

Electronic Supplementary Information – 2 for

Liquid Crucible Model for Aggregation of Phenylacetylene in the Gas Phase

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Coordinates of all the structures optimized at B97-D/aug-cc-pVDZ level of theory.

Monomer

C	0.0000000	0.0000000	-2.2564460
C	-1.2168545	0.0000000	-1.5507858
C	1.2168545	0.0000000	-1.5507858
H	-2.1671949	0.0000000	-2.0952159
H	2.1671949	0.0000000	-2.0952159
C	-1.2220794	-0.0000000	-0.1489895
C	1.2220794	-0.0000000	-0.1489895
H	-2.1669443	-0.0000000	0.4022277
H	2.1669443	-0.0000000	0.4022277
C	0.0000000	-0.0000000	0.5706280
H	0.0000000	-0.0000000	-3.3513709
C	0.0000000	-0.0000000	2.0030243
C	0.0000000	0.0000000	3.2270534
H	-0.0000000	0.0000000	4.3004195

Dimers

Dimer-01 (D1)

C	-2.5443027	1.0444820	0.8995341
C	-1.8638295	0.1042588	1.2893953
C	-1.0511935	-0.9866151	1.7362474
C	-0.8651659	-2.1262204	0.9148898
C	-0.4079804	-0.9336485	2.9981169
C	-0.0477045	-3.1790547	1.3439441
C	0.4066873	-1.9940078	3.4195777
C	0.5915408	-3.1174639	2.5945595
H	-3.1579971	1.8598243	0.5675565
H	-1.3504768	-2.1624582	-0.0635521
H	-0.5520525	-0.0555201	3.6341471
H	0.1065332	-4.0450519	0.6931572
H	0.9021341	-1.9413283	4.3950041
H	1.2417290	-3.9362524	2.9172320
C	4.1330273	-4.0131576	0.4605780
C	3.4528953	-3.0727171	0.0708412
C	2.6405716	-1.9814504	-0.3757260
C	2.4549864	-0.8420096	0.4459553
C	1.9972324	-2.0338721	-1.6375519
C	1.6378119	0.2111952	0.0172746
C	1.1828668	-0.9731333	-2.0586461
C	0.9984349	0.1501502	-1.2333002

H	4.7465292	-4.8287299	0.7924709
H	2.9404195	-0.8061911	1.4243522
H	2.1409639	-2.9118693	-2.2738405
H	1.4839196	1.0770611	0.6683188
H	0.6873203	-1.0253759	-3.0340455
H	0.3484744	0.9692310	-1.5556864

Dimer-02 (D2)

C	-0.3591684	1.0184963	-1.0943867
C	0.0680281	0.0707849	-0.4479843
C	0.5552514	-1.0450584	0.3047408
C	0.1962636	-1.2045678	1.6658267
C	1.3913878	-2.0136470	-0.3060431
C	0.6568832	-2.3098887	2.3924293
C	1.8503603	-3.1139962	0.4303372
C	1.4837027	-3.2672603	1.7795970
H	-0.7189040	1.8593423	-1.6556707
H	-0.4639513	-0.4702281	2.1334009
H	1.6696192	-1.8927282	-1.3569807
H	0.3472976	-2.4402072	3.4334039
H	2.4947403	-3.8569263	-0.0515766
H	1.8344832	-4.1340019	2.3489542
C	-2.2966498	-4.5459627	4.4104224
C	-2.4304423	-4.0058499	3.3197400
C	-2.5506268	-3.3552603	2.0501840
C	-3.2569386	-2.1320053	1.9332249
C	-1.9351761	-3.9085000	0.8996403
C	-3.3316587	-1.4764715	0.6966184
C	-2.0169463	-3.2456691	-0.3311078
C	-2.7118247	-2.0283833	-0.4376610
H	-2.2079257	-5.0339999	5.3620619
H	-3.7313821	-1.7018140	2.8200966
H	-1.3762351	-4.8432914	0.9910720
H	-3.8674566	-0.5248587	0.6196483
H	-1.5210065	-3.6721672	-1.2082353
H	-2.7512663	-1.5003321	-1.3946355

Dimer-03 (D4)

C	0.7906486	0.8211200	1.1612140
C	1.0604167	0.9081868	-0.0294038
C	1.3877438	1.0062777	-1.4190965
C	1.0742283	-0.0524236	-2.3068213
C	2.0332277	2.1623605	-1.9242143
C	1.4052173	0.0443064	-3.6644363
C	2.3591948	2.2496664	-3.2837725
C	2.0492949	1.1926706	-4.1584663
H	0.5726855	0.7400550	2.2084726
H	0.5697238	-0.9411273	-1.9189372
H	2.2573981	2.9867965	-1.2433536
H	1.1569964	-0.7804164	-4.3401668

H	2.8567788	3.1485264	-3.6623486
H	2.3083958	1.2638486	-5.2202667
C	-0.3779021	4.9934196	-1.0924713
C	-0.8487393	3.9595482	-1.5480068
C	-1.4113713	2.7560505	-2.0800347
C	-2.0118378	1.8038736	-1.2192368
C	-1.3786291	2.5027920	-3.4735422
C	-2.5689264	0.6312895	-1.7455104
C	-1.9404947	1.3282301	-3.9901013
C	-2.5384197	0.3891897	-3.1307372
H	0.0169957	5.9067711	-0.6917153
H	-2.0182840	1.9894161	-0.1426764
H	-0.9059433	3.2319787	-4.1365645
H	-3.0282638	-0.0976620	-1.0698782
H	-1.9086204	1.1440477	-5.0687516
H	-2.9772651	-0.5277618	-3.5384081

Dimer-04 (D3)

C	5.5443504	1.8432931	2.1536000
C	4.5876369	2.0453527	1.4166753
C	3.4685488	2.2840229	0.5561587
C	3.0776646	1.3142640	-0.4005599
C	2.7349097	3.4926547	0.6518427
C	1.9833500	1.5539105	-1.2416044
C	1.6404807	3.7224838	-0.1918515
C	1.2622623	2.7571433	-1.1418878
H	6.3886910	1.6728008	2.7934647
H	3.6357413	0.3768830	-0.4673473
H	3.0222427	4.2324531	1.4025994
H	1.6883790	0.7963881	-1.9752604
H	1.0758305	4.6563203	-0.1025522
H	0.4066277	2.9405548	-1.8001488
C	0.7716525	3.8891038	3.9578406
C	0.8859153	2.7653430	3.4861961
C	1.0225641	1.4515773	2.9332370
C	2.0833120	0.6068266	3.3447267
C	0.1020858	0.9804231	1.9640844
C	2.2152893	-0.6767700	2.7994098
C	0.2406400	-0.3055392	1.4262963
C	1.2952061	-1.1382805	1.8414080
H	0.6665014	4.8693538	4.3820628
H	2.8046411	0.9756835	4.0776829
H	-0.7095626	1.6355068	1.6376503
H	3.0443387	-1.3169311	3.1183220
H	-0.4738828	-0.6583049	0.6752795
H	1.4016626	-2.1422324	1.4174174

Dimer-05 (D6)

C	-0.8643322	4.6113569	2.5037277
C	-0.5075508	3.4542350	2.6830030

C	-0.0759081	2.1058429	2.8939616
C	-0.0416654	1.5597372	4.2009819
C	0.3347650	1.3041404	1.7998178
C	0.3928949	0.2436748	4.4037632
C	0.7651239	-0.0113542	2.0129451
C	0.7956091	-0.5466521	3.3129669
H	-1.1943349	5.6202708	2.3473562
H	-0.3351969	2.1837660	5.0485360
H	0.3242733	1.7292339	0.7928787
H	0.4271057	-0.1631205	5.4194547
H	1.0878969	-0.6192508	1.1616629
H	1.1370379	-1.5741405	3.4761083
C	2.7114194	2.9756981	6.3687897
C	2.9315306	2.8922370	5.1676251
C	3.1811504	2.7937737	3.7615463
C	2.8398494	3.8630427	2.8964223
C	3.7654344	1.6239091	3.2153022
C	3.0798082	3.7606684	1.5204596
C	4.0047011	1.5328442	1.8381365
C	3.6643201	2.5986916	0.9864758
H	2.5296444	3.0553588	7.4232042
H	2.3652040	4.7553325	3.3113892
H	4.0160690	0.7925994	3.8794995
H	2.7999572	4.5882675	0.8608408
H	4.4514191	0.6223377	1.4257554
H	3.8497192	2.5221744	-0.0900445

Dimer-06 (D7)

C	2.9214474	1.0936704	-1.7100465
C	2.3088408	0.9646421	-0.6579134
C	1.5617640	0.8253379	0.5552119
C	1.5289445	1.8774263	1.5033015
C	0.8219782	-0.3568255	0.8089376
C	0.7700753	1.7481988	2.6738882
C	0.0661816	-0.4754703	1.9814311
C	0.0373058	0.5740008	2.9175521
H	3.4846865	1.1974883	-2.6174283
H	2.0854728	2.7966381	1.3016212
H	0.8325535	-1.1625965	0.0707635
H	0.7370585	2.5748995	3.3899977
H	-0.5130190	-1.3867802	2.1609805
H	-0.5612873	0.4800927	3.8293839
C	-1.4255856	4.5171235	1.2230457
C	-1.5513700	3.4582396	0.6222056
C	-1.7057063	2.2251443	-0.0880461
C	-2.6219730	1.2437686	0.3661631
C	-0.9426775	1.9679241	-1.2537156
C	-2.7737913	0.0414567	-0.3366636
C	-1.0989434	0.7616353	-1.9482836
C	-2.0145574	-0.2041472	-1.4950419

H	-1.3165872	5.4465933	1.7478139
H	-3.2036265	1.4358557	1.2720428
H	-0.2151580	2.7094360	-1.5925728
H	-3.4840493	-0.7101795	0.0234061
H	-0.4893283	0.5698396	-2.8364850
H	-2.1332504	-1.1469084	-2.0392726

Dimer-07

C	-1.4554985	4.1299248	-1.4604319
C	-0.6757847	3.3732895	-0.8963090
C	0.2433131	2.4918712	-0.2406149
C	-0.1103205	1.8593639	0.9767925
C	1.5179288	2.2342292	-0.8072784
C	0.7922049	0.9961822	1.6125418
C	2.4136057	1.3689210	-0.1642514
C	2.0563034	0.7498317	1.0480654
H	-2.1309384	4.8034968	-1.9519061
H	-1.1012310	2.0320327	1.4018161
H	1.7917699	2.7175544	-1.7497891
H	0.4961658	0.4987287	2.5410371
H	3.3933859	1.1747479	-0.6135701
H	2.7589151	0.0738451	1.5468794
C	-1.1160880	-2.2953009	3.5479553
C	-1.7071503	-1.5194243	2.8081508
C	-2.3791625	-0.5972066	1.9437368
C	-3.1793267	0.4412063	2.4837071
C	-2.2358705	-0.6953852	0.5370844
C	-3.8120094	1.3592454	1.6331578
C	-2.8693814	0.2287904	-0.3036233
C	-3.6571038	1.2592540	0.2387495
H	-0.6215992	-2.9939370	4.1952110
H	-3.2907601	0.5202901	3.5688707
H	-1.6091535	-1.4878194	0.1193192
H	-4.4219086	2.1606973	2.0622054
H	-2.7320608	0.1567951	-1.3867610
H	-4.1340306	1.9899296	-0.4213282

Dimer-08

C	2.5606233	-2.0959345	5.8624070
C	2.9949360	-1.5196995	4.8735164
C	3.5071500	-0.8451547	3.7181451
C	2.6690826	-0.5937484	2.6034985
C	4.8610573	-0.4249452	3.6725983
C	3.1745976	0.0620141	1.4726435
C	5.3569237	0.2330421	2.5387057
C	4.5170413	0.4797183	1.4364926
H	2.1830196	-2.5928598	6.7353251
H	1.6294800	-0.9244701	2.6313701
H	5.5108037	-0.6194548	4.5310749
H	2.5182754	0.2349108	0.6140393

H	6.4043183	0.5522914	2.5144925
H	4.9095408	0.9939524	0.5526890
C	0.7704392	-0.6244735	-2.0191126
C	0.6129978	-1.2560750	-0.9823912
C	0.4431847	-1.9790765	0.2417317
C	-0.6028342	-1.6402312	1.1368522
C	1.3303958	-3.0297970	0.5845509
C	-0.7489565	-2.3345895	2.3463395
C	1.1771439	-3.7161598	1.7964739
C	0.1405976	-3.3715142	2.6820072
H	0.8913798	-0.0887008	-2.9410139
H	-1.2877908	-0.8288776	0.8750817
H	2.1426542	-3.2867374	-0.1006009
H	-1.5557452	-2.0594203	3.0328795
H	1.8788365	-4.5140857	2.0578239
H	0.0351555	-3.8987898	3.6349841

