

A Hybrid Metaheuristic Approach for Non-Local Optimization of Molecular Systems

Supporting Information

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1. Coordinates for Training Sets

The followings are the initial coordinates used for parameter optimizations.

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Difluoroethene

C	-0.89921	-0.11058	0.00000
H	-1.94831	0.09986	0.00000
C	0.00000	0.90332	0.00000
H	-0.34030	1.91776	0.00000
F	-0.46987	-1.39048	0.00000
F	1.32363	0.63781	0.00000

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Difluorobutadiene

C	-2.97990	-0.25080	-0.00990
H	0.00000	0.00000	0.00000
H	-4.04820	-0.25060	0.04990
C	-2.30200	0.92260	-0.02680
H	0.00000	0.00000	0.00000
H	-1.23360	0.92240	-0.08650
F	-2.30730	-1.41980	-0.06860
C	-3.06920	2.25610	0.04020
H	0.00000	0.00000	0.00000
H	-4.13760	2.25630	0.09990
C	-2.39130	3.42950	0.02330
H	0.00000	0.00000	0.00000
H	-1.32300	3.42930	-0.03650
F	-3.06390	4.59850	0.08200

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Difluorohexatriene

C	-2.97850	-0.25030	-0.01000
H	0.00000	0.00000	0.00000
H	-4.04680	-0.25110	0.04980
C	-2.30170	0.92370	-0.02670
H	0.00000	0.00000	0.00000
H	-1.23330	0.92460	-0.08650
F	-2.30480	-1.41870	-0.06870
C	-3.07020	2.25660	0.04020
H	0.00000	0.00000	0.00000
H	-4.13850	2.25570	0.10000
C	-2.39340	3.43050	0.02340
H	0.00000	0.00000	0.00000
H	-1.32500	3.43140	-0.03630
C	-3.16190	4.76340	0.09040
H	0.00000	0.00000	0.00000
H	-4.23020	4.76260	0.15020
C	-2.48510	5.93740	0.07360
H	0.00000	0.00000	0.00000
H	-1.41680	5.93820	0.01390

F	-3.15880	7.10580	0.13230
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Difluorooctatetraene			
C	-2.97710	-0.24980	-0.01010
H	0.00000	0.00000	0.00000
H	-4.04540	-0.25130	0.04970
C	-2.30100	0.92460	-0.02680
H	0.00000	0.00000	0.00000
H	-1.23260	0.92600	-0.08650
F	-2.30270	-1.41780	-0.06880
C	-3.07020	2.25700	0.04020
H	0.00000	0.00000	0.00000
H	-4.13860	2.25550	0.10000
C	-2.39410	3.43130	0.02350
H	0.00000	0.00000	0.00000
H	-1.32580	3.43280	-0.03620
C	-3.16340	4.76380	0.09050
H	0.00000	0.00000	0.00000
H	-4.23180	4.76230	0.15030
C	-2.48730	5.93810	0.07380
H	0.00000	0.00000	0.00000
H	-1.41900	5.93960	0.01400
C	-3.25660	7.27050	0.14080
H	0.00000	0.00000	0.00000
H	-4.32490	7.26910	0.20050
C	-2.58050	8.44490	0.12410
H	0.00000	0.00000	0.00000
H	-1.51220	8.44640	0.06430
F	-3.25490	9.61290	0.18280

2. Coordinates for FGG Tripeptides

2.1 Unique low energy conformations from brute force search

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O	-0.58222016	-2.02393682	-2.51145021
C	-0.11980266	-3.08783556	-2.17295947
O	0.27126192	-4.00299051	-3.11738306
H	0.11633571	-3.69107590	-4.05067856
C	0.13232044	-3.66451134	-0.79245882
H	1.16998038	-4.07732919	-0.73453811
H	-0.56016627	-4.53814772	-0.63380549
N	-0.06379389	-2.66442135	0.26246554
H	0.58356723	-1.85109673	0.23477386
C	-1.35593660	-2.46246531	0.77808614
O	-2.25615138	-3.26225880	0.61597154
C	-1.49535829	-1.18427111	1.62053644
H	-0.59692774	-1.03370837	2.26826886
H	-2.36941810	-1.29697331	2.30472481
N	-1.69694666	-0.00597227	0.75775350
H	-2.66824077	0.16192985	0.47783297
C	-0.64913308	0.48962282	-0.02135545
O	0.50043370	0.08411402	0.11820798
C	-0.99801503	1.63770783	-0.99698032
N	0.21857861	2.36290087	-1.42834761
H	0.85876112	1.73687964	-1.91638879
H	0.72572389	2.72651597	-0.62339062
H	-1.67109157	2.37634784	-0.48252902
C	-1.70931751	1.04926729	-2.23496962
H	-1.70755158	1.81332025	-3.04534710
H	-1.12164814	0.19554118	-2.64777091
C	-3.11674455	0.62675485	-1.92566557
C	-3.43762260	-0.73698355	-1.84252086
H	-2.66975022	-1.49003581	-2.04081079
C	-4.73493024	-1.13290470	-1.51077821

H	-4.97350330	-2.19414585	-1.43540180
C	-5.72274912	-0.17215349	-1.27145225
H	-6.73377109	-0.48204431	-1.01435423
C	-5.40982556	1.18742709	-1.36997209
H	-6.18078155	1.93669498	-1.19574328
C	-4.11145861	1.58891897	-1.69363959
H	-3.87443874	2.64838931	-1.77521964

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O	-1.38010078	-0.18396586	-3.25208935
C	-0.95193218	-1.11263017	-3.89718400
O	-1.60118004	-1.51902838	-5.03459573
H	-2.39877428	-0.96416814	-5.25115397
C	0.26942756	-1.99052450	-3.68376516
H	1.03931038	-1.72911307	-4.46361515
H	0.00645238	-3.06351302	-3.85457252
N	0.83224207	-1.81905054	-2.34086421
H	0.22420921	-2.12749121	-1.55873814
C	1.73159564	-0.75862376	-2.11501186
O	2.35444127	-0.23689176	-3.01689338
C	1.87920052	-0.36300760	-0.63697079
H	2.82188812	0.21922627	-0.50730092
H	1.96631875	-1.26677988	0.01496567
N	0.73184081	0.45959684	-0.21179407
H	0.76804689	1.44724659	-0.49271053
C	-0.51842986	-0.13827281	-0.02225471
O	-0.63827688	-1.35682504	0.04056557
C	-1.69848635	0.83300635	0.16695154
N	-1.63340268	1.82673249	-0.93818356
H	-2.40397592	2.48850997	-0.86625867
H	-1.71653894	1.35476593	-1.84373578
H	-1.56219630	1.38369916	1.13830192
C	-3.00903975	0.01886829	0.21869365
H	-3.16631764	-0.50908360	-0.74568447
H	-2.90323291	-0.80691595	0.95786897
C	-4.17744211	0.89628416	0.55975483
C	-5.01442328	1.38335376	-0.45564157
H	-4.83160105	1.10950009	-1.49274161
C	-6.09170895	2.21409482	-0.13596371
H	-6.74021194	2.58864673	-0.92674808
C	-6.33999344	2.56424403	1.19454390
H	-7.17893031	3.21161217	1.44135329
C	-5.50827866	2.07724788	2.20836602
H	-5.70211692	2.34587602	3.24602231
C	-4.43023634	1.24631301	1.89531816
H	-3.78899487	0.86739112	2.68889244

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O	-0.89923685	0.16983914	-3.81356431
C	-0.49165756	-0.80321889	-4.40398745
O	-0.70363616	-0.93039296	-5.75269117
H	-1.18089035	-0.15228515	-6.15009090
C	0.27345722	-2.01681873	-3.90537114
H	1.32765422	-1.96451155	-4.29899992
H	-0.17000189	-2.95121947	-4.32964398
N	0.28346255	-2.08713150	-2.44068768
H	-0.64477333	-2.21530353	-1.99400964
C	1.27122272	-1.37231237	-1.73568891
O	2.31232553	-1.02473943	-2.25439361
C	0.93222048	-1.12463218	-0.25685643
H	1.87094970	-0.88608975	0.29686637
H	0.50401579	-2.04221548	0.21649367
N	-0.01288765	-0.00067962	-0.12636854
H	0.40407807	0.93516387	-0.19082549
C	-1.35170806	-0.16813474	-0.49739900
O	-1.81102473	-1.28127934	-0.72850326

C	-2.18479588	1.12825547	-0.53404072
N	-1.48312851	2.05045792	-1.46766540
H	-2.00650038	2.91222293	-1.58919452
H	-1.37234988	1.61981581	-2.39054850
H	-2.16610109	1.59901484	0.48937994
C	-3.64656999	0.81519306	-0.92134445
H	-4.08128052	1.66103621	-1.48911321
H	-3.67726663	-0.05018371	-1.62300587
C	-4.47856186	0.51412222	0.29489646
C	-5.28987954	1.50703270	0.86261669
H	-5.32607983	2.50205640	0.42559456
C	-6.05754822	1.21797166	1.99469537
H	-6.68778941	1.99017462	2.43248659
C	-6.01838260	-0.05758498	2.56500721
H	-6.61706214	-0.28024368	3.44549658
C	-5.20703345	-1.04806103	2.00022783
H	-5.17413322	-2.04231928	2.44315829
C	-4.43906850	-0.76584370	0.86960734
H	-3.79786648	-1.53508617	0.42864409

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O	-1.27853409	0.92417592	-3.49474579
C	-1.25706014	-0.00734662	-4.26338821
O	-1.72917227	0.13691501	-5.54190122
H	-2.08584600	1.05131820	-5.71930623
C	-0.78243400	-1.43539853	-4.05656345
H	0.12886817	-1.61203565	-4.69318203
H	-1.55886815	-2.15335027	-4.41592838
N	-0.47067552	-1.69372087	-2.64589234
H	-1.28114151	-1.68758979	-2.00247984
C	0.78617779	-1.29024803	-2.15278876
O	1.74238041	-1.12781049	-2.88304669
C	0.84597353	-1.11760788	-0.62714230
H	1.91346910	-1.09215959	-0.30414347
H	0.37090925	-1.98517647	-0.10540845
N	0.18296849	0.13821035	-0.23064761
H	0.71822904	0.99694326	-0.40388940
C	-1.21469076	0.19811890	-0.20083036
O	-1.88245356	-0.82887278	-0.24300770
C	-1.81769443	1.60406000	-0.02005921
N	-1.11605528	2.52997507	-0.94870665
H	-1.54305772	3.45168525	-0.92376981
H	-1.18434418	2.19284132	-1.91600804
H	-1.58058306	1.94006952	1.03007380
C	-3.35512084	1.55721021	-0.16601574
H	-3.74669678	0.74888824	0.49452040
H	-3.78463851	2.49594765	0.23876583
C	-3.83647453	1.32951893	-1.57287109
C	-4.04063341	0.02171372	-2.04234846
H	-3.82156664	-0.82516963	-1.38544651
C	-4.50701439	-0.19336868	-3.33981051
H	-4.67284017	-1.20879235	-3.69571118
C	-4.76946690	0.89274195	-4.18234261
H	-5.14011777	0.72207406	-5.19053132
C	-4.56519685	2.19538196	-3.71904889
H	-4.77221247	3.04321901	-4.36977095
C	-4.10388450	2.41691838	-2.41791052
H	-3.95881407	3.43516907	-2.06532603

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O	-1.59493968	-2.68643812	0.26640371
C	-1.56266787	-3.81242439	-0.16971735
O	-2.27275574	-4.81338479	0.44632063
H	-2.76235090	-4.50313904	1.25510771
C	-0.83387261	-4.39260104	-1.36937072
H	-1.54828703	-4.96486176	-2.01061491

H	-0.07191377	-5.13855551	-1.00874041
N	-0.18276558	-3.34203356	-2.16016448
H	-0.82844328	-2.63966482	-2.57520869
C	1.09919338	-2.90794326	-1.76903299
O	1.85107974	-3.60402062	-1.11778893
C	1.46951965	-1.50559696	-2.28076258
H	1.17750649	-1.37992139	-3.35214810
H	2.57563814	-1.37718484	-2.22863426
N	0.80884894	-0.48989452	-1.44418760
H	1.32709683	-0.15133431	-0.62960184
C	-0.54776215	-0.22359372	-1.57850641
O	-1.20430668	-0.73226738	-2.48607366
C	-1.19576871	0.69476882	-0.52527346
N	-0.17438688	1.57771952	0.09182077
H	-0.53889875	2.00242912	0.94059603
H	0.07700222	2.33945926	-0.53932746
H	-1.57737187	-0.01413809	0.27270354
C	-2.40529824	1.43125986	-1.14053716
H	-3.01796159	0.69244833	-1.71178466
H	-3.06885831	1.78927474	-0.32912778
C	-2.00774526	2.56243172	-2.04711082
C	-1.59203623	2.29501908	-3.36102859
H	-1.56964817	1.26212329	-3.72071829
C	-1.20927301	3.34233419	-4.20010754
H	-0.88775165	3.13050416	-5.21900892
C	-1.23949751	4.66263555	-3.73701705
H	-0.94104105	5.47732103	-4.39344419
C	-1.65791292	4.93155338	-2.43092821
H	-1.68776592	5.95843222	-2.07004807
C	-2.04132745	3.88640660	-1.58520486
H	-2.37426759	4.10642756	-0.57374551

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O	-2.42240645	-2.44607946	-0.85368700
C	-1.96027848	-3.46608885	-1.30942901
O	-2.75910422	-4.57006385	-1.47267768
H	-3.69412329	-4.42556475	-1.16397882
C	-0.55677836	-3.80275825	-1.78370900
H	-0.59889471	-4.24509496	-2.80979251
H	-0.12821127	-4.60344096	-1.11776019
N	0.31300440	-2.62186878	-1.78321255
H	0.01301984	-1.85260327	-2.41365121
C	0.99258821	-2.28693923	-0.59506190
O	1.23811481	-3.10932621	0.26350263
C	1.41176391	-0.80910404	-0.50397794
H	1.84100968	-0.44932124	-1.47096056
H	2.20824101	-0.69785874	0.26713702
N	0.23137406	-0.01139076	-0.13197761
H	0.06948929	0.14549188	0.86449681
C	-0.76935220	0.24938079	-1.06325645
O	-0.59456527	0.01963167	-2.25692587
C	-2.11180887	0.74782145	-0.50251672
N	-1.88369951	1.70202945	0.60983704
H	-2.74650103	1.84073286	1.13365915
H	-1.59987202	2.61330885	0.25716176
H	-2.60757359	-0.18130846	-0.07471160
C	-2.98622016	1.29121127	-1.64952781
H	-2.66289126	2.30871099	-1.94265344
H	-2.81075348	0.67897974	-2.56855813
C	-4.44052045	1.24876453	-1.28034325
C	-5.16285431	2.43466043	-1.09026936
H	-4.67707775	3.39912898	-1.21864026
C	-6.51636054	2.37987464	-0.74285726
H	-7.07552771	3.30317995	-0.59897952
C	-7.15227399	1.14620755	-0.58105950
H	-8.20523030	1.10585100	-0.31054873
C	-6.43132673	-0.03876465	-0.76977953

H	-6.92634159	-1.00053700	-0.64474853
C	-5.08102831	0.00865342	-1.11822028
H	-4.51822264	-0.91561104	-1.26273940

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O	-1.89210905	-3.19234220	-0.16696952
C	-1.38153626	-4.06748017	-0.82522021
O	-1.88264371	-5.34454654	-0.78454927
H	-2.65650888	-5.44066796	-0.16561149
C	-0.19638741	-4.03226667	-1.77340578
H	-0.47463374	-4.49905110	-2.75036223
H	0.62974502	-4.66822515	-1.34819360
N	0.27909935	-2.66176038	-1.99257696
H	-0.40858004	-2.01909637	-2.43422054
C	1.20003404	-2.11456253	-1.07963176
O	1.90068250	-2.80436304	-0.36694507
C	1.27829662	-0.57891357	-1.11493015
H	1.28137059	-0.20298059	-2.16806681
H	2.23812224	-0.25195279	-0.65268794
N	0.13782706	-0.02020636	-0.36834494
H	0.31837701	0.26541310	0.58877752
C	-1.13351295	0.03749467	-0.93253780
O	-1.33250354	-0.33792781	-2.08239663
C	-2.24548670	0.58333595	-0.01726236
N	-2.44300267	2.00373292	-0.39648966
H	-3.15825763	2.42782337	0.19284741
H	-2.76369337	2.08223094	-1.36063735
H	-1.92862263	0.56365728	1.06085460
C	-3.47572039	-0.33536830	-0.18653727
H	-3.79557366	-0.35128391	-1.25039125
H	-3.17950799	-1.39307241	0.01911353
C	-4.59319665	0.08336029	0.72147251
C	-5.64115569	0.87909413	0.23453895
H	-5.66151620	1.17586762	-0.81195988
C	-6.66963865	1.28196608	1.09069899
H	-7.48247111	1.89786438	0.70833713
C	-6.65935605	0.89544137	2.43413255
H	-7.46060818	1.21085801	3.09916925
C	-5.61766931	0.09816920	2.92023689
H	-5.61043820	-0.20825982	3.96542761
C	-4.58733952	-0.30813836	2.06964341
H	-3.78252839	-0.93458568	2.45072642

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O	0.65618173	-3.97303517	-1.62677729
C	-0.02028978	-3.83947752	-2.61748163
O	0.22410769	-4.58928196	-3.73950066
H	1.00107856	-5.20483105	-3.63773498
C	-1.17700732	-2.89312490	-2.88196255
H	-1.62985655	-3.09594054	-3.88294597
H	-0.75302908	-1.84041431	-2.94970462
N	-2.19991701	-2.98477370	-1.83983713
H	-2.95170085	-3.65713324	-2.00906134
C	-2.07505740	-2.48545688	-0.53439769
O	-2.96759352	-2.74905200	0.25291955
C	-0.87357283	-1.61434765	-0.16370363
H	0.04794814	-1.89749861	-0.73609963
H	-0.62844825	-1.80801695	0.91109500
N	-1.17915510	-0.18480222	-0.33826455
H	-1.89171902	0.18754868	0.29569202
C	-0.87738442	0.46827699	-1.52959660
O	-0.22725944	-0.07410992	-2.41673179
C	-1.32889021	1.94473985	-1.64006369
N	-0.49164826	2.69301590	-2.60452856
H	-0.49791767	2.24156042	-3.51915832
H	0.47873728	2.71746740	-2.29760156

H	-1.23352170	2.44803569	-0.63960100
C	-2.80185096	1.99375484	-2.10305170
H	-3.06466312	3.05298176	-2.32891941
H	-2.92059553	1.46476670	-3.07084675
C	-3.72484876	1.43475173	-1.05818319
C	-4.24940650	0.14124835	-1.19960206
H	-4.02367496	-0.44876413	-2.08642801
C	-5.05584457	-0.39970114	-0.19503990
H	-5.43374924	-1.41866532	-0.29258106
C	-5.35642653	0.35100786	0.94580312
H	-5.98032677	-0.07619004	1.72918897
C	-4.85124421	1.64811823	1.07860199
H	-5.09284953	2.23790364	1.96200327
C	-4.03454387	2.18989593	0.08292289
H	-3.64502606	3.20062748	0.19073662

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O	-1.14475059	-4.19508139	0.85025389
C	-1.61624230	-4.16793437	-0.26060222
O	-2.30274216	-5.24799790	-0.75536085
H	-2.36681439	-6.00159169	-0.10722700
C	-1.61345798	-3.05290239	-1.29039567
H	-2.26104347	-2.20744687	-0.89061689
H	-2.10974061	-3.38834916	-2.23319066
N	-0.25364763	-2.59277867	-1.57024893
H	0.20810402	-3.00860257	-2.38116117
C	0.51442249	-1.76331896	-0.74335018
O	1.64468574	-1.49293717	-1.11079717
C	-0.08374356	-1.22539401	0.55830463
H	0.72479267	-1.22512057	1.33217816
H	-0.88714860	-1.89137222	0.96750469
N	-0.58272236	0.14639866	0.38093758
H	0.12924326	0.87644110	0.26610550
C	-1.89127573	0.38628357	-0.01773879
O	-2.71621791	-0.51666489	-0.11083185
C	-2.27303605	1.86817767	-0.21982249
N	-1.16169481	2.56408567	-0.91827513
H	-1.28313839	3.57393421	-0.85665844
H	-1.14599751	2.32678086	-1.90799620
H	-2.37942765	2.32250131	0.80646353
C	-3.63118334	1.94361285	-0.94761957
H	-3.54945442	1.51438162	-1.96681452
H	-4.35886193	1.26979176	-0.43705867
C	-4.14652478	3.35285807	-0.98337039
C	-4.74955077	3.90991856	0.15524637
H	-4.86267048	3.31397324	1.05925345
C	-5.21251437	5.22722625	0.12764039
H	-5.68132585	5.65585146	1.01275312
C	-5.07835894	5.99674318	-1.03290299
H	-5.44015626	7.02294067	-1.05170285
C	-4.48243521	5.44204941	-2.16927337
H	-4.38209101	6.03729552	-3.07604322
C	-4.01634663	4.12455854	-2.14759349
H	-3.56234111	3.69850970	-3.03950877

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O	1.59200679	-3.70669790	-2.51589011
C	0.44675606	-4.07572472	-2.56474072
O	0.12155060	-5.26586213	-3.17544487
H	0.91640344	-5.75164483	-3.52481336
C	-0.83067545	-3.43520090	-2.05335187
H	-1.31272961	-4.13142758	-1.31106253
H	-1.55717605	-3.32076612	-2.89429500
N	-0.56547127	-2.13529131	-1.43098778
H	-0.24902877	-1.37150955	-2.05043422
C	-0.35667595	-2.05051392	-0.05068030

O	-0.60300070	-2.97621704	0.69923580
C	0.16331881	-0.68902787	0.43686161
H	1.09760711	-0.42065493	-0.11881231
H	0.45033782	-0.78983901	1.51184858
N	-0.82605446	0.39321644	0.30115086
H	-1.53614390	0.42297471	1.03716240
C	-1.09578524	0.94696628	-0.95338839
O	-0.43460927	0.65348784	-1.94163548
C	-2.21321387	2.01654276	-0.99592667
N	-2.00312916	2.97739417	-2.10131426
H	-1.92391466	2.49331071	-2.99579241
H	-1.13755603	3.49670715	-1.97051226
H	-2.22538334	2.59600846	-0.03329713
C	-3.57520500	1.31151695	-1.18940135
H	-4.36545993	2.09090402	-1.28060214
H	-3.59667967	0.77861392	-2.16286626
C	-3.87802430	0.37716453	-0.05294701
C	-3.68234894	-1.00420191	-0.20642912
H	-3.35153850	-1.40724321	-1.16282188
C	-3.89819598	-1.86581416	0.87143916
H	-3.72213576	-2.93604207	0.75537307
C	-4.32387359	-1.35734524	2.10285052
H	-4.48748354	-2.03119187	2.94245224
C	-4.53900350	0.01614514	2.25207259
H	-4.88230125	0.41213708	3.20716236
C	-4.31478648	0.88393056	1.18002239
H	-4.48746623	1.95193111	1.30104976

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O	-2.80416523	-3.93881346	0.75540059
C	-1.68440478	-3.52099044	0.90553276
O	-1.28364799	-3.13882474	2.14558791
H	-0.38530672	-2.63006226	2.15948738
C	-0.62878612	-3.42361327	-0.20462542
H	-0.98332753	-4.00599095	-1.09010879
H	0.31398714	-3.91696323	0.13979862
N	-0.35992734	-2.03753003	-0.61417161
H	-0.76221762	-1.73016498	-1.51998669
C	0.20180774	-1.11119159	0.24564951
O	0.52169020	-1.38528430	1.40132345
C	0.46895562	0.27125649	-0.36310289
H	0.98924626	0.16446294	-1.34825029
H	1.16950410	0.82233547	0.31214319
N	-0.76253402	1.06077943	-0.53176491
H	-1.07675664	1.56332100	0.30390091
C	-1.66930567	0.75740940	-1.55182737
O	-1.43376951	-0.12259869	-2.37242295
C	-2.92641928	1.65555434	-1.63534005
N	-3.42304831	1.76787836	-3.02290487
H	-3.64699992	0.85146610	-3.41001027
H	-2.72173796	2.18484576	-3.63060447
H	-2.67820439	2.69107828	-1.27520612
C	-4.03250725	1.05009981	-0.74281735
H	-4.92864338	1.70977216	-0.79197722
H	-4.37952554	0.08201460	-1.16311237
C	-3.57442852	0.88794167	0.67856720
C	-3.36276026	2.01745923	1.48460733
H	-3.58574949	3.01119309	1.10187785
C	-2.88583811	1.86440002	2.78883651
H	-2.72588369	2.74192978	3.41397278
C	-2.62096664	0.58841173	3.29616842
H	-2.24456223	0.47000127	4.31110211
C	-2.84948749	-0.53802757	2.50051731
H	-2.65360654	-1.54164832	2.89561265
C	-3.32390697	-0.39190502	1.19457549
H	-3.51041134	-1.27980386	0.58872956

O	0.78596449	-4.31041555	-5.15009244
C	0.65947439	-3.47873011	-4.28537903
O	1.65252621	-2.55817412	-4.05691314
H	2.43663539	-2.68475679	-4.65926076
C	-0.52613321	-3.27005424	-3.36390084
H	-0.75535007	-4.25119883	-2.85751834
H	-1.42062096	-3.02248332	-3.98952834
N	-0.32440406	-2.22175570	-2.35760198
H	-0.09003623	-1.28042077	-2.71587835
C	0.03965510	-2.57593451	-1.05367704
O	-0.04330749	-3.71969419	-0.64623362
C	0.49737308	-1.40512482	-0.16954232
H	1.35957005	-0.88249592	-0.65600073
H	0.87903499	-1.82365208	0.79341581
N	-0.57329025	-0.43584836	0.11793833
H	-1.23044892	-0.72323481	0.84768245
C	-0.97127501	0.47899698	-0.86135263
O	-0.35818762	0.59867644	-1.91457773
C	-2.16691365	1.38975913	-0.49436981
N	-2.11659345	2.67211723	-1.23125694
H	-2.05796674	2.51173077	-2.23713393
H	-1.29090776	3.20724534	-0.97081746
H	-2.14838930	1.62149619	0.60487524
C	-3.48252106	0.65734543	-0.84389766
H	-4.33284410	1.35140912	-0.65436331
H	-3.52942205	0.45141288	-1.93356974
C	-3.63955309	-0.60522267	-0.04551742
C	-4.02816001	-0.54477521	1.30104302
H	-4.26788453	0.41408028	1.75748880
C	-4.11842359	-1.71743896	2.05554106
H	-4.42539105	-1.66775521	3.09966276
C	-3.81621404	-2.95306624	1.47497599
H	-3.87615158	-3.86491422	2.06717585
C	-3.43791080	-3.01663584	0.12999713
H	-3.19515168	-3.97865794	-0.32323028
C	-3.35654853	-1.84872857	-0.63165325
H	-3.06230520	-1.90601881	-1.67908402

O	-0.34217004	-5.45644812	0.05349240
C	-0.21406054	-4.38769586	-0.49301945
O	-0.67225818	-3.24616768	0.12271267
H	-1.06618073	-3.43660240	1.01735346
C	0.41238539	-4.11019542	-1.84449390
H	-0.05234874	-4.79550368	-2.59847441
H	1.50109959	-4.39915264	-1.78526120
N	0.29134634	-2.72517016	-2.31370310
H	-0.67924891	-2.36855424	-2.41245959
C	1.30212719	-1.80887509	-1.98449199
O	2.39926843	-2.15341309	-1.59082314
C	0.94210488	-0.34296590	-2.28246315
H	0.46353063	-0.26136925	-3.29010726
H	1.88558465	0.25126285	-2.32256498
N	0.05579543	0.20391024	-1.24334830
H	0.48695346	0.77717476	-0.51576355
C	-1.30232464	-0.06919811	-1.22713156
O	-1.81619381	-0.81839384	-2.05388498
C	-2.13347572	0.57936887	-0.10111725
N	-1.50731597	1.85437456	0.33338310
H	-1.89195834	2.14592722	1.23117595
H	-1.70460612	2.60180734	-0.32886243
H	-2.09800376	-0.13952574	0.76762530
C	-3.59408460	0.71942873	-0.57897626
H	-3.66369884	1.44999368	-1.40991235
H	-3.92078162	-0.24133561	-1.04456238

C	-4.49893801	1.09219846	0.55902771
C	-4.92550200	0.11068622	1.46739167
H	-4.61942624	-0.92539657	1.33384119
C	-5.75170295	0.46028614	2.53766742
H	-6.08292643	-0.30437345	3.23948665
C	-6.15772423	1.78793209	2.70953226
H	-6.80167323	2.05756322	3.54445557
C	-5.73834062	2.76566717	1.80277049
H	-6.05890841	3.79895013	1.93040624
C	-4.91109340	2.42213454	0.72983070
H	-4.59864278	3.18778282	0.02331612

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O	0.61363567	-6.10943888	-2.38096832
C	0.36697501	-4.92987165	-2.30985169
O	-0.13298674	-4.26178058	-3.40027950
H	-0.23494160	-4.85419986	-4.19511392
C	0.52179246	-4.02285452	-1.10514789
H	1.59572983	-4.07414846	-0.76363720
H	-0.09343220	-4.43884279	-0.26752680
N	0.14065517	-2.62906530	-1.35131030
H	-0.83634348	-2.45825623	-1.64635777
C	1.12435784	-1.67674288	-1.62007223
O	2.31004054	-1.89365100	-1.44832901
C	0.59977902	-0.32405014	-2.13252177
H	0.04481788	-0.49160270	-3.09030021
H	1.48243411	0.31480503	-2.37672415
N	-0.25286543	0.36461879	-1.15203645
H	0.15307138	1.16338614	-0.66151914
C	-1.59457415	0.04698879	-1.00950289
O	-2.09203411	-0.90955276	-1.59656874
C	-2.40848034	0.91241548	-0.02509060
N	-1.90274065	2.30951081	-0.04641421
H	-2.24516363	2.81871828	0.76761826
H	-2.24094829	2.80663335	-0.86785419
H	-2.22185114	0.48972766	1.00373136
C	-3.90782929	0.77422923	-0.36161947
H	-4.12076702	1.19302059	-1.36615199
H	-4.16157504	-0.30705764	-0.47008859
C	-4.75923093	1.41619676	0.69471624
C	-4.98107753	0.75814554	1.91462110
H	-4.55387273	-0.22804246	2.08792199
C	-5.75794268	1.36370228	2.90463545
H	-5.92942154	0.84933426	3.84964476
C	-6.31862569	2.62655671	2.68571154
H	-6.92401710	3.09592494	3.45878716
C	-6.10313097	3.28103216	1.46942421
H	-6.54413522	4.26151450	1.29389115
C	-5.32561538	2.68063375	0.47516861
H	-5.17165022	3.19318838	-0.47175994

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O	-2.29901101	-4.54876218	-3.07792506
C	-1.54198787	-3.62433092	-2.90640501
O	-1.97127618	-2.33278460	-3.06615423
H	-2.95632086	-2.26984909	-3.22457688
C	-0.06946911	-3.68287112	-2.55085043
H	0.51827513	-3.86379165	-3.48631941
H	0.09728229	-4.58035145	-1.89064623
N	0.44056486	-2.47243026	-1.89174781
H	0.28051647	-1.58229269	-2.40233426
C	0.51415078	-2.43632408	-0.49457984
O	0.34619396	-3.41863757	0.20395466
C	0.93770477	-1.07173536	0.07572313
H	1.70450793	-0.59035456	-0.58160273
H	1.42382373	-1.23542612	1.06641959

N	-0.21535772	-0.16868418	0.23737706
H	-0.74598992	-0.29188899	1.09782480
C	-0.81018585	0.41443593	-0.88566875
O	-0.30767132	0.30705778	-1.99634671
C	-2.04222163	1.31550282	-0.64171061
N	-2.62401888	1.76305838	-1.92888781
H	-2.96217781	0.96400853	-2.46396148
H	-1.90875621	2.21042163	-2.50463114
H	-1.67608521	2.23594315	-0.10155701
C	-3.12419202	0.64434272	0.22793234
H	-2.78356437	0.60174179	1.28164519
H	-4.00800131	1.32799422	0.24919173
C	-3.56087184	-0.71588908	-0.24460784
C	-4.54864137	-0.83014184	-1.23493691
H	-4.99301981	0.06694942	-1.66684676
C	-4.97983856	-2.09111044	-1.65529407
H	-5.75874671	-2.17354581	-2.41262477
C	-4.42703611	-3.24647665	-1.09466433
H	-4.75459203	-4.23112127	-1.42982771
C	-3.44337105	-3.13672807	-0.10646145
H	-3.00550857	-4.03581125	0.33048148
C	-3.01592714	-1.87801166	0.32290281
H	-2.26643377	-1.81598048	1.10893677

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O	-2.09639991	-1.68991386	-3.49024649
C	-1.52406137	-2.73347310	-3.70115810
O	-2.04346859	-3.63309563	-4.59734295
H	-2.89038406	-3.32037562	-5.01829628
C	-0.23666475	-3.29089827	-3.12708940
H	0.49619124	-3.46415432	-3.95498896
H	-0.43648768	-4.30329386	-2.67488012
N	0.35107096	-2.39214496	-2.12724423
H	0.49456317	-1.40994305	-2.43665278
C	0.11531699	-2.63476954	-0.76291431
O	-0.30063136	-3.70014015	-0.35357000
C	0.50657185	-1.46245915	0.15399637
H	1.44995705	-0.97616097	-0.19683847
H	0.70571499	-1.85468212	1.17828638
N	-0.58344550	-0.46896710	0.20874817
H	-1.30741803	-0.67051374	0.90059445
C	-0.86410213	0.30269477	-0.91857957
O	-0.05534380	0.36298855	-1.84268776
C	-2.15613545	1.14862160	-0.99259221
N	-2.61232160	1.21350696	-2.40528719
H	-2.75389091	0.27082684	-2.78274678
H	-1.89101563	1.64340894	-2.98734455
H	-1.85901444	2.19309051	-0.68355509
C	-3.32846258	0.71426090	-0.09089131
H	-3.22277626	1.21833987	0.89198880
H	-4.26472027	1.14642389	-0.52836080
C	-3.53559711	-0.76291927	0.09455022
C	-3.65290902	-1.62599404	-1.00311507
H	-3.62284337	-1.22453148	-2.02035704
C	-3.79986992	-3.00063692	-0.80436759
H	-3.87499186	-3.66760127	-1.66172250
C	-3.84830413	-3.52416050	0.49106326
H	-3.94431720	-4.59771722	0.64346369
C	-3.76665395	-2.66329999	1.58980954
H	-3.81839694	-3.06610666	2.60043228
C	-3.61431950	-1.28837575	1.39598985
H	-3.56454787	-0.62720367	2.25867216

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O	3.28878509	3.44440922	-2.87485883
C	3.46959727	2.32602731	-2.46582317

O	4.11757331	2.15470458	-1.28456489
H	4.16082912	1.18201962	-0.96149908
C	3.05486758	1.04589699	-3.20492993
H	3.94594340	0.37945716	-3.31693555
H	2.73160644	1.31539346	-4.24018304
N	1.96324811	0.32552489	-2.53292112
H	0.99958725	0.52591146	-2.86553144
C	2.14898260	-0.28743280	-1.30374935
O	3.23429319	-0.30297356	-0.72856588
C	0.91327820	-1.00342494	-0.74089456
H	1.25266410	-1.75934866	0.00889740
H	0.38352703	-1.56659484	-1.54952564
N	-0.01263704	-0.05758860	-0.09728079
H	0.13714028	0.12131349	0.90186109
C	-0.75355401	0.84793929	-0.85463530
O	-0.73787126	0.81691360	-2.08104940
C	-1.66121402	1.80631714	-0.05916082
N	-0.91224513	2.28986199	1.13047331
H	-1.54910678	2.73051145	1.79344525
H	-0.22491717	2.99520353	0.86774919
H	-2.54434160	1.20601848	0.30147446
C	-2.15765489	2.92387293	-0.99896917
H	-1.30183438	3.51997423	-1.37986145
H	-2.58867104	2.46902949	-1.92096432
C	-3.17003509	3.79405253	-0.31245424
C	-4.48941467	3.34413607	-0.14888298
H	-4.78732693	2.37271545	-0.53883040
C	-5.42557372	4.14741441	0.50621131
H	-6.44941426	3.79631096	0.62972577
C	-5.05368932	5.40188152	1.00088617
H	-5.78528203	6.02612318	1.51042893
C	-3.74126930	5.85370122	0.83381894
H	-3.45077864	6.83342263	1.21174294
C	-2.79967186	5.05421708	0.18006894
H	-1.78303757	5.41876818	0.04497879

2.2 PCONE, lowest energy, PM6-DH+ optimized

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O	-1.24300	-1.48500	0.28500
C	-2.21900	-2.01000	-0.20400
O	-2.45200	-3.33500	-0.15800
H	-1.71000	-3.72300	0.33000
C	-3.32100	-1.29600	-0.96200
H	-4.27300	-1.61000	-0.54100
H	-3.28700	-1.62400	-1.99900
N	-3.19400	0.13000	-0.88200
H	-2.47400	0.58200	-1.43700
C	-3.45600	0.71700	0.32500
O	-4.07100	0.16200	1.22400
C	-2.83000	2.09500	0.47500
H	-3.29000	2.60000	1.31700
H	-2.95100	2.68700	-0.43100
N	-1.41200	1.92200	0.72600
H	-1.08100	1.66600	1.64800
C	-0.55600	1.63700	-0.27700
O	-0.86300	1.69700	-1.47000
C	0.84200	1.24000	0.18800
N	0.76300	0.68000	1.53500
H	1.69700	0.57400	1.91300
H	0.36400	-0.25300	1.47500
H	1.42600	2.16300	0.25300
C	1.49200	0.32900	-0.86300
H	0.87900	-0.56800	-0.96200
H	1.48100	0.84400	-1.82200
C	2.89000	-0.03300	-0.46000

C	3.15900	-1.23300	0.20500
H	2.35000	-1.93300	0.37500
C	4.45000	-1.54100	0.63300
H	4.64000	-2.47700	1.14100
C	5.49200	-0.64600	0.40400
H	6.49500	-0.88400	0.73300
C	5.23800	0.55300	-0.25900
H	6.04500	1.24900	-0.44800
C	3.94700	0.85500	-0.68500
H	3.75600	1.78500	-1.20700

2.3 ACO conformations

First global best, PM6-DH+ optimized, identical to the PCONF lowest energy

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O	0.22480	2.73930	-3.68150
C	-0.74980	3.45300	-3.73370
O	-0.60890	4.81610	-3.68630
H	0.34030	5.11140	-3.63490
C	-2.22500	3.11160	-3.85730
H	-2.57010	3.38310	-4.89480
H	-2.82580	3.74110	-3.15560
N	-2.47590	1.69070	-3.59720
H	-2.27390	1.37100	-2.63100
C	-2.32270	0.77250	-4.65450
O	-2.38090	1.11220	-5.81840
C	-2.12300	-0.68240	-4.20020
H	-2.34810	-1.36540	-5.05290
H	-2.83200	-0.94860	-3.37810
N	-0.73230	-0.89170	-3.75720
H	-0.04340	-1.01890	-4.50880
C	-0.30420	-0.35500	-2.53850
O	-1.10580	0.07080	-1.71420
C	1.21440	-0.40230	-2.28670
N	1.88000	0.15220	-3.49610
H	2.89120	0.15270	-3.37590
H	1.58730	1.12230	-3.64730
H	1.53020	-1.47640	-2.17720
C	1.52510	0.35940	-0.98030
H	1.24920	1.42950	-1.09000
H	0.85340	-0.00510	-0.17060
C	2.96590	0.20250	-0.59190
C	3.39290	-0.95250	0.08160
H	2.67610	-1.73020	0.33820
C	4.73740	-1.10320	0.42820
H	5.06480	-2.00020	0.95220
C	5.66400	-0.10610	0.10600
H	6.71090	-0.22620	0.37700
C	5.24020	1.04620	-0.56270
H	5.95900	1.82560	-0.81170
C	3.89630	1.20300	-0.91200
H	3.57280	2.10600	-1.42560

Second global best, PM6-DH+ optimized, identical to the PCONF lowest energy

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O	1.52760	-7.33190	-2.87460
C	2.63850	-6.99230	-3.19220
O	3.65810	-7.91730	-3.25000
H	3.35620	-8.83950	-3.03330
C	3.20360	-5.63480	-3.56710
H	3.58540	-5.68230	-4.62620

H	4.08910	-5.40270	-2.92670
N	2.19200	-4.58380	-3.43880
H	1.88390	-4.33160	-2.48600
C	1.45400	-4.17770	-4.55040
O	1.72550	-4.53470	-5.68160
C	0.27480	-3.24140	-4.23500
H	-0.41290	-3.74930	-3.51230
H	-0.30340	-3.08920	-5.17770
N	0.72770	-1.94220	-3.71020
H	0.58060	-1.13330	-4.31390
C	1.03450	-1.78000	-2.36440
O	1.09470	-2.74060	-1.60460
C	1.34470	-0.33050	-1.93160
N	0.15580	0.49330	-2.27130
H	0.36470	1.48380	-2.17230
H	-0.62600	0.28610	-1.65340
H	2.21070	0.03850	-2.55280
C	1.74730	-0.29230	-0.44140
H	1.43720	0.66610	0.01810
H	1.19460	-1.08000	0.12270
C	3.22850	-0.49940	-0.27670
C	3.75760	-1.79940	-0.28920
H	3.08580	-2.65260	-0.41900
C	5.13140	-1.99560	-0.14100
H	5.53940	-3.00510	-0.14870
C	5.98530	-0.89870	0.02000
H	7.05590	-1.05410	0.13690
C	5.45970	0.39640	0.03180
H	6.12240	1.25110	0.15790
C	4.08450	0.59960	-0.11690
H	3.68430	1.61050	-0.10490

3. Coordinates for Molecular Balances (Closed Form) Optimized with PM6-DH+

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1_9_disubsti_triptycene/opt_a10_folded_opt.xyz

C	-5.03280	-0.68520	1.90790
C	-3.87340	-0.22540	2.56410
C	-3.12020	0.84180	2.04880
C	-3.52270	1.36600	0.79470
C	-4.65990	0.92170	0.12790
C	-5.42110	-0.10200	0.70460
C	-1.20410	1.76560	0.23170
C	-0.80420	1.26940	1.50460
C	0.42620	0.64460	1.63790
H	0.75900	0.25080	2.59580
C	1.26120	0.51500	0.51230
C	0.86410	1.00540	-0.72850
C	-0.38290	1.63890	-0.87690
H	-5.62590	-1.49070	2.32710
H	-6.32130	-0.45410	0.20080
H	2.22680	0.02450	0.62060
H	1.51710	0.90080	-1.59270
H	-0.68990	2.01970	-1.84760
C	-2.09840	3.02180	2.57340
C	-1.93010	3.93020	3.60860
C	-2.18780	5.29540	3.39240
C	-2.60350	5.75180	2.14460
C	-2.75920	4.84920	1.07860
C	-2.50060	3.50490	1.29690
H	-1.60560	3.59820	4.59760
H	-2.05760	5.99760	4.21370
H	-2.80470	6.80930	1.98650
H	-3.07230	5.20650	0.10110
C	-1.85260	1.50090	2.61620
C	-1.38270	0.96260	3.97430
H	-1.27530	-0.14240	3.88640

H	-0.36960	1.35890	4.18860
C	-2.29990	1.26890	5.15630
H	-3.35600	1.11180	4.89560
H	-2.19820	2.30650	5.50060
O	-3.39520	-0.78970	3.72790
C	-4.09590	-1.93410	4.27170
H	-3.48670	-2.16540	5.15500
H	-5.11350	-1.65680	4.56010
H	-4.08310	-2.76380	3.55930
H	-2.07490	0.61210	6.00270
H	-4.95080	1.35500	-0.82400
C	-2.57890	2.42220	0.23470
H	-2.88530	2.80070	-0.75820

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l_9_disubsti_triptycene/opt_al_folded_opt.xyz

C	-4.91120	-0.83250	1.81830
C	-3.84430	-0.27230	2.53630
C	-3.16710	0.87080	2.06650
C	-3.54330	1.38020	0.80770
C	-4.61320	0.82060	0.09000
C	-5.30860	-0.28200	0.59830
C	-1.25400	1.99220	0.35720
C	-0.87150	1.50870	1.64070
C	0.40090	0.99100	1.82660
H	0.72310	0.60900	2.79280
C	1.29630	0.95600	0.74100
C	0.91660	1.43220	-0.51050
C	-0.37310	1.95690	-0.71120
H	-5.43370	-1.70670	2.19850
H	-6.14130	-0.72280	0.05810
H	2.29520	0.54940	0.88950
H	1.61660	1.40040	-1.34340
H	-0.66820	2.32470	-1.69110
C	-2.35870	3.12580	2.66830
C	-2.30200	4.03120	3.71790
C	-2.66940	5.37210	3.50740
C	-3.08050	5.80750	2.25060
C	-3.11620	4.91050	1.16920
C	-2.74800	3.59100	1.38080
H	-1.97550	3.72140	4.71360
H	-2.62700	6.07200	4.34010
H	-3.36920	6.84560	2.09720
H	-3.42410	5.25180	0.18350
O	-4.87000	1.46010	-1.11040
C	-5.91700	0.91090	-1.94310
H	-5.88960	1.58480	-2.80920
H	-5.67320	-0.11390	-2.23720
H	-6.88170	0.97190	-1.43150
C	-1.98740	1.63050	2.70270
C	-1.53190	1.10780	4.07130
H	-1.32380	0.01600	3.96860
H	-0.57060	1.59160	4.34570
C	-2.53720	1.31830	5.21230
H	-3.55600	0.99350	4.89120
H	-2.61560	2.40070	5.47060
O	-3.35860	-0.79430	3.71700
C	-4.07950	-1.87610	4.35280
H	-3.54490	-1.94240	5.31860
H	-5.12690	-1.61140	4.51080
H	-3.96630	-2.79260	3.76990
C	-2.13120	0.53350	6.42150
O	-2.48950	-0.55090	6.82140
O	-1.20640	1.24250	7.16110
H	-0.90600	0.75710	7.97320
C	-2.68170	2.52310	0.30270
H	-2.98930	2.87790	-0.70160

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1_9_disubsti_triptycene/opt_a2_folded_opt.xyz

C	-4.92780	-0.81720	1.78940
C	-3.90000	-0.23110	2.54300
C	-3.20960	0.90610	2.07770
C	-3.52750	1.38020	0.78940
C	-4.55760	0.79390	0.03570
C	-5.26980	-0.30040	0.53820
C	-1.22290	1.99840	0.43570
C	-0.90070	1.55110	1.74870
C	0.36420	1.04820	2.00990
H	0.64050	0.69360	3.00050
C	1.31210	0.99220	0.97080
C	0.99130	1.43320	-0.30980
C	-0.29040	1.94250	-0.58700
H	-5.46150	-1.68590	2.16650
H	-6.07290	-0.76080	-0.02960
H	2.30500	0.59720	1.17850
H	1.73150	1.38530	-1.10630
H	-0.53930	2.28250	-1.58940
C	-2.44710	3.18230	2.65940
C	-2.44760	4.11500	3.68640
C	-2.81220	5.44730	3.42310
C	-3.16370	5.84710	2.13680
C	-3.14100	4.92210	1.07880
C	-2.77570	3.61130	1.34260
H	-2.16930	3.83270	4.70480
H	-2.81500	6.16860	4.23840
H	-3.45080	6.87860	1.94230
H	-3.40250	5.23550	0.07080
O	-4.76010	1.40050	-1.19220
C	-5.75820	0.81870	-2.06180
H	-5.69140	1.46860	-2.94400
H	-5.49170	-0.21160	-2.31400
H	-6.74840	0.88500	-1.60220
C	-2.06820	1.69140	2.75140
C	-1.67760	1.20830	4.15410
H	-1.45690	0.11600	4.09150
H	-0.73440	1.70650	4.46300
C	-2.73830	1.43920	5.23900
H	-3.73660	1.09110	4.88250
H	-2.84270	2.52640	5.46170
O	-3.46400	-0.72280	3.75500
C	-4.22210	-1.77490	4.39750
H	-3.73390	-1.80510	5.38990
H	-5.27390	-1.49930	4.49560
H	-4.08740	-2.71370	3.85660
C	-2.38030	0.69180	6.49140
O	-2.76280	-0.38260	6.89500
O	-1.49490	1.45710	7.22380
C	-1.00250	0.89760	8.46860
H	-0.18310	0.21150	8.23540
H	-0.65320	1.77940	9.01520
H	-1.80570	0.37710	9.00210
C	-2.64980	2.51650	0.29740
H	-2.91000	2.84270	-0.72960

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1_9_disubsti_triptycene/opt_a3_folded_opt.xyz

C	-4.63270	-0.70930	2.55430
C	-3.54440	0.02730	3.04630
C	-2.97770	1.07900	2.29980
C	-3.48970	1.31010	1.00670
C	-4.58060	0.57420	0.51590
C	-5.16370	-0.43240	1.29340
C	-1.29090	1.92340	0.22700
C	-0.77090	1.72240	1.53690
C	0.54290	1.31000	1.69700

H	0.97000	1.14290	2.68390
C	1.34290	1.10050	0.55800
C	0.82880	1.30090	-0.71990
C	-0.50380	1.71640	-0.89400
H	-5.06840	-1.51190	3.14400
H	-6.01080	-1.00720	0.93090
H	2.37470	0.77720	0.68610
H	1.45610	1.13590	-1.59400
H	-0.90380	1.86860	-1.89360
C	-2.26630	3.44220	2.37060
C	-2.18220	4.53870	3.21630
C	-2.65220	5.79260	2.78680
C	-3.19340	5.95080	1.51390
C	-3.26070	4.85680	0.63400
C	-2.79150	3.62430	1.06040
H	-1.75450	4.44850	4.21690
H	-2.58650	6.64460	3.46110
H	-3.56040	6.92320	1.19110
H	-3.67120	4.98150	-0.36540
O	-4.97560	0.94960	-0.75600
C	-6.05230	0.19990	-1.36430
H	-6.13620	0.68640	-2.34480
H	-5.77220	-0.85180	-1.47250
H	-6.97380	0.32160	-0.78790
C	-1.79730	2.00250	2.65730
C	-1.19360	1.78390	4.04910
H	-0.92550	0.70410	4.14090
H	-0.23980	2.34760	4.13100
C	-2.10650	2.17100	5.21840
H	-3.14160	1.78390	5.04930
H	-2.21260	3.27840	5.30140
O	-2.93270	-0.24030	4.25640
C	-3.59740	-1.14020	5.17580
H	-2.99510	-1.00380	6.08760
H	-4.62950	-0.82810	5.35330
H	-3.53160	-2.16560	4.80440
C	-1.54860	1.64020	6.50500
O	-0.42340	1.61190	6.92440
O	-2.63710	1.14220	7.23040
C	-2.55200	0.55100	8.49120
C	-1.36550	0.21740	9.14650
C	-3.82010	0.28430	9.03590
C	-1.46020	-0.40740	10.39440
H	-0.39190	0.44300	8.70550
C	-3.88260	-0.34030	10.28020
H	-4.71570	0.57020	8.49070
C	-2.70720	-0.68790	10.95990
H	-0.54760	-0.67600	10.92720
H	-4.85260	-0.55740	10.72710
H	-2.76730	-1.17450	11.93080
C	-2.74860	2.36740	0.20870
H	-3.16290	2.50070	-0.81100

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1_9_disubsti_triptycene/opt_a7_folded_opt.xyz			
C	-4.84680	-0.72490	2.10720
C	-3.72630	-0.14700	2.72220
C	-3.06800	0.95750	2.14800
C	-3.52170	1.40850	0.89180
C	-4.64030	0.82600	0.27360
C	-5.31430	-0.23680	0.88580
C	-1.26160	1.97550	0.26330
C	-0.79960	1.55260	1.54180
C	0.47810	1.03130	1.67240
H	0.85880	0.69300	2.63390
C	1.30100	0.93350	0.53470
C	0.84440	1.35110	-0.71230
C	-0.45180	1.87830	-0.85630

H	-5.36460	-1.56030	2.57260
H	-6.18670	-0.69230	0.42590
H	2.30460	0.52430	0.63870
H	1.48920	1.27060	-1.58580
H	-0.80680	2.19970	-1.83270
C	-2.21250	3.23200	2.58180
C	-2.09440	4.18330	3.58480
C	-2.47330	5.51410	3.33380
C	-2.95640	5.89240	2.08410
C	-3.05720	4.94670	1.04930
C	-2.67910	3.63700	1.30000
H	-1.71020	3.92170	4.57180
H	-2.38380	6.25190	4.12960
H	-3.25260	6.92360	1.90010
H	-3.42330	5.24350	0.06890
O	-4.96310	1.40020	-0.94240
C	-6.08400	0.83980	-1.66480
H	-6.10090	1.46440	-2.56760
H	-5.89110	-0.20670	-1.91710
H	-7.00640	0.96010	-1.08950
C	-1.84380	1.73800	2.66310
C	-1.31430	1.28520	4.02830
H	-1.10350	0.18910	3.97280
H	-0.33990	1.77580	4.22980
C	-2.27620	1.55860	5.18970
H	-3.34070	1.44260	4.85370
H	-2.20880	2.61760	5.53780
O	-3.19410	-0.60320	3.91580
C	-3.69360	-1.84980	4.45650
H	-3.00680	-2.01500	5.29940
H	-4.72170	-1.72190	4.80570
H	-3.60340	-2.65530	3.72280
C	-2.02310	0.62770	6.32530
O	-1.21750	-0.21590	6.57170
O	-3.06410	0.91400	7.27120
C	-3.22690	0.24550	8.45970
F	-3.48570	-1.04280	8.27850
F	-2.17480	0.35070	9.25670
F	-4.26760	0.78980	9.07250
C	-2.68660	2.51610	0.27470
H	-3.05650	2.82300	-0.72440

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1_9_disubsti_triptycene/opt_a8_folded_opt.xyz

C	-4.92020	-0.81360	1.89490
C	-3.80290	-0.29930	2.56880
C	-3.12080	0.83700	2.08720
C	-3.54560	1.37890	0.85800
C	-4.66210	0.85910	0.18110
C	-5.36210	-0.23190	0.70380
C	-1.26770	1.95450	0.30850
C	-0.83700	1.44170	1.56510
C	0.43260	0.89770	1.68250
H	0.78970	0.49410	2.62740
C	1.27680	0.86510	0.55660
C	0.84960	1.37040	-0.66790
C	-0.43760	1.92230	-0.79990
H	-5.45750	-1.67310	2.28640
H	-6.23290	-0.63990	0.20030
H	2.27320	0.43800	0.65200
H	1.50990	1.34090	-1.53240
H	-0.77000	2.31330	-1.75840
C	-2.24840	3.06510	2.68840
C	-2.14170	3.94660	3.75430
C	-2.49150	5.29790	3.58390
C	-2.93780	5.76720	2.35160
C	-3.03160	4.89300	1.25500
C	-2.68100	3.56320	1.42730

H	-1.79570	3.60420	4.73230
H	-2.40910	5.97870	4.42890
H	-3.21120	6.81310	2.22930
H	-3.37120	5.25920	0.28930
O	-4.95370	1.52290	-0.99840
C	-6.07430	1.03720	-1.77210
H	-6.06820	1.72370	-2.62870
H	-5.89760	0.00740	-2.09510
H	-7.00200	1.13380	-1.20100
C	-1.89880	1.56400	2.68140
C	-1.39600	1.01200	4.02160
H	-1.21490	-0.07990	3.89670
H	-0.41200	1.46830	4.25240
C	-2.33260	1.21520	5.21060
H	-3.37420	0.98500	4.94450
H	-2.30950	2.24720	5.58420
O	-3.28730	-0.85970	3.72460
C	-3.87940	-2.09090	4.19990
H	-3.25710	-2.30900	5.07760
H	-4.92040	-1.92690	4.49140
H	-3.78310	-2.87890	3.44790
H	-2.05800	0.55330	6.03810
C	-2.68530	2.51300	0.33010
H	-3.03300	2.89030	-0.65250

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1_9_disubsti_triptycene/opt_a9_folded_opt.xyz

C	-5.04900	-0.64750	1.92360
C	-3.86480	-0.20110	2.55870
C	-3.12390	0.87530	2.03860
C	-3.52650	1.42260	0.79550
C	-4.69610	0.97990	0.15600
C	-5.46050	-0.05510	0.74680
C	-1.20010	1.78660	0.24180
C	-0.80110	1.27810	1.50840
C	0.42280	0.63880	1.63420
H	0.75700	0.23820	2.58870
C	1.24990	0.50590	0.50350
C	0.85170	1.00610	-0.73360
C	-0.38790	1.65530	-0.87320
H	-5.63870	-1.45360	2.35240
H	-6.38070	-0.38580	0.24660
H	2.21150	0.00500	0.60390
H	1.49940	0.89750	-1.60210
H	-0.69800	2.04530	-1.84090
C	-2.07930	3.03700	2.59750
C	-1.90290	3.93280	3.64240
C	-2.15560	5.30100	3.44010
C	-2.57490	5.77220	2.19840
C	-2.73720	4.88230	1.12320
C	-2.48020	3.53550	1.32830
H	-1.57540	3.59040	4.62650
H	-2.01890	5.99510	4.26760
H	-2.77400	6.83250	2.05260
H	-3.05520	5.24790	0.14830
C	-1.84680	1.51460	2.61920
C	-1.38730	0.95840	3.97320
H	-1.27450	-0.14470	3.87700
H	-0.37340	1.35190	4.19440
C	-2.30610	1.25870	5.15560
H	-3.36380	1.13170	4.89150
H	-2.18400	2.28820	5.51970
O	-3.36180	-0.78760	3.68470
C	-4.05770	-1.93260	4.24470
H	-3.41450	-2.17800	5.10110
H	-5.05870	-1.64450	4.57730
H	-4.08040	-2.75500	3.52400
H	-2.09570	0.58460	5.99250

N	-5.18780	1.52640	-1.10940
O	-4.57530	2.43350	-1.65410
O	-6.21240	1.03700	-1.56710
C	-2.56150	2.46740	0.25330
H	-2.84860	2.87610	-0.74370

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1_9_disubsti_triptycene/opt_b1_folded_opt.xyz

C	-4.20680	-0.70310	2.97250
C	-3.02070	0.00340	3.23200
C	-2.62580	1.07740	2.41220
C	-3.39270	1.33910	1.25660
C	-4.56910	0.62110	0.99250
C	-4.99180	-0.39100	1.86200
C	-1.39380	2.00370	0.07140
C	-0.62370	1.78050	1.24820
C	0.69970	1.38240	1.13900
H	1.31170	1.19510	2.01780
C	1.26420	1.21350	-0.13930
C	0.50830	1.43830	-1.28630
C	-0.83710	1.83640	-1.18610
H	-4.52120	-1.51020	3.62970
H	-5.90920	-0.94320	1.68230
H	2.30390	0.90280	-0.22400
H	0.95470	1.30530	-2.27000
H	-1.42610	2.00630	-2.08440
C	-1.96880	3.44830	2.41260
C	-1.78260	4.50340	3.29430
C	-2.35630	5.75510	3.00730
C	-3.10370	5.94870	1.84850
C	-3.29410	4.89060	0.94310
C	-2.72730	3.65830	1.22800
H	-1.20780	4.37830	4.21570
H	-2.21120	6.57710	3.70570
H	-3.54450	6.92070	1.63730
H	-3.87720	5.04060	0.03830
O	-5.21460	1.01820	-0.16640
C	-6.41780	0.30460	-0.53180
H	-6.69840	0.80510	-1.46770
H	-6.19760	-0.75260	-0.70430
H	-7.18910	0.44310	0.23120
C	-1.41700	2.01690	2.54900
C	-0.54160	1.80650	3.79190
H	-0.37740	0.73100	3.99110
H	0.42370	2.33830	3.69930
O	-2.14040	-0.34980	4.23600
C	-2.62920	-1.22390	5.28400
H	-1.76620	-1.25920	5.96480
H	-3.48950	-0.77100	5.78570
H	-2.85430	-2.21250	4.87900
O	-1.19830	2.45970	4.91560
C	-1.33300	1.73730	6.08730
C	-2.54880	1.94260	6.76160
C	-0.32130	0.93750	6.63050
C	-2.74910	1.33160	7.99330
H	-3.31030	2.57370	6.30540
C	-0.53940	0.32000	7.86150
H	0.61980	0.79890	6.10630
C	-1.75380	0.49920	8.55810
H	-3.69330	1.49380	8.51060
H	0.24480	-0.31120	8.27790
N	-2.02280	-0.27590	9.74020
C	-3.11980	0.24510	10.60700
H	-4.05960	0.27370	10.02910
H	-3.28340	-0.45240	11.44450
H	-2.93070	1.24760	11.02060
C	-0.82000	-0.60190	10.56240
H	-1.11600	-1.26220	11.39330

H	-0.09710	-1.16630	9.94810
H	-0.30940	0.27930	10.98000
C	-2.83170	2.42230	0.35060
H	-3.44040	2.56990	-0.56380

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1_9_disubsti_triptycene/opt_b2_folded_opt.xyz

C	-3.85360	-0.93390	3.30410
C	-2.61930	-0.26970	3.38500
C	-2.37510	0.90110	2.64000
C	-3.34810	1.28490	1.69350
C	-4.57510	0.60920	1.60100
C	-4.84250	-0.48940	2.42530
C	-1.59310	2.02350	0.20730
C	-0.61820	1.68570	1.18970
C	0.64560	1.27860	0.79230
H	1.40860	1.00550	1.51770
C	0.94810	1.21490	-0.58100
C	-0.00620	1.55220	-1.53630
C	-1.29410	1.96010	-1.14360
H	-4.04940	-1.81020	3.91670
H	-5.79450	-1.00970	2.38190
H	1.94180	0.89670	-0.89160
H	0.23850	1.50080	-2.59560
H	-2.03860	2.21800	-1.89320
C	-1.65410	3.26710	2.71650
C	-1.24100	4.25330	3.60200
C	-1.81590	5.53430	3.53340
C	-2.78820	5.83010	2.58120
C	-3.20010	4.84920	1.66340
C	-2.62830	3.58820	1.73200
H	-0.48110	4.04630	4.36190
H	-1.49140	6.29880	4.23730
H	-3.23000	6.82360	2.53980
H	-3.95180	5.08030	0.91290
O	-5.43200	1.14030	0.65230
C	-6.67520	0.44030	0.41750
H	-7.12020	1.04010	-0.38710
H	-6.48180	-0.58240	0.08150
H	-7.30040	0.46540	1.31440
C	-1.13920	1.81760	2.63620
C	-0.05300	1.48150	3.66900
H	0.06600	0.38900	3.80050
H	0.91790	1.93670	3.37970
O	-1.55700	-0.74230	4.13050
C	-1.82080	-1.78390	5.10250
H	-0.84630	-1.87360	5.59980
H	-2.58630	-1.45860	5.81480
H	-2.09240	-2.71170	4.59370
O	-0.22150	2.10540	4.96550
C	-1.14790	1.54600	5.84400
C	-2.51160	1.83610	5.72930
C	-0.63040	0.79480	6.91430
C	-3.39530	1.34180	6.69160
H	-2.87660	2.43720	4.89430
C	-1.50300	0.31150	7.88170
H	0.44060	0.61120	6.97450
C	-2.88100	0.58340	7.75030
H	-4.45570	1.55500	6.60440
H	-1.14990	-0.26400	8.73400
O	-3.62940	0.00620	8.75890
C	-5.04720	0.29140	8.78880
H	-5.36750	-0.25380	9.68600
H	-5.21750	1.36600	8.90320
H	-5.53370	-0.10500	7.89330
C	-2.93880	2.43670	0.79260
H	-3.70540	2.67310	0.02760

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1_9_disubsti_triptycene/opt_b3_folded_opt.xyz
C      -4.61490      -0.74110      2.31470
C      -3.44650      -0.14860      2.82280
C      -2.86250       0.95870      2.18340
C      -3.42700      1.39490      0.96520
C      -4.58740      0.79380      0.45560
C      -5.19560     -0.26790      1.13840
C      -1.23870      2.03970      0.16730
C      -0.66730      1.63290      1.40630
C       0.63370      1.15540      1.44120
H       1.09650      0.82990      2.36940
C       1.37310      1.08750      0.24550
C       0.81110      1.49020     -0.96270
C      -0.50980      1.97130     -1.00900
H      -5.06900     -1.58390      2.83050
H      -6.10200     -0.73340      0.76310
H       2.39530      0.71390      0.27340
H       1.39200      1.43340     -1.88160
H      -0.94720      2.28080     -1.95550
C      -2.07810      3.25380      2.56090
C      -1.97510      4.18120      3.58730
C      -2.42670      5.49640      3.37680
C      -2.97320      5.87520      2.15320
C      -3.08200      4.94450      1.10510
C      -2.63510      3.64930      1.31350
H      -1.56350      3.90270      4.56000
H      -2.34710      6.22050      4.18560
H      -3.32070      6.89520      2.00180
H      -3.51180      5.24010      0.15150
O      -5.02480      1.34950     -0.73370
C      -6.20630      0.77640     -1.33930
H      -6.31440      1.39130     -2.24230
H      -6.03200     -0.27180     -1.59840
H      -7.06980      0.89750     -0.67910
C      -1.63300      1.78120      2.59820
C      -0.97160      1.36100      3.91500
H      -0.86950      0.25980      3.97780
H       0.00360      1.85850      4.06340
O      -2.76070     -0.66360      3.90820
C      -3.53040     -1.40020      4.89050
H      -2.79090     -1.54250      5.69150
H      -4.37150     -0.79840      5.24610
H      -3.85240     -2.35730      4.47430
O      -1.83350      1.85550      4.98470
C      -1.85470      1.17510      6.17600
C      -2.91730      1.58120      7.01280
C      -0.92550      0.20660      6.57840
C      -3.03360      0.99570      8.26740
H      -3.61500      2.33590      6.65840
C      -1.07240     -0.36530      7.84660
H      -0.11000     -0.09720      5.93170
C      -2.11720      0.01870      8.68830
H      -3.84490      1.29560      8.93070
H      -0.35690     -1.11810      8.17760
H      -2.22060     -0.43110      9.67150
C      -2.67630      2.52890      0.28680
H      -3.13170      2.82200     -0.68030
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1_9_disubsti_triptycene/opt_b4_folded_opt.xyz
C      -4.55130     -0.71910      2.46740
C      -3.37920     -0.09590      2.92490
C      -2.82300      0.99270      2.22990
C      -3.43180      1.39150      1.02120
C      -4.59840      0.76070      0.56240
C      -5.16910     -0.28980      1.29250
C      -1.28180      2.04110      0.12940
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C	-0.66090	1.66660	1.35440
C	0.64560	1.20300	1.35240
H	1.14700	0.90250	2.26860
C	1.34110	1.11640	0.13190
C	0.73090	1.48740	-1.06320
C	-0.59570	1.95440	-1.07130
H	-4.98760	-1.54880	3.01880
H	-6.07820	-0.78040	0.95620
H	2.36780	0.75350	0.12970
H	1.27870	1.41640	-2.00170
H	-1.07060	2.23910	-2.00780
C	-2.04420	3.30020	2.52590
C	-1.91180	4.24950	3.52840
C	-2.38500	5.55550	3.30740
C	-2.98150	5.90180	2.09770
C	-3.12000	4.94800	1.07400
C	-2.65200	3.66200	1.29210
H	-1.45950	3.99810	4.48860
H	-2.28200	6.29860	4.09650
H	-3.34560	6.91530	1.93790
H	-3.58850	5.21950	0.13100
O	-5.07690	1.27580	-0.62830
C	-6.27880	0.68330	-1.17340
H	-6.41910	1.27010	-2.09080
H	-6.11250	-0.37220	-1.40620
H	-7.11860	0.82510	-0.48720
C	-1.58510	1.83290	2.57600
C	-0.87130	1.44400	3.87320
H	-0.73280	0.34720	3.94280
H	0.08680	1.97890	4.00010
O	-2.66730	-0.53030	4.02970
C	-3.32280	-1.45600	4.93080
H	-2.57140	-1.56520	5.72470
H	-4.24360	-1.01590	5.32430
H	-3.50270	-2.41030	4.42900
O	-1.73300	1.91870	4.96180
C	-1.71270	1.27110	6.15120
C	-2.74020	1.70680	7.02800
C	-0.77400	0.29430	6.54070
C	-2.82430	1.15070	8.28890
C	-0.86960	-0.25480	7.81230
H	0.01200	-0.02750	5.86280
C	-1.89320	0.16190	8.68280
H	-3.60620	1.45980	8.99330
H	-0.15360	-1.01440	8.14960
N	-1.99470	-0.43150	10.01550
O	-1.18100	-1.29270	10.31990
O	-2.89000	-0.04020	10.75030
H	-3.44270	2.46530	6.68200
C	-2.71900	2.51860	0.29190
H	-3.21300	2.78620	-0.66390

