

C₁-S₀
MP2/cc-pVDZ

1				2			
N	-1.71240338	-0.52882252	-0.11908975	H	-1.05805569	2.44790801	0.80445133
C	-1.95674743	0.85198351	-0.03072566	H	1.05790687	-2.44804844	-0.80507934
C	-0.72837198	1.54199431	-0.00390801	N	4.83178130	6.78448465	-0.07668469
C	0.27259441	0.54368663	-0.10369112	C	4.26704935	5.73980078	-0.08078828
C	-0.34236019	-0.72777917	-0.14899473	N	-4.83215848	-6.78448562	0.07450970
N	1.64083862	0.34188761	-0.03242678	C	-4.26731848	-5.73985790	0.07890926
C	1.88293097	-1.04218134	-0.00829256	H	2.58539912	4.83200701	1.81195685
C	0.65511448	-1.73110823	-0.06451847	H	4.42067929	3.84754042	-1.98726800
C	3.22925824	-1.61004981	-0.09254166	H	1.41829833	2.60997181	1.81388904
C	4.22651447	-1.03706390	-0.91763860	H	3.20615873	1.65831148	-2.00620464
C	3.54503728	-2.77550326	0.64433779	C	3.58013960	4.47279105	-0.08493490
C	5.50364034	-1.60346631	-0.99432182	C	2.72133831	4.13388233	0.98179157
C	4.81582933	-3.35238583	0.55672883	C	3.76320600	3.57426535	-1.15778560
C	5.80437359	-2.76455260	-0.25545397	C	2.06390959	2.89841359	0.97959432
H	3.98837207	-0.15362788	-1.51757607	C	3.09002797	2.34803666	-1.16687150
H	2.78475008	-3.21378741	1.29881556	C	2.24729575	2.00439008	-0.09219648
H	6.26803754	-1.15873432	-1.63494357	H	-2.58637945	-4.83136484	-1.81405728
H	5.06961937	-4.25135043	1.12445040	H	-4.42036115	-3.84834898	1.98613822
C	-3.29944039	1.42496550	-0.13603542	H	-1.41913336	-2.60936712	-1.81551469
C	-3.64357967	2.54880532	0.65048466	H	-3.20531944	-1.65920929	2.00565322
C	-4.26433831	0.89929803	-1.02887894	C	-3.58040118	-4.47285013	0.08332288
C	-4.90940996	3.13718559	0.54812350	C	-2.72194493	-4.13356767	-0.98355500
C	-5.53449376	1.47578971	-1.12124451	C	-3.76312326	-3.57473330	1.15658224
C	-5.86493605	2.59527630	-0.33341639	C	-2.06443455	-2.89813137	-0.98109093
H	-2.90832784	2.94835560	1.35638787	C	-3.08978992	-2.34860138	1.16597348
H	-4.00442083	0.04895408	-1.66638919	C	-2.24748622	-2.00452424	0.09109289
H	-5.16957011	4.00354597	1.15979556	H	9.25596212	-3.37334497	-3.57696138
H	-6.28492726	1.07964915	-1.81034534	H	9.66524456	-3.22488930	-1.82511210
C	-7.23679351	3.16766394	-0.48002689	H	9.79777298	-1.79482464	-2.88882895
O	-8.08978065	2.73340841	-1.23340544	C	9.23109556	-2.71778568	-2.69883789
O	-7.42418693	4.23630744	0.33008535	O	7.84265066	-2.42431513	-2.47713587
C	-8.73228162	4.81944420	0.22111269	O	8.50914169	-1.16927098	-0.70887580
H	-8.91675451	5.17072611	-0.80437470	C	7.62181818	-1.61391032	-1.41498549
H	-9.50760467	4.08687073	0.48809082	H	-9.25462834	3.37369068	3.57948847
H	-8.73811151	5.66065247	0.92382871	H	-9.79663688	1.79491086	2.89209525
C	7.14818862	-3.41547879	-0.29658093	H	-9.66509353	3.22475289	1.82795776
O	7.44829032	-4.42039381	0.32312651	C	-9.23025389	2.71792926	2.70150199
O	8.00247912	-2.75206432	-1.11067319	O	-7.84191064	2.42464041	2.47892225
C	9.30908619	-3.34445037	-1.18111634	O	-8.50939208	1.16913119	0.71136036
H	9.77975686	-3.36597510	-0.18762128	C	-7.62166476	1.61405219	1.41678649
H	9.24902368	-4.37279251	-1.56578000	H	-6.57765924	0.11005748	-0.50281721
H	9.88271854	-2.70927550	-1.86589917	H	-5.46710153	2.52124371	2.89825530
C	-2.65425477	-1.57182321	0.03731485	H	-4.16397218	-0.40225429	-0.94060346
C	-2.52217054	-2.73170829	-0.74949046	H	-3.05717220	1.96696650	2.50979832
C	-3.69042889	-1.47232459	0.98624867	C	-6.16665603	1.33803796	1.22298123
C	-3.42148405	-3.79378832	-0.59467185	C	-5.79465774	0.50740931	0.14829775
C	-4.60498169	-2.52149012	1.13403753	C	-5.17539022	1.87929098	2.06445742
C	-4.45392041	-3.66602164	0.34172647	C	-4.44725099	0.21669637	-0.08409906
H	-1.72258006	-2.78615956	-1.49372682	C	-3.82820897	1.57317754	1.83985655
H	-3.76850180	-0.57975016	1.61136607	C	-3.44154330	0.74056339	0.76397925
H	-3.34376165	-4.70209781	-1.19372860	H	6.57687804	-0.11043075	0.50439087
H	-5.41715235	-2.47093081	1.86051305	H	5.46814401	-2.52059719	-2.89793426
C	2.57478585	1.37375743	0.21547173	H	4.16279928	0.40181942	0.94104808
C	2.47091822	2.57480456	-0.51168119	H	3.05783266	-1.96642090	-2.51053669
C	3.57533344	1.22206712	1.19536604	C	6.16670991	-1.33778192	-1.22201794
C	3.36338162	3.62570351	-0.26706957	C	5.79416293	-0.50753695	-0.14721767
C	4.48338229	2.26039295	1.43275012	C	5.17591216	-1.87881693	-2.06418655
C	4.36121588	3.44604217	0.69793390	C	4.44662910	-0.21699440	0.08462007
H	1.69916353	2.67035570	-1.28075087	C	3.82859962	-1.57284355	-1.84015461

H	3.63082533	0.29718559	1.77421922	C	3.44140332	-0.74067574	-0.76413213
H	3.30700805	4.56512971	-0.81866391	C	0.95353233	-1.38847664	-0.57379543
H	5.26797254	2.16958547	2.18518170	C	2.02225877	-0.47117566	-0.53096020
N	5.31395832	4.54686651	0.95331837	N	1.54886168	0.77399196	-0.08211614
O	5.16054911	5.58620981	0.30983151	C	-0.18883079	-0.66296305	-0.15353887
O	6.19467012	4.34773845	1.79130996	C	0.18858995	0.66291403	0.15262899
N	-5.41268232	-4.77941331	0.50388448	C	-0.95372696	1.38835983	0.57304048
O	-5.23895593	-5.77925073	-0.19455619	C	-2.02249406	0.47106825	0.53022086
O	-6.31759809	-4.62926111	1.32612472	N	-1.54903929	-0.77410816	0.08132633
H	0.55840952	-2.81444461	-0.12665167				
H	-0.63071485	2.62701806	-0.00506498				
3				4			
H	-1.16301873	2.53168156	-0.03254051	H	-1.00919245	-2.58232371	0.15373444
H	1.16308431	-2.53148380	0.03191748	H	1.04527551	2.59613255	-0.10334033
O	2.65753326	6.55867122	1.05344888	N	-2.19182371	6.25251572	-2.03752682
O	0.96426884	5.39937149	1.82102229	C	-2.44668252	5.32234924	-1.34322854
N	1.99241991	5.52682255	1.15392452	N	2.22866754	-6.23954216	2.08581507
O	-0.96523466	-5.39918888	-1.82172913	C	2.48324678	-5.30907633	1.39181501
O	-2.65873816	-6.55812943	-1.05412161	H	-4.33502121	5.22680955	0.57558884