Dimer-09

C	-0.8450032	0.9399264	2.9731820
C	0.0240115	1.5059591	2.3231757
C	1.0443348	2.1461486	1.5482952
C	0.7163353	2.8173652	0.3432653
C	2.3981913	2.1034536	1.9673563
C	1.7208321	3.4268246	-0.4212721
C	3.3955519	2.7159513	1.1958609
C	3.0617963	3.3778113	0.0004791
H	-1.6098976	0.4603485	3.5538115
H	-0.3265001	2.8458926	0.0161741
H	2.6533365	1.5807339	2.8930563
H	1.4573846	3.9355761	-1.3540870
H	4.4387483	2.6697678	1.5244184
H	3.8445266	3.8445632	-0.6051564
C	4.9122145	0.4243849	-3.0390280
C	4.0502802	-0.2281785	-2.4639407
C	3.0416023	-0.9905832	-1.7899070
C	2.2461048	-0.3931834	-0.7796378
C	2.8265873	-2.3521969	-2.1241088
C	1.2607879	-1.1425314	-0.1217746
C	1.8385873	-3.0934201	-1.4610680
C	1.0537891	-2.4924437	-0.4596125
H	5.6686162	0.9914218	-3.5466843
H	2.4092143	0.6544127	-0.5187081
H	3.4398026	-2.8145667	-2.9030535
H	0.6545688	-0.6696331	0.6573434
H	1.6807257	-4.1444268	-1.7269960
H	0.2834475	-3.0757325	0.0556823

Dimer-10

C	-3.8330542	3.0542710	-0.1516454
C	-3.3299032	2.1869935	0.5506392

C	-2.7340341	1.1681726	1.3605674
C	-3.4568611	-0.0073196	1.6824960
C	-1.4083107	1.3166799	1.8383362
C	-2.8624051	-1.0097382	2.4616191
C	-0.8246785	0.3111932	2.6187008
C	-1.5467892	-0.8540441	2.9339848
H	-4.2856601	3.8288891	-0.7403025
H	-4.4811777	-0.1218876	1.3160297
H	-0.8412285	2.2114749	1.5715447
H	-3.4297903	-1.9150474	2.7019177
H	0.2017840	0.4362198	2.9767100
H	-1.0859757	-1.6384640	3.5436024
C	2.1148011	3.7077861	-0.8251943
C	1.5250412	2.6353861	-0.8500053
C	0.8307719	1.3830170	-0.8692911
C	-0.4801912	1.2966430	-1.3996533
C	1.4401553	0.2155081	-0.3442110
C	-1.1633113	0.0734422	-1.3959051
C	0.7475850	-1.0023093	-0.3450469
C	-0.5551233	-1.0786699	-0.8695931
H	2.6357713	4.6459554	-0.8146241
H	-0.9633488	2.1978440	-1.7854045
H	2.4532765	0.2793359	0.0633257
H	-2.1840310	0.0283880	-1.7868267
H	1.2254320	-1.8953465	0.0705619
H	-1.0970902	-2.0295058	-0.8572033

Dimer-11 (D9)

C	3.8137378	-1.8639737	1.7551186
C	3.2303522	-0.8534058	2.1236250
C	2.5161538	0.3101749	2.5555749
C	1.9372201	1.1911778	1.6074737
C	2.3618865	0.5868775	3.9374990
C	1.2227644	2.3188192	2.0352713
C	1.6457810	1.7169405	4.3559410
C	1.0743094	2.5859782	3.4085501
H	4.3301966	-2.7476228	1.4317919
H	2.0497760	0.9753812	0.5416564
H	2.8020906	-0.0952763	4.6696858
H	0.7775512	2.9905905	1.2941573
H	1.5306442	1.9192090	5.4257857
H	0.5136977	3.4661856	3.7390452
C	0.1243037	-5.4660892	1.4938516
C	-0.4203621	-4.4326887	1.8609342
C	-1.0605490	-3.2250600	2.2906329
C	-2.4550737	-3.2060599	2.5494728
C	-0.3100560	-2.0339961	2.4628470
C	-3.0785879	-2.0229583	2.9696560
C	-0.9423990	-0.8555135	2.8835256
C	-2.3258575	-0.8459760	3.1377949

H	0.6012975	-6.3718899	1.1721369
H	-3.0352378	-4.1238935	2.4167569
H	0.7646053	-2.0447032	2.2641903
H	-4.1562960	-2.0197705	3.1664955
H	-0.3521235	0.0566344	3.0125707
H	-2.8171525	0.0760436	3.4662827

Dimer-12 (D10)

C	-2.1084000	-2.5993328	-4.0693490
C	-1.5570394	-2.9527582	-3.0355789
C	-0.8968348	-3.3451479	-1.8268265
C	-1.3973433	-2.9290763	-0.5672641
C	0.2735180	-4.1440445	-1.8740786
C	-0.7410119	-3.3060306	0.6126444
C	0.9227177	-4.5158459	-0.6886109
C	0.4193045	-4.0997314	0.5574465
H	-2.6017659	-2.3031635	-4.9754809
H	-2.2963663	-2.3079570	-0.5290663
H	0.6644649	-4.4605843	-2.8448781
H	-1.1349210	-2.9770423	1.5794491
H	1.8270928	-5.1305214	-0.7371277
H	0.9302718	-4.3902636	1.4809473
C	3.2429849	4.0400564	-3.3989019
C	2.8625928	2.9859610	-2.9053595
C	2.4174250	1.7525790	-2.3281097
C	1.3866221	0.9982224	-2.9450168
C	3.0012429	1.2670181	-1.1302955
C	0.9542213	-0.2081110	-2.3762060
C	2.5615118	0.0592920	-0.5696338
C	1.5386182	-0.6826401	-1.1877849
H	3.5765773	4.9639288	-3.8313111
H	0.9349144	1.3709497	-3.8689999
H	3.7963589	1.8465759	-0.6520382
H	0.1584868	-0.7829084	-2.8593724
H	3.0204515	-0.3047803	0.3557430
H	1.1972808	-1.6244978	-0.7489416

Dimer-13 (D11)

C	-0.2903567	3.3166395	1.5562591
C	-0.0487707	2.4181975	0.7600704
C	0.2340597	1.3670846	-0.1713967
C	-0.6873745	0.3054281	-0.3621158
C	1.4402486	1.3722357	-0.9173979
C	-0.4071705	-0.7213715	-1.2744380
C	1.7116142	0.3407292	-1.8274915
C	0.7918324	-0.7079263	-2.0098155
H	-0.5017255	4.1042310	2.2539610
H	-1.6179579	0.3001126	0.2128583
H	2.1527120	2.1895904	-0.7726796
H	-1.1243598	-1.5354403	-1.4148604

H	2.6466783	0.3563946	-2.3979476
H	1.0057353	-1.5114187	-2.7209406
C	1.4082549	-3.9240706	-4.7086815
C	0.3866468	-3.8734557	-4.0366982
C	-0.8013532	-3.7938461	-3.2409076
C	-0.8447303	-4.3864353	-1.9536358
C	-1.9460013	-3.1114097	-3.7249135
C	-2.0062094	-4.2971062	-1.1739671
C	-3.1029937	-3.0272111	-2.9379937
C	-3.1379442	-3.6187402	-1.6620454
H	2.2988955	-3.9828563	-5.3048668
H	0.0392298	-4.9078210	-1.5767828
H	-1.9118203	-2.6489935	-4.7149814
H	-2.0274871	-4.7561695	-0.1802377
H	-3.9801026	-2.4951537	-3.3204388
H	-4.0423569	-3.5489957	-1.0494348

Dimer-14

C	2.0810574	-0.2674870	-1.4519770
C	1.9369829	-1.2568479	-0.7460699
C	1.7603676	-2.4133041	0.0801049
C	1.8635835	-2.3122044	1.4907187
C	1.4707105	-3.6742106	-0.5006108
C	1.6800248	-3.4450487	2.2956383
C	1.2878702	-4.8014434	0.3127138
C	1.3929771	-4.6915411	1.7109540
H	2.2133343	0.5991784	-2.0710706
H	2.0821371	-1.3400040	1.9405104
H	1.3876924	-3.7533786	-1.5879043
H	1.7558570	-3.3532366	3.3838711
H	1.0600130	-5.7686292	-0.1467917
H	1.2472650	-5.5732021	2.3426766
C	-4.0831027	-5.7471584	4.6732785
C	-3.8154431	-4.9134008	3.8177014
C	-3.5006170	-3.9380535	2.8165773
C	-4.4887142	-3.0265330	2.3646888
C	-2.1968710	-3.8693165	2.2638247
C	-4.1746753	-2.0737305	1.3852678
C	-1.8909309	-2.9142076	1.2850861
C	-2.8775526	-2.0143893	0.8431378
H	-4.3197897	-6.4774299	5.4231529
H	-5.4954629	-3.0770606	2.7892440
H	-1.4296369	-4.5676914	2.6077092
H	-4.9460580	-1.3744803	1.0445250
H	-0.8804351	-2.8732739	0.8698369
H	-2.6352874	-1.2681871	0.0796012

Dimer-15 (D12)

C	-2.5749399	1.9373867	-0.0952805
C	-1.6855365	2.3449832	-0.8298447

C	-0.6262396	2.8593338	-1.6444611
C	-0.5661801	2.5824570	-3.0336672
C	0.3818964	3.6676626	-1.0582361
C	0.4764196	3.1034197	-3.8134868
C	1.4193960	4.1828160	-1.8472538
C	1.4722620	3.9043987	-3.2253670
H	-3.3370722	1.6196380	0.5904952
H	-1.3417961	1.9597792	-3.4891065
H	0.3361499	3.8816879	0.0137358
H	0.5117593	2.8835476	-4.8858523
H	2.1916084	4.8063000	-1.3838143
H	2.2846737	4.3094196	-3.8380319
C	0.5389513	4.4617678	2.7517516
C	-0.5782479	3.9680207	2.8300787
C	-1.8846300	3.3903481	2.9250769
C	-3.0289980	4.1351653	2.5454978
C	-2.0498629	2.0634043	3.3948697
C	-4.3051153	3.5633897	2.6345798
C	-3.3302273	1.4994351	3.4807378
C	-4.4619295	2.2451243	3.1012001
H	1.5187741	4.8954801	2.6932484
H	-2.9029910	5.1559514	2.1742909
H	-1.1676911	1.4848526	3.6822314
H	-5.1811388	4.1478457	2.3352947
H	-3.4453170	0.4734481	3.8451062
H	-5.4606205	1.8017427	3.1698700

Dimer-16 (D13)

C	1.9350712	-1.8882687	-5.1961718
C	1.7972838	-1.6211431	-4.0096796
C	1.6346667	-1.3072883	-2.6214672
C	0.7863811	-0.2447901	-2.2188712
C	2.3161447	-2.0580359	-1.6294928
C	0.6248473	0.0551789	-0.8588953
C	2.1499218	-1.7493974	-0.2721027
C	1.3053682	-0.6936147	0.1178874
H	2.0539547	-2.1225838	-6.2369172
H	0.2469741	0.3323562	-2.9742917
H	2.9703627	-2.8787151	-1.9375259
H	-0.0472336	0.8689810	-0.5696348
H	2.6806045	-2.3369019	0.4849881
H	1.1766753	-0.4583292	1.1794507
C	-1.8177031	2.3945413	-2.3968953
C	-2.5405874	1.4285886	-2.1887370
C	-3.3943126	0.3041325	-1.9442493
C	-4.7954305	0.4853062	-1.8186476
C	-2.8536564	-1.0016206	-1.8265261
C	-5.6313556	-0.6145751	-1.5818065
C	-3.6989610	-2.0947700	-1.5900333
C	-5.0873085	-1.9067827	-1.4668974

H	-1.1833364	3.2394997	-2.5848875
H	-5.2137169	1.4918614	-1.9096672
H	-1.7742881	-1.1446613	-1.9180074
H	-6.7120078	-0.4628174	-1.4869193
H	-3.2705708	-3.0987600	-1.5015484
H	-5.7438673	-2.7635695	-1.2825895

Dimer-17 (D14)

C	-0.3891300	2.5582635	-0.1401571
C	-0.3933638	2.8718597	1.0431821
C	-0.3913965	3.2400228	2.4279034
C	-1.1352690	4.3603680	2.8788193
C	0.3551010	2.4885160	3.3713976
C	-1.1304224	4.7146551	4.2352010
C	0.3537171	2.8503580	4.7257452
C	-0.3877050	3.9627247	5.1634209
H	-0.3896074	2.2724698	-1.1759264
H	-1.7119858	4.9428343	2.1545563
H	0.9310649	1.6246976	3.0272603
H	-1.7095416	5.5817946	4.5704151
H	0.9341450	2.2613822	5.4439669
H	-0.3865179	4.2423503	6.2222875
C	2.7560718	-0.9752858	-2.6208444
C	1.7739263	-0.2890829	-2.8710348
C	0.6257101	0.5150533	-3.1624737
C	-0.6808099	0.0180948	-2.9222783
C	0.7783799	1.8226401	-3.6906989
C	-1.8017189	0.8115720	-3.2039743
C	-0.3490490	2.6084432	-3.9691012
C	-1.6414689	2.1074171	-3.7277749
H	3.6173065	-1.5763785	-2.3994841
H	-0.8006759	-0.9869225	-2.5088961
H	1.7846943	2.2096566	-3.8721778
H	-2.8047418	0.4197783	-3.0076886
H	-0.2186247	3.6177909	-4.3720306
H	-2.5189673	2.7258309	-3.9411455