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1_9_disubsti_triptycene/opt_b5_folded_opt.xyz			
C	-4.56060	-0.70340	2.53190
C	-3.40350	-0.05140	2.98520
C	-2.83550	1.00370	2.25100
C	-3.42740	1.35300	1.01850
C	-4.57900	0.69230	0.56290
C	-5.15490	-0.33220	1.32520
C	-1.27580	2.00770	0.13460
C	-0.66720	1.68150	1.37860
C	0.64790	1.24200	1.40790
H	1.14460	0.97990	2.33790
C	1.36190	1.13050	0.20040
C	0.76200	1.45310	-1.01400
C	-0.57170	1.89620	-1.05390
H	-5.01020	-1.50630	3.11160

H	-6.05320	-0.84490	0.99190
H	2.39500	0.78720	0.22320
H	1.32430	1.36310	-1.94240
H	-1.03900	2.14460	-2.00470
C	-2.10080	3.32350	2.48870
C	-2.03350	4.29220	3.47810
C	-2.52670	5.58270	3.21200
C	-3.08170	5.89200	1.97310
C	-3.16810	4.91290	0.96740
C	-2.68380	3.64190	1.23120
H	-1.64150	4.06510	4.47200
H	-2.48240	6.33810	3.99550
H	-3.46140	6.89370	1.77900
H	-3.61480	5.15280	0.00580
O	-5.03370	1.14750	-0.66000
C	-6.25870	0.57090	-1.17050
H	-6.38830	1.12270	-2.11100
H	-6.12650	-0.49810	-1.35930
H	-7.08820	0.76820	-0.48530
C	-1.61240	1.86930	2.58300
C	-0.89070	1.51810	3.88500
H	-0.71170	0.42770	3.95840
H	0.03930	2.09990	4.01760
O	-2.72470	-0.41130	4.14100
C	-3.33990	-1.40960	4.99180
H	-2.60150	-1.51050	5.79680
H	-4.29450	-1.03810	5.37720
H	-3.45500	-2.35400	4.45210
O	-1.77480	1.96180	4.98100
C	-1.73440	1.31240	6.15080
C	-2.75310	1.68750	7.07570
C	-0.77450	0.33330	6.52090
C	-2.83340	1.05200	8.31940
C	-0.84870	-0.26960	7.75820
H	0.01660	0.05890	5.82330
C	-1.88890	0.07790	8.65640
H	-3.63920	1.32030	9.02580
H	-0.11250	-1.02500	8.06730
N	-1.96340	-0.59270	9.96000
O	-1.13020	-1.45370	10.19500
O	-2.85260	-0.25250	10.72130
N	-3.73150	2.73420	6.74120
O	-3.41890	3.55010	5.89780
O	-4.78470	2.71510	7.35670
C	-2.72060	2.46800	0.26440
H	-3.20680	2.70030	-0.70460

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Gellman/opt_b1_folded_opt.xyz

C	-0.33000	1.73870	0.71830
C	0.73580	1.85040	0.16280
C	2.01890	1.95310	-0.47440
O	2.73000	2.93970	-0.48140
C	1.62050	-0.45410	-1.14720
H	0.54090	-0.11530	-1.23300
C	1.92060	-1.31090	-2.38490
O	2.95910	-1.81490	-2.73890
O	0.73350	-1.50240	-3.03960
C	0.78220	-2.23800	-4.29460
H	1.43690	-3.11100	-4.20320
H	-0.26390	-2.51880	-4.45180
H	1.14370	-1.55420	-5.07120
C	1.79080	-1.33680	0.11260
H	2.30490	-2.29260	-0.13030
H	2.48080	-0.83770	0.82850
N	2.47160	0.75700	-1.09040
C	0.46660	-1.62630	0.76500
C	0.27020	-1.31920	2.11910

C	-0.57900	-2.19980	0.02420
C	-0.96130	-1.58340	2.72530
H	1.06930	-0.86260	2.70150
C	-1.80870	-2.45560	0.63420
H	-0.43380	-2.44350	-1.02910
C	-2.00340	-2.14850	1.98500
H	-1.11020	-1.33530	3.77600
H	-2.61790	-2.89750	0.05540
H	-2.96290	-2.34600	2.45830
C	3.79390	0.77580	-1.73660
H	4.26320	-0.24220	-1.72890
H	4.48340	1.45460	-1.16390
C	3.69910	1.26520	-3.17600
O	2.75550	1.30120	-3.92620
O	4.95630	1.68180	-3.54450
C	5.11710	2.16800	-4.90420
H	4.29890	2.84890	-5.16350
H	6.08130	2.68580	-4.86130
H	5.14180	1.30880	-5.58070
C	-1.58790	1.50380	1.34740
C	-2.68730	1.04130	0.54160
C	-2.86080	1.37050	3.30070
C	-3.87160	0.73870	1.16220
H	-2.55280	0.93170	-0.53310
C	-3.99110	0.88910	2.57820
C	-2.94050	1.53600	4.72380
H	-4.72960	0.37840	0.59300
C	-5.18610	0.57420	3.29520
C	-4.10370	1.22290	5.37660
H	-2.06060	1.91260	5.24930
C	-5.23720	0.73630	4.65660
H	-6.04840	0.20670	2.73980
H	-4.18500	1.34120	6.45770
H	-6.14360	0.49900	5.21340
N	-1.66170	1.67590	2.67160

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Gellman/opt_b2_folded_opt.xyz

C	-0.43770	1.69880	0.88030
C	0.61900	1.81070	0.30640
C	1.89040	1.91850	-0.35100
O	2.62700	2.88620	-0.30970
C	1.43610	-0.44400	-1.14080
H	0.35630	-0.09510	-1.12980
C	1.64710	-1.19910	-2.46100
O	2.64980	-1.70480	-2.90440
O	0.42640	-1.28880	-3.07230
C	0.38960	-1.90450	-4.39080
H	1.03120	-2.79140	-4.42010
H	-0.66890	-2.15450	-4.51300
H	0.72010	-1.15480	-5.11890
C	1.68050	-1.42350	0.03210
H	2.07030	-2.39960	-0.33230
H	2.49680	-1.03700	0.68080
N	2.30120	0.75390	-1.04930
C	0.42540	-1.65050	0.82960
C	0.41040	-1.39160	2.20760
C	-0.73680	-2.12160	0.19800
C	-0.75750	-1.60280	2.94640
H	1.30490	-1.02250	2.70610
C	-1.90140	-2.32490	0.94080
H	-0.73190	-2.32970	-0.87220
C	-1.91510	-2.06710	2.31580
H	-0.76520	-1.39900	4.01700
H	-2.80270	-2.68680	0.44780
H	-2.82520	-2.22550	2.89120
C	-1.66940	1.47040	1.54540
C	-1.75210	1.57620	2.91960

C	-2.80150	1.06190	0.76120
C	-2.98010	1.24320	3.56680
H	-0.90260	1.89390	3.53030
C	-3.98970	0.74620	1.36480
H	-2.68900	1.00140	-0.32340
C	-4.10180	0.82160	2.78900
H	-4.86440	0.42980	0.79140
C	-4.21750	0.98560	5.51530
C	-5.35640	0.55790	4.72660
H	-4.29540	1.04120	6.60830
H	-6.29820	0.28940	5.22160
N	-3.06280	1.31760	4.95610
N	-5.30310	0.47600	3.40450
C	3.60700	0.78420	-1.72870
H	4.04860	-0.24320	-1.80350
H	4.32880	1.40600	-1.13210
C	3.48760	1.37200	-3.12920
O	2.52410	1.49570	-3.84350
O	4.74970	1.76220	-3.51030
C	4.89030	2.32970	-4.84050
H	4.09320	3.05730	-5.02950
H	5.87560	2.80580	-4.79520
H	4.86020	1.51610	-5.57090

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Gellman/opt_c1_folded_opt.xyz

C	-1.28750	1.80920	-0.95950
C	-0.50900	2.15560	-1.81610
C	0.43280	2.59760	-2.80230
O	0.43640	3.69000	-3.34180
C	1.60840	0.37010	-2.49780
H	0.59120	-0.07450	-2.27930
C	2.34060	-0.55560	-3.47690
O	3.20530	-0.29330	-4.27410
O	1.85910	-1.82860	-3.28660
C	2.42090	-2.87830	-4.12120
H	3.51120	-2.78590	-4.16980
H	2.10770	-3.79180	-3.60510
H	1.97890	-2.80070	-5.11950
C	2.42500	0.46920	-1.18530
H	3.40640	-0.04270	-1.27560
H	2.69160	1.52960	-0.98500
C	1.64800	-0.11550	-0.03840
C	1.18430	0.67740	0.98490
C	1.37610	-1.52090	-0.03910
C	0.41680	0.11020	2.04990
H	1.37870	1.74900	0.99940
C	0.65440	-2.08730	0.97800
H	1.74820	-2.12500	-0.86940
C	0.15230	-1.28360	2.05110
C	-0.11020	0.92160	3.10450
H	0.44780	-3.15690	0.98670
C	-0.62180	-1.84700	3.11360
C	-0.85870	0.35640	4.10590
H	0.08880	1.99200	3.08920
C	-1.11470	-1.04610	4.11310
H	-0.81080	-2.91910	3.11090
H	-1.26940	0.96710	4.90840
H	-1.70680	-1.46500	4.92470
C	-2.15890	1.37120	0.06920
C	-2.72850	2.30330	0.95580
C	-2.42110	-0.00350	0.22160
C	-3.54920	1.85590	1.99270
H	-2.52490	3.36680	0.83170
C	-3.24650	-0.43670	1.26040
H	-1.97030	-0.72360	-0.46110
C	-3.80670	0.48940	2.14680
H	-3.98800	2.57390	2.68440

H	-3.44420	-1.50040	1.38720
H	-4.44170	0.14470	2.96200
N	1.43020	1.66970	-3.16590
H	2.18920	1.98940	-3.77720

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Gellman/opt_c2_folded_opt.xyz

C	-0.26670	2.99600	0.13810
C	0.65350	3.43890	-0.50770
C	1.75670	4.00380	-1.22820
O	2.12450	5.16370	-1.15740
C	2.18930	1.68920	-2.17130
H	1.07400	1.51480	-2.10110
C	2.67270	1.21360	-3.54720
O	3.63800	1.56380	-4.17790
O	1.79960	0.24940	-3.98970
C	2.08850	-0.36170	-5.27700
H	2.92260	-1.05890	-5.15540
H	1.15150	-0.87680	-5.51410
H	2.32950	0.40940	-6.01730
C	2.91290	0.87710	-1.06880
H	3.77450	0.30940	-1.47990
H	3.37520	1.57190	-0.33400
C	-1.32900	2.45850	0.90760
C	-1.95190	3.25120	1.89020
C	-1.74600	1.13030	0.70160
C	-2.97840	2.70910	2.66530
H	-1.62970	4.28180	2.04220
C	-2.76900	0.59850	1.48860
H	-1.26180	0.51770	-0.06080
C	-3.38420	1.38450	2.46840
H	-3.46280	3.31970	3.42670
H	-3.08300	-0.43620	1.34410
H	-4.18120	0.96330	3.08080
N	2.45690	3.13400	-2.08760
H	3.31860	3.47690	-2.52590
C	1.95580	-0.06090	-0.38850
C	1.63560	0.11100	0.96530
C	1.36150	-1.10460	-1.11540
C	0.72180	-0.74400	1.58370
H	2.08940	0.91900	1.53810
C	0.44940	-1.95870	-0.49820
H	1.60480	-1.23840	-2.17200
C	0.11600	-1.77950	0.85460
H	0.46430	-0.59500	2.63260
H	-0.00330	-2.77180	-1.06530
C	-0.88200	-2.65850	1.49900
C	-0.59920	-3.26970	2.73090
C	-2.12580	-2.87800	0.88380
C	-1.55440	-4.08550	3.34180
H	0.36870	-3.11360	3.20530
C	-3.07740	-3.69230	1.50170
H	-2.34780	-2.41290	-0.07540
C	-2.79490	-4.29600	2.73120
H	-1.33080	-4.55980	4.29660
H	-4.04150	-3.85860	1.02330
H	-3.53780	-4.93050	3.21070

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Gellman/opt_a1_folded_opt.xyz

C	-3.74640	-3.33630	-2.78070
C	-2.78880	-2.94630	-1.87920
C	-2.88140	-1.67350	-1.23060
C	-3.98040	-0.82380	-1.52400
C	-4.96520	-1.25880	-2.46650
C	-4.84790	-2.48090	-3.07900
H	-1.02790	-1.88530	-0.09650
H	-3.68440	-4.30190	-3.28070

H	-1.94740	-3.59460	-1.64150
C	-1.88070	-1.23070	-0.31480
C	-4.07070	0.45300	-0.88320
H	-5.80470	-0.60040	-2.68590
H	-5.59210	-2.81930	-3.79900
C	-3.09910	0.86740	-0.01110
C	-1.98020	0.01650	0.26960
H	-4.92260	1.09300	-1.11170
H	-3.14790	1.84350	0.47250
C	-0.95030	0.49490	1.11760
C	-0.02650	0.90110	1.78250
C	1.00300	1.42400	2.62230
O	0.81620	2.23710	3.51370
N	2.33290	0.97980	2.38950
C	2.79910	0.08430	1.30900
H	3.82050	-0.33300	1.61440
C	3.36470	1.43090	3.34710
H	4.19190	1.96320	2.82350
H	2.90820	2.17080	4.06820
C	3.93820	0.24240	4.10730
O	4.51040	-0.72220	3.65240
O	3.74950	0.44150	5.44410
C	4.20410	-0.61020	6.34170
H	4.13090	-0.13150	7.32410
H	3.52310	-1.46310	6.25180
H	5.23050	-0.90060	6.09730
C	1.92440	-1.16920	1.20800
O	1.23250	-1.69880	2.03930
O	2.10710	-1.73870	-0.03880
C	1.37210	-2.96430	-0.29390
H	0.29350	-2.73860	-0.28920
H	1.72920	-3.25850	-1.28550
H	1.61420	-3.71120	0.46960
C	3.01020	0.81500	-0.03310
H	3.73360	1.64300	0.12980
H	3.52440	0.10350	-0.72230
C	1.77450	1.34760	-0.70260
C	1.08060	0.57660	-1.60750
C	1.33950	2.68020	-0.41710
C	-0.08670	1.08550	-2.25350
H	1.40300	-0.44190	-1.83000
C	0.22100	3.18950	-1.02500
H	1.90360	3.27670	0.29870
C	-0.52610	2.40160	-1.95690
C	-0.83540	0.29110	-3.17990
H	-0.12000	4.20050	-0.80450
C	-1.70890	2.90120	-2.58820
C	-1.96940	0.79330	-3.76580
H	-0.49200	-0.71810	-3.39940
C	-2.41170	2.11570	-3.46660
H	-2.03790	3.91220	-2.35420
H	-2.55280	0.19060	-4.46030
H	-3.31550	2.48470	-3.94730

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Elguero_Cornago/opt_a1_folded_opt.xyz

C	0.34690	-3.50620	-0.67300
C	0.61850	-2.27770	0.01650
C	1.07430	-1.38370	-0.95500
N	1.06340	-2.08360	-2.16920
H	1.33530	-1.74720	-3.07950
H	0.49830	-2.09740	1.06270
N	0.62560	-3.36450	-2.00600
C	-0.16030	-4.76470	-0.08840
H	0.52780	-5.15270	0.67740
H	-1.14030	-4.61440	0.38860
H	-0.28220	-5.55180	-0.84990
C	1.50040	0.01210	-0.85740

C	0.56080	1.05930	-0.80170
C	2.87550	0.29720	-0.80520
C	1.01910	2.38340	-0.69560
C	3.31660	1.61570	-0.70170
H	3.59550	-0.52110	-0.83730
C	2.38480	2.65930	-0.64620
H	0.29580	3.19710	-0.63860
H	4.38220	1.83300	-0.65920
H	2.72830	3.68990	-0.56060
C	-0.92030	0.79760	-0.85450
H	-1.34970	1.30180	-1.74710
H	-1.13960	-0.28440	-1.01130
C	-1.60700	1.24740	0.40840
C	-2.64000	2.19360	0.35570
C	-1.21830	0.70830	1.64520
C	-3.27940	2.59480	1.53270
H	-2.94820	2.61700	-0.59730
C	-1.85920	1.11480	2.81650
H	-0.41210	-0.02330	1.68660
C	-2.89150	2.05830	2.76340
H	-4.08250	3.32860	1.48820
H	-1.55440	0.69650	3.77440
H	-3.38980	2.37260	3.67760

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Elguero_Cornago/opt_a2_folded_opt.xyz

C	0.66480	-3.48630	-0.92780
C	0.95730	-2.30390	-0.17710
C	1.21500	-1.31270	-1.12560
N	1.07290	-1.92850	-2.38470
H	1.19800	-1.50280	-3.29450
H	0.98010	-2.20670	0.89120
N	0.74370	-3.23250	-2.27220
C	0.32300	-4.83310	-0.39490
C	1.56840	0.09720	-0.97770
C	0.57780	1.09190	-0.87260
C	2.92920	0.44640	-0.92210
C	0.97240	2.43130	-0.71190
C	3.30530	1.77910	-0.76570
H	3.68860	-0.33320	-0.99400
C	2.32300	2.77190	-0.65910
H	0.21050	3.20530	-0.61310
H	4.35960	2.04780	-0.72080
H	2.61630	3.81390	-0.53030
C	-0.88960	0.76120	-0.92550
H	-1.36360	1.31560	-1.76480
H	-1.06460	-0.31110	-1.16660
C	-1.56290	1.08530	0.38360
C	-2.45520	2.16260	0.47530
C	-1.29450	0.30250	1.51710
C	-3.07420	2.45290	1.69470
H	-2.67040	2.77340	-0.39840
C	-1.91510	0.59890	2.73210
H	-0.60140	-0.53430	1.44800
C	-2.80580	1.67410	2.82390
H	-3.76840	3.28910	1.76340
H	-1.70550	-0.00990	3.61070
H	-3.28870	1.90210	3.77180
F	-0.81560	-5.36010	-0.87050
F	0.15950	-4.86810	0.93900
F	1.24780	-5.77760	-0.62910

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Elguero_Cornago/opt_a3_folded_opt.xyz

C	1.07840	-2.10340	-1.15710
C	0.97990	-1.13450	-0.10190
C	1.52270	0.04620	-0.61060
N	1.91870	-0.23930	-1.92660

H	2.36430	0.38220	-2.58470
H	0.56660	-1.29340	0.87150
N	1.65540	-1.52910	-2.26140
C	1.70120	1.36560	-0.00620
C	0.66860	2.32220	-0.02050
C	2.92910	1.66300	0.60970
C	0.88780	3.57140	0.58490
C	3.13310	2.90650	1.20560
H	3.71860	0.91080	0.62490
C	2.10860	3.86110	1.19240
H	0.08730	4.31190	0.58870
H	4.08420	3.13350	1.68390
H	2.26510	4.83200	1.66170
C	-0.65930	2.04210	-0.67170
H	-0.78270	2.71000	-1.55170
H	-0.69990	1.01160	-1.09440
C	-1.79510	2.21170	0.30320
C	-2.72270	3.25020	0.14080
C	-1.92460	1.32250	1.38190
C	-3.77230	3.39670	1.05260
H	-2.63060	3.94260	-0.69280
C	-2.97410	1.47570	2.28950
H	-1.20270	0.51730	1.50970
C	-3.90000	2.51260	2.12750
H	-4.49200	4.20340	0.92350
H	-3.07240	0.78580	3.12630
H	-4.71690	2.62920	2.83620
C	0.64830	-3.50160	-1.12270
C	0.22400	-4.14400	-2.29850
C	0.65980	-4.20800	0.09230
C	-0.18900	-5.47730	-2.25420
H	0.22470	-3.59850	-3.24320
C	0.24470	-5.54080	0.12730
H	0.99930	-3.71890	1.00370
C	-0.18110	-6.17700	-1.04340
H	-0.51690	-5.97260	-3.16680
H	0.25530	-6.08650	1.06930
H	-0.50370	-7.21570	-1.01220

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Cozzi_aromatic/opt_a10_folded_opt.xyz

C	-0.09900	-3.02380	1.71350
C	0.98810	-3.20430	0.89660
C	1.17820	-2.36470	-0.24400
C	0.27370	-1.29610	-0.49690
C	-0.74860	-1.01510	0.46860
C	-0.99130	-1.94410	1.47540
H	2.96730	-3.39450	-0.92780
H	-0.29760	-3.68660	2.55950
H	1.70460	-4.00260	1.08810
C	2.25570	-2.60250	-1.15770
C	0.39030	-0.58220	-1.73350
C	1.41590	-0.84570	-2.60350
C	2.37820	-1.85340	-2.29900
H	-0.36570	0.16560	-1.97860
H	1.50950	-0.29650	-3.53910
H	3.19850	-2.02270	-2.99610
C	-1.57160	0.21970	0.45800
C	-1.07340	1.50210	0.16850
C	-2.92980	0.09590	0.84180
C	-1.96620	2.59340	0.11060
C	-3.80920	1.17240	0.75890
C	-3.32320	2.42740	0.36820
H	-1.57650	3.58550	-0.12770
H	-4.86310	1.03750	1.01360
H	-4.00490	3.27470	0.29340
C	-3.38060	-1.19380	1.44150
C	-2.23530	-1.83390	2.28280

C	0.36980	1.77690	-0.01270
C	0.82320	2.48410	-1.13840
C	1.29010	1.34250	0.95530
C	2.18800	2.72870	-1.30460
H	0.11390	2.82960	-1.88830
C	2.65330	1.59060	0.78150
H	0.94090	0.80400	1.83640
C	3.10470	2.27910	-0.34880
H	2.53870	3.26910	-2.18240
H	3.36590	1.24320	1.52870
O	-4.46280	-1.69740	1.31160
O	-2.37990	-2.17580	3.42540
H	4.16860	2.46540	-0.48430

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Cozzi_aromatic/opt_a1_folded_opt.xyz

C	0.08240	-2.93510	1.54390
C	1.16100	-3.05800	0.70660
C	1.27920	-2.21860	-0.44530
C	0.31000	-1.20730	-0.67900
C	-0.69350	-0.96550	0.32270
C	-0.87330	-1.90180	1.33040
H	3.10920	-3.14650	-1.16610
H	-0.04730	-3.60440	2.39470
H	1.92790	-3.81080	0.88840
C	2.34360	-2.40260	-1.38460
C	0.34440	-0.50640	-1.92640
C	1.35940	-0.71960	-2.82400
C	2.39070	-1.66040	-2.53680
H	-0.46220	0.19010	-2.15800
H	1.39090	-0.18010	-3.76990
H	3.20230	-1.78570	-3.25290
C	-1.54710	0.24200	0.33450
C	-1.07490	1.53300	0.01960
C	-2.88280	0.10090	0.77370
C	-1.97670	2.61020	-0.03460
C	-3.77380	1.17300	0.70240
C	-3.32460	2.42410	0.26760
H	-1.61270	3.60460	-0.29720
H	-4.81580	1.04010	0.99550
H	-4.02140	3.25860	0.19580
C	-3.30940	-1.19370	1.42560
H	-4.16890	-1.04060	2.12080
C	-2.12100	-1.86810	2.18110
H	-2.42480	-2.89670	2.48820
C	0.36500	1.81270	-0.18100
C	0.80420	2.51550	-1.31790
C	1.29620	1.37380	0.77840
C	2.16370	2.73540	-1.52190
H	0.08120	2.87080	-2.05230
C	2.65730	1.58650	0.58120
H	0.94760	0.84600	1.67100
C	3.08460	2.25880	-0.57540
H	2.52290	3.26610	-2.41000
H	3.39490	1.23240	1.30990
O	-3.83820	-2.12830	0.48410
H	-3.22590	-2.23970	-0.27840
O	-1.79170	-1.10040	3.34840
H	-2.49330	-1.18920	4.02510
N	4.52760	2.46210	-0.80470
O	4.86420	3.03270	-1.83150
O	5.30330	2.04660	0.04170

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Cozzi_aromatic/opt_a2_folded_opt.xyz

C	0.16240	-2.89800	1.44070
C	1.25980	-3.04460	0.63140
C	1.45050	-2.17500	-0.48730

C	0.53630	-1.11190	-0.71490
C	-0.48800	-0.85940	0.26150
C	-0.73870	-1.81720	1.23440
H	3.25280	-3.16820	-1.18920
H	-0.02750	-3.59060	2.26180
H	1.98370	-3.83930	0.80860
C	2.53150	-2.38070	-1.40330
C	0.64200	-0.37270	-1.93630
C	1.67160	-0.60520	-2.81170
C	2.64690	-1.60540	-2.52840
H	-0.12280	0.37060	-2.16490
H	1.75790	-0.03560	-3.73580
H	3.47100	-1.74780	-3.22630
C	-1.30320	0.37550	0.27900
C	-0.78410	1.66160	0.02710
C	-2.65980	0.25570	0.66200
C	-1.65640	2.76570	-0.00680
C	-3.51810	1.35310	0.60680
C	-3.01740	2.60840	0.24440
H	-1.25600	3.75850	-0.21670
H	-4.57350	1.23700	0.85570
H	-3.68740	3.46580	0.18710
C	-3.14820	-1.05840	1.23210
H	-4.05000	-0.92900	1.87820
C	-2.01150	-1.75120	2.04740
H	-2.34940	-2.76360	2.37740
C	0.66360	1.91560	-0.14290
C	1.12810	2.65540	-1.24420
C	1.57690	1.42190	0.80640
C	2.49380	2.88340	-1.42020
H	0.41960	3.04300	-1.97680
C	2.94630	1.63700	0.65030
H	1.21390	0.85390	1.66450
C	3.37240	2.36040	-0.46740
H	2.85920	3.44770	-2.27640
H	3.65770	1.24540	1.37610
O	-3.61410	-1.94580	0.21790
H	-2.93090	-2.06660	-0.48040
O	-1.83010	-1.06130	3.28370
H	-1.43030	-0.17630	3.13250
F	4.68100	2.56460	-0.63130

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Cozzi_aromatic/opt_a3_folded_opt.xyz

C	-0.03470	-3.17950	1.60820
C	1.07140	-3.24270	0.80020
C	1.19150	-2.36870	-0.32490
C	0.19420	-1.38500	-0.56040
C	-0.84890	-1.20970	0.41330
C	-1.02090	-2.17740	1.39340
H	3.06920	-3.21690	-1.01840
H	-0.16810	-3.87830	2.43490
H	1.85760	-3.97390	0.98370
C	2.28660	-2.49270	-1.23900
C	0.24200	-0.64730	-1.78640
C	1.28810	-0.80150	-2.65960
C	2.34010	-1.71820	-2.36930
H	-0.57880	0.03250	-2.01860
H	1.32940	-0.23160	-3.58610
H	3.17340	-1.79900	-3.06550
C	-1.76450	-0.04700	0.41900
C	-1.35390	1.27630	0.15740
C	-3.10730	-0.27780	0.79970
C	-2.31830	2.30130	0.11000
C	-4.05590	0.74160	0.73160
C	-3.66180	2.03130	0.35800
H	-2.00220	3.32220	-0.10720
H	-5.09790	0.53890	0.97890

H	-4.40190	2.82790	0.29050
C	-3.48440	-1.62280	1.38210
H	-4.39560	-1.56410	2.02490
C	-2.29510	-2.20910	2.20590
H	-2.54740	-3.24180	2.54800
C	0.06570	1.64910	-0.01090
C	0.47580	2.41840	-1.10780
C	1.01960	1.23200	0.94260
C	1.82070	2.75520	-1.28610
H	-0.25730	2.74950	-1.84420
C	2.35930	1.55440	0.78870
H	0.69940	0.64080	1.80240
C	2.74890	2.31080	-0.33800
H	2.12130	3.34300	-2.14580
H	3.11250	1.23410	1.50530
O	-3.87040	-2.55700	0.37560
H	-3.17780	-2.62400	-0.32060
O	-2.17380	-1.49110	3.43380
H	-1.84360	-0.57950	3.27150
O	4.10480	2.54610	-0.37210
C	4.63340	3.30070	-1.48850
H	5.70670	3.32020	-1.25760
H	4.44440	2.77300	-2.42750
H	4.21630	4.31160	-1.49520

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Cozzi_aromatic/opt_a4_folded_opt.xyz

C	0.03170	-2.98280	1.60930
C	1.09200	-3.12650	0.75280
C	1.18780	-2.30980	-0.41740
C	0.22040	-1.29600	-0.64790
C	-0.76730	-1.03510	0.36540
C	-0.92830	-1.95410	1.39250
H	2.98850	-3.27110	-1.16420
H	-0.08210	-3.63260	2.47700
H	1.85980	-3.87740	0.93320
C	2.22760	-2.52240	-1.37800
C	0.23830	-0.61270	-1.90550
C	1.23130	-0.85010	-2.82150
C	2.25590	-1.80050	-2.54380
H	-0.56070	0.09620	-2.12700
H	1.25090	-0.31950	-3.77180
H	3.04720	-1.94880	-3.27660
C	-1.63260	0.16460	0.35990
C	-1.17950	1.45490	0.01310
C	-2.96180	0.01600	0.81680
C	-2.10070	2.51600	-0.05460
C	-3.87050	1.07170	0.73100
C	-3.44280	2.31850	0.26390
H	-1.75180	3.50870	-0.34140
H	-4.90640	0.93020	1.03660
H	-4.15150	3.14110	0.18020
C	-3.36670	-1.26880	1.50070
H	-4.22370	-1.11300	2.19750
C	-2.16420	-1.91340	2.25870
H	-2.45490	-2.93750	2.59320
C	0.25070	1.75660	-0.21260
C	0.66630	2.44920	-1.35990
C	1.20650	1.35630	0.73770
C	2.02080	2.71090	-1.57180
H	-0.06750	2.77160	-2.09700
C	2.55800	1.61820	0.52550
H	0.88580	0.82830	1.63810
C	2.97690	2.29090	-0.63510
H	2.33290	3.23870	-2.47000
H	3.29220	1.29370	1.26040
O	-3.88970	-2.23220	0.58290
H	-3.28370	-2.34340	-0.18470

O	-1.82430	-1.12750	3.41150
H	-2.56900	-1.10920	4.04510
C	4.43160	2.54580	-0.86190
H	4.62220	3.16760	-1.74550
H	4.88940	3.05700	-0.00330
H	4.97690	1.60150	-1.00680

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Cozzi_aromatic/opt_a5_folded_opt.xyz

C	0.16410	-2.90350	1.43640
C	1.25300	-3.06090	0.61780
C	1.44140	-2.19440	-0.50370
C	0.53650	-1.12160	-0.72370
C	-0.48120	-0.86230	0.25800
C	-0.73080	-1.81680	1.23450
H	3.22280	-3.21170	-1.22360
H	-0.02410	-3.59250	2.26060
H	1.97160	-3.86130	0.78980
C	2.51040	-2.41450	-1.43040
C	0.64320	-0.38100	-1.94410
C	1.66170	-0.62620	-2.82910
C	2.62480	-1.64090	-2.55690
H	-0.11100	0.37580	-2.16450
H	1.74840	-0.05450	-3.75170
H	3.43830	-1.79580	-3.26400
C	-1.29590	0.37330	0.27350
C	-0.77830	1.65810	0.01480
C	-2.65220	0.25430	0.65850
C	-1.65250	2.76060	-0.02760
C	-3.51210	1.35010	0.59610
C	-3.01330	2.60350	0.22420
H	-1.25230	3.75190	-0.24540
H	-4.56690	1.23430	0.84670
H	-3.68460	3.45910	0.16010
C	-3.13820	-1.05540	1.24020
H	-4.03730	-0.92160	1.88880
C	-1.99760	-1.74170	2.05570
H	-2.33460	-2.74980	2.39870
C	0.67050	1.91670	-0.14930
C	1.14080	2.65240	-1.24960
C	1.58020	1.43960	0.80870
C	2.50960	2.88440	-1.40040
H	0.44060	3.02930	-1.99290
C	2.94740	1.67550	0.65100
H	1.21990	0.87340	1.66670
C	3.41480	2.39400	-0.45390
H	2.87240	3.44640	-2.25930
H	3.65070	1.29390	1.38980
O	-3.60770	-1.95120	0.23450
H	-2.92780	-2.07500	-0.46630
O	-1.80760	-1.03840	3.28330
H	-1.40210	-0.15790	3.11980
H	4.48150	2.57050	-0.57740

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Cozzi_aromatic/opt_a6_folded_opt.xyz

C	-0.20390	-3.07730	1.85640
C	0.87780	-3.23120	1.02570
C	1.01090	-2.41830	-0.14130
C	0.04960	-1.40510	-0.41210
C	-0.96090	-1.13640	0.56820
C	-1.14470	-2.04300	1.60700
H	2.84790	-3.36790	-0.81810
H	-0.35860	-3.72580	2.72280
H	1.63380	-3.99040	1.22810
C	2.08870	-2.62500	-1.06280
C	0.10350	-0.73340	-1.67680
C	1.12940	-0.97000	-2.55370

C	2.15440	-1.90800	-2.22880
H	-0.70260	-0.04650	-1.93820
H	1.17550	-0.45610	-3.51350
H	2.97560	-2.05200	-2.93160
C	-1.82230	0.07170	0.54940
C	-1.37030	1.35960	0.21060
C	-3.16290	-0.07840	0.97910
C	-2.28980	2.42730	0.15880
C	-4.07200	0.97460	0.90170
C	-3.63260	2.23250	0.46870
H	-1.93650	3.42390	-0.11630
H	-5.11430	0.81830	1.19330
H	-4.33850	3.06100	0.39960
C	-3.56010	-1.36830	1.61760
C	-2.37420	-1.95460	2.44190
C	0.05910	1.65770	-0.03490
C	0.45040	2.33570	-1.20390
C	1.02590	1.26180	0.90650
C	1.79910	2.57260	-1.45620
H	-0.30040	2.65890	-1.92560
C	2.37730	1.49130	0.66070
H	0.71830	0.75690	1.82500
C	2.75640	2.13660	-0.52670
H	2.12160	3.08520	-2.36930
H	3.14330	1.17060	1.37610
O	-4.63010	-1.90350	1.52640
O	-2.47880	-2.27420	3.59470
N	4.19030	2.35560	-0.80790
O	4.48270	2.89970	-1.86110
O	4.99610	1.97590	0.02610

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Cozzi_aromatic/opt_a7_folded_opt.xyz

C	-0.08660	-2.97110	1.79610
C	1.00390	-3.16330	0.98610
C	1.18880	-2.35290	-0.17610
C	0.27330	-1.30180	-0.46040
C	-0.75070	-1.00190	0.49730
C	-0.98670	-1.90470	1.52910
H	2.99420	-3.37730	-0.82530
H	-0.28130	-3.61370	2.65840
H	1.72710	-3.95000	1.20010
C	2.27270	-2.60160	-1.07950
C	0.38210	-0.62380	-1.71790
C	1.41380	-0.89820	-2.57710
C	2.38970	-1.88270	-2.24040
H	-0.38590	0.10280	-1.98710
H	1.50210	-0.37700	-3.52940
H	3.21590	-2.05880	-2.92910
C	-1.57890	0.22860	0.45610
C	-1.08560	1.50540	0.13330
C	-2.93530	0.11030	0.84690
C	-1.98130	2.59280	0.05290
C	-3.81810	1.18200	0.74090
C	-3.33690	2.42880	0.31910
H	-1.59610	3.58050	-0.20920
H	-4.87110	1.05030	1.00170
H	-4.02150	3.27220	0.22680
C	-3.38000	-1.16680	1.47840
C	-2.23110	-1.78020	2.33440
C	0.35510	1.77530	-0.06380
C	0.79940	2.45070	-1.21360
C	1.28120	1.36050	0.91050
C	2.15990	2.68920	-1.41320
H	0.08020	2.77960	-1.96420
C	2.64570	1.58790	0.73110
H	0.93140	0.84830	1.80920
C	3.05300	2.24360	-0.43450

H	2.51090	3.20370	-2.30630
H	3.36800	1.25850	1.47730
O	-4.45990	-1.67810	1.36110
O	-2.37260	-2.09290	3.48560
F	4.35660	2.45750	-0.62090

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Cozzi_aromatic/opt_a8_folded_opt.xyz

C	-0.27250	-3.32110	1.91830
C	0.83850	-3.40270	1.11800
C	0.95920	-2.56400	-0.03290
C	-0.04600	-1.59760	-0.31430
C	-1.10270	-1.40450	0.63580
C	-1.26480	-2.33880	1.65390
H	2.85680	-3.41040	-0.67450
H	-0.41560	-3.98860	2.77160
H	1.62910	-4.12150	1.33090
C	2.06960	-2.70140	-0.92760
C	0.01340	-0.89520	-1.56160
C	1.07420	-1.06290	-2.41310
C	2.13170	-1.95940	-2.07840
H	-0.81340	-0.23510	-1.82810
H	1.12400	-0.52150	-3.35630
H	2.97670	-2.05120	-2.75990
C	-2.03950	-0.25460	0.60020
C	-1.66150	1.06640	0.29820
C	-3.38320	-0.50200	0.97480
C	-2.65470	2.06670	0.22020
C	-4.36030	0.48410	0.87120
C	-3.99180	1.77520	0.46860
H	-2.35920	3.08870	-0.02520
H	-5.39880	0.25290	1.11880
H	-4.75020	2.55280	0.37860
C	-3.71440	-1.82200	1.58690
C	-2.52230	-2.34000	2.44700
C	-0.25230	1.46880	0.11830
C	0.14270	2.20350	-1.00750
C	0.70670	1.11440	1.09220
C	1.47980	2.56420	-1.19530
H	-0.59530	2.48810	-1.75830
C	2.03870	1.46140	0.92840
H	0.39560	0.55550	1.97730
C	2.41520	2.18040	-0.22740
H	1.77000	3.12470	-2.07680
H	2.79650	1.19030	1.66080
O	-4.74170	-2.42920	1.45270
O	-2.64640	-2.68200	3.59210
O	3.76440	2.44420	-0.26810
C	4.27910	3.17440	-1.40760
H	5.35040	3.22940	-1.17230
H	4.10900	2.61020	-2.32880
H	3.83630	4.17340	-1.45030

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Cozzi_aromatic/opt_a9_folded_opt.xyz

C	-0.24310	-3.10260	1.95900
C	0.82560	-3.27720	1.11720
C	0.93650	-2.49800	-0.07570
C	-0.03020	-1.49360	-0.35900
C	-1.03370	-1.20510	0.62420
C	-1.19660	-2.08360	1.69060
H	2.75610	-3.47330	-0.75850
H	-0.38100	-3.72290	2.84800
H	1.58770	-4.02620	1.32950
C	1.99700	-2.73370	-1.00960
C	0.00990	-0.85000	-1.63840
C	1.02170	-1.11090	-2.52530
C	2.04510	-2.04760	-2.19530

H	-0.79210	-0.15790	-1.90030
H	1.05770	-0.61330	-3.49320
H	2.85180	-2.21520	-2.90820
C	-1.91550	-0.01280	0.57300
C	-1.48920	1.27250	0.19330
C	-3.25230	-0.17660	1.01300
C	-2.43560	2.31600	0.10740
C	-4.18490	0.85130	0.90210
C	-3.77330	2.10270	0.42370
H	-2.10240	3.30950	-0.20020
H	-5.22170	0.68310	1.20240
H	-4.49720	2.91180	0.32680
C	-3.61930	-1.44900	1.70030
C	-2.41700	-1.98570	2.53420
C	-0.06950	1.59790	-0.06080
C	0.31220	2.25920	-1.23850
C	0.91000	1.25090	0.88570
C	1.65680	2.54000	-1.48300
H	-0.44040	2.54170	-1.97340
C	2.25240	1.53170	0.64050
H	0.61870	0.75120	1.81040
C	2.63800	2.17140	-0.54980
H	1.94300	3.04330	-2.40430
H	3.00560	1.24810	1.37370
O	-4.67940	-2.00970	1.63810
O	-2.50710	-2.26840	3.69850
C	4.08240	2.44400	-0.81380
H	4.24120	3.09620	-1.68220
H	4.56770	2.92960	0.04480
H	4.62810	1.50840	-1.00790

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Cozzi_aromatic/opt_b1_folded_opt.xyz

C	-0.50170	-4.30360	-0.45550
C	0.85760	-4.33780	-0.28970
C	1.59010	-3.13530	-0.03180
C	0.91820	-1.88140	0.04570
C	-0.51340	-1.89230	-0.09920
C	-1.19200	-3.06710	-0.35180
H	3.48840	-4.18830	0.09210
H	-1.07030	-5.21020	-0.65920
H	1.40500	-5.27820	-0.35150
C	3.00780	-3.21250	0.14740
C	1.72580	-0.70600	0.26050
H	-2.27690	-3.06600	-0.46730
C	3.09060	-0.81790	0.43470
C	3.73970	-2.07950	0.38600
H	3.69510	0.07430	0.60490
H	4.81830	-2.12410	0.53310
C	-1.35030	-0.67470	0.04000
C	-1.78890	0.01400	-1.10330
C	-1.75000	-0.25000	1.31960
C	-2.55690	1.16880	-0.97040
H	-1.50510	-0.34160	-2.09410
C	-2.51180	0.90620	1.46290
H	-1.43920	-0.81480	2.19910
C	-2.89120	1.62180	0.31530
H	-2.88590	1.73240	-1.84950
H	-2.80210	1.27130	2.45280
C	1.16750	0.66430	0.28270
C	0.99850	1.39120	-0.92110
C	0.86320	1.26240	1.51270
C	0.46430	2.68130	-0.87760
C	0.32750	2.54920	1.57410
H	1.03370	0.70680	2.43650
C	0.11550	3.22900	0.36640
H	0.30840	3.26780	-1.78000
H	0.07670	3.00230	2.52650

C	1.38930	0.79120	-2.23050
H	1.08400	-0.26320	-2.30940
H	0.95920	1.32320	-3.08850
H	2.48400	0.81010	-2.35290
O	-0.45760	4.47280	0.31180
H	-0.74940	4.79550	1.20290
N	-3.62010	2.89410	0.46700
O	-4.19390	3.34730	-0.50870
O	-3.59640	3.42790	1.56800

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Cozzi_aromatic/opt_b2_folded_opt.xyz

C	-0.56570	-4.07260	-0.77670
C	0.78750	-4.09050	-0.56370
C	1.47560	-2.89940	-0.16820
C	0.76600	-1.67410	-0.01600
C	-0.66420	-1.71200	-0.17340
C	-1.29780	-2.87480	-0.56290
H	3.39460	-3.91180	-0.03100
H	-1.09980	-4.96740	-1.09340
H	1.36260	-5.00630	-0.69250
C	2.88540	-2.95500	0.07210
C	1.53570	-0.49240	0.28150
H	-2.38000	-2.89440	-0.69550
C	2.89290	-0.58220	0.51710
C	3.57340	-1.82520	0.42850
H	3.46740	0.31230	0.75890
H	4.64290	-1.85620	0.63190
C	-1.54210	-0.55620	0.13080
C	-1.99420	0.29070	-0.89310
C	-1.96870	-0.35660	1.45500
C	-2.84450	1.35920	-0.60040
H	-1.66740	0.12370	-1.91950
C	-2.82460	0.70030	1.76930
H	-1.62350	-1.02880	2.24080
C	-3.23300	1.54030	0.72930
H	-3.18050	2.03470	-1.38550
H	-3.15520	0.86450	2.79260
C	0.94840	0.86610	0.28710
C	0.83610	1.59010	-0.92600
C	0.55470	1.45290	1.49540
C	0.30270	2.88090	-0.91230
C	0.01440	2.73990	1.52640
H	0.66040	0.89180	2.42520
C	-0.11250	3.42640	0.31180
H	0.19490	3.46660	-1.82150
H	-0.30490	3.18330	2.46180
C	1.28760	0.98220	-2.21230
H	0.89150	-0.03730	-2.34090
H	0.98600	1.56550	-3.09080
H	2.38520	0.89520	-2.23830
O	-0.64960	4.68850	0.23340
H	-0.97220	5.01150	1.11000
F	-4.03550	2.56700	1.02320

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Cozzi_aromatic/opt_b3_folded_opt.xyz

C	0.07750	-4.49950	-0.56370
C	1.43750	-4.39810	-0.43570
C	2.04660	-3.13670	-0.14130
C	1.25020	-1.96430	0.00440
C	-0.17910	-2.11980	-0.09080
C	-0.73490	-3.35020	-0.37860
H	4.04500	-3.99140	-0.09880
H	-0.39900	-5.45070	-0.79590
H	2.07760	-5.27070	-0.55490
C	3.46890	-3.07360	0.00570
C	1.94030	-0.72020	0.23750

H	-1.81710	-3.45770	-0.45760
C	3.31330	-0.69580	0.38320
C	4.08640	-1.88130	0.27690
H	3.82690	0.24680	0.57310
H	5.16610	-1.82040	0.40450
C	-1.13000	-1.00930	0.14570
C	-1.58120	-0.21830	-0.91780
C	-1.61620	-0.78010	1.44760
C	-2.45260	0.84980	-0.68940
H	-1.23480	-0.42250	-1.93090
C	-2.48920	0.27120	1.69780
H	-1.29130	-1.42500	2.26440
C	-2.86840	1.10110	0.62300
H	-2.77490	1.47250	-1.51680
H	-2.86720	0.47810	2.69510
C	1.25380	0.59090	0.29800
C	1.05710	1.34810	-0.88250
C	0.84640	1.10160	1.53660
C	0.41210	2.58680	-0.81020
C	0.20020	2.33610	1.62690
H	1.02220	0.51930	2.44250
C	-0.02760	3.04260	0.43990
H	0.23380	3.19050	-1.69530
H	-0.13540	2.71570	2.58470
C	1.53520	0.83240	-2.19920
H	1.27470	-0.22860	-2.33940
H	1.12320	1.38700	-3.05080
H	2.63260	0.89500	-2.26640
O	-0.71600	4.23740	0.42110
H	-0.99390	4.51380	1.32900
O	-3.67740	2.14980	1.01140
C	-3.87560	3.22020	0.05510
H	-4.46750	3.93740	0.63580
H	-2.90660	3.64770	-0.23670
H	-4.43850	2.85800	-0.80890

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Cozzi_aromatic/opt_b4_folded_opt.xyz

C	-0.39560	-4.41530	-0.21020
C	0.97340	-4.42400	-0.16680
C	1.70320	-3.19970	-0.03640
C	1.01860	-1.95250	0.04740
C	-0.42070	-1.98460	0.00270
C	-1.09450	-3.18300	-0.12360
H	3.62160	-4.22170	-0.05660
H	-0.96410	-5.33880	-0.30920
H	1.52960	-5.35790	-0.22970
C	3.13270	-3.25120	0.00900
C	1.82350	-0.76300	0.17090
H	-2.18450	-3.19790	-0.15650
C	3.20120	-0.84880	0.21470
C	3.86510	-2.10060	0.13420
H	3.80270	0.05530	0.31060
H	4.95300	-2.12440	0.17280
C	-1.26580	-0.76940	0.08620
C	-1.71550	-0.14660	-1.08820
C	-1.66680	-0.27160	1.33410
C	-2.49840	1.00480	-1.01320
H	-1.43710	-0.55430	-2.05840
C	-2.45530	0.87760	1.40840
H	-1.34700	-0.77410	2.24550
C	-2.85220	1.53980	0.23630
H	-2.82030	1.49980	-1.92660
H	-2.74720	1.26800	2.38020
C	1.25480	0.60170	0.25940
C	1.00110	1.35940	-0.90930
C	1.02510	1.16070	1.52310
C	0.47540	2.65020	-0.79470

C	0.50680	2.45040	1.65640
H	1.24450	0.57500	2.41710
C	0.21750	3.16070	0.48450
H	0.24950	3.25480	-1.66870
H	0.31930	2.87270	2.63550
C	1.30370	0.79730	-2.25860
H	1.02920	-0.26680	-2.32990
H	0.77870	1.32420	-3.06510
H	2.38180	0.85950	-2.47200
O	-0.34600	4.41780	0.51130
H	-0.48420	4.74010	1.43380
C	-3.60710	2.82660	0.31000
H	-2.91460	3.67500	0.17350
H	-4.37230	2.90520	-0.47320
H	-4.11390	2.96790	1.27190

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Cozzi_aromatic/opt_b5_folded_opt.xyz

C	-0.56700	-4.06300	-0.85520
C	0.79370	-4.07610	-0.69680
C	1.48900	-2.88990	-0.29990
C	0.77810	-1.67450	-0.08440
C	-0.65570	-1.71480	-0.20030
C	-1.29610	-2.87360	-0.59130
H	3.41860	-3.89070	-0.27780
H	-1.10800	-4.95450	-1.16890
H	1.36890	-4.98420	-0.87030
C	2.90830	-2.94170	-0.12260
C	1.55110	-0.49990	0.23120
H	-2.38210	-2.89490	-0.68950
C	2.91820	-0.58600	0.40330
C	3.60390	-1.81820	0.23870
H	3.49550	0.30350	0.65610
H	4.68170	-1.84620	0.39160
C	-1.53440	-0.56650	0.13400
C	-2.01320	0.28340	-0.87320
C	-1.94680	-0.38080	1.46320
C	-2.87480	1.33340	-0.54500
H	-1.70180	0.13360	-1.90500
C	-2.81470	0.66600	1.78180
H	-1.58440	-1.05010	2.24100
C	-3.27520	1.52730	0.78050
H	-3.22910	2.00620	-1.32420
H	-3.12990	0.81310	2.81280
C	0.95580	0.85120	0.33720
C	0.78970	1.64540	-0.82430
C	0.61140	1.36170	1.59430
C	0.25800	2.93250	-0.70990
C	0.07820	2.64550	1.72680
H	0.75210	0.74370	2.48230
C	-0.10000	3.40230	0.56190
H	0.10890	3.56980	-1.57720
H	-0.19920	3.03090	2.70000
C	1.18690	1.11670	-2.16240
H	0.78500	0.10550	-2.33310
H	0.84650	1.74950	-2.99090
H	2.28210	1.03400	-2.24030
O	-0.63500	4.66960	0.58580
H	-0.87960	4.95160	1.49960
H	-3.94350	2.34760	1.03190

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Cozzi_aromatic/opt_c2_folded_opt.xyz

C	-1.01820	-4.68440	-0.50220
C	0.41310	-4.70030	-0.38490
C	1.00470	-3.48580	-0.26460
C	0.23110	-2.24180	-0.25300
C	-1.12440	-2.22390	-0.37910

C	-1.74840	-3.51600	-0.50250
H	-1.52770	-5.64330	-0.59530
H	0.95460	-5.63960	-0.39670
H	-2.83390	-3.54510	-0.59360
C	2.25820	-2.70070	-0.12590
C	3.61170	-2.70010	-0.03860
C	4.22390	-1.40600	0.07380
C	3.49150	-0.23950	0.10000
C	2.05260	-0.23420	0.01750
C	1.47670	-1.46270	-0.10350
H	4.22070	-3.59680	-0.05300
H	5.31120	-1.36610	0.13760
H	3.99260	0.72490	0.18050
C	1.28470	1.02100	0.07190
C	0.61330	1.48730	-1.08060
C	1.18820	1.74650	1.27520
C	-0.13220	2.66950	-1.02180
C	0.43580	2.92840	1.32040
C	-0.22280	3.39350	0.17590
H	-0.65450	3.02430	-1.90670
H	0.36460	3.48580	2.25000
C	-1.91890	-0.98370	-0.41470
C	-2.03200	-0.15890	0.72900
C	-2.53670	-0.61430	-1.61830
C	-2.76680	1.03330	0.64750
C	-3.26790	0.57120	-1.71520
H	-2.43930	-1.25930	-2.49270
C	-3.35920	1.36570	-0.57070
H	-2.85350	1.68840	1.51230
H	-3.74270	0.86090	-2.64890
C	0.69050	0.72300	-2.36180
H	0.22660	1.25170	-3.20250
H	1.73100	0.50460	-2.64160
H	0.17650	-0.24790	-2.26400
C	1.88070	1.28340	2.51800
H	2.87550	1.74580	2.60010
H	1.32390	1.54950	3.42570
H	2.03280	0.19490	2.54000
C	-1.37760	-0.54340	2.01190
H	-1.64770	0.11480	2.84610
H	-1.62810	-1.57330	2.30460
H	-0.27840	-0.50010	1.90960
C	-1.02600	4.65260	0.22190
H	-0.74320	5.34020	-0.58750
H	-2.09870	4.43980	0.10160
H	-0.90940	5.19880	1.16610
F	-4.05590	2.50300	-0.64570

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Cozzi_aromatic/opt_c4_folded_opt.xyz

C	-0.79830	-4.85800	-0.47580
C	0.63410	-4.87750	-0.37670
C	1.22970	-3.66430	-0.26140
C	0.45920	-2.41910	-0.23760
C	-0.89840	-2.39690	-0.34270
C	-1.52570	-3.68780	-0.46240
H	-1.31110	-5.81520	-0.56560
H	1.17340	-5.81770	-0.39710
H	-2.61240	-3.71360	-0.53930
C	2.48700	-2.88300	-0.13650
C	3.84140	-2.88600	-0.06480
C	4.45860	-1.59380	0.04070
C	3.72980	-0.42530	0.07410
C	2.29010	-0.41600	0.00740
C	1.70890	-1.64280	-0.10440
H	4.44750	-3.78440	-0.08630
H	5.54640	-1.55710	0.09250
H	4.23450	0.53760	0.14820

C	1.52600	0.84160	0.06370
C	0.84110	1.30060	-1.08230
C	1.44200	1.57330	1.26530
C	0.09330	2.48350	-1.02150
C	0.68690	2.75210	1.31350
C	0.01070	3.20790	0.17380
H	-0.44010	2.82740	-1.90330
H	0.62150	3.31350	2.24090
C	-1.69040	-1.15520	-0.35730
C	-1.78020	-0.33070	0.78460
C	-2.33500	-0.77260	-1.54260
C	-2.50650	0.86610	0.71240
C	-3.05150	0.42080	-1.60890
H	-2.26650	-1.41320	-2.42160
C	-3.13580	1.25000	-0.47860
H	-2.56350	1.51010	1.58680
H	-3.53890	0.71020	-2.53560
C	0.89910	0.52850	-2.35950
H	0.47480	1.07560	-3.20910
H	1.92900	0.25070	-2.62390
H	0.33000	-0.41230	-2.26170
C	2.15120	1.11700	2.50130
H	3.14980	1.57360	2.56440
H	1.60920	1.39220	3.41500
H	2.29630	0.02740	2.52870
C	-1.10670	-0.72020	2.05850
H	-1.36260	-0.06140	2.89590
H	-1.35870	-1.74850	2.35300
H	-0.01020	-0.68130	1.93870
C	-0.80570	4.45880	0.24780
H	-0.26260	5.26860	0.75390
H	-1.09450	4.83390	-0.74190
H	-1.73170	4.28220	0.81430
C	-3.88340	2.54240	-0.55890
H	-3.28950	3.29700	-1.09590
H	-4.83450	2.43160	-1.09670
H	-4.11880	2.95550	0.42980

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Cozzi_aromatic/opt_c5_folded_opt.xyz

C	-1.01990	-4.66910	-0.54400
C	0.40980	-4.69170	-0.41040
C	1.00480	-3.48030	-0.27660
C	0.23560	-2.23360	-0.26740
C	-1.11880	-2.20880	-0.40320
C	-1.74560	-3.49780	-0.54330
H	-1.53200	-5.62510	-0.65000
H	0.94740	-5.63310	-0.42070
H	-2.83030	-3.52150	-0.64650
C	2.25960	-2.70100	-0.11700
C	3.61190	-2.70480	-0.01010
C	4.22670	-1.41320	0.11520
C	3.49850	-0.24370	0.13220
C	2.06150	-0.23370	0.02740
C	1.48280	-1.46030	-0.10100
H	4.21800	-3.60340	-0.01850
H	5.31290	-1.37750	0.19600
H	4.00180	0.71850	0.22190
C	1.29120	1.02070	0.06220
C	0.63660	1.47440	-1.10510
C	1.16380	1.74950	1.26030
C	-0.12880	2.64470	-1.06370
C	0.38910	2.91790	1.28880
C	-0.26180	3.36350	0.13270
H	-0.64000	2.98730	-1.95940
H	0.29140	3.47580	2.21540
C	-1.91040	-0.96510	-0.42620
C	-2.03200	-0.15790	0.72510

C	-2.52350	-0.57190	-1.62480
C	-2.76400	1.03710	0.64700
C	-3.24660	0.62050	-1.68980
H	-2.42680	-1.19930	-2.50980
C	-3.36400	1.42480	-0.55230
H	-2.85070	1.67370	1.52540
H	-3.71380	0.92310	-2.62350
C	0.74500	0.70620	-2.38160
H	0.34860	1.25400	-3.24410
H	1.78550	0.43580	-2.61010
H	0.17870	-0.23800	-2.30750
C	1.84480	1.30180	2.51500
H	2.84090	1.76070	2.59850
H	1.28170	1.58100	3.41460
H	1.99130	0.21260	2.55170
C	-1.38800	-0.56000	2.01010
H	-1.65890	0.09460	2.84620
H	-1.65270	-1.58860	2.29230
H	-0.28900	-0.52640	1.91530
C	-1.10270	4.59950	0.16110
H	-0.67530	5.38180	-0.48250
H	-2.11890	4.39610	-0.20540
H	-1.19980	5.02510	1.16750
H	-3.92170	2.35780	-0.60160

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9_benzyl_triptycene/opt_b1_folded_opt.xyz

C	-1.90860	-2.41440	-0.71150
C	-0.85640	-1.82640	0.00980
C	-0.20350	-0.67750	-0.47090
C	-0.54570	-0.21370	-1.75830
C	-1.59040	-0.80880	-2.48150
C	-2.29010	-1.90080	-1.95080
C	1.75370	0.42580	-2.12690
C	2.08710	0.00150	-0.80810
C	3.35860	-0.48040	-0.54230
C	4.30470	-0.53850	-1.58340
C	3.97420	-0.12030	-2.86890
C	2.68480	0.36760	-3.15040
H	-2.42160	-3.28670	-0.31320
H	-3.11040	-2.36150	-2.49290
H	5.30330	-0.91690	-1.37310
H	4.71280	-0.16950	-3.66690
H	2.42970	0.68990	-4.15710
C	0.52530	1.62620	0.07890
C	0.52160	2.56500	1.10140
C	0.13600	3.88870	0.82530
C	-0.22910	4.27030	-0.46360
C	-0.20030	3.33730	-1.51400
C	0.18400	2.03380	-1.23950
H	0.12510	4.61800	1.63320
H	-0.53250	5.29570	-0.66510
H	-0.47180	3.63790	-2.52290
C	0.91890	0.14100	0.19140
C	1.29050	-0.30080	1.60870
H	1.55690	-1.38800	1.56680
H	2.22050	0.23160	1.90850
C	0.26910	-0.13660	2.70420
C	0.67570	-0.46060	4.01280
C	-1.04920	0.29350	2.49140
C	-0.21890	-0.35670	5.07850
H	1.69310	-0.79780	4.19770
C	-1.94040	0.39730	3.56200
H	-1.39040	0.54870	1.48740
C	-1.53160	0.07220	4.85800
H	0.10770	-0.60930	6.08570
H	-2.95910	0.73700	3.38200
H	0.80690	2.29570	2.11780

H	3.63990	-0.81720	0.45270
H	-2.22680	0.15560	5.68900
O	-0.34690	-2.38720	1.16760
O	-1.82670	-0.21440	-3.70830
C	-2.84270	-0.80790	-4.54900
H	-3.82230	-0.73950	-4.06740
H	-2.79800	-0.16680	-5.43900
H	-2.57920	-1.84000	-4.79680
C	-1.28110	-3.08510	2.02780
H	-0.67350	-3.25030	2.92740
H	-2.13950	-2.44690	2.25740
H	-1.57830	-4.03080	1.56980
C	0.31910	0.92460	-2.26920
H	0.05290	1.23280	-3.29990

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9_benzyl_triptycene/opt_b3_folded_opt.xyz

C	-1.76120	-2.42150	-1.20450
C	-0.71540	-1.82920	-0.47710
C	-0.04630	-0.69350	-0.96690
C	-0.36780	-0.24790	-2.26630
C	-1.40610	-0.84730	-2.99500
C	-2.12110	-1.92590	-2.45730
C	1.93930	0.37440	-2.61380
C	2.25240	-0.03230	-1.28450
C	3.51730	-0.51840	-0.99510
C	4.47660	-0.59760	-2.02250
C	4.16600	-0.19590	-3.31830
C	2.88350	0.29580	-3.62390
H	-2.28640	-3.28320	-0.79910
H	-2.93700	-2.38950	-3.00360
H	5.46980	-0.97940	-1.79350
H	4.91470	-0.26100	-4.10540
H	2.64370	0.60490	-4.63830
C	0.68720	1.61410	-0.44300
C	0.67320	2.56840	0.56510
C	0.29600	3.88900	0.26400
C	-0.05040	4.25250	-1.03520
C	-0.01030	3.30380	-2.07110
C	0.36560	2.00330	-1.77190
H	0.27590	4.63020	1.06100
H	-0.34790	5.27560	-1.25600
H	-0.26730	3.59000	-3.08790
C	1.07230	0.12910	-0.30230
C	1.42600	-0.29170	1.12670
H	1.67350	-1.38340	1.10710
H	2.36180	0.23300	1.42140
C	0.39850	-0.08690	2.20950
C	0.79060	-0.35660	3.52910
C	-0.92710	0.32130	1.96390
C	-0.10630	-0.23190	4.59520
H	1.81170	-0.67420	3.73840
C	-1.83860	0.45260	3.00410
H	-1.25410	0.53860	0.94430
C	-1.41550	0.17090	4.31780
H	0.22330	-0.44510	5.60530
H	-2.86270	0.77180	2.82670
H	0.94490	2.31350	1.58900
H	3.78310	-0.84260	0.00830
O	-0.23080	-2.37390	0.69880
O	-1.62010	-0.27100	-4.23450
C	-2.63410	-0.86560	-5.07690
H	-3.61780	-0.77840	-4.60710
H	-2.57230	-0.23900	-5.97610
H	-2.37990	-1.90440	-5.30580
C	-1.18810	-3.04170	1.55790
H	-0.59880	-3.19240	2.47180
H	-2.04410	-2.39000	1.75740

H	-1.48730	-3.99460	1.11630
O	-2.42460	0.33040	5.24830
C	-2.09480	0.11480	6.63970
H	-1.32630	0.82270	6.96300
H	-3.05260	0.32300	7.13360
H	-1.78770	-0.92210	6.80150
C	0.50960	0.87820	-2.78280
H	0.25870	1.17190	-3.82150

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9_benzyl_triptycene/opt_c10_folded_opt.xyz

C	-1.89990	-2.34540	-0.65380
C	-0.84660	-1.75150	0.06880
C	-0.18710	-0.60680	-0.38570
C	-0.55230	-0.11550	-1.66680
C	-1.59580	-0.70520	-2.37890
C	-2.28940	-1.81780	-1.87780
C	1.73320	0.53240	-2.07430
C	2.09700	0.07090	-0.77720
C	3.37180	-0.42820	-0.56030
C	4.28920	-0.46410	-1.62720
C	3.92860	-0.00680	-2.89140
C	2.63610	0.49750	-3.12410
H	-2.41450	-3.21540	-0.23920
H	-3.10170	-2.27300	-2.45020
H	5.29010	-0.85620	-1.45460
H	4.64590	-0.03850	-3.70970
H	2.35730	0.85030	-4.11390
C	0.56310	1.68000	0.19460
C	0.58770	2.59620	1.23720
C	0.19090	3.92460	1.00290
C	-0.21130	4.33530	-0.26570
C	-0.20790	3.42720	-1.33800
C	0.18680	2.11890	-1.10410
H	0.20040	4.63480	1.82820
H	-0.52410	5.36410	-0.43430
H	-0.50670	3.75120	-2.33150
C	0.95870	0.19310	0.26060
C	1.38630	-0.28290	1.65120
H	1.58420	-1.38250	1.59010
H	2.36540	0.19130	1.89030
C	0.45240	-0.06110	2.81100
C	0.97740	-0.24250	4.10440
C	-0.90210	0.27310	2.66830
C	0.15820	-0.10280	5.22600
H	2.02850	-0.48950	4.23590
C	-1.71890	0.40740	3.79350
H	-1.33010	0.43350	1.67740
C	-1.19460	0.21670	5.07500
H	0.57600	-0.23970	6.22220
H	-2.77210	0.65820	3.66640
H	0.90590	2.30840	2.23880
H	3.67810	-0.79500	0.41670
O	-0.36820	-2.36870	1.22970
O	-1.90690	-0.06000	-3.58160
C	-2.50520	-0.71890	-4.65590
O	-2.82110	-1.87740	-4.62280
C	-2.64300	0.28170	-5.74810
H	-2.32960	1.29300	-5.43970
H	-2.03300	-0.00640	-6.61990
H	-3.68950	0.34430	-6.08930
C	-1.24720	-2.84250	2.21400
O	-2.44050	-2.79990	2.08340
C	-0.41770	-3.36050	3.33100
H	-0.86960	-4.25990	3.77590
H	0.61060	-3.60300	3.02000
H	-0.33860	-2.59840	4.13090
H	-1.83370	0.32140	5.94850

C	0.29780	1.03800	-2.16580
H	0.00660	1.37540	-3.18000

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9_benzyl_triptycene/opt_c12_folded_opt.xyz

C	-1.89400	-2.34540	-0.64730
C	-0.83950	-1.75140	0.07330
C	-0.18160	-0.60630	-0.38230
C	-0.54910	-0.11520	-1.66280
C	-1.59410	-0.70460	-2.37290
C	-2.28640	-1.81740	-1.87020
C	1.73660	0.53000	-2.07430
C	2.10240	0.06910	-0.77760
C	3.37700	-0.43090	-0.56210
C	4.29260	-0.46840	-1.63060
C	3.93020	-0.01190	-2.89460
C	2.63780	0.49330	-3.12560
H	-2.40750	-3.21610	-0.23260
H	-3.10010	-2.27270	-2.44090
H	5.29360	-0.86120	-1.45940
H	4.64600	-0.04520	-3.71420
H	2.35770	0.84560	-4.11540
C	0.57260	1.68080	0.19510
C	0.60300	2.59830	1.23650
C	0.20600	3.92670	1.00250
C	-0.20120	4.33620	-0.26490
C	-0.20160	3.42720	-1.33640
C	0.19310	2.11880	-1.10290
H	0.21960	4.63810	1.82690
H	-0.51450	5.36500	-0.43320
H	-0.50340	3.75060	-2.32950
C	0.96580	0.19330	0.26130
C	1.39330	-0.28280	1.65230
H	1.59380	-1.38200	1.58910
H	2.37100	0.19440	1.89200
C	0.45700	-0.06260	2.81010
C	0.97770	-0.26000	4.10290
C	-0.89530	0.28690	2.66130
C	0.16840	-0.12530	5.23200
H	2.02780	-0.52060	4.23230
C	-1.72590	0.42540	3.77410
H	-1.31510	0.45580	1.66600
C	-1.17300	0.21400	5.03950
H	0.57620	-0.27340	6.23050
H	-2.77710	0.68700	3.65080
H	0.92790	2.31240	2.23620
H	3.68500	-0.79730	0.41450
O	-0.35740	-2.36910	1.23270
O	-1.90760	-0.05940	-3.57450
C	-2.50880	-0.71860	-4.64800
O	-2.82330	-1.87720	-4.61320
C	-2.65010	0.28260	-5.73890
H	-2.33340	1.29330	-5.43210
H	-2.04510	-0.00640	-6.61400
H	-3.69820	0.34730	-6.07500
C	-1.23380	-2.85360	2.21450
O	-2.42710	-2.79890	2.09180
C	-0.40090	-3.39380	3.31870
H	-0.83160	-4.32550	3.71800
H	0.63670	-3.59610	3.00940
H	-0.35430	-2.66950	4.15370
F	-1.95840	0.33970	6.11190
C	0.30150	1.03700	-2.16390
H	0.00910	1.37400	-3.17800

