	-0.216897	1.812211
	H	3.651362	1.135886	2.584580
	H	3.507636	-0.532020	3.234635

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	C	-9.384557	-1.007682	-0.407682
215	C	-8.542924	0.061781	-0.051434
	C	-9.131955	1.174834	0.570246
	C	-10.496598	1.198136	0.818050
	N	-11.288172	0.150790	0.456609
	C	-10.743967	-0.942568	-0.151936

	C	-7.093731	0.015699	-0.333824
	C	-6.379510	1.176175	-0.681063
	C	-5.030175	1.103120	-0.989465
	N	-4.366016	-0.087436	-0.955256
5	C	-5.027715	-1.224752	-0.592927
	C	-6.378094	-1.194869	-0.285271
	C	-2.908356	-0.152703	-1.336446
	C	-1.967153	-0.143565	-0.115103
	C	-0.491530	-0.165870	-0.588273
10	C	0.493433	-0.193696	0.601504
	C	1.968551	-0.161551	0.127553
	C	2.912912	-0.233758	1.344428
	N	4.369260	-0.150929	0.962086
	C	5.026837	1.042024	1.028046
15	C	6.374342	1.131241	0.717335
	C	7.094161	-0.014336	0.333205
	C	6.385080	-1.227010	0.252626
	C	5.036110	-1.273558	0.565202
	C	8.541570	0.051179	0.046038
20	C	9.390817	-1.029750	0.342136
	C	10.749270	-0.943781	0.083337
	N	11.284466	0.182022	-0.469226
	C	10.484514	1.242454	-0.773375
	C	9.122078	1.198134	-0.521638
25	C	12.758444	0.263161	-0.704458
	C	-12.761997	0.194845	0.703123
	H	8.521048	2.062011	-0.805002
	H	10.974061	2.107385	-1.221775
	H	11.446277	-1.752018	0.307933
30	H	9.016142	-1.941152	0.809036
	H	6.863402	2.099972	0.824128
	H	4.444475	1.901363	1.360281
	H	4.454888	-2.194934	0.525770
	H	6.871140	-2.148534	-0.070469
35	H	13.125510	-0.720690	-1.024652
	H	12.956212	1.008491	-1.484036
	H	13.247392	0.562136	0.235841
	H	2.789850	-1.178111	1.895798
	H	2.731100	0.596362	2.042461
40	H	2.160126	0.765903	-0.438911
	H	2.164613	-1.010664	-0.549814
	H	0.316414	-1.103106	1.202647
	H	0.301047	0.672747	1.258702
	H	-0.292697	0.725320	-1.209361
45	H	-0.320350	-1.051189	-1.226040
	H	-2.170693	-1.021230	0.522272
	H	-2.153036	0.758572	0.492431
	H	-2.723422	0.711634	-1.990456
	H	-2.784838	-1.067813	-1.935131
50	H	-4.451705	1.974668	-1.294801
	H	-6.874235	2.144912	-0.761091
	H	-6.860822	-2.127743	0.009141
	H	-4.441211	-2.143297	-0.577609
	H	-9.001486	-1.890150	-0.921548
55	H	-11.436931	-1.740753	-0.422138
	H	-10.992248	2.035962	1.307548
	H	-8.537075	2.027509	0.898408
	H	-12.994768	1.069156	1.321576
	H	-13.279626	0.270344	-0.265008
60	H	-13.064466	-0.724191	1.224765

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	C	7.853548	0.263311	-0.000112
65	C	8.587593	-0.062675	-1.212773
	C	9.828457	-0.607482	-1.193246
	N	10.522025	-0.852133	0.000247
	C	9.828711	-0.606081	1.193601
	C	8.587844	-0.061258	1.212770
70	H	8.140824	0.135898	-2.186827
	H	10.382140	-0.853629	-2.100530
	C	11.642082	-1.784452	0.000676
	H	10.382584	-0.851183	2.101055
	H	8.141278	0.138454	2.186695
75	C	6.582445	0.820280	-0.000327
	C	5.845519	1.138347	-1.213188
	C	4.603490	1.679429	-1.193532
	N	3.948243	2.031342	-0.000805
	C	4.603677	1.680793	1.192233
80	C	5.845713	1.139735	1.212294
	H	6.298253	0.951605	-2.187005
	H	4.049546	1.923393	-2.102053
	C	2.481914	2.063639	-0.000757
	H	4.049868	1.925785	2.100554
85	H	6.298607	0.954102	2.186240
	H	12.258973	-1.603685	0.894912
	H	11.318320	-2.844030	0.001059
	H	12.259123	-1.604368	-0.893612
	H	2.159215	2.630234	0.889469
90	H	2.159179	2.629025	-0.891756
	C	1.849484	0.657358	0.000148
	C	0.313654	0.702554	-0.000450
	H	2.214765	0.107057	-0.885305
	H	2.214126	0.108404	0.886695
95	C	-0.313590	-0.702402	0.000416
	H	-0.043079	1.260064	0.885526
	H	-0.042406	1.258676	-0.887571
	C	-1.849420	-0.657204	-0.000097
	H	0.043101	-1.259883	-0.885595
100	H	0.042507	-1.258552	0.887502
	C	-2.481852	-2.063489	0.000722
	H	-2.214643	-0.106980	0.885423
	H	-2.214121	-0.108176	-0.886573
	N	-3.948169	-2.031178	0.000804
105	H	-2.159174	-2.629980	-0.889579
	H	-2.159075	-2.628967	0.891646
	C	-4.603675	-1.680767	-1.192222
	C	-5.845758	-1.139820	-1.212273
	C	-6.582459	-0.820306	0.000356
110	C	-5.845440	-1.138206	1.213210
	C	-4.603376	-1.679208	1.193541
	H	-4.049881	-1.925751	-2.100551
	H	-6.298704	-0.954309	-2.186213
	C	-7.853586	-0.263387	0.000139
115	H	-6.298121	-0.951388	2.187037
	H	-4.049352	-1.923013	2.102060
	C	-8.587576	0.062767	1.212789
	C	-9.828476	0.607481	1.193242
	N	-10.522171	0.851832	-0.000248
120	C	-9.828842	0.605758	-1.193597
	C	-8.587943	0.061025	-1.212751
	H	-8.140713	-0.135531	2.186850
	H	-10.382086	0.853789	2.100522
	C	-11.642131	1.784282	-0.000754
125	H	-10.382731	0.850774	-2.101065
	H	-8.141377	-0.138679	-2.186676
	H	-12.259116	1.603405	-0.894908
	H	-12.259107	1.604436	0.893620
	H	-11.318254	2.843825	-0.001375
130				

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	C	9.525037	1.485208	-0.838897
	C	9.042298	0.543785	0.084319
135	C	9.921854	0.110360	1.093550
	C	11.214825	0.601604	1.153404
	N	11.655945	1.518086	0.243717
	C	10.824808	1.960080	-0.740363
	C	7.668780	0.007863	-0.001422
140	C	7.040791	-0.205826	-1.241460
	C	5.778949	-0.776377	-1.298310
	N	5.118127	-1.131222	-0.159646
	C	5.686053	-0.895343	1.057775
	C	6.949266	-0.335496	1.157361
145	C	3.774799	-1.811160	-0.242327
	C	2.582948	-0.833384	-0.196798
	C	1.266943	-1.647325	-0.244586
	C	-0.001194	-0.765087	-0.214388
	C	-1.268229	-1.648776	-0.249370
150	C	-2.585230	-0.836494	-0.201598
	C	-3.776104	-1.814962	-0.257760
	N	-5.119947	-1.136551	-0.171224
	C	-5.782462	-0.777789	-1.307635
	C	-7.044116	-0.207073	-1.246924
155	C	-7.670089	0.002733	-0.005222
	C	-6.949080	-0.345296	1.151265
	C	-5.686201	-0.905156	1.047843
	C	-9.042628	0.540458	0.084766
	C	-9.920341	0.106989	1.094215
160	C	-11.211595	0.604694	1.161171
	N	-11.650930	1.526881	0.258352
	C	-10.821168	1.967552	-0.729414
	C	-9.525089	1.486993	-0.834773
	C	-13.058370	2.024839	0.330344
165	C	13.061211	2.019406	0.331887
	H	3.739248	-2.520252	0.598144
	H	3.780088	-2.390031	-1.177469
	H	2.622659	-0.231414	0.727076
	H	2.632546	-0.137560	-1.051665
170	H	1.252546	-2.264987	-1.160052
	H	1.239853	-2.343895	0.612540
	H	-0.003188	-0.143850	0.697986
	H	-0.000059	-0.077839	-1.078308
	H	-1.251226	-2.263801	-1.166597
175	H	-1.242059	-2.347786	0.605807
	H	-2.628819	-0.240358	0.725947
	H	-2.632474	-0.135318	-1.052220
	H	-3.779372	-2.385426	-1.198131
	H	-3.741426	-2.531492	0.576456
180	H	-5.279720	-0.991296	-2.251378
	H	-7.551468	0.023873	-2.184476
	H	-7.357916	-0.174087	2.147564
	H	-5.101650	-1.201907	1.918370
	H	-9.624198	-0.648630	1.822893
185	H	-11.928578	0.287586	1.919392
	H	-11.232827	2.708072	-1.414911
	H	-8.891965	1.888417	-1.626875
	H	5.274723	-0.993180	-2.240517
	H	7.546964	0.021531	-2.180531
190	H	7.359632	-0.161020	2.152486
	H	5.102677	-1.188885	1.930153
	H	9.624892	-0.642147	1.825130
	H	11.935092	0.284413	1.908872
	H	11.235995	2.695645	-1.430920
195	H	8.891418	1.886216	-1.630785
	H	13.215217	2.786526	-0.434988
	H	13.224150	2.449045	1.330284
	H	13.748430	1.177059	0.163330
	H	-13.105162	3.030530	-0.105735
200	H	-13.704321	1.336494	-0.236363
	H	-13.372062	2.057269	1.381171