N	-1.99327182	-5.52649393	-1.15442429	H	4.37170078	-5.21243132	-0.52677781
H	4.05193098	5.43990586	-0.56468013	H	-4.84635117	3.25551590	2.04190480
H	-4.05147186	-5.43967895	0.56570654	H	-1.25921355	2.90530779	-1.42890274
H	4.82648709	3.40991631	-1.85127263	H	-3.53507242	1.13606816	1.80504477
H	0.96992336	3.06210706	1.30793662	C	-3.77822151	4.29152129	0.46826224
H	3.63848986	1.22880550	-1.58300070	C	-2.75352202	4.19253509	-0.49798877
C	3.56169102	4.47216979	-0.45407222	C	-4.06073043	3.18396664	1.28317985
C	2.46599171	4.34049718	0.40636994	C	-2.03190039	2.99187730	-0.65891373
C	3.98297179	3.33383751	-1.15960544	C	-3.33503729	1.98966806	1.15147051
C	1.80102743	3.12755639	0.60429258	C	-2.32680082	1.89538225	1.70854553
C	3.32667260	2.10372501	-1.00842484	H	4.88138027	-3.24122733	-1.99374305
C	2.24157171	2.00284900	-0.11506782	H	1.29580426	-2.89198234	1.47879908
H	-4.82552415	-3.40968399	1.85252778	H	3.56944711	-1.12212530	-1.75630331
H	-0.97056876	-3.06176336	-1.30867511	C	3.81437565	-4.27745091	-0.41949187
H	-3.63760636	-1.22842887	1.58350520	C	2.78991510	-4.17886612	0.54704525
C	-3.56137785	-4.47190763	0.45474404	C	4.09615705	-3.16983414	-1.23458266
C	-2.46622378	-4.34023238	-0.40638774	C	2.06820770	-2.97833146	0.70850287
C	-3.98225188	-3.33359772	1.16056487	C	3.37026033	-1.97571097	-1.10244571
C	-1.80130703	-3.12731334	-0.60460945	C	2.36264926	-1.88164587	-0.12116153
C	-3.32602938	-2.10349626	1.00902180	H	-9.46166794	-4.28369841	1.34905484
C	-2.24138364	-2.00265986	0.11510749	H	-9.62241327	-3.76417995	-0.37410247
H	9.73695394	-3.83264927	-0.59599194	H	-9.98708745	-2.60419707	0.93826808
H	9.76109496	-3.24947249	1.11214004	C	-9.34776820	-3.45049184	0.64439824
H	10.15218679	-2.11772567	-0.21456618	O	-7.95926206	-3.08336580	0.70529934
C	9.53733832	-2.98425326	0.06874712	O	-8.43422051	-1.48637859	-0.83648268
O	8.14086665	-2.69018884	-0.09174895	C	-7.63334078	-2.05449682	-0.11452023
O	8.43673510	-1.02226821	1.41685860	H	9.49573047	4.30347588	-1.29261135
C	7.71303828	-1.65369749	0.66744234	H	10.02253530	2.62425955	-0.88243850
H	-9.73694110	3.83250700	0.59582642	H	9.65543382	3.78299377	0.43034871
H	-10.15206267	2.11726450	0.21572041	C	9.38205297	3.46968838	-0.58861042
H	-9.76169469	3.24818156	-1.11190395	O	7.99398904	3.10115037	-0.65102523
C	-9.53746460	2.98369733	-0.06842608	O	8.46924529	1.50367456	0.89017479
O	-8.14088294	2.68995922	0.09169256	C	7.66839768	2.07136530	0.16778532
O	-8.43711960	1.02096529	-1.41565598	H	6.43917714	0.17047474	1.55542661
C	-7.71319957	1.65303504	-0.66699450	H	5.70490031	3.21780637	-1.41529202
H	-6.30767348	-0.22755274	-1.90163263	H	4.01821999	-0.48277561	1.49847407
H	-5.91384068	2.95661245	0.98348319	H	3.29799384	2.53385466	-1.52893569
H	-3.86667125	-0.74995644	-1.67235846	C	6.21745121	1.72474559	0.07244568
H	-3.48927451	2.40471402	1.26893586	C	5.73860382	0.67670266	0.88457514
C	-6.25691646	1.38654554	-0.47059764	C	5.33071763	2.40676011	-0.78539454
C	-5.67719556	0.33741113	-1.21005599	C	4.38920018	0.31002940	0.84037728
C	-5.46154481	2.14414880	0.41100366	C	3.98354306	2.02662898	-0.84096596
C	-4.31778587	0.04402005	-1.06960490	C	3.49070372	0.97605635	-0.03019246
C	-4.10430062	1.83758161	0.56286201	H	-6.40308935	-0.15664153	-1.50542668
C	-3.51083606	0.78600802	-0.17341991	H	-5.66959504	-3.20243728	1.46714530

H	6.30738904	0.22640912	1.90260851	H	-3.98158262	0.49501950	-1.44974867
H	5.91424276	-2.95565973	-0.98489094	H	-3.26209583	-2.52018724	1.57900444
H	3.86639173	0.74909993	1.67296083	C	-6.18183947	-1.70940574	-0.02082019
H	3.48971922	-2.40348782	-1.27059286	C	-5.70272205	-0.66241578	-0.83401488
C	6.25688642	-1.38680739	0.47058326	C	-5.29521300	-2.39181335	0.83681298
C	5.67704755	-0.33806148	1.21050539	C	-4.35303354	-0.29661778	-0.79051547
C	5.46175555	-2.14372098	-0.41181934	C	-3.94780248	-2.01242954	0.89158564
C	4.31770438	-0.04448222	1.06983519	C	-3.45465574	-0.96227012	0.08044699
C	4.10456893	-1.83697318	-0.56386881	C	-0.93142431	-1.49457090	0.15551087
C	3.51095941	-0.78588304	0.17296980	C	-2.03280654	-0.61436851	0.13068705
C	1.02980865	-1.45120186	-0.01702121	N	-1.56836946	0.70942077	0.01699042
C	2.08090101	-0.51442938	0.02508890	C	0.21876385	-0.66893529	0.07073751
N	1.54463482	0.78540438	0.05615467	C	-0.18267899	0.68278223	-0.01989049
C	-0.16288851	-0.68594871	-0.02684400	C	0.96749906	1.50838532	-0.10498652
C	0.16300646	0.68616642	0.02659498	C	2.06888490	0.62814780	-0.08032663
C	-1.02969360	1.45141197	0.01652795	N	1.60443610	-0.69562934	0.03359694
C	-2.08078325	0.51461722	-0.02553587				
N	-1.54451594	-0.78519841	-0.05648994				
5				6			
H	1.46573185	2.26117268	-0.47922850	H	5.72811144	-5.18617907	0.88807985
H	-1.62900489	-2.31312288	0.26135843	H	4.24663134	-6.15592689	0.70204181
H	4.25123469	-4.39804441	-0.16337727	H	4.71374931	-5.54993307	2.31095217
H	-2.67804736	3.87771323	3.91255407	C	4.68915336	-5.29812328	1.23860438
H	-2.57882290	8.07249212	2.48344089	H	-4.27893528	6.32348632	-0.68013206
H	-2.95255703	7.19435789	0.96041837	H	-5.76632876	5.35725586	-0.83582385
H	-1.24809695	7.33993993	1.52272542	H	-4.77102491	5.70404569	-2.27630066
C	-2.29698766	7.22117617	1.84955143	C	-4.73210613	5.46220066	-1.20203760
O	-2.46436223	6.06333986	2.65651391	H	-0.99164221	-2.34907275	0.97394875
H	4.15887149	-7.83698413	-1.26796434	H	0.94787668	2.51272833	-0.93655138
H	4.12277805	-6.68330101	0.10945405	H	2.72864155	-4.18696399	2.81781783
H	4.89636849	-6.20727624	-1.44568824	H	-4.89974807	3.75032364	0.93756609
C	4.06762931	-6.77852537	-0.98997227	H	-2.77040199	4.35178462	-2.77947932
O	2.80569992	-6.35358676	-1.48820641	H	-3.53170146	1.71191692	1.39492772
H	-1.57026476	5.56672879	0.08165552	H	-1.44125943	2.27439642	-2.34832359