Dimer-18 (D15)

C	0.0510225	0.2872865	-1.1490906
C	0.8631966	-0.6169881	-1.2967104
C	1.8130382	-1.6753497	-1.4689102
C	2.9883005	-1.7249066	-0.6762611
C	1.5902857	-2.6932861	-2.4313026
C	3.9122411	-2.7654619	-0.8454168
C	2.5201530	-3.7297596	-2.5927840
C	3.6827709	-3.7704413	-1.8022795
H	-0.6880353	1.0510568	-0.9825277
H	3.1632378	-0.9412427	0.0664445
H	0.6854257	-2.6574830	-3.0447439
H	4.8162879	-2.7925095	-0.2276530

H	2.3373357	-4.5095176	-3.3399158
H	4.4070612	-4.5815771	-1.9317098
C	-2.7474413	2.4543153	0.1458737
C	-3.0068143	1.3756500	0.6650332
C	-3.3308099	0.1231564	1.2819422
C	-4.5457286	-0.0215203	1.9996245
C	-2.4484768	-0.9826504	1.1860049
C	-4.8662860	-1.2442560	2.6050377
C	-2.7795099	-2.2009088	1.7956188
C	-3.9859102	-2.3370689	2.5057433
H	-2.5248836	3.4052391	-0.2995508
H	-5.2269476	0.8310000	2.0738208
H	-1.5123785	-0.8786366	0.6307973
H	-5.8071551	-1.3453832	3.1564961
H	-2.0911080	-3.0487637	1.7149442
H	-4.2401867	-3.2909392	2.9799758

Dimer-19 (D8)

C	0.3808224	2.2970985	2.5767165
C	1.5080895	2.4088769	1.7421879
C	-0.8624682	1.9403411	2.0247986
H	2.4785276	2.6892278	2.1651723
H	-1.7418325	1.8473564	2.6702556
C	1.3959260	2.1661061	0.3666204
C	-0.9839250	1.6940956	0.6507828
H	2.2701396	2.2493039	-0.2854907
H	-1.9448629	1.3983273	0.2220501
C	0.1463757	1.8020137	-0.1960433
H	0.4715879	2.4883789	3.6509374
C	0.0357750	1.5212333	-1.5943551
C	-0.0522313	1.2527376	-2.7846719
H	-0.1307700	0.9829311	-3.8196491
C	-0.4215748	-1.5904188	1.8439258
C	0.8035134	-1.3130395	1.2140313
C	-1.5075836	-2.0609487	1.0843692
H	1.6432194	-0.9240539	1.7972156
H	-2.4656909	-2.2751654	1.5695226
C	0.9484916	-1.5059109	-0.1656745
C	-1.3724174	-2.2570385	-0.2969683
H	1.8946988	-1.2749075	-0.6619933
H	-2.2142112	-2.6244183	-0.8911660
C	-0.1381761	-1.9848371	-0.9392691
H	-0.5334788	-1.4284698	2.9204721
C	0.0077984	-2.1941266	-2.3477851
C	0.1348366	-2.3864386	-3.5499914
H	0.2494214	-2.5582569	-4.6029259

Trimer

Trimer-01 (T1)

C	-4.7391921	-2.7049565	-5.5465996
C	-3.5750624	-2.5359914	-5.2077600
C	-2.2216651	-2.3428681	-4.7811801
C	-1.7648278	-1.0547082	-4.4068253
C	-1.3299387	-3.4431992	-4.7044958
C	-0.4478354	-0.8751892	-3.9631707
C	-0.0132049	-3.2522004	-4.2623596
C	0.4314720	-1.9697327	-3.8909873
H	-5.7500695	-2.8502284	-5.8756234
H	-2.4564541	-0.2101101	-4.4447019
H	-1.6844477	-4.4388192	-4.9855163
H	-0.1145810	0.1186354	-3.6554282
H	0.6648361	-4.1093191	-4.2001055
H	1.4560063	-1.8269859	-3.5334917
C	-4.5354077	1.8810604	-3.4668626
C	-3.4039251	1.9174156	-3.0015388
C	-2.0690233	1.9287570	-2.4835424
C	-1.0718247	2.7350841	-3.0889993
C	-1.7228126	1.1132238	-1.3778694
C	0.2399470	2.7225675	-2.5941439
C	-0.4086681	1.1064166	-0.8916929
C	0.5756312	1.9100650	-1.4945600
H	-5.5326253	1.8666163	-3.8621945
H	-1.3374530	3.3598431	-3.9464540
H	-2.4834560	0.4774345	-0.9221975
H	1.0032292	3.3455517	-3.0714883
H	-0.1497706	0.4534149	-0.0539026
H	1.6022126	1.9004881	-1.1137630
C	0.9062742	-2.5644104	0.5134828
C	-0.2812143	-2.3639692	0.2944640
C	-1.6660309	-2.1001715	0.0429284
C	-2.2327230	-2.3745025	-1.2262854
C	-2.4811866	-1.5396820	1.0592686
C	-3.5854325	-2.0993746	-1.4684250
C	-3.8319536	-1.2631964	0.8056781
C	-4.3887549	-1.5446797	-0.4560963
H	1.9389226	-2.7743354	0.7154369
H	-1.6020348	-2.7839291	-2.0169321
H	-2.0422150	-1.3216612	2.0369686
H	-4.0073195	-2.3041183	-2.4562778
H	-4.4501809	-0.8217653	1.5937915
H	-5.4423425	-1.3219842	-0.6520646

Trimer-02 (T1)

C	2.1025539	-1.3773795	2.1772573
C	1.5293979	-1.3369628	1.0971251
C	0.8681684	-1.3296335	-0.1722996

C	1.3365727	-0.5062508	-1.2271094
C	-0.2503645	-2.1701239	-0.3964038
C	0.6978745	-0.5279527	-2.4751909
C	-0.8841268	-2.1804449	-1.6456153
C	-0.4155445	-1.3620003	-2.6887724
H	2.5849707	-1.4129926	3.1345304
H	2.2035630	0.1385456	-1.0575821
H	-0.5983664	-2.8231507	0.4049844
H	1.0736023	0.1048627	-3.2854572
H	-1.7358880	-2.8476340	-1.8058181
H	-0.9065837	-1.3808340	-3.6668579
C	2.2696049	-5.1352421	3.4712283
C	1.3162324	-5.1526241	2.7040952
C	0.1943288	-5.1894075	1.8149758
C	0.3554317	-5.6140601	0.4727301
C	-1.0936898	-4.8047508	2.2675275
C	-0.7462825	-5.6566381	-0.3920545
C	-2.1910284	-4.8545977	1.3959281
C	-2.0221931	-5.2828905	0.0656908
H	3.1043228	-5.1265083	4.1450545
H	1.3468749	-5.8973372	0.1174184
H	-1.2187557	-4.4696153	3.3009273
H	-0.6006979	-5.9670156	-1.4306650
H	-3.1804903	-4.5563331	1.7567917
H	-2.8819142	-5.3178834	-0.6116389
C	0.2883641	-5.4442239	-4.5232646
C	1.1303667	-5.3459337	-3.6400218
C	2.0952805	-5.2457823	-2.5864485
C	2.3011904	-4.0146296	-1.9159347
C	2.8387198	-6.3851989	-2.1861286
C	3.2249898	-3.9301807	-0.8657879
C	3.7636422	-6.2890625	-1.1368314
C	3.9593537	-5.0633436	-0.4735382
H	-0.4211981	-5.5245909	-5.3240445
H	1.7194957	-3.1403680	-2.2114621
H	2.6768588	-7.3368268	-2.7003750
H	3.3507993	-2.9827665	-0.3352922
H	4.3255356	-7.1767453	-0.8294114
H	4.6712885	-4.9964434	0.3549912

Trimer-03 (T3)

C	-0.1388440	-1.9750228	5.5526116
C	1.2256811	-1.6768800	5.7949594
C	-0.4655041	-3.0487374	4.6855736
C	2.2340920	-2.4216762	5.1712102
C	0.5525011	-3.7946090	4.0734422
C	1.9038642	-3.4819318	4.3083945
C	1.3963806	-0.1256407	1.2607825
C	1.8067970	1.1621996	0.8317602
C	0.8108726	-0.2740952	2.5422252

C	1.6271659	2.2730567	1.6679741
C	0.6276720	0.8436191	3.3675727
C	1.0328460	2.1191628	2.9350693
C	1.5923761	-1.2662124	0.4174912
C	1.7895966	-2.2452055	-0.2900665
C	-1.1711976	-1.1856300	6.1536804
C	-2.0517666	-0.4912857	6.6445455
H	1.4811316	-0.8473473	6.4600316
H	-1.5173823	-3.2771067	4.4931918
H	3.2809718	-2.1614301	5.3419445
H	0.2876928	-4.6157202	3.3998577
H	2.2673900	1.2756833	-0.1536477
H	0.5156116	-1.2668403	2.8857541
H	1.9515050	3.2619951	1.3283872
H	0.1690845	0.7110479	4.3515906
H	0.8890573	2.9910969	3.5816513
H	1.9446961	-3.1005169	-0.9187937
H	-2.8287611	0.0955304	7.0955860
H	2.6970466	-4.0495976	3.8129165
C	5.2048306	-2.3881585	3.3060726
C	4.3867369	-1.3806079	2.7374865
C	5.9099975	-2.1130355	4.5053999
C	4.2728580	-0.1298154	3.3591518
C	5.7938361	-0.8565780	5.1171274
C	4.9757036	0.1372984	4.5473770
C	5.2976621	-3.6785362	2.6919622
C	5.3580254	-4.7897519	2.1820369
H	3.8307757	-1.5972944	1.8230165
H	6.5363443	-2.8925155	4.9480739
H	3.6192836	0.6294450	2.9223489
H	6.3408853	-0.6552849	6.0438652
H	5.4389461	-5.7539686	1.7183817
H	4.8827249	1.1148963	5.0316336

Trimer-04 (T6)

C	-4.9864586	-2.1766642	3.2464910
C	-3.8979928	-2.4521492	2.7588754
C	-2.6123603	-2.7489514	2.2022877
C	-2.3489094	-2.5039332	0.8319133
C	-1.5812011	-3.2718318	3.0236180
C	-1.0834854	-2.7809200	0.2980719
C	-0.3180488	-3.5449437	2.4798612
C	-0.0657927	-3.3031178	1.1162536
H	-5.9496387	-1.9655185	3.6692562
H	-3.1337055	-2.0817130	0.2023127
H	-1.7826102	-3.4552880	4.0827770
H	-0.8863599	-2.5662053	-0.7556377
H	0.4722310	-3.9442165	3.1237163
H	0.9228234	-3.5147799	0.6957285
C	-2.3960109	5.5295015	1.5841948

C	-2.0371123	4.3688385	1.7338176
C	-1.6209041	3.0092441	1.9039272
C	-2.4632892	2.0752974	2.5601157
C	-0.3639884	2.5734395	1.4114999
C	-2.0610959	0.7410903	2.7071305
C	0.0301431	1.2369928	1.5681859
C	-0.8158921	0.3162426	2.2110768
H	-2.7074121	6.5482330	1.4554958
H	-3.4319506	2.4098842	2.9424374
H	0.2859345	3.2903545	0.9021613
H	-2.7293604	0.0243538	3.1920922
H	0.9951433	0.9088348	1.1701443
H	-0.5163611	-0.7297203	2.3094187
C	0.3092106	-0.0405578	-2.4751290
C	-0.8748438	-0.0885789	-2.1683356
C	-2.2559474	-0.1727382	-1.8003565
C	-3.1165452	-1.0877734	-2.4586166
C	-2.7755760	0.6422024	-0.7646181
C	-4.4642498	-1.1822450	-2.0841525
C	-4.1250026	0.5427888	-0.4012022
C	-4.9738816	-0.3666606	-1.0563668
H	1.3379642	0.0323815	-2.7703825
H	-2.7155069	-1.7203269	-3.2556238
H	-2.1145671	1.3353681	-0.2431390
H	-5.1173885	-1.8979150	-2.5935145
H	-4.5063655	1.1713908	0.4085474
H	-6.0255321	-0.4472966	-0.7634563

Trimer-05 (T4)