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9_benzyl_triptycene/opt_c13_folded_opt.xyz

C	-1.84460	-2.35090	-0.75880
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C	-0.79480	-1.75300	-0.03460
C	-0.12790	-0.61600	-0.49650
C	-0.48100	-0.13710	-1.78560
C	-1.52170	-0.72990	-2.49950
C	-2.22280	-1.83490	-1.99110
C	1.81130	0.49500	-2.18180
C	2.16320	0.04640	-0.87690
C	3.43380	-0.45560	-0.64350
C	4.35950	-0.50720	-1.70260
C	4.01080	-0.06290	-2.97480
C	2.72240	0.44400	-3.22380
H	-2.36540	-3.21520	-0.33980
H	-3.03290	-2.29360	-2.56470
H	5.35770	-0.90120	-1.51770
H	4.73460	-0.10700	-3.78710
H	2.45320	0.78650	-4.22010
C	0.63050	1.67430	0.06410
C	0.65550	2.60250	1.09610
C	0.26630	3.93000	0.84440
C	-0.12770	4.32750	-0.43090
C	-0.12230	3.40730	-1.49280
C	0.26490	2.09980	-1.24200
H	0.27570	4.65040	1.66120
H	-0.43490	5.35610	-0.61300
H	-0.41360	3.72160	-2.49200
C	1.01660	0.18590	0.14860
C	1.42650	-0.27700	1.54900
H	1.62720	-1.37780	1.49910
H	2.40310	0.19910	1.79700
C	0.47590	-0.04720	2.69110
C	0.97650	-0.24110	3.99430
C	-0.87150	0.30890	2.52580
C	0.14880	-0.09190	5.10380
H	2.02290	-0.50650	4.14060
C	-1.70970	0.45480	3.63010
H	-1.27930	0.47690	1.52510
C	-1.20240	0.25110	4.92400
H	0.54500	-0.23710	6.10970
H	-2.75930	0.72130	3.48810
H	0.97070	2.32720	2.10140
H	3.73140	-0.81280	0.33960
O	-0.32800	-2.36120	1.13690
O	-1.82110	-0.09660	-3.71020
C	-2.42200	-0.76280	-4.78060
O	-2.74300	-1.91910	-4.73490
C	-2.55240	0.22870	-5.88120
H	-2.21340	1.23650	-5.58880
H	-1.96180	-0.08240	-6.75870
H	-3.60220	0.31110	-6.20890
C	-1.21960	-2.82440	2.11580
O	-2.41050	-2.73920	1.98880
C	-0.40440	-3.38200	3.22450
H	-0.84370	-4.31910	3.60270
H	0.63680	-3.58520	2.92790
H	-0.37000	-2.67240	4.07160
C	-2.05760	0.39700	6.06190
N	-2.74650	0.51450	6.98340
C	0.37900	1.00640	-2.29050
H	0.09760	1.33390	-3.31080

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9_benzyl_triptycene/opt_c14_folded_opt.xyz			
C	-1.76920	-2.36450	-0.96280
C	-0.72410	-1.76430	-0.23330
C	-0.04670	-0.63570	-0.70030
C	-0.38590	-0.16670	-1.99690
C	-1.42250	-0.76120	-2.71510
C	-2.13320	-1.85860	-2.20340

C	1.91190	0.45300	-2.37940
C	2.25080	0.01350	-1.06810
C	3.51690	-0.49300	-0.82020
C	4.45100	-0.55800	-1.87120
C	4.11510	-0.12200	-3.14970
C	2.83140	0.38940	-3.41340
H	-2.29830	-3.22250	-0.54110
H	-2.93970	-2.31900	-2.78050
H	5.44540	-0.95590	-1.67500
H	4.84530	-0.17620	-3.95560
H	2.57210	0.72540	-4.41450
C	0.71640	1.65560	-0.15290
C	0.73410	2.59160	0.87230
C	0.35120	3.91820	0.60650
C	-0.02920	4.30690	-0.67560
C	-0.01670	3.37840	-1.73020
C	0.36390	2.07170	-1.46550
H	0.35470	4.64480	1.41780
H	-0.33170	5.33480	-0.86860
H	-0.29770	3.68570	-2.73450
C	1.09640	0.16670	-0.05330
C	1.49460	-0.28590	1.35370
H	1.69430	-1.38760	1.31330
H	2.47000	0.19070	1.60620
C	0.53570	-0.04910	2.48650
C	1.02360	-0.24270	3.79490
C	-0.80860	0.30970	2.31220
C	0.18310	-0.09550	4.89430
H	2.06840	-0.50710	3.95250
C	-1.65750	0.45160	3.41070
H	-1.20860	0.48170	1.30900
C	-1.16690	0.24340	4.70590
H	0.57980	-0.24520	5.90080
H	-2.70360	0.71810	3.23970
H	1.03850	2.32340	1.88280
H	3.80480	-0.84370	0.16800
O	-0.27480	-2.36120	0.95070
O	-1.70870	-0.13720	-3.93390
C	-2.29910	-0.81180	-5.00480
O	-2.62130	-1.96750	-4.95290
C	-2.41740	0.17050	-6.11500
H	-2.08220	1.18080	-5.82690
H	-1.81660	-0.14740	-6.98310
H	-3.46340	0.24970	-6.45540
C	-1.18230	-2.81410	1.92100
O	-2.37070	-2.72800	1.77380
C	-0.38620	-3.36230	3.04760
H	-0.81070	-4.31570	3.40170
H	0.66900	-3.53340	2.78230
H	-0.39970	-2.66330	3.90450
C	-2.05320	0.37050	5.90820
F	-1.61870	1.25110	6.82850
F	-2.19130	-0.77210	6.60710
F	-3.31980	0.75480	5.68510
C	0.48280	0.96930	-2.50400
H	0.21110	1.28950	-3.52930

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9_benzyl_triptycene/opt_c15_folded_opt.xyz

C	-1.59030	-2.25180	-1.01290
C	-0.55690	-1.62260	-0.29120
C	0.04930	-0.44470	-0.73710
C	-0.36090	0.05480	-2.00110
C	-1.38840	-0.56690	-2.70900
C	-2.02060	-1.72110	-2.22180
C	1.88290	0.80990	-2.44440
C	2.29480	0.33520	-1.16670
C	3.59380	-0.11540	-0.99050

C	4.48710	-0.08900	-2.07790
C	4.07910	0.38140	-3.32270
C	2.76190	0.83620	-3.51470
H	-2.05960	-3.15220	-0.60930
H	-2.81710	-2.20340	-2.79350
H	5.50690	-0.44300	-1.93670
H	4.77790	0.39820	-4.15710
H	2.44550	1.19940	-4.48930
C	0.71900	1.85750	-0.12390
C	0.73070	2.75300	0.93670
C	0.27130	4.06750	0.74060
C	-0.17920	4.48630	-0.50880
C	-0.16210	3.60150	-1.60030
C	0.29370	2.30700	-1.40400
H	0.26980	4.75990	1.58090
H	-0.54050	5.50350	-0.64770
H	-0.49820	3.93250	-2.57960
C	1.17730	0.38760	-0.09960
C	1.66300	-0.10300	1.26770
H	1.87690	-1.19710	1.17970
H	2.64190	0.38570	1.47630
C	0.77050	0.09040	2.46460
C	1.35440	-0.02250	3.73400
C	-0.61320	0.34010	2.36910
C	0.58930	0.09600	4.89940
H	2.42450	-0.20510	3.82790
C	-1.39610	0.45710	3.50900
H	-1.08390	0.44670	1.38840
C	-0.78220	0.33170	4.77230
H	1.06590	0.00750	5.86890
H	-2.46750	0.64080	3.44770
H	1.08730	2.45960	1.92370
H	3.93750	-0.49120	-0.02940
O	-0.04750	-2.22340	0.86350
O	-1.75200	0.08660	-3.89150
O	-1.67860	0.45380	5.81440
C	-1.15860	0.37670	7.16180
H	-0.44410	1.18490	7.34160
H	-2.06780	0.51660	7.76140
H	-0.71740	-0.60700	7.34390
C	-2.31020	-0.58090	-4.98210
O	-2.54970	-1.75720	-4.97680
C	-2.52680	0.46050	-6.04740
H	-2.22830	1.46740	-5.67780
H	-3.61710	0.52370	-6.26110
C	-0.89540	-2.78620	1.83170
O	-2.08590	-2.82720	1.68790
C	-0.00820	-3.28510	2.93670
H	0.36170	-4.29880	2.66800
H	0.90020	-2.64410	3.01610
C	-1.74950	0.09490	-7.30470
H	-1.95190	0.80870	-8.11310
H	-0.66570	0.09500	-7.12900
H	-2.02160	-0.90530	-7.67310
C	-0.76200	-3.30870	4.25850
H	-1.68350	-3.90400	4.19040
H	-0.14460	-3.73210	5.05840
H	-1.06030	-2.29620	4.57050
C	0.42610	1.25540	-2.49220
H	0.09680	1.60170	-3.49170

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9_benzyl_triptycene/opt_c16_folded_opt.xyz

C	-1.58620	-2.23590	-0.83300
C	-0.54010	-1.61170	-0.12540
C	0.06790	-0.43880	-0.58100
C	-0.34530	0.05410	-1.84650
C	-1.38190	-0.56530	-2.54320

C	-2.02170	-1.70940	-2.04190
C	1.90320	0.79150	-2.30130
C	2.31570	0.32680	-1.02010
C	3.61290	-0.12800	-0.84180
C	4.50400	-0.11620	-1.93130
C	4.09550	0.34390	-3.17980
C	2.78010	0.80330	-3.37360
H	-2.05940	-3.12890	-0.41850
H	-2.82760	-2.18800	-2.60360
H	5.52250	-0.47340	-1.78870
H	4.79260	0.34930	-4.01580
H	2.46350	1.15860	-4.35100
C	0.74910	1.86570	0.01170
C	0.76600	2.76900	1.06570
C	0.31530	4.08480	0.85910
C	-0.13290	4.49660	-0.39360
C	-0.12280	3.60290	-1.47780
C	0.32490	2.30700	-1.27140
H	0.31930	4.78410	1.69360
H	-0.48690	5.51510	-0.54060
H	-0.45770	3.92800	-2.45940
C	1.20030	0.39360	0.04770
C	1.68190	-0.08530	1.42000
H	1.90910	-1.17730	1.33930
H	2.65340	0.41490	1.63540
C	0.77640	0.10140	2.60850
C	1.34570	-0.04010	3.88590
C	-0.59660	0.37180	2.50770
C	0.56010	0.07580	5.03330
H	2.41050	-0.23960	3.98900
C	-1.38420	0.48230	3.65280
H	-1.06240	0.50040	1.52880
C	-0.81470	0.33310	4.92710
H	1.02010	-0.03280	6.01320
H	-2.45010	0.68300	3.55250
H	1.11910	2.48010	2.05540
H	3.95670	-0.49590	0.12230
O	-0.01740	-2.21930	1.01960
O	-1.74400	0.08020	-3.73060
C	-2.31860	-0.59060	-4.81040
O	-2.58260	-1.76150	-4.78880
C	-2.51610	0.44020	-5.88980
H	-2.20930	1.44810	-5.53030
H	-3.60380	0.51230	-6.11330
C	-0.85400	-2.75840	2.01010
O	-2.04920	-2.75980	1.90200
C	0.05030	-3.29470	3.08330
H	0.38910	-4.31220	2.78900
H	0.97550	-2.67610	3.14680
C	-1.73270	0.05060	-7.13610
H	-1.91890	0.75800	-7.95410
H	-0.65050	0.03910	-6.95080
H	-2.01420	-0.95000	-7.49590
C	-0.66560	-3.32110	4.42570
H	-1.61450	-3.87260	4.37010
H	-0.04510	-3.79360	5.19550
H	-0.90460	-2.30410	4.77260
C	-1.66760	0.45520	6.14770
H	-2.59810	-0.12190	6.05210
H	-1.16180	0.10500	7.05600
H	-1.95420	1.50320	6.32100
C	0.44870	1.24490	-2.35040
H	0.11950	1.58410	-3.35240

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9_benzyl_triptycene/opt_c17_folded_opt.xyz

C	-1.67370	-2.21390	-0.56060
C	-0.61690	-1.60430	0.14370

C	-0.02790	-0.41250	-0.28690
C	-0.47090	0.11660	-1.52740
C	-1.51810	-0.48830	-2.22100
C	-2.13900	-1.65240	-1.74250
C	1.76320	0.88300	-2.00460
C	2.20510	0.38260	-0.74680
C	3.50860	-0.06820	-0.60890
C	4.37680	-0.01750	-1.71570
C	3.93950	0.47680	-2.94110
C	2.61750	0.93290	-3.09380
H	-2.13140	-3.12340	-0.16490
H	-2.95360	-2.11910	-2.30170
H	5.40030	-0.37180	-1.60480
H	4.61910	0.51180	-3.79080
H	2.27860	1.31510	-4.05350
C	0.64970	1.87790	0.36330
C	0.68260	2.74890	1.44380
C	0.21840	4.06690	1.28700
C	-0.25900	4.51320	0.05720
C	-0.26500	3.65310	-1.05400
C	0.19620	2.35520	-0.89670
H	0.23500	4.74050	2.14230
H	-0.62350	5.53300	-0.05110
H	-0.62270	4.00550	-2.01800
C	1.11110	0.40870	0.34450
C	1.62280	-0.10900	1.69140
H	1.85440	-1.19700	1.57320
H	2.59660	0.38910	1.90190
C	0.74180	0.03600	2.90400
C	1.34560	-0.13400	4.16410
C	-0.63440	0.29750	2.83960
C	0.58440	-0.04450	5.33050
H	2.41280	-0.33110	4.23530
C	-1.39320	0.37970	4.00950
H	-1.12400	0.44360	1.87550
C	-0.78890	0.20990	5.25820
H	1.06290	-0.17200	6.30010
H	-2.46330	0.57550	3.94300
H	1.05860	2.43350	2.41670
H	3.87470	-0.46240	0.33630
O	-0.06280	-2.24330	1.25640
O	-1.91090	0.19180	-3.37870
C	-2.50040	-0.44970	-4.46860
O	-2.74970	-1.62390	-4.48030
C	-2.73290	0.61450	-5.50770
H	-2.42030	1.61180	-5.12430
H	-3.82690	0.68840	-5.69740
C	-0.87070	-2.82630	2.24580
O	-2.06790	-2.83670	2.16550
C	0.06430	-3.38940	3.27840
H	0.39030	-4.40090	2.95030
H	0.99320	-2.77550	3.32890
C	-1.98410	0.27010	-6.78810
H	-2.19790	1.00230	-7.57710
H	-0.89700	0.25930	-6.63490
H	-2.27080	-0.72010	-7.17180
C	-0.61170	-3.44600	4.64030
H	-1.56150	-3.99760	4.60060
H	0.03100	-3.93520	5.38100
H	-0.84150	-2.43740	5.01650
H	-1.38160	0.28030	6.16690
C	0.30510	1.32770	-2.01030
H	-0.04660	1.69510	-2.99450

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9_benzyl_triptycene/opt_c19_folded_opt.xyz

C	-1.66190	-2.22080	-0.56280
C	-0.60630	-1.61030	0.14250

C	-0.02070	-0.41600	-0.28560
C	-0.46460	0.11440	-1.52520
C	-1.51090	-0.49100	-2.21970
C	-2.12890	-1.65770	-1.74300
C	1.76890	0.88490	-2.00010
C	2.21130	0.38330	-0.74280
C	3.51550	-0.06510	-0.60460
C	4.38440	-0.01070	-1.71070
C	3.94690	0.48500	-2.93550
C	2.62400	0.93830	-3.08850
H	-2.11730	-3.13270	-0.16970
H	-2.94290	-2.12500	-2.30290
H	5.40860	-0.36300	-1.59990
H	4.62710	0.52310	-3.78460
H	2.28500	1.32130	-4.04790
C	0.65400	1.87500	0.36820
C	0.68820	2.74530	1.44920
C	0.22190	4.06280	1.29450
C	-0.25770	4.50950	0.06570
C	-0.26350	3.65070	-1.04640
C	0.19920	2.35310	-0.89100
H	0.23890	4.73590	2.15030
H	-0.62380	5.52910	-0.04110
H	-0.62200	4.00400	-2.01000
C	1.11650	0.40620	0.34730
C	1.62650	-0.11340	1.69470
H	1.86130	-1.20050	1.57330
H	2.59840	0.38760	1.90800
C	0.74110	0.02810	2.90390
C	1.34040	-0.15200	4.16490
C	-0.63530	0.29770	2.83070
C	0.58750	-0.06750	5.33710
H	2.40810	-0.35660	4.23600
C	-1.41140	0.38210	3.98760
H	-1.11650	0.44870	1.86080
C	-0.77900	0.19880	5.21940
H	1.05580	-0.20160	6.31040
H	-2.48070	0.58330	3.92280
H	1.06890	2.43090	2.42020
H	3.88220	-0.46020	0.34000
O	-0.04930	-2.25030	1.25330
O	-1.90620	0.19010	-3.37540
C	-2.49590	-0.45160	-4.46620
O	-2.73800	-1.62710	-4.47960
C	-2.73770	0.61460	-5.50070
H	-2.41720	1.61050	-5.12010
H	-3.83400	0.69260	-5.67610
C	-0.85380	-2.84870	2.23680
O	-2.05110	-2.85260	2.16280
C	0.08570	-3.42980	3.25510
H	0.40410	-4.43840	2.90900
H	1.01860	-2.82340	3.30710
C	-2.00710	0.26930	-6.79130
H	-2.23210	1.00100	-7.57760
H	-0.91790	0.25840	-6.65370
H	-2.29940	-0.72110	-7.17050
C	-0.58070	-3.50680	4.62060
H	-1.53990	-4.04250	4.57600
H	0.05850	-4.02500	5.34480
H	-0.79290	-2.50640	5.02490
F	-1.51040	0.27990	6.33420
C	0.31000	1.32720	-2.00590
H	-0.04160	1.69550	-2.98990

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9_benzyl_triptycene/opt_c1_folded_opt.xyz

C	-1.76100	-2.42170	-1.20450
C	-0.71530	-1.82930	-0.47700

C	-0.04610	-0.69360	-0.96680
C	-0.36760	-0.24810	-2.26620
C	-1.40580	-0.84750	-2.99500
C	-2.12090	-1.92610	-2.45730
C	1.93950	0.37410	-2.61360
C	2.25260	-0.03250	-1.28430
C	3.51740	-0.51860	-0.99480
C	4.47680	-0.59780	-2.02210
C	4.16630	-0.19610	-3.31790
C	2.88380	0.29550	-3.62360
H	-2.28620	-3.28340	-0.79910
H	-2.93670	-2.38970	-3.00370
H	5.47000	-0.97950	-1.79300
H	4.91510	-0.26130	-4.10500
H	2.64400	0.60460	-4.63810
C	0.68740	1.61400	-0.44300
C	0.67360	2.56840	0.56500
C	0.29640	3.88900	0.26390
C	-0.05000	4.25240	-1.03530
C	-0.01000	3.30360	-2.07120
C	0.36590	2.00310	-1.77190
H	0.27650	4.63020	1.06080
H	-0.34740	5.27560	-1.25620
H	-0.26700	3.58980	-3.08800
C	1.07240	0.12900	-0.30210
C	1.42590	-0.29170	1.12690
H	1.67330	-1.38340	1.10740
H	2.36170	0.23300	1.42170
C	0.39820	-0.08680	2.20950
C	0.79000	-0.35660	3.52920
C	-0.92730	0.32150	1.96370
C	-0.10710	-0.23170	4.59510
H	1.81100	-0.67430	3.73870
C	-1.83890	0.45300	3.00370
H	-1.25400	0.53890	0.94400
C	-1.41610	0.17120	4.31750
H	0.22240	-0.44500	5.60530
H	-2.86300	0.77240	2.82610
H	0.94530	2.31360	1.58900
H	3.78320	-0.84280	0.00860
O	-0.23070	-2.37420	0.69880
O	-1.61970	-0.27140	-4.23460
C	-2.63360	-0.86600	-5.07700
H	-3.61740	-0.77850	-4.60730
H	-2.57160	-0.23950	-5.97630
H	-2.37960	-1.90480	-5.30580
C	-1.18810	-3.04140	1.55810
H	-0.59850	-3.19310	2.47170
H	-2.04340	-2.38890	1.75830
H	-1.48860	-3.99390	1.11630
O	-2.42540	0.33080	5.24780
C	-2.09590	0.11520	6.63920
H	-1.32760	0.82330	6.96270
H	-3.05390	0.32330	7.13290
H	-1.78860	-0.92160	6.80120
C	0.50980	0.87800	-2.78270
H	0.25910	1.17160	-3.82150

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9_benzyl_triptycene/opt_c20_folded_opt.xyz

C	-1.61540	-2.22340	-0.66260
C	-0.56880	-1.60230	0.04700
C	0.02330	-0.41580	-0.39260
C	-0.40870	0.09900	-1.64320
C	-1.44750	-0.51570	-2.34090
C	-2.06920	-1.67710	-1.85560
C	1.82800	0.86490	-2.10930
C	2.26040	0.37710	-0.84340

C	3.56320	-0.07050	-0.68990
C	4.44060	-0.02860	-1.78970
C	4.01290	0.45390	-3.02330
C	2.69150	0.90620	-3.19160
H	-2.07500	-3.13020	-0.26270
H	-2.87640	-2.15310	-2.41840
H	5.46380	-0.38020	-1.66720
H	4.69980	0.48240	-3.86750
H	2.36030	1.27900	-4.15780
C	0.69490	1.88230	0.23880
C	0.72120	2.76460	1.31020
C	0.25510	4.07990	1.13720
C	-0.21630	4.51200	-0.10000
C	-0.21360	3.64070	-1.20240
C	0.24920	2.34530	-1.02920
H	0.26620	4.76320	1.98510
H	-0.58260	5.53010	-0.22090
H	-0.56560	3.98300	-2.17250
C	1.15690	0.41330	0.23730
C	1.65620	-0.09040	1.59410
H	1.89690	-1.17870	1.48500
H	2.62540	0.41460	1.81250
C	0.75900	0.05380	2.79210
C	1.34300	-0.13570	4.06060
C	-0.61440	0.33010	2.70890
C	0.57170	-0.05830	5.21710
H	2.40950	-0.34080	4.14380
C	-1.39650	0.40220	3.86050
H	-1.08610	0.49310	1.73590
C	-0.80580	0.20540	5.11960
H	1.03150	-0.20170	6.19570
H	-2.46640	0.60630	3.78240
H	1.09620	2.46280	2.28700
H	3.92270	-0.45570	0.26140
O	-0.03140	-2.22660	1.17740
O	-1.83140	0.15040	-3.50840
C	-2.41580	-0.50440	-4.59550
O	-2.65870	-1.67970	-4.59450
C	-2.64920	0.54890	-5.64450
H	-2.33460	1.55010	-5.27290
H	-3.74400	0.62260	-5.83180
C	-0.86020	-2.79810	2.15830
O	-2.05610	-2.77430	2.06990
C	0.05230	-3.38710	3.19590
H	0.37010	-4.39840	2.85610
H	0.98930	-2.79010	3.26880
C	-1.60330	0.27250	6.30550
N	-2.24590	0.32370	7.26580
C	-0.64520	-3.46110	4.54610
H	-1.59700	-4.00860	4.48310
H	-0.01820	-3.96800	5.28910
H	-0.87980	-2.46130	4.93850
C	-1.90530	0.18990	-6.92370
H	-2.12230	0.91300	-7.72020
H	-0.81760	0.18080	-6.77510
H	-2.19360	-0.80450	-7.29550
C	0.36910	1.30670	-2.13130
H	0.02500	1.66380	-3.12230

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9_benzyl_triptycene/opt_c21_folded_opt.xyz

C	-1.57180	-2.25350	-0.87140
C	-0.53530	-1.63180	-0.14770
C	0.07430	-0.45470	-0.58850
C	-0.32930	0.04950	-1.85260
C	-1.35750	-0.56630	-2.56520
C	-1.99720	-1.71770	-2.07960
C	1.92090	0.79530	-2.28340

C	2.32570	0.31690	-1.00470
C	3.62200	-0.13860	-0.82230
C	4.52030	-0.11380	-1.90560
C	4.11960	0.35960	-3.15170
C	2.80500	0.81970	-3.34940
H	-2.04630	-3.15230	-0.47070
H	-2.79640	-2.19460	-2.65310
H	5.53850	-0.47150	-1.76030
H	4.82260	0.37480	-3.98300
H	2.49480	1.18540	-4.32530
C	0.75170	1.84450	0.03270
C	0.76580	2.73860	1.09460
C	0.31100	4.05480	0.89960
C	-0.13620	4.47650	-0.35010
C	-0.11920	3.59360	-1.44300
C	0.33230	2.29730	-1.24790
H	0.31150	4.74690	1.74050
H	-0.49440	5.49530	-0.48800
H	-0.45150	3.92760	-2.42280
C	1.20230	0.37220	0.05450
C	1.67190	-0.12300	1.42520
H	1.89220	-1.21760	1.33570
H	2.64880	0.36440	1.65000
C	0.76160	0.05880	2.60750
C	1.33030	-0.08170	3.88930
C	-0.61000	0.33150	2.50210
C	0.54600	0.05010	5.03190
H	2.39460	-0.28770	3.99390
C	-1.40220	0.45620	3.64380
H	-1.07340	0.45550	1.51950
C	-0.82840	0.31400	4.91410
H	1.00770	-0.05070	6.01640
H	-2.46880	0.66380	3.52730
H	1.12270	2.44630	2.08100
H	3.96060	-0.51700	0.13940
O	-0.02530	-2.24490	1.00110
O	-1.70850	0.08860	-3.74910
C	-2.28800	-0.56960	-4.83660
O	-2.55860	-1.73870	-4.82250
C	-2.47690	0.47290	-5.90540
H	-2.12280	1.46720	-5.55130
H	-3.56760	0.58760	-6.09620
C	-0.87640	-2.80300	1.97080
O	-2.06990	-2.78130	1.85410
C	0.01240	-3.37610	3.03750
H	0.30190	-4.40910	2.74080
H	0.96580	-2.80420	3.09510
C	-1.64870	0.46230	6.15980
F	-1.38110	1.57660	6.86460
F	-1.48080	-0.52590	7.05940
F	-2.98110	0.50560	5.99810
C	-1.74640	0.06050	-7.17610
H	-1.93040	0.77840	-7.98550
H	-0.66040	0.00720	-7.02440
H	-2.07630	-0.92700	-7.53140
C	-0.69720	-3.37510	4.38330
H	-1.65970	-3.90520	4.33720
H	-0.08710	-3.85960	5.15470
H	-0.91360	-2.35400	4.72790
C	0.46600	1.24710	-2.33750
H	0.14340	1.59680	-3.33820

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9_benzyl_triptycene/opt_c22_folded_opt.xyz			
C	-1.70970	-2.20990	-0.81930
C	-0.62350	-1.64440	-0.12520
C	0.04000	-0.50480	-0.59540
C	-0.33960	-0.02040	-1.87310

C	-1.40410	-0.59660	-2.56730
C	-2.11420	-1.68400	-2.04040
C	1.95510	0.58450	-2.31310
C	2.32180	0.15000	-1.00730
C	3.59120	-0.36000	-0.78570
C	4.50150	-0.43340	-1.85700
C	4.13840	-0.00280	-3.12980
C	2.85080	0.51210	-3.36710
H	-2.22560	-3.08300	-0.40820
H	-2.96490	-2.11090	-2.57940
H	5.49840	-0.83380	-1.68110
H	4.84970	-0.06400	-3.95150
H	2.56960	0.84300	-4.36390
C	0.80470	1.79690	-0.06770
C	0.83970	2.73860	0.95210
C	0.45250	4.06440	0.68830
C	0.05100	4.45010	-0.58820
C	0.04590	3.51750	-1.63900
C	0.43020	2.21190	-1.37450
H	0.46870	4.79250	1.49780
H	-0.25410	5.47710	-0.77940
H	-0.25050	3.82050	-2.63960
C	1.18960	0.30690	0.03170
C	1.61880	-0.12450	1.43600
H	1.78130	-1.23720	1.43100
H	2.61460	0.32950	1.64120
C	0.70370	0.18130	2.59180
C	1.25750	0.17580	3.87970
C	-0.67440	0.43530	2.44170
C	0.46860	0.41060	5.01130
H	2.32140	-0.01560	4.01560
C	-1.47950	0.67180	3.54770
H	-1.12200	0.45010	1.44550
C	-0.89550	0.65530	4.83090
H	0.92150	0.40190	5.99580
H	-2.54430	0.87060	3.44540
H	1.15980	2.47480	1.95990
H	3.89860	-0.70620	0.19820
O	-0.19080	-2.17350	1.09700
O	-1.62690	-0.02600	-3.82360
O	-1.81100	0.89490	5.83510
C	-1.32380	0.92550	7.19670
H	-0.59510	1.73130	7.32220
H	-2.24270	1.13630	7.75940
H	-0.90910	-0.04730	7.47460
C	-2.83870	-0.11740	-4.49900
O	-3.77800	-0.74080	-4.08300
C	-2.72390	0.68940	-5.78880
H	-3.69600	0.55570	-6.33640
C	-0.29100	-3.53350	1.39080
O	-0.76600	-4.33220	0.62770
C	0.28660	-3.79680	2.77730
H	0.15770	-4.89800	2.96580
C	-1.58370	0.13870	-6.64220
H	-1.75320	-0.90870	-6.92120
H	-1.47050	0.71190	-7.56990
H	-0.62380	0.18240	-6.10710
C	-2.53840	2.16600	-5.44360
H	-3.38180	2.55680	-4.86050
H	-1.62680	2.32940	-4.85190
H	-2.45590	2.77610	-6.35110
C	-0.50430	-3.01730	3.82280
H	-0.48280	-1.93370	3.62130
H	-1.55790	-3.31860	3.84930
H	-0.09210	-3.16380	4.82730
C	1.77640	-3.46260	2.78180
H	2.19450	-3.53120	3.79270
H	2.34750	-4.14170	2.13830

H	1.95410	-2.43160	2.42200
C	0.52560	1.10530	-2.40890
H	0.23380	1.41760	-3.43130

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9_benzyl_triptycene/opt_c23_folded_opt.xyz

C	-1.69900	-2.20520	-0.66120
C	-0.61060	-1.63730	0.02760
C	0.05710	-0.50480	-0.45420
C	-0.31880	-0.03280	-1.73760
C	-1.38660	-0.61060	-2.42520
C	-2.10140	-1.68940	-1.88730
C	1.98060	0.55490	-2.17980
C	2.34250	0.13530	-0.86780
C	3.60950	-0.37650	-0.63630
C	4.52210	-0.46670	-1.70410
C	4.16380	-0.05090	-2.98320
C	2.87870	0.46560	-3.23040
H	-2.21840	-3.07230	-0.24200
H	-2.95420	-2.11730	-2.42180
H	5.51720	-0.86820	-1.52060
H	4.87700	-0.12520	-3.80220
H	2.60140	0.78490	-4.23200
C	0.83100	1.80040	0.04740
C	0.86860	2.75420	1.05580
C	0.49100	4.07910	0.77430
C	0.09550	4.45150	-0.50800
C	0.08670	3.50590	-1.54710
C	0.46210	2.20140	-1.26530
H	0.51050	4.81720	1.57460
H	-0.20170	5.47820	-0.71290
H	-0.20490	3.79840	-2.55220
C	1.20830	0.30970	0.16600
C	1.62950	-0.10470	1.57720
H	1.79350	-1.21740	1.58760
H	2.62350	0.35210	1.78460
C	0.70560	0.21190	2.72330
C	1.25160	0.20800	4.01870
C	-0.66360	0.47670	2.56800
C	0.44740	0.45550	5.13190
H	2.31160	0.00920	4.16320
C	-1.46850	0.72470	3.67950
H	-1.11040	0.49230	1.57300
C	-0.92200	0.71380	4.97250
H	0.88860	0.44940	6.12620
H	-2.52850	0.92940	3.53910
H	1.18320	2.50070	2.06800
H	3.91290	-0.71100	0.35300
O	-0.17810	-2.15580	1.25410
O	-1.60880	-0.05310	-3.68780
C	-2.83110	-0.12580	-4.34610
O	-3.77700	-0.72620	-3.91130
C	-2.71900	0.66710	-5.64470
H	-3.69890	0.54260	-6.18030
C	-0.29320	-3.50990	1.56810
O	-0.77770	-4.31480	0.81740
C	0.28080	-3.75860	2.95880
H	0.14990	-4.85750	3.15920
C	-1.59630	0.09330	-6.50590
H	-1.78450	-0.95350	-6.77530
H	-1.48440	0.65810	-7.43890
H	-0.63020	0.12630	-5.98120
C	-2.50900	2.14400	-5.31440
H	-3.33900	2.55100	-4.72320
H	-1.58710	2.29990	-4.73660
H	-2.43080	2.74530	-6.22810
C	-0.51350	-2.96640	3.99210
H	-0.49190	-1.88490	3.77740

H	-1.56620	-3.26920	4.02060
H	-0.10250	-3.09830	4.99940
C	1.77090	-3.42650	2.96580
H	2.18480	-3.48520	3.97920
H	2.34380	-4.11270	2.33150
H	1.95190	-2.39920	2.59720
C	-1.79270	0.98420	6.15620
H	-2.72550	0.40500	6.11470
H	-1.30340	0.73880	7.10710
H	-2.07250	2.04710	6.20130
C	0.55370	1.08130	-2.28550
H	0.26590	1.38210	-3.31250

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9_benzyl_triptycene/opt_c24_folded_opt.xyz

C	-1.78200	-2.16440	-0.39920
C	-0.69120	-1.60150	0.29000
C	-0.03470	-0.45680	-0.17780
C	-0.42290	0.03380	-1.45050
C	-1.49250	-0.53920	-2.13930
C	-2.19710	-1.63070	-1.61330
C	1.87020	0.64110	-1.89940
C	2.24400	0.20260	-0.59690
C	3.51540	-0.30540	-0.38250
C	4.42090	-0.37320	-1.45820
C	4.05090	0.06080	-2.72790
C	2.76120	0.57380	-2.95770
H	-2.29260	-3.04150	0.00980
H	-3.05190	-2.05450	-2.14800
H	5.41960	-0.77180	-1.28830
H	4.75860	0.00380	-3.55310
H	2.47480	0.90740	-3.95210
C	0.73050	1.84460	0.35550
C	0.77150	2.78260	1.37840
C	0.38470	4.10980	1.12100
C	-0.02300	4.50020	-0.15210
C	-0.03490	3.57120	-1.20600
C	0.34950	2.26430	-0.94790
H	0.40680	4.83540	1.93260
H	-0.32730	5.52840	-0.33830
H	-0.33600	3.87790	-2.20400
C	1.11610	0.35410	0.44720
C	1.54840	-0.08060	1.84870
H	1.71860	-1.19280	1.84060
H	2.54190	0.37730	2.05700
C	0.63080	0.21180	3.00640
C	1.19090	0.18780	4.29740
C	-0.73940	0.47540	2.86390
C	0.39240	0.41980	5.41870
H	2.25170	-0.01240	4.42860
C	-1.53410	0.70700	3.98910
H	-1.19400	0.50350	1.87310
C	-0.97340	0.67900	5.26920
H	0.83610	0.40040	6.41250
H	-2.59660	0.91170	3.86430
H	1.09580	2.51560	2.38400
H	3.82810	-0.65400	0.59890
O	-0.24440	-2.13930	1.50310
O	-1.72700	0.03650	-3.39130
C	-2.95450	-0.03150	-4.04110
O	-3.89460	-0.64110	-3.60680
C	-2.85480	0.77910	-5.32960
H	-3.84050	0.66360	-5.85650
C	-0.34020	-3.50160	1.78830
O	-0.82200	-4.29530	1.02440
C	0.25030	-3.77260	3.16780
H	0.12820	-4.87600	3.34910
C	-1.74230	0.21470	-6.21010

H	-1.93540	-0.82800	-6.49150
H	-1.63900	0.79160	-7.13670
H	-0.77060	0.23900	-5.69540
C	-2.63840	2.25110	-4.98200
H	-3.46220	2.65220	-4.37820
H	-1.71100	2.39740	-4.41060
H	-2.56690	2.86410	-5.88850
C	-0.53700	-3.00490	4.22480
H	-0.52350	-1.91950	4.03140
H	-1.58790	-3.31400	4.25800
H	-0.11530	-3.15590	5.22500
C	1.73840	-3.43170	3.16410
H	2.16460	-3.50940	4.17120
H	2.30770	-4.10160	2.50930
H	1.90960	-2.39620	2.81500
H	-1.59470	0.86100	6.14260
C	0.43970	1.16130	-1.98650
H	0.14290	1.47680	-3.00650

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9_benzyl_triptycene/opt_c26_folded_opt.xyz

C	-1.78230	-2.15830	-0.38980
C	-0.68930	-1.59650	0.29700
C	-0.03060	-0.45450	-0.17310
C	-0.42180	0.03730	-1.44460
C	-1.49410	-0.53370	-2.13100
C	-2.19890	-1.62460	-1.60320
C	1.87070	0.63930	-1.90140
C	2.24850	0.19830	-0.60100
C	3.51910	-0.31440	-0.39240
C	4.41970	-0.38430	-1.47190
C	4.04590	0.05230	-2.73960
C	2.75710	0.57000	-2.96350
H	-2.29270	-3.03480	0.02060
H	-3.05490	-2.04810	-2.13660
H	5.41780	-0.78670	-1.30660
H	4.75000	-0.00650	-3.56790
H	2.46770	0.90560	-3.95650
C	0.74390	1.84410	0.35890
C	0.79380	2.78160	1.38190
C	0.40770	4.10960	1.12780
C	-0.00700	4.50150	-0.14250
C	-0.02600	3.57340	-1.19710
C	0.35750	2.26560	-0.94230
H	0.43600	4.83480	1.93970
H	-0.31110	5.53040	-0.32620
H	-0.33160	3.88170	-2.19350
C	1.12530	0.35250	0.44740
C	1.56210	-0.08560	1.84710
H	1.72780	-1.19860	1.83570
H	2.55830	0.36890	2.05070
C	0.65020	0.20960	3.00790
C	1.21560	0.18090	4.29670
C	-0.72140	0.47740	2.86510
C	0.43320	0.40980	5.42980
H	2.27840	-0.02310	4.42120
C	-1.52510	0.71000	3.98240
H	-1.17440	0.50820	1.87160
C	-0.92670	0.66950	5.24400
H	0.87410	0.38820	6.42460
H	-2.58790	0.91830	3.86600
H	1.12660	2.51450	2.38430
H	3.83490	-0.66520	0.58720
O	-0.24710	-2.13370	1.51230
O	-1.73100	0.04370	-3.38110
C	-2.95640	-0.03350	-4.03540
O	-3.89260	-0.65050	-3.60380
C	-2.85840	0.77850	-5.32310

H	-3.84220	0.65690	-5.85250
C	-0.32550	-3.50100	1.78490
O	-0.78810	-4.29310	1.00810
C	0.25580	-3.77520	3.16740
H	0.13350	-4.87920	3.34530
C	-1.74030	0.22120	-6.20100
H	-1.92580	-0.82290	-6.48260
H	-1.63930	0.79830	-7.12790
H	-0.76980	0.25240	-5.68470
C	-2.65230	2.25160	-4.97450
H	-3.48010	2.64720	-4.37240
H	-1.72700	2.40400	-4.40140
H	-2.58320	2.86540	-5.88070
C	-0.53760	-3.01140	4.22260
H	-0.52960	-1.92720	4.02940
H	-1.58730	-3.32640	4.25360
H	-0.11900	-3.16220	5.22450
C	1.74390	-3.43360	3.17190
H	2.16380	-3.50800	4.18200
H	2.31730	-4.10710	2.52390
H	1.91800	-2.40050	2.81850
F	-1.68710	0.88660	6.32030
C	0.44120	1.16350	-1.98250
H	0.14140	1.48100	-3.00110

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9_benzyl_triptycene/opt_c27_folded_opt.xyz

C	-1.74980	-2.16090	-0.47750
C	-0.65680	-1.59840	0.20850
C	0.01030	-0.46540	-0.27040
C	-0.37220	0.01650	-1.54820
C	-1.44530	-0.55450	-2.23350
C	-2.15820	-1.63640	-1.69760
C	1.92670	0.59900	-1.99980
C	2.29600	0.16870	-0.69330
C	3.56210	-0.34980	-0.47300
C	4.46720	-0.43640	-1.54760
C	4.10200	-0.01060	-2.82140
C	2.81760	0.51310	-3.05680
H	-2.26610	-3.03100	-0.06120
H	-3.01430	-2.06110	-2.23070
H	5.46200	-0.84350	-1.37370
H	4.80960	-0.08250	-3.64590
H	2.53520	0.84030	-4.05470
C	0.79740	1.83370	0.24300
C	0.84890	2.78020	1.25750
C	0.47250	4.10820	0.98900
C	0.06610	4.49040	-0.28700
C	0.04570	3.55240	-1.33280
C	0.41960	2.24460	-1.06400
H	0.50240	4.84150	1.79370
H	-0.23030	5.51970	-0.48190
H	-0.25330	3.85340	-2.33360
C	1.16830	0.34040	0.34690
C	1.59200	-0.08600	1.75370
H	1.75780	-1.20020	1.75360
H	2.58750	0.36790	1.96370
C	0.66850	0.21500	2.90190
C	1.21600	0.17410	4.19950
C	-0.69700	0.50260	2.74640
C	0.41680	0.40650	5.31630
H	2.27430	-0.04210	4.33810
C	-1.50450	0.73590	3.85800
H	-1.13890	0.54600	1.74810
C	-0.95030	0.68500	5.14800
H	0.84760	0.37340	6.31750
H	-2.56500	0.95760	3.72670
H	1.17650	2.52180	2.26340

H	3.87150	-0.69270	0.51130
O	-0.22480	-2.12690	1.43170
O	-1.67460	0.01450	-3.48810
C	-2.89260	-0.07540	-4.15610
O	-3.82880	-0.69610	-3.73010
C	-2.78490	0.72910	-5.44750
H	-3.76150	0.59690	-5.98780
C	-0.29840	-3.49530	1.70590
O	-0.74210	-4.29040	0.92210
C	0.26090	-3.76210	3.09870
H	0.13750	-4.86580	3.27970
C	-1.65250	0.17470	-6.30850
H	-1.82670	-0.87260	-6.58550
H	-1.54540	0.74650	-7.23810
H	-0.68820	0.21690	-5.78150
C	-2.59390	2.20590	-5.10580
H	-3.43270	2.59990	-4.51820
H	-1.67770	2.36880	-4.52120
H	-2.51670	2.81420	-6.01520
C	-0.55100	-2.99600	4.13820
H	-0.54410	-1.91310	3.94130
H	-1.60010	-3.31530	4.15410
H	-0.14860	-3.14380	5.14730
C	1.74850	-3.41920	3.12520
H	2.15160	-3.48590	4.14280
H	2.33270	-4.09910	2.49330
H	1.92970	-2.39020	2.76570
C	-1.77710	0.91650	6.29260
N	-2.44480	1.10140	7.21880
C	0.50100	1.13170	-2.09290
H	0.20810	1.44110	-3.11600

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9_benzyl_triptycene/opt_c28_folded_opt.xyz

C	-1.70500	-2.18080	-0.64920
C	-0.60730	-1.62320	0.03370
C	0.06690	-0.49670	-0.45060
C	-0.31410	-0.01670	-1.72960
C	-1.39110	-0.58370	-2.41190
C	-2.11070	-1.65870	-1.87120
C	1.98730	0.55230	-2.18620
C	2.35610	0.12330	-0.87920
C	3.61980	-0.40100	-0.65920
C	4.52320	-0.49460	-1.73470
C	4.15860	-0.06980	-3.00900
C	2.87650	0.45950	-3.24420
H	-2.22730	-3.04530	-0.22870
H	-2.97010	-2.07960	-2.40180
H	5.51630	-0.90600	-1.56090
H	4.86490	-0.14690	-3.83410
H	2.59450	0.78580	-4.24240
C	0.86800	1.79910	0.05480
C	0.92590	2.74780	1.06690
C	0.55630	4.07710	0.79540
C	0.15030	4.45820	-0.48110
C	0.12350	3.51750	-1.52450
C	0.49060	2.20850	-1.25270
H	0.59110	4.81230	1.59830
H	-0.14070	5.48850	-0.67830
H	-0.17540	3.81750	-2.52560
C	1.23080	0.30410	0.16200
C	1.65430	-0.12070	1.56920
H	1.81570	-1.23570	1.57160
H	2.65180	0.32960	1.77790
C	0.73260	0.18460	2.71710
C	1.27800	0.13380	4.01560
C	-0.62960	0.48370	2.56500
C	0.47650	0.36280	5.13090

H	2.33470	-0.08850	4.15550
C	-1.43660	0.71360	3.67940
H	-1.07240	0.53750	1.56770
C	-0.88830	0.64920	4.96710
H	0.91590	0.31600	6.12930
H	-2.49430	0.94030	3.52910
H	1.25300	2.49040	2.07320
H	3.92870	-0.74320	0.32550
O	-0.17800	-2.14950	1.25870
O	-1.61710	-0.01950	-3.66950
C	-2.83780	-0.10020	-4.33360
O	-3.77960	-0.70760	-3.90100
C	-2.72470	0.69450	-5.63050
H	-3.70420	0.56960	-6.16740
C	-0.26690	-3.51560	1.54170
O	-0.71590	-4.31060	0.76080
C	0.28410	-3.77990	2.93820
H	0.15530	-4.88260	3.12200
C	-1.60100	0.12170	-6.49100
H	-1.78750	-0.92540	-6.76040
H	-1.49020	0.68600	-7.42470
H	-0.63480	0.15680	-5.96700
C	-2.51640	2.17130	-5.29930
H	-3.34880	2.57810	-4.71110
H	-1.59630	2.32810	-4.71920
H	-2.43610	2.77280	-6.21290
C	-0.53130	-3.00790	3.97030
H	-0.52240	-1.92590	3.76930
H	-1.58100	-3.32560	3.98390
H	-0.13430	-3.15090	4.98240
C	1.77290	-3.44320	2.97230
H	2.16840	-3.50400	3.99330
H	2.35850	-4.13040	2.34970
H	1.96140	-2.41790	2.60670
C	-1.73160	0.86880	6.18660
F	-1.27170	1.81880	7.02100
F	-1.84250	-0.21650	6.97610
F	-3.00770	1.23200	5.97790
C	0.56440	1.09220	-2.27860
H	0.27150	1.40040	-3.30220

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9_benzyl_triptycene/opt_c29_folded_opt.xyz

C	-1.90210	-2.48550	-1.26970
C	-0.86310	-1.87920	-0.53910
C	-0.17020	-0.76350	-1.01660
C	-0.48140	-0.31990	-2.32820
C	-1.50910	-0.92560	-3.05130
C	-2.23960	-2.00320	-2.52840
C	1.82910	0.27700	-2.67340
C	2.13730	-0.13480	-1.34540
C	3.39620	-0.63840	-1.05840
C	4.35290	-0.72960	-2.08690
C	4.04650	-0.32200	-3.38200
C	2.77070	0.18750	-3.68520
H	-2.44690	-3.32810	-0.83730
H	-3.04360	-2.46770	-3.10600
H	5.34160	-1.12510	-1.85970
H	4.79390	-0.39650	-4.17010
H	2.53510	0.50290	-4.69870
C	0.59460	1.53320	-0.49990
C	0.59550	2.48860	0.50740
C	0.23190	3.81280	0.20610
C	-0.11460	4.17890	-1.09240
C	-0.08770	3.22910	-2.12760
C	0.27440	1.92470	-1.82800
H	0.22240	4.55530	1.00270
H	-0.40230	5.20530	-1.31310

H	-0.34340	3.51850	-3.14380
C	0.96240	0.04460	-0.35840
C	1.32540	-0.38110	1.06680
H	1.56680	-1.47230	1.04250
H	2.26970	0.13770	1.34930
C	0.31860	-0.16300	2.16580
C	0.72710	-0.44810	3.47650
C	-1.00150	0.27680	1.94390
C	-0.14890	-0.30950	4.55800
H	1.74570	-0.78470	3.66820
C	-1.89090	0.42380	2.99920
H	-1.34220	0.50550	0.93090
C	-1.45240	0.12890	4.30670
H	0.19320	-0.53370	5.56200
H	-2.91500	0.75700	2.83920
H	0.86860	2.23210	1.53090
H	3.66070	-0.96640	-0.05560
O	-0.43210	-2.44540	0.66580
O	-1.75180	-0.33740	-4.29970
O	-2.43590	0.31890	5.25380
C	-2.10170	0.05160	6.63580
H	-1.30070	0.71690	6.96980
H	-3.04610	0.28790	7.14390
H	-1.84080	-1.00210	6.76720
C	-2.42950	-0.96540	-5.32790
O	-2.89560	-2.06850	-5.26250
C	-1.31990	-2.88880	1.63770
O	-2.50940	-2.91020	1.49210
H	-2.42310	-0.23660	-6.14400
H	-0.68610	-3.18840	2.47580
C	0.40620	0.79940	-2.84050
H	0.15990	1.10050	-3.87770

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9_benzyl_triptycene/opt_c2_folded_opt.xyz

C	-1.75010	-2.43860	-1.02490
C	-0.70710	-1.84150	-0.29740
C	-0.04050	-0.70540	-0.78930
C	-0.35760	-0.26680	-2.09210
C	-1.39280	-0.87120	-2.82100
C	-2.10790	-1.94850	-2.28050
C	1.95120	0.35350	-2.43250
C	2.25860	-0.04400	-1.09910
C	3.52240	-0.52670	-0.80010
C	4.48670	-0.61200	-1.82240
C	4.18170	-0.22010	-3.12240
C	2.90020	0.26820	-3.43760
H	-2.27360	-3.30030	-0.61730
H	-2.92120	-2.41580	-2.82730
H	5.47930	-0.99090	-1.58590
H	4.93410	-0.29030	-3.90560
H	2.66490	0.56960	-4.45540
C	0.68880	1.60650	-0.27560
C	0.67030	2.56700	0.72660
C	0.29580	3.88600	0.41540
C	-0.04370	4.24170	-0.88780
C	0.00040	3.28650	-1.91750
C	0.37380	1.98760	-1.60840
H	0.27310	4.63220	1.20750
H	-0.33880	5.26380	-1.11660
H	-0.25110	3.56670	-2.93740
C	1.07340	0.12240	-0.12390
C	1.41730	-0.28960	1.30950
H	1.67530	-1.37910	1.29740
H	2.34540	0.24370	1.61300
C	0.37700	-0.09130	2.38130
C	0.75460	-0.37880	3.70590
C	-0.93690	0.33230	2.13390

C	-0.15720	-0.24720	4.75240
H	1.76840	-0.71110	3.92100
C	-1.85080	0.46540	3.18020
H	-1.25950	0.56120	1.11700
C	-1.47070	0.17760	4.49900
H	0.15430	-0.47400	5.76970
H	-2.86390	0.79940	2.96590
H	0.93550	2.31780	1.75370
H	3.78360	-0.84370	0.20690
O	-0.22010	-2.38640	0.87760
O	-1.60430	-0.30090	-4.06370
C	-2.60930	-0.90560	-4.90960
H	-3.59660	-0.82060	-4.44700
H	-2.54440	-0.28390	-5.81200
H	-2.34850	-1.94440	-5.13080
C	-1.18090	-3.03230	1.74940
H	-0.58510	-3.19050	2.65800
H	-2.02120	-2.36230	1.95490
H	-1.50340	-3.98080	1.31500
C	-2.45410	0.30750	5.61730
H	-3.00120	-0.63410	5.76730
H	-1.96890	0.55770	6.56980
H	-3.19960	1.09010	5.42400
C	0.52210	0.85610	-2.61150
H	0.27620	1.14320	-3.65320

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9_benzyl_triptycene/opt_c30_folded_opt.xyz

C	-1.89640	-2.49240	-1.05560
C	-0.85560	-1.87950	-0.33310
C	-0.16110	-0.77080	-0.82420
C	-0.47150	-0.34330	-2.14130
C	-1.50030	-0.95610	-2.85670
C	-2.23310	-2.02540	-2.32020
C	1.84020	0.24650	-2.49310
C	2.14730	-0.14740	-1.15950
C	3.40600	-0.64720	-0.86470
C	4.36310	-0.75340	-1.89150
C	4.05740	-0.36400	-3.19230
C	2.78210	0.14210	-3.50320
H	-2.44230	-3.32830	-0.61210
H	-3.03820	-2.49540	-2.89180
H	5.35150	-1.14610	-1.65820
H	4.80490	-0.45030	-3.97910
H	2.54730	0.44350	-4.52120
C	0.60410	1.53190	-0.33690
C	0.60230	2.49940	0.65880
C	0.24120	3.82020	0.34010
C	-0.10090	4.17050	-0.96400
C	-0.07300	3.20780	-1.98720
C	0.28670	1.90680	-1.67040
H	0.23060	4.57260	1.12710
H	-0.38570	5.19470	-1.19840
H	-0.32600	3.48480	-3.00760
C	0.97170	0.04520	-0.17610
C	1.33300	-0.36050	1.25480
H	1.59320	-1.44780	1.24260
H	2.26650	0.17580	1.54070
C	0.31440	-0.15300	2.34480
C	0.70650	-0.46670	3.65810
C	-0.99600	0.29540	2.12160
C	-0.19170	-0.34610	4.71880
H	1.72120	-0.80690	3.85630
C	-1.89500	0.41660	3.18060
H	-1.32960	0.54980	1.11390
C	-1.50400	0.09330	4.48950
H	0.13150	-0.59220	5.72830
H	-2.91060	0.75910	2.98560

H	0.87040	2.25440	1.68640
H	3.67000	-0.96100	0.14270
O	-0.42490	-2.43500	0.87700
O	-1.74010	-0.38360	-4.11300
C	-2.42430	-1.01960	-5.13170
O	-2.90150	-2.11680	-5.05040
C	-1.31320	-2.85020	1.86060
O	-2.50400	-2.85850	1.72160
H	-2.41090	-0.30270	-5.95830
H	-0.67910	-3.14430	2.70080
C	-2.48020	0.21700	5.61300
H	-3.37010	-0.40510	5.43710
H	-2.05930	-0.08840	6.57900
H	-2.82760	1.25420	5.72570
C	0.41790	0.76800	-2.66800
H	0.17260	1.05560	-3.70920

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9_benzyl_triptycene/opt_c31_folded_opt.xyz

C	-2.06130	-2.47870	-0.75810
C	-1.01240	-1.87980	-0.03570
C	-0.33290	-0.75330	-0.50650
C	-0.66820	-0.29000	-1.80530
C	-1.70530	-0.88860	-2.52070
C	-2.42230	-1.97770	-2.00290
C	1.63360	0.32450	-2.17910
C	1.96600	-0.10630	-0.86310
C	3.23240	-0.60690	-0.60460
C	4.17220	-0.67700	-1.65020
C	3.84200	-0.25140	-2.93360
C	2.55870	0.25570	-3.20770
H	-2.59470	-3.33070	-0.33010
H	-3.23420	-2.43640	-2.57410
H	5.16660	-1.07060	-1.44560
H	4.57640	-0.30980	-3.73530
H	2.30460	0.58520	-4.21220
C	0.42770	1.53880	0.03470
C	0.43810	2.47720	1.05780
C	0.06390	3.80440	0.78370
C	-0.30320	4.19010	-0.50340
C	-0.28770	3.25750	-1.55440
C	0.08500	1.95020	-1.28170
H	0.06300	4.53380	1.59230
H	-0.59800	5.21880	-0.70310
H	-0.56010	3.56230	-2.56180
C	0.80640	0.05040	0.14540
C	1.19450	-0.39550	1.55690
H	1.45650	-1.48180	1.50900
H	2.13310	0.13340	1.84060
C	0.19760	-0.22190	2.67270
C	0.62520	-0.56230	3.97020
C	-1.11940	0.22140	2.48640
C	-0.25050	-0.46370	5.05210
H	1.64550	-0.90150	4.13560
C	-1.99310	0.31700	3.57270
H	-1.47740	0.49310	1.49220
C	-1.56480	-0.02700	4.85730
H	0.09180	-0.72650	6.05190
H	-3.01600	0.65720	3.41150
H	0.72600	2.20530	2.07300
H	3.51560	-0.94860	0.38830
O	-0.55820	-2.46660	1.15100
O	-1.97000	-0.28200	-3.75560
C	-2.66980	-0.89220	-4.77990
O	-3.13980	-1.99400	-4.72150
C	-1.42850	-2.91940	2.13470
O	-2.62120	-2.92720	2.01510
H	-2.67500	-0.15160	-5.58540

H	-0.77930	-3.23930	2.95360
H	-2.24820	0.04630	5.70020
C	0.20550	0.84180	-2.31420
H	-0.05940	1.15810	-3.34230

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9_benzyl_triptycene/opt_c33_folded_opt.xyz

C	-2.05580	-2.49400	-0.78300
C	-1.01140	-1.89650	-0.05270
C	-0.33430	-0.76450	-0.51340
C	-0.66630	-0.29420	-1.81060
C	-1.69940	-0.89080	-2.53360
C	-2.41450	-1.98570	-2.02520
C	1.63560	0.32560	-2.17290
C	1.96450	-0.11210	-0.85830
C	3.23050	-0.61280	-0.59850
C	4.17370	-0.67590	-1.64140
C	3.84710	-0.24350	-2.92350
C	2.56410	0.26350	-3.19890
H	-2.58750	-3.35140	-0.36360
H	-3.22320	-2.44340	-2.60230
H	5.16810	-1.06920	-1.43570
H	4.58430	-0.29660	-3.72310
H	2.31270	0.59810	-4.20260
C	0.42170	1.52670	0.04290
C	0.43100	2.46080	1.07000
C	0.05410	3.78850	0.80200
C	-0.31310	4.17950	-0.48350
C	-0.29400	3.25210	-1.53890
C	0.08100	1.94410	-1.27220
H	0.05160	4.51430	1.61400
H	-0.61030	5.20860	-0.67840
H	-0.56520	3.56140	-2.54540
C	0.80120	0.03800	0.14660
C	1.18370	-0.41540	1.55780
H	1.43330	-1.50470	1.50770
H	2.12870	0.10280	1.84090
C	0.18800	-0.22930	2.67190
C	0.62290	-0.54000	3.97460
C	-1.13410	0.20090	2.47520
C	-0.23960	-0.43070	5.06570
H	1.64820	-0.86950	4.14120
C	-2.01720	0.31760	3.55020
H	-1.49160	0.44890	1.47250
C	-1.54810	-0.00210	4.82610
H	0.10140	-0.66860	6.07190
H	-3.04420	0.64550	3.38930
H	0.72250	2.18670	2.08330
H	3.51110	-0.95990	0.39330
O	-0.55860	-2.49150	1.13100
O	-1.96180	-0.27680	-3.76480
C	-2.65520	-0.88340	-4.79640
O	-3.11980	-1.98770	-4.74640
C	-1.43090	-2.96740	2.10230
O	-2.62340	-2.96280	1.98340
H	-2.66040	-0.13700	-5.59660
H	-0.78330	-3.31260	2.91190
F	-2.38340	0.10420	5.86200
C	0.20720	0.84170	-2.31020
H	-0.05460	1.16320	-3.33750

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9_benzyl_triptycene/opt_c34_folded_opt.xyz

C	-1.98860	-2.49850	-0.90390
C	-0.95030	-1.89590	-0.16900
C	-0.26530	-0.77120	-0.63490
C	-0.58160	-0.31410	-1.94080
C	-1.60860	-0.91560	-2.66850

C	-2.33240	-2.00290	-2.15530
C	1.72620	0.29630	-2.28410
C	2.03930	-0.12830	-0.96140
C	3.30060	-0.63020	-0.68180
C	4.25540	-0.70660	-1.71330
C	3.94460	-0.28610	-3.00330
C	2.66620	0.22130	-3.29870
H	-2.52730	-3.35000	-0.48140
H	-3.13630	-2.46470	-2.73600
H	5.24620	-1.10100	-1.49260
H	4.69090	-0.34900	-3.79380
H	2.42740	0.54640	-4.30860
C	0.49050	1.52460	-0.09550
C	0.49090	2.46980	0.92140
C	0.11930	3.79510	0.63500
C	-0.23400	4.17240	-0.65850
C	-0.20520	3.23350	-1.70350
C	0.16490	1.92800	-1.41860
H	0.11010	4.53030	1.43860
H	-0.52780	5.19990	-0.86770
H	-0.46530	3.53230	-2.71630
C	0.86510	0.03610	0.02770
C	1.22830	-0.40250	1.44830
H	1.48190	-1.49240	1.41260
H	2.16940	0.11830	1.74110
C	0.21610	-0.20990	2.54430
C	0.62650	-0.51970	3.85650
C	-1.10050	0.22510	2.32830
C	-0.25720	-0.39970	4.92560
H	1.64690	-0.85290	4.04250
C	-1.99390	0.34550	3.39210
H	-1.44270	0.47390	1.32020
C	-1.57530	0.03120	4.69510
H	0.06930	-0.63720	5.93910
H	-3.01800	0.67820	3.21060
H	0.77190	2.20760	1.94040
H	3.56930	-0.96810	0.31630
O	-0.51190	-2.48170	1.02550
O	-1.85620	-0.31500	-3.90860
C	-2.53960	-0.93240	-4.94170
O	-3.00530	-2.03550	-4.88340
C	-1.39760	-2.94680	1.99050
O	-2.58900	-2.91740	1.86670
H	-2.53470	-0.19460	-5.74970
H	-0.76040	-3.30690	2.80170
C	-2.48750	0.15240	5.79110
N	-3.22250	0.25100	6.67850
C	0.30050	0.81400	-2.44290
H	0.05110	1.12480	-3.47680

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9_benzyl_triptycene/opt_c36_folded_opt.xyz

C	-1.90640	-2.43290	-1.19020
C	-0.85610	-1.82560	-0.47710
C	-0.16710	-0.70870	-0.95360
C	-0.49470	-0.26350	-2.26280
C	-1.53470	-0.86810	-2.96550
C	-2.26320	-1.94560	-2.44160
C	1.81210	0.32320	-2.63860
C	2.13540	-0.08860	-1.31470
C	3.39540	-0.59860	-1.04340
C	4.33780	-0.69500	-2.08430
C	4.01680	-0.28590	-3.37560
C	2.73980	0.22950	-3.66280
H	-2.44250	-3.28040	-0.75580
H	-3.07540	-2.40660	-3.00950
H	5.32780	-1.09540	-1.86980
H	4.75420	-0.36340	-4.17340

H	2.49370	0.54760	-4.67340
C	0.60780	1.58720	-0.45120
C	0.62320	2.54410	0.55480
C	0.25900	3.86860	0.25570
C	-0.10230	4.23380	-1.03910
C	-0.09040	3.28270	-2.07330
C	0.27240	1.97810	-1.77530
H	0.26110	4.61270	1.05130
H	-0.38970	5.26120	-1.25800
H	-0.35700	3.57180	-3.08740
C	0.97630	0.09880	-0.31110
C	1.35480	-0.32380	1.11000
H	1.59300	-1.41570	1.09300
H	2.30720	0.19040	1.37650
C	0.36490	-0.09000	2.22090
C	0.79970	-0.34600	3.53060
C	-0.96190	0.33130	2.01370
C	-0.06310	-0.21240	4.62090
H	1.82660	-0.66540	3.71170
C	-1.84000	0.47300	3.08020
H	-1.31900	0.55420	1.00590
C	-1.38080	0.19410	4.38340
H	0.29610	-0.42540	5.62250
H	-2.87050	0.79100	2.93140
H	0.90860	2.28910	1.57570
H	3.67180	-0.92700	-0.04350
O	-0.38990	-2.41810	0.71330
O	-1.81080	-0.25730	-4.20590
O	-2.35500	0.36630	5.34150
C	-2.00970	0.06680	6.71510
H	-1.22320	0.74130	7.06450
H	-2.95760	0.26620	7.23220
H	-1.72310	-0.98410	6.81570
C	-2.33470	-0.98210	-5.25720
O	-2.65030	-2.13760	-5.22920
C	-1.29120	-2.81400	1.68810
O	-2.48420	-2.76550	1.59250
C	-2.42580	-0.05390	-6.38400
C	-0.49750	-3.31550	2.80860
N	-2.50500	0.65690	-7.28650
N	0.10510	-3.70900	3.70770
C	0.38950	0.85200	-2.78850
H	0.13230	1.15490	-3.82300

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9_benzyl_triptycene/opt_c37_folded_opt.xyz

C	-1.71750	-2.58520	-0.99200
C	-0.70200	-1.92050	-0.27990
C	-0.05140	-0.78820	-0.77380
C	-0.37650	-0.38770	-2.09770
C	-1.37420	-1.05640	-2.80400
C	-2.06990	-2.14680	-2.26270
C	1.91250	0.28450	-2.44860
C	2.22840	-0.07700	-1.10830
C	3.50400	-0.52300	-0.80030
C	4.46930	-0.60580	-1.82120
C	4.15510	-0.24700	-3.12910
C	2.86250	0.20330	-3.45330
H	-2.23050	-3.43840	-0.54130
H	-2.86910	-2.64020	-2.82190
H	5.47170	-0.95570	-1.57790
H	4.91010	-0.31380	-3.91120
H	2.62090	0.48080	-4.47720
C	0.61240	1.55200	-0.31800
C	0.56460	2.53340	0.66300
C	0.15320	3.83370	0.32170
C	-0.19230	4.15140	-0.98990
C	-0.11860	3.17570	-1.99830

C	0.28920	1.89480	-1.65840
H	0.10700	4.59690	1.09760
H	-0.51480	5.16050	-1.24180
H	-0.37110	3.42880	-3.02530
C	1.04290	0.08510	-0.13190
C	1.40960	-0.28240	1.30700
H	1.70120	-1.36140	1.32520
H	2.33010	0.28320	1.58170
C	0.38370	-0.07060	2.38930
C	0.79890	-0.27780	3.71690
C	-0.95190	0.27990	2.14740
C	-0.10380	-0.15730	4.77270
H	1.83350	-0.54340	3.92990
C	-1.85640	0.40150	3.20270
H	-1.30130	0.46580	1.13100
C	-1.44390	0.17840	4.52500
H	0.23550	-0.33010	5.79290
H	-2.89190	0.66740	2.99360
H	0.83560	2.31600	1.69650
H	3.77530	-0.81150	0.21320
O	-0.22920	-2.46780	0.92910
O	-1.54900	-0.58230	-4.12050
C	-2.76790	-0.67890	-4.76010
O	-3.75460	-1.20020	-4.32410
C	-1.12500	-2.86700	1.90740
O	-2.31850	-2.85480	1.80420
C	-2.59510	-0.03010	-6.05970
C	-0.32340	-3.32370	3.04120
N	-2.48470	0.47750	-7.08740
N	0.28680	-3.68350	3.94920
C	-2.42550	0.29170	5.64440
H	-3.20970	-0.47560	5.56160
H	-1.96120	0.17100	6.63160
H	-2.92760	1.26970	5.64220
C	0.47200	0.74840	-2.63840
H	0.22440	1.01030	-3.68650