H	-2.16352571	1.57381934	3.04039428	C	-3.93589884	4.20158416	-0.95474109
H	-1.12027043	3.28482038	-0.79073808	C	-4.13836549	3.43691996	0.21367900
C	-2.16621201	4.86836676	2.06666558	C	-2.94395208	3.77719356	-1.86212992
C	-2.33529195	3.72950314	2.88402134	C	-3.37933374	2.28762957	0.47706404
C	-1.71215660	4.70861793	0.74224999	C	-2.18860596	2.61786710	-1.62529212
C	-2.05276016	2.45120732	2.39631803	C	-2.40778959	1.87164594	-0.45272537
C	-1.44883342	3.41904850	0.24525439	H	4.85402494	-3.58793800	-0.90187432
C	-1.61827855	2.29125027	1.06399469	H	1.39928843	-2.10953825	2.38689495
H	0.61854232	-5.37864746	-2.30758776	H	3.48594899	-1.54939473	-1.35877074
H	3.44948010	-2.07231135	0.13932646	C	3.89213929	-4.03792780	-0.99180782
H	-0.16382643	-2.99470331	-2.04787490	C	2.90129880	-3.61288913	1.89999419
C	2.47820546	-5.04684933	-1.26678308	C	4.09353141	-3.27392091	-0.17731208
C	3.28303750	-4.11402385	-0.58138059	C	2.14584433	-2.45352845	1.66329078
C	1.22754271	-4.63936650	-1.77860225	C	3.33450407	-2.12465589	-0.44046434
C	2.83626133	-2.79231811	-0.41083231	C	2.36400053	-1.70796952	0.49017946
C	0.79427331	-3.31849709	-1.62799985	H	-9.38001067	-3.84221215	2.65697701
C	1.60195348	-2.38740532	-0.94366594	H	-9.56346270	-3.85460481	0.85954120
H	-10.09986116	1.42906862	2.41289950	H	-9.95242377	-2.37055030	1.77870251
H	-9.60813271	0.56405415	3.92106835	C	-9.29108351	-3.24952786	1.73777266
H	-10.08828543	-0.37656169	2.47771974	O	-7.91373382	-2.84759509	1.67139437
C	-9.59353251	0.54501814	2.82057894	O	-8.44390585	-1.78614566	-0.26311355
O	-8.24605850	0.61274183	2.32824191	C	-7.62012952	-2.09504017	0.58085969
O	-7.86571058	-1.31674498	3.46041577	H	9.33664295	4.00252344	-2.62291202
C	-7.46556413	-0.41815096	2.74008046	H	9.90858335	2.53035644	-1.74517754
H	9.75722378	2.07953103	-3.05146796	H	9.52131552	4.01459212	-0.82559865
H	9.08017864	1.60116988	-4.65685215	C	9.24790410	3.40980697	-1.70371013
H	9.70102131	0.34312732	-3.54779899	O	7.87032098	3.00884297	-1.63645272
C	9.18974304	1.31659261	-3.59920407	O	8.40095545	1.94699196	0.29773035
O	7.90831221	1.25346278	-2.95375384	C	7.57689911	2.25639254	-0.54578431
O	7.36336923	-0.34864180	-4.46559490	H	6.41167285	0.80613383	1.34930578

C	7.06463597	0.34735922	-3.51014571	H	5.57031559	2.84966544	-2.36107299
H	6.21529908	1.82411880	-1.32538006	H	4.01145471	0.10455682	1.51932781
H	5.00486831	-1.19555666	-4.16596636	H	3.18346210	2.10453902	-2.23364570
H	3.98658513	1.66080391	-0.19776816	C	6.13683252	1.86325149	-0.51376220
H	2.74845079	-1.32451507	-3.08329105	C	5.69242940	1.08211128	0.57232656
C	5.74586836	0.31447381	-2.81135175	C	5.22401456	2.24714912	-1.51740837
C	5.45449099	1.13617656	-1.70315227	C	4.35347080	0.68598619	0.65715985
C	4.76656230	-0.57627226	-3.29594647	C	3.88790314	1.83486497	-1.43894456
C	4.20380839	1.04762365	-1.07949285	C	3.42772422	1.05130892	-0.35265345
C	3.51165885	-0.65017674	-2.68204460	H	-6.45478695	-0.64398773	-1.31354157
C	3.20995686	0.15869134	-1.55726789	H	-5.61411279	-2.68748241	2.39700836
H	-6.38159077	1.52569172	1.09140394	H	-4.05474170	0.05862533	-1.48248357
H	-5.49200014	-2.13359034	3.20525828	H	-3.22751890	-1.94121123	2.27071153
H	-4.04164456	1.61308549	0.23220300	C	-6.18025623	-1.70114255	0.54955272
H	-3.11405339	-2.02711400	2.39063955	C	-5.73574486	-0.91971293	-0.53628767
C	-6.07583803	-0.31056756	2.20500001	C	-5.26771108	-2.08468556	1.55357850
C	-5.66370020	0.75124589	1.37357718	C	-4.39690753	-0.52303481	-0.62052942
C	-5.15643679	-1.31972846	2.55555391	C	-3.93175209	-1.67178149	1.47574101
C	-4.34693482	0.80129474	0.90019757	C	-3.47144719	-0.88804165	0.38964684
C	-3.83701005	-1.25908667	2.09404891	C	-0.93938242	-1.31717042	0.62528926
C	-3.40895984	-0.19992060	1.25638819	C	-2.05871658	-0.51269568	0.31690445
C	-1.27951787	-1.28052245	0.28239516	N	-1.62150737	0.71230119	-0.21609521
C	-2.03285096	-0.18395237	0.75814485	C	0.19355079	-0.54021847	0.27789160
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C	-0.08850873	-0.72207249	-0.24421707	C	0.89559836	1.48084009	-0.58787404
C	-0.10870343	0.68075234	-0.05203439	C	2.01492535	0.67636097	-0.27946481
C	1.14302593	1.22051805	-0.43834105	N	1.57766500	-0.54859209	0.25357589
C	1.90113181	0.12221711	-0.90335466				
N	1.14104784	-1.05352450	-0.78530001				
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H	1.44565211	-2.34492745	0.43565726	N	1.40123424	0.99558952	0.23539756
H	-1.44552428	2.34594989	-0.43379033	C	2.12111169	-0.08028296	-0.31728627
O	-3.11035692	-6.97636297	1.10816661	C	1.22928097	-1.12493416	-0.63058865
O	-4.49406155	-6.46885484	-0.51334466	C	-0.05883478	-0.65050047	-0.26862910
N	-3.59077477	-6.19914964	0.28075871	C	0.05878682	0.65012416	0.26942153
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O	3.11168380	6.97679748	-1.10802891	C	-2.12116471	0.07994561	0.31800682
N	3.59168647	6.19975598	-0.28021276	C	-1.22930800	1.12451381	0.63150907
H	1.68111071	5.20817559	-1.87600861	C	-3.58557924	0.09466568	0.39603076
H	-1.68136111	-5.20709718	1.87764460	C	-4.38960699	-0.38994736	-0.66461385
H	-9.60762098	4.17673946	1.44308841	C	-4.22463263	0.63323289	1.53619483
H	-7.84913788	4.42621870	1.66337449	C	-5.78690305	-0.34852471	-0.57564473
H	-8.84132920	3.78982195	3.03294277	C	-5.62491446	0.68884572	1.61205415
C	-8.70552918	3.79453906	1.94432875	C	-6.42211925	0.18474609	0.56648155
H	8.83996023	-3.79270211	-3.03389704	H	-3.91323930	-0.78186979	-1.56976949
H	7.84773355	-4.42810297	-1.66388877	H	-3.61261341	0.99709710	2.36919999
H	9.60631235	-4.17901055	-1.44391951	H	-6.39988746	-0.71250610	-1.40795126
C	8.70427664	-3.79681783	-1.94526642	H	-6.10485252	1.11110459	2.50245955
O	8.46278324	-2.42570919	-1.58213012	C	3.58552284	-0.09496738	-0.39547868