C	-3.8166071	-0.9167778	2.3002181
C	-2.9160301	-1.7279050	2.4709192
C	-1.8662756	-2.6808804	2.6712135
C	-2.1541568	-3.9659789	3.1990396
C	-0.5259916	-2.3586404	2.3383478
C	-1.1241565	-4.9004206	3.3813892
C	0.4945577	-3.3000218	2.5245839
C	0.2013978	-4.5735090	3.0434436
H	-4.6070087	-0.2059593	2.1538635
H	-3.1867167	-4.2170851	3.4569660
H	-0.3031028	-1.3759250	1.9156246
H	-1.3604215	-5.8908022	3.7844441
H	1.5198103	-3.0461912	2.2474237
H	0.9990796	-5.3119597	3.1625438
C	-0.9035914	-1.4929761	-1.4933112
C	-0.7725243	-2.7095300	-1.4705916
C	-0.6011697	-4.1302509	-1.4350006
C	-0.0366872	-4.8143905	-2.5413450
C	-0.9796519	-4.8682232	-0.2862906
C	0.1448624	-6.2038543	-2.4935143
C	-0.7938112	-6.2562520	-0.2487403

C	-0.2328269	-6.9300786	-1.3484063
H	-1.0631022	-0.4324970	-1.5208529
H	0.2575263	-4.2462428	-3.4283198
H	-1.4037301	-4.3452342	0.5711759
H	0.5863467	-6.7208907	-3.3513952
H	-1.0764388	-6.8090459	0.6519966
H	-0.0833463	-8.0137242	-1.3126538
C	2.8912250	-7.6042094	2.0235595
C	3.0519072	-6.4586003	1.6235105
C	3.2223368	-5.1082437	1.1780843
C	4.0654665	-4.2203756	1.8934774
C	2.5353777	-4.6378806	0.0316884
C	4.2152035	-2.8936683	1.4656363
C	2.6900150	-3.3096474	-0.3863312
C	3.5299243	-2.4342243	0.3250824
H	2.7790942	-8.6180619	2.3565114
H	4.5923233	-4.5814501	2.7811445
H	1.8721566	-5.3140802	-0.5090725
H	4.8660335	-2.2156601	2.0270475
H	2.1331093	-2.9525766	-1.2568017
H	3.6458030	-1.3960754	-0.0026043

Trimer-06 (T5)

C	4.0846412	-0.1501883	3.1940883
C	3.5921556	-0.1664178	2.0737995
C	2.9806587	-0.2009220	0.7794200
C	2.1035582	0.8359947	0.3747989
C	3.2210733	-1.2866573	-0.1006328
C	1.4778471	0.7826100	-0.8777398
C	2.5981823	-1.3259584	-1.3561746
C	1.7259933	-0.2931232	-1.7484438
H	4.5383118	-0.1245143	4.1660918
H	1.8994880	1.6603038	1.0610864
H	3.8907372	-2.0918354	0.2143833
H	0.7811200	1.5743889	-1.1637603
H	2.7919248	-2.1683982	-2.0281288
H	1.2373644	-0.3302784	-2.7276623
C	-0.5590374	0.1903775	5.9597340
C	-0.7855915	-0.2456367	4.8388096
C	-1.0594648	-0.7764669	3.5374363
C	-2.3822463	-1.1426729	3.1793752
C	-0.0157640	-0.9499397	2.5942476
C	-2.6464228	-1.6826213	1.9123200
C	-0.2905716	-1.4888306	1.3298698
C	-1.6021531	-1.8612491	0.9861770
H	-0.3650685	0.5671664	6.9453656
H	-3.1895364	-1.0017787	3.9035272
H	1.0011294	-0.6536362	2.8599324
H	-3.6714639	-1.9636980	1.6495222
H	0.5204948	-1.6049303	0.6074572

H	-1.8116002	-2.2795569	-0.0036772
C	0.3368629	2.8326258	3.4233574
C	-0.1772472	2.8381065	2.3135205
C	-0.7606984	2.7915075	1.0076925
C	-1.6176579	1.7194396	0.6549622
C	-0.4741736	3.7928287	0.0458859
C	-2.1703526	1.6540104	-0.6305670
C	-1.0335445	3.7187428	-1.2379539
C	-1.8834411	2.6505221	-1.5813585
H	0.7562379	2.8137525	4.4100284
H	-1.8299022	0.9415431	1.3901259
H	0.1893468	4.6192786	0.3159157
H	-2.8243053	0.8156193	-0.8905811
H	-0.8038129	4.4968427	-1.9730562
H	-2.3181944	2.5968106	-2.5849495

Trimer-07

C	0.2325864	-1.7020091	-4.3058385
C	1.0088718	-2.0430644	-3.4231528
C	1.8986915	-2.4415278	-2.3743506
C	2.9116133	-1.5627551	-1.9178509
C	1.7625022	-3.7163095	-1.7680836
C	3.7702899	-1.9539567	-0.8815482
C	2.6243118	-4.0979983	-0.7301663
C	3.6317889	-3.2206229	-0.2857057
H	-0.4251262	-1.4169037	-5.1042417
H	3.0061609	-0.5748044	-2.3701972
H	0.9777795	-4.3935699	-2.1167919
H	4.5418497	-1.2613775	-0.5328714
H	2.5082413	-5.0828050	-0.2664563
H	4.3037493	-3.5238060	0.5237804
C	0.2046965	2.5047308	3.8259446
C	0.0046272	1.7230718	2.9053514
C	-0.2212406	0.8163225	1.8205686
C	0.6503870	-0.2813355	1.6067287
C	-1.3143652	1.0081773	0.9366227
C	0.4445441	-1.1502694	0.5276009
C	-1.5159005	0.1276960	-0.1363207
C	-0.6356021	-0.9487057	-0.3490022
H	0.3742360	3.1859307	4.6375556
H	1.4936986	-0.4324719	2.2864555
H	-1.9898727	1.8524389	1.1000559
H	1.1364361	-1.9785294	0.3620052
H	-2.3606069	0.2884447	-0.8142186
H	-0.7771704	-1.6164708	-1.2033467
C	6.3537413	1.1771130	0.5198595
C	5.3602883	1.4010934	-0.1595270
C	4.1932781	1.6286063	-0.9576264
C	4.3103060	1.8772665	-2.3492377
C	2.9041339	1.5842105	-0.3709364

C	3.1610529	2.0730526	-3.1281230
C	1.7613790	1.7730479	-1.1586031
C	1.8848622	2.0196492	-2.5371194
H	7.2283792	1.0172024	1.1206302
H	5.3039936	1.9069643	-2.8046980
H	2.8064037	1.3858464	0.6986783
H	3.2626668	2.2583494	-4.2021724
H	0.7747793	1.7093281	-0.6942723
H	0.9901222	2.1578871	-3.1519807

Trimer-08

C	-1.1476795	3.4217540	-3.2472235
C	-0.7045967	3.6560383	-2.1305406
C	-0.1762731	3.9442556	-0.8315428
C	1.1793413	3.6559380	-0.5278053
C	-0.9964841	4.5249005	0.1682551
C	1.6964710	3.9505831	0.7424984
C	-0.4693068	4.8198928	1.4318290
C	0.8760536	4.5359835	1.7240214
H	-1.5279281	3.2163783	-4.2293477
H	1.8132197	3.2011269	-1.2941711
H	-2.0477243	4.7271789	-0.0495869
H	2.7433794	3.7203349	0.9656743
H	-1.1140510	5.2603818	2.1939523
H	1.2770723	4.7572849	2.7180408
C	-3.1724027	1.5272066	-0.6889526
C	-2.6332494	1.1820205	0.3536296
C	-1.9955182	0.8310236	1.5857897
C	-2.6601213	0.0244567	2.5439947
C	-0.6951675	1.3161377	1.8733542
C	-2.0374413	-0.2792160	3.7632931
C	-0.0843135	1.0103174	3.0959255
C	-0.7504001	0.2148846	4.0453809
H	-3.6008283	1.8212522	-1.6270130
H	-3.6644192	-0.3489817	2.3247820
H	-0.1849124	1.9434637	1.1415427
H	-2.5611721	-0.8971480	4.4994848
H	0.9117796	1.4073719	3.3139152
H	-0.2744989	-0.0107437	5.0047468
C	-0.4962920	3.8806425	6.5664648
C	-1.2954635	4.1592717	5.6821054
C	-2.2113603	4.4875960	4.6311756
C	-2.7230761	3.4725016	3.7850516
C	-2.5990911	5.8339759	4.4087811
C	-3.5906877	3.8000666	2.7349418
C	-3.4710688	6.1508739	3.3572462
C	-3.9669207	5.1368699	2.5163985
H	0.1877374	3.6362690	7.3561791
H	-2.4198930	2.4375999	3.9477130
H	-2.2044833	6.6195329	5.0593695

H	-3.9520335	3.0101932	2.0709072
H	-3.7600561	7.1933747	3.1899866
H	-4.6377965	5.3906401	1.6892756

Trimer-09

C	-1.2051736	0.3557707	5.1003506
C	-0.9417126	0.0115626	3.9555952
C	-0.5958761	-0.3763026	2.6216039
C	-0.5091151	0.5950525	1.5935937
C	-0.3069263	-1.7310188	2.3161850
C	-0.1339047	0.2224413	0.2971173
C	0.0630448	-2.0955262	1.0138306
C	0.1535362	-1.1215922	0.0016070
H	-1.4615339	0.6497420	6.0999066
H	-0.7159340	1.6426641	1.8243186
H	-0.3683789	-2.4816101	3.1091025
H	-0.0500424	0.9882920	-0.4766809
H	0.2867457	-3.1437975	0.7903268
H	0.4542058	-1.4074004	-1.0113222
C	2.6113303	4.5347269	4.6476413
C	2.9876400	3.5383365	4.0442861
C	3.4135647	2.3852583	3.3095277
C	4.7125204	2.3335599	2.7420758
C	2.5329096	1.2913996	3.1201084
C	5.1129906	1.2126078	2.0014710
C	2.9379214	0.1814664	2.3669063
C	4.2273760	0.1357465	1.8088427
H	2.2969878	5.3953805	5.2060615
H	5.3912746	3.1790797	2.8841604
H	1.5324579	1.3255942	3.5570064
H	6.1152652	1.1860642	1.5625724
H	2.2359103	-0.6398560	2.2026110
H	4.5379570	-0.7294099	1.2149400
C	3.9401513	0.8374358	-2.6416598
C	3.1189402	1.5572915	-2.0888885
C	2.1488772	2.3900238	-1.4436127
C	2.3079692	2.7554686	-0.0840828
C	1.0078739	2.8447438	-2.1529757
C	1.3474999	3.5555014	0.5493633
C	0.0492441	3.6397989	-1.5089244
C	0.2157105	3.9986213	-0.1576829
H	4.6704386	0.2244189	-3.1336675
H	3.1774501	2.3966191	0.4674194
H	0.8825914	2.5620133	-3.2020099
H	1.4860888	3.8246534	1.6006028
H	-0.8304245	3.9805523	-2.0643131
H	-0.5351212	4.6214407	0.3396012

Trimer-10

C	-1.5881943	0.3147550	-3.8755863
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C	-0.4848574	-0.2147593	-3.8901211
C	0.7941864	-0.8583038	-3.9039595
C	1.7231320	-0.6353260	-2.8578955
C	1.1381977	-1.7414539	-4.9590201
C	2.9708445	-1.2738043	-2.8750784
C	2.3862469	-2.3799694	-4.9645580
C	3.3076483	-2.1450487	-3.9265002
H	-2.5429524	0.8043512	-3.8788260
H	1.4528485	0.0266706	-2.0334941
H	0.4186957	-1.9201310	-5.7631338
H	3.6762064	-1.0963360	-2.0581421
H	2.6396607	-3.0636391	-5.7810765
H	4.2826766	-2.6432064	-3.9363808
C	-3.3622219	-5.0338220	1.8628923
C	-2.5381302	-4.7635852	0.9988363
C	-1.5711111	-4.4436351	-0.0074289
C	-0.2295765	-4.8881619	0.1176962
C	-1.9361594	-3.6715113	-1.1402093
C	0.7154940	-4.5624902	-0.8652510
C	-0.9806134	-3.3467556	-2.1127261
C	0.3476235	-3.7880169	-1.9797387
H	-4.0847251	-5.2735267	2.6190779
H	0.0543895	-5.4846692	0.9893107
H	-2.9692773	-3.3261592	-1.2385758
H	1.7485678	-4.9082352	-0.7559452
H	-1.2679113	-2.7284942	-2.9672350
H	1.0917104	-3.5165003	-2.7321069
C	5.2721838	-0.6414955	0.6463100
C	4.0606509	-0.4679907	0.6225225
C	2.6437598	-0.2710258	0.5580521
C	2.1021494	1.0371714	0.4735634
C	1.7647962	-1.3826574	0.5502287
C	0.7147850	1.2200755	0.3849886
C	0.3806682	-1.1901983	0.4567955
C	-0.1491187	0.1091693	0.3761924
H	6.3337580	-0.7880293	0.7022135
H	2.7786983	1.8963228	0.4699839
H	2.1762669	-2.3937303	0.5968720
H	0.3076550	2.2337290	0.3145377
H	-0.2806378	-2.0586521	0.4258702
H	-1.2307017	0.2557187	0.2955094