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9_benzyl_triptycene/opt_c38_folded_opt.xyz

C	-2.02450	-2.44580	-0.67960
C	-0.96360	-1.84210	0.02060
C	-0.30110	-0.70540	-0.44610
C	-0.66740	-0.23370	-1.73550
C	-1.71750	-0.83490	-2.42600
C	-2.41910	-1.93380	-1.90960
C	1.62180	0.39320	-2.15380
C	1.98370	-0.04530	-0.84860
C	3.25690	-0.54360	-0.62050
C	4.17450	-0.60130	-1.68620
C	3.81580	-0.16630	-2.95900
C	2.52500	0.33720	-3.20240
H	-2.53820	-3.31030	-0.25190
H	-3.23950	-2.39190	-2.46790
H	5.17510	-0.99210	-1.50570
H	4.53430	-0.21400	-3.77620
H	2.24950	0.67560	-4.19880
C	0.45570	1.58840	0.09230
C	0.48310	2.52130	1.12030
C	0.09520	3.84760	0.86160
C	-0.30210	4.23850	-0.41500
C	-0.30380	3.31210	-1.47150
C	0.08260	2.00580	-1.21350
H	0.10810	4.57290	1.67430
H	-0.60710	5.26700	-0.60240
H	-0.59900	3.62140	-2.47160
C	0.84740	0.10210	0.18700
C	1.26500	-0.34820	1.58780
H	1.51950	-1.43610	1.54080

H	2.21690	0.17160	1.84600
C	0.29840	-0.15740	2.72730
C	0.77350	-0.43910	4.02210
C	-1.03480	0.24300	2.56470
C	-0.07470	-0.33340	5.12470
H	1.80690	-0.74770	4.16990
C	-1.88070	0.34820	3.67260
H	-1.42610	0.48390	1.57610
C	-1.40730	0.05640	4.95370
H	0.30230	-0.56010	6.12170
H	-2.91660	0.65600	3.53070
H	0.79560	2.24670	2.12790
H	3.56260	-0.89190	0.36400
O	-0.45880	-2.45890	1.18250
O	-2.03300	-0.19860	-3.64380
C	-2.57380	-0.90520	-4.69910
O	-2.87360	-2.06520	-4.69080
C	-1.32760	-2.88200	2.17550
O	-2.52310	-2.82970	2.12100
C	-2.70510	0.04840	-5.80020
C	-0.49610	-3.41520	3.25280
N	-2.81590	0.77980	-6.68280
N	0.13860	-3.83440	4.11740
H	-2.06920	0.13350	5.81360
C	0.18910	0.90560	-2.25600
H	-0.09770	1.22930	-3.27640

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9_benzyl_triptycene/opt_c3_folded_opt.xyz

C	-1.90340	-2.41730	-0.71560
C	-0.85290	-1.82810	0.00730
C	-0.20180	-0.67750	-0.47170
C	-0.54390	-0.21290	-1.75900
C	-1.58690	-0.80930	-2.48360
C	-2.28490	-1.90320	-1.95460
C	1.75450	0.43140	-2.12510
C	2.08770	0.00630	-0.80650
C	3.35990	-0.47350	-0.54020
C	4.30700	-0.52850	-1.58050
C	3.97680	-0.10960	-2.86590
C	2.68660	0.37610	-3.14790
H	-2.41500	-3.29100	-0.31860
H	-3.10390	-2.36490	-2.49790
H	5.30630	-0.90490	-1.36970
H	4.71610	-0.15650	-3.66330
H	2.43170	0.69880	-4.15450
C	0.52210	1.62710	0.08090
C	0.51580	2.56490	1.10450
C	0.12780	3.88810	0.82940
C	-0.23710	4.27030	-0.45940
C	-0.20570	3.33840	-1.51070
C	0.18110	2.03540	-1.23730
H	0.11470	4.61650	1.63810
H	-0.54220	5.29530	-0.66020
H	-0.47700	3.63940	-2.51950
C	0.91850	0.14250	0.19230
C	1.28980	-0.30000	1.60940
H	1.55820	-1.38670	1.56660
H	2.21860	0.23380	1.91050
C	0.26720	-0.13880	2.70430
C	0.67360	-0.46340	4.01280
C	-1.05180	0.28890	2.49090
C	-0.22200	-0.36240	5.07800
H	1.69150	-0.79870	4.19810
C	-1.94390	0.38980	3.56100
H	-1.39280	0.54430	1.48700
C	-1.53540	0.06420	4.85700
H	0.10440	-0.61540	6.08520

H	-2.96320	0.72770	3.38070
H	0.80090	2.29520	2.12080
H	3.64100	-0.81080	0.45470
O	-0.34340	-2.38910	1.16480
O	-1.82340	-0.21390	-3.70990
C	-2.83730	-0.80880	-4.55220
H	-3.81750	-0.74270	-4.07160
H	-2.79290	-0.16680	-5.44160
H	-2.57150	-1.84010	-4.80060
C	-1.27700	-3.08960	2.02360
H	-0.67020	-3.25410	2.92380
H	-2.13710	-2.45340	2.25260
H	-1.57160	-4.03570	1.56460
H	-2.23130	0.14540	5.68770
C	0.31910	0.92760	-2.26800
H	0.05310	1.23630	-3.29860

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9_benzyl_triptycene/opt_c40_folded_opt.xyz

C	-2.01610	-2.46140	-0.69910
C	-0.96110	-1.85500	0.00730
C	-0.30310	-0.71260	-0.45240
C	-0.66580	-0.23860	-1.74170
C	-1.71040	-0.84240	-2.43880
C	-2.40860	-1.94640	-1.92860
C	1.62320	0.39610	-2.14800
C	1.98100	-0.04460	-0.84230
C	3.25450	-0.53990	-0.60980
C	4.17660	-0.59300	-1.67190
C	3.82210	-0.15600	-2.94520
C	2.53110	0.34490	-3.19290
H	-2.52710	-3.33070	-0.27750
H	-3.22500	-2.40660	-2.49140
H	5.17750	-0.98180	-1.48820
H	4.54410	-0.20020	-3.75960
H	2.25900	0.68500	-4.18970
C	0.44530	1.58300	0.09520
C	0.46990	2.51470	1.12440
C	0.07870	3.84030	0.86750
C	-0.31800	4.23220	-0.40910
C	-0.31440	3.30780	-1.46730
C	0.07500	2.00200	-1.21090
H	0.08900	4.56460	1.68130
H	-0.62610	5.26020	-0.59520
H	-0.60730	3.61840	-2.46780
C	0.83960	0.09730	0.18800
C	1.25080	-0.35530	1.59060
H	1.50630	-1.44300	1.54200
H	2.20140	0.16530	1.85290
C	0.27820	-0.16460	2.72450
C	0.74910	-0.44360	4.02250
C	-1.05460	0.23760	2.55060
C	-0.09170	-0.33700	5.12960
H	1.78370	-0.75440	4.17190
C	-1.91700	0.35240	3.64330
H	-1.43760	0.47260	1.55510
C	-1.41480	0.06010	4.91270
H	0.27480	-0.56010	6.13130
H	-2.95280	0.66030	3.50080
H	0.78490	2.24080	2.13110
H	3.55740	-0.88940	0.37500
O	-0.45510	-2.47130	1.16880
O	-2.02240	-0.20390	-3.65580
C	-2.56330	-0.90750	-4.71390
O	-2.86460	-2.06700	-4.70780
C	-1.32260	-2.91910	2.15250
O	-2.51810	-2.88080	2.09350
C	-2.69090	0.04900	-5.81270

C	-0.48580	-3.44620	3.22830
N	-2.79870	0.78270	-6.69370
N	0.15560	-3.85970	4.09080
F	-2.23040	0.16300	5.96380
C	0.18940	0.90460	-2.25540
H	-0.09380	1.23000	-3.27650

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9_benzyl_triptycene/opt_c41_folded_opt.xyz

C	-1.96640	-2.45990	-0.82060
C	-0.91800	-1.85020	-0.10740
C	-0.24630	-0.71840	-0.57310
C	-0.59040	-0.25740	-1.87220
C	-1.62930	-0.86370	-2.57580
C	-2.33970	-1.95800	-2.06140
C	1.70630	0.36110	-2.25940
C	2.04700	-0.06740	-0.94520
C	3.31520	-0.56660	-0.69280
C	4.24910	-0.63530	-1.74360
C	3.91140	-0.21010	-3.02540
C	2.62580	0.29420	-3.29330
H	-2.48780	-3.32160	-0.39590
H	-3.15140	-2.42120	-2.62920
H	5.24600	-1.02700	-1.54430
H	4.64270	-0.26620	-3.83090
H	2.36660	0.62480	-4.29690
C	0.50950	1.57880	-0.04250
C	0.52790	2.52170	0.97660
C	0.14630	3.84630	0.70080
C	-0.23450	4.22590	-0.58430
C	-0.22420	3.28980	-1.63210
C	0.15600	1.98510	-1.35720
H	0.15190	4.57990	1.50650
H	-0.53510	5.25350	-0.78500
H	-0.50470	3.59100	-2.63920
C	0.89450	0.09210	0.06990
C	1.28780	-0.34750	1.48140
H	1.54090	-1.43730	1.44660
H	2.23890	0.17020	1.75000
C	0.30430	-0.14470	2.60160
C	0.75510	-0.42160	3.90740
C	-1.02430	0.26390	2.41230
C	-0.10370	-0.30340	4.99690
H	1.78530	-0.73770	4.07370
C	-1.89220	0.38630	3.49720
H	-1.39480	0.49930	1.41210
C	-1.43550	0.09860	4.79310
H	0.25200	-0.52560	6.00480
H	-2.92550	0.70130	3.33780
H	0.83140	2.25880	1.98930
H	3.60550	-0.90750	0.29870
O	-0.43360	-2.45280	1.07090
O	-1.92080	-0.23800	-3.80370
C	-2.46000	-0.94830	-4.85920
O	-2.77500	-2.10380	-4.84090
C	-1.32020	-2.88850	2.04350
O	-2.51400	-2.83760	1.96710
C	-2.56420	-0.00370	-5.97030
C	-0.50420	-3.41350	3.13620
N	-2.65370	0.72090	-6.86080
N	0.12050	-3.82380	4.01230
C	-2.32370	0.21910	5.90900
N	-3.04050	0.31830	6.81100
C	0.27650	0.87580	-2.38840
H	0.00660	1.19140	-3.41620

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9_benzyl_triptycene/opt_c42_folded_opt.xyz

C	-1.87550	-2.47570	-1.03140
C	-0.83510	-1.85940	-0.31210
C	-0.15460	-0.73530	-0.78380
C	-0.48090	-0.29000	-2.09290
C	-1.51200	-0.90290	-2.80230
C	-2.23140	-1.98910	-2.28340
C	1.82180	0.32020	-2.45850
C	2.14490	-0.09240	-1.13480
C	3.40890	-0.58990	-0.85970
C	4.35630	-0.67270	-1.89730
C	4.03590	-0.26300	-3.18860
C	2.75460	0.23940	-3.47940
H	-2.40480	-3.33060	-0.60280
H	-3.03660	-2.45780	-2.85590
H	5.35010	-1.06290	-1.68010
H	4.77760	-0.33000	-3.98370
H	2.50910	0.55800	-4.49020
C	0.59830	1.56710	-0.27240
C	0.60410	2.52210	0.73550
C	0.22890	3.84400	0.43830
C	-0.13310	4.20860	-0.85650
C	-0.11050	3.25970	-1.89260
C	0.26300	1.95770	-1.59660
H	0.22420	4.58720	1.23510
H	-0.42820	5.23440	-1.07400
H	-0.37680	3.54890	-2.90700
C	0.97950	0.08130	-0.13690
C	1.35410	-0.34110	1.28480
H	1.60980	-1.43090	1.26600
H	2.30040	0.18140	1.56130
C	0.35440	-0.12890	2.38820
C	0.78250	-0.39990	3.70270
C	-0.96970	0.28090	2.17850
C	-0.09630	-0.27580	4.77520
H	1.80910	-0.71610	3.88920
C	-1.85500	0.40830	3.25060
H	-1.32580	0.51390	1.17250
C	-1.42400	0.12480	4.55180
H	0.25280	-0.49760	5.78700
H	-2.88210	0.72520	3.05350
H	0.89270	2.27120	1.75550
H	3.68600	-0.91870	0.13970
O	-0.36820	-2.44730	0.88040
O	-1.78620	-0.29190	-4.04170
C	-2.31320	-1.01410	-5.09510
O	-2.63130	-2.16860	-5.06670
C	-1.26910	-2.87630	1.84380
O	-2.46150	-2.82660	1.74840
C	-2.40040	-0.08310	-6.21910
C	-0.46840	-3.39240	2.95160
N	-2.47630	0.63050	-7.11970
N	0.14440	-3.79660	3.83880
C	-2.35180	0.23800	5.72530
F	-2.55110	-0.91940	6.38070
F	-1.92690	1.07870	6.68600
F	-3.59690	0.66850	5.46440
C	0.39470	0.83530	-2.61220
H	0.13830	1.13850	-3.64710

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9_benzyl_triptycene/opt_c43_folded_opt.xyz

C	-1.79340	-2.36260	-1.03840
C	-0.73590	-1.74840	-0.33990
C	-0.06270	-0.62690	-0.82480
C	-0.42200	-0.17830	-2.12610
C	-1.47000	-0.78800	-2.81120
C	-2.17850	-1.87520	-2.28060
C	1.86910	0.43070	-2.55280

C	2.22580	0.01490	-1.23910
C	3.49560	-0.48720	-1.00000
C	4.41430	-0.57070	-2.06290
C	4.06050	-0.15730	-3.34430
C	2.77330	0.34940	-3.59900
H	-2.31260	-3.21770	-0.59940
H	-2.99790	-2.34110	-2.83440
H	5.41200	-0.96470	-1.87350
H	4.77990	-0.22500	-4.15920
H	2.50050	0.67030	-4.60200
C	0.70330	1.67440	-0.33180
C	0.73260	2.62780	0.67710
C	0.34750	3.94950	0.39210
C	-0.04750	4.31630	-0.89240
C	-0.04910	3.36950	-1.93060
C	0.33410	2.06780	-1.64610
H	0.35990	4.69010	1.19080
H	-0.35090	5.34130	-1.10010
H	-0.34210	3.65920	-2.93730
C	1.08900	0.18890	-0.20740
C	1.50790	-0.23720	1.20060
H	1.73980	-1.32890	1.17310
H	2.47320	0.26890	1.43570
C	0.55790	0.00930	2.34270
C	1.05270	-0.17910	3.64220
C	-0.78520	0.39440	2.17400
C	0.23600	-0.00470	4.76220
H	2.09220	-0.47180	3.79210
C	-1.62000	0.57020	3.26970
H	-1.18850	0.56550	1.17380
C	-1.09870	0.36540	4.56330
H	0.64180	-0.15890	5.75620
H	-2.66290	0.85890	3.15110
H	1.04510	2.37270	1.69010
H	3.79740	-0.81960	-0.00870
O	-0.26350	-2.36110	0.84310
O	-1.76890	-0.17560	-4.04700
O	-2.03290	0.57310	5.55410
C	-1.62900	0.33010	6.92260
H	-0.83360	1.02210	7.21250
H	-2.55610	0.54450	7.47060
H	-1.33140	-0.71450	7.05180
C	-2.37740	-0.86230	-5.06370
O	-2.76110	-1.99190	-5.05890
C	-2.45860	0.17120	-6.21840
C	-1.16370	-2.74110	1.81160
O	-2.34550	-2.57740	1.79640
C	-0.32700	-3.46660	2.89480
F	-1.77800	-0.20820	-7.30330
F	-1.96990	1.36840	-5.88770
F	-3.70810	0.39270	-6.63350
F	0.99130	-3.40460	2.69980
F	-0.61180	-4.77290	2.95760
F	-0.53420	-2.99930	4.12720
C	0.43950	0.94770	-2.66680
H	0.15650	1.25340	-3.69390

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9_benzyl_triptycene/opt_c44_folded_opt.xyz

C	-1.80190	-2.35980	-0.87320
C	-0.73950	-1.75330	-0.17550
C	-0.05530	-0.63960	-0.66310
C	-0.40820	-0.19240	-1.96660
C	-1.46150	-0.79400	-2.65060
C	-2.18090	-1.87280	-2.11750
C	1.88950	0.39640	-2.38990
C	2.23940	-0.01720	-1.07370
C	3.50450	-0.52830	-0.82920

C	4.42560	-0.62270	-1.88910
C	4.07860	-0.21110	-3.17300
C	2.79610	0.30450	-3.43330
H	-2.32930	-3.20860	-0.43190
H	-3.00390	-2.33280	-2.67080
H	5.41970	-1.02350	-1.69540
H	4.79980	-0.28710	-3.98550
H	2.52880	0.62400	-4.43820
C	0.72640	1.65740	-0.17670
C	0.75810	2.61370	0.82940
C	0.38490	3.93750	0.53810
C	-0.00150	4.30310	-0.74930
C	-0.00670	3.35270	-1.78420
C	0.36490	2.04900	-1.49370
H	0.40040	4.68070	1.33420
H	-0.29510	5.32990	-0.96190
H	-0.29350	3.64120	-2.79300
C	1.10130	0.16950	-0.04590
C	1.51270	-0.25290	1.36490
H	1.74170	-1.34550	1.34380
H	2.47890	0.24990	1.60380
C	0.55780	-0.00060	2.50160
C	1.04640	-0.18860	3.80690
C	-0.77920	0.38400	2.33080
C	0.21510	-0.00800	4.91120
H	2.08330	-0.48230	3.96340
C	-1.61420	0.56030	3.43470
H	-1.18260	0.55860	1.33280
C	-1.12750	0.36290	4.73540
H	0.61040	-0.16130	5.91380
H	-2.65280	0.84960	3.28000
H	1.06270	2.35950	1.84500
H	3.80090	-0.85930	0.16420
O	-0.27410	-2.36780	1.00930
O	-1.75410	-0.18150	-3.88790
C	-2.37100	-0.86310	-4.90270
O	-2.76660	-1.98860	-4.89600
C	-2.44340	0.17000	-6.05840
C	-1.17730	-2.73180	1.98060
O	-2.35710	-2.55190	1.96770
C	-0.34940	-3.46740	3.06390
F	-1.76710	-0.21650	-7.14350
F	-1.94340	1.36300	-5.72890
F	-3.69110	0.40280	-6.47280
F	0.96990	-3.41160	2.87510
F	-0.64210	-4.77260	3.11690
F	-0.56110	-3.00660	4.29770
C	-2.03360	0.53050	5.91050
H	-2.70910	-0.33330	6.00710
H	-1.48680	0.61970	6.85790
H	-2.66390	1.42550	5.81760
C	0.46420	0.92400	-2.50970
H	0.18640	1.22790	-3.53880

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9_benzyl_triptycene/opt_c45_folded_opt.xyz

C	-1.89760	-2.35630	-0.60610
C	-0.83590	-1.75240	0.09470
C	-0.18310	-0.60830	-0.36470
C	-0.56710	-0.12360	-1.64560
C	-1.61950	-0.72310	-2.33320
C	-2.30770	-1.83430	-1.82610
C	1.71100	0.52540	-2.08570
C	2.09170	0.07380	-0.79070
C	3.37060	-0.41990	-0.58510
C	4.27480	-0.45930	-1.66290
C	3.89750	-0.01080	-2.92580
C	2.60090	0.48760	-3.14660

H	-2.39980	-3.23100	-0.18640
H	-3.13080	-2.29200	-2.38140
H	5.27980	-0.84660	-1.49990
H	4.60590	-0.04440	-3.75240
H	2.30990	0.83590	-4.13530
C	0.56260	1.68590	0.18900
C	0.59460	2.60780	1.22670
C	0.19110	3.93320	0.98780
C	-0.22570	4.33490	-0.27920
C	-0.23140	3.42050	-1.34600
C	0.17040	2.11520	-1.10720
H	0.20710	4.64920	1.80860
H	-0.54280	5.36240	-0.45110
H	-0.54170	3.73760	-2.33920
C	0.96780	0.20200	0.26130
C	1.41060	-0.26120	1.64950
H	1.65940	-1.34820	1.58690
H	2.37230	0.25000	1.88970
C	0.47200	-0.06630	2.81110
C	0.99190	-0.29010	4.09970
C	-0.87400	0.29910	2.67500
C	0.17680	-0.15380	5.22380
H	2.03500	-0.57370	4.22570
C	-1.68800	0.43030	3.80390
H	-1.29950	0.49620	1.69110
C	-1.16830	0.20310	5.08010
H	0.58890	-0.33030	6.21660
H	-2.73460	0.70890	3.68240
H	0.92290	2.32590	2.22730
H	3.69070	-0.77890	0.39100
O	-0.33650	-2.39800	1.24870
O	-1.94390	-0.07480	-3.54390
C	-2.57240	-0.73070	-4.56880
O	-2.95330	-1.86090	-4.59180
C	-2.68090	0.33910	-5.68770
C	-1.21410	-2.81730	2.22170
O	-2.39670	-2.65900	2.23790
C	-0.34950	-3.57730	3.25870
F	-2.03740	-0.01080	-6.80460
F	-2.17230	1.52180	-5.33510
F	-3.94080	0.58270	-6.05610
F	-0.62200	-4.88760	3.27420
F	-0.53520	-3.16110	4.51230
F	0.96360	-3.49450	3.03820
H	-1.80440	0.30270	5.95680
C	0.27380	1.02830	-2.16350
H	-0.02730	1.36210	-3.17660

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9_benzyl_triptycene/opt_c47_folded_opt.xyz

C	-1.91420	-2.35890	-0.60300
C	-0.85120	-1.75790	0.09820
C	-0.18890	-0.62100	-0.36530
C	-0.56540	-0.14100	-1.65020
C	-1.62010	-0.73650	-2.33790
C	-2.31700	-1.84070	-1.82700
C	1.71900	0.48650	-2.08780
C	2.09260	0.03890	-0.78940
C	3.36650	-0.46510	-0.57750
C	4.27310	-0.51820	-1.65270
C	3.90320	-0.07320	-2.91890
C	2.61150	0.43510	-3.14600
H	-2.42340	-3.22850	-0.18090
H	-3.14140	-2.29620	-2.38260
H	5.27420	-0.91360	-1.48490
H	4.61360	-0.11720	-3.74340
H	2.32630	0.78040	-4.13750
C	0.57620	1.67070	0.17630

C	0.61830	2.60010	1.20700
C	0.22520	3.92700	0.95940
C	-0.19010	4.32300	-0.31000
C	-0.20310	3.40150	-1.37050
C	0.18870	2.09480	-1.12300
H	0.24860	4.64890	1.77500
H	-0.49980	5.35180	-0.48850
H	-0.51100	3.71440	-2.36600
C	0.96710	0.18360	0.25870
C	1.40240	-0.27570	1.65120
H	1.63500	-1.36680	1.59580
H	2.37180	0.22350	1.88640
C	0.46670	-0.05630	2.81010
C	0.98830	-0.26610	4.10160
C	-0.87660	0.32180	2.66620
C	0.18920	-0.10690	5.23300
H	2.03070	-0.56000	4.22640
C	-1.69950	0.48290	3.78320
H	-1.29760	0.50540	1.67550
C	-1.14600	0.26450	5.04600
H	0.59530	-0.27120	6.23030
H	-2.74430	0.76980	3.66400
H	0.94900	2.32430	2.20820
H	3.68110	-0.82190	0.40110
O	-0.36080	-2.39770	1.25940
O	-1.93630	-0.09200	-3.55200
C	-2.56850	-0.74740	-4.57580
O	-2.95770	-1.87480	-4.59370
C	-2.66610	0.31890	-5.69890
C	-1.24600	-2.81110	2.22850
O	-2.42760	-2.64580	2.23650
C	-0.38900	-3.56330	3.27700
F	-2.01310	-0.03510	-6.80880
F	-2.15930	1.50200	-5.34490
F	-3.92250	0.56240	-6.07880
F	0.92440	-3.50060	3.04960
F	-0.67800	-4.86850	3.32170
F	-0.56350	-3.11560	4.52160
F	-1.92190	0.41670	6.12110
C	0.28620	1.00090	-2.17250
H	-0.00930	1.33110	-3.18850

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9_benzyl_triptycene/opt_c48_folded_opt.xyz

C	-1.85470	-2.36910	-0.72000
C	-0.80370	-1.75860	-0.00910
C	-0.13240	-0.62910	-0.47750
C	-0.48790	-0.16590	-1.77440
C	-1.53050	-0.77100	-2.47240
C	-2.23620	-1.86800	-1.95800
C	1.80280	0.45610	-2.18480
C	2.15660	0.02460	-0.87550
C	3.42680	-0.47710	-0.63800
C	4.34930	-0.54440	-1.69880
C	3.99860	-0.11550	-2.97600
C	2.71090	0.39080	-3.22890
H	-2.37160	-3.23290	-0.29510
H	-3.05130	-2.33150	-2.52100
H	5.34770	-0.93810	-1.51120
H	4.72120	-0.17060	-3.78940
H	2.44070	0.72370	-4.22890
C	0.62600	1.66890	0.04700
C	0.65230	2.61070	1.06680
C	0.26240	3.93430	0.79700
C	-0.13350	4.31440	-0.48330
C	-0.13000	3.38000	-1.53260
C	0.25820	2.07650	-1.26330
H	0.27310	4.66650	1.60380

H	-0.44070	5.34100	-0.67920
H	-0.42240	3.68080	-2.53650
C	1.01500	0.18270	0.15270
C	1.42860	-0.25880	1.55710
H	1.66710	-1.35050	1.51820
H	2.39360	0.24470	1.80350
C	0.47370	-0.03310	2.69700
C	0.96810	-0.24200	3.99940
C	-0.86620	0.34670	2.52970
C	0.14230	-0.07850	5.10840
H	2.00690	-0.53730	4.14730
C	-1.70270	0.50930	3.63400
H	-1.26960	0.53170	1.53180
C	-1.20110	0.29510	4.92740
H	0.53210	-0.24320	6.11430
H	-2.74570	0.79920	3.49150
H	0.96880	2.34880	2.07580
H	3.72720	-0.82170	0.34930
O	-0.33500	-2.38190	1.17020
O	-1.82300	-0.14450	-3.70120
C	-2.44670	-0.81080	-4.72410
O	-2.84750	-1.93410	-4.72790
C	-2.51400	0.23710	-5.86640
C	-1.23910	-2.78480	2.12680
O	-2.41910	-2.60980	2.11520
C	-0.40340	-3.53400	3.19450
F	-1.84530	-0.14270	-6.95820
F	-2.00090	1.42060	-5.52310
F	-3.76100	0.48690	-6.27210
F	0.91430	-3.46790	2.99380
F	-0.69060	-4.83900	3.23770
F	-0.60420	-3.08140	4.43360
C	-2.05550	0.45900	6.06390
N	-2.74470	0.59280	6.98280
C	0.37170	0.96970	-2.29750
H	0.09180	1.28740	-3.32200

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9_benzyl_triptycene/opt_c49_folded_opt.xyz

C	-1.79120	-2.38610	-0.92270
C	-0.75010	-1.76510	-0.20620
C	-0.08110	-0.63470	-0.67610
C	-0.42870	-0.18090	-1.97840
C	-1.46120	-0.79680	-2.68190
C	-2.16460	-1.89510	-2.16710
C	1.86070	0.45310	-2.37540
C	2.20730	0.03030	-1.06130
C	3.47850	-0.46300	-0.81210
C	4.40900	-0.53070	-1.86580
C	4.06530	-0.11020	-3.14770
C	2.77670	0.38760	-3.41250
H	-2.30690	-3.25030	-0.49700
H	-2.97140	-2.36710	-2.73480
H	5.40810	-0.91800	-1.66890
H	4.79400	-0.16560	-3.95550
H	2.51190	0.71390	-4.41610
C	0.65970	1.67020	-0.15830
C	0.67200	2.61710	0.85720
C	0.27690	3.93710	0.57750
C	-0.11060	4.30860	-0.70790
C	-0.09350	3.36900	-1.75240
C	0.29980	2.06900	-1.47340
H	0.27700	4.67330	1.38080
H	-0.42190	5.33240	-0.91140
H	-0.37980	3.66310	-2.76010
C	1.05720	0.18710	-0.04230
C	1.46380	-0.24410	1.36710
H	1.71220	-1.33410	1.33540

H	2.42250	0.26870	1.61910
C	0.49790	-0.02310	2.49810
C	0.98060	-0.22840	3.80550
C	-0.84270	0.34570	2.32130
C	0.13970	-0.07510	4.90420
H	2.02040	-0.51330	3.96510
C	-1.69160	0.49710	3.41960
H	-1.23980	0.53110	1.32100
C	-1.20510	0.28370	4.71440
H	0.53130	-0.24100	5.91080
H	-2.73360	0.77800	3.24770
H	0.98100	2.36210	1.87020
H	3.77360	-0.80090	0.17920
O	-0.28900	-2.37750	0.98170
O	-1.74800	-0.18010	-3.91710
C	-2.34340	-0.86360	-4.94560
O	-2.72410	-1.99380	-4.94840
C	-2.41110	0.17600	-6.09530
C	-1.20080	-2.78510	1.93000
O	-2.38180	-2.61990	1.90320
C	-0.37100	-3.52330	3.00970
F	-3.65550	0.40010	-6.52330
F	-1.71730	-0.19780	-7.17360
F	-1.92570	1.37090	-5.75120
F	0.94840	-3.44260	2.82530
F	-0.64390	-4.83150	3.04970
F	-0.59280	-3.07210	4.24550
C	-2.09150	0.42450	5.91650
F	-1.65240	1.31500	6.82480
F	-3.35570	0.81450	5.68620
F	-2.23720	-0.70790	6.62740
C	0.42750	0.95760	-2.50100
H	0.15290	1.26840	-3.52910

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9_benzyl_triptycene/opt_c5_folded_opt.xyz

C	-1.90540	-2.41800	-0.72360
C	-0.86180	-1.82580	0.00610
C	-0.20500	-0.67750	-0.47260
C	-0.54140	-0.21370	-1.76120
C	-1.57960	-0.81160	-2.49200
C	-2.27820	-1.90640	-1.96670
C	1.75720	0.43090	-2.12170
C	2.08700	0.00370	-0.80300
C	3.35830	-0.47770	-0.53470
C	4.30740	-0.53220	-1.57310
C	3.98040	-0.11100	-2.85860
C	2.69130	0.37630	-3.14260
H	-2.42100	-3.29120	-0.33110
H	-3.09220	-2.37110	-2.51520
H	5.30590	-0.91010	-1.36080
H	4.72150	-0.15730	-3.65440
H	2.43880	0.70080	-4.14930
C	0.52110	1.62530	0.08320
C	0.51450	2.56250	1.10720
C	0.12620	3.88570	0.83280
C	-0.23810	4.26850	-0.45590
C	-0.20500	3.33760	-1.50800
C	0.18190	2.03450	-1.23530
H	0.11270	4.61400	1.64190
H	-0.54390	5.29370	-0.65600
H	-0.47520	3.63950	-2.51700
C	0.91580	0.14040	0.19340
C	1.28670	-0.30410	1.61060
H	1.55270	-1.39130	1.56590
H	2.21700	0.22840	1.91030
C	0.26490	-0.14020	2.70520
C	0.67360	-0.46100	4.01420

C	-1.05670	0.28170	2.48500
C	-0.21280	-0.36920	5.08800
H	1.69580	-0.79040	4.19800
C	-1.96280	0.38280	3.54230
H	-1.39330	0.53350	1.47650
C	-1.51830	0.05190	4.82380
H	0.10810	-0.61720	6.09770
H	-2.98440	0.71440	3.36530
H	0.80180	2.29330	2.12280
H	3.63750	-0.81680	0.46010
O	-0.36720	-2.36700	1.17900
O	-1.80920	-0.21670	-3.71960
C	-2.82260	-0.80830	-4.56500
H	-3.80390	-0.74060	-4.08690
H	-2.77440	-0.16520	-5.45350
H	-2.55830	-1.83990	-4.81420
C	-1.28050	-3.14970	1.98650
H	-0.69820	-3.29010	2.90680
H	-2.19390	-2.58400	2.19140
H	-1.48680	-4.10570	1.49950
F	-2.37900	0.13990	5.84230
C	0.32230	0.92780	-2.26690
H	0.05850	1.23770	-3.29780

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9_benzyl_triptycene/opt_c6_folded_opt.xyz

C	-1.85120	-2.41230	-0.82540
C	-0.81310	-1.81360	-0.09400
C	-0.14420	-0.67720	-0.58480
C	-0.46630	-0.22980	-1.88240
C	-1.50050	-0.83350	-2.61470
C	-2.20840	-1.91760	-2.08010
C	1.83890	0.39540	-2.23300
C	2.15600	-0.01600	-0.90630
C	3.42210	-0.50140	-0.62120
C	4.37870	-0.57620	-1.65140
C	4.06400	-0.17090	-2.94510
C	2.78040	0.32060	-3.24590
H	-2.37670	-3.27680	-0.42670
H	-3.01870	-2.38750	-2.63010
H	5.37330	-0.95720	-1.42640
H	4.81090	-0.23300	-3.73470
H	2.53770	0.63280	-4.25900
C	0.59420	1.62770	-0.05400
C	0.58670	2.57810	0.95770
C	0.20900	3.90000	0.66300
C	-0.14360	4.26790	-0.63330
C	-0.10910	3.32290	-1.67280
C	0.26740	2.02100	-1.38030
H	0.19490	4.63950	1.46210
H	-0.44130	5.29240	-0.84930
H	-0.36990	3.61350	-2.68780
C	0.97750	0.14170	0.07790
C	1.33180	-0.28770	1.50360
H	1.60490	-1.37460	1.47170
H	2.25690	0.24970	1.81220
C	0.29500	-0.12190	2.58130
C	0.67710	-0.45950	3.89550
C	-1.01590	0.32640	2.34890
C	-0.22800	-0.35950	4.94870
H	1.69000	-0.80770	4.09340
C	-1.92810	0.43000	3.39660
H	-1.33520	0.59230	1.33820
C	-1.53850	0.08400	4.70140
H	0.07610	-0.62330	5.96210
H	-2.94320	0.78010	3.20480
H	0.86560	2.32150	1.97850
H	3.69220	-0.82840	0.38000

O	-0.33650	-2.32770	1.09880
O	-1.71510	-0.25550	-3.85260
C	-2.72650	-0.85130	-4.69780
H	-3.71100	-0.76940	-4.22850
H	-2.66630	-0.22080	-5.59460
H	-2.46810	-1.88810	-4.93070
C	-1.23520	-3.15630	1.87580
H	-0.67330	-3.27610	2.81150
H	-2.17970	-2.63540	2.05640
H	-1.38260	-4.11820	1.37850
C	-2.47530	0.18210	5.77790
N	-3.23390	0.25870	6.64790
C	0.40850	0.89970	-2.39600
H	0.15470	1.19760	-3.43300

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9_benzyl_triptycene/opt_c7_folded_opt.xyz

C	-1.72270	-2.44900	-0.99800
C	-0.69160	-1.82970	-0.27360
C	-0.02990	-0.69710	-0.78200
C	-0.35010	-0.27550	-2.08880
C	-1.37600	-0.90060	-2.81440
C	-2.07830	-1.98010	-2.26280
C	1.95090	0.36610	-2.44000
C	2.26590	-0.01880	-1.10480
C	3.53560	-0.48540	-0.80520
C	4.49800	-0.56790	-1.82950
C	4.18540	-0.18890	-3.13160
C	2.89800	0.28350	-3.44700
H	-2.24370	-3.30960	-0.58480
H	-2.88330	-2.46550	-2.80720
H	5.49560	-0.93410	-1.59300
H	4.93670	-0.25690	-3.91640
H	2.65700	0.57520	-4.46660
C	0.68380	1.62350	-0.28850
C	0.66130	2.59070	0.70700
C	0.27230	3.90360	0.38780
C	-0.07720	4.24570	-0.91640
C	-0.02830	3.28350	-1.93950
C	0.35970	1.99060	-1.62290
H	0.24650	4.65630	1.17410
H	-0.38380	5.26340	-1.15140
H	-0.28750	3.55400	-2.96030
C	1.08110	0.14390	-0.12930
C	1.43230	-0.25740	1.30520
H	1.72720	-1.33910	1.29060
H	2.34380	0.30240	1.61450
C	0.38280	-0.09870	2.37110
C	0.74890	-0.43770	3.68870
C	-0.92770	0.34400	2.12690
C	-0.17170	-0.34970	4.73090
H	1.76110	-0.77990	3.89980
C	-1.85110	0.43440	3.16570
H	-1.23860	0.61310	1.11440
C	-1.47940	0.08370	4.47320
H	0.13980	-0.62250	5.74060
H	-2.86530	0.77900	2.95230
H	0.93640	2.35400	1.73360
H	3.80440	-0.79170	0.20290
O	-0.21520	-2.32170	0.92860
O	-1.59000	-0.34720	-4.06360
C	-2.58870	-0.97040	-4.90410
H	-3.57730	-0.89000	-4.44350
H	-2.52870	-0.35710	-5.81280
H	-2.31740	-2.00880	-5.11470
C	-1.11970	-3.12500	1.72600
H	-0.55850	-3.22620	2.66430
H	-2.06030	-2.59290	1.89480

H	-1.27450	-4.09740	1.25190
C	-2.50090	0.17430	5.56480
F	-2.07660	-0.10180	6.80990
F	-3.07660	1.38310	5.69640
F	-3.54910	-0.65660	5.40590
C	0.51640	0.85310	-2.61820
H	0.26460	1.13050	-3.66150

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9_benzyl_triptycene/opt_c8_folded_opt.xyz

C	-1.78250	-2.37270	-1.14820
C	-0.74340	-1.77110	-0.41170
C	-0.07140	-0.63410	-0.86830
C	-0.40980	-0.15910	-2.16280
C	-1.44030	-0.75580	-2.88790
C	-2.14600	-1.86040	-2.38670
C	1.88460	0.47700	-2.53460
C	2.22180	0.03180	-1.22470
C	3.49060	-0.46810	-0.97680
C	4.42820	-0.52140	-2.02530
C	4.09330	-0.08040	-3.30230
C	2.80720	0.42470	-3.56640
H	-2.30780	-3.23640	-0.73330
H	-2.94740	-2.32160	-2.96950
H	5.42420	-0.91410	-1.82820
H	4.82570	-0.12590	-4.10630
H	2.54830	0.76470	-4.56610
C	0.67440	1.65770	-0.30380
C	0.68150	2.58760	0.72700
C	0.29200	3.91360	0.46800
C	-0.08490	4.30850	-0.81330
C	-0.06260	3.38650	-1.87350
C	0.32440	2.08050	-1.61510
H	0.28640	4.63420	1.28420
H	-0.39280	5.33540	-1.00120
H	-0.34160	3.69800	-2.87680
C	1.06430	0.17090	-0.21020
C	1.46550	-0.28930	1.19420
H	1.65630	-1.39040	1.14960
H	2.44300	0.18350	1.44170
C	0.51490	-0.04290	2.33520
C	1.01110	-0.20180	3.63610
C	-0.84250	0.29540	2.15910
C	0.18360	-0.04780	4.75440
H	2.06020	-0.45120	3.79260
C	-1.68430	0.45410	3.25020
H	-1.24580	0.43750	1.15300
C	-1.15910	0.27940	4.54790
H	0.59390	-0.17150	5.75000
H	-2.73640	0.70660	3.12650
H	0.98070	2.31170	1.73800
H	3.77690	-0.82250	0.01090
O	-0.29050	-2.36890	0.76900
O	-1.72660	-0.12530	-4.10460
O	-2.10580	0.45980	5.53400
C	-1.67880	0.32970	6.91000
H	-0.91830	1.07930	7.14590
H	-2.61130	0.53200	7.45360
H	-1.32600	-0.68670	7.10450
C	-2.29900	-0.79880	-5.18370
O	-2.61140	-1.95810	-5.14400
C	-2.41700	0.18860	-6.29030
H	-2.10790	1.20320	-5.98870
H	-1.79270	-0.11080	-7.14790
H	-3.45750	0.24810	-6.64980
C	-1.18890	-2.84650	1.73390
O	-2.37810	-2.83230	1.56670
C	-0.38270	-3.32880	2.88380

H	-0.82960	-4.23010	3.32970
H	0.65910	-3.55420	2.60690
H	-0.34350	-2.55220	3.67240
C	0.45290	0.98560	-2.66030
H	0.18230	1.31060	-3.68410

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9_benzyl_triptycene/opt_c9_folded_opt.xyz

C	-1.76630	-2.38050	-0.95920
C	-0.72760	-1.77020	-0.22920
C	-0.05610	-0.63810	-0.69800
C	-0.39430	-0.17790	-1.99790
C	-1.42340	-0.78390	-2.71720
C	-2.12910	-1.88300	-2.20390
C	1.89950	0.45830	-2.37510
C	2.23640	0.02810	-1.06010
C	3.50580	-0.46680	-0.80570
C	4.44440	-0.52960	-1.85270
C	4.11000	-0.10300	-3.13470
C	2.82320	0.39680	-3.40550
H	-2.29100	-3.23930	-0.53410
H	-2.92980	-2.35140	-2.78190
H	5.44100	-0.91840	-1.65050
H	4.84330	-0.15560	-3.93740
H	2.56470	0.72570	-4.40890
C	0.68470	1.66110	-0.15830
C	0.68740	2.60160	0.86280
C	0.29680	3.92420	0.58860
C	-0.07770	4.30490	-0.69770
C	-0.05240	3.37160	-1.74780
C	0.33590	2.06890	-1.47460
H	0.28910	4.65360	1.39690
H	-0.38570	5.32950	-0.89730
H	-0.33000	3.67190	-2.75480
C	1.07780	0.17610	-0.04830
C	1.47860	-0.26640	1.36130
H	1.67850	-1.36660	1.32940
H	2.45170	0.21570	1.60840
C	0.52170	-0.01890	2.49670
C	1.01420	-0.17570	3.80370
C	-0.83020	0.31430	2.32040
C	0.17230	-0.02240	4.90640
H	2.06270	-0.41870	3.96490
C	-1.67300	0.46470	3.42030
H	-1.23580	0.45910	1.31720
C	-1.18190	0.29280	4.72460
H	0.57360	-0.14350	5.91040
H	-2.72210	0.71270	3.26230
H	0.98340	2.33670	1.87760
H	3.79190	-0.80990	0.18610
O	-0.27580	-2.35900	0.95680
O	-1.70720	-0.16770	-3.94190
C	-2.28580	-0.85030	-5.01180
O	-2.60990	-2.00570	-4.95670
C	-2.39320	0.12300	-6.13190
H	-2.08790	1.14160	-5.83990
H	-1.75900	-0.18620	-6.97880
H	-3.42970	0.17660	-6.50350
C	-1.17670	-2.80630	1.93330
O	-2.36700	-2.76920	1.77430
C	-0.37370	-3.29340	3.08300
H	-0.82720	-4.18970	3.53190
H	0.66620	-3.52800	2.80640
H	-0.32670	-2.51490	3.87000
C	-2.09830	0.44770	5.89390
H	-2.96160	-0.22920	5.81700
H	-1.60670	0.23730	6.85180
H	-2.49490	1.47180	5.95320

C	0.46700	0.96270	-2.50750
H	0.19650	1.27580	-3.53510

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shimizu/opt_al_folded_opt.xyz

C	-2.41790	-3.33420	1.24460
C	-1.11580	-2.99000	1.60830
C	-0.76250	-1.64050	1.76050
C	-1.72890	-0.61880	1.51730
C	-3.05920	-0.98980	1.17300
C	-3.38570	-2.34780	1.03740
C	0.55060	-1.20380	2.14610
C	-1.37360	0.78130	1.60380
C	-0.03530	1.18240	1.89150
C	0.90200	0.13140	2.17190
C	0.29930	2.54510	1.91290
H	1.32970	2.84750	2.09480
C	-0.68420	3.50930	1.69250
C	-2.00640	3.13480	1.43980
C	-2.36400	1.77930	1.38290
H	-2.68280	-4.38430	1.11940
H	-0.36750	-3.76780	1.75890
H	-4.40020	-2.63620	0.76550
H	-0.41830	4.56580	1.71450
H	-2.76210	3.90090	1.27240
C	1.73620	-2.02090	2.62570
H	1.52190	-3.02370	3.01140
C	2.34830	0.23190	2.61360
H	2.69220	1.20360	2.98320
C	2.31680	-0.96310	3.62990
O	2.62310	-1.03920	4.77420
C	2.87490	-1.94560	1.57400
H	3.73290	-2.58380	1.87670
C	3.24840	-0.41720	1.52530
H	4.32210	-0.23450	1.74140
C	2.43670	-2.32250	0.16200
O	2.08210	-3.39400	-0.24670
C	2.93380	0.03550	0.09840
O	3.00150	1.14190	-0.36670
N	2.59600	-1.14590	-0.64760
C	2.24250	-1.11530	-2.04330
C	0.98810	-0.62680	-2.46920
C	3.15850	-1.57520	-3.00160
C	0.66670	-0.55240	-3.83070
C	2.83170	-1.51640	-4.35760
H	4.12300	-1.97170	-2.68320
C	1.59570	-1.00200	-4.76870
H	-0.29920	-0.15670	-4.14130
H	3.54520	-1.87140	-5.09970
H	1.35430	-0.95520	-5.83110
O	0.07820	-0.29690	-1.47190
C	-0.64060	0.89730	-1.69500
C	0.02990	2.12230	-1.61610
C	-2.01630	0.78390	-1.90720
C	-0.72700	3.28520	-1.76260
H	1.10640	2.15010	-1.42790
C	-2.74940	1.96580	-2.04940
H	-2.48920	-0.19510	-1.93750
C	-2.10880	3.20790	-1.98390
H	-0.23930	4.25740	-1.70070
H	-3.82500	1.91500	-2.21180
H	-2.68750	4.12140	-2.10150
C	-3.72370	1.36360	1.08240
H	-4.46720	2.14720	0.93880
C	-4.04980	0.05430	0.97290
H	-5.06650	-0.25810	0.73550

shimizu/opt_a2_folded_opt.xyz			
C	-2.43920	-3.40580	1.19290
C	-1.19600	-2.99210	1.62390
C	-0.91610	-1.60840	1.77470
C	-1.91050	-0.64130	1.47120
C	-3.18370	-1.10200	1.03710
C	-3.44230	-2.45050	0.90120
C	0.36170	-1.13020	2.20400
C	-1.61580	0.78320	1.58020
C	-0.30630	1.22150	1.90720
C	0.66320	0.22000	2.22520
C	-0.00290	2.60840	1.93660
H	1.01940	2.92220	2.14410
C	-0.99110	3.53970	1.69610
C	-2.31180	3.11430	1.41520
C	-2.61440	1.76970	1.35280
H	-2.65840	-4.46520	1.06650
H	-0.41070	-3.71840	1.83380
H	-3.95850	-0.36970	0.80310
H	-4.41900	-2.79430	0.56320
H	-0.76770	4.60490	1.71740
H	-3.08370	3.86190	1.23870
H	-3.63070	1.44850	1.11810
C	1.56590	-1.89700	2.71920
H	1.38170	-2.90370	3.11010
C	2.09390	0.37740	2.69940
H	2.39360	1.36390	3.06810
C	2.08300	-0.80920	3.72520
O	2.36540	-0.86380	4.87710
C	2.72370	-1.78780	1.69110
H	3.59830	-2.39020	2.01820
C	3.04040	-0.24660	1.63580
H	4.10180	-0.02180	1.87190
C	2.33110	-2.19340	0.27370
O	2.02790	-3.28120	-0.13320
C	2.73780	0.18170	0.19900
O	2.77130	1.28560	-0.27600
N	2.46160	-1.01800	-0.54320
C	2.14230	-1.01220	-1.94740
C	0.87810	-0.58640	-2.40930
C	3.10420	-1.43220	-2.87900
C	0.58970	-0.53280	-3.77920
C	2.81120	-1.39460	-4.24340
H	4.07760	-1.78100	-2.53310
C	1.56370	-0.94130	-4.69010
H	-0.38560	-0.18520	-4.11680
H	3.56050	-1.71820	-4.96450
H	1.34890	-0.91050	-5.75870
O	-0.07700	-0.29980	-1.44060
C	-0.83370	0.86700	-1.67610
C	-0.20830	2.11670	-1.61780
C	-2.20650	0.70120	-1.87620
C	-1.00800	3.24910	-1.77610
H	0.86720	2.18740	-1.43390
C	-2.98320	1.85320	-2.02870
H	-2.64060	-0.29590	-1.89510
C	-2.38740	3.11860	-1.98710
H	-0.55560	4.23930	-1.73040
H	-4.05690	1.76210	-2.18520
H	-2.99950	4.00890	-2.11460

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shimizu/opt_a3_folded_opt.xyz			
C	-1.27890	-1.97660	2.04750
C	-2.42440	-1.37120	1.48910
C	-0.28680	-1.15000	2.53170
C	-2.54930	0.01440	1.42380
C	-1.52840	0.86370	1.89940

C	-0.40890	0.27550	2.44900
C	1.02390	-1.45540	3.22760
H	1.12070	-2.44780	3.68240
C	0.83350	0.87300	3.07580
H	0.77140	1.91880	3.39680
C	1.04550	-0.21430	4.18370
O	1.17750	-0.12600	5.36120
C	2.20050	-1.03630	2.30600
H	3.17300	-1.34230	2.74870
C	2.06140	0.52850	2.18930
H	2.96710	1.06200	2.54950
C	2.10610	-1.57630	0.88070
O	2.16140	-2.71430	0.50480
C	1.86440	0.81600	0.70290
O	1.67970	1.87490	0.16300
N	2.01120	-0.43340	0.01060
C	1.92820	-0.53860	-1.42380
C	0.68950	-0.50940	-2.09720
C	3.10860	-0.65490	-2.17590
C	0.62230	-0.54010	-3.49600
C	3.04200	-0.70470	-3.56910
H	4.07260	-0.70020	-1.66830
C	1.80650	-0.63880	-4.22590
H	-0.34620	-0.49760	-3.99240
H	3.95990	-0.79230	-4.14950
H	1.76880	-0.66940	-5.31530
O	-0.47120	-0.55090	-1.32710
C	-1.40290	0.47330	-1.56530
C	-1.03650	1.81970	-1.46640
C	-2.71830	0.05310	-1.79160
C	-2.04300	2.77850	-1.58680
H	0.00350	2.10240	-1.27800
C	-3.70570	1.03510	-1.90420
H	-2.94850	-1.00680	-1.86450
C	-3.37160	2.39010	-1.80310
H	-1.79060	3.83610	-1.50860
H	-4.74050	0.74120	-2.07730
H	-4.14750	3.14730	-1.89570
H	-1.62620	1.94420	1.81910
H	-3.44290	0.45910	0.98410
H	-3.21920	-2.00580	1.09810
H	-1.18700	-3.06010	2.08340

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motherwell/opt_all_folded_opt.xyz

C	-3.85050	-0.36100	0.69790
C	-2.64240	-0.29430	1.40530
C	-1.43850	-0.22600	0.70580
C	-1.43850	-0.22600	-0.70580
C	-2.64240	-0.29420	-1.40530
C	-3.85050	-0.36100	-0.69790
C	0.86120	-1.09940	-0.70680
C	0.86120	-1.09940	0.70680
C	1.71490	-1.95030	1.40600
C	2.57150	-2.80480	0.69770
C	2.57150	-2.80480	-0.69770
C	1.71490	-1.95030	-1.40600
H	-4.79120	-0.41600	1.24250
H	-4.79120	-0.41600	-1.24250
H	3.24030	-3.46820	1.24230
H	3.24030	-3.46820	-1.24230
H	1.72520	-1.95200	-2.49330
C	-0.09010	-0.14270	1.39400
H	1.72520	-1.95200	2.49330
H	-2.65000	-0.29900	-2.49300
H	-2.65000	-0.29900	2.49300
H	-0.19580	-0.41890	2.47180
C	-0.09010	-0.14270	-1.39400

H	-0.19580	-0.41890	-2.47180
C	0.42840	1.31190	1.32100
H	-0.41890	1.99490	1.53510
H	1.15140	1.46480	2.14940
C	0.42840	1.31190	-1.32100
H	1.15140	1.46470	-2.14940
H	-0.41890	1.99490	-1.53510
C	1.09650	1.75260	0.00000
C	1.27350	3.28070	0.00000
H	1.83080	3.62820	-0.87900
H	0.30850	3.79770	0.00000
H	1.83080	3.62820	0.87900
F	2.37420	1.22660	0.00000

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motherwell/opt_a12_folded_opt.xyz

C	-4.00180	-0.38640	0.69780
C	-2.79270	-0.33480	1.40530
C	-1.58820	-0.28150	0.70600
C	-1.58820	-0.28150	-0.70600
C	-2.79270	-0.33480	-1.40530
C	-4.00180	-0.38640	-0.69780
C	0.69450	-1.19130	-0.70750
C	0.69450	-1.19130	0.70750
C	1.52620	-2.06250	1.40660
C	2.36250	-2.93760	0.69720
C	2.36250	-2.93760	-0.69720
C	1.52620	-2.06250	-1.40660
H	-4.94280	-0.42970	1.24240
H	-4.94270	-0.42970	-1.24240
H	3.01460	-3.61630	1.24190
H	3.01460	-3.61640	-1.24190
H	1.53740	-2.06480	-2.49300
C	-0.23760	-0.21420	1.39230
H	1.53740	-2.06480	2.49300
H	-2.80030	-0.33950	-2.49280
H	-2.80030	-0.33950	2.49270
H	-0.34560	-0.48360	2.47110
C	-0.23760	-0.21420	-1.39230
H	-0.34560	-0.48360	-2.47110
C	0.29670	1.23580	1.31310
H	-0.55360	1.92470	1.49020
H	0.99300	1.39140	2.16020
C	0.29670	1.23580	-1.31310
H	0.99300	1.39140	-2.16020
H	-0.55360	1.92470	-1.49010
C	1.01260	1.65660	0.00000
C	1.09530	3.21120	0.00000
H	1.62040	3.58920	-0.88140
H	0.10040	3.66740	0.00000
H	1.62040	3.58920	0.88140
N	2.38640	1.07210	0.00000
H	2.91710	1.33650	-0.82040
H	2.91710	1.33650	0.82040

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motherwell/opt_a13_folded_opt.xyz

C	-3.93970	-0.23180	0.69800
C	-2.73140	-0.17180	1.40560
C	-1.52740	-0.10940	0.70560
C	-1.52740	-0.10940	-0.70560
C	-2.73140	-0.17170	-1.40560
C	-3.93970	-0.23180	-0.69800
C	0.76350	-1.00180	-0.70720
C	0.76350	-1.00180	0.70720
C	1.60480	-1.86370	1.40670
C	2.45070	-2.72890	0.69740
C	2.45070	-2.72890	-0.69750

C	1.60480	-1.86370	-1.40670
H	-4.88100	-0.28090	1.24250
H	-4.88100	-0.28090	-1.24250
H	3.11020	-3.40150	1.24210
H	3.11020	-3.40140	-1.24210
H	1.61440	-1.86760	-2.49360
C	-0.17800	-0.03430	1.39320
H	1.61440	-1.86760	2.49360
H	-2.73940	-0.17650	-2.49340
H	-2.73930	-0.17650	2.49340
H	-0.28470	-0.30560	2.47230
C	-0.17800	-0.03420	-1.39320
H	-0.28470	-0.30560	-2.47230
C	0.34710	1.41910	1.31840
H	-0.50870	2.10610	1.49140
H	1.04150	1.58390	2.16670
C	0.34710	1.41910	-1.31840
H	1.04150	1.58390	-2.16670
H	-0.50870	2.10620	-1.49130
C	1.06050	1.82420	0.00000
N	2.44720	1.29910	0.00000
H	2.97220	1.55700	-0.82650
H	2.97220	1.55690	0.82650
C	1.10410	3.32750	0.00000
N	1.16080	4.47910	0.00000

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motherwell/opt_a1_folded_opt.xyz

C	-3.50200	-1.45390	0.79500
C	-2.39350	-0.92560	1.47040
C	-1.31390	-0.43140	0.73940
C	-1.33860	-0.46570	-0.67110
C	-2.44280	-0.99380	-1.33890
C	-3.52650	-1.48780	-0.60030
C	1.12230	-0.41110	-0.71690
C	1.14710	-0.37670	0.69640
C	2.27590	-0.81610	1.38600
C	3.38340	-1.29140	0.67030
C	3.35890	-1.32550	-0.72460
C	2.22660	-0.88460	-1.42340
H	-4.34520	-1.84100	1.36410
H	-4.38880	-1.90120	-1.12000
H	4.26480	-1.63600	1.20840
H	4.22120	-1.69670	-1.27590
H	2.21500	-0.91430	-2.51110
C	-0.08320	0.16370	1.39390
H	2.30250	-0.79270	2.47360
H	-2.46770	-1.02650	-2.42590
H	-2.38020	-0.90530	2.55790
H	-0.05910	-0.11090	2.47720
C	-0.13210	0.09570	-1.39640
H	-0.14560	-0.23130	-2.46530
C	-0.14010	1.70340	1.28850
H	-1.15870	2.03690	1.57100
H	0.54410	2.13500	2.05060
C	-0.18650	1.63880	-1.36420
H	0.47030	2.03220	-2.16980
H	-1.21460	1.95910	-1.62680
C	0.23230	2.34450	-0.06110
H	-0.17180	3.39030	-0.07960
O	1.64380	2.61150	-0.09230
H	2.16620	1.78260	-0.08100

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motherwell/opt_a2_folded_opt.xyz

C	-3.50630	-1.71800	0.79850
C	-2.38460	-1.22000	1.47520
C	-1.29310	-0.75140	0.74520

C	-1.31880	-0.78120	-0.66520
C	-2.43590	-1.27930	-1.33450
C	-3.53170	-1.74750	-0.59690
C	1.14310	-0.78650	-0.71140
C	1.16880	-0.75660	0.70170
C	2.28610	-1.22640	1.39020
C	3.38120	-1.72730	0.67290
C	3.35590	-1.75670	-0.72220
C	2.23500	-1.28560	-1.41960
H	-4.35910	-2.08480	1.36650
H	-4.40440	-2.13740	-1.11750
H	4.25390	-2.09530	1.20990
H	4.20870	-2.14750	-1.27450
H	2.22260	-1.31160	-2.50740
C	-0.04780	-0.18730	1.39910
H	2.31320	-1.20660	2.47780
H	-2.46160	-1.30810	-2.42150
H	-2.37070	-1.20280	2.56270
H	-0.02980	-0.46560	2.48210
C	-0.09860	-0.24620	-1.38740
H	-0.11990	-0.56990	-2.45760
C	-0.07200	1.35270	1.30300
H	-1.08070	1.70000	1.60470
H	0.62850	1.76400	2.06090
C	-0.12030	1.29660	-1.35550
H	0.55210	1.67480	-2.15500
H	-1.13950	1.63180	-1.63490
C	0.30150	2.00710	-0.04790
O	1.73580	2.19800	-0.07790
H	2.21540	1.34710	-0.06950
C	-0.20610	3.45830	-0.06920
H	0.18790	4.01960	0.78770
H	0.15590	3.98270	-0.96280
H	-1.29670	3.51650	-0.05050

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motherwell/opt_a3_folded_opt.xyz

C	-3.78760	-2.61410	0.48660
C	-2.61490	-2.23950	1.15630
C	-1.50190	-1.83560	0.42000
C	-1.55760	-1.80620	-0.98940
C	-2.72560	-2.18150	-1.65190
C	-3.84250	-2.58550	-0.90800
C	0.89440	-2.01390	-1.09250
C	0.94990	-2.04530	0.31960
C	2.03720	-2.63410	0.96330
C	3.07280	-3.19280	0.20170
C	3.01820	-3.16130	-1.19250
C	1.92700	-2.57110	-1.84490
H	-4.65730	-2.93030	1.05940
H	-4.75510	-2.87950	-1.42310
H	3.92200	-3.65360	0.70340
H	3.82500	-3.59720	-1.77930
H	1.89140	-2.55040	-2.93230
C	-0.20050	-1.40510	1.06570
H	2.08650	-2.66250	2.04990
H	-2.77500	-2.16410	-2.73830
H	-2.57850	-2.26670	2.24310
H	-0.18500	-1.72730	2.13650
C	-0.31080	-1.34480	-1.71680
H	-0.37990	-1.62000	-2.79850
C	-0.09460	0.13420	1.03070
H	-1.06330	0.55290	1.37130
H	0.65550	0.44830	1.78840
C	-0.20400	0.19200	-1.62220
H	0.48220	0.54390	-2.42230
H	-1.19840	0.61710	-1.86590
C	0.30460	0.81570	-0.29790

O	1.74730	0.88290	-0.36500
H	2.14840	-0.00780	-0.38800
C	-0.10380	2.31280	-0.28070
H	0.20730	2.77060	-1.24220
H	-1.20460	2.39660	-0.23440
C	0.54240	3.09670	0.86750
H	0.18320	2.72310	1.84400
H	1.63860	2.91350	0.85550
C	0.25670	4.59980	0.74900
H	-0.83600	4.77760	0.73010
H	0.64300	4.98060	-0.21710
C	0.88770	5.38280	1.89820
H	0.68890	6.45590	1.80290
H	0.49720	5.06060	2.87000
H	1.97600	5.25160	1.92340

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motherwell/opt_a4_folded_opt.xyz

C	-3.52630	-1.47530	0.82290
C	-2.39920	-0.98450	1.49540
C	-1.30200	-0.53640	0.76070
C	-1.32750	-0.57980	-0.64880
C	-2.45030	-1.07070	-1.31420
C	-3.55160	-1.51800	-0.57250
C	1.13480	-0.61680	-0.69380
C	1.16030	-0.57310	0.71890
C	2.27090	-1.05070	1.41290
C	3.35950	-1.57270	0.70120
C	3.33450	-1.61550	-0.69380
C	2.22030	-1.13720	-1.39660
H	-4.38460	-1.82570	1.39400
H	-4.42980	-1.90180	-1.08950
H	4.22720	-1.94780	1.24240
H	4.18270	-2.02390	-1.24180
H	2.20740	-1.17600	-2.48450
C	-0.04980	0.01670	1.41130
H	2.29720	-1.02250	2.50080
H	-2.47660	-1.10970	-2.40130
H	-2.38590	-0.95690	2.58300
H	-0.03610	-0.25180	2.49740
C	-0.10020	-0.06980	-1.37720
H	-0.12550	-0.40530	-2.44430
C	-0.05410	1.55620	1.30310
H	-1.06290	1.92140	1.59170
H	0.64400	1.97220	2.06290
C	-0.10160	1.47340	-1.36490
H	0.56910	1.84020	-2.17330
H	-1.12020	1.82170	-1.63990
C	0.34530	2.16690	-0.05860
O	1.77380	2.35950	-0.09010
H	2.24540	1.49550	-0.07150
C	-0.15590	3.56930	-0.09320
N	-0.54840	4.65300	-0.11970

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motherwell/opt_a5_folded_opt.xyz

C	-3.53060	-1.58130	0.82620
C	-2.39550	-1.10920	1.49880
C	-1.29030	-0.68000	0.76490
C	-1.31630	-0.72290	-0.64500
C	-2.44700	-1.19530	-1.31030
C	-3.55610	-1.62420	-0.56900
C	1.14420	-0.80060	-0.68970
C	1.17050	-0.75790	0.72300
C	2.27330	-1.25370	1.41660
C	3.35320	-1.79360	0.70470
C	3.32720	-1.83590	-0.69020
C	2.22100	-1.33880	-1.39260

H	-4.39430	-1.91720	1.39710
H	-4.43960	-1.99380	-1.08630
H	4.21470	-2.18200	1.24560
H	4.16830	-2.25740	-1.23830
H	2.20770	-1.37550	-2.48020
C	-0.02920	-0.14760	1.41540
H	2.30080	-1.22440	2.50410
H	-2.47330	-1.23380	-2.39710
H	-2.38210	-1.08110	2.58620
H	-0.01980	-0.41780	2.50090
C	-0.08090	-0.23170	-1.37260
H	-0.11140	-0.56630	-2.43950
C	-0.00820	1.39100	1.30880
H	-1.00760	1.77390	1.60400
H	0.70280	1.79420	2.06220
C	-0.05820	1.31050	-1.35930
H	0.62330	1.66740	-2.16180
H	-1.06870	1.67560	-1.63900
C	0.38870	2.01300	-0.05310
O	1.82860	2.17010	-0.08480
H	2.27670	1.29800	-0.06720
C	-0.09010	3.39930	-0.08620
C	-0.47300	4.54020	-0.11390
H	-0.80200	5.51920	-0.13770

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motherwell/opt_a6_folded_opt.xyz

C	-3.75060	-1.85740	1.01000
C	-2.61710	-1.34870	1.65860
C	-1.53170	-0.90700	0.90320
C	-1.57650	-0.97430	-0.50600
C	-2.70500	-1.48310	-1.14720
C	-3.79420	-1.92450	-0.38350
C	0.88260	-1.00360	-0.58690
C	0.92960	-0.93610	0.82480
C	2.05120	-1.40130	1.50830
C	3.12850	-1.93550	0.78670
C	3.07990	-2.00520	-0.60580
C	1.95360	-1.53900	-1.29900
H	-4.59790	-2.20350	1.59860
H	-4.67540	-2.32310	-0.88220
H	4.00600	-2.29520	1.31970
H	3.91780	-2.42240	-1.15970
H	1.92280	-1.59750	-2.38370
C	-0.27280	-0.33820	1.52610
H	2.10060	-1.34370	2.59280
H	-2.74460	-1.54170	-2.23240
H	-2.58870	-1.30330	2.74500
H	-0.24130	-0.58860	2.61490
C	-0.36250	-0.46420	-1.25730
H	-0.40270	-0.80580	-2.32030
C	-0.28120	1.20110	1.39130
H	-1.28680	1.57880	1.65580
H	0.42270	1.61530	2.14710
C	-0.37660	1.08120	-1.24740
H	0.20830	1.44080	-2.11590
H	-1.41830	1.41620	-1.43300
C	0.14210	1.78940	0.02280
O	1.58580	1.73770	0.16510
C	2.40240	2.05220	-0.97040
H	2.18080	3.05060	-1.35300
H	3.41340	2.01150	-0.54480
H	2.28890	1.28550	-1.74370
C	-0.26570	3.27500	-0.04320
H	-1.34350	3.41180	0.07780
H	0.23740	3.84280	0.74920
H	0.02300	3.73600	-0.99210

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motherwell/opt_a7_folded_opt.xyz

C	-3.88170	-2.63610	1.35030
C	-2.75160	-2.14540	2.01850
C	-1.61830	-1.79380	1.28680
C	-1.61110	-1.93360	-0.11770
C	-2.73640	-2.42430	-0.77820
C	-3.87420	-2.77480	-0.03850
C	0.84380	-2.08300	-0.09270
C	0.84080	-1.93490	1.31320
C	1.91200	-2.41060	2.06690
C	2.98650	-3.03920	1.42140
C	2.98460	-3.19330	0.03480
C	1.91030	-2.71500	-0.72890
H	-4.76680	-2.91190	1.92030
H	-4.75320	-3.15890	-0.55220
H	3.82490	-3.40730	2.00910
H	3.81870	-3.68610	-0.45950
H	1.91520	-2.83980	-1.80850
C	-0.35950	-1.24670	1.92930
H	1.92420	-2.28970	3.14730
H	-2.73640	-2.53850	-1.85970
H	-2.76340	-2.04370	3.10140
H	-0.38200	-1.43710	3.03070
C	-0.34480	-1.52080	-0.84140
H	-0.35980	-1.91600	-1.88650
C	-0.29690	0.28120	1.71210
H	-1.29600	0.70860	1.91930
H	0.39590	0.70450	2.47360
C	-0.28270	0.02230	-0.91480
H	0.35840	0.29840	-1.77450
H	-1.29880	0.39200	-1.16910
C	0.20510	0.78630	0.33110
O	1.63640	0.70180	0.55990
C	2.53710	0.80110	-0.55020
H	2.37130	1.73300	-1.10770
H	3.51510	0.80910	-0.05310
H	2.44660	-0.07950	-1.19360
C	-0.16580	2.29420	0.22300
H	-1.23260	2.42820	0.48360
H	0.41130	2.82940	1.00620
C	0.10700	2.95060	-1.13330
H	1.15480	2.74260	-1.44680
H	-0.54170	2.51220	-1.91480
C	-0.11850	4.46820	-1.07160
H	0.53910	4.91550	-0.30000
H	-1.15510	4.68280	-0.74550
C	0.14620	5.13160	-2.42100
H	-0.02050	6.21350	-2.36890
H	1.17910	4.97590	-2.75250
H	-0.51270	4.73680	-3.20270