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205	C	-3.827133	-3.001410	0.102276
	N	-5.071567	-2.233300	0.106232
	H	-3.861848	-3.687939	-0.761031
	C	-2.560782	-2.122622	0.033416
	H	-3.808860	-3.618829	1.017048
210	C	-1.277033	-2.967375	0.026332
	H	-2.611692	-1.495283	-0.873724
	H	-2.560236	-1.434239	0.897011
	C	-0.000004	-2.110414	-0.000030
	H	-1.258153	-3.617841	0.920648
215	H	-1.282617	-3.639309	-0.852155
	C	1.277026	-2.967374	-0.026358
	H	-0.017618	-1.450198	-0.885848
	H	0.017608	-1.450164	0.885761
	C	2.560774	-2.122619	-0.033441

	H	1.282599	-3.639286	0.852146
	H	1.258159	-3.617862	-0.920658
	C	3.827129	-3.001408	-0.102227
	H	2.560249	-1.434270	-0.897063
5	H	2.611660	-1.495244	0.873677
	N	5.071561	-2.233295	-0.106176
	H	3.861817	-3.687901	0.761109
	H	3.808885	-3.618865	-1.016974
	C	5.572149	-1.731529	1.104451
10	C	6.477083	-0.723754	1.154681
	C	6.958376	-0.040253	-0.036479
	C	6.343738	-0.531764	-1.260205
	C	5.444113	-1.545437	-1.271011
	H	5.210531	-2.248552	1.995532
15	H	6.849451	-0.429645	2.135808
	C	7.901756	0.976923	-0.007680
	H	6.612251	-0.086458	-2.218288
	H	4.987942	-1.922353	-2.188462
	C	8.373614	1.669435	-1.197104
20	C	9.289595	2.667146	-1.148843
	N	9.819009	3.142861	0.059459
	C	9.445611	2.455434	1.223000
	C	8.530132	1.456159	1.213893
	H	7.981170	1.394342	-2.176051
25	H	9.643164	3.190444	-2.039028
	C	11.058215	3.909027	0.045160
	H	9.920620	2.814361	2.137687
	H	8.266811	1.006941	2.171514
	C	-5.444076	-1.545383	1.271047
30	C	-6.343696	-0.531706	1.260222
	C	-6.958377	-0.040253	0.036495
	C	-6.477127	-0.723812	-1.154649
	C	-5.572194	-1.731587	-1.104403
	H	-4.987876	-1.922258	2.188500
35	H	-6.612174	-0.086353	2.218293
	C	-7.901755	0.976923	0.007679
	H	-6.849525	-0.429746	-2.135778
	H	-5.210606	-2.248654	-1.995471
	C	-8.530181	1.456093	-1.213895
40	C	-9.445656	2.455371	-1.223020
	N	-9.819003	3.142864	-0.059502
	C	-9.289541	2.667215	1.148805
	C	-8.373563	1.669503	1.197084
	H	-8.266903	1.006819	-2.171502
45	H	-9.920704	2.814247	-2.137707
	C	-11.058197	3.909048	-0.045195
	H	-9.643071	3.190566	2.038975
	H	-7.981079	1.394463	2.176031
	H	-11.020383	4.637129	0.780507
50	H	-11.149764	4.459963	-0.994408
	H	-11.955878	3.271791	0.083735
	H	11.149747	4.460001	0.994342
	H	11.955892	3.271749	-0.083688
	H	11.020448	4.637055	-0.780591
55				

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72

	C	4.238444	-1.357589	0.704836
	H	4.122541	-2.341026	0.226711
60	C	3.245623	-0.330563	0.127683
	H	4.100789	-1.482942	1.788713
	N	5.678870	-0.957087	0.507028
	H	3.406786	0.653626	0.599793
	H	3.415109	-0.212282	-0.956475
65	C	1.795959	-0.808368	0.385130
	C	0.745476	0.174628	-0.172899
	H	1.647638	-1.800081	-0.077668
	H	1.637702	-0.931403	1.471441
	C	-0.694203	-0.321328	0.088637
70	H	0.883440	1.166791	0.291790
	H	0.897628	0.301508	-1.259523
	C	-1.752757	0.659648	-0.455904
	H	-0.830362	-1.310639	-0.383237
	H	-0.842669	-0.457001	1.174857
75	C	-3.196776	0.145477	-0.216806
	H	-1.625507	1.642327	0.031101
	H	-1.591645	0.808600	-1.538436
	C	-4.198337	1.162003	-0.772938
	H	-3.304308	-0.830777	-0.718656
80	H	-3.359940	0.001327	0.865406
	N	-5.661316	0.843948	-0.520081
	H	-4.036350	2.152891	-0.323637
	H	-4.103327	1.255302	-1.867134
	C	6.324127	-0.234828	1.466642
85	C	7.656753	0.114615	1.319877
	C	8.372328	-0.277300	0.174373
	C	7.673684	-0.998005	-0.811099
	C	6.339322	-1.321896	-0.628790
	H	5.743068	0.022654	2.351801
90	H	8.140060	0.656218	2.133297
	C	9.807459	0.034475	0.021672
	H	8.156399	-1.303099	-1.740425
	H	5.765684	-1.888428	-1.363115
	C	10.673908	-0.853113	-0.642668
95	C	12.021140	-0.558068	-0.762065
	N	12.530793	0.598312	-0.247080
	C	11.714708	1.479335	0.395060
	C	10.360936	1.215683	0.541916
	H	10.319408	-1.802127	-1.045198
100	H	12.731301	-1.222140	-1.256696
	C	13.991403	0.881239	-0.387359
	H	12.182212	2.387433	0.775973
	H	9.745035	1.963062	1.043131
	C	-6.572173	1.853606	-0.644266
105	C	-7.925172	1.621887	-0.469903
	C	-8.391117	0.328733	-0.169830
	C	-7.432801	-0.690670	-0.046529
	C	-6.083827	-0.414143	-0.219690
	H	-6.172625	2.837852	-0.892131
110	H	-8.613629	2.457089	-0.604067
	C	-9.832384	0.058713	0.004254
	H	-7.719282	-1.709971	0.214055
	H	-5.314909	-1.177678	-0.121977
	C	-10.400624	-1.158944	-0.411546
115	C	-11.756775	-1.387608	-0.251880
	N	-12.561829	-0.444108	0.318161
	C	-12.037870	0.741222	0.735337
	C	-10.686048	1.011751	0.583639
	H	-9.802044	-1.931373	-0.895659
120	H	-12.244204	-2.309985	-0.570849
	C	-14.019675	-0.728824	0.481442
	H	-12.732348	1.448258	1.188346
	H	-10.308993	1.965164	0.953834
	H	-14.507877	0.147588	0.923449
125	H	-14.453254	-0.940546	-0.506487
	H	-14.139148	-1.598572	1.143920
	H	14.204623	1.871297	0.031951
	H	14.555660	0.112828	0.161179
	H	14.257318	0.860179	-1.453524
130				

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72

	C	3.903249	-2.227299	0.141380
	H	3.663980	-2.894458	-0.704340
135	C	3.091722	-0.919433	0.038613
	H	3.643220	-2.762584	1.071605
	N	5.351445	-2.013631	0.141513
	H	3.380159	-0.259210	0.875845
	H	3.376643	-0.396455	-0.891750
140	C	1.576380	-1.173381	0.062691
	C	0.758167	0.126900	-0.012401
	H	1.296984	-1.829397	-0.782778
	H	1.307883	-1.718439	0.987296
	C	-0.758403	-0.126268	0.011725
145	H	1.034973	0.782034	0.833941
	H	1.024762	0.674033	-0.935532
	C	-1.576624	1.173999	-0.063501
	H	-1.035221	-0.781507	-0.834539
	H	-1.024980	-0.673291	0.934924
150	C	-3.091964	0.920043	-0.039171
	H	-1.297144	1.830186	0.781809
	H	-1.308229	1.718877	-0.988250
	C	-3.903532	2.227852	-0.142367
	H	-3.380494	0.259480	-0.876113
155	H	-3.376767	0.397428	0.891438
	N	-5.351723	2.014104	-0.142350
	H	-3.664279	2.895347	0.703098
	H	-3.643545	2.762792	-1.072811
	C	5.954094	-1.490858	1.296501
160	C	7.166048	-0.884965	1.275343
	C	7.918195	-0.678347	0.047095
	C	7.215999	-1.152418	-1.135323
	C	6.001920	-1.751547	-1.074616
	H	5.388556	-1.652719	2.216441
165	H	7.580660	-0.553221	2.227211
	C	9.171291	-0.083670	0.006886
	H	7.669811	-1.032532	-2.118753
	H	5.471738	-2.108683	-1.959817
	C	9.929109	0.113141	-1.219579
170	C	11.144905	0.711516	-1.239909
	N	11.744817	1.234319	-0.085310
	C	11.085062	0.994268	1.129126
	C	9.869153	0.398830	1.188266
	H	9.519415	-0.226734	-2.170575
175	H	11.718037	0.857039	-2.157338
	C	13.177052	1.501394	-0.080504
	H	11.611746	1.356321	2.013854
	H	9.410104	0.290264	2.170524
	C	-6.002113	1.752541	1.073944
180	C	-7.216057	1.153184	1.135017
	C	-7.918212	0.678346	-0.047121
	C	-7.166152	0.884465	-1.275505
	C	-5.954314	1.490575	-1.297025
	H	-5.471987	2.110299	1.958945
185	H	-7.669832	1.033771	2.118510
	C	-9.171184	0.083433	-0.006552
	H	-7.580700	0.552075	-2.227178
	H	-5.388811	1.651974	-2.217070
	C	-9.869103	-0.399584	-1.187685
190	C	-11.084863	-0.995286	-1.128186
	N	-11.744399	-1.235129	0.086410
	C	-11.144482	-0.711748	1.240753
	C	-9.928819	-0.113112	1.220071
	H	-9.410246	-0.291136	-2.170039
195	H	-11.611617	-1.357668	-2.012756
	C	-13.176625	-1.502341	0.081852
	H	-11.717464	-0.857095	2.158312
	H	-9.519077	0.227166	2.170903
	H	-13.456889	-1.969293	1.039322
200	H	-13.784797	-0.586202	-0.057588
	H	-13.407655	-2.206819	-0.732730
	H	13.408064	2.205809	0.734114
	H	13.785120	0.585186	0.059016
	H	13.457509	1.968347	-1.037901
205				