Trimer-11

C	-2.6648955	2.4608536	-0.0630061
C	-1.8117099	2.2753235	0.7950325
C	-0.8293310	2.0333158	1.8084329
C	0.4692309	1.5880342	1.4584606
C	-1.1544069	2.2154698	3.1765406
C	1.4184262	1.3314719	2.4559748
C	-0.1978659	1.9549789	4.1676214

C	1.0894786	1.5132918	3.8108397
H	-3.4056025	2.6531544	-0.8150491
H	0.7158003	1.4307040	0.4080527
H	-2.1572955	2.5584146	3.4473298
H	2.4142525	0.9776810	2.1750204
H	-0.4563071	2.1000213	5.2219687
H	1.8333527	1.3101446	4.5880204
C	0.3604897	-3.6583925	-2.2689173
C	0.0694062	-3.1853491	-1.1777206
C	-0.2419533	-2.5959642	0.0892600
C	-1.3849507	-1.7704319	0.2370081
C	0.6036106	-2.8121973	1.2070105
C	-1.6726638	-1.1813944	1.4747670
C	0.3056618	-2.2170299	2.4399306
C	-0.8313489	-1.4026479	2.5781598
H	0.6001976	-4.0992078	-3.2173604
H	-2.0297762	-1.5899957	-0.6273995
H	1.4927054	-3.4385917	1.0914920
H	-2.5391530	-0.5215957	1.5707658
H	0.9696874	-2.3788433	3.2948758
H	-1.0423135	-0.9127442	3.5325098
C	5.0404136	-0.3873008	1.1423671
C	4.2068118	0.0144858	0.3407778
C	3.2119259	0.4920350	-0.5719710
C	3.1718143	1.8616497	-0.9382434
C	2.2429676	-0.3947211	-1.1037991
C	2.1821096	2.3267005	-1.8150308
C	1.2560717	0.0803506	-1.9777943
C	1.2219178	1.4396839	-2.3362346
H	5.7911716	-0.7444499	1.8206531
H	3.9131565	2.5486831	-0.5210016
H	2.2609463	-1.4478603	-0.8179917
H	2.1537990	3.3866337	-2.0866187
H	0.5114005	-0.6183535	-2.3687796
H	0.4451127	1.8101623	-3.0120071

Trimer-12

C	1.9920745	3.2023152	-2.2613272
C	0.9402951	2.6000693	-2.4324739
C	-0.2877322	1.8889411	-2.6241957
C	-1.4955821	2.3714424	-2.0572822
C	-0.3143773	0.6868922	-3.3766593
C	-2.6918148	1.6618423	-2.2369353
C	-1.5147920	-0.0150926	-3.5467033
C	-2.7064627	0.4666404	-2.9776622
H	2.9138676	3.7315418	-2.1135236
H	-1.4785604	3.2981771	-1.4768224
H	0.6159104	0.3091191	-3.8102609
H	-3.6158883	2.0396468	-1.7872497
H	-1.5156906	-0.9572975	-4.1008474

H	-3.6343241	-0.0977745	-3.0964440
C	1.6553714	-4.9959467	-1.5208981
C	0.9081955	-4.1843519	-0.9905620
C	0.0512135	-3.2305990	-0.3537151
C	-0.6825546	-3.5870185	0.8069076
C	-0.0679482	-1.9144125	-0.8657036
C	-1.5027104	-2.6421694	1.4406799
C	-0.8879008	-0.9766408	-0.2251201
C	-1.6038159	-1.3346686	0.9307487
H	2.3151460	-5.7095979	-1.9755037
H	-0.5988553	-4.6036351	1.2010674
H	0.4755783	-1.6387519	-1.7716011
H	-2.0633838	-2.9290817	2.3362627
H	-0.9755197	0.0305969	-0.6379452
H	-2.2470610	-0.6002972	1.4259977
C	-1.0299398	-4.0604514	-3.9512799
C	-2.0997547	-3.5942678	-3.5842418
C	-3.3261308	-3.0179783	-3.1239051
C	-4.3486664	-2.6569059	-4.0371591
C	-3.5194602	-2.7813089	-1.7400650
C	-5.5372297	-2.0761177	-3.5719311
C	-4.7089261	-2.1970465	-1.2859359
C	-5.7222932	-1.8446552	-2.1959304
H	-0.0899580	-4.4916249	-4.2350554
H	-4.1979181	-2.8313465	-5.1061846
H	-2.7276027	-3.0439942	-1.0368689
H	-6.3207599	-1.8013675	-4.2853876
H	-4.8408494	-2.0104309	-0.2154628
H	-6.6511101	-1.3893999	-1.8369492

Trimer-13 (T7)

C	-2.0819480	-3.1832757	2.5015211
C	-1.0914454	-2.6928157	1.9745971
C	0.0519538	-2.1227584	1.3284840
C	0.2128391	-0.7171657	1.2658680
C	1.0202025	-2.9582838	0.7172048
C	1.3154374	-0.1646386	0.6006427
C	2.1191333	-2.3950874	0.0568079
C	2.2720698	-0.9979429	-0.0040779
H	-2.9222582	-3.6196982	3.0056362
H	-0.5394087	-0.0706215	1.7211830
H	0.8871206	-4.0427331	0.7504251
H	1.4097514	0.9227743	0.5322773
H	2.8491380	-3.0482686	-0.4308329
H	3.1199162	-0.5628259	-0.5414429
C	2.4743068	-0.4482991	-4.0315746
C	1.5755907	-1.1493216	-3.5841618
C	0.5394971	-1.9836233	-3.0535164
C	-0.4165668	-1.4560180	-2.1512224
C	0.4710648	-3.3537243	-3.4109969

C	-1.4081619	-2.2853776	-1.6139271
C	-0.5308492	-4.1732662	-2.8720763
C	-1.4718793	-3.6436461	-1.9704009
H	3.2559073	0.1618758	-4.4407320
H	-0.3501088	-0.4071689	-1.8609340
H	1.2084436	-3.7624553	-4.1079835
H	-2.1146925	-1.8774525	-0.8861136
H	-0.5748317	-5.2302057	-3.1555906
H	-2.2434172	-4.2891113	-1.5383039
C	0.1195092	2.3471068	-2.4165758
C	-0.5773269	2.2016496	-1.4216388
C	-1.3775802	1.9582899	-0.2608280
C	-2.4427969	1.0243948	-0.3161155
C	-1.1010736	2.6166933	0.9629586
C	-3.2027815	0.7510681	0.8287518
C	-1.8686082	2.3386113	2.1027918
C	-2.9197201	1.4048304	2.0417056
H	0.7223268	2.4574824	-3.2970292
H	-2.6572053	0.5173068	-1.2597607
H	-0.2792384	3.3366176	1.0081839
H	-4.0142048	0.0185640	0.7772710
H	-1.6419443	2.8483815	3.0444395
H	-3.5114316	1.1851217	2.9356746

Trimer-14 (T8)

C	-0.9051551	5.6558625	-5.0394684
C	-0.9230786	4.4578604	-5.2858358
C	-0.9663898	3.0447247	-5.5081879
C	-2.1941697	2.4080812	-5.8167955
C	0.2071559	2.2589064	-5.3811139
C	-2.2429799	1.0182800	-5.9872916
C	0.1469603	0.8688980	-5.5520131
C	-1.0766843	0.2430163	-5.8550160
H	-0.9018884	6.7059160	-4.8208256
H	-3.1035367	3.0053986	-5.8953991
H	1.1536644	2.7477823	-5.1343897
H	-3.2015438	0.5403957	-6.2118212
H	1.0567628	0.2703534	-5.4415118
H	-1.1199990	-0.8434489	-5.9824397
C	-0.3198093	5.8593479	0.1697214
C	-0.7341868	4.7544046	-0.1572367
C	-1.2240074	3.4636010	-0.5384140
C	-1.1396389	3.0310736	-1.8859688
C	-1.7999921	2.6033866	0.4305053
C	-1.6099467	1.7619660	-2.2478784
C	-2.2734710	1.3376408	0.0569135
C	-2.1759510	0.9122425	-1.2804889
H	0.0670246	6.8166178	0.4618703
H	-0.7213432	3.7011006	-2.6398941
H	-1.8683404	2.9373861	1.4698487

H	-1.5431386	1.4394439	-3.2888085
H	-2.7145510	0.6801345	0.8136623
H	-2.5447051	-0.0776573	-1.5694493
C	-3.2713219	5.9263229	-2.0590285
C	-3.8542860	5.1813460	-2.8341383
C	-4.5323416	4.2875357	-3.7210159
C	-4.7178037	2.9300564	-3.3554170
C	-5.0188170	4.7362668	-4.9749850
C	-5.3728398	2.0485981	-4.2259335
C	-5.6741624	3.8464267	-5.8381927
C	-5.8539681	2.5004260	-5.4680538
H	-2.7042137	6.5161278	-1.3646532
H	-4.3279808	2.5791068	-2.3973314
H	-4.8690807	5.7804767	-5.2622600
H	-5.5022892	1.0009027	-3.9357925
H	-6.0428477	4.2035565	-6.8050239
H	-6.3626468	1.8081348	-6.1467348

Trimer-15

C	-1.9113656	-5.4914156	3.5531023
C	-0.8518033	-4.9389085	3.8177531
C	0.3755060	-4.2682913	4.1246306
C	1.2845249	-3.9253843	3.0925215
C	0.6913878	-3.9268790	5.4642548
C	2.4782641	-3.2565224	3.3966243
C	1.8879372	-3.2580478	5.7584252
C	2.7852198	-2.9207863	4.7278586
H	-2.8282419	-6.0000747	3.3247513
H	1.0516373	-4.1800149	2.0557110
H	-0.0096709	-4.1883584	6.2615104
H	3.1611021	-2.9968652	2.5825469
H	2.1179551	-2.9964209	6.7962091
H	3.7182003	-2.3980632	4.9620441
C	-4.2865023	2.5252370	1.8294717
C	-3.4204495	1.7951442	2.2935044
C	-2.4028181	0.9425949	2.8303964
C	-1.2437270	1.4974721	3.4307645
C	-2.5335902	-0.4681594	2.7620701
C	-0.2434463	0.6578670	3.9417272
C	-1.5288300	-1.2977411	3.2781759
C	-0.3804177	-0.7400190	3.8683331
H	-5.0504702	3.1645801	1.4306177
H	-1.1404111	2.5847083	3.4858863
H	-3.4256595	-0.8988243	2.2991795
H	0.6490637	1.0985828	4.3973738
H	-1.6396330	-2.3838520	3.2172087
H	0.4021248	-1.3919277	4.2638515
C	3.0667648	-4.1006979	-0.0937177
C	2.4203024	-3.0808796	-0.2955671
C	1.6612538	-1.8906406	-0.5402088

C	0.9435555	-1.2626216	0.5085865
C	1.6146944	-1.3283065	-1.8416184
C	0.1973121	-0.1031863	0.2587491
C	0.8677282	-0.1666618	-2.0807208
C	0.1569879	0.4491805	-1.0336693
H	3.6280117	-4.9973326	0.0860254
H	0.9699482	-1.6860391	1.5145729
H	2.1659701	-1.8120619	-2.6531841
H	-0.3555501	0.3635707	1.0771005
H	0.8395837	0.2577700	-3.0899686
H	-0.4290106	1.3543472	-1.2248492

Trimer-16

C	1.4048487	2.0514285	-0.0459402
C	0.2021875	1.8353260	0.0120676
C	-1.2055557	1.5941648	0.1041102
C	-2.1293660	2.6547301	-0.0764646
C	-1.6952185	0.2998319	0.4022878
C	-3.5056585	2.4213079	0.0457405
C	-3.0726544	0.0759254	0.5215001
C	-3.9835444	1.1320656	0.3463088
H	2.4588488	2.2468659	-0.0565920
H	-1.7546346	3.6566168	-0.3047307
H	-0.9986405	-0.5248307	0.5569785
H	-4.2093554	3.2487645	-0.0944341
H	-3.4315299	-0.9291979	0.7648932
H	-5.0597974	0.9550449	0.4436715
C	-1.2262507	-3.3579407	0.8621083
C	-0.1756458	-2.9546654	1.3437596
C	1.0407085	-2.4618529	1.9163516
C	1.7304984	-1.3775780	1.3181686
C	1.5607926	-3.0439579	3.1000177
C	2.9083277	-0.8886337	1.8966860
C	2.7432594	-2.5489170	3.6682220
C	3.4202103	-1.4703146	3.0696489
H	-2.1315021	-3.7250031	0.4185607
H	1.3300969	-0.9055228	0.4183135
H	1.0271420	-3.8776179	3.5650906
H	3.4127453	-0.0296185	1.4469998
H	3.1333825	-3.0020856	4.5851525
H	4.3318249	-1.0732976	3.5263657
C	3.1037838	2.5519984	3.3491699
C	1.9445952	2.1702147	3.4473620
C	0.5858713	1.7323458	3.5541653
C	-0.4776850	2.6448454	3.3414246
C	0.2860854	0.3826410	3.8654379
C	-1.8068405	2.2146015	3.4417363
C	-1.0467043	-0.0381826	3.9576977
C	-2.0959526	0.8737387	3.7486607
H	4.1185561	2.8947857	3.2904842