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Diederich/opt_a1_folded_opt.xyz

C	2.26570	1.58270	4.00780
C	2.35790	0.35220	3.35420
C	1.18700	-0.35130	3.03790
C	-0.08180	0.19680	3.33480
C	-0.15310	1.42180	4.00550
C	1.01560	2.10980	4.34580
H	3.17310	2.12710	4.26440
H	3.32960	-0.07540	3.11010
H	-1.12360	1.84720	4.25930
H	0.95040	3.05850	4.87480
C	-1.35300	-0.52620	2.95320
H	-1.93550	-0.77970	3.87080
N	1.32580	-1.69160	2.47910
N	-1.12760	-1.81900	2.22440

C	0.09380	-2.49550	2.77760
H	0.18800	-3.51090	2.33110
H	-0.00990	-2.61610	3.87980
C	1.56130	-1.67550	0.99810
H	2.22560	-0.82030	0.73540
H	2.13090	-2.60470	0.75770
C	0.29650	-1.61910	0.17240
C	-0.97740	-1.62700	0.78810
C	0.38200	-1.55540	-1.21860
C	-2.14060	-1.52320	0.01220
C	-0.78330	-1.45150	-1.99440
H	1.35740	-1.57450	-1.70600
C	-2.04190	-1.43380	-1.37640
H	-3.11670	-1.52340	0.49800
H	-2.94360	-1.33870	-1.98070
H	-2.00250	0.13970	2.34070
C	-0.67970	-1.30790	-3.46400
C	0.01280	-0.21920	-4.03090
C	-1.26660	-2.25760	-4.31410
C	0.11660	-0.08310	-5.42230
C	-1.16490	-2.11800	-5.69950
H	-1.79870	-3.10720	-3.88520
C	-0.47510	-1.03360	-6.25510
H	0.66000	0.76280	-5.84820
H	-1.62500	-2.86000	-6.35370
H	-0.39870	-0.93190	-7.33710
C	0.66920	0.78690	-3.15980
C	-0.04200	1.94250	-1.10010
C	1.23140	2.25440	-0.61730
C	-1.21990	2.23160	-0.39000
C	1.33300	2.89900	0.62000
H	2.12640	2.01410	-1.19450
C	-1.05510	2.87860	0.83150
H	-2.19090	1.95290	-0.79380
C	0.19320	3.23350	1.35520
H	2.31970	3.14580	1.01600
H	0.27890	3.74180	2.31340
O	-0.31000	1.28630	-2.29630
O	1.81040	1.16200	-3.14100
F	-2.14680	3.17180	1.54030

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Diederich/opt_a2_folded_opt.xyz

C	1.82720	1.74000	4.11750
C	2.06580	0.54410	3.43810
C	0.98690	-0.28610	3.09950
C	-0.33760	0.10100	3.40530
C	-0.55500	1.29370	4.10320
C	0.52240	2.10870	4.46110
H	2.66340	2.38340	4.38730
H	3.08180	0.24220	3.18520
H	-1.56820	1.59180	4.36840
H	0.34460	3.03310	5.00680
C	-1.51370	-0.75680	2.99780
H	-2.05320	-1.11680	3.90620
N	1.28500	-1.58430	2.50520
N	-1.13480	-1.98090	2.21680
C	0.15150	-2.53410	2.76110
H	0.36400	-3.51520	2.27960
H	0.05390	-2.70640	3.85670
C	1.53280	-1.49750	1.02830
H	2.09290	-0.56130	0.79730
H	2.21120	-2.34470	0.76940
C	0.27710	-1.56260	0.18950
C	-0.99430	-1.71350	0.79170
C	0.36810	-1.46250	-1.19940
C	-2.15590	-1.68560	0.00700
C	-0.79430	-1.44250	-1.98620

H	1.34720	-1.38680	-1.67500
C	-2.05420	-1.54240	-1.37660
H	-3.13190	-1.79160	0.48050
H	-2.95740	-1.50350	-1.98520
H	-2.24410	-0.15380	2.41360
C	-0.70100	-1.28880	-3.45540
C	-0.00040	-0.21620	-4.04040
C	-1.32060	-2.23070	-4.29400
C	0.07250	-0.08480	-5.43490
C	-1.24870	-2.09630	-5.68100
H	-1.85450	-3.07300	-3.85320
C	-0.55510	-1.02340	-6.25400
H	0.62340	0.74980	-5.87360
H	-1.73430	-2.83250	-6.32290
H	-0.50260	-0.92290	-7.33730
C	0.71370	0.78060	-3.20130
C	0.18290	2.01090	-1.14900
C	1.39060	2.69000	-0.99060
C	-0.80240	1.95500	-0.15000
C	1.61480	3.34310	0.22660
H	2.13880	2.70550	-1.78480
C	-0.55460	2.62480	1.04570
H	-1.71970	1.39680	-0.32390
C	0.65090	3.31490	1.23690
H	2.55190	3.87730	0.38140
H	-1.29800	2.60370	1.84200
H	0.83700	3.82050	2.18230
O	-0.20080	1.32280	-2.30760
O	1.87180	1.10740	-3.23930

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Diederich/opt_a3_folded_opt.xyz

C	0.92460	1.82540	4.34520
C	1.31630	0.63860	3.72270
C	0.34020	-0.21380	3.18720
C	-1.02890	0.12940	3.25270
C	-1.40030	1.32920	3.86850
C	-0.42890	2.17110	4.41700
H	1.67710	2.48050	4.77950
H	2.36960	0.36650	3.65250
H	-2.45090	1.60900	3.92470
H	-0.72820	3.09760	4.90240
C	-2.09150	-0.79240	2.69930
H	-2.75930	-1.13220	3.52690
N	0.77940	-1.49320	2.64010
N	-1.55950	-2.03820	2.05210
C	-0.32590	-2.49880	2.77470
H	0.00270	-3.47640	2.35550
H	-0.55860	-2.65000	3.85280
C	1.19440	-1.38190	1.20220
H	1.68650	-0.39330	1.03040
H	1.97900	-2.15800	1.04050
C	0.07060	-1.57300	0.21000
C	-1.24990	-1.83480	0.64240
C	0.33140	-1.48920	-1.15880
C	-2.29120	-1.97520	-0.28590
C	-0.71040	-1.63220	-2.08740
H	1.34190	-1.27720	-1.51460
C	-2.02000	-1.87340	-1.65040
H	-3.30420	-2.17490	0.06330
H	-2.82700	-1.97670	-2.37520
H	-2.73640	-0.24360	1.97650
C	-0.42510	-1.49150	-3.53400
C	-0.25080	-0.21700	-4.10730
C	-0.33550	-2.62550	-4.35420
C	0.01490	-0.07730	-5.47520
C	-0.06730	-2.48530	-5.71760
H	-0.47140	-3.61570	-3.91880

C	0.10830	-1.21510	-6.27900
H	0.14580	0.91590	-5.90790
H	0.00540	-3.37170	-6.34890
H	0.31640	-1.11300	-7.34320
C	-0.38840	0.99540	-3.25930
C	0.72000	1.72280	-1.18270
C	-0.41930	2.23940	-0.56560
C	1.99930	1.77820	-0.61780
C	-0.25790	2.85130	0.68260
H	-1.39670	2.18160	-1.03970
C	2.12530	2.38950	0.64340
H	2.84470	1.35110	-1.14500
C	0.99370	2.94710	1.28370
H	-1.13180	3.26110	1.19210
H	1.09270	3.42260	2.25500
O	0.70060	1.00840	-2.38170
O	-1.22490	1.85510	-3.27120
N	3.37100	2.36980	1.30760
H	4.19330	2.26160	0.73230
H	3.50170	3.04280	2.04840

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Diederich/opt_a4_folded_opt.xyz

C	2.11050	1.30720	4.44790
C	2.10030	0.09490	3.75460
C	0.89620	-0.38530	3.21970
C	-0.29630	0.36260	3.35040
C	-0.26820	1.56870	4.05820
C	0.92950	2.03990	4.60430
H	3.04080	1.67300	4.88090
H	3.01440	-0.48830	3.63990
H	-1.18410	2.14430	4.18650
H	0.93840	2.97240	5.16570
C	-1.59350	-0.12870	2.75070
H	-2.36310	-0.23740	3.55190
N	0.89480	-1.71290	2.61800
N	-1.50230	-1.46610	2.07610
C	-0.47190	-2.31690	2.76070
H	-0.47940	-3.33750	2.31540
H	-0.72320	-2.41430	3.84100
C	1.29970	-1.69540	1.17260
H	2.05150	-0.88890	1.00230
H	1.82400	-2.66300	0.98600
C	0.15320	-1.53690	0.20020
C	-1.17180	-1.35940	0.66050
C	0.39670	-1.57520	-1.17470
C	-2.22330	-1.16960	-0.24690
C	-0.65960	-1.40770	-2.08280
H	1.41070	-1.72760	-1.54550
C	-1.96580	-1.19610	-1.61710
H	-3.23720	-1.01820	0.12330
H	-2.77760	-1.04220	-2.32750
H	-1.98430	0.62820	2.03120
C	-0.39800	-1.41760	-3.54110
C	0.34780	-0.38750	-4.14720
C	-0.89230	-2.45990	-4.33930
C	0.59350	-0.39770	-5.52670
C	-0.64890	-2.46700	-5.71430
H	-1.46520	-3.26500	-3.87850
C	0.09150	-1.43860	-6.30950
H	1.17630	0.40510	-5.98260
H	-1.03770	-3.28030	-6.32870
H	0.27780	-1.45080	-7.38270
C	0.91230	0.70330	-3.31570
C	-0.02820	1.91110	-1.39160
C	-1.23500	2.47280	-0.93290
C	1.13560	1.88070	-0.62910
C	-1.25890	3.02420	0.34610

H	-2.11170	2.46170	-1.57310
C	1.05410	2.43300	0.65840
H	2.07680	1.47190	-0.99570
C	-0.12170	3.01290	1.16020
H	-2.18040	3.47250	0.72020
H	-0.14810	3.44600	2.15310
O	-0.15560	1.31130	-2.63690
O	2.04670	1.07410	-3.19650
O	2.21070	2.36820	1.38620
H	2.07950	2.65720	2.32910

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Zoltewicz/opt_a2_folded_opt.xyz

C	0.06050	-4.71880	-0.15970
C	1.42470	-4.68660	-0.04000
C	2.11510	-3.43730	0.06540
C	1.39520	-2.20810	0.02940
C	-0.04060	-2.28450	-0.04460
C	-0.67630	-3.50500	-0.14970
H	4.05690	-4.39790	0.24650
H	-0.47700	-5.66130	-0.25250
H	2.00710	-5.60660	-0.02480
C	3.53910	-3.44080	0.20730
C	2.16090	-0.98970	0.06980
H	-1.76380	-3.55420	-0.21710
C	3.53340	-1.02770	0.21240
C	4.23100	-2.26160	0.29380
H	4.10640	-0.10040	0.25400
H	5.31330	-2.24870	0.41350
C	1.55980	0.35930	-0.08510
C	1.12160	1.07660	1.03500
C	1.49780	0.93490	-1.36360
C	0.57720	2.35880	0.87370
H	1.18530	0.62640	2.02290
C	0.96830	2.21860	-1.51640
H	1.85240	0.37930	-2.22810
C	0.50320	2.92840	-0.40810
H	0.91050	2.66530	-2.50760
H	0.07150	3.91770	-0.53850
C	-0.92010	-1.09280	0.03820
C	-1.30080	-0.39700	-1.08460
C	-1.41800	-0.71620	1.32780
C	-2.14810	0.74900	-0.96750
H	-0.93990	-0.68740	-2.07030
C	-2.25020	0.36400	1.45820
H	-1.11440	-1.30260	2.19380
C	-2.62120	1.13790	0.31230
C	-2.50670	1.53050	-2.11130
H	-2.63360	0.65850	2.43340
C	-3.44120	2.30390	0.42870
C	-3.28910	2.64890	-1.97010
H	-2.13800	1.22340	-3.08860
C	-3.76220	3.04080	-0.68370
H	-3.80170	2.59260	1.41420
H	-3.56110	3.25330	-2.83350
H	-4.38170	3.93220	-0.60430
C	0.05860	3.11790	2.05210
H	0.57510	4.08040	2.16880
H	-1.01430	3.33280	1.93350
H	0.17530	2.56940	2.99500

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Zoltewicz/opt_a3_folded_opt.xyz

C	-0.04940	-5.05290	-0.58050
C	1.31290	-5.07310	-0.43730
C	2.04390	-3.85290	-0.27830
C	1.36660	-2.59980	-0.29500
C	-0.07090	-2.62400	-0.36250

C	-0.74640	-3.81680	-0.52370
H	3.94860	-4.88020	-0.07120
H	-0.61650	-5.97170	-0.72150
H	1.86300	-6.01290	-0.44510
C	3.46320	-3.90610	-0.10300
C	2.17270	-1.40890	-0.24280
H	-1.83460	-3.82770	-0.59350
C	3.53840	-1.49350	-0.06450
C	4.19060	-2.75190	0.02440
H	4.14160	-0.58610	-0.00770
H	5.26870	-2.77720	0.17610
C	1.62040	-0.04520	-0.45350
C	1.24080	0.74210	0.63470
C	1.55120	0.45380	-1.76360
C	0.74770	2.04920	0.42180
H	1.32040	0.33330	1.63890
C	1.07590	1.75000	-1.97080
H	1.86130	-0.16320	-2.60110
C	0.66830	2.54360	-0.90120
H	1.01710	2.14650	-2.98410
H	0.29460	3.54560	-1.09420
C	-0.90950	-1.41320	-0.18510
C	-1.31310	-0.64010	-1.24760
C	-1.35430	-1.10710	1.14240
C	-2.14090	0.50580	-1.03030
H	-0.98590	-0.87020	-2.26120
C	-2.17630	-0.03470	1.36670
H	-1.02400	-1.74600	1.96060
C	-2.58100	0.80930	0.28390
C	-2.52280	1.36520	-2.10890
H	-2.53500	0.19380	2.36870
C	-3.41020	1.95520	0.49610
C	-3.30640	2.46720	-1.87520
H	-2.17020	1.12970	-3.11200
C	-3.76000	2.76340	-0.55670
H	-3.75750	2.16880	1.50530
H	-3.59640	3.12940	-2.68900
H	-4.39030	3.63780	-0.40530
N	0.46240	2.91080	1.52530
C	-0.51890	4.00030	1.25640
H	-1.51110	3.63400	0.94460
H	-0.63880	4.62330	2.15590
H	-0.12500	4.65590	0.46000
C	0.18480	2.24400	2.82810
H	-0.74370	1.65180	2.83470
H	1.02550	1.57680	3.08840
H	0.12340	3.00690	3.62050

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Zoltewicz/opt_a5_folded_opt.xyz

C	-0.18990	-4.85900	-0.29420
C	1.17180	-4.92520	-0.16030
C	1.94560	-3.73030	-0.01210
C	1.31220	-2.45440	-0.02400
C	-0.12540	-2.42860	-0.10160
C	-0.84230	-3.59830	-0.24980
H	3.81480	-4.82510	0.17230
H	-0.78990	-5.75880	-0.42160
H	1.68900	-5.88360	-0.16610
C	3.36400	-3.83410	0.14860
C	2.16020	-1.29320	0.04320
H	-1.93030	-3.57080	-0.32170
C	3.52400	-1.42640	0.20500
C	4.13340	-2.70740	0.27280
H	4.15890	-0.54160	0.27090
H	5.21170	-2.77150	0.41060
C	1.64990	0.09280	-0.11580
C	1.28360	0.84640	0.99700

C	1.59600	0.65120	-1.40880
C	0.80330	2.15520	0.78770
H	1.33000	0.44230	2.00500
C	1.13930	1.95620	-1.58130
H	1.90220	0.05620	-2.26480
C	0.72860	2.72660	-0.48740
H	1.09180	2.38560	-2.58190
H	0.35270	3.73090	-0.64150
C	-0.91910	-1.18260	0.03340
C	-1.30320	-0.44640	-1.06210
C	-1.32870	-0.79140	1.34980
C	-2.06700	0.75090	-0.89180
H	-1.00720	-0.74460	-2.06680
C	-2.07910	0.33980	1.53200
H	-1.02090	-1.40610	2.19480
C	-2.45500	1.15020	0.41310
C	-2.42500	1.57230	-2.00740
H	-2.38590	0.65150	2.52930
C	-3.19620	2.36160	0.58150
C	-3.12690	2.73590	-1.81620
H	-2.12150	1.25770	-3.00460
C	-3.51870	3.13540	-0.50540
H	-3.49800	2.65200	1.58640
H	-3.39810	3.36950	-2.65870
H	-4.08130	4.05940	-0.38710
O	0.43710	2.77770	1.96220
C	-0.22860	4.05910	1.85970
H	-0.47470	4.27080	2.90740
H	0.45810	4.80900	1.45790
H	-1.13550	3.96790	1.25180

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Zoltewicz/opt_a6_folded_opt.xyz

C	-0.28980	-4.87170	-0.44200
C	1.06490	-4.98370	-0.27130
C	1.86880	-3.81830	-0.06160
C	1.27350	-2.52430	-0.05030
C	-0.15980	-2.45240	-0.16460
C	-0.90630	-3.59420	-0.37260
H	3.69920	-4.97350	0.14270
H	-0.91170	-5.74830	-0.61710
H	1.55340	-5.95680	-0.29390
C	3.27810	-3.96910	0.13710
C	2.15200	-1.39100	0.07530
H	-1.99060	-3.53160	-0.47260
C	3.50590	-1.57000	0.27320
C	4.07540	-2.87010	0.31960
H	4.16430	-0.70720	0.38410
H	5.14680	-2.97060	0.48750
C	1.68770	0.01190	-0.06040
C	1.33090	0.76030	1.06760
C	1.66560	0.60100	-1.33710
C	0.92230	2.08760	0.89770
H	1.35420	0.29860	2.05530
C	1.26400	1.92910	-1.48160
H	1.95420	0.01510	-2.20750
C	0.88550	2.68140	-0.36300
H	1.23920	2.38480	-2.47010
H	0.56630	3.71240	-0.49610
C	-0.91960	-1.18850	-0.00320
C	-1.26640	-0.40910	-1.08120
C	-1.33970	-0.82760	1.31830
C	-2.00860	0.79780	-0.88640
H	-0.96100	-0.68320	-2.08970
C	-2.07270	0.31110	1.52280
H	-1.05740	-1.47310	2.14900
C	-2.41810	1.16000	0.42280
C	-2.33000	1.66140	-1.98100

H	-2.38950	0.59940	2.52460
C	-3.15350	2.37130	0.61470
C	-3.02440	2.82560	-1.76650
H	-2.00720	1.37730	-2.98110
C	-3.44430	3.18420	-0.45250
H	-3.47390	2.63140	1.62260
H	-3.26910	3.49040	-2.59290
H	-4.00320	4.10790	-0.31640
C	-0.47950	4.36170	1.85270
H	-0.97070	4.77080	2.74550
H	0.14640	5.14670	1.41550
H	-1.25990	4.08390	1.13160
S	0.49540	2.93630	2.37870

4. Coordinates for Lowest-Energy Molecular Balances Conformation Found by ACO, subsequently optimized with PM-DH+

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1_9_disubsti_triptycene_pm6/opt_a1_folded_opt_7.xyz
C      -5.77520      1.62560      1.94620
C      -4.49140      1.19340      2.30820
C      -3.34090      1.90900      1.91970
C      -3.52120      3.03030      1.08640
C      -4.80750      3.46470      0.72500
C      -5.94000      2.76940      1.16200
C      -1.45750      2.52910     -0.05610
C      -1.25340      1.41130      0.80220
C      -0.56810      0.30230      0.33110
H      -0.40070     -0.57060      0.95830
C      -0.08020      0.30280     -0.98930
C      -0.28070      1.40000     -1.82190
C      -0.97810      2.52910     -1.35570
H      -6.65470      1.07300      2.26650
H      -6.94100      3.09560      0.89560
H      0.45830     -0.56910     -1.35660
H      0.10060      1.39000     -2.84130
H      -1.13710      3.38310     -2.00980
C      -1.22620      2.91000      2.70980
C      -0.45160      3.09220      3.84620
C      0.06260      4.36590      4.14730
C      -0.18790      5.44960      3.31020
C      -0.94760      5.27750      2.14040
C      -1.44760      4.01880      1.84530
H      -0.23240      2.26010      4.51980
H      0.66380      4.49760      5.04530
H      0.20860      6.43360      3.55330
H      -1.13370      6.12020      1.47850
O      -4.80610      4.59510     -0.07390
C      -6.08680      5.07950     -0.53890
H      -5.79070      5.94530     -1.14540
H      -6.58140      4.32230     -1.15390
H      -6.70670      5.38910      0.30720
C      -1.86060      1.59690      2.21130
C      -1.60930      0.37500      3.10520
H      -2.14500     -0.49610      2.65590
H      -0.52710      0.12910      3.08680
C      -2.06190      0.53490      4.56260
H      -3.10020      0.94750      4.59810
H      -1.41620      1.27050      5.09910
O      -4.24280      0.05800      3.04970
C      -5.35100     -0.78070      3.44930
H      -4.81860     -1.55570      4.03140
H      -6.04850     -0.22710      4.08080
H      -5.83790     -1.21020      2.57100
C      -2.04210     -0.78350      5.27180
O      -2.75760     -1.75480      5.18520
O      -1.00540     -0.80230      6.18500

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H	-0.94890	-1.65370	6.69140
C	-2.23450	3.66770	0.59450
H	-2.41550	4.52890	-0.07980

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1_9_disubsti_triptycene_pm6/opt_a2_folded_opt_9.xyz

C	0.17140	6.37340	5.21940
C	-0.46100	5.31420	5.88720
C	-1.84370	5.08160	5.74440
C	-2.58440	6.00350	4.97820
C	-1.95060	7.06300	4.30840
C	-0.56770	7.24520	4.41740
C	-4.47020	5.73580	6.45840
C	-3.73850	4.77930	7.21830
C	-3.98590	4.64880	8.57600
H	-3.44040	3.93200	9.18590
C	-4.96210	5.46320	9.18040
C	-5.67580	6.39400	8.43110
C	-5.43060	6.53740	7.05330
H	1.24120	6.53320	5.32750
H	-0.06220	8.05580	3.90100
H	-5.15480	5.35860	10.24660
H	-6.42860	7.01880	8.90810
H	-5.98690	7.26840	6.47140
C	-3.56290	3.38000	5.24520
C	-3.72630	2.03720	4.93720
C	-4.55470	1.65960	3.86550
C	-5.22500	2.61990	3.11270
C	-5.09360	3.98310	3.42860
C	-4.28000	4.34960	4.48930
H	-3.21910	1.26030	5.51460
H	-4.67000	0.60330	3.62930
H	-5.85930	2.32010	2.28090
H	-5.62680	4.73390	2.85010
O	-2.81900	7.85450	3.57640
C	-2.25900	9.00610	2.90480
H	-3.14890	9.44500	2.43520
H	-1.81970	9.69590	3.63100
H	-1.53420	8.69070	2.14900
C	-2.71320	3.98120	6.38170
C	-1.95460	2.95610	7.23440
H	-1.36020	3.51590	7.99540
H	-2.68470	2.33480	7.79500
C	-1.01340	2.03010	6.45220
H	-0.37630	2.62620	5.75680
H	-1.59580	1.32100	5.81930
O	0.18990	4.45300	6.74490
C	1.63440	4.49850	6.82020
H	1.83820	3.59660	7.42780
H	2.08390	4.40350	5.82990
H	1.95140	5.40780	7.33480
C	-0.12570	1.26660	7.39260
O	1.00980	1.48800	7.74660
O	-0.81250	0.15830	7.84630
C	-0.11880	-0.72240	8.76710
H	0.43370	-0.14020	9.51260
H	-0.93370	-1.29730	9.21880
H	0.56000	-1.35900	8.19210
C	-4.08450	5.77220	4.98420
H	-4.63580	6.53310	4.39590

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1_9_disubsti_triptycene_pm6/opt_a3_folded_opt_6.xyz

C	-6.09340	4.36900	4.15730
C	-5.00370	3.52760	4.42880
C	-3.69330	4.03680	4.51900
C	-3.50600	5.40680	4.24410
C	-4.59730	6.24880	3.97490

C	-5.89790	5.73410	3.94110
C	-1.36510	4.92950	3.23990
C	-1.53190	3.54830	3.54190
C	-0.95850	2.59230	2.71780
H	-1.07050	1.52840	2.91780
C	-0.21610	3.00590	1.59580
C	-0.05520	4.35810	1.30740
C	-0.63510	5.33640	2.13520
H	-7.10170	3.96640	4.10070
H	-6.75320	6.37240	3.73950
H	0.23390	2.25340	0.95030
H	0.52100	4.66690	0.43710
H	-0.51090	6.39190	1.90530
C	-1.64870	4.10100	5.90180
C	-1.10770	3.62030	7.08540
C	-0.46300	4.50280	7.97040
C	-0.35050	5.85690	7.66770
C	-0.86810	6.35600	6.46000
C	-1.49810	5.48120	5.58880
H	-1.17180	2.56210	7.34670
H	-0.04750	4.11530	8.89910
H	0.14470	6.53450	8.36060
H	-0.76960	7.41130	6.21580
O	-4.23990	7.56800	3.75890
C	-5.29660	8.49330	3.41410
H	-4.73880	9.43010	3.28500
H	-5.77770	8.19280	2.47910
H	-6.01330	8.57600	4.23610
C	-2.37620	3.29230	4.81030
C	-2.52220	1.79510	5.10430
H	-3.08810	1.33320	4.25990
H	-1.51890	1.31810	5.10170
C	-3.23270	1.46110	6.42120
H	-4.14700	2.09310	6.54160
H	-2.58910	1.69770	7.30110
O	-5.12280	2.15990	4.58700
C	-6.44990	1.60070	4.73870
H	-6.21750	0.56470	5.03080
H	-6.99940	2.10530	5.53730
H	-6.97930	1.63630	3.78370
C	-3.58920	0.00510	6.45960
O	-2.96530	-0.96830	6.13440
O	-4.88010	-0.06970	6.99520
C	-5.59420	-1.25110	7.19670
C	-5.18990	-2.51960	6.77750
C	-6.81440	-1.02350	7.85670
C	-6.04550	-3.59660	7.03170
H	-4.23300	-2.67140	6.27270
C	-7.64620	-2.11590	8.09510
H	-7.08160	-0.01810	8.17130
C	-7.26630	-3.40060	7.68340
H	-5.75120	-4.59790	6.71580
H	-8.59720	-1.96880	8.60650
H	-7.92290	-4.24650	7.87470
C	-2.05740	5.86010	4.22840
H	-1.94960	6.93550	3.98130

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l_9_disubsti_triptycene_pm6/opt_a7_folded_opt_13.xyz

C	-4.36810	5.27030	2.11380
C	-4.36060	4.01650	2.74290
C	-3.91480	2.86430	2.06720
C	-3.55670	2.99940	0.71040
C	-3.57010	4.25390	0.07900
C	-3.96550	5.39690	0.78330
C	-4.41200	0.78990	0.24990
C	-4.74780	0.63330	1.62460
C	-5.82740	-0.15910	1.98210

H	-6.11440	-0.29350	3.02290
C	-6.57210	-0.80210	0.97550
C	-6.23680	-0.64780	-0.36670
C	-5.14570	0.15760	-0.74040
H	-4.68800	6.15860	2.65340
H	-3.97230	6.37600	0.31280
H	-7.41950	-1.42490	1.25760
H	-6.81960	-1.14970	-1.13720
H	-4.88920	0.27940	-1.79020
C	-2.40640	0.91490	2.20370
C	-1.48360	0.30160	3.03870
C	-0.23730	-0.10120	2.52670
C	0.07870	0.09880	1.18560
C	-0.85500	0.69450	0.32040
C	-2.08380	1.08610	0.82840
H	-1.70400	0.12150	4.09190
H	0.48280	-0.57550	3.19150
H	1.04810	-0.21080	0.79890
H	-0.61390	0.84040	-0.73020
O	-3.17260	4.21260	-1.24490
C	-3.18940	5.45690	-1.98240
H	-2.85030	5.13160	-2.97470
H	-4.20520	5.85960	-2.02920
H	-2.48520	6.16930	-1.54330
C	-3.81610	1.41360	2.57590
C	-4.19410	1.21630	4.04820
H	-5.21990	1.63240	4.20190
H	-4.26570	0.13190	4.27090
C	-3.22480	1.87950	5.03270
H	-2.82380	2.83650	4.60480
H	-2.31810	1.25010	5.20280
O	-4.77670	3.81830	4.04810
C	-5.43590	4.91180	4.73060
H	-5.76560	4.42450	5.65980
H	-4.71900	5.71070	4.93810
H	-6.29550	5.26660	4.15580
C	-3.89660	2.17370	6.32980
O	-4.96930	1.95520	6.80210
O	-2.91740	2.89390	7.09330
C	-3.14190	3.39520	8.35190
F	-4.09740	4.31520	8.36140
F	-3.45920	2.45630	9.23010
F	-2.01610	3.97010	8.74790
C	-3.21020	1.69650	0.01220
H	-2.96280	1.83960	-1.05920

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1_9_disubsti_triptycene_pm6/opt_a8_folded_opt_18.xyz

C	-5.33730	5.02560	5.16450
C	-4.60090	3.87390	4.85100
C	-3.30070	3.67930	5.36070
C	-2.73550	4.72380	6.11890
C	-3.47250	5.87980	6.42720
C	-4.78180	6.02970	5.96170
C	-0.55570	4.21950	5.21590
C	-1.11490	3.13990	4.47480
C	-0.54830	2.77690	3.26290
H	-0.95470	1.95980	2.67090
C	0.57450	3.48010	2.78730
C	1.11700	4.53290	3.51850
C	0.54860	4.91240	4.74800
H	-6.34920	5.15630	4.79080
H	-5.36980	6.91090	6.19880
H	1.01780	3.19210	1.83600
H	1.98530	5.07020	3.14220
H	0.97210	5.73740	5.31560
C	-1.82170	2.10600	6.55390
C	-1.80350	0.84130	7.12360

C	-1.27590	0.66190	8.41480
C	-0.76170	1.74040	9.12920
C	-0.75250	3.02510	8.55910
C	-1.26940	3.19540	7.28450
H	-2.20200	-0.02170	6.58530
H	-1.27230	-0.33390	8.85360
H	-0.35990	1.59410	10.12960
H	-0.34310	3.86720	9.11160
O	-2.77380	6.79340	7.19810
C	-3.44430	8.03110	7.52830
H	-2.67650	8.55080	8.11590
H	-3.68530	8.58910	6.61910
H	-4.33260	7.83300	8.13480
C	-2.34160	2.49080	5.15490
C	-2.90910	1.32540	4.33410
H	-3.28180	1.73570	3.36800
H	-2.08460	0.62830	4.08110
C	-4.04040	0.54270	4.99710
H	-4.58340	-0.05520	4.25820
H	-4.77100	1.21550	5.46850
O	-5.07580	2.86800	4.02740
C	-6.35810	3.06760	3.38860
H	-6.44860	2.15320	2.78790
H	-7.15360	3.12250	4.13670
H	-6.33470	3.95400	2.74870
H	-3.67190	-0.13870	5.77510
C	-1.28740	4.50820	6.52100
H	-0.87030	5.36430	7.08830

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1_9_disubsti_triptycene_pm6/opt_a9_folded_opt_18.xyz

C	-4.61050	-1.53390	2.10640
C	-3.56250	-0.79200	2.70320
C	-2.98010	0.30340	2.04070
C	-3.38630	0.57030	0.71000
C	-4.42020	-0.16610	0.10870
C	-5.03720	-1.21460	0.83320
C	-1.12300	1.24890	0.19150
C	-0.72820	1.02190	1.53860
C	0.57460	0.63570	1.81380
H	0.90780	0.45310	2.83310
C	1.48480	0.47700	0.75240
C	1.09060	0.70130	-0.56410
C	-0.22860	1.09180	-0.85520
H	-5.08330	-2.35440	2.63990
H	-5.85380	-1.77650	0.36010
H	2.50810	0.17510	0.97000
H	1.80310	0.57560	-1.37780
H	-0.53560	1.26600	-1.88490
C	-2.35220	2.67570	2.27410
C	-2.39730	3.74050	3.16280
C	-2.86300	4.99390	2.72840
C	-3.27400	5.18410	1.41140
C	-3.21380	4.12300	0.49230
C	-2.74760	2.89150	0.92610
H	-2.08150	3.61890	4.20120
H	-2.89940	5.82170	3.43470
H	-3.63880	6.15670	1.08550
H	-3.52470	4.27010	-0.54050
C	-1.86930	1.24050	2.55520
C	-1.41210	0.99190	3.99860
H	-1.11010	-0.07550	4.08970
H	-0.49500	1.58720	4.18910
C	-2.44270	1.30660	5.08070
H	-3.44430	0.95350	4.80370
H	-2.52090	2.38580	5.27250
O	-3.04350	-1.09730	3.92890
C	-3.57310	-2.24500	4.64400

H	-2.95660	-2.23550	5.55340
H	-4.62830	-2.08970	4.88510
H	-3.40910	-3.16110	4.06940
H	-2.17530	0.82130	6.02520
N	-4.91270	0.08070	-1.24710
O	-4.42370	0.98240	-1.91240
O	-5.81130	-0.64420	-1.65430
C	-2.57740	1.67160	0.03950
H	-2.86310	1.86280	-1.02130

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1_9_disubsti_triptycene_pm6/opt_a10_folded_opt_4.xyz

C	-0.51950	5.42720	4.21780
C	-0.76980	4.06250	3.97030
C	0.24820	3.10270	4.08890
C	1.55270	3.58070	4.37050
C	1.82180	4.92410	4.61140
C	0.76810	5.84360	4.54610
C	2.48060	1.82690	2.98620
C	1.17170	1.32850	2.73140
C	0.90450	0.69640	1.52670
H	-0.08630	0.30880	1.29980
C	1.93380	0.55450	0.57740
C	3.21180	1.04200	0.83520
C	3.49460	1.68760	2.05250
H	-1.31730	6.15900	4.15290
H	0.95950	6.89830	4.74330
H	1.72070	0.05700	-0.36700
H	4.00100	0.92670	0.09490
H	4.49360	2.06780	2.24960
C	0.87340	0.94920	5.10970
C	0.38210	-0.05500	5.93140
C	1.15990	-0.52710	7.00350
C	2.42680	-0.00410	7.24760
C	2.94950	0.99850	6.41290
C	2.17930	1.45790	5.35580
H	-0.60910	-0.48220	5.76210
H	0.76110	-1.31090	7.64470
H	3.02060	-0.37190	8.08180
H	3.94330	1.39880	6.59580
C	0.17780	1.58020	3.88770
C	-1.21790	1.02080	3.58090
H	-1.62540	1.57730	2.70660
H	-1.12070	-0.03630	3.26080
C	-2.22700	1.10640	4.72400
H	-3.24860	0.98480	4.34990
H	-2.18000	2.08180	5.22820
O	-2.00400	3.58280	3.58580
C	-3.07580	4.53520	3.38450
H	-3.89760	3.87830	3.07120
H	-3.31670	5.04270	4.32260
H	-2.81530	5.24150	2.59120
H	-2.05490	0.33480	5.48600
H	2.82940	5.25670	4.84060
C	2.62580	2.50000	4.34520
H	3.64350	2.88920	4.53420

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1_9_disubsti_triptycene_pm6/opt_b1_folded_opt_19.xyz

C	2.84520	-3.86060	19.24300
C	2.22690	-3.85310	17.98590
C	0.82550	-3.90670	17.86750
C	0.05570	-3.95580	19.04490
C	0.67810	-3.96220	20.30520
C	2.07300	-3.91670	20.40680
C	-1.68300	-5.19110	17.90910
C	-0.92700	-5.15010	16.70470
C	-1.05780	-6.16900	15.77350

H	-0.50820	-6.14120	14.83060
C	-1.92970	-7.23890	16.04500
C	-2.65900	-7.27980	17.23070
C	-2.54070	-6.24600	18.17690
H	3.92750	-3.82180	19.33220
H	2.56740	-3.92280	21.37390
H	-2.03230	-8.03900	15.31430
H	-3.32940	-8.11320	17.43100
H	-3.11490	-6.27890	19.09920
C	-0.97870	-2.71450	16.75470
C	-1.14290	-1.64690	15.88710
C	-2.06860	-0.63570	16.20540
C	-2.81400	-0.69650	17.37920
C	-2.65240	-1.77340	18.26980
C	-1.74260	-2.76960	17.95600
H	-0.57690	-1.57740	14.96010
H	-2.19790	0.19900	15.51860
H	-3.52790	0.09010	17.61540
H	-3.23390	-1.81680	19.18730
O	-0.21220	-4.01570	21.36180
C	0.34130	-4.01020	22.69800
H	-0.56630	-4.05240	23.31450
H	0.96280	-4.89600	22.85690
H	0.89330	-3.08350	22.87860
C	-0.02810	-3.90950	16.58600
C	0.85070	-3.88930	15.33160
H	1.42970	-2.95070	15.25570
H	1.54720	-4.75310	15.31270
O	2.90920	-3.78760	16.78100
C	4.35490	-3.76160	16.82240
H	4.60790	-3.72260	15.75480
H	4.70440	-2.86390	17.34030
H	4.73930	-4.67680	17.28160
O	-0.00050	-4.10650	14.17140
C	0.04260	-3.21370	13.12600
C	-0.98070	-3.43370	12.18020
C	0.99480	-2.20060	12.96290
C	-1.03710	-2.61780	11.05840
H	-1.70330	-4.22850	12.35140
C	0.92140	-1.38670	11.83030
H	1.77920	-2.04740	13.70070
C	-0.08920	-1.58940	10.87900
H	-1.82040	-2.77160	10.31740
H	1.65040	-0.58860	11.67980
N	-0.07890	-0.68040	9.73530
C	-1.33470	0.12710	9.67700
H	-1.22160	0.89490	8.89520
H	-2.24880	-0.44790	9.47180
H	-1.46630	0.65180	10.63770
C	0.14820	-1.42290	8.45880
H	-0.66000	-2.10970	8.17000
H	0.29180	-0.69090	7.64820
H	1.08040	-2.00510	8.54620
C	-1.44650	-3.99170	18.81570
H	-2.02200	-4.02420	19.76190

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1_9_disubsti_triptycene_pm6/opt_b2_folded_opt_20.xyz

C	1.12740	-0.38610	0.74840
C	-0.02630	-0.19970	1.52090
C	-1.16240	0.43380	0.98380
C	-1.11450	0.87760	-0.35120
C	0.04420	0.68930	-1.12420
C	1.16650	0.05770	-0.57660
C	-2.64790	2.67550	0.15270
C	-2.72180	2.23810	1.50490
C	-2.98590	3.14890	2.51560
H	-3.08490	2.81980	3.55060

C	-3.15330	4.50630	2.18600
C	-3.06330	4.93350	0.86350
C	-2.81200	4.01280	-0.17000
H	2.00400	-0.87530	1.16430
H	2.06850	-0.09440	-1.16230
H	-3.35880	5.22400	2.97810
H	-3.19250	5.98640	0.62030
H	-2.75070	4.35050	-1.20140
C	-3.56850	0.08800	0.75960
C	-4.54720	-0.81600	1.14130
C	-5.44160	-1.30500	0.17180
C	-5.35430	-0.88450	-1.15300
C	-4.37410	0.04540	-1.54510
C	-3.49320	0.52880	-0.59140
H	-4.64050	-1.13030	2.18150
H	-6.20990	-2.01660	0.46850
H	-6.05010	-1.27110	-1.89510
H	-4.31570	0.37630	-2.57890
O	-0.06450	1.17870	-2.41280
C	1.08310	1.02750	-3.28000
H	0.72280	1.49090	-4.20790
H	1.94010	1.57470	-2.87750
H	1.30780	-0.03170	-3.43420
C	-2.50870	0.72650	1.66880
C	-2.51730	0.22860	3.11510
H	-2.38130	-0.86820	3.16750
H	-1.74810	0.73960	3.72460
O	-0.15660	-0.60570	2.84020
C	0.97240	-1.26520	3.45890
H	0.58940	-1.46460	4.46810
H	1.20120	-2.19850	2.93650
H	1.83390	-0.59210	3.49400
O	-3.83540	0.56470	3.64140
C	-4.09910	0.22030	4.95110
C	-5.39470	0.59410	5.35540
C	-3.20960	-0.42950	5.81990
C	-5.81030	0.31300	6.65410
H	-6.04960	1.09680	4.64500
C	-3.62600	-0.71050	7.11930
H	-2.21140	-0.71470	5.49990
C	-4.92070	-0.33690	7.52300
H	-6.80820	0.59800	6.97370
H	-2.96930	-1.21300	7.82690
O	-5.18680	-0.68210	8.83690
C	-6.49040	-0.34790	9.36460
H	-6.42050	-0.72780	10.39220
H	-6.63840	0.73570	9.35820
H	-7.27310	-0.87060	8.80750
C	-2.38820	1.54820	-0.83900
H	-2.31750	1.88530	-1.89190

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1_9_disubsti_triptycene_pm6/opt_b3_folded_opt_14.xyz

C	-0.90160	6.15930	3.53590
C	-1.83380	5.32980	4.17260
C	-2.67460	4.48070	3.42930
C	-2.54830	4.47330	2.02730
C	-1.61240	5.30650	1.39050
C	-0.78900	6.15180	2.14260
C	-4.88170	3.90030	1.77510
C	-5.03480	3.89670	3.18940
C	-6.26250	4.21190	3.75120
H	-6.40770	4.18550	4.83290
C	-7.33700	4.54730	2.90760
C	-7.17870	4.56050	1.52400
C	-5.94010	4.23190	0.94450
H	-0.25510	6.81620	4.11160
H	-0.06210	6.80170	1.66380

H	-8.30090	4.79510	3.34820
H	-8.01650	4.82280	0.88100
H	-5.82160	4.23850	-0.13600
C	-3.35160	2.14480	3.36710
C	-3.12590	0.97340	4.07180
C	-2.76390	-0.19270	3.37180
C	-2.62970	-0.17880	1.98640
C	-2.85460	1.00550	1.26120
C	-3.21210	2.15310	1.94950
H	-3.23240	0.93400	5.15430
H	-2.59190	-1.11260	3.92810
H	-2.35050	-1.08640	1.45490
H	-2.74770	1.01320	0.17930
O	-1.61220	5.18690	0.01300
C	-0.68390	6.01410	-0.72580
H	-0.90120	5.72100	-1.76140
H	-0.90510	7.07310	-0.56520
H	0.34650	5.76460	-0.45720
C	-3.75350	3.51040	3.94420
C	-3.87830	3.57490	5.46910
H	-2.95410	3.22860	5.96760
H	-4.11920	4.60180	5.81300
O	-2.00750	5.26140	5.54640
C	-1.20300	6.13320	6.37410
H	-1.55830	5.87560	7.38050
H	-0.14210	5.89300	6.26020
H	-1.41430	7.18090	6.14190
O	-5.04070	2.79070	5.86180
C	-4.91580	1.84550	6.85080
C	-6.08780	1.07780	7.01910
C	-3.77840	1.64420	7.64250
C	-6.09980	0.09860	8.00550
H	-6.94470	1.26240	6.37620
C	-3.82170	0.65000	8.62530
H	-2.88400	2.24520	7.50060
C	-4.97060	-0.12030	8.81080
H	-6.99370	-0.50760	8.15350
H	-2.94560	0.47980	9.25080
H	-4.99460	-0.89040	9.57660
C	-3.48420	3.51080	1.31450
H	-3.35430	3.52500	0.21430

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1_9_disubsti_triptycene_pm6/opt_b4_folded_opt_6.xyz

C	2.02470	1.24180	4.38290
C	1.02610	1.20970	3.40040
C	-0.06260	2.09870	3.44740
C	-0.12950	3.02480	4.50590
C	0.87290	3.05510	5.49020
C	1.95130	2.16390	5.43010
C	-2.54410	3.00390	4.42120
C	-2.50140	2.07530	3.34370
C	-3.54020	1.17630	3.16110
H	-3.53820	0.48020	2.32330
C	-4.61950	1.18550	4.06350
C	-4.65180	2.08710	5.12440
C	-3.60730	3.01110	5.30950
H	2.86620	0.55460	4.34580
H	2.73360	2.17650	6.18430
H	-5.43620	0.47940	3.92320
H	-5.49140	2.08440	5.81760
H	-3.64050	3.71670	6.13630
C	-1.24830	3.68260	2.01720
C	-1.22590	4.14510	0.71090
C	-1.23140	5.53230	0.47610
C	-1.26430	6.43310	1.53760
C	-1.29940	5.97170	2.86610
C	-1.29520	4.60600	3.09900

H	-1.22150	3.45170	-0.12910
H	-1.21280	5.89830	-0.54910
H	-1.26660	7.50450	1.34420
H	-1.33060	6.67960	3.69090
O	0.66720	4.01700	6.46040
C	1.64960	4.11660	7.51790
H	1.24070	4.93660	8.12340
H	1.68630	3.18730	8.09340
H	2.62690	4.38480	7.10690
C	-1.24580	2.21590	2.47120
C	-1.12930	1.19290	1.34160
H	-0.21990	1.35640	0.73280
H	-1.15880	0.15490	1.72370
O	1.01420	0.33210	2.32620
C	2.10070	-0.61760	2.21820
H	2.10910	-1.28550	3.08470
H	1.83290	-1.16370	1.30490
H	3.05280	-0.09310	2.09490
O	-2.30590	1.40960	0.49090
C	-2.45620	0.62890	-0.60890
C	-3.62760	0.93990	-1.34490
C	-1.57360	-0.38970	-1.01480
C	-3.90720	0.22160	-2.49140
C	-1.86750	-1.10440	-2.17030
H	-0.67790	-0.62200	-0.44530
C	-3.02660	-0.80340	-2.90710
H	-4.80330	0.43260	-3.08770
H	-1.20290	-1.90510	-2.51710
N	-3.32740	-1.56170	-4.12270
O	-2.54540	-2.44250	-4.45250
O	-4.34150	-1.27400	-4.74080
H	-4.27990	1.73810	-0.98930
C	-1.34280	3.93960	4.46800
H	-1.36480	4.65500	5.31410

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1_9_disubsti_triptycene_pm6/opt_b5_folded_opt_9.xyz

C	-8.39770	2.59450	11.93080
C	-7.14830	3.13270	11.59570
C	-6.06220	3.05080	12.48500
C	-6.25440	2.40230	13.72000
C	-7.50820	1.86250	14.05480
C	-8.58230	1.95980	13.16160
C	-4.57950	3.79780	14.76380
C	-4.35870	4.46480	13.52730
C	-3.92830	5.78220	13.52240
H	-3.71360	6.30890	12.58750
C	-3.72890	6.44360	14.74760
C	-3.95970	5.79010	15.95550
C	-4.38840	4.45070	15.97090
H	-9.23590	2.65960	11.24150
H	-9.55740	1.54810	13.40800
H	-3.37980	7.47590	14.74040
H	-3.80260	6.31240	16.89770
H	-4.56170	3.94180	16.91580
C	-3.73290	2.34640	12.49520
C	-2.79330	1.83960	11.61230
C	-2.05730	0.69380	11.96820
C	-2.26700	0.06540	13.19210
C	-3.22360	0.56610	14.09370
C	-3.94700	1.69450	13.74410
H	-2.60700	2.30580	10.65040
H	-1.31580	0.30170	11.27380
H	-1.69070	-0.81900	13.45950
H	-3.38790	0.07090	15.04830
O	-7.53710	1.26020	15.29710
C	-8.79430	0.69180	15.73320
H	-8.52790	0.30050	16.72430

H	-9.55770	1.47090	15.81380
H	-9.10020	-0.11680	15.06350
C	-4.62700	3.58030	12.30030
C	-4.49670	4.30170	10.95900
H	-4.64300	3.61700	10.10320
H	-5.20240	5.15740	10.88490
O	-6.86800	3.75880	10.38870
C	-7.97150	4.00910	9.48650
H	-7.47690	4.54760	8.66820
H	-8.39360	3.06320	9.13450
H	-8.72410	4.63920	9.97000
O	-3.18350	4.97070	10.90960
C	-2.36560	4.77670	9.86760
C	-1.11900	5.46360	9.94610
C	-2.65100	3.96140	8.74220
C	-0.16330	5.28220	8.93760
C	-1.71090	3.80400	7.74630
H	-3.62120	3.46070	8.67480
C	-0.45820	4.45960	7.84730
H	0.81510	5.79180	9.00850
H	-1.91190	3.17410	6.86830
N	0.53710	4.27000	6.78340
O	1.59910	4.85780	6.89150
O	0.23240	3.53480	5.85760
N	-0.81180	6.36890	11.06280
O	0.35460	6.69750	11.19960
O	-1.73520	6.74590	11.75850
C	-5.01970	2.34980	14.60400
H	-5.20420	1.82880	15.56490

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Gellman_pm6/opt_a1_folded_opt_11.xyz

C	-4.35720	7.86630	-2.41850
C	-3.42940	7.07830	-1.78790
C	-2.91300	7.45430	-0.50650
C	-3.37120	8.65170	0.10490
C	-4.34060	9.45360	-0.57780
C	-4.81870	9.06920	-1.80490
H	-1.59590	5.72310	-0.29990
H	-4.75600	7.59140	-3.39440
H	-3.06720	6.15360	-2.25380
C	-1.94920	6.65390	0.17180
C	-2.85380	9.02680	1.38580
H	-4.68750	10.37120	-0.10360
H	-5.55630	9.67430	-2.33190
C	-1.92690	8.24510	2.02580
C	-1.46770	7.03710	1.41000
H	-3.21230	9.94970	1.84320
H	-1.52620	8.52220	3.00170
C	-0.51720	6.21480	2.06590
C	0.28480	5.45270	2.55290
C	1.23340	4.57230	3.16130
O	1.82120	4.79490	4.20490
N	1.47990	3.34560	2.48700
C	0.84560	2.88700	1.23090
H	1.26520	1.85820	0.97340
C	2.42850	2.39900	3.11150
H	2.73110	2.78030	4.12830
H	1.94950	1.40150	3.26340
C	3.67870	2.26700	2.25210
O	4.76240	2.76800	2.38740
O	3.39260	1.40110	1.21190
C	4.44700	1.14960	0.24650
H	4.46560	1.97880	-0.46680
H	5.41520	1.05180	0.75170
H	4.13700	0.20900	-0.22030
C	-0.65060	2.63950	1.49070
O	-1.11060	1.69650	2.08760

O	-1.44090	3.61710	0.94440
C	-2.88220	3.45480	1.07010
H	-3.24230	4.46390	1.29600
H	-3.23760	3.09430	0.09990
H	-3.13670	2.74940	1.87120
C	1.16390	3.81700	0.04810
H	0.79770	4.84680	0.24310
H	2.26810	3.92100	-0.04180
C	0.58550	3.29120	-1.23580
C	-0.51620	3.89550	-1.79580
C	1.18150	2.15880	-1.87320
C	-1.07670	3.40920	-3.01400
H	-0.99330	4.74770	-1.29720
C	0.65880	1.67080	-3.04340
H	2.05040	1.69210	-1.41080
C	-0.48550	2.28470	-3.64600
C	-2.22210	4.02710	-3.60910
H	1.10420	0.80600	-3.53450
C	-1.05170	1.79530	-4.86550
C	-2.74390	3.53690	-4.77880
H	-2.66540	4.89670	-3.11200
C	-2.15110	2.40600	-5.41490
H	-0.59330	0.93160	-5.34530
H	-3.61460	3.99920	-5.24140
H	-2.58850	2.03990	-6.34250

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Gellman_pm6/opt_b1_folded_opt_5.xyz

C	2.27600	0.04780	-4.31770
C	2.70190	-0.92420	-3.74290
C	3.18560	-2.11920	-3.10340
O	2.76280	-3.23420	-3.35880
C	4.89340	-3.07320	-1.49800
H	5.83530	-2.68950	-0.99590
C	3.98670	-3.60720	-0.37580
O	3.23840	-2.98530	0.33640
O	4.20380	-4.95430	-0.21890
C	3.41770	-5.63430	0.79780
H	3.32000	-5.01070	1.69320
H	2.43550	-5.85970	0.36980
H	3.99930	-6.54170	0.98900
C	5.29520	-4.17770	-2.49150
H	5.75210	-5.02100	-1.92560
H	4.38160	-4.62170	-2.95770
N	4.20360	-1.92980	-2.14590
C	6.24120	-3.66780	-3.54090
C	5.77270	-3.40100	-4.83630
C	7.59370	-3.45510	-3.23410
C	6.65130	-2.93240	-5.81560
H	4.72030	-3.56150	-5.07590
C	8.46760	-2.98480	-4.21720
H	7.96420	-3.64570	-2.22820
C	8.00040	-2.72620	-5.51000
H	6.28340	-2.73080	-6.82020
H	9.51580	-2.81940	-3.97300
H	8.68570	-2.37280	-6.27670
C	4.66020	-0.58980	-1.73310
H	4.67450	-0.51040	-0.61660
H	3.96360	0.21160	-2.08800
C	6.06700	-0.34590	-2.27300
O	7.11290	-0.66070	-1.75810
O	5.97360	0.32300	-3.45940
C	7.21050	0.56700	-4.18580
H	8.03510	0.77130	-3.49480
H	7.41650	-0.32410	-4.79080
H	6.96500	1.43630	-4.80360
C	1.78480	1.20840	-4.98410
C	1.17980	1.07640	-6.28180

C	1.45150	3.52180	-4.97740
C	0.71660	2.20590	-6.90700
H	1.10150	0.08930	-6.73550
C	0.84090	3.47610	-6.26510
C	1.59260	4.77830	-4.29830
H	0.25020	2.15300	-7.89210
C	0.38090	4.69390	-6.85490
C	1.13860	5.92440	-4.89610
H	2.06260	4.78240	-3.31290
C	0.52720	5.88280	-6.18650
H	-0.08530	4.65530	-7.83910
H	1.23540	6.88910	-4.39670
H	0.17930	6.81730	-6.62680
N	1.92130	2.37830	-4.34730

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Gellman_pm6/opt_b2_folded_opt_7.xyz

C	3.89000	-3.84490	4.72130
C	3.40190	-4.67630	3.99300
C	2.86050	-5.69350	3.14350
O	2.53250	-6.81040	3.50130
C	2.29070	-6.36560	0.81350
H	1.95070	-7.27570	1.40600
C	1.10210	-5.83690	-0.00360
O	1.02710	-4.83040	-0.67140
O	0.07510	-6.72690	0.12580
C	-1.12700	-6.48400	-0.65610
H	-1.31850	-5.41000	-0.75570
H	-0.98300	-6.95360	-1.63420
H	-1.90550	-6.98660	-0.07210
C	3.41990	-6.77490	-0.14940
H	3.74390	-5.90800	-0.76850
H	4.32680	-7.03480	0.44090
N	2.70290	-5.32240	1.78140
C	2.99530	-7.93000	-1.01100
C	3.02380	-9.23620	-0.50000
C	2.55540	-7.70400	-2.32380
C	2.61570	-10.30670	-1.29930
H	3.35880	-9.41670	0.52060
C	2.14910	-8.77920	-3.11810
H	2.52640	-6.69160	-2.72440
C	2.17830	-10.08100	-2.60850
H	2.63690	-11.31960	-0.89970
H	1.80870	-8.60120	-4.13700
H	1.86070	-10.91680	-3.22860
C	4.48680	-2.84080	5.52440
C	5.32340	-1.90840	4.93960
C	4.21060	-2.81570	6.93260
C	5.91840	-0.90370	5.76100
H	5.54440	-1.92110	3.86060
C	4.77250	-1.85790	7.73490
H	3.54510	-3.57660	7.34640
C	5.64220	-0.87690	7.16290
H	4.57870	-1.81590	8.80970
C	7.29280	0.95530	5.98350
C	7.01270	0.98380	7.40610
H	7.96000	1.70480	5.53970
H	7.46720	1.75500	8.04060
N	6.76400	0.04170	5.18300
N	6.21280	0.09690	7.98100
C	3.12920	-4.00740	1.27770
H	2.68130	-3.19890	1.91180
H	2.72700	-3.83830	0.23860
C	4.64090	-3.81370	1.27030
O	5.27470	-2.99710	1.89620
O	5.23160	-4.68640	0.39450
C	6.68150	-4.63080	0.28260
H	7.11280	-5.16030	1.13740

H	6.87100	-5.15180	-0.66190
H	7.02460	-3.59050	0.25360

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Gellman_pm6/opt_c1_folded_opt_10.xyz

C	-2.98900	1.72940	-9.61630
C	-3.34390	1.48690	-8.48720
C	-3.82670	1.22590	-7.16110
O	-4.90940	1.57350	-6.72230
C	-3.25930	0.14670	-4.98020
H	-4.36220	0.33890	-4.80160
C	-2.96070	-1.35000	-4.80260
O	-1.96450	-1.96000	-5.11020
O	-4.04590	-1.92740	-4.20570
C	-3.93290	-3.32210	-3.81020
H	-3.29220	-3.87640	-4.50470
H	-3.52660	-3.33930	-2.79340
H	-4.96970	-3.67320	-3.84070
C	-2.41930	0.94730	-3.96220
H	-1.33530	0.80350	-4.15380
H	-2.59890	2.03330	-4.12020
C	-2.77650	0.55300	-2.55580
C	-1.99500	-0.33410	-1.85160
C	-3.96280	1.09230	-1.96610
C	-2.36300	-0.73120	-0.52910
H	-1.09000	-0.75580	-2.28840
C	-4.33340	0.72630	-0.69840
H	-4.56690	1.79140	-2.54420
C	-3.54200	-0.19910	0.05400
C	-1.57200	-1.66000	0.21980
H	-5.23740	1.13040	-0.24360
C	-3.91130	-0.60270	1.37590
C	-1.95030	-2.03040	1.48560
H	-0.66830	-2.06210	-0.23570
C	-3.13500	-1.49510	2.07160
H	-4.81770	-0.18800	1.81470
H	-1.35470	-2.73590	2.06300
H	-3.40790	-1.80800	3.07800
C	-2.56880	2.01520	-10.94010
C	-3.28350	2.94920	-11.71350
C	-1.44220	1.36560	-11.47850
C	-2.86770	3.22840	-13.01660
H	-4.15720	3.44890	-11.29290
C	-1.03750	1.65370	-12.78310
H	-0.89210	0.64100	-10.87840
C	-1.74750	2.58300	-13.55130
H	-3.41900	3.95110	-13.61810
H	-0.16610	1.15230	-13.20370
H	-1.42730	2.80420	-14.56940
N	-2.91580	0.51170	-6.36460
H	-2.00020	0.22730	-6.70780

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Gellman_pm6/opt_c2_folded_opt_4.xyz

C	-0.24900	3.50060	-3.04650
C	0.37230	3.77270	-2.04700
C	1.10080	4.15240	-0.86950
O	1.47810	5.28110	-0.60400
C	2.03140	3.30810	1.28490
H	2.34260	4.39730	1.35460
C	0.99730	3.03520	2.38770
O	-0.09910	2.54310	2.30390
O	1.53020	3.45950	3.58340
C	0.69500	3.31620	4.76360
H	0.18950	2.34420	4.75990
H	1.41510	3.40380	5.58360
H	-0.03330	4.13320	4.77090
C	3.27450	2.41870	1.48560

H	4.02430	2.67520	0.70540
H	3.75120	2.69460	2.45300
C	-0.98280	3.17180	-4.21540
C	-0.30450	2.78940	-5.38760
C	-2.38880	3.23100	-4.19870
C	-1.03480	2.46720	-6.53310
H	0.78450	2.74850	-5.39820
C	-3.10660	2.90650	-5.35130
H	-2.91070	3.53080	-3.28950
C	-2.43260	2.52490	-6.51640
H	-0.51300	2.17130	-7.44280
H	-4.19540	2.95200	-5.34210
H	-2.99770	2.27310	-7.41350
N	1.40390	3.06970	-0.02510
H	0.99150	2.14680	-0.16920
C	2.96390	0.94820	1.45270
C	3.02470	0.23960	0.24380
C	2.60490	0.27850	2.63250
C	2.72370	-1.12270	0.21280
H	3.30900	0.75190	-0.67470
C	2.30680	-1.08370	2.60330
H	2.55370	0.82450	3.57440
C	2.36310	-1.79150	1.39240
H	2.77370	-1.67150	-0.72710
H	2.02180	-1.60030	3.51940
C	2.04410	-3.23560	1.36020
C	2.83740	-4.14710	2.07420
C	0.94750	-3.69680	0.61560
C	2.53440	-5.51030	2.03970
H	3.69060	-3.78980	2.64850
C	0.64870	-5.06120	0.58810
H	0.32810	-2.98890	0.06710
C	1.44080	-5.96920	1.29820
H	3.15210	-6.21690	2.59170
H	-0.20420	-5.41760	0.01260
H	1.20640	-7.03150	1.27410

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Elguero_Cornago_pm6/opt_a1_folded_opt_3.xyz

C	-2.52050	1.23370	1.31910
C	-1.16790	1.06130	0.87720
C	-1.05700	1.79010	-0.31040
N	-2.30790	2.37990	-0.52980
H	-2.60800	2.90290	-1.34160
H	-0.40600	0.49370	1.36490
N	-3.20100	2.03250	0.43800
C	-3.14500	0.66600	2.53220
H	-4.20910	0.94030	2.61210
H	-3.08620	-0.43210	2.53370
H	-2.64440	1.02880	3.44230
C	0.08420	1.98790	-1.20450
C	0.20980	1.25800	-2.40400
C	1.07340	2.91430	-0.83950
C	1.32960	1.47340	-3.22150
C	2.18210	3.12020	-1.66200
H	0.97030	3.47080	0.09300
C	2.30850	2.39850	-2.85310
H	1.43740	0.91510	-4.15030
H	2.94660	3.84010	-1.37540
H	3.17380	2.55710	-3.49590
C	-0.83500	0.25460	-2.81280
H	-0.44580	-0.42670	-3.60130
H	-1.05890	-0.41190	-1.94790
C	-2.09300	0.91420	-3.31470
C	-2.02610	1.94870	-4.26010
C	-3.34190	0.49690	-2.82980
C	-3.19750	2.56200	-4.71010
H	-1.05940	2.27610	-4.63990

C	-4.50980	1.11580	-3.28190
H	-3.40460	-0.29780	-2.08750
C	-4.44090	2.14950	-4.22120
H	-3.14090	3.36440	-5.44420
H	-5.47610	0.79490	-2.89390
H	-5.35210	2.63070	-4.57010

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Elguero_Cornago_pm6/opt_a2_folded_opt_9.xyz

C	-3.78320	-3.27200	-0.46790
C	-2.76230	-2.97750	-1.42530
C	-3.10060	-1.73260	-1.95920
N	-4.29670	-1.34430	-1.32500
H	-4.77430	-0.45320	-1.41530
H	-1.91940	-3.58970	-1.67940
N	-4.70200	-2.25500	-0.41830
C	-3.88490	-4.47470	0.40010
C	-2.44280	-0.90660	-2.97010
C	-1.50640	0.08280	-2.60460
C	-2.75380	-1.11820	-4.32240
C	-0.90200	0.85230	-3.61020
C	-2.14300	-0.34690	-5.31200
H	-3.47300	-1.89160	-4.59590
C	-1.21800	0.63910	-4.95340
H	-0.17940	1.62240	-3.34230
H	-2.38520	-0.51410	-6.36040
H	-0.74050	1.24300	-5.72510
C	-1.14000	0.31480	-1.16350
H	-0.73680	-0.63310	-0.73790
H	-0.30190	1.04180	-1.07610
C	-2.30130	0.81330	-0.34410
C	-3.10040	1.86660	-0.81400
C	-2.59640	0.21250	0.88910
C	-4.19340	2.30310	-0.06180
H	-2.86730	2.34370	-1.76450
C	-3.69290	0.65180	1.63490
H	-1.98460	-0.60800	1.26160
C	-4.49530	1.69430	1.16020
H	-4.81030	3.12270	-0.42780
H	-3.92750	0.17230	2.58540
H	-5.35100	2.03140	1.74220
F	-3.56060	-4.25450	1.68580
F	-3.07440	-5.48400	0.03640
F	-5.09730	-5.04490	0.46080

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Elguero_Cornago_pm6/opt_a3_folded_opt_9.xyz

C	4.79180	-1.32210	-3.42870
C	4.19630	-1.14420	-2.13540
C	4.46310	0.17620	-1.76780
N	5.21080	0.73320	-2.81590
H	5.49080	1.69980	-2.92240
H	3.67230	-1.88300	-1.56760
N	5.39650	-0.15460	-3.82460
C	4.10440	0.92690	-0.56480
C	2.96270	1.75410	-0.53710
C	4.91120	0.80330	0.57660
C	2.65260	2.45070	0.64040
C	4.59110	1.50150	1.74210
H	5.78860	0.15570	0.54770
C	3.46150	2.32530	1.77170
H	1.77460	3.09420	0.67380
H	5.21920	1.40300	2.62580
H	3.21030	2.87100	2.68080
C	2.07760	1.89200	-1.74670
H	1.78900	0.87600	-2.10280
H	1.11550	2.38410	-1.48360
C	2.73960	2.67320	-2.85170

C	3.36050	3.90150	-2.57930
C	2.74540	2.16670	-4.16030
C	3.98720	4.61090	-3.60640
H	3.35580	4.29960	-1.56590
C	3.37700	2.87920	-5.18240
H	2.27590	1.20880	-4.38080
C	4.00000	4.10100	-4.90830
H	4.46680	5.56460	-3.39130
H	3.39010	2.47490	-6.19430
H	4.49240	4.65270	-5.70630
C	4.79190	-2.53300	-4.24940
C	3.75320	-3.47060	-4.11620
C	5.82580	-2.76680	-5.17270
C	3.75600	-4.63020	-4.89430
H	2.94420	-3.29080	-3.41060
C	5.82030	-3.92870	-5.94720
H	6.62750	-2.03490	-5.28260
C	4.78830	-4.86240	-5.80900
H	2.95060	-5.35480	-4.78860
H	6.62300	-4.10650	-6.66110
H	4.78770	-5.76740	-6.41290

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Cozzi_aromatic_pm6/opt_a1_folded_opt_6.xyz