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75

	C	-10.491933	1.598025	-1.042040
	C	-10.161168	0.714999	-0.000565
210	C	-11.123619	0.502340	1.002549
	C	-12.348133	1.146474	0.944162
	N	-12.639580	2.002513	-0.078207
	C	-11.725315	2.230120	-1.061317
	C	-8.851392	0.034962	0.031519
215	C	-8.206523	-0.261716	1.245195
	C	-6.983613	-0.913570	1.246610
	N	-6.388104	-1.287950	0.078869
	C	-6.984425	-1.000252	-1.112782
	C	-8.203330	-0.344073	-1.157607

	C	-5.063080	-2.006999	0.101281
	C	-3.861904	-1.042187	0.058334
	C	-2.546995	-1.856517	0.051678
	C	-1.290845	-0.959871	0.022053
5	C	-0.001990	-1.808708	0.001120
	C	1.284445	-0.956183	-0.020536
	C	2.542980	-1.849471	-0.049367
	C	3.855983	-1.032068	-0.057455
	C	5.058817	-1.994735	-0.099247
10	N	6.383193	-1.274382	-0.078546
	C	6.981701	-0.987515	1.112115
	C	8.201712	-0.333186	1.155080
	C	8.848821	0.044380	-0.035003
	C	8.200655	-0.249572	-1.247649
15	C	6.976803	-0.899542	-1.247197
	C	10.162256	0.717381	-0.004951
	C	11.120497	0.500407	-1.008320
	C	12.353548	1.132776	-0.948127
	N	12.653964	1.978844	0.075847
20	C	11.739667	2.214204	1.061283
	C	10.501833	1.595905	1.040413
	C	13.983518	2.658090	0.132041
	C	-13.977027	2.667406	-0.118892
	H	1.276883	-0.296049	-0.905779
25	H	1.311204	-0.304036	0.870285
	H	0.013928	-2.467285	0.887922
	H	-0.015996	-2.468057	-0.885133
	H	-1.285126	-0.298911	0.906696
	H	-1.319409	-0.308570	-0.869349
30	H	-2.534081	-2.525299	-0.827214
	H	-2.508362	-2.501648	0.947275
	H	-3.887027	-0.371965	0.934618
	H	2.531979	-2.517185	0.830350
	H	2.505750	-2.495824	-0.944139
35	H	3.879415	-0.363104	-0.934707
	H	3.911482	-0.400505	0.845831
	H	5.060876	-2.669870	0.768879
	H	6.459162	-1.320143	2.009452
	H	8.659938	-0.161943	2.129367
40	H	8.630971	0.041474	-2.206840
	H	6.442177	-1.150300	-2.163601
	H	10.938181	-0.189881	-1.832574
	H	13.128769	0.980972	-1.698368
	H	12.043084	2.909017	1.845537
45	H	9.796023	1.833013	1.836968
	H	13.831729	3.744579	0.054089
	H	14.599698	2.306422	-0.703541
	H	-5.055397	-2.617818	1.015403
	H	-5.063908	-2.683559	-0.765731
50	H	-6.451136	-1.165730	2.163902
	H	-8.638179	0.029216	2.203832
	H	-8.659901	-0.171773	-2.132510
	H	-6.460742	-1.333326	-2.009269
	H	-9.783714	1.832348	-1.837250
55	H	-12.016968	2.930301	-1.844372
	H	-13.127778	1.002878	1.692406
	H	-10.946950	-0.191989	1.824669
	H	-14.181188	3.118840	0.861730
	H	-13.966164	3.443554	-0.893225
60	H	-14.740464	1.911171	-0.355740
	H	14.470068	2.409212	1.086304
	H	-3.918506	-0.412052	-0.845892
	H	5.051711	-2.607167	-1.012292

65 1BP9BP1

75

	C	-9.800023	1.618695	-1.224215
	C	-9.166534	1.133380	-0.007254
	C	-9.637240	1.816107	1.187738
70	C	-10.555436	2.813313	1.149620
	N	-11.089272	3.295583	-0.054432
	C	-10.717623	2.615667	-1.223192
	C	-8.220655	0.117092	0.012772
	C	-7.601498	-0.380616	1.232028
75	C	-6.700853	-1.391536	1.232710
	N	-6.328716	-2.070747	0.062762
	C	-6.833588	-1.563127	-1.143445
	C	-7.741423	-0.556383	-1.183795
	C	-5.084197	-2.840135	0.052334
80	C	-3.818051	-1.961682	-0.011171
	C	-2.534690	-2.805476	-0.010499
	C	-1.257175	-1.947525	-0.031945
	C	0.021181	-2.802477	-0.025939
	C	1.305794	-1.956978	-0.030551
85	C	2.576997	-2.824292	-0.006996
	C	3.866463	-1.989854	-0.006076
	C	5.127935	-2.877316	0.057192
	N	6.376429	-2.117856	0.068592
	C	6.753539	-1.443505	1.240736
90	C	7.648558	-0.426042	1.238127
	C	8.255276	0.083486	0.018398
	C	7.780677	-0.593300	-1.178884
	C	6.879095	-1.605661	-1.136651
	C	9.188984	1.110903	-0.001083
95	C	9.804940	1.613307	-1.219275
	C	10.729169	2.605657	-1.216747
	N	11.199659	3.191912	-0.032815
	C	10.578854	2.787198	1.158280
	C	9.653144	1.796840	1.194650
100	C	11.845436	4.498275	-0.090515
	C	-12.329286	4.059644	-0.031907
	H	1.319438	-1.308720	-0.925427
	H	1.306350	-1.284428	0.846614
	H	0.018274	-3.456599	0.865528
105	H	0.019184	-3.470392	-0.907084
	H	-1.253442	-1.274597	0.844927
	H	-1.263741	-1.299598	-0.927101
	H	-2.534064	-3.480047	-0.886937
	H	-2.518975	-3.453388	0.885770
110	H	-3.822767	-1.271499	0.852334
	H	2.555811	-3.472707	0.888820
	H	2.573740	-3.498217	-0.883924
	H	3.918243	-1.361270	-0.912450
	H	3.876249	-1.302829	0.858641
115	H	5.105154	-3.501844	0.967004
	H	6.302676	-1.834225	2.155216
	H	7.922141	0.006282	2.201220
	H	8.156397	-0.293405	-2.156620
	H	6.524290	-2.117701	-2.032461
120	H	9.534189	1.181258	-2.182783
	H	11.195235	2.982455	-2.129053
	H	10.928147	3.304005	2.053669
	H	9.257115	1.515342	2.170106
	H	11.120652	5.332019	-0.171786
125	H	12.517293	4.526155	-0.962911
	H	-5.066663	-3.463455	0.963080
	H	-5.121114	-3.520989	-0.815258
	H	-6.240387	-1.773810	2.146713
	H	-7.868656	0.058894	2.193599
130	H	-8.116409	-0.256360	-2.162227
	H	-6.472631	-2.072981	-2.038626
	H	-9.540718	1.174492	-2.185271
	H	-11.197428	2.979743	-2.134352
	H	-10.907468	3.329907	2.044028
135	H	-9.241958	1.536518	2.163985
	H	-12.292234	4.781315	0.799302
	H	-12.425388	4.616460	-0.976615
	H	-13.225850	3.419239	0.094000
	H	12.448248	4.640044	0.820954
140	H	-3.865351	-1.334328	-0.918575
	H	5.158353	-3.558417	-0.811648