O	8.31040708	-3.13512611	0.57045965	C	4.38967011	0.38988025	0.66497597
C	8.26662623	-2.24325595	-0.25594279	C	4.22445676	-0.63362906	-1.53566150
O	-8.46360367	2.42369352	1.58050357	C	5.78695312	0.34865147	0.57576143
O	-8.31112202	3.13428591	-0.57169953	C	5.62473773	-0.68893773	-1.61181274
C	-8.26721101	2.24199706	0.25424007	C	6.42204826	-0.18457476	-0.56645569
H	-8.34917751	0.55367835	-1.03594129	H	3.91340901	0.78188359	1.57015100
H	-8.37471559	0.13764482	0.71293325	H	3.61234208	-0.99785525	-2.36843990
C	-7.92748724	0.79502873	-0.04714810	H	6.40003203	0.71277224	1.40794196
H	8.34988237	-0.55417379	1.03311583	H	6.10457893	-1.11107818	-2.50232596
H	8.37431107	-0.13921502	-0.71601708	C	1.88751788	2.29738520	0.50304075
C	7.92742953	-0.79602544	0.04476174	C	1.43091297	2.97110361	1.65341848
H	-4.30354301	-4.25132130	-1.41615294	C	2.79045898	2.92805204	-0.37689874
H	-3.34849462	-1.91753796	-1.51138889	C	1.87433313	4.27101525	1.92809987
H	-0.76006449	-2.85172300	1.82818326	C	3.24988421	4.22007711	-0.09457902
C	-3.03752843	-4.82798740	0.23788119	C	2.79251278	4.89755278	1.05745088

C	-3.53089122	-3.92757251	-0.71594573	H	0.74193457	2.46208535	2.33485614
C	-2.03426207	-4.47422435	1.14933455	H	3.12051269	2.40687773	-1.27971182
C	-3.00032276	-2.63178563	-0.76030111	H	1.52545498	4.79856442	2.82095956
C	-1.52308585	-3.16985296	1.11078148	C	-1.88765733	-2.29759687	-0.50273597
C	-2.00369565	-2.24750104	0.15993410	C	-2.79076538	-2.92833038	0.37698697
H	4.30463714	4.25183277	1.41654729	C	-1.43096860	-2.97115503	-1.65317301
H	0.75924400	2.85308652	-1.82603548	C	-3.25035557	-4.22022320	0.09433218
H	3.34932290	1.91827034	1.51213613	C	-1.87446343	-4.27098610	-1.92812314
C	3.03810552	4.82876588	-0.23700311	C	-2.79274625	-4.89761753	-1.05765279
C	2.03426582	4.47521319	-1.14791306	H	-3.12076052	-2.40732874	1.27992062
C	3.53164442	3.92825090	0.71663912	H	-0.74187905	-2.46206752	-2.33444642
C	1.52276504	3.17098852	-1.10907109	H	-1.52558870	-4.79838585	-2.82107296
C	3.00095662	2.63252158	0.76114623	C	7.93708647	-0.23959215	-0.63309248
C	2.00388281	2.24840671	-0.15868572	H	8.26645178	-0.56247134	-1.63185735
H	6.33768325	0.65792387	-1.67703316	H	8.36826519	0.74765233	-0.40370310
H	6.15664390	-1.92813863	1.78466335	C	-7.93715615	0.24008532	0.63284830
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H	3.67033932	-1.65380014	1.85678286	H	-8.36848864	-0.74711636	0.40353430
C	6.41822820	-0.63563437	0.06324364	C	-8.43654772	1.21413567	-0.41691983
C	5.75517739	0.15088102	-0.89914161	O	-8.65756050	0.93426228	-1.57987146
C	5.65033522	-1.30153114	1.04195540	O	-8.55025186	2.45946390	0.10066054
C	4.35888340	0.28287738	-0.88234554	C	8.43682730	-1.21372694	0.41642034
C	4.25637572	-1.15930073	1.07386301	O	8.65805262	-0.93402514	1.57937045
C	3.58842232	-0.36516599	0.11181175	O	8.55051781	-2.45896024	-0.10140631
H	-6.33828932	-0.65787345	1.67607264	C	8.93364012	-3.45196828	0.86664731
H	-6.15602936	1.92736188	-1.78618579	H	9.91272101	-3.20928350	1.30667447
H	-3.85881515	-0.87525174	1.65575492	H	8.18766787	-3.51355781	1.67358641
H	-3.66956200	1.65401842	-1.85660387	H	8.98292676	-4.39799883	0.31328250
C	-6.41822279	0.63513788	-0.06463856	C	-8.93304725	3.45234563	-0.86765453
C	-5.75548305	-0.15082321	0.89841186	H	-8.98242098	4.39846664	-0.31445332
C	-5.64996607	1.30106620	-1.04304402	H	-8.18685879	3.51375648	-1.67440720
C	-4.35912015	-0.28223961	0.88256650	H	-9.91202510	3.20964760	-1.30790369
C	-4.25592134	1.15942237	-1.07398649	H	-3.95228616	-4.71584323	0.77173531
C	-3.58829360	0.36575921	-0.11132184	H	3.95145261	4.71575372	-0.77231532
C	-1.18654462	1.29521916	-0.29945859	C	3.26050345	6.23223187	1.34271111
C	-2.12600651	0.25744834	-0.14133015	N	3.64543848	7.33155285	1.57790243
N	-1.44816560	-0.94617397	0.12852914	C	-3.26054642	-6.23234072	-1.34301209
C	0.08619720	0.68825443	-0.13461778	N	-3.64525937	-7.33172887	-1.57825625
C	-0.08603679	-0.68727711	0.13591538	H	-1.53299253	2.10679179	0.99483762
C	1.18668008	-1.29423954	0.30095717	H	1.53300326	-2.10730436	-0.99363666
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H	1.44059034	2.26829392	-0.74645511	H	1.28478660	-2.70363686	0.76484982
H	-1.44133499	-2.27002332	0.74627789	H	-1.48226868	2.08258378	0.05267386
O	0.72123280	-5.16205005	2.50094705	N	1.19162961	6.44638396	1.19899756
O	2.00100028	-6.68951069	1.58738554	C	1.58531376	5.44671464	0.69289542
N	1.51395870	-5.55855952	1.64377435	N	-1.37670690	-7.07811883	-0.29505082
O	-1.99662142	6.68650750	-1.59274530	C	-1.76847701	-6.07278372	0.20126075
O	-0.71913655	5.15606287	-2.50453604	H	3.53246724	5.25152829	-1.15375157
N	-1.51148565	5.55467697	-1.64795288	H	-3.68547669	-5.86201789	2.07756500
H	-3.02156620	6.08510648	0.50866104	H	10.41479753	0.98664039	-1.53509363
H	3.02103085	-6.08637124	-0.51513124	H	8.85043437	1.29123530	-2.34367750
H	-9.87109247	-3.68327857	0.60840241	H	9.96425609	0.02987693	-2.99810913
H	-8.19899287	-4.02548556	0.06984755	C	9.59001168	0.51778563	-2.09075572
H	-9.39435029	-3.34323878	-1.10091508	H	-8.40767275	1.98845399	-3.99319695
C	-9.05938685	-3.35077605	-0.05622013	H	-7.60230115	3.18472664	-2.90809098
H	9.39871203	3.34663303	1.10126904	H	-9.37877045	2.99211170	-2.85070955
H	8.19866119	4.02781273	-0.06530924	C	-8.42690968	2.46370475	-3.00558395
H	9.86953659	3.68836349	-0.60935142	O	-8.27890143	1.39314839	-2.05877605
C	9.06043976	3.35430368	0.05764190	O	-8.40158655	2.96413326	-0.42163599
O	8.68680253	1.99629737	-0.23602705	C	-8.26866566	1.80757790	-0.76989299
O	8.16903967	2.70594726	-2.33108337	O	8.98370076	-0.52802627	-1.31260770
C	8.23510330	1.82037175	-1.49946972	O	8.49899287	1.05812867	0.23537526

O	-8.68469250	-1.99316574	0.23782810	C	8.46048874	-0.09726268	-0.14218894