C	-2.18150	-2.45090	1.32100
C	-1.14980	-2.43420	0.41730
C	-1.13480	-1.47330	-0.64120
C	-2.15810	-0.49070	-0.71180
C	-3.10590	-0.40220	0.36500
C	-3.18690	-1.44600	1.27630
H	0.68720	-2.23020	-1.55680
H	-2.23780	-3.21660	2.09630
H	-0.34530	-3.16770	0.47270
C	-0.12150	-1.50600	-1.65230
C	-2.23120	0.33390	-1.87980
C	-1.26430	0.26440	-2.84980
C	-0.17650	-0.64780	-2.72020
H	-3.08240	1.00630	-1.99290
H	-1.31470	0.89690	-3.73540
H	0.59490	-0.65860	-3.48990
C	-4.00690	0.75570	0.55780
C	-3.61300	2.09460	0.36170
C	-5.30480	0.49920	1.05770
C	-4.55840	3.12650	0.50530
C	-6.23930	1.52750	1.17990
C	-5.87050	2.84290	0.87820
H	-4.25510	4.16140	0.33750
H	-7.25300	1.30890	1.52010
H	-6.60230	3.64650	0.96060
C	-5.63870	-0.89090	1.55370
H	-6.47920	-0.88600	2.28980
C	-4.38100	-1.55420	2.19770
H	-4.61050	-2.61670	2.45820
C	-2.21210	2.47300	0.06590
C	-1.92280	3.31960	-1.02040
C	-1.16900	1.98810	0.87570
C	-0.60300	3.64090	-1.32550
H	-2.73200	3.70830	-1.63930
C	0.15410	2.30120	0.57610
H	-1.39530	1.34490	1.72800
C	0.43000	3.11990	-0.53050
H	-0.36100	4.28540	-2.17760
H	0.97770	1.91320	1.18600
O	-6.13850	-1.72700	0.51360
H	-5.51900	-1.74300	-0.25130
O	-4.13630	-0.96370	3.47310
H	-3.82160	-0.03820	3.37470
N	1.83230	3.43300	-0.86960

O	2.03550	4.12520	-1.85520
O	2.70630	2.98010	-0.14780

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Cozzi_aromatic_pm6/opt_a2_folded_opt_18.xyz

C	-2.02290	-2.39050	1.37370
C	-0.95660	-2.46830	0.51470
C	-0.83740	-1.54480	-0.57020
C	-1.78990	-0.50060	-0.71200
C	-2.77880	-0.32210	0.31570
C	-2.96180	-1.32910	1.25340
H	0.96190	-2.45070	-1.38860
H	-2.15860	-3.12400	2.16950
H	-0.20390	-3.24800	0.62610
C	0.21000	-1.67690	-1.53750
C	-1.75620	0.29490	-1.90180
C	-0.75780	0.13250	-2.82770
C	0.25630	-0.84940	-2.62980
H	-2.55060	1.02430	-2.06510
H	-0.72600	0.74510	-3.72750
H	1.05420	-0.93590	-3.36630
C	-3.62600	0.88650	0.42310
C	-3.15320	2.19710	0.20970
C	-4.96140	0.71020	0.85550
C	-4.05570	3.27590	0.26260
C	-5.85070	1.78380	0.88650
C	-5.40000	3.06810	0.56210
H	-3.69150	4.28820	0.08220
H	-6.89090	1.62600	1.17320
H	-6.09480	3.90740	0.57220
C	-5.38930	-0.64180	1.38390
H	-6.26640	-0.56820	2.07140
C	-4.20070	-1.33680	2.11960
H	-4.49650	-2.37250	2.41620
C	-1.72130	2.50010	-0.00730
C	-1.32340	3.30040	-1.09230
C	-0.75610	1.99140	0.88070
C	0.02730	3.57410	-1.31380
H	-2.07210	3.69990	-1.77680
C	0.59940	2.25160	0.67850
H	-1.06750	1.37660	1.72680
C	0.95870	3.03450	-0.42240
H	0.34120	4.18530	-2.15810
H	1.35090	1.84890	1.35620
O	-5.87300	-1.49600	0.34970
H	-5.21670	-1.56540	-0.38070
O	-3.98680	-0.69790	3.37780
H	-3.61820	0.20430	3.25130
F	2.25360	3.28190	-0.63090

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Cozzi_aromatic_pm6/opt_a3_folded_opt_15.xyz

C	-4.27480	4.97340	-0.97020
C	-3.14560	5.56260	-0.46240
C	-2.39420	4.91110	0.56480
C	-2.78310	3.61880	1.00810
C	-3.84930	2.94220	0.32060
C	-4.64980	3.66670	-0.55190
H	-0.95860	6.52700	0.79570
H	-4.89080	5.48390	-1.71140
H	-2.82160	6.54290	-0.80900
C	-1.27300	5.55720	1.17760
C	-2.12840	3.06800	2.15600
C	-1.07110	3.71630	2.74140
C	-0.61910	4.96680	2.22850
H	-2.49530	2.12520	2.56410
H	-0.56400	3.28920	3.60520
H	0.24080	5.44510	2.69510

C	-4.14790	1.50390	0.50300
C	-3.15980	0.50370	0.61090
C	-5.50750	1.11310	0.47430
C	-3.54880	-0.82710	0.85770
C	-5.87990	-0.20400	0.73860
C	-4.89390	-1.17260	0.95750
H	-2.78310	-1.59770	0.95510
H	-6.93370	-0.48180	0.76380
H	-5.18060	-2.20050	1.17720
C	-6.55330	2.12190	0.05130
H	-7.47530	1.63310	-0.34630
C	-5.96640	3.09190	-1.02150
H	-6.71180	3.88980	-1.25570
C	-1.72190	0.78210	0.41800
C	-1.28580	1.49560	-0.70850
C	-0.77820	0.33190	1.36400
C	0.06670	1.79270	-0.88890
H	-2.01130	1.83590	-1.44940
C	0.57120	0.61520	1.20740
H	-1.11340	-0.23120	2.23590
C	0.97970	1.35760	0.07900
H	0.38390	2.35630	-1.75960
H	1.31470	0.28690	1.92970
O	-7.05040	2.87850	1.15360
H	-6.30960	3.28290	1.66010
O	-5.84330	2.40080	-2.26470
H	-5.12960	1.72650	-2.21730
O	2.33800	1.58060	0.05680
C	2.87710	2.36140	-1.03700
H	3.94590	2.38890	-0.78740
H	2.70990	1.84780	-1.98800
H	2.44730	3.36720	-1.03370

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Cozzi_aromatic_pm6/opt_a4_folded_opt_17.xyz

C	-4.05560	3.66530	-1.26230
C	-3.02550	4.40370	-0.73900
C	-2.29880	3.92280	0.39450
C	-2.60100	2.64320	0.93220
C	-3.54860	1.80920	0.24420
C	-4.34330	2.37210	-0.74500
H	-1.03920	5.68600	0.56660
H	-4.65620	4.04530	-2.08960
H	-2.76440	5.37510	-1.15690
C	-1.29240	4.72810	1.01790
C	-1.98680	2.26230	2.16800
C	-1.04250	3.06150	2.76000
C	-0.67040	4.30090	2.16290
H	-2.29350	1.32650	2.63760
H	-0.56670	2.76440	3.69300
H	0.10180	4.90230	2.63990
C	-3.73210	0.37170	0.54560
C	-2.67020	-0.51590	0.81310
C	-5.04600	-0.14730	0.46810
C	-2.95580	-1.84860	1.16600
C	-5.31810	-1.46420	0.83650
C	-4.26900	-2.30990	1.21340
H	-2.13350	-2.52980	1.38900
H	-6.34210	-1.83780	0.82050
H	-4.47860	-3.33540	1.51540
C	-6.14230	0.71430	-0.11980
H	-6.98500	0.10560	-0.52760
C	-5.56520	1.63390	-1.24150
H	-6.35910	2.33260	-1.60060
C	-1.25060	-0.12290	0.67760
C	-0.80280	0.50640	-0.49670
C	-0.33750	-0.38010	1.71230
C	0.52840	0.89860	-0.61940

H	-1.50340	0.70110	-1.30880
C	0.99560	0.01290	1.58890
H	-0.67240	-0.87440	2.62320
C	1.43710	0.66210	0.42590
H	0.86270	1.39760	-1.52710
H	1.69170	-0.18170	2.40190
O	-6.78530	1.51780	0.86790
H	-6.12330	2.03690	1.37890
O	-5.29000	0.84690	-2.40030
H	-4.52040	0.25580	-2.24330
C	2.85600	1.11000	0.29400
H	3.29850	0.78080	-0.65670
H	2.92330	2.20800	0.32060
H	3.49940	0.72790	1.09670

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Cozzi_aromatic_pm6/opt_a5_folded_opt_19.xyz

C	-2.06070	-2.45360	1.43750
C	-0.98230	-2.59740	0.60280
C	-0.79800	-1.70150	-0.49610
C	-1.69540	-0.61510	-0.67560
C	-2.69920	-0.37410	0.32480
C	-2.94780	-1.35370	1.27630
H	0.96630	-2.71330	-1.26400
H	-2.24620	-3.16380	2.24420
H	-0.26920	-3.40870	0.74430
C	0.25860	-1.90470	-1.44060
C	-1.59620	0.15820	-1.87630
C	-0.59020	-0.07120	-2.77960
C	0.36690	-1.10130	-2.54660
H	-2.34610	0.92730	-2.06670
H	-0.50920	0.52490	-3.68710
H	1.17090	-1.24370	-3.26710
C	-3.50000	0.86910	0.38560
C	-2.97050	2.15500	0.15840
C	-4.85300	0.75380	0.78320
C	-3.83230	3.26790	0.15870
C	-5.70050	1.86080	0.76430
C	-5.19160	3.11880	0.42310
H	-3.42340	4.26050	-0.03570
H	-6.75340	1.74970	1.02490
H	-5.85360	3.98350	0.39260
C	-5.34700	-0.56770	1.33030
H	-6.23800	-0.44430	1.99200
C	-4.20540	-1.29050	2.11250
H	-4.54980	-2.30520	2.42750
C	-1.52060	2.40090	-0.01560
C	-1.05370	3.15900	-1.10190
C	-0.60600	1.88750	0.91870
C	0.31630	3.37670	-1.26360
H	-1.75770	3.56420	-1.82650
C	0.76220	2.10950	0.75040
H	-0.96340	1.30380	1.76620
C	1.22610	2.84970	-0.34160
H	0.67630	3.95590	-2.11220
H	1.46930	1.69990	1.47050
O	-5.83610	-1.42760	0.30300
H	-5.16440	-1.53770	-0.40810
O	-3.99570	-0.62780	3.35920
H	-3.58220	0.25290	3.21900
H	2.29360	3.01440	-0.47400

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Cozzi_aromatic_pm6/opt_a6_folded_opt_9.xyz

C	-0.23710	-3.22670	1.44050
C	0.82850	-3.32210	0.58070
C	0.95340	-2.41400	-0.51480
C	0.00160	-1.36950	-0.68090

C	-0.98860	-1.17340	0.33660
C	-1.16760	-2.16330	1.29720
H	2.76550	-3.32450	-1.30290
H	-0.38640	-3.94530	2.25080
H	1.57720	-4.10520	0.70410
C	2.01260	-2.55420	-1.46970
C	0.04360	-0.59270	-1.88430
C	1.05110	-0.76610	-2.79660
C	2.06840	-1.74100	-2.57130
H	-0.75720	0.12410	-2.07150
H	1.08810	-0.17270	-3.70970
H	2.87550	-1.83440	-3.29850
C	-1.83370	0.04230	0.43620
C	-1.36980	1.34890	0.20070
C	-3.16900	-0.12790	0.87480
C	-2.27570	2.42810	0.25630
C	-4.06490	0.93870	0.90340
C	-3.61570	2.22370	0.57180
H	-1.91350	3.44030	0.06120
H	-5.10440	0.77060	1.19860
H	-4.31150	3.06350	0.58580
C	-3.57300	-1.46270	1.40790
C	-2.38180	-2.13160	2.15820
C	0.05910	1.65000	-0.04370
C	0.43950	2.42280	-1.15600
C	1.03640	1.16210	0.84210
C	1.78680	2.66550	-1.41070
H	-0.31900	2.81650	-1.83340
C	2.38630	1.39680	0.59320
H	0.73780	0.58240	1.71840
C	2.75370	2.13910	-0.54000
H	2.10060	3.25250	-2.28110
H	3.16010	1.00610	1.26410
O	-4.65160	-1.97520	1.29000
O	-2.47160	-2.54710	3.28120
N	4.18550	2.36570	-0.82630
O	4.46730	2.99580	-1.83350
O	5.00010	1.90620	-0.04250

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Cozzi_aromatic_pm6/opt_a7_folded_opt_9.xyz

C	-0.10350	-3.10350	1.41770
C	0.97280	-3.24070	0.57800
C	1.14770	-2.34350	-0.52020
C	0.23790	-1.26590	-0.70700
C	-0.76880	-1.03370	0.28700
C	-0.99770	-2.01250	1.24880
H	2.93320	-3.32900	-1.27600
H	-0.29100	-3.80980	2.23050
H	1.69180	-4.04760	0.71860
C	2.21550	-2.52960	-1.45710
C	0.33460	-0.49200	-1.90900
C	1.35100	-0.70640	-2.80280
C	2.32220	-1.72250	-2.55970
H	-0.43030	0.25980	-2.10860
H	1.43070	-0.11220	-3.71210
H	3.13630	-1.85090	-3.27290
C	-1.58610	0.20280	0.35480
C	-1.08600	1.49690	0.12520
C	-2.93780	0.06490	0.75550
C	-1.97300	2.59420	0.14340
C	-3.81250	1.14840	0.74620
C	-3.32620	2.42060	0.41580
H	-1.58270	3.59640	-0.04630
H	-4.86290	1.00490	1.01110
H	-4.00440	3.27390	0.39950
C	-3.38470	-1.25410	1.29230
C	-2.22890	-1.94140	2.08040

C	0.35400	1.77030	-0.07260
C	0.78660	2.53110	-1.17240
C	1.29130	1.27250	0.85080
C	2.14600	2.77430	-1.37430
H	0.05890	2.92380	-1.88320
C	2.65480	1.50320	0.66820
H	0.95100	0.69330	1.71160
C	3.04990	2.24590	-0.44840
H	2.48770	3.35520	-2.22960
H	3.38560	1.11030	1.37440
O	-4.47060	-1.74630	1.15190
O	-2.35650	-2.34190	3.20570
F	4.35240	2.46410	-0.63810

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Cozzi_aromatic_pm6/opt_a8_folded_opt_9.xyz

C	-3.16360	5.52190	-1.22130
C	-2.10330	6.18440	-0.65740
C	-1.31060	5.54930	0.34800
C	-1.58380	4.20400	0.72130
C	-2.57720	3.47280	-0.01060
C	-3.42130	4.16930	-0.86970
H	-0.02840	7.27340	0.68160
H	-3.81910	6.00370	-1.95090
H	-1.86700	7.20810	-0.94530
C	-0.25630	6.25980	1.00800
C	-0.88860	3.65430	1.84690
C	0.10080	4.36310	2.47700
C	0.44020	5.67550	2.03400
H	-1.17430	2.66330	2.20360
H	0.63850	3.93980	3.32420
H	1.24970	6.20470	2.53610
C	-2.75740	2.00350	0.09130
C	-1.70040	1.07840	0.17010
C	-4.08290	1.50750	0.02400
C	-1.99470	-0.29170	0.34210
C	-4.36530	0.15840	0.21920
C	-3.30840	-0.74430	0.40140
H	-1.17130	-1.00530	0.41450
H	-5.40050	-0.19000	0.21250
H	-3.51930	-1.80160	0.56160
C	-5.17150	2.45030	-0.36670
C	-4.64300	3.50060	-1.38970
C	-0.28600	1.47380	0.01920
C	0.11030	2.26010	-1.07330
C	0.67380	1.06400	0.96730
C	1.43710	2.67030	-1.21540
H	-0.62740	2.56470	-1.81870
C	1.99810	1.46020	0.84830
H	0.37040	0.44240	1.81060
C	2.36550	2.27440	-0.24480
H	1.72380	3.28650	-2.06100
H	2.75340	1.16540	1.57300
O	-6.30330	2.43410	0.03420
O	-5.17880	3.70890	-2.44490
O	3.70010	2.60710	-0.23020
C	4.19770	3.45800	-1.29140
H	5.25560	3.56290	-1.01670
H	4.09190	2.95870	-2.25870
H	3.68940	4.42640	-1.27200

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Cozzi_aromatic_pm6/opt_a9_folded_opt_17.xyz

C	-2.92830	5.56290	-1.68790
C	-1.84410	6.24920	-1.20310
C	-1.04310	5.68630	-0.16200
C	-1.33170	4.38250	0.32860
C	-2.35490	3.61310	-0.31790

C	-3.20460	4.25150	-1.21560
H	0.27360	7.40890	0.00210
H	-3.58930	5.99390	-2.44390
H	-1.59390	7.23920	-1.58300
C	0.03440	6.43110	0.41790
C	-0.62260	3.91570	1.48270
C	0.38830	4.65840	2.03480
C	0.73940	5.92360	1.47820
H	-0.91490	2.96200	1.92500
H	0.93370	4.29850	2.90580
H	1.56500	6.48010	1.92090
C	-2.56290	2.16260	-0.08480
C	-1.52400	1.22460	0.05110
C	-3.89960	1.69290	-0.07870
C	-1.84110	-0.11800	0.34970
C	-4.20430	0.37230	0.24050
C	-3.16210	-0.53440	0.47780
H	-1.03050	-0.84030	0.46700
H	-5.24640	0.04790	0.28740
H	-3.39030	-1.56860	0.73530
C	-4.97740	2.62210	-0.52690
C	-4.45170	3.56770	-1.64890
C	-0.10380	1.57050	-0.17130
C	0.28040	2.23570	-1.34700
C	0.87190	1.23000	0.78020
C	1.61520	2.58270	-1.55340
H	-0.46910	2.49030	-2.09730
C	2.20580	1.57740	0.57290
H	0.58490	0.70580	1.69080
C	2.58710	2.26390	-0.59230
H	1.89970	3.10760	-2.46380
H	2.95430	1.31820	1.31900
O	-6.09980	2.66560	-0.10210
O	-5.00840	3.69570	-2.70590
C	4.01770	2.63730	-0.80280
H	4.15430	3.34000	-1.63540
H	4.44990	3.11120	0.08970
H	4.62730	1.74940	-1.02740

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Cozzi_aromatic_pm6/opt_a10_folded_opt_9.xyz

C	-0.11150	-3.14310	1.33950
C	0.96130	-3.26800	0.49380
C	1.14070	-2.34470	-0.58200
C	0.24080	-1.25390	-0.73810
C	-0.76430	-1.04090	0.26210
C	-0.99880	-2.04240	1.19880
H	2.91130	-3.33070	-1.37040
H	-0.30210	-3.86720	2.13560
H	1.67400	-4.08370	0.61210
C	2.20270	-2.51860	-1.52770
C	0.34470	-0.44760	-1.91790
C	1.35570	-0.64970	-2.82080
C	2.31450	-1.68430	-2.60940
H	-0.40910	0.32160	-2.09340
H	1.44020	-0.03030	-3.71240
H	3.12320	-1.80450	-3.32970
C	-1.57800	0.19630	0.35850
C	-1.07450	1.49390	0.15960
C	-2.93140	0.05220	0.75240
C	-1.96010	2.59190	0.19790
C	-3.80400	1.13730	0.76390
C	-3.31450	2.41530	0.46200
H	-1.56660	3.59690	0.02980
H	-4.85530	0.99010	1.02300
H	-3.99110	3.26990	0.46120
C	-3.38250	-1.27630	1.26000
C	-2.22930	-1.98580	2.03200

C	0.36790	1.77250	-0.02260
C	0.80910	2.56140	-1.09760
C	1.29980	1.25850	0.89390
C	2.17300	2.80930	-1.26650
H	0.09100	2.96840	-1.80720
C	2.66200	1.51060	0.71790
H	0.96030	0.65560	1.73620
C	3.10100	2.28150	-0.36310
H	2.51420	3.41340	-2.10570
H	3.38350	1.10180	1.42420
O	-4.47040	-1.76170	1.10970
O	-2.35890	-2.41250	3.14760
H	4.16400	2.47100	-0.50090

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Cozzi_aromatic_pm6/opt_b1_folded_opt_8.xyz

C	11.65870	0.94230	0.45370
C	12.19760	1.43080	1.61430
C	11.41570	2.24610	2.49360
C	10.06030	2.55370	2.18080
C	9.54240	2.05150	0.93560
C	10.31890	1.26370	0.11040
H	13.05850	2.50230	3.89490
H	12.24040	0.31480	-0.22060
H	13.22840	1.20790	1.88950
C	12.01690	2.74760	3.69140
C	9.31890	3.33970	3.13590
H	9.91650	0.88070	-0.82860
C	9.93210	3.81130	4.27930
C	11.29340	3.52180	4.55940
H	9.36800	4.41200	4.99430
H	11.74040	3.91790	5.47060
C	8.17760	2.36250	0.44260
C	7.94820	3.56330	-0.25250
C	7.13600	1.43620	0.61760
C	6.66640	3.87760	-0.69500
H	8.77220	4.25760	-0.42010
C	5.85090	1.73920	0.17310
H	7.32890	0.49100	1.12560
C	5.61970	2.97140	-0.45780
H	6.46250	4.82330	-1.20650
H	5.02180	1.04030	0.32410
C	7.88420	3.66470	2.97430
C	6.88790	2.76380	3.42340
C	7.51760	4.90150	2.42730
C	5.53950	3.08850	3.25570
C	6.17580	5.24090	2.25120
H	8.29430	5.60400	2.12000
C	5.20650	4.31030	2.65090
H	4.74460	2.41920	3.57640
H	5.89570	6.19140	1.81130
C	7.26800	1.47620	4.07500
H	8.09890	0.97850	3.55230
H	7.60830	1.65120	5.10800
H	6.43640	0.76200	4.12560
O	3.86430	4.52070	2.47060
H	3.67460	5.36220	1.98140
N	4.24550	3.34000	-0.84330
O	3.40990	2.45440	-0.90830
O	4.02200	4.52250	-1.06600

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Cozzi_aromatic_pm6/opt_b2_folded_opt_4.xyz

C	-0.02190	7.36260	-0.78440
C	1.16200	7.47700	-0.10460
C	1.58150	6.45020	0.80000
C	0.78560	5.28380	0.98540
C	-0.48620	5.23510	0.31320

C	-0.85900	6.23780	-0.55900
H	3.38460	7.52340	1.36870
H	-0.34610	8.12850	-1.48750
H	1.80400	8.34620	-0.24040
C	2.81060	6.61000	1.51570
C	1.31680	4.24350	1.82960
H	-1.81700	6.18860	-1.07760
C	2.50090	4.43340	2.51320
C	3.24800	5.63230	2.36990
H	2.88950	3.64980	3.16410
H	4.17200	5.74820	2.93470
C	-1.48870	4.16980	0.55630
C	-2.37480	4.30450	1.63890
C	-1.59710	3.07410	-0.31420
C	-3.35340	3.33750	1.87470
H	-2.29200	5.16690	2.30060
C	-2.56370	2.09070	-0.09300
H	-0.91310	2.98160	-1.15800
C	-3.41490	2.24570	1.00400
H	-4.03940	3.43180	2.71370
H	-2.63860	1.22580	-0.75010
C	0.67900	2.91450	1.96190
C	0.96370	1.89910	1.01520
C	-0.16040	2.64670	3.04960
C	0.37890	0.63870	1.15830
C	-0.75770	1.39430	3.20470
H	-0.36040	3.43170	3.78050
C	-0.48300	0.41400	2.24230
H	0.56800	-0.16470	0.45130
H	-1.42030	1.19710	4.03880
C	1.88570	2.16940	-0.12700
H	1.88490	1.36880	-0.87680
H	1.62740	3.10670	-0.64430
H	2.92210	2.28490	0.22710
O	-1.03550	-0.84280	2.29470
H	-1.67130	-0.93960	3.04530
F	-4.33460	1.30430	1.23330

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Cozzi_aromatic_pm6/opt_b3_folded_opt_19.xyz

C	-2.71440	4.80160	-4.25460
C	-3.30300	3.56480	-4.23860
C	-2.87870	2.57130	-3.29980
C	-1.82560	2.84640	-2.38040
C	-1.26370	4.17320	-2.39630
C	-1.69350	5.10780	-3.31680
H	-4.34160	1.12670	-4.00610
H	-3.02080	5.56430	-4.96880
H	-4.10070	3.31550	-4.93650
C	-3.53160	1.29760	-3.29910
C	-1.41140	1.77550	-1.50880
H	-1.25710	6.10700	-3.32790
C	-2.06850	0.56100	-1.52790
C	-3.14410	0.31960	-2.42180
H	-1.75850	-0.23970	-0.85620
H	-3.64020	-0.64950	-2.40090
C	-0.24100	4.62830	-1.42670
C	1.12270	4.51620	-1.72310
C	-0.65060	5.21870	-0.21520
C	2.08720	4.91300	-0.79330
H	1.43750	4.09640	-2.67850
C	0.29020	5.62810	0.72150
H	-1.71410	5.33980	-0.00840
C	1.65630	5.43250	0.43260
H	3.14080	4.79690	-1.02250
H	0.00020	6.07260	1.66930
C	-0.26030	1.87990	-0.58230
C	1.04060	1.53010	-1.01910

C	-0.47380	2.27550	0.74390
C	2.11720	1.62560	-0.13170
C	0.58970	2.37700	1.64300
H	-1.48350	2.52310	1.07540
C	1.87320	2.07300	1.17390
H	3.13020	1.37620	-0.43350
H	0.42300	2.70730	2.66160
C	1.26660	1.05960	-2.41760
H	0.87310	0.04020	-2.55390
H	0.74430	1.69540	-3.14980
H	2.32710	1.04060	-2.69640
O	2.99260	2.20670	1.96810
H	2.76050	2.51460	2.87870
O	2.48570	5.81050	1.46910
C	3.86620	5.37570	1.40200
H	4.26210	5.72580	2.36260
H	3.91230	4.28050	1.32810
H	4.37740	5.86270	0.56780

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Cozzi_aromatic_pm6/opt_b4_folded_opt_7.xyz

C	-1.18520	6.53750	-3.39290
C	-1.89520	5.45670	-3.84420
C	-1.73240	4.17380	-3.23080
C	-0.82830	3.99920	-2.14310
C	-0.10150	5.15960	-1.69550
C	-0.28210	6.38320	-2.30880
H	-3.17610	3.24070	-4.56140
H	-1.29900	7.51960	-3.84940
H	-2.59410	5.55280	-4.67360
C	-2.49500	3.07010	-3.72940
C	-0.71750	2.67650	-1.58070
H	0.27190	7.25650	-1.96280
C	-1.47080	1.63410	-2.08420
C	-2.36790	1.82790	-3.16650
H	-1.38270	0.63720	-1.65180
H	-2.94320	0.97940	-3.53360
C	0.86900	5.12990	-0.57530
C	2.23620	4.95290	-0.83740
C	0.43470	5.33340	0.74230
C	3.14930	4.90420	0.21530
H	2.58030	4.83510	-1.86340
C	1.35000	5.29050	1.79510
H	-0.62110	5.50700	0.94350
C	2.70840	5.04520	1.54140
H	4.20400	4.73740	0.00850
H	1.00300	5.43040	2.81590
C	0.18170	2.34120	-0.45250
C	1.51660	1.93090	-0.68500
C	-0.32560	2.37610	0.85280
C	2.33810	1.60710	0.39940
C	0.47840	2.04960	1.94670
H	-1.36230	2.67370	1.01800
C	1.80960	1.69520	1.69410
H	3.37320	1.30670	0.26220
H	0.08470	2.09040	2.95440
C	2.04770	1.82740	-2.07620
H	1.70610	0.89630	-2.55360
H	1.69610	2.65510	-2.71180
H	3.14420	1.83170	-2.11260
O	2.69610	1.40980	2.70970
H	2.26780	1.45970	3.59750
C	3.67420	4.88770	2.66990
H	3.82970	3.81540	2.88110
H	4.65770	5.31730	2.43980
H	3.32500	5.35770	3.59690

Cozzi_aromatic_pm6/opt_b5_folded_opt_16.xyz

C	-1.34550	-2.76750	-2.64670
C	-0.24240	-3.32410	-2.05490
C	0.46050	-2.62110	-1.02540
C	0.03500	-1.32460	-0.61670
C	-1.16250	-0.79920	-1.21750
C	-1.81420	-1.49950	-2.21290
H	1.88460	-4.23780	-0.73530
H	-1.88300	-3.28520	-3.43990
H	0.11900	-4.30610	-2.35590
C	1.59680	-3.23880	-0.41230
C	0.83810	-0.64070	0.36510
H	-2.71440	-1.09060	-2.67320
C	1.92360	-1.26840	0.94280
C	2.30100	-2.58320	0.56280
H	2.51880	-0.75090	1.69540
H	3.15850	-3.04660	1.04830
C	-1.80120	0.47020	-0.78940
C	-1.56690	1.66030	-1.49300
C	-2.70560	0.45660	0.28450
C	-2.21050	2.83710	-1.10140
H	-0.87400	1.66880	-2.33200
C	-3.35130	1.63530	0.66420
H	-2.89580	-0.47130	0.82040
C	-3.10090	2.82730	-0.02350
H	-2.01160	3.76550	-1.63420
H	-4.04810	1.62580	1.49990
C	0.59260	0.76120	0.77180
C	1.15150	1.82520	0.02140
C	-0.14430	1.02890	1.93140
C	0.94310	3.14400	0.43320
C	-0.36280	2.34070	2.35720
H	-0.56250	0.20060	2.50560
C	0.17900	3.37650	1.58580
H	1.34910	3.98740	-0.11870
H	-0.94480	2.54310	3.24760
C	1.96590	1.54250	-1.19710
H	1.46100	0.82550	-1.86380
H	2.18160	2.44230	-1.78580
H	2.93130	1.08850	-0.92480
O	0.00450	4.70180	1.91180
H	-0.54660	4.81460	2.72300
H	-3.59730	3.74620	0.27970

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Cozzi_aromatic_pm6/opt_c2_folded_opt_3.xyz

C	1.18710	3.14890	2.73180
C	0.21770	4.09910	3.20100
C	-1.05150	3.63460	3.31410
C	-1.40490	2.25350	2.97690
C	-0.48620	1.34840	2.54050
C	0.85920	1.84730	2.42030
H	2.21690	3.48950	2.62550
H	0.51530	5.11380	3.44110
H	1.62370	1.15640	2.06580
C	-2.46690	3.90110	3.67970
C	-3.39210	4.77940	4.14110
C	-4.72600	4.26330	4.26930
C	-5.05420	2.96540	3.94320
C	-4.07800	2.03010	3.44540
C	-2.81240	2.52160	3.33340
H	-3.17260	5.80700	4.40750
H	-5.49430	4.93950	4.64390
H	-6.07700	2.60830	4.06140
C	-4.43790	0.64870	3.08520
C	-3.97730	-0.42530	3.87750
C	-5.20180	0.38550	1.93030
C	-4.28000	-1.74230	3.51120

C	-5.49360	-0.93680	1.57340
C	-5.02990	-2.00260	2.35730
H	-3.91740	-2.56750	4.11870
H	-6.07990	-1.13930	0.68170
C	-0.81960	-0.05120	2.22300
C	-1.63190	-0.36670	1.10840
C	-0.34970	-1.06780	3.06660
C	-1.96470	-1.70560	0.85600
C	-0.67830	-2.40460	2.83140
H	0.27540	-0.81010	3.92270
C	-1.48580	-2.68410	1.72720
H	-2.59890	-1.96700	0.01140
H	-0.32070	-3.19220	3.48920
C	-3.15880	-0.16770	5.10040
H	-3.63100	0.57780	5.75600
H	-2.98860	-1.07100	5.69760
H	-2.16890	0.23250	4.82420
C	-5.71330	1.49880	1.07170
H	-5.79930	1.20460	0.01790
H	-6.71410	1.81290	1.40380
H	-5.07180	2.39090	1.10710
C	-2.13980	0.70830	0.20900
H	-2.63800	0.31910	-0.68670
H	-2.87640	1.33600	0.74180
H	-1.33350	1.37840	-0.12230
C	-5.33500	-3.40800	1.95200
H	-4.85910	-4.15110	2.60570
H	-6.41650	-3.60210	1.97190
H	-4.98420	-3.61370	0.93050
F	-1.81530	-3.95660	1.49020

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Cozzi_aromatic_pm6/opt_c4_folded_opt_11.xyz

C	-3.51060	-3.21440	2.03080
C	-4.34050	-3.33430	3.19660
C	-5.39390	-2.48190	3.25550
C	-5.66290	-1.50420	2.19890
C	-4.88330	-1.39490	1.08760
C	-3.76510	-2.30080	1.03120
H	-2.65230	-3.88100	1.95160
H	-4.11230	-4.06920	3.96010
H	-3.11130	-2.23920	0.16150
C	-6.59030	-2.00420	3.99530
C	-7.39490	-2.12120	5.08100
C	-8.51510	-1.22370	5.12100
C	-8.75960	-0.29900	4.12950
C	-7.90360	-0.16400	2.97800
C	-6.84790	-1.02400	2.93850
H	-7.23380	-2.83500	5.88060
H	-9.18770	-1.29430	5.97550
H	-9.62460	0.36060	4.19140
C	-8.16840	0.84100	1.93460
C	-7.97320	2.21100	2.19530
C	-8.58230	0.42640	0.64870
C	-8.19230	3.15420	1.18110
C	-8.80190	1.37840	-0.35270
C	-8.60050	2.74120	-0.09220
H	-8.03810	4.20950	1.38570
H	-9.10930	1.05710	-1.34430
C	-5.15300	-0.44070	-0.00150
C	-5.03570	0.95230	0.20190
C	-5.56780	-0.92730	-1.24830
C	-5.34660	1.82680	-0.84650
C	-5.88130	-0.05020	-2.28700
H	-5.65410	-2.00250	-1.40390
C	-5.77750	1.33400	-2.08680
H	-5.27270	2.90060	-0.68960
H	-6.21000	-0.44240	-3.24520

C	-7.53490	2.68750	3.54420
H	-6.93290	3.60310	3.48510
H	-8.40630	2.91030	4.17720
H	-6.93300	1.94030	4.08150
C	-8.77620	-1.02340	0.34650
H	-7.80220	-1.54240	0.32780
H	-9.38780	-1.52270	1.11090
H	-9.25270	-1.19690	-0.62510
C	-4.59120	1.49300	1.52040
H	-5.35380	1.29240	2.29270
H	-3.66030	1.01860	1.86070
H	-4.42700	2.57630	1.50420
C	-8.81200	3.73970	-1.18490
H	-8.10480	3.55720	-2.01810
H	-9.82750	3.67210	-1.59830
H	-8.66380	4.77410	-0.85260
C	-6.13150	2.29140	-3.17900
H	-6.98100	2.93310	-2.87220
H	-5.29000	2.95570	-3.41850
H	-6.42360	1.78850	-4.10870

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Cozzi_aromatic_pm6/opt_c5_folded_opt_6.xyz

C	2.58420	-0.85440	-7.39950
C	3.34620	-0.92090	-6.18330
C	2.66260	-0.63810	-5.04670
C	1.24010	-0.28760	-5.06690
C	0.51140	-0.24010	-6.21500
C	1.24410	-0.53480	-7.41930
H	3.10490	-1.06850	-8.33240
H	4.39800	-1.18280	-6.20890
H	0.70040	-0.49270	-8.36260
C	2.66830	-0.50020	-3.56680
C	3.36240	-0.57540	-2.40370
C	2.61170	-0.28410	-1.21440
C	1.27690	0.05710	-1.24310
C	0.53660	0.14820	-2.47570
C	1.24930	-0.14180	-3.59900
H	4.41240	-0.83670	-2.33990
H	3.13610	-0.34260	-0.26090
H	0.74030	0.26400	-0.31770
C	-0.88480	0.53180	-2.50260
C	-1.87500	-0.43940	-2.76310
C	-1.25800	1.87760	-2.31630
C	-3.22300	-0.06460	-2.80450
C	-2.61060	2.24030	-2.36180
C	-3.59310	1.27280	-2.60690
H	-3.98480	-0.81130	-3.01010
H	-2.89580	3.27750	-2.21370
C	-0.92520	0.09100	-6.23230
C	-1.90240	-0.88310	-6.51880
C	-1.31540	1.40080	-5.91140
C	-3.25840	-0.51850	-6.49500
C	-2.66580	1.75070	-5.89140
H	-0.55520	2.14230	-5.66620
C	-3.63700	0.78860	-6.18590
H	-4.02020	-1.26340	-6.71390
H	-2.96110	2.76460	-5.63090
C	-1.49090	-1.86090	-3.01480
H	-0.98630	-1.94890	-3.99220
H	-0.78760	-2.23530	-2.25790
H	-2.35150	-2.53910	-3.03130
C	-0.21480	2.92440	-2.08970
H	-0.63190	3.93620	-2.02620
H	0.34030	2.73920	-1.15860
H	0.52580	2.92500	-2.90450
C	-1.52810	-2.29280	-6.84650
H	-2.25480	-3.01420	-6.45120

H	-1.47960	-2.44010	-7.93520
H	-0.54490	-2.57310	-6.44160
C	-5.03740	1.65560	-2.66810
H	-5.49240	1.33610	-3.61620
H	-5.60610	1.17890	-1.85690
H	-5.19440	2.73790	-2.58120
H	-4.69110	1.05760	-6.16640

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9_benzyl_triptycene_pm6/opt_b1_folded_opt_11.xyz

C	-1.89880	-2.54720	-1.19530
C	-1.42950	-1.52890	-0.34920
C	-0.76550	-0.40430	-0.87050
C	-0.46790	-0.39360	-2.24930
C	-0.92950	-1.41680	-3.09120
C	-1.66510	-2.48910	-2.56910
C	1.61070	0.74310	-1.78050
C	1.28500	0.77460	-0.39360
C	2.29840	0.74710	0.55090
C	3.63830	0.69320	0.12200
C	3.95050	0.66530	-1.23390
C	2.92900	0.68920	-2.20130
H	-2.43420	-3.39750	-0.77960
H	-2.04110	-3.27990	-3.21100
H	4.43340	0.67230	0.86500
H	4.98950	0.62340	-1.55510
H	3.17730	0.66340	-3.25960
C	-0.69190	2.07220	-0.91660
C	-1.32020	3.19960	-0.40550
C	-1.67020	4.25030	-1.27180
C	-1.38200	4.17780	-2.63260
C	-0.71870	3.05580	-3.15790
C	-0.37120	2.02310	-2.30060
H	-2.17220	5.12720	-0.86700
H	-1.66350	4.99360	-3.29560
H	-0.48100	3.00480	-4.21750
C	-0.23400	0.83250	-0.12470
C	-0.57490	0.88340	1.36630
H	-0.19580	-0.06110	1.83400
H	0.00740	1.71050	1.83020
C	-2.01970	1.02860	1.76870
C	-2.29040	1.17080	3.14320
C	-3.09290	1.00790	0.86550
C	-3.60450	1.28720	3.59780
H	-1.47200	1.18720	3.85930
C	-4.40650	1.12630	1.32560
H	-2.91110	0.89680	-0.20420
C	-4.66900	1.26490	2.69100
H	-3.80090	1.39760	4.66280
H	-5.22900	1.11300	0.61210
H	-1.55360	3.28530	0.65520
H	2.08010	0.76350	1.61610
H	-5.69190	1.35850	3.04570
O	-1.50850	-1.61460	1.02940
O	-0.58770	-1.23990	-4.42020
C	-0.96760	-2.28240	-5.34760
H	-2.05670	-2.36910	-5.39720
H	-0.56170	-1.89870	-6.29270
H	-0.49320	-3.22910	-5.07390
C	-2.65520	-2.30710	1.58200
H	-2.57400	-2.05550	2.64780
H	-3.58320	-1.90610	1.16380
H	-2.55740	-3.38250	1.41870
C	0.39360	0.77240	-2.69970
H	0.64630	0.72420	-3.77770

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9_benzyl_triptycene_pm6/opt_b3_folded_opt_3.xyz

C	-1.09620	-5.41190	-2.70150
C	-0.01520	-5.05140	-1.87990
C	0.74730	-3.90120	-2.15070
C	0.47510	-3.19490	-3.34120
C	-0.59870	-3.56300	-4.16580
C	-1.40180	-4.66350	-3.83780
C	2.82670	-2.70190	-3.57790
C	3.09430	-3.37630	-2.35160
C	4.31440	-4.00650	-2.16690
C	5.27430	-3.96480	-3.19600
C	5.00830	-3.30190	-4.39040
C	3.77120	-2.66190	-4.59000
H	-1.69240	-6.28970	-2.46310
H	-2.24520	-4.95050	-4.45860
H	6.23230	-4.45990	-3.04910
H	5.75700	-3.27540	-5.17980
H	3.56560	-2.14850	-5.52610
C	1.65640	-1.80030	-1.20420
C	1.70930	-1.05570	-0.03380
C	1.43960	0.32360	-0.07720
C	1.13400	0.95230	-1.28190
C	1.10850	0.21640	-2.47880
C	1.37820	-1.14270	-2.43340
H	1.47110	0.89990	0.84570
H	0.91970	2.01890	-1.30330
H	0.88400	0.70920	-3.42150
C	1.92160	-3.31090	-1.34940
C	2.22870	-4.02180	-0.02860
H	2.38520	-5.10670	-0.25600
H	3.20260	-3.64130	0.35170
C	1.21440	-3.94110	1.08260
C	1.57660	-4.48090	2.32570
C	-0.07310	-3.39070	0.92930
C	0.68730	-4.48400	3.40520
H	2.56780	-4.91240	2.46260
C	-0.97630	-3.38120	1.98480
H	-0.37620	-2.96370	-0.02960
C	-0.58370	-3.93320	3.22000
H	0.99350	-4.90600	4.35530
H	-1.97060	-2.95420	1.87950
H	1.95200	-1.52000	0.92160
H	4.54470	-4.53490	-1.24470
O	0.41110	-5.84270	-0.82820
O	-0.75350	-2.74880	-5.27360
C	-1.79350	-3.09990	-6.21520
H	-2.77600	-3.02980	-5.73990
H	-1.67230	-2.32280	-6.98100
H	-1.61070	-4.09350	-6.63380
C	-0.60510	-6.58380	-0.10820
H	-0.04090	-6.94770	0.76040
H	-1.41200	-5.91720	0.21110
H	-0.96980	-7.41140	-0.72030
O	-1.58090	-3.86720	4.17430
C	-1.27590	-4.36020	5.49900
H	-0.45430	-3.78740	5.93870
H	-2.21600	-4.17010	6.03260
H	-1.05410	-5.43030	5.46500
C	1.44270	-2.06400	-3.64000
H	1.22530	-1.56000	-4.60280

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9_benzyl_triptycene_pm6/opt_c1_folded_opt_17.xyz			
C	-2.58240	-2.06440	-1.39460
C	-1.52070	-1.61600	-0.59130
C	-0.65080	-0.60620	-1.03960
C	-0.79730	-0.15100	-2.36690
C	-1.85220	-0.60800	-3.17100
C	-2.76220	-1.55360	-2.67970

C	1.59710	0.11180	-2.53240
C	1.73940	-0.30380	-1.17700
C	2.88960	-0.96590	-0.77900
C	3.90420	-1.21280	-1.72330
C	3.76100	-0.80150	-3.04510
C	2.59550	-0.13180	-3.46080
H	-3.26250	-2.82710	-1.02230
H	-3.59230	-1.90450	-3.28540
H	4.80730	-1.73260	-1.40900
H	4.55110	-0.99720	-3.76750
H	2.48580	0.18430	-4.49540
C	0.37870	1.57820	-0.48730
C	0.42920	2.54880	0.50390
C	0.27950	3.90290	0.15600
C	0.09520	4.28130	-1.17170
C	0.07370	3.31170	-2.18860
C	0.22510	1.97760	-1.84300
H	0.30830	4.65850	0.93910
H	-0.02690	5.33160	-1.42920
H	-0.05630	3.60760	-3.22660
C	0.52330	0.05640	-0.29650
C	0.69610	-0.37700	1.16170
H	0.77600	-1.49360	1.17610
H	1.67470	0.00850	1.52450
C	-0.36990	0.00620	2.15520
C	-0.12660	-0.28590	3.50560
C	-1.59560	0.60130	1.79830
C	-1.07450	-0.00200	4.49420
H	0.81560	-0.74700	3.80050
C	-2.55490	0.89310	2.75980
H	-1.80570	0.83930	0.75280
C	-2.28240	0.58450	4.10690
H	-0.86020	-0.23660	5.53030
H	-3.50240	1.35680	2.49630
H	0.57820	2.28200	1.54970
H	3.02350	-1.30120	0.24690
O	-1.21970	-2.19570	0.62830
O	-1.87730	-0.03860	-4.43170
C	-2.89380	-0.50270	-5.34960
H	-3.88970	-0.26010	-4.96820
H	-2.66550	0.08280	-6.24970
H	-2.77740	-1.57350	-5.53970
C	-2.33230	-2.69180	1.41340
H	-1.84780	-2.90460	2.37530
H	-3.09430	-1.91550	1.53190
H	-2.73440	-3.60090	0.96130
O	-3.32500	0.91630	4.95100
C	-3.14140	0.68670	6.36690
H	-2.30230	1.27890	6.74300
H	-4.09230	1.04790	6.77930
H	-3.00840	-0.38040	6.56510
C	0.27750	0.81880	-2.82420
H	0.15650	1.12060	-3.88360

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9_benzyl_triptycene_pm6/opt_c2_folded_opt_8.xyz

C	3.22480	-4.66460	2.40620
C	2.91660	-3.37440	1.94330
C	2.33980	-3.17970	0.67600
C	2.20750	-4.30220	-0.16840
C	2.52570	-5.58840	0.29240
C	3.01710	-5.77700	1.59130
C	2.69720	-2.90760	-2.07830
C	2.78050	-1.76660	-1.22860
C	3.62240	-0.71910	-1.56570
C	4.38070	-0.79830	-2.74930
C	4.29320	-1.91390	-3.57670
C	3.44400	-2.98490	-3.24190

H	3.64470	-4.79970	3.40030
H	3.25240	-6.76840	1.96610
H	5.04130	0.02540	-3.01300
H	4.88380	-1.96560	-4.48940
H	3.38170	-3.85630	-3.88920
C	0.47690	-2.12360	-0.57140
C	-0.65440	-1.33760	-0.39890
C	-1.86060	-1.71460	-1.01520
C	-1.92930	-2.85900	-1.80620
C	-0.78440	-3.64680	-2.01390
C	0.40450	-3.27050	-1.40800
H	-2.74680	-1.10010	-0.86760
H	-2.86950	-3.14550	-2.27320
H	-0.83400	-4.53250	-2.64230
C	1.87680	-1.86720	0.01880
C	1.95780	-0.63060	0.91700
H	3.01180	-0.54680	1.28570
H	1.77840	0.27000	0.28870
C	1.05810	-0.56150	2.12370
C	1.07960	0.62880	2.87490
C	0.23260	-1.61080	2.55090
C	0.29860	0.76240	4.02120
H	1.71450	1.45570	2.56240
C	-0.55130	-1.47850	3.69880
H	0.19520	-2.54610	1.99010
C	-0.52550	-0.29290	4.44530
H	0.32630	1.69020	4.58850
H	-1.18830	-2.30470	4.00820
H	-0.62810	-0.43490	0.21080
H	3.71160	0.16120	-0.93330
O	3.24830	-2.23570	2.65590
O	2.30290	-6.58470	-0.64150
C	2.67920	-7.93260	-0.27680
H	2.08130	-8.27780	0.57130
H	2.42500	-8.48940	-1.18800
H	3.75200	-7.98770	-0.07120
C	3.16950	-2.31900	4.10060
H	3.28640	-1.26640	4.39040
H	2.18860	-2.69350	4.40870
H	3.98720	-2.93120	4.48650
C	-1.36430	-0.13940	5.67290
H	-1.87060	-1.07030	5.95780
H	-0.76300	0.17880	6.53520
H	-2.14620	0.61900	5.52220
C	1.73700	-3.98110	-1.57560
H	1.69000	-4.87820	-2.22450

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9_benzyl_triptycene_pm6/opt_c3_folded_opt_5.xyz

C	-0.37660	-2.67410	-1.45210
C	-0.32330	-1.82440	-0.33490
C	-0.61750	-0.45430	-0.45360
C	-0.83640	0.06420	-1.74700
C	-0.87820	-0.78490	-2.86320
C	-0.66810	-2.16250	-2.71640
C	0.25540	2.11770	-1.09740
C	0.43300	1.61000	0.22210
C	1.52300	2.01760	0.97410
C	2.43730	2.93430	0.42090
C	2.25710	3.42910	-0.86730
C	1.15570	3.01890	-1.64090
H	-0.17360	-3.73640	-1.33910
H	-0.71310	-2.83320	-3.56920
H	3.29290	3.25400	1.01290
H	2.96980	4.13730	-1.28580
H	1.02070	3.40510	-2.64830
C	-1.97160	1.41800	0.44080
C	-2.92260	1.72320	1.40500

C	-4.05820	2.47050	1.04590
C	-4.23240	2.91800	-0.26150
C	-3.26250	2.64220	-1.24030
C	-2.14190	1.90860	-0.88240
H	-4.80560	2.69780	1.80390
H	-5.11820	3.49000	-0.53040
H	-3.39140	3.00300	-2.25780
C	-0.67110	0.61870	0.64830
C	-0.48230	0.09220	2.07280
H	0.48790	-0.46680	2.10270
H	-0.35570	0.96330	2.75360
C	-1.53610	-0.81800	2.64860
C	-1.38360	-1.20330	3.99430
C	-2.63010	-1.31170	1.92230
C	-2.30490	-2.06310	4.59350
H	-0.54100	-0.83250	4.57340
C	-3.55010	-2.17130	2.52710
H	-2.77050	-1.03030	0.87790
C	-3.39230	-2.55190	3.86230
H	-2.17670	-2.35280	5.63490
H	-4.39660	-2.54330	1.95190
H	-2.80980	1.39020	2.43620
H	1.68830	1.64200	1.98120
O	0.10390	-2.25760	0.90760
O	-1.13960	-0.12760	-4.05230
C	-1.12640	-0.91720	-5.26390
H	-1.92200	-1.66710	-5.23760
H	-1.33030	-0.15600	-6.02820
H	-0.14200	-1.36920	-5.41500
C	-0.19900	-3.62800	1.26810
H	0.06200	-3.63970	2.33470
H	-1.26490	-3.83320	1.13270
H	0.43110	-4.31350	0.69730
H	-4.11060	-3.21950	4.33040
C	-0.98180	1.57420	-1.80500
H	-1.10690	1.95100	-2.83970

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9_benzyl_triptycene_pm6/opt_c5_folded_opt_6.xyz

C	-2.73150	-1.38230	-1.55690
C	-1.68990	-1.09020	-0.66140
C	-0.45610	-0.59630	-1.12280
C	-0.25470	-0.52180	-2.51650
C	-1.29420	-0.82250	-3.41020
C	-2.54390	-1.23670	-2.93160
C	2.06420	-1.11720	-2.20690
C	1.87110	-1.14830	-0.79550
C	2.63120	-2.00620	-0.01700
C	3.58840	-2.83240	-0.63620
C	3.77440	-2.79580	-2.01490
C	3.00550	-1.93080	-2.81510
H	-3.68890	-1.73970	-1.18540
H	-3.36170	-1.45930	-3.61070
H	4.18520	-3.50550	-0.02330
H	4.51700	-3.43880	-2.48390
H	3.15140	-1.90820	-3.89250
C	1.24050	1.18970	-0.85920
C	1.52910	2.33060	-0.12290
C	1.94250	3.49820	-0.78820
C	2.07820	3.51820	-2.17430
C	1.82020	2.36100	-2.92860
C	1.41660	1.21000	-2.26960
H	2.15750	4.39310	-0.20670
H	2.39180	4.42950	-2.68010
H	1.94010	2.37200	-4.00930
C	0.77880	-0.17260	-0.30770
C	0.59250	-0.20110	1.21160
H	0.25800	-1.23270	1.49230

H	1.58880	-0.06050	1.68730
C	-0.37920	0.76690	1.83430
C	-0.44930	0.78640	3.24080
C	-1.22170	1.61370	1.09530
C	-1.34210	1.62810	3.90540
H	0.19830	0.13380	3.82530
C	-2.12310	2.46580	1.73620
H	-1.18350	1.61210	0.00340
C	-2.16340	2.45160	3.13180
H	-1.39190	1.64020	4.99240
H	-2.77020	3.12260	1.15750
H	1.43900	2.34180	0.96250
H	2.50230	-2.05690	1.06160
O	-1.77780	-1.33860	0.69650
O	-0.94670	-0.66480	-4.73990
C	-1.93700	-1.02190	-5.73170
H	-2.81310	-0.37310	-5.64500
H	-1.39580	-0.82680	-6.66680
H	-2.20020	-2.07990	-5.64570
C	-3.09700	-1.30510	1.29430
H	-2.85620	-1.34630	2.36480
H	-3.60630	-0.36850	1.05010
H	-3.67140	-2.18120	0.98410
F	-3.02640	3.25940	3.75530
C	1.15270	-0.13210	-2.93140
H	1.28630	-0.12510	-4.03160

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9_benzyl_triptycene_pm6/opt_c6_folded_opt_6.xyz

C	5.05260	-3.71600	2.51110
C	4.10350	-3.01440	1.75080
C	3.32340	-3.67180	0.78200
C	3.60510	-5.02720	0.51530
C	4.55930	-5.72540	1.27170
C	5.27470	-5.07480	2.28520
C	3.08880	-4.67060	-1.81590
C	2.76230	-3.31160	-1.53920
C	2.95710	-2.34580	-2.51340
C	3.47220	-2.72680	-3.76710
C	3.78720	-4.05610	-4.03260
C	3.59640	-5.04410	-3.04910
H	5.63410	-3.20290	3.27350
H	6.00700	-5.60520	2.88720
H	3.62410	-1.96730	-4.53220
H	4.18520	-4.34020	-5.00520
H	3.84730	-6.08110	-3.25970
C	1.01860	-4.06670	-0.03690
C	-0.30690	-3.73790	0.21190
C	-1.27760	-4.75440	0.24680
C	-0.92590	-6.08310	0.02120
C	0.40690	-6.42540	-0.26390
C	1.36150	-5.42060	-0.30150
H	-2.31430	-4.49260	0.45260
H	-1.68420	-6.86330	0.05750
H	0.67900	-7.46080	-0.45480
C	2.21220	-3.09610	-0.11330
C	1.84930	-1.63640	0.16970
H	2.78710	-1.02960	0.07250
H	1.17120	-1.28020	-0.63850
C	1.23530	-1.29480	1.50020
C	0.84640	0.04500	1.70170
C	1.04870	-2.22010	2.54060
C	0.29250	0.45190	2.91250
H	0.98340	0.77520	0.90510
C	0.49460	-1.82220	3.75520
H	1.34450	-3.26380	2.40810
C	0.11690	-0.48260	3.94740
H	-0.00500	1.49060	3.05970

H	0.35330	-2.54950	4.55580
H	-0.61240	-2.70700	0.38350
H	2.72340	-1.29980	-2.33020
O	3.92230	-1.64610	1.84690
O	4.69120	-7.05370	0.91000
C	5.70200	-7.83100	1.59280
H	5.46970	-7.90440	2.65900
H	5.60070	-8.80780	1.10180
H	6.69440	-7.40630	1.41740
C	4.30340	-1.00750	3.08990
H	3.90270	0.00530	2.95090
H	3.82200	-1.50010	3.93940
H	5.39200	-0.99120	3.18470
C	-0.44510	-0.06960	5.19620
N	-0.89680	0.26490	6.20730
C	2.82790	-5.61660	-0.64810
H	3.10420	-6.66980	-0.85550

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9_benzyl_triptycene_pm6/opt_c7_folded_opt_10.xyz

C	3.08810	-4.78380	1.81600
C	2.74270	-3.44300	1.58330
C	2.38440	-3.00130	0.29650
C	2.49800	-3.91470	-0.77150
C	2.85070	-5.25300	-0.53800
C	3.13020	-5.69610	0.76130
C	3.18130	-2.11580	-2.23000
C	3.02390	-1.18540	-1.16250
C	3.81740	-0.05050	-1.11690
C	4.76740	0.16630	-2.13320
C	4.91570	-0.74500	-3.17450
C	4.11680	-1.90210	-3.22860
H	3.34000	-5.12010	2.81900
H	3.39190	-6.73170	0.95900
H	5.39000	1.05850	-2.09680
H	5.65340	-0.56830	-3.95520
H	4.23850	-2.61320	-4.04230
C	0.68050	-1.78210	-1.02570
C	-0.52490	-1.10430	-0.90440
C	-1.57450	-1.39390	-1.79400
C	-1.41290	-2.34190	-2.80160
C	-0.18740	-3.01230	-2.95490
C	0.84720	-2.72220	-2.07890
H	-2.52140	-0.86700	-1.68830
H	-2.23420	-2.56340	-3.48090
H	-0.05660	-3.74210	-3.75050
C	1.93460	-1.59940	-0.15050
C	1.76190	-0.58760	0.98470
H	2.73970	-0.52130	1.52950
H	1.59400	0.41840	0.53770
C	0.69660	-0.84190	2.01570
C	0.53780	0.12740	3.02710
C	-0.12390	-1.98070	2.03730
C	-0.40570	-0.04590	4.03560
H	1.16200	1.01980	3.02690
C	-1.07120	-2.15800	3.04490
H	-0.02110	-2.74810	1.26600
C	-1.21370	-1.19440	4.05190
H	-0.51160	0.71500	4.81140
H	-1.69380	-3.05460	3.03360
H	-0.67720	-0.35290	-0.13120
H	3.72430	0.67500	-0.31250
O	2.79880	-2.46880	2.56400
O	2.88270	-6.02720	-1.68350
C	3.30360	-7.40400	-1.54290
H	2.60010	-7.95430	-0.91170
H	3.25760	-7.75770	-2.58130
H	4.32600	-7.45370	-1.15780

C	2.68000	-2.90030	3.94190
H	2.58440	-1.94080	4.46760
H	1.78020	-3.50650	4.07960
H	3.58570	-3.42940	4.24820
C	-2.21160	-1.36030	5.15640
F	-1.66850	-1.39770	6.38850
F	-3.11840	-0.37010	5.24410
F	-2.96870	-2.47010	5.12180
C	2.24430	-3.31640	-2.14360
H	2.38300	-4.05170	-2.96140

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9_benzyl_triptycene_pm6/opt_c8_folded_opt_17.xyz

C	-4.14680	0.65240	-2.71240
C	-4.29490	1.75160	-1.84520
C	-5.34770	2.66190	-1.97530
C	-6.21550	2.49250	-3.08500
C	-6.06080	1.40650	-3.94790
C	-5.03570	0.46710	-3.76380
C	-6.44000	4.88480	-3.27890
C	-5.59650	5.05730	-2.14470
C	-4.79720	6.18580	-2.05090
C	-4.83840	7.14760	-3.07780
C	-5.66870	6.97500	-4.18140
C	-6.48060	5.83120	-4.28950
H	-3.33630	-0.06140	-2.54520
H	-4.93550	-0.39390	-4.43180
H	-4.21040	8.03360	-3.00170
H	-5.69340	7.72490	-4.97010
H	-7.12460	5.69780	-5.15520
C	-7.19500	3.82080	-0.80280
C	-7.78810	3.96100	0.44450
C	-9.18550	3.85990	0.56360
C	-9.98220	3.63720	-0.55680
C	-9.39840	3.52900	-1.83030
C	-8.02040	3.63140	-1.94450
H	-9.64270	3.95680	1.54700
H	-11.06230	3.55250	-0.45220
H	-10.02120	3.37170	-2.70710
C	-5.69130	3.89940	-1.12560
C	-4.79500	4.12570	0.09530
H	-3.73220	4.09110	-0.25140
H	-4.96760	5.16460	0.45740
C	-4.91780	3.18670	1.26570
C	-4.31990	3.57470	2.47210
C	-5.56230	1.93460	1.19500
C	-4.33790	2.73910	3.59500
H	-3.82720	4.54350	2.54950
C	-5.59480	1.08740	2.29290
H	-6.04660	1.61890	0.26720
C	-4.97750	1.50110	3.49220
H	-3.87190	3.06550	4.51760
H	-6.08170	0.11430	2.24770
H	-7.19290	4.14610	1.33840
H	-4.13690	6.34320	-1.20110
O	-3.31940	2.01290	-0.87710
O	-6.98240	1.39640	-5.00100
O	-5.08040	0.56090	4.49540
C	-4.51160	0.88630	5.78510
H	-3.43010	1.02200	5.70090
H	-5.00340	1.76720	6.20740
H	-4.75000	-0.01330	6.36810
C	-7.20690	0.29190	-5.82070
O	-6.60660	-0.74330	-5.71840
C	-8.28060	0.68330	-6.77410
H	-9.17690	0.05820	-6.62700
H	-8.58640	1.73650	-6.66180
H	-7.94910	0.53770	-7.81530

C	-2.79820	0.98820	-0.07440
O	-3.10100	-0.16390	-0.22640
C	-1.87080	1.62080	0.89770
H	-2.38400	1.77430	1.86710
H	-0.99660	0.97930	1.08510
H	-1.51640	2.60890	0.56520
C	-7.24790	3.59220	-3.25190
H	-7.88630	3.44670	-4.14550

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9_benzyl_triptycene_pm6/opt_c9_folded_opt_20.xyz

C	-7.69780	-0.69340	1.08130
C	-7.62020	-0.48370	-0.30890
C	-8.32470	0.54250	-0.94440
C	-9.21040	1.31050	-0.14450
C	-9.29350	1.09250	1.23120
C	-8.52820	0.10050	1.86220
C	-10.73680	1.49010	-2.00200
C	-9.83430	0.74970	-2.81740
C	-10.32930	-0.04970	-3.83580
C	-11.71900	-0.11120	-4.05080
C	-12.59540	0.61820	-3.25250
C	-12.10440	1.42930	-2.21330
H	-7.09090	-1.47600	1.54300
H	-8.58160	-0.04560	2.94520
H	-12.10560	-0.73920	-4.85160
H	-13.66850	0.56370	-3.42710
H	-12.79250	1.99430	-1.58920
C	-8.16070	2.47460	-2.48320
C	-7.25920	3.17450	-3.27350
C	-7.21560	4.57790	-3.19930
C	-8.07670	5.27420	-2.35470
C	-9.01760	4.58070	-1.57480
C	-9.05940	3.19700	-1.65190
H	-6.49710	5.11960	-3.81230
H	-8.02960	6.36020	-2.29960
H	-9.70050	5.12480	-0.92750
C	-8.35150	0.94730	-2.42990
C	-7.40370	0.16290	-3.34090
H	-7.59040	-0.92670	-3.17020
H	-7.69800	0.36360	-4.39610
C	-5.92130	0.38860	-3.20770
C	-5.09530	-0.12090	-4.22420
C	-5.32480	1.03530	-2.11420
C	-3.70680	-0.00510	-4.14020
H	-5.53650	-0.61200	-5.08940
C	-3.93840	1.14950	-2.02740
H	-5.94270	1.45620	-1.31850
C	-3.11460	0.62560	-3.03670
H	-3.08460	-0.40240	-4.93950
H	-3.49400	1.64530	-1.16490
H	-6.57860	2.65890	-3.95080
H	-9.66650	-0.63240	-4.47160
O	-6.89840	-1.37760	-1.10710
O	-10.23240	1.90940	1.87140
C	-10.26590	2.10870	3.25030
O	-9.51250	1.57130	4.01600
C	-11.37400	3.06680	3.51370
H	-11.94000	3.32320	2.60300
H	-12.08450	2.64920	4.24570
H	-10.98240	4.00590	3.93850
C	-5.61270	-1.80150	-0.74280
O	-5.10000	-1.48010	0.29500
C	-5.10620	-2.66360	-1.84030
H	-4.52930	-3.51230	-1.44360
H	-5.91240	-3.05610	-2.47950
H	-4.43130	-2.08180	-2.49880
C	-1.62990	0.74690	-2.92660

H	-1.09890	0.23480	-3.73850
H	-1.31650	1.80090	-2.95050
H	-1.26300	0.32230	-1.98080
C	-10.05050	2.31130	-0.91640
H	-10.75410	2.86880	-0.26730

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9_benzyl_triptycene_pm6/opt_c10_folded_opt_8.xyz

C	-0.85030	-5.61700	-2.19410
C	-1.68710	-6.53100	-1.52440
C	-3.05320	-6.62740	-1.80100
C	-3.59520	-5.68930	-2.71860
C	-2.76390	-4.78690	-3.38080
C	-1.38230	-4.74700	-3.13670
C	-5.63980	-5.61940	-1.44310
C	-5.11220	-6.58600	-0.54040
C	-5.50840	-6.57120	0.78780
C	-6.43290	-5.60220	1.22100
C	-6.94810	-4.66300	0.33230
C	-6.54960	-4.66580	-1.01680
H	0.22010	-5.60610	-1.97540
H	-0.74360	-4.03030	-3.65940
H	-6.74320	-5.59260	2.26450
H	-7.66280	-3.91790	0.67740
H	-6.95180	-3.92820	-1.70690
C	-4.91350	-8.15470	-2.38020
C	-5.20690	-9.49340	-2.60150
C	-5.95160	-9.86200	-3.73580
C	-6.41120	-8.89890	-4.63070
C	-6.15120	-7.53720	-4.40070
C	-5.41900	-7.17700	-3.27980
H	-6.16690	-10.91500	-3.91010
H	-6.98010	-9.19580	-5.50980
H	-6.52310	-6.78400	-5.09050
C	-4.11660	-7.56540	-1.20140
C	-3.58690	-8.61010	-0.21590
H	-2.97580	-8.07500	0.55380
H	-4.45760	-9.04010	0.32970
C	-2.74740	-9.74290	-0.74390
C	-2.51390	-10.82890	0.12070
C	-2.16340	-9.75190	-2.01890
C	-1.70380	-11.89200	-0.28210
H	-2.96860	-10.84610	1.10860
C	-1.35010	-10.81590	-2.41590
H	-2.34050	-8.92910	-2.71360
C	-1.11370	-11.88700	-1.54970
H	-1.53430	-12.72960	0.39260
H	-0.89540	-10.80430	-3.40650
H	-4.86950	-10.26980	-1.91540
H	-5.11880	-7.29160	1.50350
O	-1.17170	-7.30530	-0.47930
O	-3.42000	-3.98830	-4.32480
C	-2.94380	-2.73550	-4.71200
O	-1.92910	-2.25670	-4.28300
C	-3.91600	-2.19510	-5.70000
H	-4.37800	-1.26740	-5.32470
H	-3.41030	-1.94680	-6.64780
H	-4.72760	-2.90540	-5.92970
C	0.05190	-7.97750	-0.60970
O	0.74040	-7.87390	-1.58860
C	0.25970	-8.75660	0.63690
H	1.31990	-8.75630	0.93190
H	-0.33810	-8.37670	1.48030
H	-0.04120	-9.81100	0.48080
H	-0.47930	-12.71310	-1.86200
C	-5.10430	-5.74990	-2.86460
H	-5.49680	-4.98410	-3.56210