H	-0.2467730	3.6816425	3.0826592
H	1.1014480	-0.3256789	4.0201822
H	-2.6207150	2.9210545	3.2547525
H	-1.2652945	-1.0877807	4.1777355
H	-3.1356664	0.5376729	3.8022729

Trimer-17 (T9)

C	-8.1534583	0.4724908	3.6209812
C	-6.9444646	0.6398585	3.7184150
C	-5.5281526	0.8082804	3.8416268
C	-4.6817693	0.6235910	2.7203356
C	-4.9525140	1.1385286	5.0946340
C	-3.2949806	0.7711069	2.8523985
C	-3.5641114	1.2844396	5.2156921
C	-2.7326945	1.1073871	4.0959716
H	-9.2157744	0.3518765	3.5305358
H	-5.1224802	0.3481592	1.7591513
H	-5.6041749	1.2738409	5.9625966
H	-2.6427231	0.6235855	1.9873533
H	-3.1294820	1.5340394	6.1888088
H	-1.6500877	1.2315406	4.1835248
C	-0.0841807	1.9906519	1.7497330
C	0.3126768	0.8481764	1.9370765
C	0.7719045	-0.4896237	2.1622308
C	0.1966700	-1.2833842	3.1863184
C	1.8063569	-1.0396195	1.3625605
C	0.6495594	-2.5921885	3.4032310
C	2.2506889	-2.3500073	1.5868918
C	1.6759950	-3.1302924	2.6070914
H	-0.4466325	2.9881533	1.5920108
H	-0.6116780	-0.8813961	3.8013575
H	2.2513789	-0.4305350	0.5703823
H	0.1852612	-3.1892615	4.1937110
H	3.0493344	-2.7642475	0.9624641
H	2.0265861	-4.1534056	2.7780674
C	-1.7220058	-2.2133862	6.1540739
C	-2.5336760	-2.3649160	5.2504312
C	-3.4898562	-2.5365159	4.1986099
C	-4.8762427	-2.4416979	4.4743768
C	-3.0662532	-2.7987788	2.8710828
C	-5.8136924	-2.6047101	3.4464107
C	-4.0117546	-2.9579047	1.8495892
C	-5.3860616	-2.8609160	2.1321737
H	-1.0072810	-2.0823565	6.9433140
H	-5.2042331	-2.2222077	5.4935037
H	-1.9988784	-2.8661164	2.6500489
H	-6.8795993	-2.5022184	3.6674547
H	-3.6735262	-3.1551266	0.8270312
H	-6.1214657	-2.9780141	1.3295505

Trimer-18

C	-3.3899547	3.2622334	0.5052337
C	-2.5219457	2.6503090	-0.1031014
C	-1.5049341	1.9395894	-0.8185267
C	-0.2642102	2.5626280	-1.1122373
C	-1.7214684	0.6027525	-1.2367661
C	0.7287682	1.8614934	-1.8119509
C	-0.7204269	-0.0906585	-1.9304056
C	0.5046024	0.5342968	-2.2227159
H	-4.1503553	3.8040263	1.0340218
H	-0.0934485	3.5931543	-0.7880055
H	-2.6686961	0.1152093	-1.0006396
H	1.6829330	2.3516213	-2.0303480
H	-0.8921984	-1.1303426	-2.2229758
H	1.2870950	-0.0125211	-2.7584732
C	0.6871882	-0.1698084	1.2870595
C	0.8966030	-1.1862254	1.9351969
C	1.0877148	-2.4080403	2.6576736
C	0.8230970	-3.6512185	2.0264147
C	1.5234816	-2.4010941	4.0070799
C	0.9897805	-4.8507832	2.7320161
C	1.6863523	-3.6069103	4.7035271
C	1.4212402	-4.8353655	4.0706268
H	0.4963390	0.7078717	0.6981463
H	0.4787769	-3.6617490	0.9883850
H	1.7296923	-1.4450031	4.4970643
H	0.7779661	-5.8027151	2.2336647
H	2.0201755	-3.5879672	5.7464591
H	1.5494048	-5.7747570	4.6188862
C	-0.8605760	-4.2593405	-1.4474682
C	-1.7146365	-3.5449984	-0.9384406
C	-2.7072715	-2.6845259	-0.3679920
C	-3.9080363	-2.4158407	-1.0727920
C	-2.4938224	-2.0745553	0.8931722
C	-4.8683918	-1.5534856	-0.5253063
C	-3.4583545	-1.2111248	1.4290747
C	-4.6469530	-0.9473068	0.7253312
H	-0.1242956	-4.9104696	-1.8778334
H	-4.0721453	-2.8834291	-2.0477453
H	-1.5654799	-2.2657314	1.4333176
H	-5.7898291	-1.3491427	-1.0795637
H	-3.2718271	-0.7302655	2.3938354
H	-5.3936974	-0.2655328	1.1441174

Trimer-19

C	-0.1676483	-2.5283482	1.7760977
C	-0.4428799	-1.3570605	2.0004696
C	-0.7739929	0.0163491	2.2327166
C	0.1435747	1.0421658	1.8945336
C	-2.0319531	0.3710643	2.7830537

C	-0.1951057	2.3871582	2.0930403
C	-2.3603896	1.7197709	2.9798628
C	-1.4469876	2.7310533	2.6318817
H	0.0798029	-3.5579040	1.6004994
H	1.1140412	0.7693059	1.4708773
H	-2.7439664	-0.4182633	3.0393063
H	0.5171722	3.1699656	1.8166496
H	-3.3367098	1.9841704	3.3974016
H	-1.7137827	3.7824246	2.7748450
C	-3.8542393	4.3788568	-0.6890445
C	-3.2980441	3.3854048	-1.1395510
C	-2.6398474	2.2280520	-1.6660845
C	-2.2546239	1.1713133	-0.8046680
C	-2.3501404	2.1340985	-3.0499835
C	-1.6026260	0.0431403	-1.3196307
C	-1.6931448	1.0049025	-3.5551604
C	-1.3227110	-0.0444733	-2.6947722
H	-4.3705040	5.2381016	-0.3066403
H	-2.4569636	1.2524425	0.2646673
H	-2.6246925	2.9595135	-3.7117878
H	-1.3052322	-0.7636694	-0.6427612
H	-1.4542756	0.9504172	-4.6216370
H	-0.8091192	-0.9243292	-3.0954888
C	1.9088957	2.7527960	-6.1917575
C	1.5146472	3.0631836	-5.0747745
C	1.0416016	3.4193643	-3.7708729
C	0.3853104	4.6580936	-3.5571571
C	1.2043801	2.5282780	-2.6806780
C	-0.0999860	4.9883351	-2.2845853
C	0.7155604	2.8688459	-1.4138402
C	0.0611374	4.0947580	-1.2119522
H	2.2699320	2.4905016	-7.1678489
H	0.2561178	5.3452878	-4.3985180
H	1.6924605	1.5645136	-2.8470677
H	-0.6230976	5.9374148	-2.1322175
H	0.8085239	2.1589326	-0.5893057
H	-0.3582421	4.3366279	-0.2317909

Trimer-20

C	-0.0018001	-0.2768725	-3.6339887
C	0.0374861	-1.3418514	-3.0320833
C	0.0994325	-2.5821411	-2.3173874
C	-1.0839935	-3.3049526	-2.0179113
C	1.3479950	-3.1039391	-1.8906785
C	-1.0157102	-4.5134035	-1.3106796
C	1.4057848	-4.3133906	-1.1839595
C	0.2268380	-5.0221192	-0.8908226
H	-0.0146722	0.6732833	-4.1367309
H	-2.0487064	-2.9066261	-2.3449870
H	2.2644766	-2.5522873	-2.1156520

H	-1.9367278	-5.0617237	-1.0850934
H	2.3758424	-4.7047630	-0.8598647
H	0.2757202	-5.9662486	-0.3380182
C	0.0861531	3.9983551	-0.5380002
C	0.2705579	3.7239387	-1.7162965
C	0.4852564	3.3970347	-3.0939007
C	-0.5953683	3.4127321	-4.0135277
C	1.7782385	3.0422546	-3.5541775
C	-0.3815248	3.0799207	-5.3588349
C	1.9813015	2.7064218	-4.9000375
C	0.9055222	2.7248931	-5.8060970
H	-0.0781517	4.2460073	0.4932752
H	-1.5944398	3.6814436	-3.6592128
H	2.6101947	3.0171220	-2.8471277
H	-1.2224210	3.0933659	-6.0599011
H	2.9808463	2.4147398	-5.2362898
H	1.0664636	2.4591000	-6.8557104
C	5.6030893	0.4928093	-5.5125366
C	5.1323957	0.6541912	-4.3937087
C	4.5599576	0.8635279	-3.0979278
C	3.3821338	0.1747187	-2.7143035
C	5.1468217	1.7843133	-2.1924055
C	2.8068337	0.4037455	-1.4578011
C	4.5637828	2.0057411	-0.9366033
C	3.3942440	1.3172332	-0.5651836
H	6.0324068	0.3318750	-6.4828388
H	2.9057072	-0.5097543	-3.4193633
H	6.0521500	2.3215656	-2.4886212
H	1.8829190	-0.1151226	-1.1896101
H	5.0208698	2.7236001	-0.2476735
H	2.9339375	1.5050451	0.4096739

Trimer-21 (T10)

C	3.7103246	-0.5175235	-0.2970176
C	3.5274657	-1.6975062	-0.5660933
C	3.2737358	-3.0648504	-0.9066900
C	1.9583377	-3.4807637	-1.2373649
C	4.3238861	-4.0172953	-0.9291009
C	1.7063160	-4.8159127	-1.5815516
C	4.0613017	-5.3494435	-1.2778276
C	2.7541776	-5.7544055	-1.6048430
H	3.8205899	0.5327054	-0.0946050
H	1.1480838	-2.7468189	-1.2278397
H	5.3384071	-3.6998700	-0.6714161
H	0.6863995	-5.1245719	-1.8335330
H	4.8812647	-6.0753307	-1.2947000
H	2.5534452	-6.7960152	-1.8765628
C	-1.6104000	1.2834762	-6.6457793
C	-1.1362096	1.0443902	-5.5425202
C	-0.5718331	0.7819079	-4.2530537

C	-1.1561995	1.3376838	-3.0873374
C	0.5887691	-0.0218420	-4.1259200
C	-0.5834692	1.0996290	-1.8299802
C	1.1521912	-0.2539349	-2.8655019
C	0.5708894	0.3053331	-1.7144657
H	-2.0446627	1.4720409	-7.6087253
H	-2.0558228	1.9525355	-3.1827187
H	1.0488114	-0.4399962	-5.0246117
H	-1.0389132	1.5406379	-0.9373618
H	2.0577348	-0.8580047	-2.7747445
H	1.0289968	0.1304428	-0.7373847
C	3.1479828	3.1249838	0.0668118
C	3.1386972	2.8866732	-1.1342658
C	3.1335722	2.6003988	-2.5370194
C	4.1236365	1.7574282	-3.1005043
C	2.1383948	3.1576352	-3.3775523
C	4.1204153	1.4919953	-4.4765096
C	2.1387927	2.8785468	-4.7496112
C	3.1313867	2.0514575	-5.3049805
H	3.1653459	3.3622629	1.1131356
H	4.8814392	1.3111570	-2.4513363
H	1.3656627	3.7950929	-2.9406412
H	4.8930375	0.8437763	-4.9027288
H	1.3507871	3.2922909	-5.3856405
H	3.1272712	1.8362409	-6.3783481

Trimer-22 (T11)

C	1.9489064	0.0863079	1.6916815
C	1.4467769	-1.0794970	1.0875298
C	2.4461983	1.1296096	0.8909954
H	1.0434235	-1.8859277	1.7071989
H	2.8388106	2.0399459	1.3566316
C	1.4376943	-1.2061388	-0.3069659
C	2.4401736	1.0132563	-0.5061307
H	1.0305194	-2.1024048	-0.7809592
H	2.8223765	1.8233109	-1.1337465
C	1.9308936	-0.1572594	-1.1223186
H	1.9381182	0.1862062	2.7814130
C	1.8991209	-0.2714001	-2.5495286
C	1.8539865	-0.3611247	-3.7694456
H	1.8348855	-0.4487353	-4.8391418
C	-1.7668950	0.0016388	1.1517058
C	-2.2637768	-1.2061963	0.6035865
C	-1.3080611	1.0186221	0.2791246
H	-2.6305482	-1.9855071	1.2757792
H	-0.9113818	1.9448397	0.7015959
C	-2.3007718	-1.3867027	-0.7846070
C	-1.3448960	0.8261310	-1.1074015
H	-2.7025648	-2.3157290	-1.1997576
H	-0.9726058	1.6099372	-1.7736808