O	-8.17419883	-2.70236624	2.33482876	H	8.15247814	-1.16662411	1.66138577
C	-8.23648967	-1.81718090	1.50253344	H	8.11899750	-2.19764151	0.19658979
H	-7.96689050	-0.12883470	2.76635915	C	7.80390924	-1.23353337	0.61792364
H	-8.33082340	0.28968022	1.05588003	H	-8.41248666	0.89147831	1.14337957
C	-7.76994205	-0.39000383	1.71432548	H	-8.47898466	-0.26476451	-0.23159019
H	7.96765203	0.13126687	-2.76273456	C	-7.99386231	0.64184483	0.15780034
H	8.33119459	-0.28630817	-1.05195752	H	4.31397975	3.13478722	-2.24857123
C	7.77000559	0.39265587	-1.71086503	H	3.28441777	0.94255542	-1.62776618
H	-3.67009205	4.43421520	2.30956105	H	0.71973964	2.95334833	1.22071448
H	-2.89029500	2.06282831	2.17608021	C	3.09184887	4.28822914	-0.88538792
H	-0.88810503	2.95446124	-1.57459025	C	3.53109331	3.09930555	-1.48590855
C	-2.70727317	5.04074339	0.46739205	C	2.06182374	4.23277451	0.07678230
C	-3.06314014	4.11016924	1.45830186	C	2.96447989	1.86477156	-1.13722006
C	-1.91104525	4.59352937	-0.59454952	C	1.49895462	2.99797282	0.45511596
C	-2.63486941	2.77546767	1.38753577	C	1.95784940	1.81708942	-0.15294980
C	-1.48394806	3.26715567	-0.71467121	H	-4.49691469	-3.72987757	3.11809599
C	-1.85244494	2.35478918	0.29150484	H	-0.92366390	-3.58253879	-0.37417414
H	3.66823473	-4.43340038	-2.31454444	H	-3.49025662	-1.53976639	2.44851100
H	0.88914538	-2.95819784	1.57356936	C	-3.26302487	-4.89923783	1.77972253
H	2.88803350	-2.06229934	-2.17787837	C	-2.24411392	-4.85232806	0.80515428
C	2.70695110	-5.04200143	-0.47227442	C	-3.71377947	-3.70222062	2.35529848
C	1.91167639	-4.59606096	0.59091205	C	-1.69379524	-3.62034432	0.40085306
C	3.06185051	-4.11037773	-1.46248970	C	-3.16034748	-2.46965823	1.97961774
C	1.48441214	-3.26989059	0.71288029	C	-2.15589953	-2.43209814	0.99233661
C	2.63359133	-2.77579930	-1.38978886	H	-6.44724801	-1.34094869	-0.97206159
C	1.85212408	-2.35638112	-0.29261027	H	-6.19780312	2.24084099	1.43294318
H	6.49908982	-1.00203111	0.30053235	H	-3.97460005	-1.59602543	-0.86269307
H	5.73733303	1.63484635	-3.04226941	H	-3.71722481	1.96888211	1.57915538
H	4.06059312	-1.09682747	0.79265917	C	-6.49365274	0.45191534	0.24516493
H	3.27968321	1.48713514	-2.59646248	C	-5.85157593	-0.62098741	-0.40120352
C	6.28337745	0.30770251	-1.41612409	C	-5.70852506	1.39387893	0.93991933
C	5.79473351	-0.45773135	-0.33919331	C	-4.45963682	-0.76814890	-0.33620111
C	5.36465140	1.02375956	-2.21256551	C	-4.31791231	1.24666626	1.01676382
C	4.42031082	-0.52021086	-0.06651146	C	-3.67229726	0.16017953	0.38304944
C	3.98878448	0.95183157	-1.95489183	H	5.98156965	-2.88481399	-0.60852778
C	3.49519020	0.17863564	-0.87747707	H	6.27093145	0.73861033	1.72857576
H	-6.49896551	1.00263757	-0.29850824	H	3.50886146	-2.58949126	-0.76328132
H	-5.73755510	-1.63243223	3.04581331	H	3.79240934	0.97041475	1.68267512
H	-4.06064342	1.09456859	-0.79236079	C	6.29664984	-1.09099543	0.56828088
H	-3.28003332	-1.48758135	2.59816537	C	5.50420909	-2.02860940	-0.11999737
C	-6.28341169	-0.30625498	1.41879445	C	5.66295419	0.00038359	1.19763679
C	-5.79472128	0.45799896	0.34105139	C	4.11301764	-1.87195432	-0.19863805
C	-5.36484171	-1.02249021	2.21526229	C	4.27194602	0.14600033	1.14590118
C	-4.42039925	0.51910882	0.06757045	C	3.47529131	-0.78230025	0.43430125
C	-3.98904645	-0.95192189	1.95678382	C	1.05304475	-1.66024513	0.55340343
C	-3.49541666	-0.17974518	0.87866981	C	2.01792955	-0.65214053	0.36853700
C	-1.16266624	-1.23366702	0.55245525	N	1.37147135	0.58927483	0.23040570
C	-2.05563598	-0.14586401	0.60234071	C	-0.20193475	-1.00150770	0.50845669
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O	-7.72665631	-2.32199383	3.64701304	H	-1.25174753	2.35983082	0.78356485
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H	6.87645716	3.42763280	-3.52110467	H	-7.49126161	5.03905150	-0.64200021
C	6.79972218	3.41923911	-2.42198364	H	-9.26542947	4.88440582	-0.48621130
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H	-6.97022954	-4.15700650	2.18046040	O	-8.23181928	3.08510601	-0.78211043
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H	5.30443637	-4.86149243	1.27900499	O	8.08218899	-3.58147016	-1.42257278
C	5.22562867	-5.31983410	0.27582491	C	8.08407370	-2.76750876	-0.51818030
O	5.40096841	-4.34477261	-0.75257193	H	8.19225280	-0.99956531	-1.68611965
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H	-3.75271184	6.21621160	1.79333251	C	7.82880573	-1.28588815	-0.68733572
H	-4.02345480	5.40918727	3.37615155	H	-8.19266810	0.97474816	1.67068057
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H	-0.60248937	-2.59613987	0.09627587	H	3.26184145	1.92396666	-1.58842935
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H	1.31100199	-2.58841041	-1.87181938	C	3.37090409	4.63904797	0.52857361
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C	4.43883028	-3.35504865	-0.68789936	C	2.45030006	4.17472338	1.48848486
C	3.20992520	-3.51965160	-1.35132264	C	3.05012061	2.55266819	-0.71965361
C	4.70114267	-2.16983923	0.02213249	C	1.84817077	2.91387204	1.36827859
C	2.25675433	-2.49020238	-1.32872058	C	2.14830008	2.10123592	0.26055289
C	3.74545876	-1.14451601	0.06477757	H	-4.39038572	-4.14052562	1.32399914
C	2.52306959	-1.30369576	-0.61762155	H	-1.13491169	-2.55573792	-2.10789147
H	-3.74246274	4.63215946	-0.42816811	H	-3.28100453	-1.92129257	1.58707993
H	-3.16966995	0.63655349	2.53129645	C	-3.38477084	-4.63340771	-0.53343337
H	-2.21853225	2.74368125	-1.12503273	C	-2.44709588	-4.17653437	-1.48008306
C	-4.31495493	3.67670600	1.42582973	C	-3.67660960	-3.80055072	0.56577050
C	-4.16275966	2.55250971	2.25663695	C	-1.83762339	-2.91984567	-1.35243437
C	-3.59961877	3.75979141	0.21777774	C	-3.06146298	-2.55120038	0.72116462