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9_benzyl_triptycene_pm6/opt_c12_folded_opt_7.xyz
C -3.23340 -3.60570 -0.16260
C -2.11290 -4.18260 0.46670
C -0.96820 -4.54870 -0.24540
C -1.01370 -4.41270 -1.65800
C -2.12370 -3.84040 -2.27770
C -3.24030 -3.41930 -1.53850
C 0.32380 -6.40400 -1.89490
C 0.40010 -6.52420 -0.47800
C 0.50320 -7.78030 0.09890
C 0.53690 -8.91840 -0.72880
C 0.46630 -8.79360 -2.11330
C 0.35730 -7.52400 -2.70920
H -4.09060 -3.29630 0.44010
H -4.10600 -2.97740 -2.03880
H 0.61800 -9.90430 -0.27390
H 0.49310 -9.68030 -2.74440
H 0.29910 -7.43140 -3.79100
C 1.49760 -4.36320 -0.38270
C 2.59700 -3.81890 0.26720
C 3.55830 -3.10810 -0.47270
C 3.42880 -2.95830 -1.85140
C 2.34050 -3.53550 -2.52720
C 1.39580 -4.23810 -1.79490
H 4.41130 -2.67220 0.04510
H 4.17460 -2.39900 -2.41350
H 2.24810 -3.43310 -3.60550
C 0.34960 -5.16620 0.25670
C 0.46080 -5.32070 1.77600
H -0.45070 -5.86470 2.13040
H 1.32250 -5.99370 1.98960
C 0.60100 -4.08180 2.61920
C 0.96490 -4.26090 3.96710
C 0.35340 -2.78390 2.14220
C 1.07050 -3.17200 4.83390
H 1.17040 -5.26140 4.34650
C 0.44950 -1.67910 2.98920
H 0.08120 -2.62360 1.09550
C 0.80610 -1.89940 4.32180
H 1.35790 -3.31400 5.87420
H 0.24590 -0.67560 2.61490
H 2.73330 -3.92890 1.34240
H 0.55670 -7.90620 1.17780
O -2.16780 -4.49670 1.82930
O -1.99210 -3.68320 -3.66200
C -3.09100 -3.64360 -4.52170
O -4.22680 -3.71580 -4.13780
C -2.55060 -3.49990 -5.90000
H -2.79980 -4.38330 -6.51050
H -2.99150 -2.62280 -6.40200
H -1.45450 -3.37990 -5.91650
C -2.67390 -3.58290 2.76500
O -3.11650 -2.51420 2.44260
C -2.54000 -4.20750 4.10540
H -2.39800 -5.29850 4.05440
H -1.66310 -3.79150 4.63650
H -3.42590 -4.00180 4.72650
F 0.89790 -0.85080 5.14320
C 0.19890 -4.96510 -2.38370
H 0.11650 -4.87260 -3.48450

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9_benzyl_triptycene_pm6/opt_c13_folded_opt_9.xyz
C 6.34740 -3.04380 0.75240
C 6.87680 -3.13160 2.05470
C 6.36420 -4.01640 3.00610
C 5.21070 -4.76050 2.64330

C	4.68930	-4.67230	1.35310
C	5.25730	-3.82360	0.38970
C	4.39300	-4.60130	4.90550
C	5.56420	-3.88360	5.28110
C	5.49630	-2.94320	6.29700
C	4.26790	-2.71770	6.94630
C	3.12770	-3.42570	6.57740
C	3.18440	-4.37920	5.54460
H	6.80650	-2.36730	0.02770
H	4.83490	-3.76050	-0.61690
H	4.21610	-1.97890	7.74450
H	2.18240	-3.24370	7.08630
H	2.29030	-4.92740	5.25740
C	6.90810	-5.79820	4.63820
C	7.97260	-6.50830	5.17650
C	7.89610	-7.90930	5.26800
C	6.75890	-8.59030	4.84040
C	5.65960	-7.88110	4.32760
C	5.73710	-6.49940	4.24150
H	8.73960	-8.46180	5.67960
H	6.71350	-9.67600	4.90830
H	4.76530	-8.41120	4.00950
C	6.81120	-4.27200	4.45670
C	8.06270	-3.50770	4.89610
H	7.89860	-2.42380	4.66590
H	8.13530	-3.57520	6.00610
C	9.38910	-3.89460	4.30320
C	10.54490	-3.36070	4.90800
C	9.52980	-4.71680	3.17450
C	11.80870	-3.63380	4.39170
H	10.45400	-2.73040	5.79180
C	10.79050	-4.99110	2.64650
H	8.64850	-5.15290	2.69600
C	11.93500	-4.44670	3.25190
H	12.69910	-3.22260	4.86910
H	10.88640	-5.62310	1.76100
H	8.87050	-6.00510	5.53200
H	6.37080	-2.37360	6.60270
O	7.88200	-2.24300	2.45460
O	3.61050	-5.52890	1.11060
C	2.64710	-5.26960	0.13310
O	2.68470	-4.30720	-0.58410
C	1.66200	-6.38160	0.19940
H	1.56450	-6.87470	-0.78220
H	1.94070	-7.15410	0.93540
H	0.66340	-6.00260	0.47290
C	8.99060	-1.98780	1.63370
O	9.12000	-2.49940	0.55530
C	9.86460	-1.03240	2.36040
H	10.26600	-0.26790	1.67580
H	9.34270	-0.51800	3.18280
H	10.72910	-1.56100	2.80250
C	13.23200	-4.72170	2.71370
N	14.28160	-4.94240	2.28110
C	4.61680	-5.58990	3.76650
H	3.70070	-6.13160	3.45860

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9_benzyl_triptycene_pm6/opt_c14_folded_opt_5.xyz

C	1.50990	-3.42510	-1.12330
C	2.86770	-3.14450	-1.37260
C	3.33160	-2.79380	-2.64250
C	2.39190	-2.82370	-3.70650
C	1.04830	-3.09960	-3.45610
C	0.58930	-3.39240	-2.16210
C	4.11060	-3.59310	-5.21130
C	5.06380	-3.53530	-4.15510
C	6.13230	-4.41810	-4.14650

C	6.26040	-5.35520	-5.18900
C	5.32760	-5.40350	-6.22100
C	4.23690	-4.51530	-6.23720
H	1.18460	-3.65690	-0.10630
H	-0.46620	-3.61320	-1.98120
H	7.10070	-6.04770	-5.18120
H	5.43630	-6.13200	-7.02290
H	3.50860	-4.55870	-7.04350
C	4.64830	-1.15380	-3.94940
C	5.41540	-0.00450	-3.81580
C	5.18330	1.08730	-4.67090
C	4.20470	1.02260	-5.65980
C	3.44600	-0.14790	-5.82980
C	3.67930	-1.22370	-4.98700
H	5.77980	1.99090	-4.55270
H	4.02770	1.87680	-6.31130
H	2.69370	-0.20450	-6.61270
C	4.75490	-2.44040	-3.11010
C	5.80870	-2.38140	-2.00160
H	5.75370	-3.34220	-1.42780
H	6.81430	-2.37160	-2.48200
C	5.74270	-1.26170	-1.00120
C	6.85850	-1.08460	-0.15790
C	4.63170	-0.42190	-0.83830
C	6.85330	-0.10280	0.82840
H	7.73690	-1.71740	-0.27760
C	4.61840	0.55950	0.15380
H	3.75930	-0.52800	-1.48920
C	5.72670	0.71930	0.99500
H	7.72870	0.02300	1.46920
H	3.73140	1.18860	0.26350
H	6.19700	0.07380	-3.06170
H	6.87360	-4.40480	-3.35100
O	3.80790	-3.31090	-0.34850
O	0.22320	-3.00390	-4.58160
C	-0.98250	-3.69990	-4.69310
O	-1.41040	-4.41160	-3.82570
C	-1.54660	-3.36510	-6.02780
H	-0.94570	-2.61440	-6.56770
H	-1.60740	-4.26460	-6.66240
H	-2.57030	-2.96700	-5.92950
C	3.56480	-2.81550	0.94220
O	2.54450	-2.25090	1.22800
C	4.75720	-3.13140	1.76790
H	4.45980	-3.50860	2.75980
H	5.41620	-3.87910	1.29920
H	5.36180	-2.22060	1.93540
C	5.74280	1.75280	2.08080
F	6.76980	2.61930	2.00780
F	5.85190	1.23960	3.32090
F	4.66800	2.55230	2.16760
C	2.98590	-2.57230	-5.07990
H	2.23100	-2.63240	-5.88880

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9_benzyl_triptycene_pm6/opt_c15_folded_opt_20.xyz

C	-1.90240	-8.33640	-2.20520
C	-2.93010	-7.43850	-2.54600
C	-3.74120	-6.83470	-1.57790
C	-3.51040	-7.19210	-0.22520
C	-2.48900	-8.08200	0.10920
C	-1.67300	-8.66070	-0.87350
C	-5.85960	-6.97860	0.25410
C	-6.09910	-6.60050	-1.09730
C	-7.31020	-6.92010	-1.69160
C	-8.28570	-7.60780	-0.94560
C	-8.04570	-7.97010	0.37680
C	-6.81910	-7.65560	0.98900

H	-1.29280	-8.79280	-2.99070
H	-0.86840	-9.34760	-0.59730
H	-9.23590	-7.85690	-1.41490
H	-8.80670	-8.50190	0.94510
H	-6.63250	-7.94440	2.02040
C	-4.65060	-4.67660	-0.78930
C	-4.68410	-3.32360	-1.09730
C	-4.41540	-2.37660	-0.09300
C	-4.13220	-2.77980	1.20950
C	-4.12850	-4.14490	1.54310
C	-4.39550	-5.07610	0.55130
H	-4.43040	-1.31740	-0.34480
H	-3.91860	-2.03890	1.97760
H	-3.92360	-4.45880	2.56330
C	-4.91380	-5.85070	-1.74940
C	-5.23010	-5.43700	-3.19040
H	-5.31900	-6.36940	-3.79910
H	-6.23990	-4.96660	-3.19380
C	-4.27930	-4.52090	-3.91410
C	-4.74170	-3.89860	-5.08180
C	-2.94960	-4.29830	-3.50240
C	-3.90720	-3.07550	-5.84660
H	-5.76810	-4.05360	-5.41270
C	-2.10150	-3.48550	-4.24180
H	-2.57480	-4.77150	-2.59180
C	-2.59260	-2.87900	-5.41620
H	-4.29010	-2.60510	-6.74490
H	-1.07340	-3.30550	-3.93470
H	-4.91320	-2.97640	-2.10460
H	-7.52330	-6.65190	-2.72380
O	-3.14000	-7.03390	-3.86500
O	-2.41400	-8.38150	1.47390
O	-1.64120	-2.11090	-6.05590
C	-2.04080	-1.40300	-7.25240
H	-2.83880	-0.69060	-7.02490
H	-1.11420	-0.88050	-7.52420
H	-2.33460	-2.11030	-8.03270
C	-1.24320	-8.82500	2.09000
O	-0.22010	-9.01610	1.49180
C	-1.56950	-8.97080	3.55220
H	-2.65510	-8.80020	3.73010
H	-1.03880	-8.16780	4.11100
C	-2.81140	-7.80340	-4.98160
O	-2.37370	-8.91890	-4.90390
C	-3.11240	-6.95300	-6.18610
H	-3.12950	-5.87180	-5.90420
H	-2.28210	-7.06850	-6.91630
C	-1.15060	-10.34590	4.05360
H	-1.72870	-11.14790	3.57570
H	-0.08760	-10.54460	3.85130
H	-1.30160	-10.43280	5.13680
C	-4.44250	-7.36040	-6.80530
H	-4.65430	-6.75970	-7.69910
H	-4.44540	-8.41630	-7.10900
H	-5.27680	-7.21240	-6.10720
C	-4.48150	-6.57770	0.76600
H	-4.28380	-6.89370	1.80920

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9_benzyl_triptycene_pm6/opt_c16_folded_opt_19.xyz

C	12.82910	-3.23700	3.94830
C	12.30000	-2.52970	2.85060
C	12.34600	-1.13530	2.77410
C	12.86630	-0.44290	3.89910
C	13.39130	-1.14610	4.98220
C	13.38880	-2.54920	5.01680
C	11.28460	1.33970	3.54380
C	10.78010	0.66420	2.39630

C	9.44780	0.81380	2.04440
C	8.61630	1.63830	2.82560
C	9.11730	2.29950	3.94330
C	10.46660	2.15120	4.31250
H	12.80550	-4.32920	3.94640
H	13.79610	-3.08550	5.87720
H	7.57030	1.75440	2.54710
H	8.46590	2.93500	4.54050
H	10.85350	2.66640	5.18820
C	12.97840	0.80890	1.37900
C	13.49660	1.14460	0.13570
C	14.54020	2.08290	0.04950
C	15.04940	2.69000	1.19490
C	14.51160	2.38480	2.45670
C	13.48060	1.46140	2.53780
H	14.95020	2.33220	-0.92780
H	15.86250	3.40930	1.11760
H	14.89840	2.86950	3.34930
C	11.84250	-0.19010	1.66800
C	11.27760	-0.87860	0.42280
H	10.51150	-1.61970	0.76190
H	10.72520	-0.11490	-0.17050
C	12.22510	-1.60280	-0.49580
C	11.73930	-1.98120	-1.75920
C	13.53750	-1.95420	-0.14450
C	12.53770	-2.71170	-2.64080
H	10.73050	-1.70480	-2.06000
C	14.33500	-2.68660	-1.02210
H	13.94730	-1.65680	0.82290
C	13.84140	-3.07840	-2.27700
H	12.14450	-2.99260	-3.61560
H	15.34720	-2.96000	-0.72620
H	13.11380	0.69320	-0.77940
H	9.03000	0.30580	1.17820
O	11.62130	-3.22350	1.84410
O	13.95290	-0.33830	5.97700
C	14.01710	-0.72490	7.31590
O	13.63360	-1.79290	7.70810
C	14.64600	0.42470	8.05710
H	14.94640	1.22990	7.34950
H	15.58640	0.06590	8.53130
C	12.14490	-4.40140	1.28940
O	13.15990	-4.90040	1.69190
C	11.21010	-4.81120	0.18830
H	10.25060	-4.25320	0.25920
H	11.66490	-4.49540	-0.78280
C	13.68190	0.96160	9.10660
H	12.77510	1.38100	8.65120
H	13.36350	0.17420	9.80560
H	14.15040	1.75710	9.69970
C	10.97310	-6.31370	0.21300
H	10.42780	-6.62680	1.11260
H	10.38640	-6.63320	-0.65690
H	11.92120	-6.87170	0.19580
C	14.70230	-3.87400	-3.20270
H	15.60400	-3.31220	-3.48690
H	15.03900	-4.80800	-2.72980
H	14.18840	-4.14900	-4.13210
C	12.75980	1.06850	3.81600
H	13.14770	1.57400	4.72220

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9_benzyl_triptycene_pm6/opt_c17_folded_opt_18.xyz

C	-5.45580	-4.21200	5.29280
C	-5.14500	-4.35050	3.92590
C	-6.12730	-4.59720	2.96330
C	-7.45220	-4.80420	3.42910
C	-7.75650	-4.66570	4.78300

C	-6.76640	-4.35650	5.72840
C	-7.81850	-6.42570	1.68350
C	-6.50110	-6.19760	1.19350
C	-5.81290	-7.22870	0.57340
C	-6.43260	-8.48460	0.43200
C	-7.72260	-8.69920	0.90870
C	-8.42850	-7.66150	1.54420
H	-4.66050	-3.97840	6.00460
H	-7.01840	-4.25410	6.78730
H	-5.89050	-9.29290	-0.05590
H	-8.19310	-9.67410	0.79390
H	-9.43450	-7.83420	1.91830
C	-7.08130	-3.87550	0.79610
C	-6.90920	-2.95220	-0.22620
C	-8.01640	-2.22510	-0.69780
C	-9.28540	-2.43140	-0.16230
C	-9.48020	-3.38750	0.84890
C	-8.38690	-4.10500	1.30950
H	-7.87200	-1.49340	-1.49110
H	-10.13430	-1.85750	-0.52920
H	-10.47300	-3.55980	1.25650
C	-5.99470	-4.75830	1.43790
C	-4.58860	-4.53460	0.87540
H	-3.88180	-5.17610	1.45910
H	-4.56930	-4.92770	-0.16660
C	-4.02490	-3.13860	0.86940
C	-2.87110	-2.91320	0.09540
C	-4.55990	-2.07890	1.61600
C	-2.26290	-1.65680	0.08220
H	-2.44890	-3.71900	-0.50080
C	-3.94510	-0.82480	1.60340
H	-5.46260	-2.22370	2.21220
C	-2.79350	-0.60930	0.84120
H	-1.37340	-1.49210	-0.52390
H	-4.36680	-0.01340	2.19670
H	-5.93110	-2.77430	-0.67220
H	-4.80280	-7.08880	0.19500
O	-3.80840	-4.33760	3.51570
O	-9.11500	-4.81340	5.08130
C	-9.58390	-5.16980	6.34650
O	-8.85980	-5.35700	7.28530
C	-11.08170	-5.26060	6.22670
H	-11.37630	-6.33010	6.31580
H	-11.41430	-4.93470	5.21530
C	-2.90910	-3.36900	3.98810
O	-3.22620	-2.54760	4.80390
C	-1.60880	-3.60780	3.27610
H	-1.60550	-4.60770	2.78910
H	-1.53530	-2.87030	2.43970
C	-11.75000	-4.42370	7.30880
H	-12.83940	-4.55310	7.28970
H	-11.40160	-4.70630	8.31330
H	-11.54420	-3.35260	7.18140
C	-0.43520	-3.46140	4.23290
H	0.51960	-3.52450	3.69660
H	-0.45830	-2.49270	4.75420
H	-0.43440	-4.24430	5.00210
H	-2.31680	0.36800	0.83490
C	-8.44350	-5.20720	2.35340
H	-9.45920	-5.39020	2.75580

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9_benzyl_triptycene_pm6/opt_c19_folded_opt_18.xyz

C	2.65240	12.58010	-0.55900
C	1.55150	11.79080	-0.94580
C	1.32010	10.52430	-0.40340
C	2.29980	10.01280	0.48780
C	3.38740	10.79730	0.87000

C	3.57070	12.09280	0.36130
C	1.92700	7.79140	-0.37050
C	0.92080	8.29550	-1.24290
C	0.70040	7.67820	-2.46420
C	1.47260	6.55610	-2.81890
C	2.45110	6.06520	-1.95930
C	2.68660	6.68690	-0.71950
H	2.77140	13.58140	-0.97960
H	4.43100	12.69460	0.66610
H	1.29770	6.07230	-3.77840
H	3.04240	5.19630	-2.24300
H	3.45430	6.30230	-0.05260
C	-0.33830	9.04570	0.69010
C	-1.65990	8.99930	1.11240
C	-1.95960	8.52960	2.40340
C	-0.94800	8.09540	3.25650
C	0.39050	8.10230	2.82880
C	0.68220	8.56320	1.55410
H	-2.99720	8.50830	2.73310
H	-1.19020	7.74140	4.25700
H	1.17860	7.74790	3.48840
C	0.17940	9.52760	-0.67790
C	-0.91520	10.03150	-1.62260
H	-0.41600	10.40930	-2.55010
H	-1.52550	9.15450	-1.93790
C	-1.84470	11.11200	-1.13930
C	-2.99780	11.35840	-1.90820
C	-1.59960	11.89620	0.00020
C	-3.88880	12.37540	-1.56190
H	-3.20570	10.74930	-2.78740
C	-2.47350	12.92070	0.36600
H	-0.71600	11.71110	0.61700
C	-3.60220	13.13900	-0.42770
H	-4.78170	12.56010	-2.15660
H	-2.27150	13.53240	1.24560
H	-2.47490	9.32040	0.46480
H	-0.05530	8.04330	-3.15600
O	0.70940	12.23270	-1.97100
O	4.22030	10.20060	1.82140
C	5.56590	10.54250	1.97440
O	6.10330	11.38990	1.31610
C	6.10270	9.64780	3.05890
H	6.76550	8.88670	2.58950
H	5.27660	9.07710	3.54010
C	0.23740	13.55440	-2.01000
O	0.55900	14.37000	-1.19070
C	-0.67480	13.64880	-3.19930
H	-0.53650	12.77290	-3.87070
H	-1.72770	13.58200	-2.83380
C	6.86570	10.46600	4.09140
H	6.20680	11.15960	4.63050
H	7.33870	9.81560	4.83780
H	7.66080	11.06690	3.62550
C	-0.44600	14.95270	-3.94940
H	-1.18260	15.07900	-4.75250
H	-0.53370	15.82310	-3.28180
H	0.55110	14.99260	-4.40640
F	-4.44390	14.11900	-0.09030
C	2.06580	8.57950	0.92720
H	2.86440	8.20240	1.59600

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9_benzyl_triptycene_pm6/opt_c20_folded_opt_10.xyz

C	-10.97510	-3.27270	4.86640
C	-10.79360	-4.42400	4.07510
C	-11.08120	-4.43680	2.70830
C	-11.66430	-3.26520	2.15790
C	-11.83970	-2.12610	2.94280

C	-11.48750	-2.11240	4.30180
C	-12.99170	-4.62090	0.67040
C	-12.38450	-5.79670	1.19650
C	-13.10280	-6.98150	1.23460
C	-14.42230	-7.00340	0.74480
C	-15.00840	-5.85180	0.22740
C	-14.29000	-4.64290	0.18830
H	-10.69930	-3.29650	5.92330
H	-11.63560	-1.21390	4.90700
H	-14.98520	-7.93500	0.77500
H	-16.02970	-5.87970	-0.14920
H	-14.75320	-3.74500	-0.21360
C	-10.22570	-4.98110	0.44840
C	-9.12380	-5.50650	-0.21280
C	-8.59780	-4.83160	-1.32850
C	-9.17910	-3.65200	-1.78720
C	-10.31690	-3.12880	-1.14990
C	-10.83490	-3.79830	-0.05190
H	-7.72560	-5.24210	-1.83520
H	-8.75890	-3.13320	-2.64720
H	-10.78070	-2.21690	-1.51800
C	-10.93490	-5.57320	1.68050
C	-10.29430	-6.85650	2.21560
H	-10.85520	-7.15830	3.13700
H	-10.47310	-7.66680	1.47170
C	-8.83250	-6.83970	2.56660
C	-8.07760	-5.66510	2.70910
C	-8.21160	-8.08330	2.79940
C	-6.73870	-5.72170	3.09280
H	-8.53400	-4.68940	2.51970
C	-6.87290	-8.15060	3.17680
H	-8.77940	-9.00530	2.67990
C	-6.13270	-6.96600	3.33250
H	-6.16510	-4.80000	3.21230
H	-6.39770	-9.11710	3.34980
H	-8.65390	-6.43340	0.11230
H	-12.67070	-7.89470	1.63670
O	-10.40570	-5.62390	4.68090
O	-12.33560	-1.02030	2.24690
C	-13.02390	0.02500	2.86860
O	-13.23090	0.05760	4.05020
C	-13.40440	0.98370	1.77310
H	-14.50660	0.93130	1.62750
H	-12.95280	0.67140	0.80440
C	-9.36030	-5.66160	5.61800
O	-8.76540	-4.67320	5.94730
C	-9.20140	-7.09830	6.02570
H	-10.09120	-7.69300	5.72270
H	-8.34420	-7.52810	5.45490
C	-4.76010	-7.03110	3.73160
N	-3.65090	-7.08660	4.05450
C	-8.95860	-7.20670	7.52390
H	-8.73220	-8.24080	7.81250
H	-8.10940	-6.58290	7.84190
H	-9.83270	-6.88590	8.10510
C	-12.97400	2.39830	2.13630
H	-11.88150	2.48930	2.19900
H	-13.32040	3.12000	1.38580
H	-13.38430	2.71050	3.10810
C	-12.08760	-3.39380	0.70650
H	-12.56750	-2.47360	0.31880

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9_benzyl_triptycene_pm6/opt_c21_folded_opt_12.xyz			
C	-5.79380	-6.95370	6.05000
C	-6.96660	-6.23960	5.73420
C	-7.64920	-6.43090	4.53070
C	-7.06150	-7.31260	3.58550

C	-5.90200	-8.01930	3.90190
C	-5.26090	-7.85700	5.14040
C	-7.85150	-5.92080	1.78340
C	-8.46790	-5.04880	2.72540
C	-8.58860	-3.69920	2.43350
C	-8.10440	-3.21390	1.20410
C	-7.50740	-4.07250	0.28550
C	-7.37540	-5.44310	0.57350
H	-5.31400	-6.80000	7.01940
H	-4.34900	-8.41360	5.37290
H	-8.20040	-2.15350	0.97620
H	-7.13660	-3.68690	-0.66280
H	-6.90520	-6.10970	-0.14540
C	-9.84650	-6.89440	3.48780
C	-11.18620	-7.09400	3.79160
C	-11.87090	-8.18350	3.22480
C	-11.22520	-9.05390	2.35010
C	-9.87960	-8.84220	2.00510
C	-9.20810	-7.76530	2.56340
H	-12.91840	-8.34220	3.47730
H	-11.76250	-9.89920	1.92330
H	-9.38010	-9.51200	1.30950
C	-8.93660	-5.76720	4.01010
C	-9.62050	-4.81260	4.99190
H	-8.85070	-4.07900	5.34490
H	-10.37210	-4.21550	4.42550
C	-10.28280	-5.38550	6.21330
C	-11.12080	-4.52760	6.95440
C	-10.08190	-6.69580	6.67050
C	-11.72630	-4.96740	8.12800
H	-11.30230	-3.51110	6.60800
C	-10.68070	-7.13960	7.85030
H	-9.44990	-7.38660	6.10540
C	-11.50000	-6.27520	8.58740
H	-12.37540	-4.28980	8.68690
H	-10.49230	-8.16230	8.18670
H	-11.72390	-6.42470	4.46150
H	-9.04730	-3.00550	3.13410
O	-7.41970	-5.23960	6.60150
O	-5.48660	-8.91530	2.91280
C	-4.15990	-9.33260	2.77440
O	-3.28310	-8.97120	3.50960
C	-4.13230	-10.24360	1.57720
H	-3.63520	-9.70590	0.73890
H	-5.16660	-10.46240	1.22770
C	-7.48350	-5.45510	7.98870
O	-7.14380	-6.49260	8.48610
C	-8.04000	-4.19920	8.59510
H	-8.01680	-3.36390	7.86120
H	-9.11930	-4.37210	8.82160
C	-12.14590	-6.71150	9.86800
F	-11.74970	-6.00900	10.94610
F	-11.94970	-7.98700	10.23750
F	-13.48560	-6.58540	9.88570
C	-3.39120	-11.53150	1.90830
H	-3.91870	-12.12230	2.66900
H	-3.28390	-12.16400	1.01800
H	-2.38080	-11.33040	2.29420
C	-7.27860	-3.83330	9.86090
H	-6.23690	-3.56050	9.64880
H	-7.74650	-2.98070	10.36880
H	-7.25820	-4.67000	10.57590
C	-7.77530	-7.37080	2.24780
H	-7.27450	-8.04570	1.52590

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9_benzyl_triptycene_pm6/opt_c22_folded_opt_6.xyz
C -12.86500 9.60880 -4.97720

C	-13.37190	8.60690	-4.12170
C	-14.24730	7.61750	-4.56590
C	-14.64490	7.68920	-5.93080
C	-14.13370	8.67250	-6.77730
C	-13.23100	9.64300	-6.31430
C	-16.82750	6.84600	-5.37080
C	-16.43270	6.75720	-4.00690
C	-17.37680	6.94960	-3.00950
C	-18.71350	7.20940	-3.36480
C	-19.09460	7.27920	-4.70200
C	-18.14350	7.09970	-5.72220
H	-12.17970	10.35110	-4.56790
H	-12.84630	10.41560	-6.98540
H	-19.45170	7.36130	-2.57900
H	-20.13150	7.47920	-4.96530
H	-18.44120	7.16420	-6.76540
C	-14.68510	5.18590	-4.65070
C	-14.18830	3.97020	-4.20030
C	-14.02870	2.90550	-5.10480
C	-14.37760	3.04980	-6.44520
C	-14.91270	4.26330	-6.90910
C	-15.07010	5.30990	-6.01340
H	-13.62750	1.95960	-4.74460
H	-14.24440	2.22140	-7.13820
H	-15.20060	4.37280	-7.95140
C	-14.92710	6.45680	-3.81360
C	-14.57810	6.29630	-2.33100
H	-14.74130	7.27630	-1.82590
H	-15.33790	5.61050	-1.88620
C	-13.21280	5.78810	-1.95650
C	-12.09060	5.89390	-2.78670
C	-13.06980	5.18910	-0.68700
C	-10.83830	5.42830	-2.37270
H	-12.18000	6.34600	-3.77640
C	-11.83800	4.71820	-0.25090
H	-13.93660	5.09120	-0.03320
C	-10.72540	4.84700	-1.10670
H	-9.98570	5.52310	-3.03620
H	-11.71380	4.25430	0.72410
H	-13.91640	3.81790	-3.15580
H	-17.10530	6.91570	-1.95620
O	-12.81380	8.65140	-2.83370
O	-14.58320	8.56890	-8.09530
O	-9.56500	4.34960	-0.54890
C	-8.35980	4.40260	-1.34770
H	-8.48120	3.81020	-2.25910
H	-8.09570	5.44060	-1.56850
H	-7.62360	3.94330	-0.67560
C	-14.50560	9.60190	-9.03050
O	-13.98440	10.65760	-8.80080
C	-15.19120	9.07040	-10.28460
H	-15.43460	7.98410	-10.13340
C	-13.45750	9.36640	-1.82510
O	-14.61610	9.67840	-1.91180
C	-12.48050	9.65020	-0.69070
H	-13.08920	10.06530	0.15750
C	-14.22870	9.21440	-11.46100
H	-13.91090	10.25720	-11.60360
H	-13.32250	8.61140	-11.32240
H	-14.69970	8.88800	-12.39640
C	-16.48740	9.85430	-10.48320
H	-17.01630	9.51640	-11.38300
H	-17.17220	9.73050	-9.63450
H	-16.30120	10.93100	-10.60190
C	-11.49010	10.71370	-1.16770
H	-10.78880	10.98160	-0.36810
H	-10.89340	10.35190	-2.01670
H	-11.99670	11.63440	-1.48130

C	-11.78320	8.37500	-0.23290
H	-12.49090	7.64460	0.17890
H	-11.26460	7.87570	-1.06770
H	-11.03540	8.58080	0.54060
C	-15.67740	6.65940	-6.35140
H	-15.97540	6.76250	-7.41360

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9_benzyl_triptycene_pm6/opt_c23_folded_opt_20.xyz

C	12.02330	-8.55760	-9.26860
C	12.03960	-7.47890	-8.36510
C	12.86290	-6.36890	-8.55160
C	13.65100	-6.32630	-9.73050
C	13.62150	-7.39040	-10.63370
C	12.81770	-8.51950	-10.40820
C	15.33170	-5.00130	-8.62440
C	14.57080	-5.06060	-7.42470
C	15.22650	-5.08050	-6.20200
C	16.63030	-5.00530	-6.16940
C	17.36680	-4.92250	-7.34870
C	16.71560	-4.92610	-8.59430
H	11.39280	-9.42290	-9.06130
H	12.81770	-9.35560	-11.11460
H	17.14040	-5.01360	-5.20760
H	18.45280	-4.86090	-7.31170
H	17.29240	-4.87640	-9.51410
C	12.70260	-3.95610	-8.59030
C	11.71270	-3.00420	-8.39350
C	11.52540	-1.99530	-9.35500
C	12.31440	-1.95010	-10.50190
C	13.30520	-2.92270	-10.72280
C	13.48830	-3.91780	-9.77520
H	10.75310	-1.24500	-9.19470
H	12.16370	-1.16260	-11.23800
H	13.91000	-2.89270	-11.62540
C	13.05050	-5.12640	-7.65540
C	12.21870	-5.20440	-6.37480
H	11.14570	-5.31150	-6.66990
H	12.47300	-6.16750	-5.87180
C	12.32230	-4.10000	-5.36010
C	11.64050	-4.28970	-4.14290
C	13.04310	-2.91470	-5.54990
C	11.66970	-3.31560	-3.14870
H	11.08560	-5.21800	-3.97380
C	13.07470	-1.93530	-4.55410
H	13.59540	-2.74520	-6.47630
C	12.38790	-2.12390	-3.34740
H	11.13610	-3.47740	-2.21470
H	13.64080	-1.02110	-4.72330
H	11.08320	-3.02310	-7.50410
H	14.67360	-5.14900	-5.26550
O	11.12370	-7.45940	-7.30470
O	14.44190	-7.19470	-11.74620
C	14.69520	-8.15770	-12.72230
O	14.20270	-9.25140	-12.71430
C	15.66720	-7.50300	-13.69870
H	15.83930	-6.43890	-13.38290
C	11.02960	-8.51960	-6.39840
O	11.75980	-9.46940	-6.44490
C	9.88350	-8.17030	-5.45570
H	9.32890	-7.28590	-5.87130
C	15.03710	-7.52220	-15.08960
H	14.79780	-8.54460	-15.41560
H	14.10710	-6.94080	-15.12370
H	15.71840	-7.09510	-15.83570
C	16.98850	-8.26710	-13.63880
H	17.43790	-8.22530	-12.63840
H	16.86040	-9.32750	-13.89810

H	17.71710	-7.84720	-14.34320
C	10.46320	-7.80300	-4.09130
H	10.97240	-6.82360	-4.11240
H	9.67180	-7.73660	-3.33380
H	11.18560	-8.54930	-3.73370
C	8.94090	-9.37060	-5.38930
H	9.45790	-10.27520	-5.03790
H	8.10940	-9.18150	-4.69950
H	8.50590	-9.60220	-6.36960
C	12.41570	-1.08230	-2.27630
H	12.88940	-1.46610	-1.36150
H	12.97190	-0.18410	-2.57380
H	11.40070	-0.75770	-2.00750
C	14.48410	-5.06300	-9.88540
H	15.07390	-5.05390	-10.82280

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9_benzyl_triptycene_pm6/opt_c24_folded_opt_6.xyz

C	-3.07400	3.41960	-9.94790
C	-3.93730	3.68990	-11.02770
C	-4.33780	4.98400	-11.35090
C	-3.80210	6.04660	-10.57510
C	-2.93930	5.77760	-9.51170
C	-2.56990	4.46290	-9.18250
C	-5.76670	7.38970	-10.95530
C	-6.32950	6.32710	-11.71300
C	-7.70340	6.13120	-11.69850
C	-8.51790	7.00840	-10.96090
C	-7.96010	8.06170	-10.24000
C	-6.56820	8.25670	-10.22880
H	-2.80600	2.38710	-9.72550
H	-1.90090	4.26460	-8.33930
H	-9.59570	6.85460	-10.95560
H	-8.60040	8.73650	-9.67500
H	-6.13350	9.07030	-9.65410
C	-4.41990	6.45930	-13.26640
C	-4.10790	6.37970	-14.61590
C	-3.29760	7.37160	-15.19640
C	-2.79820	8.42160	-14.42970
C	-3.08620	8.49850	-13.05590
C	-3.88410	7.51960	-12.48440
H	-3.06200	7.31140	-16.25760
H	-2.17590	9.18670	-14.89010
H	-2.68310	9.31080	-12.45660
C	-5.28840	5.47690	-12.46280
C	-5.88640	4.32670	-13.27200
H	-5.03860	3.69710	-13.63970
H	-6.45030	3.67570	-12.56130
C	-6.79290	4.63200	-14.43220
C	-7.26450	3.53160	-15.17380
C	-7.19410	5.92210	-14.80250
C	-8.11520	3.72200	-16.26190
H	-6.96100	2.51850	-14.89270
C	-8.04710	6.10910	-15.89430
H	-6.84520	6.79240	-14.24410
C	-8.51000	5.01380	-16.62720
H	-8.47380	2.86400	-16.82790
H	-8.35080	7.11770	-16.17160
H	-4.48430	5.56530	-15.23430
H	-8.16260	5.31110	-12.25020
O	-4.27210	2.59240	-11.84030
O	-2.49910	6.92580	-8.85230
C	-1.70880	6.92750	-7.70260
O	-1.30220	5.92720	-7.18040
C	-1.52590	8.39670	-7.33610
H	-2.01410	9.03200	-8.12340
C	-5.27110	1.70930	-11.43110
O	-5.98910	1.95320	-10.49880

C	-5.26480	0.47710	-12.32810
H	-6.23160	-0.06230	-12.13360
C	-0.02980	8.69990	-7.29720
H	0.49890	8.05770	-6.57830
H	0.44160	8.55300	-8.27710
H	0.15270	9.73950	-6.99820
C	-2.21310	8.64070	-5.99400
H	-2.08840	9.68220	-5.67270
H	-3.29110	8.44090	-6.04610
H	-1.79830	8.00450	-5.19930
C	-4.09680	-0.41290	-11.90100
H	-3.13170	0.09300	-12.04430
H	-4.16800	-0.70270	-10.84530
H	-4.07020	-1.33690	-12.49170
C	-5.18980	0.85610	-13.80350
H	-6.06370	1.44860	-14.12510
H	-4.29040	1.45190	-14.01990
H	-5.14980	-0.03630	-14.43940
H	-9.17360	5.16300	-17.47540
C	-4.24810	7.43470	-11.00960
H	-3.80160	8.23840	-10.39200

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9_benzyl_triptycene_pm6/opt_c26_folded_opt_10.xyz

C	6.86490	11.86860	-5.92050
C	6.79350	10.84560	-4.95510
C	7.65640	10.80150	-3.85620
C	8.68050	11.78200	-3.79700
C	8.74590	12.79600	-4.75200
C	7.83450	12.85750	-5.81760
C	10.17980	10.16530	-2.82520
C	9.14560	9.18670	-2.85440
C	9.47240	7.84920	-3.01300
C	10.82500	7.47940	-3.13550
C	11.83120	8.44040	-3.10100
C	11.51080	9.80140	-2.94560
H	6.14650	11.88590	-6.74380
H	7.90410	13.65350	-6.56330
H	11.07950	6.42810	-3.25940
H	12.87440	8.14390	-3.19600
H	12.29950	10.54940	-2.92260
C	7.81320	10.59300	-1.39400
C	7.04250	10.41720	-0.25290
C	7.25050	11.25050	0.86050
C	8.23190	12.23830	0.83820
C	9.04480	12.40270	-0.29600
C	8.83880	11.57760	-1.39100
H	6.63270	11.11580	1.74710
H	8.37900	12.88340	1.70250
H	9.82240	13.16230	-0.30790
C	7.72900	9.78510	-2.70240
C	6.63950	8.70830	-2.71050
H	6.61870	8.25130	-3.73170
H	6.95840	7.89520	-2.01890
C	5.23070	9.10750	-2.36120
C	4.33370	8.07700	-2.02220
C	4.77350	10.43540	-2.38270
C	3.00380	8.35710	-1.70480
H	4.67590	7.04280	-2.00020
C	3.44710	10.74140	-2.07500
H	5.45770	11.24920	-2.63680
C	2.59010	9.69120	-1.73770
H	2.31530	7.55800	-1.43620
H	3.09760	11.77360	-2.09910
H	6.27580	9.64530	-0.19780
H	8.70570	7.07850	-3.04700
O	5.90610	9.78020	-5.12250
O	9.74560	13.74430	-4.51960

C	10.33940	14.48900	-5.54070
O	10.01380	14.39230	-6.69130
C	11.39180	15.35780	-4.86140
H	11.33470	15.19710	-3.75110
C	4.60010	9.96450	-5.59910
O	4.17480	11.04660	-5.89290
C	3.96490	8.58130	-5.64620
H	4.45480	7.93590	-4.86830
C	11.08430	16.82020	-5.17620
H	11.07100	17.01140	-6.25870
H	10.10930	17.12640	-4.77660
H	11.84030	17.48390	-4.73880
C	12.76670	14.92280	-5.36520
H	13.55980	15.53620	-4.92000
H	12.98050	13.87640	-5.11400
H	12.85310	15.02390	-6.45650
C	4.22260	7.98700	-7.03070
H	5.29690	7.91390	-7.24510
H	3.80310	6.97620	-7.10600
H	3.76340	8.58630	-7.82790
C	2.47800	8.71140	-5.33050
H	1.97270	7.74110	-5.39580
H	2.31090	9.10050	-4.31660
H	1.97030	9.39670	-6.02380
F	1.31950	9.97190	-1.43630
C	9.66990	11.59280	-2.66250
H	10.47190	12.35720	-2.66390

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9_benzyl_triptycene_pm6/opt_c27_folded_opt_11.xyz

C	-0.72090	8.46670	-5.68230
C	0.27400	9.25680	-6.28600
C	-0.02690	10.20760	-7.26790
C	-1.37620	10.29620	-7.69390
C	-2.35960	9.50500	-7.09950
C	-2.04600	8.59190	-6.08160
C	-0.63950	10.81160	-9.93090
C	0.71630	10.75750	-9.49930
C	1.70270	10.35630	-10.38670
C	1.34650	10.01370	-11.70470
C	0.01960	10.07220	-12.12120
C	-0.99000	10.47390	-11.22780
H	-0.44780	7.74060	-4.91050
H	-2.83070	7.99450	-5.60970
H	2.12260	9.69960	-12.40080
H	-0.24530	9.80500	-13.14290
H	-2.02620	10.51370	-11.55560
C	0.26490	12.56860	-7.94670
C	0.88310	13.75070	-7.56280
C	0.14410	14.94700	-7.54840
C	-1.19540	14.96190	-7.92940
C	-1.82450	13.77870	-8.35250
C	-1.09250	12.60130	-8.36760
H	0.63180	15.86890	-7.23490
H	-1.76010	15.89250	-7.90800
H	-2.86540	13.79320	-8.66590
C	0.90710	11.17040	-8.02300
C	2.37850	11.13860	-7.60060
H	2.73530	10.07270	-7.65430
H	2.96570	11.69530	-8.36680
C	2.75390	11.65640	-6.23900
C	1.82600	11.91680	-5.21810
C	4.12530	11.85670	-5.98390
C	2.25230	12.35270	-3.96500
H	0.75770	11.77300	-5.39760
C	4.56060	12.29290	-4.73500
H	4.85780	11.67010	-6.76780
C	3.62280	12.53860	-3.71790

H	1.52310	12.54790	-3.17680
H	5.62360	12.44530	-4.54530
H	1.93180	13.77570	-7.27060
H	2.74650	10.29950	-10.08830
O	1.61100	9.17810	-5.89840
O	-3.63440	9.65570	-7.65150
C	-4.80620	9.42630	-6.92580
O	-4.80170	9.04330	-5.78920
C	-5.95240	9.75990	-7.87340
H	-5.52890	10.01050	-8.88310
C	2.21130	8.02180	-5.38790
O	1.60370	7.01000	-5.17920
C	3.68340	8.37670	-5.21480
H	3.74980	9.44380	-4.86280
C	-6.68930	10.97750	-7.31830
H	-6.03490	11.85570	-7.25340
H	-7.53860	11.24740	-7.95820
H	-7.08950	10.78980	-6.31180
C	-6.85120	8.53120	-7.99350
H	-7.71680	8.73830	-8.63480
H	-6.31780	7.67690	-8.42920
H	-7.24030	8.21200	-7.01590
C	4.35720	8.26080	-6.58280
H	4.34040	7.23250	-6.96590
H	3.85340	8.90570	-7.32470
H	5.40760	8.57060	-6.52960
C	4.30500	7.45840	-4.16880
H	5.38140	7.64360	-4.06990
H	3.85430	7.60620	-3.17870
H	4.17500	6.39720	-4.42460
C	4.06580	12.97960	-2.43080
N	4.42560	13.33460	-1.39040
C	-1.61270	11.25620	-8.84500
H	-2.67050	11.27450	-9.17450

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9_benzyl_triptycene_pm6/opt_c28_folded_opt_6.xyz

C	-10.19290	1.68230	-0.13030
C	-10.05540	1.70170	-1.53200
C	-10.25760	2.86470	-2.28000
C	-10.69910	4.01750	-1.58010
C	-10.83030	3.99630	-0.19200
C	-10.56970	2.83300	0.54940
C	-12.04280	4.66270	-3.47290
C	-11.58160	3.52250	-4.19050
C	-12.40750	2.92250	-5.12800
C	-13.68910	3.45640	-5.36010
C	-14.13170	4.57440	-4.65910
C	-13.30370	5.18850	-3.70180
H	-9.99040	0.76010	0.42000
H	-10.68510	2.82920	1.63640
H	-14.33640	2.98400	-6.09720
H	-15.12450	4.98000	-4.84670
H	-13.65440	6.05960	-3.15390
C	-9.31270	4.36320	-4.01010
C	-8.22440	4.51670	-4.85800
C	-7.56650	5.75770	-4.92500
C	-8.00490	6.83880	-4.16430
C	-9.12900	6.70860	-3.33120
C	-9.77690	5.48450	-3.26950
H	-6.70480	5.86710	-5.58190
H	-7.48300	7.79270	-4.21720
H	-9.48220	7.55720	-2.75050
C	-10.15130	3.08890	-3.79910
C	-9.67050	1.87790	-4.60350
H	-10.29720	0.99840	-4.30540
H	-9.90380	2.06430	-5.67730
C	-8.22960	1.46520	-4.48950

C	-7.72320	0.60100	-5.48090
C	-7.38160	1.87130	-3.44880
C	-6.40250	0.16350	-5.43360
H	-8.36420	0.27500	-6.29880
C	-6.05960	1.42920	-3.39200
H	-7.74810	2.54770	-2.67180
C	-5.56360	0.57360	-4.38440
H	-6.02530	-0.49730	-6.21700
H	-5.42630	1.76050	-2.56530
H	-7.86460	3.69690	-5.47770
H	-12.08820	2.04620	-5.68740
O	-9.79890	0.51820	-2.22910
O	-11.18690	5.22330	0.37220
C	-11.86660	5.33380	1.58790
O	-12.16450	4.38270	2.25520
C	-12.09380	6.82600	1.80020
H	-11.59500	7.39220	0.96800
C	-8.89220	-0.44220	-1.75330
O	-8.28310	-0.29020	-0.73190
C	-8.90840	-1.58280	-2.76170
H	-9.19700	-1.17090	-3.76560
C	-11.46130	7.22450	3.13170
H	-11.63420	8.28620	3.34700
H	-11.87900	6.65060	3.97120
H	-10.37580	7.06320	3.13170
C	-13.59810	7.08900	1.75990
H	-14.13330	6.52250	2.53520
H	-13.81520	8.15110	1.92830
H	-14.03440	6.81410	0.79150
C	-9.95850	-2.59860	-2.31260
H	-10.95720	-2.14710	-2.24920
H	-10.02010	-3.43500	-3.02000
H	-9.72300	-3.02680	-1.32920
C	-7.50860	-2.18350	-2.84500
H	-6.77000	-1.44790	-3.19050
H	-7.16040	-2.55030	-1.86900
H	-7.47970	-3.02860	-3.54240
C	-4.14410	0.09250	-4.36370
F	-3.41100	0.42880	-3.29020
F	-3.40040	0.52450	-5.39850
F	-4.01240	-1.24660	-4.42020
C	-11.03460	5.20310	-2.46520
H	-11.40160	6.07540	-1.88890

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9_benzyl_triptycene_pm6/opt_c29_folded_opt_20.xyz

C	4.57290	-3.91320	-0.31130
C	3.29360	-3.52100	-0.74790
C	2.22260	-4.41620	-0.81380
C	2.49890	-5.77810	-0.52550
C	3.76930	-6.16450	-0.09800
C	4.81560	-5.23840	0.02830
C	0.89690	-6.45480	-2.19640
C	0.59140	-5.08940	-2.46130
C	0.19000	-4.71060	-3.73270
C	0.08590	-5.68640	-4.74180
C	0.38280	-7.02000	-4.47550
C	0.79470	-7.41490	-3.18960
H	5.36800	-3.16840	-0.23260
H	5.80630	-5.55470	0.36650
H	-0.23040	-5.38730	-5.73980
H	0.29890	-7.76680	-5.26310
H	1.02760	-8.45740	-2.98670
C	-0.12830	-4.83300	-0.16060
C	-1.20190	-4.25240	0.50110
C	-1.91520	-5.00110	1.45360
C	-1.56550	-6.32080	1.73000
C	-0.50110	-6.93050	1.04450

C	0.19820	-6.19070	0.10320
H	-2.74980	-4.53730	1.97710
H	-2.12030	-6.88930	2.47420
H	-0.23830	-7.96540	1.24930
C	0.76090	-4.17210	-1.23020
C	0.40130	-2.71480	-1.53130
H	1.10320	-2.34950	-2.32090
H	-0.61400	-2.69810	-1.98860
C	0.43100	-1.71740	-0.40330
C	0.88690	-2.00740	0.88800
C	0.00380	-0.40490	-0.69810
C	0.94400	-1.01770	1.87390
H	1.21540	-3.01720	1.14590
C	0.05030	0.59620	0.26240
H	-0.36720	-0.16800	-1.69530
C	0.52990	0.27740	1.54980
H	1.31150	-1.26910	2.86400
H	-0.27550	1.61150	0.04910
H	-1.50170	-3.22390	0.29980
H	-0.04500	-3.67490	-3.96820
O	3.09050	-2.21980	-1.22200
O	3.87390	-7.52620	0.21470
O	0.53550	1.36210	2.40050
C	1.06930	1.16700	3.73220
H	2.11710	0.85580	3.68020
H	0.97840	2.17350	4.16030
H	0.45690	0.44860	4.28430
C	5.07360	-8.20510	0.31740
O	6.15400	-7.70580	0.17030
C	3.56060	-1.10350	-0.54280
O	4.23910	-1.16290	0.44410
H	4.78490	-9.23420	0.55240
H	3.18140	-0.25080	-1.11160
C	1.33190	-6.71990	-0.75910
H	1.58920	-7.77850	-0.55860

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9_benzyl_triptycene_pm6/opt_c30_folded_opt_13.xyz

C	-1.80200	-1.18450	-1.85800
C	-0.55710	-1.41790	-1.24440
C	0.65280	-1.19390	-1.90680
C	0.58340	-0.82030	-3.27410
C	-0.65230	-0.59450	-3.88060
C	-1.85640	-0.75910	-3.17960
C	2.58450	-2.08980	-3.72140
C	2.67660	-2.43650	-2.34330
C	3.24640	-3.64570	-1.97690
C	3.73020	-4.51050	-2.97670
C	3.64030	-4.16410	-4.32180
C	3.06070	-2.94080	-4.70500
H	-2.72150	-1.32960	-1.28620
H	-2.81800	-0.57710	-3.66740
H	4.17790	-5.45980	-2.68720
H	4.01810	-4.83990	-5.08720
H	2.99090	-2.67520	-5.75710
C	2.86170	-0.08320	-1.79190
C	3.65350	0.69890	-0.96180
C	4.28950	1.83860	-1.48440
C	4.14460	2.18330	-2.82620
C	3.37130	1.38310	-3.68420
C	2.74830	0.25770	-3.16680
H	4.90060	2.45440	-0.82630
H	4.63570	3.07190	-3.21870
H	3.27020	1.64440	-4.73460
C	2.09630	-1.36040	-1.39910
C	2.22950	-1.74310	0.07670
H	1.65010	-2.68620	0.23500
H	3.29530	-2.00060	0.27210

C	1.78080	-0.75730	1.12350
C	1.98060	-1.11420	2.46880
C	1.15220	0.46350	0.83640
C	1.55350	-0.27730	3.49990
H	2.47450	-2.05240	2.71500
C	0.72510	1.30150	1.86590
H	0.98450	0.76960	-0.19790
C	0.91760	0.93860	3.20810
H	1.71870	-0.57070	4.53460
H	0.23240	2.24210	1.62230
H	3.78810	0.45000	0.09080
H	3.32650	-3.94180	-0.93340
O	-0.50510	-1.97750	0.03720
O	-0.56380	-0.16360	-5.21100
C	-1.60800	-0.23130	-6.11400
O	-2.70390	-0.64620	-5.85860
C	-1.30870	-1.52680	1.07660
O	-2.16790	-0.70140	0.94370
H	-1.19070	0.16710	-7.04390
H	-0.97290	-2.08980	1.95110
C	0.44490	1.84010	4.30100
H	-0.64160	2.00140	4.24050
H	0.65710	1.44410	5.30190
H	0.92280	2.82820	4.23730
C	1.92830	-0.73630	-3.97230
H	1.83810	-0.47570	-5.04510

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9_benzyl_triptycene_pm6/opt_c31_folded_opt_8.xyz

C	-2.09610	-2.51150	-0.73490
C	-1.38360	-1.61170	0.07960
C	-0.97270	-0.35760	-0.37960
C	-1.20780	-0.05910	-1.74690
C	-1.91090	-0.95480	-2.55260
C	-2.37480	-2.18210	-2.05570
C	0.86620	1.16830	-1.83410
C	1.08680	0.90080	-0.45290
C	2.38270	0.79090	0.02600
C	3.46190	0.95090	-0.86350
C	3.23960	1.21550	-2.21180
C	1.92820	1.32580	-2.70920
H	-2.43640	-3.46300	-0.31970
H	-2.92590	-2.87440	-2.69840
H	4.47940	0.86460	-0.48570
H	4.08140	1.33790	-2.89130
H	1.75930	1.53070	-3.76360
C	-0.96710	2.07570	0.07450
C	-1.37860	3.01820	1.00720
C	-2.05210	4.17350	0.57340
C	-2.29860	4.38860	-0.78060
C	-1.85970	3.45800	-1.73760
C	-1.19250	2.32140	-1.30700
H	-2.38220	4.90410	1.31020
H	-2.82730	5.28310	-1.10490
H	-2.03930	3.63340	-2.79540
C	-0.21850	0.76100	0.36120
C	0.04250	0.49840	1.84610
H	0.59560	-0.47030	1.92690
H	0.74200	1.28180	2.21790
C	-1.13150	0.42650	2.78710
C	-0.84410	0.27300	4.15680
C	-2.47100	0.47090	2.37530
C	-1.87740	0.16260	5.08810
H	0.18890	0.24360	4.49630
C	-3.50220	0.35860	3.31160
H	-2.72290	0.59050	1.32050
C	-3.21110	0.20130	4.66900
H	-1.64350	0.04770	6.14550

H	-4.53870	0.38890	2.97580
H	-1.19470	2.87880	2.07230
H	2.58440	0.58200	1.07420
O	-0.98450	-1.99890	1.36400
O	-2.12890	-0.49610	-3.85840
C	-2.46140	-1.31810	-4.91890
O	-2.61600	-2.50470	-4.83850
C	-1.84540	-2.64040	2.24580
O	-2.95450	-2.99050	1.95590
H	-2.53870	-0.64080	-5.77490
H	-1.27540	-2.73050	3.17380
H	-4.01620	0.11170	5.39470
C	-0.60770	1.25350	-2.21620
H	-0.77940	1.44150	-3.29430

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9_benzyl_triptycene_pm6/opt_c33_folded_opt_19.xyz

C	-2.89790	-1.73400	0.62360
C	-1.93960	-2.72360	0.33500
C	-1.33460	-2.82960	-0.92000
C	-1.80360	-1.96250	-1.94080
C	-2.75640	-0.98510	-1.65270
C	-3.30370	-0.84930	-0.36790
C	-1.47920	-3.70960	-3.57100
C	-0.97430	-4.56960	-2.55440
C	-1.15590	-5.93940	-2.66170
C	-1.83420	-6.45880	-3.78050
C	-2.32200	-5.61320	-4.77270
C	-2.14640	-4.22110	-4.67190
H	-3.31220	-1.65990	1.63190
H	-4.04920	-0.07770	-0.15520
H	-1.97570	-7.53520	-3.86370
H	-2.84490	-6.02540	-5.63420
H	-2.53110	-3.56420	-5.44840
C	0.81350	-2.98490	-2.14180
C	2.18670	-3.04460	-1.94580
C	3.03100	-2.21300	-2.70210
C	2.50680	-1.34230	-3.65460
C	1.12180	-1.29660	-3.88700
C	0.29190	-2.12030	-3.14180
H	4.10650	-2.25540	-2.53580
H	3.16930	-0.69730	-4.22950
H	0.71440	-0.62860	-4.64200
C	-0.25930	-3.81460	-1.41240
C	0.29700	-4.75880	-0.34360
H	-0.56850	-5.29930	0.11470
H	0.90740	-5.53710	-0.85660
C	1.11470	-4.17780	0.77950
C	1.71500	-5.08930	1.66930
C	1.27920	-2.80010	0.99540
C	2.46300	-4.64320	2.75920
H	1.59960	-6.16100	1.50930
C	2.02200	-2.32820	2.07910
H	0.82350	-2.07550	0.31560
C	2.59930	-3.26420	2.94000
H	2.92840	-5.35120	3.44300
H	2.13970	-1.25720	2.24480
H	2.62620	-3.72230	-1.21460
H	-0.78740	-6.62230	-1.89970
O	-1.63480	-3.69950	1.29140
O	-3.07040	-0.15780	-2.73820
C	-4.21470	0.61570	-2.81240
O	-5.05110	0.67630	-1.95540
C	-1.41560	-3.38550	2.62710
O	-1.52600	-2.27990	3.07610
H	-4.14500	1.11220	-3.78500
H	-1.14850	-4.33590	3.09540
F	3.31080	-2.82520	3.98080

C	-1.21380	-2.23020	-3.31320
H	-1.62470	-1.56020	-4.09400

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9_benzyl_triptycene_pm6/opt_c34_folded_opt_17.xyz

C	1.56780	-6.10540	2.92260
C	1.74090	-5.18130	1.87510
C	0.75270	-4.95240	0.91460
C	-0.40460	-5.77240	0.96690
C	-0.57200	-6.69010	2.00400
C	0.40250	-6.85780	2.99990
C	-0.51590	-5.76420	-1.44240
C	0.62320	-4.91130	-1.49640
C	1.48590	-4.98540	-2.57850
C	1.21730	-5.90300	-3.61150
C	0.10040	-6.73180	-3.55470
C	-0.77990	-6.66690	-2.45920
H	2.34910	-6.22050	3.67770
H	0.25830	-7.58040	3.80860
H	1.89560	-5.96040	-4.46150
H	-0.09820	-7.43800	-4.35940
H	-1.65010	-7.31790	-2.41840
C	-0.60660	-3.23750	-0.24510
C	-0.80790	-1.86620	-0.32610
C	-2.11690	-1.35500	-0.28580
C	-3.21240	-2.20890	-0.18070
C	-3.02440	-3.60050	-0.13210
C	-1.73240	-4.10190	-0.17540
H	-2.26890	-0.27770	-0.33830
H	-4.22170	-1.80170	-0.14290
H	-3.88080	-4.26750	-0.06650
C	0.74470	-3.97530	-0.27430
C	1.96090	-3.05040	-0.36130
H	2.87630	-3.69460	-0.38020
H	1.93300	-2.53400	-1.34880
C	2.15880	-2.01560	0.71240
C	3.22710	-1.11230	0.54180
C	1.36880	-1.92400	1.86860
C	3.50040	-0.14340	1.50340
H	3.84630	-1.16560	-0.35300
C	1.63660	-0.95910	2.83900
H	0.53290	-2.61130	2.02360
C	2.70550	-0.06620	2.66030
H	4.32640	0.55520	1.36210
H	1.01940	-0.90230	3.73810
H	0.02790	-1.17420	-0.41910
H	2.36710	-4.35180	-2.64710
O	2.97020	-4.52870	1.71800
O	-1.79170	-7.37620	1.96710
C	-2.02950	-8.56300	2.63840
O	-1.22800	-9.12230	3.33250
C	3.65670	-3.97340	2.79160
O	3.27660	-4.03630	3.92620
H	-3.06140	-8.81920	2.37980
H	4.54390	-3.51610	2.34720
C	2.98560	0.92600	3.65280
N	3.21280	1.72950	4.45290
C	-1.36650	-5.57660	-0.19050
H	-2.24120	-6.25460	-0.13950

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9_benzyl_triptycene_pm6/opt_c36_folded_opt_16.xyz

C	-4.78150	-3.15910	-2.22270
C	-5.29780	-2.36640	-1.18080
C	-5.03260	-1.00020	-1.06940
C	-4.11340	-0.44720	-2.00140
C	-3.60480	-1.23560	-3.03130
C	-3.93680	-2.59100	-3.16840

C	-3.26600	1.02310	-0.29090
C	-4.21070	0.49590	0.63460
C	-3.89690	0.44960	1.98390
C	-2.64750	0.93170	2.41700
C	-1.73010	1.45010	1.50740
C	-2.03670	1.49820	0.13540
H	-5.05150	-4.21600	-2.28930
H	-3.52580	-3.19270	-3.98300
H	-2.40240	0.89560	3.47770
H	-0.76670	1.82190	1.85370
H	-1.31640	1.90390	-0.57150
C	-6.00660	1.25960	-0.80750
C	-7.21730	1.92040	-0.64810
C	-7.50310	3.04300	-1.44450
C	-6.58070	3.50790	-2.37920
C	-5.33810	2.86890	-2.52700
C	-5.05860	1.76360	-1.73800
H	-8.45980	3.54990	-1.32420
H	-6.81560	4.37410	-2.99600
H	-4.61160	3.24200	-3.24530
C	-5.52350	0.02280	-0.02780
C	-6.53440	-0.51440	0.98750
H	-6.08420	-1.41050	1.48120
H	-6.64900	0.24910	1.79140
C	-7.90740	-0.90100	0.50400
C	-8.85910	-1.23720	1.47920
C	-8.26890	-0.97420	-0.85430
C	-10.14240	-1.66050	1.12550
H	-8.59980	-1.17950	2.53700
C	-9.53830	-1.39090	-1.23320
H	-7.55190	-0.70100	-1.63150
C	-10.46960	-1.73620	-0.23290
H	-10.85630	-1.92320	1.89940
H	-9.82700	-1.45810	-2.28070
H	-7.95540	1.58410	0.08050
H	-4.59490	0.04800	2.71560
O	-6.02090	-2.97570	-0.13620
O	-2.78740	-0.52790	-3.93630
O	-11.68230	-2.13750	-0.74760
C	-12.70590	-2.55570	0.18680
H	-12.99210	-1.72260	0.83470
H	-13.52720	-2.82860	-0.48900
H	-12.36660	-3.42320	0.76020
C	-1.76890	-1.15890	-4.62130
O	-1.50320	-2.32620	-4.57200
C	-7.03690	-3.87100	-0.42860
O	-7.33280	-4.25240	-1.52490
C	-1.10440	-0.11960	-5.40730
C	-7.62910	-4.25930	0.85020
N	-0.56330	0.68110	-6.03350
N	-8.11790	-4.57540	1.84390
C	-3.74440	1.00100	-1.73870
H	-3.00140	1.39450	-2.46080

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9_benzyl_triptycene_pm6/opt_c37_folded_opt_8.xyz

C	-0.63700	2.91390	-1.60800
C	-1.33380	3.02000	-2.82610
C	-1.37850	4.20060	-3.56980
C	-0.77790	5.34910	-2.98670
C	-0.09010	5.23980	-1.78010
C	0.00470	4.02800	-1.08100
C	-2.50110	6.73470	-3.94620
C	-3.08300	5.59020	-4.56120
C	-4.45150	5.54860	-4.77710
C	-5.24330	6.64540	-4.38840
C	-4.66730	7.76370	-3.79220
C	-3.28000	7.81460	-3.56470

H	-0.59720	1.95570	-1.08430
H	0.54860	3.96380	-0.13510
H	-6.31860	6.61200	-4.55940
H	-5.28920	8.60770	-3.49700
H	-2.83460	8.69060	-3.09840
C	-1.01920	5.23590	-5.78800
C	-0.66000	4.93140	-7.09410
C	0.30560	5.71710	-7.74740
C	0.89460	6.80370	-7.10490
C	0.51740	7.14180	-5.79430
C	-0.43750	6.36670	-5.15430
H	0.59160	5.46700	-8.76830
H	1.64620	7.40150	-7.61820
H	0.96600	7.99970	-5.29850
C	-2.05490	4.49540	-4.92170
C	-2.69710	3.28790	-5.60680
H	-3.42200	2.82850	-4.89040
H	-3.31100	3.66300	-6.45820
C	-1.80400	2.18740	-6.11690
C	-2.41070	1.16710	-6.87210
C	-0.43030	2.10480	-5.85290
C	-1.66560	0.08310	-7.33210
H	-3.47550	1.21450	-7.09670
C	0.31760	1.01980	-6.31320
H	0.07400	2.88920	-5.28710
C	-0.29260	-0.00510	-7.05040
H	-2.15430	-0.70070	-7.90890
H	1.38300	0.97180	-6.09150
H	-1.10830	4.09080	-7.62440
H	-4.92750	4.68630	-5.23970
O	-2.11800	1.93810	-3.27270
O	0.53890	6.43510	-1.37540
C	0.74100	6.71760	-0.03970
O	0.47050	6.00100	0.88160
C	-1.58520	0.65930	-3.29410
O	-0.49800	0.35310	-2.89490
C	1.34990	8.04680	0.00590
C	-2.61560	-0.21010	-3.85850
N	1.82790	9.09260	0.06780
N	-3.40950	-0.91420	-4.30600
C	0.50880	-1.16630	-7.53940
H	-0.10190	-2.06890	-7.67540
H	0.97300	-0.93910	-8.51060
H	1.31950	-1.43150	-6.84680
C	-0.99030	6.63460	-3.76450
H	-0.54060	7.51780	-3.26870

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9_benzyl_triptycene_pm6/opt_c38_folded_opt_16.xyz

C	-3.58240	-3.67010	-2.52890
C	-4.05560	-2.40130	-2.14620
C	-3.33360	-1.22750	-2.36940
C	-2.02560	-1.37120	-2.90600
C	-1.56070	-2.62930	-3.28290
C	-2.32880	-3.79060	-3.11590
C	-1.27490	0.48660	-1.56670
C	-2.59310	0.65530	-1.05600
C	-2.77440	1.15530	0.22390
C	-1.64770	1.49430	0.99640
C	-0.36150	1.33150	0.48930
C	-0.16610	0.82110	-0.80690
H	-4.20370	-4.55490	-2.36940
H	-1.94490	-4.76870	-3.41720
H	-1.79130	1.88790	2.00190
H	0.50330	1.59860	1.09510
H	0.84090	0.69550	-1.19860
C	-3.38530	1.05900	-3.31420
C	-4.22720	1.96760	-3.94150

C	-3.78190	2.64450	-5.09040
C	-2.50320	2.42460	-5.59730
C	-1.62980	1.53140	-4.95400
C	-2.07110	0.86810	-3.81930
H	-4.45050	3.34820	-5.58480
H	-2.17100	2.94960	-6.49160
H	-0.62590	1.37170	-5.34090
C	-3.69690	0.23490	-2.05120
C	-5.10470	0.45000	-1.49330
H	-5.22130	-0.19650	-0.58840
H	-5.17040	1.49950	-1.12270
C	-6.28670	0.19130	-2.39070
C	-7.55530	0.54610	-1.89440
C	-6.19420	-0.40660	-3.65480
C	-8.70380	0.29380	-2.64520
H	-7.64780	1.01530	-0.91650
C	-7.34780	-0.65670	-4.40380
H	-5.22400	-0.67680	-4.07200
C	-8.60490	-0.31330	-3.90170
H	-9.68110	0.56700	-2.24820
H	-7.26130	-1.12680	-5.38330
H	-5.23060	2.16550	-3.56440
H	-3.76840	1.29100	0.64520
O	-5.24950	-2.30020	-1.40480
O	-0.28970	-2.60500	-3.89240
C	0.56580	-3.68450	-3.80200
O	0.32630	-4.73110	-3.27010
C	-6.38390	-2.97740	-1.82240
O	-6.44310	-3.72190	-2.75900
C	1.79530	-3.28590	-4.48660
C	-7.44680	-2.62100	-0.88470
N	2.77440	-2.99460	-5.01810
N	-8.30180	-2.34960	-0.16250
H	-9.50150	-0.51420	-4.48400
C	-1.23070	-0.08090	-2.98150
H	-0.20390	-0.22920	-3.37140

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9_benzyl_triptycene_pm6/opt_c40_folded_opt_4.xyz

C	-3.35940	-1.56710	0.30640
C	-3.69090	-1.84540	1.64510
C	-5.00450	-2.05530	2.06920
C	-6.02930	-1.85900	1.10510
C	-5.69760	-1.57280	-0.21770
C	-4.36750	-1.44060	-0.64180
C	-7.45800	-0.95240	2.82310
C	-6.44690	-1.19060	3.79670
C	-6.34910	-0.36070	4.90250
C	-7.25840	0.70400	5.04600
C	-8.24680	0.92970	4.09210
C	-8.35260	0.09560	2.96430
H	-2.31180	-1.45830	0.01430
H	-4.12660	-1.24380	-1.68990
H	-7.18170	1.35520	5.91590
H	-8.94560	1.75650	4.21330
H	-9.12560	0.27720	2.22040
C	-6.55160	-3.55980	3.28380
C	-6.59040	-4.74610	4.00410
C	-7.58010	-5.70100	3.71260
C	-8.53020	-5.46380	2.72190
C	-8.52300	-4.25330	2.00850
C	-7.54660	-3.31310	2.29990
H	-7.59880	-6.63520	4.27310
H	-9.28900	-6.21320	2.50050
H	-9.27670	-4.06080	1.24840
C	-5.55070	-2.40360	3.46640
C	-4.48620	-2.66050	4.53520
H	-3.81700	-1.76550	4.57870