C	-1.8415373	-0.3740566	-1.6440807
H	-1.8696828	-0.5197519	-2.7275454
C	-1.7286983	0.1920061	2.5694790
C	-1.6952499	0.3546783	3.7830221
H	-1.6661425	0.4973608	4.8458915
C	-5.4402635	0.1043528	1.9037183
C	-5.9689426	-1.1159643	1.4476133
C	-4.9863413	1.0588904	0.9769625
H	-6.3238067	-1.8631240	2.1655940
H	-4.5593236	2.0026228	1.3292425
C	-6.0420863	-1.3855573	0.0737387
C	-5.0561320	0.7998762	-0.3973631
H	-6.4487365	-2.3348869	-0.2862793
H	-4.6874756	1.5314309	-1.1203792
C	-5.5817475	-0.4297727	-0.8663831
H	-5.3683285	0.3058709	2.9769372
C	-5.6307744	-0.7097965	-2.2696881
C	-5.6549594	-0.9569876	-3.4688072
H	-5.6964645	-1.1648899	-4.5207785

Trimer-23 (T12)

C	2.5825912	-3.8066575	1.2016213
C	2.6276715	-2.9506948	2.0750907
C	2.6780321	-1.9417488	3.0890613
C	3.3461026	-0.7145909	2.8472409
C	2.0547775	-2.1499785	4.3454203
C	3.3854232	0.2763911	3.8379432
C	2.0995785	-1.1536468	5.3304287
C	2.7628341	0.0622413	5.0816310
H	2.5307353	-4.5450621	0.4246043
H	3.8247651	-0.5499294	1.8779835
H	1.5342772	-3.0931003	4.5324773
H	3.9017015	1.2208971	3.6387684
H	1.6121238	-1.3244553	6.2955649
H	2.7948076	0.8383964	5.8528193
C	-3.3809839	-2.8151483	-4.3642051
C	-2.4328110	-2.5713529	-3.6288013
C	-1.3306104	-2.2734053	-2.7646425
C	-0.2936386	-1.4080909	-3.1956925
C	-1.2671839	-2.8290328	-1.4621508
C	0.7747752	-1.1063098	-2.3391785
C	-0.1956966	-2.5207624	-0.6148120
C	0.8277535	-1.6599325	-1.0476737
H	-4.2032078	-3.0428527	-5.0153306
H	-0.3404192	-0.9793015	-4.2008965
H	-2.0737780	-3.4843039	-1.1238789
H	1.5694013	-0.4354456	-2.6829936
H	-0.1571976	-2.9386726	0.3946776
H	1.6570772	-1.4268271	-0.3740275
C	-0.2012102	0.1363905	2.6723288

C	-1.1056819	-0.0025188	1.8593960
C	-2.1523307	-0.1842988	0.8989759
C	-2.0996593	0.4718414	-0.3564957
C	-3.2455233	-1.0428111	1.1788391
C	-3.1088918	0.2651748	-1.3050902
C	-4.2513583	-1.2417170	0.2227543
C	-4.1868178	-0.5913810	-1.0218783
H	0.6004955	0.2407436	3.3794546
H	-1.2509769	1.1226494	-0.5813935
H	-3.2900230	-1.5509067	2.1465210
H	-3.0473747	0.7618853	-2.2782271
H	-5.0886858	-1.9106775	0.4489489
H	-4.9635929	-0.7624992	-1.7734930

Trimer-24

C	0.5975521	-3.2553559	-0.0000755
C	0.0609977	-3.7390751	-1.2207907
C	0.0647253	-3.7386663	1.2224304
C	-0.9828829	-4.6751051	-1.2143613
C	-0.9791865	-4.6746606	1.2194972
C	-1.5085703	-5.1454098	0.0034571
C	1.6443919	-2.2789310	-0.0018321
C	2.5306750	-1.4355937	-0.0033205
H	0.4642978	-3.3635541	-2.1652488
H	0.4709981	-3.3629513	2.1655449
H	-1.3938631	-5.0346912	-2.1631079
H	-1.3872297	-5.0339525	2.1696259
H	-2.3268775	-5.8722198	0.0048505
H	3.2786796	-0.6646909	-0.0045082
C	2.5194108	2.1454005	-0.0027875
C	3.2067917	1.9239016	1.2181676
C	3.2045315	1.9241596	-1.2250616
C	4.5392351	1.4874558	1.2121278
C	4.5369906	1.4877128	-1.2215814
C	5.2091346	1.2653018	-0.0053676
C	1.1508656	2.5654606	-0.0014860
C	-0.0218374	2.9141172	-0.0003905
H	2.6804934	2.0877444	2.1625286
H	2.6764801	2.0881964	-2.1684057
H	5.0562332	1.3125836	2.1610542
H	5.0522275	1.3130280	-2.1714952
H	6.2472766	0.9186735	-0.0063556
H	-1.0608104	3.1864369	0.0005875
C	-3.1153703	1.1092079	0.0015175
C	-3.2687715	1.8148818	-1.2193336
C	-3.2658925	1.8129532	1.2238486
C	-3.5577052	3.1868931	-1.2131933
C	-3.5548319	3.1849478	1.2206333
C	-3.6997825	3.8780862	0.0044446
C	-2.7946340	-0.2859642	0.0004036

C	-2.5104013	-1.4759673	0.0003629
H	-3.1476024	1.2772046	-2.1637361
H	-3.1424690	1.2736858	2.1670493
H	-3.6662176	3.7218458	-2.1620855
H	-3.6610813	3.7183286	2.1706638
H	-3.9199774	4.9502132	0.0055660
H	-2.2259945	-2.5116358	0.0001704

Trimer-25 (T14)

C	0.5327581	-4.6172225	1.8274191
C	1.5112104	-3.8876607	1.9175776
C	2.6417707	-3.0155072	2.0241661
C	3.1836875	-2.3976285	0.8691580
C	3.2252074	-2.7466243	3.2882154
C	4.2816424	-1.5339672	0.9800830
C	4.3238699	-1.8815854	3.3885357
C	4.8560600	-1.2729823	2.2371417
H	-0.3163403	-5.2687034	1.7489609
H	2.7287589	-2.5958827	-0.1051357
H	2.8052944	-3.2183225	4.1809498
H	4.6881941	-1.0579156	0.0823455
H	4.7651852	-1.6791247	4.3694818
H	5.7119182	-0.5953990	2.3199135
C	0.0055901	5.1097152	1.9111149
C	0.0272174	3.8855121	1.8953039
C	0.0513473	2.4528637	1.8755161
C	-1.0882903	1.7226558	1.4527752
C	1.2143286	1.7464721	2.2777381
C	-1.0599770	0.3210742	1.4341581
C	1.2328548	0.3450290	2.2541826
C	0.0977202	-0.3721208	1.8332255
H	-0.0081618	6.1824468	1.9269787
H	-1.9858785	2.2624080	1.1432112
H	2.0944054	2.3089068	2.6038782
H	-1.9463255	-0.2295205	1.1039982
H	2.1356271	-0.1906681	2.5606096
H	0.1190011	-1.4660041	1.8169565
C	-4.6403719	-1.5289809	-0.0807102
C	-4.5709381	-0.3134098	0.0443602
C	-4.4662580	1.1062919	0.1991177
C	-4.8113259	1.7220468	1.4287540
C	-4.0010145	1.9134368	-0.8697414
C	-4.6895591	3.1101006	1.5814004
C	-3.8830697	3.3007038	-0.7067803
C	-4.2250014	3.9037872	0.5171040
H	-4.7175351	-2.5929406	-0.1967665
H	-5.1639744	1.1003810	2.2562944
H	-3.7278993	1.4394937	-1.8165549
H	-4.9502550	3.5740866	2.5376018
H	-3.5144996	3.9132958	-1.5352894

H -4.1194499 4.9854437 0.6444688

Trimer-26 (T15)

C 2.2499452 -1.5439993 1.0130185
C 1.7667670 -0.5041162 1.4420998
C 1.2075011 0.7186829 1.9380854
C 2.0512146 1.7629328 2.3961853
C -0.1982333 0.9061462 1.9788726
C 1.4986490 2.9575963 2.8798988
C -0.7414272 2.1046705 2.4624735
C 0.1033237 3.1344733 2.9149455
H 2.6697935 -2.4617685 0.6449463
H 3.1356757 1.6226420 2.3661176
H -0.8510646 0.1024821 1.6257565
H 2.1617768 3.7559351 3.2305433
H -1.8266128 2.2402014 2.4840513
H -0.3251905 4.0685878 3.2905812
C -1.8280928 6.6952721 4.2326216
C -2.4571359 5.8282529 3.6402368
C -3.1724999 4.8002597 2.9463000
C -3.1324440 4.7276515 1.5311067
C -3.9189030 3.8329442 3.6657660
C -3.8236065 3.7122567 0.8565457
C -4.6074184 2.8212303 2.9818953
C -4.5628716 2.7569916 1.5772013
H -1.2899997 7.4644950 4.7526702
H -2.5504355 5.4680070 0.9757072
H -3.9466937 3.8849568 4.7575624
H -3.7815702 3.6633207 -0.2363067
H -5.1785948 2.0780067 3.5475269
H -5.0987861 1.9634431 1.0467054
C 7.1842857 -3.3325064 -0.2738040
C 6.0419268 -3.7614365 -0.1821411
C 4.7050447 -4.2627179 -0.0748347
C 3.8344782 -4.2366832 -1.1946008
C 4.2298579 -4.7886101 1.1539273
C 2.5248881 -4.7248906 -1.0831487
C 2.9186703 -5.2743339 1.2549568
C 2.0624396 -5.2451459 0.1393117
H 8.1853127 -2.9533960 -0.3533129
H 4.1966547 -3.8266081 -2.1412911
H 4.8968758 -4.8034406 2.0201480
H 1.8604627 -4.6938223 -1.9526367
H 2.5611584 -5.6709271 2.2105913
H 1.0372942 -5.6189462 0.2241186

Trimer-27 (T13)

C 1.7816841 -1.2605702 5.2425287
C 1.8638839 0.0889846 4.8185876
C 0.5454078 -1.7537784 5.7320200

H	2.8093109	0.4645493	4.4195239
H	0.4786578	-2.7955536	6.0590132
C	0.7379775	0.9198010	4.8839893
C	-0.5740977	-0.9133313	5.7962141
H	0.8081276	1.9545452	4.5359716
H	-1.5239761	-1.3061365	6.1739563
C	-0.4828251	0.4243069	5.3726193
C	0.5860208	-0.4142088	1.7167662
C	0.4706317	0.9348703	1.3023893
C	-0.5681289	-1.0962416	2.1726068
H	1.3581065	1.4567705	0.9364315
H	-0.4776791	-2.1333268	2.5048865
C	-0.7707641	1.5819317	1.3436630
C	-1.8056029	-0.4412316	2.2106072
H	-0.8496598	2.6220223	1.0115405
H	-2.6894507	-0.9764196	2.5723772
C	-1.9132894	0.8986738	1.7972578
H	-2.8823692	1.4072029	1.8285675
C	1.8507434	-1.0781889	1.6720089
C	2.9336628	-1.6442664	1.6300419
H	3.8829377	-2.1400104	1.5973377
C	1.7739468	-0.7796384	-1.9435021
C	1.4251972	0.5202549	-2.3906982
C	0.7565576	-1.6318966	-1.4471687
H	2.2080603	1.1807516	-2.7747977
H	1.0274650	-2.6251209	-1.0810821
C	0.0921071	0.9494201	-2.3414140
C	-0.5725680	-1.1920448	-1.4000625
H	-0.1648373	1.9565758	-2.6860695
H	-1.3457124	-1.8512741	-0.9952344
C	-0.9101466	0.0971411	-1.8453878
C	3.1346438	-1.2224237	-1.9928616
C	4.2972255	-1.6017117	-2.0447729
H	5.3164006	-1.9339710	-2.0943640
H	-1.9473421	0.4411101	-1.7921814
C	2.9287530	-2.1145128	5.1778130
C	3.9096419	-2.8452838	5.1319732
H	4.7695990	-3.4854645	5.0940904
H	-1.3627236	1.0736823	5.4095922

Tetramer

Tetramer-01 (Te1)

C	4.3693764	1.6087143	1.2471760
C	3.2308719	1.4869810	1.6786463
C	1.8873652	1.3342197	2.1487684
C	1.2119162	2.4089564	2.7810951
C	1.2073558	0.1048727	1.9637851