145

C60@1BP1BP14+

150 88

	C	4.834902	-0.514963	0.361670
	C	4.444860	-0.164713	1.719269
	C	3.738835	-1.302763	2.292648
	C	3.693344	-2.358014	1.288096
155	C	4.371116	-1.869449	0.094294
	C	4.031454	1.134386	2.013187
	C	2.889014	1.352617	2.889423
	C	2.212931	0.263627	3.439400
	C	2.648156	-1.093018	3.135658
160	C	2.140599	2.494493	2.379542
	C	0.748181	2.504126	2.445978
	C	0.040171	1.364978	3.017454
	C	0.758016	0.268117	3.500501
	C	1.461345	-1.927503	3.007189
165	C	0.292601	-1.086609	3.234474
	C	-0.874509	-1.296094	2.499024
	C	-1.616284	-0.151432	1.985136
	C	-1.170034	1.149433	2.238693
	C	-1.209518	2.158837	1.181852
170	C	-0.025475	2.994788	1.311824
	C	2.821372	2.980048	1.184795
	C	2.080596	3.453380	0.100921
	C	0.626421	3.455419	0.163849
	C	0.118529	3.109746	-1.158883
175	C	-1.026619	2.319380	-1.287332
	C	-1.693182	1.824480	-0.088265
	C	-2.106454	-0.499279	0.659474
	C	-2.136662	0.464919	-0.352765
	C	-1.072086	1.261688	-2.293285
180	C	-1.768516	0.119074	-1.715651
	C	-1.354920	-1.185599	-2.007962
	C	-1.314956	-2.196002	-0.951170
	C	-1.690204	-1.860306	0.357041
	C	-0.919923	-2.352047	1.493108
185	C	0.204435	-3.148355	1.267984
	C	1.417685	-2.937300	2.045958
	C	2.558571	-3.159321	1.167813
	C	4.796192	0.448933	-0.647936
	C	4.363988	1.805033	-0.342736
190	C	3.988647	2.140604	0.958957
	C	0.596401	-3.498373	-0.092457
	C	-0.149281	-3.037440	-1.180834
	C	0.530234	-2.550710	-2.376408
	C	-0.216138	-1.406917	-2.886275
195	C	2.050458	-3.505523	-0.153451
	C	3.887222	-2.204398	-1.170373
	C	2.699685	-3.036218	-1.296532
	C	1.923301	-2.546004	-2.428430
	C	2.632076	-1.408135	-3.000053
200	C	3.845263	-1.196907	-2.223651
	C	4.289561	0.099839	-1.967602
	C	1.917230	-0.315586	-3.492819
	C	0.462867	-0.312695	-3.427875
	C	0.028274	1.045118	-3.124778
205	C	1.215986	1.879902	-2.998444
	C	2.383211	1.038539	-3.227412
	C	3.541986	1.241204	-2.479377
	C	3.587949	2.295347	-1.474343
	C	1.260795	2.890119	-2.037009
210	C	2.472888	3.104017	-1.258347
	C	-4.992525	0.834720	-0.029361
	C	-4.994893	1.593689	-1.216253
	C	-4.763520	2.953645	-1.179069
	N	-4.554281	3.595962	0.007591
215	C	-4.595918	2.895921	1.178018
	C	-4.826688	1.534178	1.180905
	C	-4.156566	5.027442	0.016979
	C	-5.066644	-0.633631	-0.050059
	C	-5.424049	-1.373242	1.094305

C	-5.354259	-2.752259	1.088903
N	-4.946689	-3.427210	-0.025434
C	-4.633230	-2.739824	-1.162827
C	-4.706413	-1.361338	-1.199913
C	-4.749864	-4.899933	0.017285
H	-4.514407	5.496079	0.942366
H	-4.600459	5.532118	-0.850292
H	-3.057085	5.080524	-0.034785
H	-4.419315	3.467395	2.089024
H	-4.799005	1.016975	2.139486
H	-4.731274	3.572434	-2.074704
H	-5.166342	1.131483	-2.187276
H	-5.764974	-0.882915	2.005536
H	-5.609313	-3.359912	1.955794
H	-4.406088	-0.860883	-2.119317
H	-4.315274	-3.337033	-2.016762
H	-3.674601	-5.101779	0.143954
H	-5.312650	-5.313865	0.862790
H	-5.110529	-5.341216	-0.920941

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C	3.818300	4.934295	0.031872
H	4.060561	5.497095	-0.880900
H	4.168706	5.499054	0.907800
H	2.722732	4.794650	0.095724
N	4.497142	3.636657	-0.008578
C	4.651993	2.916812	1.165676
C	4.914896	1.579105	1.166563
C	4.957734	0.813677	-0.047051
C	4.810681	1.596161	-1.246752
C	4.549857	2.931698	-1.205529
H	4.381929	3.528148	-2.102679
H	4.857699	1.120548	-2.225495
H	4.552082	3.496967	2.083404
H	5.011374	1.089039	2.134265
C	5.020793	-0.600023	-0.049535
H	4.756270	-0.904059	-2.212215
C	4.855470	-1.385519	-1.240875
C	4.739839	-2.744291	-1.195772
H	4.553524	-3.350062	-2.082538
N	4.847329	-3.447291	-0.007566
C	5.070007	-2.730642	1.159428
C	5.178271	-1.373956	1.155920
H	5.364899	-0.880563	2.108231
H	5.154072	-3.330119	2.065751
C	4.438018	-4.852271	0.052725
H	3.341064	-4.932988	0.143105
H	4.768449	-5.366524	-0.861686
H	4.912318	-5.327181	0.923379
C	-1.513207	-1.489399	-3.231474
C	-0.114035	-1.095422	-3.177899
C	0.228971	0.265173	-3.198087
C	-0.813444	1.276492	-3.267127
C	-0.407558	2.406779	-2.433035
C	0.882073	2.094425	-1.848514
C	1.170605	2.480808	-0.529795
C	1.860548	1.574376	0.369442
C	2.231606	0.293086	-0.079189
C	1.928282	-0.112584	-1.443184
C	1.271099	0.763126	-2.309062
C	1.579722	-1.529375	-1.432640
C	0.575237	-2.008294	-2.282703
C	-0.398239	-2.970467	-1.776818
C	-1.690762	-2.651149	-2.368130
C	-2.857078	-2.789466	-1.613927
C	-3.899670	-1.773196	-1.689245
C	-3.729243	-0.662272	-2.517091
C	-2.513220	-0.516796	-3.302785
C	-2.157538	0.898179	-3.320552
C	-4.265264	1.941807	0.061164
C	1.653640	-1.993064	-0.053636
C	2.044782	-0.859363	0.777411
C	1.515065	-0.713596	2.061951
C	0.724947	-2.921864	0.429948
C	-0.325662	-3.419672	-0.457558
C	-1.239885	-3.152240	1.699406
C	-1.541425	-3.561526	0.330360
C	-2.780556	-3.252969	-0.234874
C	-3.489774	-2.137674	1.852227
C	-2.199117	-2.455338	2.441533
C	-1.793789	-1.325565	3.273261
C	-0.450531	-0.946440	3.328613
C	-0.094760	0.470146	3.312752
C	-1.099351	1.443489	3.244140
C	-2.495234	1.044422	3.185676
C	-2.837865	-0.313776	3.203611
C	-3.880324	-0.810856	2.316020
C	-4.544585	0.063130	1.454613
C	-4.190468	1.477765	1.438962
C	-3.187850	1.956154	2.286384
C	-2.216541	2.919861	1.785515
C	-1.071532	3.510161	-0.323611
C	-1.370469	3.106184	-1.693263
C	-3.334914	2.865933	-0.419023
C	-4.671457	0.814817	-0.772564
C	-4.846790	-0.343757	0.089488
C	1.284238	1.725692	1.695918
C	1.118965	0.617315	2.531213
C	0.550165	-1.675741	2.561571
C	0.242247	2.743437	1.624025
C	0.167103	3.208188	0.244968
C	-2.288610	3.364857	0.464845
C	-4.123427	0.663243	-2.049593
C	-0.924344	2.602550	2.379591
C	-2.765965	2.708775	-1.751041
C	-3.157016	1.626162	-2.552216
C	0.159186	-2.762934	1.759662
C	-3.777615	-2.527261	0.539214
C	-4.471386	-1.616118	-0.358706