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C	-2.75341689	2.71012843	-0.17016208	H	-6.46493790	-0.15527656	-1.24759773
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H	-4.61307061	-3.98974058	2.53468394	H	-4.01754550	-0.55335993	-1.41094823
H	-6.56051010	-1.11910004	-0.04891748	H	-3.40880561	1.72946959	2.21500399
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H	-4.35546160	-0.07986442	-0.56613468	C	-5.79733867	0.25604522	-0.48286971
C	-5.73701578	-2.63177658	1.27005239	C	-5.45660232	1.57163021	1.52381844
C	-4.55771573	-3.13178097	1.85453960	C	-4.41789840	0.02577470	-0.57355276
C	-5.64737108	-1.51830190	0.40737549	C	-4.07963740	1.33006864	1.44732347
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C	-4.40948727	-0.92545255	0.12763882	H	6.48235381	0.20288911	1.20063737
C	-3.22198861	-1.42218422	0.71919281	H	5.85103619	-2.22090977	-2.32056372
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H	5.13441694	4.30291571	-0.42138090	H	3.39731162	-1.77394183	-2.18261094
H	3.34783845	0.23276274	-2.70207440	C	6.33732486	-1.02548682	-0.58046934
H	2.99978766	3.27065362	0.36516537	C	5.80830941	-0.23448347	0.45622569
C	5.46690177	2.83881717	-1.98761777	C	5.45037275	-1.59452432	-1.51684734
C	4.95417433	1.68125822	-2.61107428	C	4.42891156	-0.00694653	0.55773359
C	4.74332756	3.40971798	-0.92228219	C	4.07385475	-1.35445430	-1.43086143
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C	3.02266024	1.67836996	-1.10832305	C	2.09022563	-0.36134943	-0.30231409
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H	3.34458940	-2.15309463	1.29719489	C	5.47424738	-1.38983767	-2.19517324
C	6.23138480	-0.67258221	0.23770194	C	6.05316934	-0.16593533	-0.16101692
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H	-3.70426103	1.85208307	-1.57574655	C	-4.91209462	1.26733835	2.28978568
C	-6.48858341	0.58449867	-0.03404667	C	-5.57845341	-0.31094837	0.54357101
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C	-4.48209255	-0.50237942	0.80542416	C	-3.21508627	0.20748350	0.87809438
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C	-3.68598724	0.29072658	-0.05922927	C	-1.80642253	0.07224648	0.55046971
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C	-0.04240959	0.67379255	-0.07148452	C	1.26168879	-1.31982382	-0.72081252
C	-0.19609047	-0.75042470	0.13711668	C	2.28533580	-0.34642780	-0.48205153
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C	5.36183617	-2.28876923	-0.28515143	C	-4.41838399	-0.13765282	-0.59359744
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H	3.34851030	-2.62382193	-0.97785459	C	-6.16256417	-1.73186758	0.03196711
H	4.00733459	0.99665088	1.37163604	H	-3.13484820	-2.72957722	1.29436095
H	5.75233264	-3.20584486	-0.73407939	H	-4.11589238	0.75329437	-1.15238809
H	6.41888384	0.40077365	1.56501628	H	-5.51326406	-3.43940937	1.21603026
C	-3.48861001	0.75203184	-0.14345084	H	-6.49810376	0.03333683	-1.17473349
C	-4.01311656	1.96211028	0.41572514	C	3.46980338	0.93039969	-0.05418064
C	-4.38640489	-0.10215305	-0.86553179	C	3.89973512	2.14166088	-0.69017509
C	-5.36134143	2.28786076	0.29005736	C	4.45380682	0.15267056	0.64428544
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C	-6.24052185	1.42267969	-0.41191917	C	5.78363994	0.56179256	0.67883801
H	-3.34860147	2.62276636	0.98453665	C	6.19811058	1.74722535	0.01995831
H	-4.00491092	-0.99520389	-1.36954073	H	3.17112048	2.74417444	-1.24492112
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H	-6.41680286	-0.40082899	-1.56221828	H	5.54939907	3.45434489	-1.16505224
C	-7.68715086	1.71183331	-0.58014498	H	6.53307311	-0.01765808	1.22724336
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O	-8.03860565	2.88591610	0.00938604	O	8.49713726	1.45949580	0.65566570
C	-9.43175084	3.20358567	-0.13236724	O	7.88942740	3.27869521	-0.56748402
H	-9.70564391	3.29348585	-1.19480825	C	9.27007009	3.66847300	-0.52304029
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C	7.68862832	-1.71169716	0.58187186	H	9.32763930	4.61154942	-1.08171341
O	8.48114615	-0.99337036	1.17330509	C	-7.59828557	-2.09684735	-0.03369647
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H	9.70815357	-3.29251726	1.19474571	H	-9.87200435	-2.88714706	1.04626499
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C	1.69245259	3.17137617	0.67388326	C	-3.26831450	2.11261301	1.07848380
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O	2.35165693	6.64469760	1.11808407	H	1.04887620	2.55843783	-0.34495995
H	1.17152855	-2.51100415	-0.18466460	H	-1.01311221	-2.54401451	0.39342195
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H	4.81537602	-6.30596031	-1.16039673	H	0.94451350	2.43883260	-1.07904640
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C	-2.02883097	7.23500900	1.98867196	H	-5.55575427	5.53423226	-0.92806666
H	-0.98681780	7.32398102	1.63246401	H	-4.02219570	6.43030895	-0.80116340
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C	7.74465920	-0.78871048	0.41821150	C	7.91742203	-1.12841741	-1.69958907
H	8.26247626	0.06071496	-0.04859478	H	8.05259022	-1.61978587	-2.67350491
H	8.04347278	-0.85955713	1.47748093	H	8.47202328	-0.17334584	-1.71228253
C	-8.01417119	0.84134979	0.09918236	C	-7.35839803	-0.02273659	1.64301434
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H	-8.42177213	0.66782705	-0.91034501	H	-7.64109188	-1.01880748	1.25104345
C	-8.36078480	2.26833272	0.48867116	C	-8.32859590	0.97639130	1.03217906
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O	-8.76354634	2.33382066	1.77476632	O	-9.49067832	0.97802121	1.72902501
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O	7.93604572	-3.19775275	0.19359057	O	8.54337171	-1.69288252	0.57828987