H	-4.99820	-2.70120	5.52500
C	-3.61140	-3.87920	4.40370
C	-2.75260	-4.16730	5.48250
C	-3.58750	-4.70460	3.26930
C	-1.87480	-5.24930	5.43210
H	-2.76350	-3.53570	6.37150
C	-2.71760	-5.79470	3.19430
H	-4.25450	-4.50910	2.42680
C	-1.87660	-6.04270	4.28070
H	-1.20720	-5.46460	6.26610
H	-2.69980	-6.42850	2.30760
H	-5.86740	-4.95600	4.79220
H	-5.58480	-0.51310	5.66170
O	-2.69020	-1.80500	2.63560
O	-6.81580	-1.35400	-1.04740
C	-6.76690	-1.62990	-2.39960
O	-5.80680	-2.01070	-3.00620
C	-1.48040	-2.44980	2.43200
O	-1.15910	-3.02380	1.43150
C	-8.10680	-1.35440	-2.91690
C	-0.70570	-2.26240	3.65700
N	-9.15440	-1.14660	-3.34740
N	-0.08170	-2.13250	4.61610
F	-1.03880	-7.07940	4.21900
C	-7.43920	-1.93940	1.66030
H	-8.21590	-1.73860	0.89520

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9_benzyl_triptycene_pm6/opt_c41_folded_opt_11.xyz

C	0.32610	4.03180	1.24990
C	0.40480	3.06320	2.26700
C	1.48700	2.97720	3.14490
C	2.58000	3.85180	2.90340
C	2.50290	4.80390	1.88820
C	1.37710	4.92120	1.06060
C	4.10960	2.12810	3.61070
C	3.01330	1.26410	3.89060
C	3.16880	-0.10700	3.76030
C	4.41490	-0.62260	3.35710
C	5.48420	0.22740	3.08850
C	5.33580	1.62060	3.21380
H	-0.56240	4.08750	0.61560
H	1.32310	5.69080	0.28520
H	4.53680	-1.70050	3.25580
H	6.44460	-0.18250	2.77800
H	6.17380	2.28120	3.00060
C	2.19810	2.87300	5.51440
C	1.70050	2.83290	6.81010
C	2.24240	3.68700	7.78650
C	3.28190	4.55980	7.47290
C	3.81820	4.58550	6.17450
C	3.28270	3.74040	5.21460
H	1.84070	3.65970	8.79890
H	3.68990	5.22160	8.23590
H	4.64310	5.25310	5.93540
C	1.73530	2.01550	4.32200
C	0.57660	1.06980	4.64350
H	0.32050	0.50660	3.71070
H	0.94950	0.30180	5.36170
C	-0.69980	1.65000	5.18900
C	-1.68510	0.73900	5.61830
C	-0.96790	3.02530	5.25750
C	-2.91270	1.19080	6.09500
H	-1.49320	-0.33340	5.57450
C	-2.19430	3.48790	5.73430
H	-0.21570	3.75310	4.94510
C	-3.17260	2.57140	6.15070
H	-3.67290	0.47790	6.42020

H	-2.39380	4.56060	5.77920
H	0.89660	2.15310	7.08990
H	2.34990	-0.79420	3.96150
O	-0.58180	2.06050	2.35330
O	3.68090	5.56200	1.74030
C	3.65850	6.83130	1.19590
O	2.69550	7.39350	0.75870
C	-1.92460	2.39880	2.28710
O	-2.35440	3.50310	2.11620
C	5.03470	7.32120	1.26220
C	-2.66970	1.15290	2.45430
N	6.11040	7.72990	1.30550
N	-3.27610	0.18380	2.59300
C	-4.43390	3.04160	6.63730
N	-5.45220	3.42120	7.03250
C	3.78860	3.60850	3.78810
H	4.63900	4.27890	3.55020

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9_benzyl_triptycene_pm6/opt_c42_folded_opt_5.xyz

C	-6.93260	2.25490	-4.21760
C	-6.79270	0.95250	-3.70370
C	-6.91120	-0.18900	-4.49870
C	-7.29310	0.00890	-5.85290
C	-7.43040	1.30030	-6.35820
C	-7.24110	2.43770	-5.56000
C	-8.57820	-2.02870	-5.78820
C	-8.16940	-2.24770	-4.44220
C	-9.01150	-2.91850	-3.56920
C	-10.25830	-3.37830	-4.03310
C	-10.65010	-3.16540	-5.35180
C	-9.80480	-2.48210	-6.24480
H	-6.79300	3.11890	-3.56270
H	-7.35500	3.44310	-5.97450
H	-10.91940	-3.90620	-3.34660
H	-11.61660	-3.52720	-5.70070
H	-10.11580	-2.31800	-7.27440
C	-5.86090	-2.32240	-5.18730
C	-4.75270	-3.12590	-4.95510
C	-4.02970	-3.63960	-6.04590
C	-4.42120	-3.36440	-7.35410
C	-5.56110	-2.58140	-7.60290
C	-6.27370	-2.07920	-6.52480
H	-3.15400	-4.26030	-5.85840
H	-3.84930	-3.76170	-8.19180
H	-5.87650	-2.38120	-8.62480
C	-6.77020	-1.67650	-4.12570
C	-6.33740	-1.94590	-2.68350
H	-7.06230	-1.43160	-2.00270
H	-6.46460	-3.03620	-2.48370
C	-4.95210	-1.54360	-2.25790
C	-4.53950	-1.93080	-0.96770
C	-4.07830	-0.78440	-3.04850
C	-3.29070	-1.55650	-0.47960
H	-5.20170	-2.52450	-0.33710
C	-2.82390	-0.40760	-2.56470
H	-4.36410	-0.48290	-4.05870
C	-2.42740	-0.78720	-1.27710
H	-2.99200	-1.86010	0.52710
H	-2.16780	0.18840	-3.20390
H	-4.42740	-3.36850	-3.94410
H	-8.73180	-3.09730	-2.53320
O	-6.63810	0.76370	-2.31590
O	-7.71440	1.34100	-7.73750
C	-8.42680	2.38790	-8.29040
O	-8.82100	3.35620	-7.70570
C	-5.72640	1.53190	-1.60680
O	-5.04770	2.40330	-2.06860

C	-8.58370	2.06560	-9.70790
C	-5.78650	1.06530	-0.22360
N	-8.72250	1.83260	-10.82710
N	-5.81300	0.70690	0.87050
C	-1.09280	-0.38760	-0.72040
F	-1.16620	0.40650	0.36270
F	-0.33440	-1.41940	-0.30770
F	-0.27690	0.28560	-1.54780
C	-7.55540	-1.26960	-6.62680
H	-7.88280	-1.08310	-7.66930

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9_benzyl_triptycene_pm6/opt_c43_folded_opt_17.xyz

C	-2.12360	2.65180	3.35990
C	-2.99000	3.21100	4.31900
C	-2.65120	3.32360	5.66760
C	-1.41260	2.74790	6.06530
C	-0.55840	2.19890	5.11230
C	-0.88870	2.15050	3.75060
C	-2.38650	2.09640	8.16980
C	-3.61730	2.70120	7.78900
C	-4.81190	2.18220	8.26330
C	-4.78550	1.06720	9.12160
C	-3.57770	0.48410	9.49480
C	-2.35990	0.99940	9.01540
H	-2.42300	2.61770	2.30990
H	-0.20550	1.71330	3.01770
H	-5.72500	0.66080	9.49430
H	-3.56900	-0.37740	10.16110
H	-1.41840	0.54000	9.30840
C	-2.47910	4.83960	7.61590
C	-2.72110	6.14810	8.01200
C	-1.72720	6.85500	8.71130
C	-0.51040	6.25360	9.02440
C	-0.26540	4.91890	8.65980
C	-1.24920	4.22430	7.97290
H	-1.91860	7.88520	9.00910
H	0.25490	6.81280	9.56040
H	0.67800	4.44340	8.91860
C	-3.44310	3.91520	6.84950
C	-4.77830	4.56450	6.48140
H	-5.37840	3.81620	5.91030
H	-5.34190	4.74240	7.42700
C	-4.76300	5.84800	5.69470
C	-3.62810	6.36260	5.06070
C	-5.98480	6.54850	5.58590
C	-3.69120	7.53950	4.30690
H	-2.66570	5.85450	5.14740
C	-6.07320	7.72140	4.85150
H	-6.87610	6.16230	6.08130
C	-4.91470	8.20670	4.20690
H	-2.79670	7.91000	3.81650
H	-7.00770	8.27030	4.75580
H	-3.66710	6.64280	7.78960
H	-5.77010	2.61710	7.98560
O	-4.29770	3.56620	3.91700
O	0.66930	1.75260	5.64610
O	-5.14410	9.36960	3.50510
C	-4.04150	9.92740	2.75040
H	-3.70000	9.21540	1.99310
H	-4.51020	10.80330	2.28330
H	-3.23400	10.22670	3.42430
C	1.41650	0.78500	5.02900
O	1.19040	0.23030	3.99730
C	2.62810	0.58520	5.97790
C	-4.47090	4.34230	2.79490
O	-3.61410	4.80760	2.10590
C	-6.00300	4.44280	2.59030

F	2.70820	-0.65650	6.46350
F	2.59810	1.38730	7.04440
F	3.80040	0.81830	5.38310
F	-6.43710	5.69550	2.44540
F	-6.72080	3.92030	3.58600
F	-6.40460	3.79610	1.48940
C	-1.15900	2.76490	7.56120
H	-0.20240	2.28120	7.84310

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9_benzyl_triptycene_pm6/opt_c44_folded_opt_13.xyz

C	-5.34520	1.30270	-0.04230
C	-4.59510	1.70050	1.08100
C	-3.76770	2.82380	1.07580
C	-3.62800	3.50950	-0.16250
C	-4.36620	3.10660	-1.27280
C	-5.24340	2.01400	-1.23100
C	-1.32380	3.98310	0.35820
C	-1.47110	3.33060	1.61450
C	-0.38230	2.69180	2.18720
C	0.85480	2.70510	1.51620
C	0.99280	3.34860	0.28940
C	-0.10650	3.99630	-0.30280
H	-6.01020	0.43860	0.02490
H	-5.83210	1.72590	-2.10630
H	1.70980	2.20350	1.96760
H	1.95490	3.35320	-0.22090
H	0.00440	4.49570	-1.26300
C	-3.18580	4.94090	2.21800
C	-3.50420	5.70980	3.32940
C	-3.73320	7.08830	3.17500
C	-3.62950	7.69310	1.92440
C	-3.27540	6.93290	0.79710
C	-3.04820	5.57420	0.95370
H	-3.99440	7.68420	4.04860
H	-3.81540	8.76050	1.81550
H	-3.17680	7.40830	-0.17610
C	-2.89910	3.42810	2.19570
C	-3.02320	2.74470	3.55800
H	-2.81600	1.65660	3.41700
H	-2.19910	3.12370	4.20640
C	-4.31690	2.87610	4.31720
C	-4.32720	2.43640	5.65280
C	-5.50080	3.38500	3.76540
C	-5.49490	2.49360	6.41260
H	-3.41770	2.04190	6.10360
C	-6.67140	3.43870	4.52250
H	-5.52060	3.75320	2.73920
C	-6.68190	2.99030	5.85190
H	-5.48380	2.14570	7.44400
H	-7.58350	3.82890	4.07280
H	-3.58500	5.26650	4.32230
H	-0.46320	2.17900	3.14350
O	-4.59290	0.86360	2.22000
O	-4.08810	3.85830	-2.43470
C	-4.97520	3.94020	-3.47430
O	-6.03170	3.39680	-3.58300
C	-4.28410	4.89600	-4.48290
C	-5.78860	0.41550	2.73150
O	-6.88340	0.68740	2.34170
C	-5.41190	-0.55370	3.88000
F	-4.98660	6.00900	-4.70930
F	-4.09180	4.33860	-5.68100
F	-3.07990	5.30640	-4.07870
F	-6.04170	-0.28990	5.02580
F	-4.11100	-0.57200	4.17460
F	-5.72380	-1.82200	3.58660
C	-7.94480	3.03680	6.64740

H	-7.79970	2.74090	7.69420
H	-8.37970	4.04620	6.65490
H	-8.70210	2.36010	6.22360
C	-2.60600	4.63120	-0.15200
H	-2.49230	5.12180	-1.13940

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9_benzyl_triptycene_pm6/opt_c45_folded_opt_2.xyz

C	-1.91820	-7.14410	0.00530
C	-2.55230	-5.89640	0.16230
C	-2.35650	-4.83440	-0.72080
C	-1.39280	-5.02710	-1.74920
C	-0.76960	-6.26330	-1.90040
C	-1.02670	-7.34100	-1.04130
C	-0.74340	-2.71350	-1.57990
C	-1.72980	-2.50880	-0.57450
C	-1.51530	-1.56060	0.41360
C	-0.32490	-0.80980	0.40040
C	0.63310	-1.01110	-0.58940
C	0.42790	-1.97410	-1.59390
H	-2.13250	-7.95590	0.70420
H	-0.52650	-8.30370	-1.17590
H	-0.15780	-0.06440	1.17700
H	1.55000	-0.42330	-0.59100
H	1.17970	-2.12910	-2.36470
C	-3.44590	-3.14940	-2.16930
C	-4.69350	-2.67820	-2.55550
C	-4.96760	-2.48280	-3.92050
C	-3.99850	-2.74190	-4.88700
C	-2.72080	-3.18670	-4.50770
C	-2.45340	-3.37510	-3.16050
H	-5.95220	-2.12450	-4.21830
H	-4.22440	-2.59420	-5.94200
H	-1.95870	-3.37380	-5.26100
C	-2.96740	-3.42030	-0.73090
C	-4.02430	-3.15930	0.34260
H	-3.57600	-3.40790	1.33500
H	-4.21830	-2.06140	0.37120
C	-5.34940	-3.86790	0.24210
C	-6.37410	-3.43580	1.10480
C	-5.60270	-4.93030	-0.63580
C	-7.62180	-4.05990	1.08800
H	-6.19660	-2.61170	1.79310
C	-6.85300	-5.55540	-0.64620
H	-4.83410	-5.27440	-1.32790
C	-7.86510	-5.12560	0.21480
H	-8.40760	-3.71830	1.76060
H	-7.03370	-6.38470	-1.32980
H	-5.47000	-2.45900	-1.82240
H	-2.24630	-1.38460	1.20030
O	-3.32590	-5.67520	1.32430
O	0.09130	-6.32880	-3.01670
C	1.13730	-7.21130	-3.06990
O	1.44310	-8.03520	-2.26310
C	1.82540	-6.89600	-4.42460
C	-4.26970	-6.60500	1.69510
O	-4.56390	-7.60190	1.10880
C	-4.82810	-6.10910	3.05240
F	1.21770	-5.92440	-5.10900
F	1.86540	-7.94700	-5.24680
F	3.09240	-6.49800	-4.28260
F	-4.39370	-4.89970	3.41090
F	-4.48590	-6.91940	4.06120
F	-6.15990	-6.04260	3.08650
H	-8.83630	-5.61550	0.20710
C	-1.11000	-3.79560	-2.58930
H	-0.33270	-3.96760	-3.36050

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9_benzyl_triptycene_pm6/opt_c47_folded_opt_7.xyz

C	-4.03200	-2.68010	-0.17660
C	-3.02120	-3.50950	0.34550
C	-2.25050	-4.35380	-0.45430
C	-2.59770	-4.42270	-1.83170
C	-3.60410	-3.60570	-2.34200
C	-4.32450	-2.71470	-1.53400
C	-2.03430	-6.76500	-1.85800
C	-1.65180	-6.69060	-0.48910
C	-1.79760	-7.80280	0.32530
C	-2.31630	-8.99190	-0.22030
C	-2.68360	-9.05940	-1.56150
C	-2.54490	-7.93520	-2.39540
H	-4.58120	-2.00670	0.48590
H	-5.09610	-2.06430	-1.95560
H	-2.42940	-9.86570	0.42020
H	-3.08280	-9.98530	-1.97360
H	-2.83620	-7.99080	-3.44230
C	0.04040	-5.05290	-1.08190
C	1.37770	-4.83060	-0.78200
C	2.29530	-4.61690	-1.82550
C	1.88190	-4.64270	-3.15550
C	0.53850	-4.90260	-3.47460
C	-0.36310	-5.11450	-2.44280
H	3.34100	-4.43020	-1.58340
H	2.60030	-4.46930	-3.95550
H	0.21940	-4.94220	-4.51370
C	-1.10010	-5.30720	-0.07890
C	-0.66930	-5.26210	1.38810
H	-1.57680	-5.42840	2.01780
H	-0.01150	-6.14310	1.57620
C	0.03360	-4.03240	1.89810
C	0.63710	-4.12090	3.16770
C	0.09880	-2.82260	1.19060
C	1.29260	-3.02550	3.72870
H	0.59320	-5.05550	3.72730
C	0.74450	-1.70910	1.73280
H	-0.34790	-2.73650	0.19800
C	1.32950	-1.83630	2.99390
H	1.75750	-3.09690	4.71120
H	0.78480	-0.76990	1.18110
H	1.73490	-4.81660	0.24760
H	-1.52150	-7.77700	1.37750
O	-2.85630	-3.57330	1.74790
O	-3.85890	-3.81930	-3.71300
C	-4.45910	-2.86930	-4.49650
O	-4.87180	-1.80020	-4.16590
C	-4.48490	-3.51130	-5.90910
C	-2.77830	-2.40680	2.47390
O	-2.78520	-1.29390	2.04420
C	-2.71890	-2.84740	3.95790
F	-3.78030	-2.81880	-6.80760
F	-5.71730	-3.61140	-6.41290
F	-3.98330	-4.74810	-5.93350
F	-3.80630	-2.47060	4.63950
F	-1.68370	-2.33020	4.62180
F	-2.63610	-4.16830	4.12850
F	1.95110	-0.77990	3.52160
C	-1.83000	-5.46350	-2.62540
H	-2.14780	-5.51960	-3.68600

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9_benzyl_triptycene_pm6/opt_c48_folded_opt_9.xyz

C	3.36350	3.47300	-1.02780
C	4.68780	3.50600	-0.55560
C	5.35830	2.36830	-0.10990
C	4.64720	1.13770	-0.14920

C	3.33760	1.10920	-0.62390
C	2.67730	2.26510	-1.06580
C	5.87260	0.31130	1.75160
C	6.57330	1.54580	1.81830
C	6.96490	2.04260	3.05380
C	6.69640	1.29550	4.21410
C	6.03430	0.07220	4.13670
C	5.60890	-0.42820	2.89420
H	2.87940	4.38950	-1.37450
H	1.64490	2.22300	-1.42520
H	7.01250	1.68380	5.18190
H	5.83720	-0.50110	5.04180
H	5.08000	-1.37720	2.83770
C	7.41740	1.15030	-0.46960
C	8.55500	1.29740	-1.25080
C	8.99810	0.21670	-2.03340
C	8.30280	-0.99050	-2.03990
C	7.13570	-1.14300	-1.27190
C	6.69960	-0.07580	-0.50180
H	9.89600	0.33170	-2.63980
H	8.65800	-1.82270	-2.64660
H	6.58620	-2.08200	-1.28990
C	6.78950	2.21330	0.44850
C	7.55350	3.53710	0.50520
H	7.57290	3.97020	-0.52240
H	6.94670	4.25590	1.11000
C	8.95920	3.53940	1.04120
C	9.61650	4.78420	1.10310
C	9.63670	2.38960	1.47230
C	10.92070	4.87750	1.58200
H	9.10460	5.68890	0.77600
C	10.94340	2.47270	1.95360
H	9.14940	1.41170	1.43850
C	11.59000	3.71730	2.00930
H	11.42260	5.84520	1.62660
H	11.46100	1.57140	2.28610
H	9.11490	2.23190	-1.26520
H	7.48020	2.99860	3.14250
O	5.36960	4.74100	-0.43800
O	2.78340	-0.18640	-0.66710
C	1.42880	-0.39650	-0.64850
O	0.56220	0.42290	-0.63300
C	1.28960	-1.94170	-0.65920
C	5.26350	5.68510	-1.43060
O	4.65100	5.60000	-2.44990
C	6.11000	6.88300	-0.92770
F	2.46440	-2.57410	-0.69910
F	0.59850	-2.39520	-1.70740
F	0.66270	-2.41330	0.42160
F	7.33870	6.91100	-1.45310
F	6.28560	6.88880	0.39550
F	5.56320	8.06350	-1.22370
C	12.93120	3.80640	2.50170
N	14.01480	3.87800	2.89930
C	5.43610	-0.06550	0.34470
H	4.85880	-1.01050	0.29340

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9_benzyl_triptycene_pm6/opt_c49_folded_opt_16.xyz

C	-4.29750	-1.02800	-2.28560
C	-3.23780	-0.26900	-1.75500
C	-2.22590	0.27000	-2.55050
C	-2.25210	-0.06320	-3.93210
C	-3.30230	-0.81860	-4.45280
C	-4.34330	-1.29990	-3.64740
C	0.15620	-0.11740	-3.96910
C	0.18760	0.24900	-2.59430
C	1.22850	-0.18980	-1.79070

C	2.24270	-0.98720	-2.35320
C	2.20840	-1.33790	-3.70010
C	1.15430	-0.90200	-4.52310
H	-5.08660	-1.39910	-1.62690
H	-5.17010	-1.88040	-4.06950
H	3.06080	-1.33090	-1.72130
H	2.99950	-1.95460	-4.12520
H	1.12990	-1.18040	-5.57480
C	-0.96370	2.31430	-3.14930
C	-0.83450	3.65880	-2.82790
C	-0.81120	4.61730	-3.85610
C	-0.89940	4.23260	-5.19210
C	-0.99370	2.87280	-5.53290
C	-1.01390	1.93030	-4.51620
H	-0.72190	5.67210	-3.59760
H	-0.88770	4.98450	-5.98010
H	-1.04340	2.57100	-6.57700
C	-1.00670	1.12990	-2.16650
C	-0.93420	1.53470	-0.69380
H	-0.99540	0.60350	-0.07740
H	0.08480	1.94760	-0.50190
C	-1.94730	2.50940	-0.16060
C	-1.72100	3.03200	1.12780
C	-3.09940	2.89970	-0.85710
C	-2.62850	3.91670	1.70380
H	-0.83070	2.74270	1.68580
C	-4.01490	3.78390	-0.28270
H	-3.29150	2.52580	-1.86500
C	-3.78500	4.29300	1.00060
H	-2.43720	4.31020	2.70500
H	-4.90710	4.06280	-0.84870
H	-0.75030	3.99190	-1.79400
H	1.27930	0.06670	-0.73460
O	-3.13350	-0.14260	-0.35070
O	-3.17080	-1.05560	-5.83640
C	-4.14970	-1.65370	-6.58400
O	-5.20820	-2.06470	-6.21890
C	-3.56060	-1.67700	-8.02000
C	-4.24480	0.21530	0.37950
O	-5.31900	0.50630	-0.04990
C	-3.80960	0.12710	1.86350
F	-4.30260	-0.99630	-8.89680
F	-3.45190	-2.91170	-8.51630
F	-2.33710	-1.14870	-8.09600
F	-4.07110	1.23670	2.55660
F	-2.50630	-0.10660	2.03110
F	-4.43310	-0.85990	2.51520
C	-4.75210	5.23580	1.65340
F	-4.21320	6.41390	2.01780
F	-5.82150	5.59600	0.92540
F	-5.29170	4.76800	2.79310
C	-1.05270	0.42590	-4.72270
H	-1.08380	0.12270	-5.78860

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shimizu_pm6/opt_a1_folded_opt_5.xyz

C	7.69150	2.33790	-1.39710
C	6.73150	2.02470	-0.43470
C	6.44200	0.68360	-0.14010
C	7.12340	-0.36160	-0.83240
C	8.09910	-0.02290	-1.81210
C	8.37250	1.32720	-2.08010
C	5.44780	0.28020	0.81470
C	6.82260	-1.75200	-0.56720
C	5.83510	-2.12100	0.39450
C	5.16010	-1.04640	1.06700
C	5.54250	-3.47570	0.61470
H	4.77300	-3.75540	1.33400

C	6.22260	-4.46310	-0.09840
C	7.19650	-4.11980	-1.03940
C	7.50500	-2.77320	-1.28660
H	7.90870	3.38260	-1.62250
H	6.19590	2.82180	0.08040
H	9.11880	1.59010	-2.82920
H	5.98670	-5.51350	0.07570
H	7.71640	-4.90410	-1.58900
C	4.49140	1.13660	1.62540
H	4.78000	2.17610	1.81090
C	4.00590	-1.10350	2.05190
H	3.86800	-2.03370	2.61250
C	4.35350	0.18900	2.86320
O	4.47200	0.38520	4.02820
C	3.06730	0.93620	1.02580
H	2.33120	1.63120	1.47850
C	2.73840	-0.57440	1.31630
H	1.82550	-0.70430	1.93230
C	3.06270	1.08010	-0.49570
O	3.25520	2.06980	-1.14910
C	2.55030	-1.23550	-0.04990
O	2.26830	-2.37690	-0.28900
N	2.75490	-0.21320	-1.04100
C	2.81600	-0.49280	-2.45230
C	1.65290	-0.64980	-3.23420
C	4.07560	-0.61790	-3.06570
C	1.74330	-0.93440	-4.60790
C	4.16330	-0.89920	-4.42740
H	4.98280	-0.49640	-2.46760
C	3.00000	-1.06030	-5.19360
H	0.82710	-1.05710	-5.18460
H	5.14130	-0.99720	-4.89630
H	3.07870	-1.28320	-6.25820
O	0.34560	-0.65650	-2.76820
C	0.00750	0.13280	-1.65990
C	0.20410	1.51810	-1.66450
C	-0.62280	-0.54310	-0.60800
C	-0.24490	2.24550	-0.56060
H	0.70260	2.00650	-2.50120
C	-1.06560	0.21000	0.48090
H	-0.75710	-1.62300	-0.65770
C	-0.87030	1.59590	0.51040
H	-0.10520	3.32680	-0.53710
H	-1.56640	-0.28710	1.31160
H	-1.21860	2.17340	1.36440
C	8.50420	-2.39160	-2.27000
H	9.01840	-3.19360	-2.80050
C	8.78510	-1.09110	-2.51870
H	9.53470	-0.80450	-3.25660

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shimizu_pm6/opt_a2_folded_opt_14.xyz

C	7.10960	3.05560	-0.11650
C	6.06620	2.58570	0.65310
C	5.88100	1.18900	0.83150
C	6.76240	0.26680	0.20850
C	7.83190	0.78500	-0.57260
C	8.00230	2.14490	-0.73120
C	4.80110	0.65490	1.60180
C	6.55550	-1.16930	0.35600
C	5.46610	-1.66470	1.11940
C	4.60090	-0.70750	1.73580
C	5.24700	-3.06370	1.22720
H	4.39080	-3.42420	1.79750
C	6.09900	-3.95020	0.60260
C	7.19700	-3.46710	-0.14910
C	7.41830	-2.11060	-0.26990
H	7.25450	4.12550	-0.26210

H	5.36560	3.27750	1.12100
H	8.52320	0.08820	-1.05090
H	8.82390	2.53230	-1.33320
H	5.93400	-5.02470	0.67610
H	7.86220	-4.18070	-0.63460
H	8.26520	-1.74530	-0.85420
C	3.67190	1.37320	2.31870
H	3.84060	2.41640	2.60470
C	3.33190	-0.92340	2.54060
H	3.20050	-1.89810	3.02150
C	3.45300	0.33240	3.46700
O	3.39680	0.45490	4.64670
C	2.36310	1.10430	1.51820
H	1.51450	1.70220	1.90890
C	2.13490	-0.44530	1.66590
H	1.16180	-0.69240	2.13680
C	2.54360	1.36040	0.02300
O	2.72950	2.40820	-0.53490
C	2.19290	-1.01680	0.24870
O	2.05550	-2.15710	-0.09820
N	2.42700	0.09070	-0.63950
C	2.68280	-0.07260	-2.04690
C	1.64190	-0.27580	-2.97680
C	4.01190	-0.02950	-2.50520
C	1.92170	-0.44230	-4.34410
C	4.28710	-0.19260	-3.86130
H	4.82400	0.13060	-1.79100
C	3.24480	-0.40240	-4.77560
H	1.09720	-0.60520	-5.03750
H	5.31750	-0.15910	-4.21140
H	3.47080	-0.53210	-5.83450
O	0.29670	-0.44180	-2.67740
C	-0.25030	0.23520	-1.57850
C	-0.18210	1.62860	-1.47050
C	-0.94480	-0.56600	-0.66390
C	-0.83230	2.23320	-0.39290
H	0.37140	2.21710	-2.20160
C	-1.58960	0.06580	0.40100
H	-0.97250	-1.64670	-0.79830
C	-1.52700	1.45710	0.54260
H	-0.79600	3.31760	-0.28380
H	-2.14460	-0.53080	1.12490
H	-2.03260	1.93940	1.37680

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shimizu_pm6/opt_a3_folded_opt_6.xyz

C	5.23790	1.76710	1.09580
C	6.20410	0.78330	0.79690
C	4.11050	1.37250	1.78500
C	6.02700	-0.54260	1.18390
C	4.87530	-0.95060	1.88960
C	3.92850	0.00770	2.18430
C	2.88480	2.14260	2.23350
H	2.98480	3.23030	2.31940
C	2.58910	-0.08410	2.88750
H	2.43200	-0.94580	3.54600
C	2.58850	1.33720	3.54200
O	2.41530	1.68990	4.66320
C	1.67420	1.65310	1.38970
H	0.77240	2.27540	1.57440
C	1.47220	0.15600	1.83300
H	0.46450	-0.02620	2.26320
C	1.96780	1.60940	-0.10790
O	2.20510	2.52350	-0.85080
C	1.64900	-0.68590	0.57050
O	1.59190	-1.87850	0.45380
N	1.88910	0.23210	-0.51210
C	2.07600	-0.18980	-1.87580

C	0.98780	-0.58340	-2.68480
C	3.37160	-0.20930	-2.41900
C	1.18810	-0.99940	-4.01030
C	3.56920	-0.61990	-3.73700
H	4.21790	0.09690	-1.80090
C	2.48200	-1.01760	-4.52680
H	0.32880	-1.30580	-4.60650
H	4.57530	-0.63350	-4.15370
H	2.64770	-1.34060	-5.55520
O	-0.32840	-0.72060	-2.25780
C	-0.84980	0.21050	-1.35150
C	-0.75910	1.58950	-1.57110
C	-1.53900	-0.34260	-0.26460
C	-1.37920	2.44010	-0.65370
H	-0.21510	1.98280	-2.42920
C	-2.15390	0.53140	0.63340
H	-1.58980	-1.42420	-0.14600
C	-2.06620	1.91630	0.44790
H	-1.32520	3.51960	-0.80100
H	-2.70560	0.13020	1.48380
H	-2.54820	2.58870	1.15500
H	4.74170	-1.99220	2.17680
H	6.78610	-1.28570	0.93810
H	7.10200	1.07390	0.25130
H	5.38100	2.79860	0.77930

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motherwell_pm6/opt_a1_folded_opt_20.xyz

C	-3.50200	-1.44860	0.81800
C	-2.39390	-0.91570	1.49040
C	-1.31400	-0.42620	0.75680
C	-1.33790	-0.46990	-0.65350
C	-2.44160	-1.00270	-1.31840
C	-3.52570	-1.49180	-0.57710
C	1.12300	-0.41530	-0.69820
C	1.14700	-0.37150	0.71480
C	2.27550	-0.80610	1.40800
C	3.38340	-1.28610	0.69610
C	3.35980	-1.32940	-0.69860
C	2.22780	-0.89340	-1.40100
H	-4.34550	-1.83200	1.38910
H	-4.38770	-1.90880	-1.09450
H	4.26460	-1.62690	1.23700
H	4.22240	-1.70410	-1.24690
H	2.21680	-0.93030	-2.48840
C	-0.08380	0.17340	1.40800
H	2.30140	-0.77550	2.49540
H	-2.46590	-1.04260	-2.40510
H	-2.38130	-0.88820	2.57780
H	-0.06020	-0.09400	2.49320
C	-0.13100	0.08680	-1.38180
H	-0.14390	-0.24730	-2.44850
C	-0.14080	1.71230	1.29240
H	-1.15960	2.04750	1.57210
H	0.54290	2.14910	2.05190
C	-0.18570	1.63000	-1.35980
H	0.47150	2.01820	-2.16770
H	-1.21370	1.94840	-1.62520
C	0.23230	2.34450	-0.06130
H	-0.17190	3.39010	-0.08690
O	1.64380	2.61150	-0.09350
H	2.16630	1.78270	-0.07640

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motherwell_pm6/opt_a2_folded_opt_20.xyz

C	-3.49830	-1.70800	0.87510
C	-2.37060	-1.20260	1.53600
C	-1.28570	-0.74220	0.79090

C	-1.32420	-0.78770	-0.61870
C	-2.44730	-1.29320	-1.27230
C	-3.53640	-1.75300	-0.51960
C	1.13710	-0.79370	-0.68720
C	1.17570	-0.74820	0.72520
C	2.29920	-1.21040	1.40870
C	3.38770	-1.71930	0.68710
C	3.34970	-1.76410	-0.70730
C	2.22250	-1.30070	-1.39980
H	-4.34600	-2.06840	1.45490
H	-4.41370	-2.14860	-1.02790
H	4.26520	-2.08140	1.22010
H	4.19760	-2.16110	-1.26300
H	2.20020	-1.33880	-2.48700
C	-0.03450	-0.17110	1.42730
H	2.33610	-1.17850	2.49570
H	-2.48290	-1.33410	-2.35860
H	-2.34680	-1.17340	2.62310
H	-0.00670	-0.43720	2.51310
C	-0.11070	-0.26080	-1.35780
H	-0.14170	-0.59640	-2.42410
C	-0.05970	1.36780	1.31420
H	-1.06570	1.71850	1.62120
H	0.64760	1.78740	2.06120
C	-0.13210	1.28220	-1.34290
H	0.53300	1.65150	-2.15260
H	-1.15370	1.61430	-1.61670
C	0.30160	2.00720	-0.04720
O	1.73560	2.19760	-0.09230
H	2.21520	1.34680	-0.07890
C	-0.20640	3.45810	-0.08000
H	0.19530	4.02880	0.76700
H	0.14740	3.97240	-0.98270
H	-1.29670	3.51630	-0.05200

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motherwell_pm6/opt_a3_folded_opt_8.xyz

C	-6.34340	2.00300	6.24970
C	-6.24330	1.56040	4.92390
C	-5.90240	2.46640	3.92030
C	-5.66190	3.81940	4.23950
C	-5.76420	4.25600	5.55970
C	-6.10540	3.34180	6.56560
C	-6.19130	4.46220	1.91920
C	-6.43240	3.10690	1.59950
C	-7.24810	2.77870	0.51770
C	-7.82590	3.80000	-0.24860
C	-7.58770	5.13860	0.06710
C	-6.76850	5.47420	1.15370
H	-6.61030	1.29760	7.03440
H	-6.18610	3.68070	7.59660
H	-8.46400	3.54470	-1.09290
H	-8.03960	5.92810	-0.53080
H	-6.58740	6.51990	1.39390
C	-5.75820	2.06560	2.46620
H	-7.43810	1.73740	0.26550
H	-5.58280	5.29820	5.81280
H	-6.43250	0.51630	4.68490
H	-6.23420	1.06740	2.29980
C	-5.28260	4.73960	3.09710
H	-5.39120	5.80550	3.41760
C	-4.26080	1.94470	2.11770
H	-3.76890	1.34510	2.91410
H	-4.16120	1.34610	1.18710
C	-3.80580	4.50220	2.72110
H	-3.44450	5.37600	2.13780
H	-3.20800	4.49920	3.65820
C	-3.44990	3.24240	1.89930

O	-3.54120	3.59020	0.49440
H	-4.45760	3.81290	0.23890
C	-1.93380	2.94290	2.02360
H	-1.66790	2.15420	1.29170
H	-1.36810	3.83430	1.68650
C	-1.51570	2.53600	3.43780
H	-1.78020	3.33950	4.15640
H	-2.09570	1.64720	3.76280
C	-0.01330	2.23770	3.51550
H	0.56480	3.12460	3.18880
H	0.24790	1.43000	2.80350
C	0.40830	1.83790	4.92730
H	0.20110	2.63360	5.65200
H	-0.11960	0.93990	5.26820
H	1.48210	1.62400	4.97400

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motherwell_pm6/opt_a4_folded_opt_8.xyz

C	5.13330	3.42560	-2.36740
C	3.78930	3.32180	-2.74950
C	2.96090	2.40350	-2.10530
C	3.47470	1.58420	-1.07870
C	4.81340	1.68910	-0.70280
C	5.64190	2.61480	-1.35070
C	1.69160	-0.06240	-1.49860
C	1.17660	0.75910	-2.52720
C	0.40410	0.20250	-3.54530
C	0.14200	-1.17430	-3.54110
C	0.65020	-1.98540	-2.52510
C	1.42780	-1.43120	-1.49930
H	5.78250	4.14200	-2.86850
H	6.68760	2.69920	-1.05890
H	-0.46010	-1.61070	-4.33700
H	0.44460	-3.05510	-2.52760
H	1.82220	-2.07080	-0.71160
C	1.49500	2.23700	-2.45220
H	0.00580	0.82800	-4.34230
H	5.21800	1.05880	0.08660
H	3.40110	3.95520	-3.54450
H	1.28020	2.72370	-3.43660
C	2.51180	0.61540	-0.42190
H	3.08250	-0.15010	0.16130
C	0.63300	2.93560	-1.37950
H	1.06860	3.93870	-1.18350
H	-0.37970	3.12530	-1.79930
C	1.60540	1.38340	0.56300
H	1.16420	0.66040	1.28440
H	2.24590	2.05860	1.16990
C	0.43410	2.18950	-0.04130
O	-0.72420	1.33690	-0.14270
H	-0.57340	0.61540	-0.79540
C	-0.00450	3.18640	0.97500
N	-0.33940	3.96020	1.76130

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motherwell_pm6/opt_a5_folded_opt_16.xyz

C	4.30050	0.32800	3.32000
C	4.12540	0.49110	1.93930
C	2.85600	0.33480	1.38400
C	1.75710	0.01270	2.20800
C	1.93600	-0.15050	3.58120
C	3.21310	0.00930	4.13550
C	0.58240	-0.94720	0.26850
C	1.68320	-0.62410	-0.55740
C	1.89640	-1.32490	-1.74340
C	1.01330	-2.34960	-2.11020
C	-0.07350	-2.66870	-1.29470
C	-0.29260	-1.96750	-0.10110

H	5.29060	0.44930	3.75560
H	3.35510	-0.11790	5.20720
H	1.17940	-2.89810	-3.03600
H	-0.75610	-3.46630	-1.58390
H	-1.14200	-2.22230	0.52970
C	2.58110	0.50410	-0.09680
H	2.74180	-1.08200	-2.38420
H	1.09390	-0.40100	4.22270
H	4.97790	0.73700	1.30980
H	3.54380	0.48050	-0.66600
C	0.40820	-0.13330	1.53270
H	-0.30640	-0.64910	2.22160
C	1.91860	1.87550	-0.34100
H	2.48710	2.64240	0.22560
H	2.03520	2.14570	-1.41300
C	-0.16110	1.26530	1.21800
H	-1.25740	1.17920	1.05500
H	-0.04070	1.90110	2.12010
C	0.41210	2.01650	-0.00930
O	-0.35390	1.63810	-1.17940
H	-0.23050	0.68760	-1.38670
C	0.10140	3.44300	0.13470
C	-0.15990	4.61300	0.24440
H	-0.38380	5.61710	0.33900

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motherwell_pm6/opt_a6_folded_opt_2.xyz

C	-3.34700	-2.39600	1.16000
C	-2.40110	-1.61370	1.83650
C	-1.27670	-1.15030	1.15480
C	-1.09390	-1.46990	-0.20780
C	-2.03580	-2.25050	-0.87630
C	-3.16540	-2.71270	-0.18720
C	1.33160	-1.13490	0.03500
C	1.15050	-0.81380	1.40010
C	2.20240	-0.97400	2.29970
C	3.43720	-1.45520	1.84130
C	3.61410	-1.77550	0.49520
C	2.55900	-1.61660	-0.41480
H	-4.22460	-2.75900	1.69120
H	-3.90110	-3.32310	-0.70700
H	4.26000	-1.57680	2.54270
H	4.57360	-2.15040	0.14610
H	2.70430	-1.86910	-1.46180
C	-0.21210	-0.29400	1.81050
H	2.07550	-0.71960	3.34920
H	-1.89920	-2.50410	-1.92500
H	-2.54720	-1.37440	2.88740
H	-0.31810	-0.34110	2.92210
C	0.14730	-0.91950	-0.88230
H	0.31570	-1.44470	-1.85400
C	-0.39580	1.17750	1.37630
H	-1.47020	1.43560	1.42930
H	0.12280	1.82190	2.12070
C	-0.06330	0.58290	-1.17760
H	0.60030	0.86960	-2.01620
H	-1.09700	0.71640	-1.55880
C	0.15720	1.57440	-0.01460
O	1.55610	1.77030	0.32030
C	2.49250	2.00530	-0.73920
H	2.21400	2.88360	-1.32530
H	3.42450	2.18240	-0.18690
H	2.59070	1.11260	-1.36540
C	-0.42040	2.94460	-0.42250
H	-1.51240	2.93300	-0.47080
H	-0.12300	3.71320	0.30170
H	-0.04840	3.27080	-1.39790

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motherwell_pm6/opt_a7_folded_opt_15.xyz

C	3.14050	9.69300	0.79470
C	3.20660	8.49640	1.52140
C	2.03950	7.94690	2.05050
C	0.80080	8.59410	1.85420
C	0.73980	9.78590	1.13350
C	1.91550	10.33390	0.60270
C	-0.10520	7.47640	3.85290
C	1.13470	6.82740	4.05200
C	1.48780	6.37250	5.32110
C	0.60680	6.56510	6.39480
C	-0.61460	7.21030	6.19860
C	-0.97540	7.66960	4.92390
H	4.05080	10.12330	0.38190
H	1.87000	11.26460	0.04070
H	0.88040	6.20690	7.38500
H	-1.29250	7.35920	7.03600
H	-1.92800	8.17220	4.77900
C	2.02390	6.65280	2.83830
H	2.43450	5.86250	5.48140
H	-0.21060	10.29250	0.98290
H	4.16520	8.00470	1.67050
H	3.06180	6.39330	3.16230
C	-0.42510	7.92510	2.44380
H	-1.28040	8.64410	2.45680
C	1.50620	5.51040	1.93830
H	2.01040	5.57230	0.95230
H	1.82210	4.54460	2.39340
C	-0.81820	6.72590	1.55340
H	-1.89290	6.51160	1.70930
H	-0.73630	7.04720	0.49070
C	-0.02310	5.41490	1.72040
O	-0.38710	4.66270	2.91200
C	-1.77130	4.53190	3.25880
H	-2.34850	4.09960	2.43870
H	-1.73030	3.84390	4.11320
H	-2.17510	5.49950	3.57510
C	-0.32780	4.47930	0.51690
H	0.11270	3.48510	0.72990
H	-1.41750	4.30130	0.45910
C	0.19150	5.01800	-0.81830
H	-0.24750	6.01730	-1.01930
H	1.28720	5.18470	-0.75690
C	-0.12760	4.06290	-1.97530
H	-1.22090	3.89630	-2.03710
H	0.31780	3.06820	-1.77600
C	0.38840	4.60150	-3.30750
H	-0.06250	5.56950	-3.55460
H	1.47540	4.74190	-3.29300
H	0.15820	3.91360	-4.12870

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motherwell_pm6/opt_a11_folded_opt_20.xyz

C	2.43400	-1.16310	-4.36360
C	1.26500	-0.79350	-3.68450
C	1.30840	-0.57660	-2.30810
C	2.52240	-0.73120	-1.60460
C	3.68230	-1.10090	-2.28390
C	3.63450	-1.31550	-3.66810
C	1.26790	-1.15140	0.46930
C	0.05220	-0.99580	-0.23510
C	-1.11420	-1.58880	0.24380
C	-1.07230	-2.33950	1.42710
C	0.12770	-2.49320	2.12240
C	1.30410	-1.89830	1.64510
H	2.40150	-1.33410	-5.43790
H	4.53880	-1.60540	-4.19970

H	-1.98280	-2.80120	1.80380
H	0.15380	-3.07480	3.04170
H	2.23400	-2.01810	2.19570
C	0.09280	-0.16560	-1.50070
H	-2.05440	-1.46920	-0.28910
H	4.62040	-1.22610	-1.74790
H	0.33210	-0.68100	-4.23240
H	-0.83610	-0.33640	-2.09830
C	2.49020	-0.47200	-0.11110
H	3.41520	-0.87990	0.36550
C	0.18380	1.34360	-1.17820
H	0.53100	1.87390	-2.08840
H	-0.84270	1.72030	-0.98670
C	2.45530	1.05320	0.13930
H	2.85300	1.24700	1.15740
H	3.17040	1.53680	-0.55700
C	1.08560	1.75430	0.00660
C	1.28960	3.27900	-0.00930
H	1.84580	3.60130	-0.89550
H	0.33490	3.81980	-0.00760
H	1.84570	3.62680	0.87030
F	0.38010	1.48190	1.16300

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motherwell_pm6/opt_a12_folded_opt_10.xyz

C	-0.87070	6.81110	-0.65580
C	-0.07980	5.89770	-1.36660
C	0.69200	4.96940	-0.67020
C	0.67750	4.95220	0.74150
C	-0.10890	5.86350	1.44430
C	-0.88510	6.79410	0.73970
C	2.89510	3.90060	0.75280
C	2.90930	3.91640	-0.66210
C	4.12150	3.90040	-1.34850
C	5.32420	3.86560	-0.62830
C	5.31030	3.85050	0.76650
C	4.09330	3.86950	1.46300
H	-1.47360	7.53720	-1.19790
H	-1.49940	7.50680	1.28670
H	6.27180	3.85280	-1.16410
H	6.24690	3.82600	1.32080
H	4.09130	3.86170	2.55090
C	1.56630	3.94010	-1.36010
H	4.14140	3.91660	-2.43610
H	-0.12330	5.85810	2.53180
H	-0.07170	5.91890	-2.45410
H	1.69950	4.21420	-2.43510
C	1.53820	3.90680	1.42410
H	1.64950	4.15510	2.50780
C	0.86890	2.56140	-1.29720
H	-0.21710	2.71770	-1.45960
H	1.20540	1.95130	-2.15830
C	0.84370	2.52940	1.31440
H	1.16530	1.89840	2.16640
H	-0.24520	2.68090	1.46040
C	1.05920	1.72420	0.00070
C	0.01140	0.58470	-0.02410
H	0.13260	-0.07480	0.84350
H	-1.01260	0.96270	-0.02860
H	0.14840	-0.05230	-0.90590
N	2.39360	1.03780	0.00740
H	2.94830	1.27320	-0.81000
H	2.95110	1.29230	0.81720

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motherwell_pm6/opt_a13_folded_opt_18.xyz

C	6.30770	0.25880	0.36960
C	5.37370	0.95040	1.15300

C	4.36950	1.69030	0.53060
C	4.29690	1.74290	-0.87770
C	5.22920	1.05530	-1.65320
C	6.23590	0.31090	-1.02350
C	3.09680	3.88140	-0.73790
C	3.16970	3.82880	0.67410
C	3.09690	5.00210	1.42170
C	2.94760	6.23210	0.76530
C	2.87580	6.28400	-0.62710
C	2.95220	5.10680	-1.38490
H	7.09290	-0.32020	0.85320
H	6.96520	-0.22740	-1.62690
H	2.89110	7.15020	1.34860
H	2.76320	7.24270	-1.13170
H	2.90200	5.15710	-2.47090
C	3.31480	2.45900	1.30300
H	3.15880	4.97150	2.50790
H	5.18150	1.09280	-2.73950
H	5.43800	0.90670	2.23820
H	3.62380	2.55890	2.37270
C	3.17130	2.56270	-1.47840
H	3.36910	2.74310	-2.56380
C	1.98330	1.67440	1.25920
H	2.21330	0.59120	1.35460
H	1.38470	1.92180	2.15990
C	1.84840	1.77200	-1.35650
H	1.16140	2.08320	-2.17000
H	2.06330	0.69980	-1.55520
C	1.10070	1.89520	-0.00020
N	0.30170	3.15240	0.08810
H	0.52690	3.69550	0.91680
H	0.44090	3.75560	-0.71760
C	0.07220	0.81270	0.01230
N	-0.72850	-0.01750	0.02240

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Diederich_pm6/opt_a1_folded_opt_19.xyz

C	1.81500	7.67710	-1.14010
C	0.76960	7.45660	-2.03920
C	1.06060	7.07550	-3.35690
C	2.39940	6.90060	-3.77490
C	3.43230	7.11680	-2.85690
C	3.14220	7.50470	-1.54570
H	1.59310	7.98910	-0.12040
H	-0.26720	7.59050	-1.73030
H	4.46910	6.98720	-3.16420
H	3.95280	7.67860	-0.84060
C	2.72720	6.51760	-5.20000
H	3.28470	7.35070	-5.69200
N	-0.05450	6.94030	-4.28810
N	1.52550	6.24890	-6.05860
C	0.42170	7.19730	-5.68770
H	-0.42400	7.07540	-6.40160
H	0.78610	8.24650	-5.76660
C	-0.68900	5.58230	-4.21540
H	-0.71330	5.23830	-3.15530
H	-1.75240	5.71340	-4.52830
C	-0.02510	4.53920	-5.08470
C	1.05960	4.87420	-5.92790
C	-0.48460	3.22150	-5.06070
C	1.68300	3.89280	-6.71200
C	0.14190	2.23970	-5.84280
H	-1.31580	2.93930	-4.40970
C	1.22290	2.57680	-6.66890
H	2.51630	4.16630	-7.35980
H	1.70820	1.81000	-7.27260
H	3.40230	5.63290	-5.21800
C	-0.32140	0.83580	-5.76260

C	-0.02680	0.05640	-4.62680
C	-1.04810	0.25980	-6.81380
C	-0.45790	-1.27230	-4.53660
C	-1.47870	-1.06610	-6.72350
H	-1.27990	0.85500	-7.69750
C	-1.18610	-1.83160	-5.58900
H	-0.22520	-1.86520	-3.65080
H	-2.04770	-1.50710	-7.54310
H	-1.52560	-2.86490	-5.52540
C	0.78230	0.64900	-3.53210
C	0.40930	2.47280	-1.93520
C	1.63780	3.11980	-2.11070
C	-0.50470	2.82760	-0.93360
C	1.96990	4.16080	-1.24090
H	2.32250	2.81050	-2.90030
C	-0.11980	3.87540	-0.09680
H	-1.45120	2.30190	-0.83030
C	1.09690	4.55270	-0.22000
H	2.92110	4.68410	-1.36520
H	1.36170	5.36570	0.45280
O	-0.06920	1.49810	-2.80710
O	1.93350	0.49410	-3.23680
F	-0.96100	4.25030	0.86720

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Diederich_pm6/opt_a2_folded_opt_18.xyz

C	6.71640	-0.84540	-0.13470
C	6.46610	-1.38720	-1.39710
C	5.44080	-2.33100	-1.55300
C	4.63860	-2.70720	-0.45150
C	4.91680	-2.16750	0.80830
C	5.95310	-1.24250	0.96740
H	7.51740	-0.11840	-0.00830
H	7.07260	-1.09940	-2.25510
H	4.31840	-2.46200	1.66930
H	6.16410	-0.82960	1.95180
C	3.49700	-3.68390	-0.61530
H	3.68100	-4.59130	0.00740
N	5.28770	-2.96450	-2.85780
N	3.29920	-4.16960	-2.02220
C	4.63410	-4.30620	-2.69590
H	4.49720	-4.78160	-3.69320
H	5.29470	-4.96740	-2.09060
C	4.48200	-2.12930	-3.80840
H	4.73740	-1.05420	-3.66770
H	4.82140	-2.40330	-4.83590
C	2.98790	-2.32710	-3.69280
C	2.44540	-3.27700	-2.79630
C	2.12580	-1.56310	-4.48080
C	1.05680	-3.43080	-2.67780
C	0.73620	-1.71530	-4.35810
H	2.53000	-0.83540	-5.18540
C	0.20450	-2.65030	-3.45860
H	0.65130	-4.16510	-1.98160
H	-0.87540	-2.75570	-3.35890
H	2.55180	-3.22670	-0.24200
C	-0.17080	-0.84220	-5.13750
C	-0.19020	0.54700	-4.90160
C	-1.01700	-1.37930	-6.11780
C	-1.04110	1.38510	-5.63250
C	-1.86700	-0.54210	-6.84430
H	-1.00480	-2.45210	-6.31110
C	-1.88090	0.83670	-6.60400
H	-1.04410	2.46010	-5.44270
H	-2.52340	-0.96620	-7.60520
H	-2.54580	1.48340	-7.17520
C	0.72350	1.13320	-3.88690
C	1.28200	0.54410	-1.56700

C	2.64690	0.82970	-1.64330
C	0.65200	0.13170	-0.38280
C	3.40490	0.69840	-0.47690
H	3.10430	1.15840	-2.57580
C	1.43510	0.01140	0.76480
H	-0.41290	-0.08550	-0.38080
C	2.80540	0.29620	0.72110
H	4.47580	0.90520	-0.50580
H	0.97460	-0.30380	1.70030
H	3.40890	0.20080	1.62100
O	0.41310	0.54890	-2.66170
O	1.58800	1.95800	-4.02040

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Diederich_pm6/opt_a3_folded_opt_17.xyz

C	-3.06410	-5.63100	2.59430
C	-2.92530	-4.25510	2.40370
C	-1.64400	-3.70010	2.26840
C	-0.49790	-4.52700	2.31360
C	-0.65720	-5.90220	2.51170
C	-1.93420	-6.45310	2.65020
H	-4.05760	-6.06370	2.70320
H	-3.80130	-3.60770	2.37390
H	0.21690	-6.55050	2.55330
H	-2.04850	-7.52470	2.80110
C	0.88820	-3.94390	2.15730
H	1.43880	-4.01350	3.12490
N	-1.54220	-2.25130	2.13320
N	0.88840	-2.49550	1.76000
C	-0.17900	-1.78060	2.54290
H	-0.09430	-0.68060	2.37040
H	-0.03510	-1.96410	3.63070
C	-1.79990	-1.79920	0.72590
H	-2.67110	-2.35220	0.31030
H	-2.10450	-0.72530	0.78450
C	-0.60030	-1.93810	-0.18330
C	0.65860	-2.33180	0.32910
C	-0.72550	-1.64970	-1.54320
C	1.75060	-2.50680	-0.53430
C	0.38390	-1.76550	-2.39400
H	-1.68470	-1.32330	-1.94670
C	1.61210	-2.22140	-1.89270
H	2.70960	-2.83750	-0.13700
H	2.46710	-2.32460	-2.56040
H	1.47560	-4.53030	1.41650
C	0.27210	-1.37430	-3.81760
C	0.02140	-0.04050	-4.19120
C	0.41800	-2.34800	-4.81920
C	-0.08150	0.30990	-5.54640
C	0.31930	-1.99430	-6.16540
H	0.60500	-3.38410	-4.53670
C	0.07030	-0.66600	-6.53130
H	-0.28460	1.34680	-5.82400
H	0.43500	-2.75670	-6.93660
H	-0.00740	-0.39470	-7.58330
C	-0.17580	1.03600	-3.18460
C	0.87770	1.72450	-1.08680
C	0.44810	3.04790	-0.99430
C	1.41370	1.00990	-0.01490
C	0.58250	3.68150	0.24750
H	0.00820	3.55710	-1.84810
C	1.50610	1.66110	1.22910
H	1.73730	-0.01820	-0.15540
C	1.10880	3.01480	1.35180
H	0.26320	4.72010	0.34960
H	1.19070	3.52280	2.30710
O	0.88020	0.99100	-2.28390
O	-1.06400	1.84460	-3.11030

N	1.90370	0.93090	2.36720
H	2.30290	0.01350	2.20670
H	2.34630	1.43860	3.11620

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Diederich_pm6/opt_a4_folded_opt_1.xyz

C	-2.94150	-5.44750	-1.30970
C	-2.34630	-4.25500	-0.89400
C	-1.00640	-3.99950	-1.22070
C	-0.26180	-4.93570	-1.97350
C	-0.87380	-6.12700	-2.37630
C	-2.20820	-6.38200	-2.04770
H	-3.98060	-5.65050	-1.05480
H	-2.90850	-3.52840	-0.30850
H	-0.31100	-6.85940	-2.95330
H	-2.67690	-7.31040	-2.36790
C	1.18150	-4.67030	-2.33480
H	1.84250	-5.39250	-1.79840
N	-0.40830	-2.76520	-0.72140
N	1.66030	-3.29780	-1.96400
C	1.08330	-2.91030	-0.63340
H	1.54030	-1.94350	-0.30370
H	1.33430	-3.68420	0.12500
C	-0.73790	-1.59960	-1.60770
H	-1.79700	-1.67010	-1.94100
H	-0.67000	-0.68460	-0.96860
C	0.18160	-1.45390	-2.79850
C	1.30190	-2.30190	-2.96560
C	-0.04500	-0.43660	-3.72610
C	2.14830	-2.15230	-4.07380
C	0.83560	-0.25280	-4.80260
H	-0.89120	0.24300	-3.60220
C	1.91620	-1.12560	-4.98910
H	3.00330	-2.81780	-4.19510
H	2.59040	-0.98670	-5.83390
H	1.34790	-4.83910	-3.42200
C	0.65850	0.91280	-5.69750
C	0.96660	2.20540	-5.22590
C	0.20160	0.75820	-7.01260
C	0.81200	3.32480	-6.05020
C	0.04840	1.87690	-7.83620
H	-0.03870	-0.23750	-7.38570
C	0.35170	3.15650	-7.35880
H	1.04970	4.32070	-5.67350
H	-0.31120	1.75060	-8.85810
H	0.22920	4.02380	-8.00630
C	1.48880	2.35900	-3.84320
C	0.43800	2.07960	-1.63650
C	-0.62270	2.61030	-0.88080
C	1.38610	1.20610	-1.10640
C	-0.73440	2.23350	0.45660
H	-1.32850	3.29270	-1.34580
C	1.21970	0.84410	0.23850
H	2.22260	0.81840	-1.68860
C	0.17560	1.34120	1.03380
H	-1.54800	2.63580	1.06290
H	0.07130	1.04390	2.07090
O	0.37130	2.39580	-2.98700
O	2.60770	2.45890	-3.43070
O	2.13340	-0.06160	0.71650
H	1.99830	-0.25530	1.67880

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Zoltewicz_pm6/opt_a2_folded_opt_11.xyz

C	-0.04300	2.95370	0.77130
C	0.60880	2.09810	-0.07710
C	0.05910	0.81010	-0.37280
C	-1.16280	0.39120	0.22820

C	-1.84780	1.34040	1.06620
C	-1.28920	2.57310	1.33590
H	1.67550	0.30590	-1.73630
H	0.36970	3.93150	1.01520
H	1.55400	2.37970	-0.53880
C	0.75330	-0.05120	-1.28060
C	-1.61580	-0.94640	-0.05060
H	-1.80810	3.28270	1.98150
C	-0.92650	-1.74970	-0.93650
C	0.26140	-1.29700	-1.56890
H	-1.28250	-2.75760	-1.15430
H	0.77140	-1.95810	-2.26800
C	-2.78900	-1.56660	0.61580
C	-4.05780	-1.50710	0.02630
C	-2.59620	-2.27570	1.81130
C	-5.14980	-2.12590	0.65250
H	-4.19600	-0.96170	-0.90450
C	-3.68420	-2.90270	2.42340
H	-1.60670	-2.32990	2.25830
C	-4.95670	-2.82660	1.85470
H	-3.53870	-3.45030	3.35310
H	-5.80090	-3.30410	2.34550
C	-3.19210	1.08740	1.64030
C	-4.32080	1.43120	0.93130
C	-3.30250	0.53940	2.95710
C	-5.61750	1.19880	1.48490
H	-4.24280	1.86520	-0.06440
C	-4.53690	0.31240	3.50720
H	-2.38940	0.29390	3.49760
C	-5.72820	0.62310	2.77710
C	-6.80840	1.51390	0.75630
H	-4.63250	-0.11840	4.50260
C	-7.02750	0.35650	3.31250
C	-8.04240	1.24900	1.29520
H	-6.71230	1.96320	-0.23060
C	-8.15340	0.65910	2.58820
H	-7.10210	-0.09250	4.30160
H	-8.95360	1.48530	0.74860
H	-9.14570	0.45840	2.98770
C	-6.51830	-2.02060	0.06370
H	-7.06950	-2.96730	0.12420
H	-7.10800	-1.26250	0.60720
H	-6.50440	-1.71800	-0.99060

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Zoltewicz_pm6/opt_a3_folded_opt_2.xyz

C	-10.69690	-9.11480	1.05580
C	-11.78160	-8.43820	0.56380
C	-11.71900	-7.02460	0.34910
C	-10.53260	-6.29770	0.65750
C	-9.40150	-7.04860	1.13490
C	-9.49530	-8.41170	1.33380
H	-13.75220	-6.93940	-0.41560
H	-10.73280	-10.18860	1.23280
H	-12.70800	-8.96040	0.32940
C	-12.86600	-6.35220	-0.18020
C	-10.56080	-4.87180	0.46580
H	-8.63690	-8.97340	1.70450
C	-11.68190	-4.25380	-0.05040
C	-12.84360	-4.99790	-0.38580
H	-11.69150	-3.17300	-0.20110
H	-13.70560	-4.47380	-0.79590
C	-9.43470	-3.97370	0.83180
C	-8.42540	-3.70720	-0.09660
C	-9.44150	-3.35100	2.08820
C	-7.37590	-2.82380	0.23700
H	-8.45900	-4.19720	-1.06590
C	-8.40480	-2.47280	2.41470

H	-10.23880	-3.55360	2.79620
C	-7.37620	-2.21280	1.51410
H	-8.39950	-1.98690	3.39000
H	-6.57990	-1.52620	1.79110
C	-8.07390	-6.44560	1.41180
C	-7.07830	-6.49850	0.46240
C	-7.81430	-5.88340	2.70180
C	-5.78010	-5.97410	0.74900
H	-7.26730	-6.93240	-0.51800
C	-6.57960	-5.36510	2.99220
H	-8.62180	-5.86290	3.43310
C	-5.53030	-5.39320	2.01920
C	-4.72210	-6.02700	-0.21320
H	-6.37800	-4.91870	3.96480
C	-4.23350	-4.85870	2.29940
C	-3.48530	-5.51180	0.08420
H	-4.91710	-6.49230	-1.17810
C	-3.23780	-4.91780	1.35630
H	-4.05460	-4.40930	3.27510
H	-2.67400	-5.55210	-0.64040
H	-2.24620	-4.52020	1.56400
N	-6.40070	-2.43310	-0.73100
C	-5.05430	-2.09350	-0.18830
H	-4.53100	-2.95520	0.25860
H	-4.42850	-1.68100	-0.99500
H	-5.15100	-1.30820	0.58110
C	-6.29180	-3.29240	-1.94270
H	-5.56440	-2.84960	-2.64150
H	-5.98310	-4.32780	-1.72730
H	-7.26520	-3.31440	-2.46290

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Zoltewicz_pm6/opt_a5_folded_opt_19.xyz

C	2.07170	-0.88680	-1.34600
C	2.04970	-2.23850	-1.56700
C	0.84310	-2.98520	-1.38030
C	-0.35250	-2.33460	-0.95840
C	-0.29270	-0.91190	-0.74490
C	0.88750	-0.22130	-0.93310
H	1.78580	-4.85970	-1.94900
H	2.98270	-0.30620	-1.48290
H	2.94580	-2.76780	-1.88770
C	0.85560	-4.39520	-1.62480
C	-1.52340	-3.15250	-0.78090
H	0.92550	0.85640	-0.76860
C	-1.47920	-4.50970	-1.02690
C	-0.28120	-5.14040	-1.45460
H	-2.37270	-5.12160	-0.89390
H	-0.28720	-6.21350	-1.63990
C	-2.83070	-2.61600	-0.32280
C	-3.78330	-2.21870	-1.26070
C	-3.11940	-2.57050	1.05390
C	-5.01490	-1.72080	-0.79220
H	-3.58870	-2.26170	-2.32900
C	-4.35320	-2.08600	1.48680
H	-2.37370	-2.89960	1.77230
C	-5.31710	-1.64720	0.57290
H	-4.57140	-2.04110	2.55370
H	-6.26330	-1.25560	0.92600
C	-1.46190	-0.10120	-0.32460
C	-2.31600	0.44080	-1.25680
C	-1.65020	0.16420	1.06950
C	-3.42980	1.23370	-0.83880
H	-2.17290	0.25370	-2.32050
C	-2.70470	0.93140	1.49000
H	-0.94640	-0.26610	1.78070
C	-3.63210	1.47480	0.54450
C	-4.35800	1.77350	-1.78480

H	-2.86060	1.13280	2.54840
C	-4.76300	2.24570	0.96000
C	-5.43380	2.51140	-1.35860
H	-4.19720	1.57560	-2.84380
C	-5.63990	2.74870	0.03170
H	-4.91140	2.42260	2.02380
H	-6.14190	2.92880	-2.07170
H	-6.50060	3.33950	0.33930
O	-5.85560	-1.34140	-1.81630
C	-7.07700	-0.65070	-1.45920
H	-7.49400	-0.40620	-2.44380
H	-7.74040	-1.31970	-0.90530
H	-6.84520	0.25960	-0.89460

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Zoltewicz_pm6/opt_a6_folded_opt_3.xyz

C	-0.78380	-4.50580	-1.64310
C	0.41150	-4.86300	-1.07700
C	1.22590	-3.88460	-0.42290
C	0.81470	-2.52180	-0.37140
C	-0.47740	-2.19790	-0.91720
C	-1.23610	-3.16290	-1.54750
H	2.73470	-5.34530	0.13990
H	-1.40680	-5.23650	-2.15670
H	0.76360	-5.89290	-1.11560
C	2.45860	-4.29250	0.17930
C	1.72320	-1.57660	0.22280
H	-2.20820	-2.90790	-1.97150
C	2.90140	-2.00270	0.80140
C	3.26860	-3.37450	0.79410
H	3.57840	-1.28340	1.26440
H	4.20170	-3.67290	1.26980
C	1.49510	-0.11050	0.19970
C	0.86650	0.53290	1.27260
C	1.97140	0.63580	-0.89270
C	0.69200	1.92010	1.22160
H	0.50350	-0.05120	2.11880
C	1.79530	2.01950	-0.91740
H	2.46790	0.12900	-1.71780
C	1.14970	2.67140	0.14010
H	2.15690	2.59820	-1.76590
H	1.01280	3.74950	0.09900
C	-1.09640	-0.85630	-0.78400
C	-0.96720	0.10120	-1.76190
C	-1.89360	-0.60270	0.37930
C	-1.58890	1.37940	-1.60280
H	-0.37260	-0.08840	-2.65400
C	-2.51760	0.60610	0.53840
H	-1.98350	-1.38660	1.13010
C	-2.37240	1.63380	-0.44780
C	-1.42120	2.41700	-2.57360
H	-3.11860	0.81250	1.42340
C	-2.98720	2.91510	-0.28900
C	-2.01060	3.64260	-2.38900
H	-0.81390	2.21380	-3.45400
C	-2.80650	3.89440	-1.23380
H	-3.59780	3.09340	0.59510
H	-1.88460	4.43880	-3.12050
H	-3.27030	4.87250	-1.12170
C	-0.68790	4.24810	2.07270
H	-1.40400	4.61120	2.82180
H	0.13100	4.97170	2.00210
H	-1.20390	4.19720	1.10450
S	-0.11080	2.62710	2.61870