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C	-0.303738	-1.118433	-3.059841
C	-1.160370	-0.086056	-2.494450
C	-0.305152	0.991125	-2.015270
C	1.079143	0.627328	-2.287502
C	1.079370	-0.679128	-2.929832
C	-2.645253	-1.842720	-1.588832
C	-1.816861	-2.831784	-2.121548
C	-0.624228	-2.462473	-2.872425
C	1.171708	-4.708759	1.704039
C	0.421145	-3.429091	-2.560534
C	1.745887	-3.009728	-2.444216
C	2.080167	-1.602816	-2.629464
C	3.126650	-1.258275	-1.673536
C	3.435698	-2.451713	-0.897055
C	2.583663	-3.533567	-1.374579
C	2.056317	-4.452170	-0.465980
C	0.674675	-4.895143	-0.592336
C	0.126944	-5.053175	0.749584
C	-1.508392	-4.024911	-1.346697
C	-2.032270	-4.176777	-0.062972
C	-2.887563	-3.140374	0.500231
C	-3.196398	-2.001033	-0.248474
C	-2.645136	0.275740	-0.551322
C	-2.306427	-0.438019	-1.776527
C	-3.196850	-0.691419	0.395150
C	-1.825829	1.312629	-0.095477
C	-0.630337	1.680513	-0.846238
C	2.084686	0.963422	-1.377059
C	0.669292	1.359089	2.479072
C	2.052838	0.992217	2.210127
C	2.579385	1.148900	0.924169
C	3.136666	0.001999	-1.064586
C	3.725156	-1.033826	1.106449
C	3.437083	0.113877	0.359447
C	3.730724	-2.342689	0.464792
C	3.186706	-3.309811	1.410866
C	0.849066	-4.028034	2.876832
C	1.703753	-2.948812	3.352132
C	2.848159	-2.597785	2.635454
C	3.179955	-1.191882	2.448344
C	2.361662	-0.199741	2.988905
C	1.170943	-0.567156	3.742411
C	0.847037	-1.913004	3.914070
C	-0.535507	-2.353461	3.786246
C	-0.534341	-3.661636	3.146544
C	-1.197209	-4.703242	1.008522
C	-1.535011	-3.991190	2.233232
C	-2.893745	-0.584801	1.758925
C	-2.585547	-1.774900	2.538847
C	-2.580068	-3.025721	1.919856
C	-1.539422	-1.431231	3.494553
C	-2.034432	0.494681	2.233034
C	-1.199440	-0.027786	3.306754
C	-1.515186	1.425189	1.325830
C	-0.131368	1.866959	1.451772
C	0.415103	2.023979	0.109961
C	0.124726	0.394963	3.425875
C	-0.125630	-4.394945	-1.618599
C	2.364293	-4.339166	0.953757
C	1.745553	1.677618	-0.150257
C	-3.171047	4.272564	1.615223
H	-2.834233	3.611350	2.427028
H	-3.675999	5.145512	2.060328
C	-1.982097	4.684720	0.727418
H	-1.690655	3.833474	0.089903
H	-2.253831	5.528092	0.071281
C	-0.784767	5.083882	1.617393
H	-0.588900	4.269761	2.338159
H	-1.029507	5.983947	2.207195
C	0.496974	5.341308	0.796311
H	0.633592	4.521745	0.067398
H	0.391963	6.283105	0.229198
C	1.718670	5.425656	1.732089
H	1.862170	4.463803	2.257995
H	1.528373	6.183792	2.510827
C	3.027583	5.839491	1.034621
H	3.746134	6.255144	1.754354
H	2.854809	6.594305	0.254288
N	3.738326	4.686943	0.372692
C	4.557241	3.896278	1.124139
C	5.309980	2.893481	0.538500
C	5.243867	2.671210	-0.848616
C	4.343423	3.458187	-1.587603
C	3.606203	4.453037	-0.962704
H	4.612303	4.128388	2.188183
H	5.989562	2.323047	1.172169
H	4.206075	3.307685	-2.658864
H	2.926848	5.110593	-1.505540
C	6.137545	1.689810	-1.493049
C	6.558491	0.529594	-0.817230
C	7.461894	-0.335928	-1.407999
N	7.963278	-0.081109	-2.651968
C	7.561261	1.025360	-3.336866
C	6.652237	1.913107	-2.781284
H	6.165468	0.272861	0.166945
H	7.819564	-1.242670	-0.919408
H	8.002838	1.174152	-4.322030
H	6.389242	2.802201	-3.354281
C	8.995045	-0.987240	-3.238672
H	8.789104	-2.018192	-2.923979
H	9.985990	-0.672680	-2.876074
H	8.956063	-0.914681	-4.332342
N	-4.228905	3.491598	0.875544
C	-4.695069	2.326098	1.403396
C	-5.668331	1.587007	0.751001
C	-6.203491	2.038081	-0.466826

C	-5.707173	3.246010	-0.987826
C	-4.723323	3.948183	-0.310707
H	-4.261125	2.013528	2.352531
H	-6.025912	0.673709	1.227372
H	-6.065359	3.643017	-1.938065
H	-4.311427	4.885583	-0.681354
C	-7.254987	1.265308	-1.154798
C	-7.251686	-0.139393	-1.121205
C	-8.264075	-0.855120	-1.741648
N	-9.276108	-0.213429	-2.389016
C	-9.299363	1.150156	-2.445056
C	-8.303239	1.901139	-1.843709
H	-6.446150	-0.692186	-0.635246
H	-8.301397	-1.944342	-1.743158
H	-10.140630	1.598413	-2.975357
H	-8.378356	2.988051	-1.889137
C	-10.380669	-0.991755	-3.027208
H	-10.134106	-2.058963	-2.987986
H	-11.312623	-0.802190	-2.473893
H	-10.487272	-0.669810	-4.072771

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C	-6.697407	-2.739572	-2.601264
H	-6.953937	-2.822677	-3.667775
H	-7.504745	-3.185999	-2.002071
H	-5.756216	-3.284460	-2.407778
N	-6.564796	-1.325776	-2.250092
C	-5.984466	-0.435862	-3.144141
C	-5.566672	0.800498	-2.759365
C	-5.645583	1.243389	-1.387961
C	-6.295185	0.308896	-0.506390
C	-6.694593	-0.923268	-0.927098
H	-5.893169	-0.798867	-4.167969
H	-5.126144	1.442591	-3.520173
H	-6.431658	0.548545	0.546894
H	-7.136330	-1.660050	-0.256614
C	-5.065754	2.449375	-0.939530
C	-4.315776	3.321038	-1.803742
C	-3.573035	4.357840	-1.319777
N	-3.541426	4.677342	0.028372
C	-4.307359	3.896054	0.886999
C	-5.069485	2.860144	0.442011
H	-5.636876	2.299209	1.183181
H	-2.969252	4.992581	-1.966711
H	-4.252626	4.172130	1.939964
C	-2.470633	5.540430	0.571417
H	-2.781721	6.598566	0.511911
H	-2.379015	5.275085	1.636826
C	-1.108632	5.329952	-0.131761
H	-1.031795	5.980120	-1.020456
H	-1.047377	4.285830	-0.478056
C	0.066225	5.606156	0.822562
H	-0.007310	6.630429	1.235160
H	-0.000653	4.904506	1.673681
C	1.436614	5.431488	0.141249
H	1.554967	6.200363	-0.646033
H	1.477106	4.444278	-0.352356
C	2.586637	5.547609	1.156492
H	2.465523	6.475037	1.745278
H	2.538889	4.700713	1.864189
C	3.980768	5.585622	0.502673
H	3.995979	6.311563	-0.327847
H	4.738406	5.901586	1.237503
N	4.418511	4.288375	-0.030927
C	5.089314	3.386977	0.789505
C	5.500501	2.172400	0.336731
C	5.241154	1.731095	-1.011854
C	4.538493	2.693241	-1.824410
C	4.140190	3.901239	-1.333353
H	3.591499	4.630487	-1.930305
H	4.266100	2.450793	-2.850429
H	6.011707	1.518108	1.041666
H	5.260342	3.726771	1.811374
C	5.615816	0.455481	-1.485047
C	6.187792	-0.555315	-0.631456
C	6.373743	-1.835164	-1.057852
N	6.094059	-2.219049	-2.359408
C	5.614745	-1.256238	-3.238423
C	5.400558	0.028679	-2.844054
H	5.028641	0.730909	-3.588203
H	5.425533	-1.605587	-4.253393
H	6.434489	-0.330109	0.404147
H	6.743281	-2.626457	-0.405817
C	6.055289	-3.635815	-2.726291
H	6.308875	-3.739881	-3.792029
H	5.054377	-4.062616	-2.544424
H	6.796767	-4.182507	-2.125606
H	-4.282982	3.142086	-2.877549
C	0.266584	2.152366	-0.470272
C	1.504014	1.607761	-0.825427
C	2.436925	1.203021	0.219099
C	3.119199	0.002923	-0.226124
C	3.450347	-1.001906	0.704379
C	3.229221	-2.397742	0.356849
C	2.726431	-2.748249	-0.903680
C	2.397768	-1.700889	-1.872562
C	2.663526	-2.123022	2.624647
C	2.577527	-0.358109	-1.524989
C	1.596287	0.640582	-1.908283
C	0.435076	0.252448	-2.598684
C	-0.941699	1.747516	-1.187739
C	-0.850669	0.820194	-2.233587
C	-0.077683	2.324503	0.930872
C	-1.495730	2.025377	1.079513
C	-2.025942	1.674906	-0.228864
C	-2.990233	0.656455	-0.343496
C	-2.887241	-0.317778	-1.414434
C	-1.853516	-0.239188	-2.348921
C	-1.182778	-1.452036	-2.792460
C	0.230786	-1.149981	-2.941725
C	1.194360	-2.104589	-2.581350
C	0.776359	-3.398063	-2.055983
C	1.796342	-4.109519	1.430452
C	1.722730	-3.792366	-1.019178
C	1.268270	-4.468713	0.123237
C	0.705904	-4.184585	2.392763
C	-0.584795	-3.688072	-1.911743
C	-0.497964	-4.589427	1.676713
C	-1.057455	-4.389236	-0.723831
C	-0.148000	-4.763630	0.272999
C	-1.586759	-2.700701	-2.288303
C	-2.346264	-3.823397	-0.355873
C	-2.681055	-3.655145	0.989252
C	-2.672902	-2.778901	-1.327120
C	-1.736182	-4.048084	2.028601
C	-1.826960	-3.073061	3.107913
C	-3.319329	-1.611955	-0.899121
C	-3.355210	-2.439969	1.433499
C	-3.666368	-1.438400	0.504546
C	-2.826771	-2.081561	2.739661
C	-3.450721	-0.038267	0.847144
C	-2.953579	0.308495	2.107479
C	-1.948574	1.361287	2.227890
C	0.830981	1.955323	1.934692
C	2.119364	1.385268	1.564545
C	-0.672237	-2.683650	3.793845
C	1.618387	-2.195965	3.548847
C	1.356951	0.262143	3.489862
C	2.446414	0.339563	2.533565
C	0.950512	-0.983580	3.996378
C	-0.464477	-1.281236	4.139184
C	0.358047	1.257374	3.120298
C	-1.007018	0.967354	3.261050
C	-1.426576	-0.328037	3.784662
C	-2.629592	-0.733978	3.074177
C	0.616968	-3.251356	3.428851
C	3.089163	-0.827272	2.100460
C	2.755730	-3.094501	1.545656