O	8.76674674	-1.84917072	-1.43322061	O	9.09582208	-3.09675518	-1.11771974
C	9.14554758	-3.04460425	-2.14202625	C	9.71526097	-3.94327803	-0.12780742
H	9.84539375	-3.64495622	-1.54161693	H	10.51937388	-3.40264286	0.39324388
H	8.25869105	-3.65459849	-2.37102224	H	8.97251881	-4.27763981	0.61167018
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H	-3.47673709	1.15491886	2.03093396	H	3.40841682	-2.61565513	-0.40200449
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C	3.61716844	-0.02682874	-0.53410403	C	-3.63143007	0.20693450	0.47552159
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H	2.63785142	3.48883066	-0.41915137	H	3.12836579	-2.00022230	-2.28868729
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H	-3.49437936	5.52122248	3.51705274	H	8.34543095	-0.80482033	-0.82980358
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C	4.78732269	-5.44680437	0.81435758	O	8.19431267	-2.64170530	0.82677879
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N	-2.717659670	6.280950832	-2.123304794	N	-4.16301009	7.20255495	-0.17121553
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C	-5.34565436	-2.07751691	-1.07036775	C	-5.155883682	2.014003993	1.855308026
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H	-1.30277725	-2.45304287	-0.06527420				
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H	4.369684574	-4.173471792	1.009057651	H	-3.39326370	1.71334100	-2.11116765
H	1.130449295	-2.429659331	2.381903663	H	-4.04847346	-1.49154144	0.78281172
H	3.293547845	-1.964808786	1.337745369	H	-5.84439975	1.87539635	-2.47076163
C	3.342842993	-4.585036251	0.878200586	H	-6.49631291	-1.32388943	0.37570118
C	2.416029890	-4.085604884	1.819216166	C	3.51532850	-0.08238760	0.65471772
C	3.661207997	-3.813889243	0.259947573	C	4.06871365	-1.05462090	1.55268118
C	1.827129226	-2.830560722	1.638024486	C	4.42746463	0.77904978	-0.04370874
C	3.056002194	-2.561315439	0.451844791	C	5.44151093	-1.14110578	1.76776723
C	2.150748918	-2.065723182	0.499977751	C	5.79849896	0.67972041	0.16868255
H	-2.186150296	4.698723318	2.695698515	C	6.32996511	-0.26967674	1.08242918
H	-3.293547845	1.964808786	1.337745369	H	3.39326370	-1.71334100	2.11116765
H	-1.130449295	2.429659331	2.381903663	H	4.04847346	1.49154144	-0.78281172
C	-3.342842993	4.585036251	0.878200586	H	5.84439975	-1.87539635	2.47076163
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C	-2.416029890	4.085604884	1.819216166	C	7.79585534	-0.30952234	1.26790684
C	-3.056002194	2.561315439	0.451844791	O	8.60017394	0.42144981	0.70376567

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C	-2.150748918	2.065723182	0.499977751	C	9.58716522	-1.34168722	2.36259743
H	9.623435883	3.596675898	1.880305765	H	10.10949958	-1.56843029	1.42001936
H	10.078212703	1.912356132	-1.412112063	H	9.97479564	-0.38862862	2.75527747
H	9.840467870	3.148396398	0.143996192	H	9.74290620	-2.14836046	3.09107854
C	9.495590885	2.803800068	1.131459223	C	-7.79585534	0.30952234	-1.26790684
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O	8.576424685	0.967841702	0.485794399	O	-8.17007548	1.27386086	-2.15951768
C	7.753016019	1.536036108	0.220844938	C	-9.58716522	1.34168722	-2.36259743
H	-9.623435883	-3.596675898	1.880305765	H	-9.97479564	0.38862862	-2.75527747
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C	-7.753016019	-1.536036108	0.220844938	C	2.89342745	4.31522148	0.96819845
H	-5.767241915	-2.712377778	1.764330658	C	1.88072849	4.55222323	-1.21834893
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C	-4.20940053	1.30725394	-0.69724033	H	7.62735437	4.22830996	2.17339246
C	-4.35991462	-0.71705836	0.66679147	H	8.20483026	5.50009203	1.02677078
C	-5.59847297	1.44883103	-0.64467934	C	8.32692239	4.46084706	1.35613769
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H	-3.61297263	2.02654753	-1.26918696	H	-9.35461132	-4.28397220	-1.70758066
H	-3.88703640	-1.54537306	1.20115125	C	-8.32692239	-4.46084706	-1.35613769
H	-6.08635605	2.29019488	-1.14735785	O	-8.03911273	-3.65391213	-0.19926722
H	-6.34946749	-1.27982563	1.28840747	O	-8.45985682	-1.83410809	-1.49378109
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C	5.59847297	-1.44883103	0.64467934	C	8.13970177	2.32440867	0.42809835
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C	2.82081014	2.76554725	1.04076814	H	1.16591960	-2.66760201	1.90084727
C	1.45553825	3.31854740	-0.93126476	H	3.41785678	-1.76931064	-1.71043019
C	3.31829917	4.06863986	1.06209450	C	3.53045015	-4.57067055	0.28397532
C	1.94311856	4.62664520	-0.90927619	C	2.54728711	-4.20333984	1.24251561
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H	3.12990880	2.04120470	1.80241160	C	1.90173256	-2.96917044	-1.14644132
H	0.75124204	3.00274182	-1.71041917	C	3.19109187	-2.44695142	-0.88147049
H	4.02462658	4.39791006	1.82752176	C	2.21968993	-2.08317981	0.08623044
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C	7.89311869	-0.67444166	-0.11025549	H	-5.67840107	-2.49596127	2.37909518
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H	8.29746573	-0.73066045	0.91359324	H	-3.24577879	-1.97876507	-2.19583558
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O	8.15739913	-3.07871892	-0.29027859	H	5.67840107	2.49596127	-2.37909518
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C	8.86452352	-2.97179086	-2.82682822	H	3.24577879	1.97876507	-2.19583558
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H	9.13436049	-2.64343930	-3.83787095	C	5.32242097	1.82046105	-1.59290016
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C	5.68794382	0.87230011	0.81041623	C	-5.39788075	-2.21467607	-0.13903221
C	6.39309347	-0.20696853	0.23822509	C	-6.20476712	-1.37411660	-0.94459675