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129

C	6.370680	1.617614	-1.821497
C	6.254684	2.380166	-0.645352
C	7.219680	2.177111	0.356633
C	8.236874	1.256015	0.171612
N	8.321129	0.528343	-0.978629
C	7.395609	0.701206	-1.966319
C	5.160550	3.354010	-0.478558
C	4.657302	3.690515	0.788795
C	3.641853	4.628105	0.914637
N	3.124379	5.249225	-0.180157
C	3.576820	4.919900	-1.426760
C	4.581080	3.987398	-1.595101
C	2.094607	6.341862	-0.053886
C	0.697431	5.910515	-0.537773
C	-0.123882	5.157785	0.525410
C	-1.511207	4.758384	-0.019914
C	-2.436570	4.194965	1.078544
C	-3.691072	3.524542	0.473735
C	-4.488592	2.813799	1.581519
N	-5.771444	2.216789	1.064746
C	-5.735738	1.065660	0.332637
C	-6.903389	0.504282	-0.160158
C	-8.148163	1.109366	0.094672
C	-8.150638	2.298185	0.843958
C	-6.961038	2.833212	1.311592
C	-9.410488	0.520217	-0.395579
C	-10.591991	0.608323	0.362448
C	-11.769649	0.051260	-0.108050
N	-11.807788	-0.583824	-1.314740
C	-10.679394	-0.681199	-2.072189
C	-9.478938	-0.145259	-1.630920
C	-13.100559	-1.141978	-1.814813
C	9.459359	-0.416532	-1.173753
C	3.238929	1.031619	-0.839745
C	2.929310	0.405986	-2.119930
C	3.387918	-0.887381	-2.384063
C	4.190044	-1.598416	-1.394009
C	4.502387	-0.990214	-0.173741
C	4.005507	0.348905	0.110349
C	1.568708	0.785925	-2.483707
C	0.729621	-0.146883	-3.094577
C	1.212011	-1.491037	-3.381041
C	2.514525	-1.854770	-3.035436
C	0.113931	-2.422157	-3.158713
C	-1.047291	-1.652479	-2.735223
C	-0.667843	-0.246096	-2.696213
C	0.363761	-3.671263	-2.591153
C	-0.539611	-4.210740	-1.583585
C	-1.655091	-3.475614	-1.181324
C	-1.913642	-2.168662	-1.770074
C	-2.432430	-1.298978	-0.721623
C	-2.077514	0.053471	-0.689780
C	-1.173044	0.591711	-1.699952
C	1.722985	-4.050073	-2.228036
C	2.775074	-3.161827	-2.446463
C	-0.293202	1.554857	-1.050553
C	1.047070	1.655468	-1.435371
C	0.262918	-4.921469	-0.596215
C	1.660288	-4.821834	-0.994285
C	2.653123	-4.671643	-0.025530
C	3.748696	-3.738989	-0.250245
C	3.811404	-3.003456	-1.435261
C	-2.494026	-2.071031	0.514920
C	-2.013326	-3.415862	0.229159
C	-0.081614	-4.862663	0.754368
C	-1.243176	-4.092344	1.175904
C	-2.189766	-1.463346	1.735653

	C	-1.391063	-2.171927	2.726731
	C	-0.925478	-3.456637	2.449343
	C	0.434212	-3.835170	2.812437
	C	0.954424	-4.705417	1.765462
5	C	2.292419	-4.613007	1.384470
	C	-1.807633	-0.057872	1.772874
	C	-1.752505	0.684246	0.586971
	C	-0.647201	1.603862	0.360448
	C	-0.514448	-1.205575	3.375284
10	C	-0.770665	0.101455	2.785496
	C	0.342912	1.758220	1.334033
	C	0.280909	0.993610	2.571052
	C	0.789114	-1.567865	3.718607
	C	1.272206	-2.911195	3.433670
15	C	2.669425	-2.813334	3.035283
	C	3.167265	-3.644458	2.032194
	C	1.887084	-0.636838	3.492026
	C	1.640453	0.620426	2.938719
	C	1.739572	1.862674	0.936235
20	C	2.081929	1.808900	-0.419896
	C	4.067990	-3.104923	1.022352
	C	4.442485	-1.761197	1.062832
	C	2.543618	1.156185	1.928984
	C	3.657191	0.414037	1.523308
25	C	3.921719	-0.893022	2.111098
	C	3.049824	-1.407950	3.072192
	H	2.483543	7.183671	-0.646144
	H	2.083489	6.644916	1.002362
	H	0.787675	5.304822	-1.457772
30	H	0.162754	6.831813	-0.824564
	H	0.409296	4.246850	0.854120
	H	-0.247538	5.806326	1.411667
	H	-1.378351	4.005317	-0.817132
	H	-1.992948	5.637274	-0.484670
35	H	-1.883888	3.459880	1.690014
	H	-2.741143	5.010895	1.757009
	H	-3.384240	2.786074	-0.289473
	H	-4.322190	4.281020	-0.023287
	H	-4.771598	3.508287	2.385456
40	H	-3.908111	1.984702	2.015763
	H	-9.075819	2.836826	1.052478
	H	-6.920997	3.751301	1.897647
	H	-6.832747	-0.432835	-0.713606
	H	-4.750681	0.622617	0.174612
45	H	-10.605637	1.082816	1.344711
	H	-12.704874	0.086634	0.451779
	H	-10.779819	-1.193202	-3.029217
	H	-8.608614	-0.227888	-2.282569
	H	-13.630880	-1.620061	-0.980872
50	H	-13.704468	-0.318069	-2.225358
	H	-12.892475	-1.880854	-2.597861
	H	3.233289	4.925115	1.881061
	H	5.029199	3.209624	1.693688
	H	3.127588	5.460210	-2.260256
55	H	4.937516	3.792752	-2.606779
	H	7.212737	2.754642	1.280811
	H	5.632647	1.692442	-2.620216
	H	7.515733	0.083089	-2.856309
	H	9.013436	1.077918	0.915454
60	H	9.173259	-1.173531	-1.914119
	H	9.694403	-0.898133	-0.215723
	H	10.330843	0.150796	-1.534923

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65 129

	C	2.671413	5.121419	1.369638
	C	1.684943	5.419683	0.228982
	C	0.249823	5.631509	0.745523
	C	-0.745975	5.717846	-0.425901
70	C	-2.209377	5.537368	0.012808
	C	-3.170983	5.730264	-1.171197
	C	-4.651539	5.531746	-0.798409
	H	-5.306265	5.937780	-1.586916
	H	-4.889575	6.058908	0.139948
75	H	-2.907536	5.024406	-1.979834
	H	-3.049990	6.749855	-1.578015
	H	-2.330718	4.523845	0.437096
	H	-2.457366	6.263861	0.810118
	H	-0.504955	4.922791	-1.155402
80	H	-0.627171	6.684891	-0.949096
	H	-0.023255	4.766982	1.376764
	H	0.181595	6.537584	1.374095
	H	1.662478	4.545432	-0.441935
	H	2.013252	6.292698	-0.360779
85	H	2.166690	4.481708	2.116384
	H	2.990809	6.049782	1.876499
	N	3.869324	4.366179	0.926686
	C	4.194422	4.202214	-0.412307
	H	5.232565	3.139411	-1.900750
90	C	5.023596	3.206215	-0.833826
	C	5.553352	2.227086	0.080015
	C	5.354522	2.553965	1.470797
	C	4.523220	3.560389	1.851700
	C	6.148281	1.018571	-0.340461
95	C	6.321265	0.664810	-1.725761
	C	6.718847	-0.579285	-2.108239
	N	7.025086	-1.566450	-1.177000
	C	6.908481	-1.255104	0.165622
	C	6.522414	-0.017248	0.586409
100	C	7.179547	-2.959166	-1.601987
	H	3.752931	4.919103	-1.101061
	H	4.301011	3.779766	2.896223
	H	5.824620	1.959522	2.253298
	H	6.815428	-0.877591	-3.151913
105	H	6.092303	1.385633	-2.509664
	H	6.443429	0.146763	1.659225
	H	7.133144	-2.068339	0.855802
	H	7.672633	-2.982865	-2.585124
	H	7.808175	-3.490429	-0.872334
110	H	6.198717	-3.459462	-1.671902
	N	-5.013281	4.119499	-0.617765
	C	-5.033149	3.516856	0.630242
	C	-5.376573	2.207512	0.790136
	C	-5.707205	1.361409	-0.330833
115	C	-5.627672	2.018345	-1.609939
	C	-5.286662	3.330155	-1.728720
	C	-6.040346	-0.000929	-0.187379
	C	-6.105144	-0.656015	1.098733
	C	-6.215319	-2.007329	1.206760
120	N	-6.359661	-2.822966	0.092607
	C	-6.391767	-2.220066	-1.158181
	C	-6.272231	-0.871812	-1.308304
	H	-4.765227	4.163219	1.466266
	H	-5.354506	1.799736	1.799088
125	H	-5.822313	1.461641	-2.525467
	H	-5.217407	3.840013	-2.690000
	H	-6.021710	-0.078738	2.017269
	H	-6.198710	-2.527661	2.164578
	H	-6.510942	-2.902171	-2.000014
130	H	-6.303866	-0.473011	-2.321415
	C	-6.139169	-4.265473	0.196635
	H	-5.076539	-4.512763	0.013369
	H	-6.416119	-4.596813	1.207662
	H	-6.769631	-4.785491	-0.540794
135	C	1.513296	-2.533641	3.113184
	C	2.667877	-2.246737	2.380071
	C	3.054692	-0.860632	2.133558
	C	2.264736	0.178939	2.640493
	C	1.990067	1.350967	1.809789
140	C	0.626787	1.780783	2.065527
	C	-0.169306	2.262655	1.006798
	C	-1.558876	1.865554	0.897015
	C	-1.875073	1.706945	-0.528110
	C	-2.704872	0.657270	-0.932503
145	C	-2.396087	-0.108466	-2.134572
	C	-2.777318	-1.495299	-1.888607
	C	-1.987495	-2.536675	-2.390485
	C	-1.716925	-3.704650	-1.561307
	C	-0.350471	-4.129847	-1.810699
150	C	0.438539	-4.613203	-0.757644
	C	-0.118645	-4.692983	0.588656
	C	0.935603	-4.351658	1.534467
	C	0.625386	-3.607702	2.680428
	C	0.693357	-1.451054	3.637683
155	C	1.065071	-0.119529	3.398899
	C	0.049220	0.866299	3.038859
	C	-1.289639	0.478086	2.928887
	C	-1.674228	-0.905284	3.174621
	C	-0.699336	-1.849939	3.516128
160	C	-0.740645	-3.185325	2.932674
	C	-1.754767	-3.512802	2.021796
	C	-1.432895	-4.286345	0.826463
	C	-2.256262	-3.789356	-0.269412
	C	-3.070225	-2.698304	0.252380
165	C	-3.315768	-1.573610	-0.541339
	C	-3.284791	-0.242313	0.041384
	C	-2.111868	0.984680	1.836142
	C	-3.006717	-0.082168	1.412263
	C	-2.730474	-1.250230	2.229860
170	C	-2.770222	-2.538784	1.670341
	C	0.230409	-3.216451	-2.786816
	C	1.566923	-2.828180	-2.676554
	C	1.950201	-1.445372	-2.925795
	C	0.972616	-0.501777	-3.275215
175	C	-0.417787	-0.904815	-3.390608
	C	-0.785668	-2.234455	-3.151475
	C	2.136663	-4.048631	0.772085
	C	2.987582	-3.017974	1.186821
	C	3.569470	-2.108024	0.208142
180	C	3.620264	-0.780396	0.796703
	C	3.348492	0.348641	-0.002567
	C	3.030963	0.178526	-1.413961
	C	3.003733	-1.098899	-1.984213
	C	3.281952	-2.273149	-1.157574
185	C	2.390790	-3.336784	-1.583048
	C	1.830895	-4.216364	-0.643578
	C	2.020392	1.158492	-1.776114
	C	1.695544	1.921479	-0.580371
	C	0.382144	2.335235	-0.340488
190	C	1.007871	0.830803	-2.687588
	C	-0.360421	1.257931	-2.440355
	C	-0.673590	2.003627	-1.290914
	C	-1.242864	0.182457	-2.868403
	C	2.509641	1.411199	0.513482

195

C60@1BP8BP14+

132

	N	8.419401	-1.438877	0.911456
	C	8.664715	-0.165519	1.337299
200	C	7.870698	0.887103	0.914809
	C	6.807725	0.658586	0.022790
	C	6.573212	-0.661890	-0.392464
	C	7.381576	-1.690375	0.064657
	C	5.993521	1.777928	-0.486696
205	C	5.648086	2.864459	0.333907
	C	4.966197	3.948900	-0.195297
	N	4.622876	3.981016	-1.513034
	C	4.891779	2.912201	-2.316144
	C	5.571487	1.809806	-1.826902
210	C	3.962729	5.202157	-2.098589
	C	2.430494	5.133869	-2.024233
	C	1.859648	5.288834	-0.603833
	C	0.320172	5.382813	-0.634828
	C	-0.307420	5.296950	0.767366
215	C	-1.842954	5.149618	0.707702
	C	-2.442670	4.971426	2.113432
	C	-3.974928	5.055339	2.161340
	N	-4.651629	3.873410	1.514460
	C	-4.830711	2.728739	2.232247

	C	-5.537326	1.661417	1.703187
	C	-6.077832	1.741167	0.408103
	C	-5.830176	2.911983	-0.329484
	C	-5.121341	3.958878	0.238181
5	C	-6.913932	0.650756	-0.128399
	C	-8.007372	0.922364	-0.967176
	C	-8.814376	-0.108810	-1.422971
	N	-8.554837	-1.400015	-1.077803
	C	-7.491393	-1.694553	-0.272773
10	C	-6.669164	-0.692859	0.211241
	C	-9.449019	-2.500581	-1.546761
	C	9.308979	-2.546307	1.373321
	C	3.356078	-2.574135	0.218840
	C	3.357152	-1.608432	1.228477
15	C	3.270847	-0.195132	0.883549
	C	3.188228	0.192966	-0.457292
	C	3.195078	-0.812620	-1.515393
	C	3.269198	-2.169671	-1.179348
	C	2.443548	0.464480	1.887442
20	C	1.570780	1.486836	1.508402
	C	1.483411	1.888338	0.108594
	C	2.278224	1.260289	-0.855359
	C	0.228226	1.540174	2.074860
	C	-0.685495	1.974171	1.026636
25	C	0.087788	2.184130	-0.187684
	C	1.714984	0.910067	-2.155720
	C	0.376075	1.199374	-2.435428
	C	-0.452462	1.851297	-1.429957
	C	-1.795042	1.292101	-1.514646
30	C	-2.540992	1.090391	-0.349701
	C	-1.974764	1.440262	0.948971
	C	-2.400402	0.432779	1.913612
	C	-1.519539	0.005862	2.910961
	C	-0.179848	0.571662	2.992836
35	C	0.733868	-0.490183	3.394213
	C	2.017650	-0.543792	2.850760
	C	-0.451965	0.229100	-3.137140
	C	-1.792707	0.285445	-2.567913
	C	-2.530455	-0.888141	-2.410428
40	C	-3.305818	-1.103372	-1.195897
	C	-3.315976	-0.134122	-0.187809
	C	-3.229672	-0.540395	1.211939
	C	-3.139673	-1.897150	1.540101
	C	-3.141454	-2.906535	0.486990
45	C	-3.223512	-2.517474	-0.852936
	C	-2.396087	-3.175616	-1.856563
	C	-1.968021	-2.168793	-2.818455
	C	-0.684693	-2.222782	-3.361086
	C	0.089419	-0.998131	-3.519692
50	C	1.482938	-1.305470	-3.224201
	C	2.281053	-0.370537	-2.561830
	C	-2.225525	-2.338345	2.586087
	C	-1.433869	-1.406466	3.257571
	C	-0.041042	-1.713168	3.555431
55	C	-2.228230	-3.970428	0.884793
	C	-1.663012	-3.618824	2.180586
	C	-0.328376	-3.909978	2.461166
	C	0.498616	-2.937104	3.161700
	C	1.838667	-2.993489	2.593238
60	C	2.582631	-1.823138	2.443799
	C	2.582748	-3.799523	0.379213
	C	1.840184	-4.002859	1.541971
	C	0.500309	-4.568132	1.460448
	C	1.568491	-2.718658	-2.879786
65	C	2.443830	-3.144026	-1.879852
	C	2.019419	-4.151001	-0.917111
	C	-0.039503	-4.903642	0.219541
	C	0.735221	-4.689836	-0.995135
	C	-0.178224	-4.246359	-2.040254
70	C	0.229420	-3.284960	-2.963520
	C	-1.518737	-4.189881	-1.472814
	C	-1.433305	-4.595672	-0.075623
	H	-10.040171	-2.864499	-0.692940
	H	0.120725	4.436928	1.315595
75	H	-0.051642	6.200478	1.347894
	H	0.024057	6.330547	-1.117845
	H	-0.079015	4.567890	-1.265132
	H	2.271467	6.197952	-0.128527
	H	2.157014	4.423990	0.019812
80	H	2.074622	4.193773	-2.483989
	H	2.059443	5.955380	-2.661680
	H	4.356684	6.067548	-1.545149
	H	-2.269610	6.052135	0.231779
	H	-2.102475	4.285711	0.064967
85	H	-2.099441	4.022832	2.563658
	H	-2.079993	5.780084	2.771944
	H	-4.344459	5.086032	3.196504
	H	-4.344196	5.949136	1.637576
	H	-4.426057	2.723591	3.244916
90	H	-5.702539	0.787653	2.333927
	H	-6.184277	3.022503	-1.354929
	H	-4.934691	4.896366	-0.286004
	H	-8.272619	1.942956	-1.244167
	H	-9.683479	0.060709	-2.059168
95	H	-7.341466	-2.749377	-0.040704
	H	-5.822092	-0.971893	0.839061
	H	-8.832771	-3.312670	-1.956430
	H	-10.118163	-2.111616	-2.323235
	H	4.314069	5.268939	-3.137819
100	H	4.578292	2.996874	-3.357249
	H	4.712716	4.829764	0.393651
	H	5.904647	2.876949	1.393667
	H	8.120439	1.892679	1.255720
	H	9.515620	-0.034894	2.007505
105	H	5.742799	-0.907302	-1.057375
	H	7.234120	-2.730342	-0.227404
	H	8.956172	-3.490420	0.942983
	H	10.335306	-2.342534	1.034073
	H	9.275919	-2.596899	2.471069
110	H	5.807826	0.997393	-2.515206