H	3.73229522	-1.96135695	-1.02835177	H	-3.87022536	1.02116760	-1.71920987
H	3.76210382	1.78039419	1.19230915	H	-3.46342089	-2.55367447	0.75296894
H	6.21579860	-2.08200024	-0.84275189	H	-6.24548850	0.45380774	-2.11576153
H	6.23825488	1.66283616	1.33210776	H	-5.83138081	-3.12140289	0.29861865
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C	-1.23634405	-3.39555448	-0.69690783	C	1.59923174	-3.16320448	0.97602412
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C	-1.60822576	-4.74872248	-0.53325685	C	2.19463086	-4.43876214	0.91229225
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H	-0.55233530	-3.11215747	-1.50114416	H	0.72798030	-2.99271172	1.61658255
H	-3.77563300	-4.45122621	2.09760040	H	4.78773242	-3.73601946	-1.21255448
C	1.78475928	2.45223620	-0.17614260	C	-2.15335389	2.10245314	-0.23617399
C	1.23634405	3.39555448	0.69690783	C	-1.59923174	3.16320448	-0.97602412
C	2.69552943	2.79466038	-1.20160839	C	-3.30962341	2.30250917	0.55790144
C	1.60822576	4.74872248	0.53325685	C	-2.19463086	4.43876214	-0.91229225
C	3.06804018	4.15509460	-1.31500719	C	-3.89485235	3.57796431	0.59857162
C	2.54207517	5.13261352	-0.46403202	C	-3.35400901	4.65229712	-0.12510499
H	0.55233530	3.11215747	1.50114416	H	-0.72798030	2.99271172	-1.61658255
H	3.07163295	2.03348432	-1.89187523	H	-3.71458983	1.47767482	1.15043972
H	3.77563300	4.45122621	-2.09760040	H	-4.78773242	3.73601946	1.21255448
C	-7.90497570	0.28355890	-0.32871361	C	7.66730361	1.68126446	1.18252936
H	-8.30930567	-0.62037268	-0.80599907	H	7.88831063	2.73207414	0.94110184
H	-8.33369295	0.38900807	0.68116308	H	7.94376487	1.47324015	2.22838389
C	7.90497570	-0.28355890	0.32871361	C	-7.66730361	-1.68126446	-1.18252936
H	8.30930567	0.62037268	0.80599907	H	-7.88831063	-2.73207414	-0.94110184
H	8.33369295	-0.38900807	-0.68116308	H	-7.94376487	-1.47324015	-2.22838389
C	8.30058422	-1.51691716	1.12263631	C	-8.49069686	-0.76278611	-0.29752368
O	8.29918213	-2.65037055	0.68240747	O	-8.87617754	0.34814541	-0.60659412
O	8.61000195	-1.19138138	2.39571226	O	-8.68496858	-1.32610915	0.91930541
C	-8.30058422	1.51691716	-1.12263631	C	8.49069686	0.76278611	0.29752368
O	-8.29918213	2.65037055	-0.68240747	O	8.87617754	-0.34814541	0.60659412
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C	-8.93491294	2.32840565	-3.21994630	C	9.37573651	0.46987545	-1.84596812
H	-9.80522012	2.86466693	-2.81318753	H	10.37382625	0.20673871	-1.46404161
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C	8.93491294	-2.32840565	3.21994630	C	-9.37573651	-0.46987545	1.84596812
H	9.16194596	-1.91579055	4.21039436	H	-9.45837286	-1.04783110	2.77491579
H	8.08210140	-3.02176805	3.27335074	H	-8.80634696	0.45678853	2.01589783
H	9.80522012	-2.86466693	2.81318753	H	-10.37382625	-0.20673871	1.46404161
H	-2.81915809	-6.18558384	0.55075991	H	3.81103492	-5.64538439	0.08778572
H	2.81915809	6.18558384	-0.55075991	H	-3.81103492	5.64538439	-0.08778572
N	1.03328848	5.73397956	1.41129649	C	1.61861155	-5.52231049	1.66938165
O	0.18177499	5.34453082	2.24127163	N	1.13544430	-6.41409307	2.29044637
O	1.41371512	6.91585321	1.29034772	C	-1.61861155	5.52231049	-1.66938165
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O	-0.18177499	-5.34453082	-2.24127163	H	-1.22882421	-2.48028070	0.20088185
H	1.59981034	-2.26367962	0.02302392				
H	-1.59981034	2.26367962	-0.02302392				
11				12			
N	-1.278441411	-1.169406776	0.235508059	N	-1.47582149	-0.91925135	-0.18352334
C	-2.080759579	-0.250344762	-0.470483353	C	-2.11240583	0.23814442	0.30755944
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C	0.000709080	-0.636514748	0.340137792	C	-0.11019242	-0.67046011	-0.24424244
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C	4.141072225	-0.368279773	1.688064784	C	4.45663772	0.36740984	0.40125730
C	5.698616245	1.276348837	0.025039734	C	5.45004415	-1.63186718	-1.31995155
C	5.518044250	-0.283214878	1.886056922	C	5.82891700	0.14082688	0.30558254
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H	3.879169372	1.758423492	-1.020608524	H	3.39588435	-2.03631137	-1.83908527
H	3.536459136	-0.992471404	2.356179000	H	4.08287469	1.10246592	1.12063160
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C	-3.493082628	-0.388201942	-0.654318403	C	-3.53163581	0.40741046	0.37822700
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C	-1.546324700	-2.545745902	0.473126155	C	-2.01116580	-2.23503163	-0.25374726
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H	-2.985331216	-5.308143224	-0.953324897	C	-7.84749127	1.08519617	0.65649037
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C	-1.309321238	-7.463395136	0.585968948	C	7.84749127	-1.08519617	-0.65649037
H	-1.356833253	-7.350826411	-0.512691458	H	8.40855305	-0.15625099	-0.46364544
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C	1.309321238	7.463395136	-0.585968948	O	8.27509620	-1.54614407	1.61823350
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H	-8.219684715	-1.593496549	-0.982796080	H	-9.46263811	3.00764817	-2.54254235
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H	8.219684715	1.593496549	0.982796080	C	8.50380262	-2.48508364	2.68146777
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C	8.453818597	-0.459606007	0.384775919	H	-1.31924962	2.25918143	0.92351874
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O	-8.591379849	-0.003594482	0.884775573	C	-3.49417697	-6.31009464	-0.46761686
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C	-9.072262562	0.986316020	1.808558690	H	-2.84820943	-6.97924843	0.12813320
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H	-8.379884733	1.840888428	1.857070535	C	3.49417697	6.31009464	0.46761686
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