C60@1BP8BP1

132

	N	-6.407088	-2.043604	-1.545143
115	C	-6.115218	-0.928547	-2.318143
	C	-5.969812	0.310223	-1.769838
	C	-6.008835	0.511089	-0.346231
	C	-6.419364	-0.647618	0.410228
	C	-6.574374	-1.863244	-0.175840
120	C	-5.621122	1.718721	0.271316
	C	-5.327820	2.921937	-0.459684
	C	-4.895240	4.056296	0.158966
	N	-4.707761	4.108671	1.534508
	C	-4.958694	2.965254	2.273376
125	C	-5.423823	1.823070	1.694589
	C	-4.112092	5.290201	2.175224
	C	-2.573210	5.248353	2.182879
	C	-1.973628	5.319135	0.769986
	C	-0.442339	5.447108	0.789069
130	C	0.144137	5.481885	-0.630825
	C	1.680474	5.456229	-0.637026
	C	2.240939	5.382397	-2.066380
	C	3.775086	5.501903	-2.121064
	N	4.461184	4.328155	-1.564793
135	C	4.714604	3.225801	-2.367812
	C	5.237153	2.073138	-1.863101
	C	5.507244	1.906420	-0.459437
	C	5.187565	3.060242	0.342439
	C	4.686233	4.205021	-0.201398
140	C	5.994986	0.700364	0.087862
	C	6.113365	0.478543	1.505008
	C	6.403686	-0.748170	2.018686
	N	6.704331	-1.838112	1.210731
	C	6.627401	-1.652033	-0.166308
145	C	6.337022	-0.443580	-0.718635
	C	6.549419	-3.189797	1.752552
	C	-6.140569	-3.387530	-2.060509
	C	-3.296844	-2.573428	0.030261
	C	-3.441587	-1.349302	-0.629053
150	C	-3.309757	-0.100281	0.097009
	C	-3.012819	-0.116985	1.475134
	C	-2.835767	-1.389236	2.153751
	C	-2.984112	-2.597174	1.454119
	C	-2.648879	0.850208	-0.777706
155	C	-1.724752	1.765179	-0.266501
	C	-1.401009	1.745415	1.167216
	C	-2.029117	0.813185	2.003670
	C	-0.502198	2.042254	-1.000555
	C	0.576252	2.181910	-0.028110
160	C	0.018516	2.004833	1.306458
	C	-1.253539	0.118325	3.027517
	C	0.113078	0.375666	3.165818
	C	0.768969	1.338221	2.295223
	C	2.090995	0.829064	1.984109
165	C	2.622135	0.997024	0.699420
	C	1.854360	1.693767	-0.323969
	C	2.107236	1.036998	-1.602091
	C	1.072015	0.896685	-2.536725
	C	-0.257112	1.409283	-2.231737
170	C	-1.228034	0.470991	-2.766727
	C	-2.403588	0.198411	-2.059633
	C	1.039854	-0.727614	3.405547
	C	2.263398	-0.448227	2.677754
	C	2.958693	-1.491211	2.052265
175	C	3.521167	-1.310257	0.723404
	C	3.346326	-0.084075	0.058676
	C	3.022478	-0.067268	-1.358048
	C	2.888739	-1.265632	-2.067548
	C	3.062515	-2.541610	-1.379710
180	C	3.366910	-2.555354	-0.008282
	C	2.708406	-3.515939	0.869318
	C	2.455177	-2.856774	2.146131
	C	1.278897	-3.124192	2.850497
	C	0.554001	-2.038432	3.497753
185	C	-0.867966	-2.301935	3.349899
	C	-1.757508	-1.243584	3.123874
	C	1.815859	-1.413343	-3.039756
	C	0.922889	-0.353422	-3.267447
	C	-0.497810	-0.620973	-3.411251
190	C	2.085427	-3.470009	-1.912785
	C	1.312892	-2.774029	-2.940005
	C	-0.052877	-3.031748	-3.079131
	C	-0.979039	-1.930380	-3.319745
	C	-2.206564	-2.213287	-2.589416
195	C	-2.901003	-1.166934	-1.966547
	C	-2.580637	-3.665177	-0.615808
	C	-2.035956	-3.483059	-1.897303
	C	-0.710271	-3.992678	-2.204784
	C	-1.022632	-3.554023	2.620381
200	C	-2.058615	-3.690859	1.686799
	C	-1.805944	-4.351316	0.409518
	C	0.031993	-4.658070	-1.217822
	C	-0.529805	-4.838905	0.115344
	C	0.547136	-4.695898	1.085474
205	C	0.302959	-4.062406	2.311225
	C	1.770377	-4.413923	0.351270
	C	1.451858	-4.395878	-1.073211
	H	7.130004	-3.893181	1.138051
	H	-0.230227	4.605356	-1.189591
210	H	-0.214084	6.383691	-1.161869
	H	-0.148130	6.359109	1.341593
	H	-0.019443	4.583019	1.332023
	H	-2.406702	6.181369	0.225950
	H	-2.245657	4.405559	0.210436
215	H	-2.235196	4.322350	2.680773
	H	-2.211746	6.100233	2.786336
	H	-4.468564	6.178892	1.628205
	H	2.068730	6.360898	-0.130194
	H	2.026030	4.579359	-0.060878

	H	1.931119	4.430208	-2.534693
	H	1.813331	6.199896	-2.674087
	H	4.120561	5.615811	-3.160358
	H	4.111857	6.385369	-1.553269
5	H	4.472759	3.351717	-3.422954
	H	5.405264	1.251684	-2.556847
	H	5.342922	3.040929	1.419441
	H	4.451564	5.088846	0.391052
	H	5.898130	1.279974	2.210066
10	H	6.430964	-0.945340	3.090273
	H	6.833876	-2.539120	-0.764932
	H	6.321357	-0.377015	-1.805200
	H	5.485506	-3.492251	1.747121
	H	6.931239	-3.210668	2.783522
15	H	-4.508744	5.341176	3.201000
	H	-4.752744	3.044354	3.340772
	H	-4.683178	4.981569	-0.375236
	H	-5.454324	2.951380	-1.540792
	H	-5.738393	1.136854	-2.439894
20	H	-6.007518	-1.118651	-3.385642
	H	-6.588676	-0.573214	1.483103
	H	-6.835480	-2.763140	0.380959
	H	-6.857625	-4.096671	-1.619709
	H	-6.260742	-3.382668	-3.152934
25	H	-5.111615	-3.706031	-1.805970
	H	-5.584745	0.960158	2.336994

C60@1BP9BP14+

135

30	C	-6.848701	-1.412696	-1.034685
	C	-6.533434	-0.454695	-0.057750
	C	-6.343437	-0.900093	1.261495
	C	-6.452667	-2.244910	1.565153
	N	-6.769626	-3.154531	0.597239
35	C	-6.968895	-2.748974	-0.687598
	C	-6.381553	0.971407	-0.397151
	C	-6.794337	1.977475	0.493763
	C	-6.623361	3.310733	0.164939
	N	-6.046852	3.670867	-1.017529
40	C	-5.639037	2.717394	-1.899126
	C	-5.805961	1.370679	-1.614535
	C	-5.830407	5.134485	-1.302498
	C	-4.683462	5.694604	-0.444565
	C	-3.287867	5.195720	-0.860907
45	C	-2.209489	5.659636	0.140670
	C	-0.774006	5.415165	-0.365713
	C	0.259223	5.566485	0.765851
	C	1.719560	5.386547	0.300502
	C	2.678776	5.441408	1.504420
50	C	4.169571	5.476147	1.132290
	N	4.726908	4.129971	0.737052
	C	5.136284	3.269990	1.713376
	C	5.787270	2.090760	1.396071
	C	6.024562	1.752999	0.052178
55	C	5.519781	2.615661	-0.934795
	C	4.882270	3.793583	-0.573989
	C	6.813217	0.557746	-0.303758
	C	7.913809	0.166592	0.479567
	C	8.679328	-0.927931	0.113776
60	N	8.372731	-1.651339	-1.001822
	C	7.302889	-1.302853	-1.771240
	C	6.521413	-0.205604	-1.445522
	C	9.227517	-2.818281	-1.372892
	C	-6.865815	-4.598706	0.957888
65	C	3.393603	0.108526	-0.143675
	C	2.637194	1.253141	0.350188
	C	1.830805	1.764020	-0.751329
	C	2.094275	0.944376	-1.926061
	C	3.060710	-0.079224	-1.552237
70	C	1.053621	0.632144	-2.802591
	C	-0.290066	1.133425	-2.546442
	C	-0.541089	1.923950	-1.425595
	C	0.542195	2.238453	-0.505453
	C	-1.238920	0.100930	-2.940501
75	C	-2.400717	-0.099535	-2.192656
	C	-2.657238	0.723533	-1.015554
	C	-1.751095	1.717509	-0.640389
	C	-2.854359	-1.455061	-1.900227
	C	-2.120542	-2.548318	-2.366548
80	C	-0.912331	-2.337085	-3.152773
	C	-0.481925	-1.040727	-3.434502
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	C	-3.267942	-0.122757	0.002965
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	C	-1.995376	1.095106	1.740567
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	C	-1.644528	-0.774535	3.132295
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	C	0.164343	0.894885	2.920780
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	C	2.339910	0.082258	2.511844
	C	1.130515	-0.128952	3.296808
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	C	3.163376	-2.529098	-1.211568
	C	2.942629	-1.372818	-2.071720
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	C	2.214004	-3.564248	-1.601625
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	C	-0.328965	-4.712675	0.644700
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135

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