C	-0.1163863	2.2545301	3.2040517
C	-0.1185931	-0.0392538	2.3915381
C	-0.7872647	1.0327920	3.0081188
H	5.3712316	1.7113032	0.8783189
H	1.7344955	3.3590487	2.9213505
H	1.7222187	-0.7220211	1.4750809
H	-0.6326518	3.0957311	3.6770823
H	-0.6387274	-0.9866352	2.2315460
H	-1.8296790	0.9154083	3.3188572
C	4.0689325	0.0071618	-2.5666599
C	3.4457872	-0.7521756	-1.8364148
C	2.7250664	-1.6376870	-0.9727795
C	1.3229361	-1.7977444	-1.1064095
C	3.4097140	-2.3631075	0.0355006
C	0.6271128	-2.6672246	-0.2555981
C	2.7046060	-3.2289659	0.8829939
C	1.3132996	-3.3858711	0.7391474
H	4.6165715	0.6629644	-3.2150227
H	0.7859143	-1.2247230	-1.8644498
H	4.4893071	-2.2323561	0.1462011
H	-0.4541251	-2.7740388	-0.3655270
H	3.2433597	-3.7790853	1.6608841
H	0.7647151	-4.0587558	1.4058681
C	-3.4137607	3.5548523	0.1877992
C	-2.4573479	3.1790833	-0.4770102
C	-1.3501417	2.7086768	-1.2531726
C	-0.2069641	2.1679979	-0.6130011
C	-1.3921153	2.7565813	-2.6699930
C	0.8624216	1.6772033	-1.3730721
C	-0.3167527	2.2619187	-3.4219851
C	0.8102904	1.7175171	-2.7776318
H	-4.2439302	3.9117071	0.7659927
H	-0.1740250	2.1284753	0.4759705
H	-2.2736534	3.1742631	-3.1639551
H	1.7368280	1.2570375	-0.8705865
H	-0.3612104	2.2993784	-4.5153869
H	1.6453233	1.3191055	-3.3614714
C	-3.5638931	-1.4825702	3.0285963
C	-3.3041757	-1.5728797	1.8359215
C	-2.9842296	-1.6910512	0.4451309
C	-2.3936529	-0.6087684	-0.2542566
C	-3.2520902	-2.8996906	-0.2480517
C	-2.0763677	-0.7378560	-1.6130840
C	-2.9311301	-3.0181748	-1.6075370
C	-2.3420224	-1.9393587	-2.2932271
H	-3.8153003	-1.3966138	4.0679790
H	-2.1863771	0.3237009	0.2730989
H	-3.7119113	-3.7331711	0.2902024
H	-1.6172347	0.1026739	-2.1375415
H	-3.1403208	-3.9559249	-2.1319669

H -2.0881332 -2.0374556 -3.3536000

Tetramer-02 (Te2)

C	2.3363047	1.7360888	2.2140270
C	1.5073863	0.5928935	2.3398449
C	1.7622205	2.9578695	1.7777441
C	0.1457005	0.6699050	2.0194343
C	0.3974461	3.0228943	1.4604821
C	-0.4150071	1.8796386	1.5740573
C	1.2405120	1.0683039	-2.5199949
C	1.8112468	0.5008793	-3.6873706
C	1.9386034	0.9644017	-1.2906552
C	3.0479160	-0.1571102	-3.6177762
C	3.1757360	0.3099504	-1.2316979
C	3.7341376	-0.2557879	-2.3925236
C	-0.0283219	1.7292387	-2.5619932
C	-1.1150303	2.2921929	-2.5563393
C	3.7352404	1.6507050	2.5075949
C	4.9340932	1.5662473	2.7407554
H	1.9368838	-0.3526550	2.6808223
H	2.3994019	3.8409481	1.6794915
H	-0.4758199	-0.2229514	2.1068510
H	-0.0296850	3.9667776	1.1084827
H	1.2761429	0.5809160	-4.6379054
H	1.4971638	1.3953477	-0.3927011
H	3.4786688	-0.5939520	-4.5245953
H	3.7018391	0.2433882	-0.2744005
H	4.6998170	-0.7692026	-2.3453738
H	-2.0873201	2.7473847	-2.5091760
H	5.9807622	1.5028611	2.9682148
H	-1.4746509	1.9230264	1.3091013
C	-3.8035361	1.0841549	-0.1877430
C	-3.0308963	0.0713596	-0.8100092
C	-4.1091132	0.9702935	1.1927752
C	-2.5751832	-1.0249790	-0.0666876
C	-3.6489131	-0.1321512	1.9268907
C	-2.8836709	-1.1328142	1.3005875
C	-4.2655530	2.2130907	-0.9381504
C	-4.6481215	3.1871037	-1.5745415
H	-2.7801138	0.1618985	-1.8690211
H	-4.7035333	1.7517870	1.6743210
H	-1.9694879	-1.7925157	-0.5530168
H	-3.8864623	-0.2069678	2.9928005
H	-5.0143271	4.0275954	-2.1322084
H	-2.5116558	-1.9842588	1.8779758
C	0.3145578	-2.7323718	3.4941774
C	0.2463561	-2.9034680	2.2841486
C	0.1407877	-3.0881526	0.8685974
C	0.8177225	-2.2208081	-0.0247681
C	-0.6564291	-4.1372979	0.3444028

C	0.7013474	-2.4026501	-1.4093136
C	-0.7712155	-4.3083633	-1.0420167
C	-0.0930278	-3.4438823	-1.9221063
H	0.4071423	-2.5979030	4.5545403
H	1.4177182	-1.3992589	0.3694144
H	-1.1815487	-4.8050147	1.0330883
H	1.2262508	-1.7235227	-2.0850270
H	-1.3933062	-5.1181367	-1.4362788
H	-0.1869522	-3.5797791	-3.0043122

Tetramer-03 (Te5)

C	1.0146850	-2.7010947	1.5366915
C	-0.1358949	-1.9473927	1.1937080
C	1.8422370	-2.2585170	2.6003142
C	-0.4465659	-0.7753607	1.8952953
C	1.5229022	-1.0831347	3.2950303
C	0.3815945	-0.3383953	2.9440847
C	3.2194920	1.2118147	-0.3772882
C	3.6746593	1.5791421	-1.6695860
C	2.4925746	0.0060170	-0.2165909
C	3.3991575	0.7566029	-2.7713529
C	2.2269071	-0.8116210	-1.3224725
C	2.6751026	-0.4386369	-2.6015695
C	3.4656757	2.0592165	0.7503198
C	3.6471252	2.7925567	1.7130728
C	1.3454005	-3.8837750	0.7999327
C	1.6350162	-4.8813729	0.1520295
H	-0.7644043	-2.2833059	0.3684415
H	2.7338848	-2.8355005	2.8605925
H	-1.3309707	-0.1958056	1.6209588
H	2.1726133	-0.7402992	4.1063226
H	4.2330925	2.5108570	-1.7956944
H	2.1340494	-0.2748083	0.7734588
H	3.7531016	1.0471349	-3.7659427
H	1.6630339	-1.7365358	-1.1806503
H	2.4630007	-1.0766575	-3.4657535
H	3.8234875	3.4312943	2.5569662
H	1.8816016	-5.7717775	-0.3931870
H	0.1396161	0.5881800	3.4715421
C	-1.4414674	2.7362252	0.6992927
C	-0.1872988	2.3612190	0.1539870
C	-2.4504389	3.2381997	-0.1625815
C	0.0472266	2.4893158	-1.2220452
C	-2.2034210	3.3659556	-1.5362590
C	-0.9553277	2.9935188	-2.0689571
C	-1.6991144	2.6028136	2.1014631
C	-1.9358148	2.4851015	3.2963284
H	0.5888781	1.9654911	0.8112986
H	-3.4220904	3.5131405	0.2563911
H	1.0134843	2.1872639	-1.6324918

H	-2.9890588	3.7499021	-2.1943933
H	-2.1397650	2.3862407	4.3449146
H	-0.7690940	3.0879227	-3.1433245
C	-4.8451536	-0.3118753	0.9998089
C	-4.0330929	-0.7472186	0.1946827
C	-3.0597841	-1.2513361	-0.7266832
C	-3.0337682	-2.6266791	-1.0730037
C	-2.0905140	-0.3802566	-1.2829727
C	-2.0506689	-3.1136212	-1.9464012
C	-1.1107982	-0.8773242	-2.1512522
C	-1.0846713	-2.2428253	-2.4837289
H	-5.5635273	0.0705668	1.6989659
H	-3.7777861	-3.3012399	-0.6406212
H	-2.1040274	0.6753905	-1.0143306
H	-2.0306496	-4.1781474	-2.1995650
H	-0.3531023	-0.1978347	-2.5488760
H	-0.3073966	-2.6319664	-3.1488782

Tetramer-04 (Te3)

C	5.2361464	-2.6578910	1.3872992
C	4.0232711	-2.5751036	1.2414394
C	2.6095032	-2.4561895	1.0466614
C	1.9090373	-1.3337694	1.5542765
C	1.8953029	-3.4445449	0.3222793
C	0.5315375	-1.2038143	1.3366313
C	0.5164213	-3.3018054	0.1085214
C	-0.1708599	-2.1824784	0.6125279
H	6.2939749	-2.7522769	1.5394441
H	2.4528322	-0.5579915	2.0977159
H	2.4344639	-4.3096715	-0.0735509
H	0.0082840	-0.3264831	1.7225309
H	-0.0225356	-4.0644751	-0.4624507
H	-1.2429956	-2.0684288	0.4362033
C	2.0594420	1.8347196	3.4154874
C	1.2287086	2.2071602	2.5977362
C	0.2428402	2.6528896	1.6592274
C	-0.7875053	3.5337238	2.0790136
C	0.2788767	2.2219416	0.3090543
C	-1.7596368	3.9672862	1.1669348
C	-0.6975329	2.6640405	-0.5939950
C	-1.7178782	3.5343200	-0.1713359
H	2.8001142	1.5172444	4.1238445
H	-0.8123689	3.8672541	3.1200626
H	1.0622754	1.5358981	-0.0182042
H	-2.5525751	4.6427970	1.5031694
H	-0.6656213	2.3140789	-1.6280309
H	-2.4829147	3.8685150	-0.8794099
C	-1.1599664	-0.4648371	-3.0776008
C	-0.0229066	-0.0620057	-2.8698631
C	1.2887285	0.4176330	-2.5570966

C	2.1403189	-0.3468532	-1.7213405
C	1.7380994	1.6733748	-3.0376404
C	3.4039915	0.1423373	-1.3634206
C	3.0038451	2.1542926	-2.6758426
C	3.8390951	1.3934773	-1.8365831
H	-2.1507139	-0.8449514	-3.2476361
H	1.7939078	-1.3109640	-1.3477836
H	1.0838072	2.2639584	-3.6852538
H	4.0424905	-0.4538389	-0.7045086
H	3.3381558	3.1284794	-3.0470721
H	4.8252935	1.7757373	-1.5534363
C	-4.6385554	-1.7719941	-2.8718381
C	-4.2673668	-1.5090616	-1.7349004
C	-3.8367447	-1.2075172	-0.4025178
C	-3.1184426	-0.0169833	-0.1255512
C	-4.1301880	-2.1008213	0.6597574
C	-2.7211184	0.2774654	1.1854574
C	-3.7210876	-1.8002612	1.9662730
C	-3.0216919	-0.6093221	2.2339893
H	-4.9798713	-1.9986611	-3.8635909
H	-2.8624733	0.6615519	-0.9417496
H	-4.6776394	-3.0230663	0.4457067
H	-2.1659667	1.1968564	1.3824387
H	-3.9480459	-2.4997770	2.7770856
H	-2.7016008	-0.3788177	3.2549962

Tetramer-05 (Te3)

C	0.4960119	3.2798717	-1.3289988
C	0.7532859	1.9487899	-1.7436665
C	1.3421009	3.8792918	-0.3619996
C	1.8366163	1.2413980	-1.2072022
C	2.4239564	3.1615694	0.1676107
C	2.6769165	1.8430875	-0.2532993
C	-0.9350822	0.5043555	2.7740601
C	-2.2459782	0.3288187	3.2885773
C	-0.7413038	1.3318914	1.6381070
C	-3.3345275	0.9698469	2.6813298
C	-1.8384398	1.9683209	1.0409141
C	-3.1339093	1.7920301	1.5575878
C	0.1689123	-0.1495527	3.4100165
C	1.0908850	-0.7167803	3.9812298
C	-0.6114850	4.0114891	-1.8681458
C	-1.5673718	4.6385843	-2.3073544
H	0.0877255	1.4733094	-2.4672515
H	1.1399020	4.9035973	-0.0369638
H	2.0201281	0.2135925	-1.5264442
H	3.0711664	3.6344525	0.9129803
H	-2.3934682	-0.3084840	4.1649418
H	0.2618283	1.4652926	1.2267101
H	-4.3411880	0.8253910	3.0861392

H	-1.6841991	2.5925816	0.1593153
H	-3.9849001	2.2858775	1.0788592
H	1.9083740	-1.2018151	4.4785564
H	-2.3805529	5.2096916	-2.7121457
H	3.5179669	1.2824327	0.1643722
C	3.5473311	-1.6471361	-0.1095671
C	2.4493079	-1.4919848	0.7730963
C	3.3278181	-2.2143483	-1.3907737
C	1.1651562	-1.8883131	0.3802691
C	2.0377122	-2.6116507	-1.7719828
C	0.9523092	-2.4502832	-0.8907111
C	4.8545864	-1.2126970	0.2809769
C	5.9638064	-0.8129760	0.6113540
H	2.6059562	-1.0402520	1.7547409
H	4.1727010	-2.3299100	-2.0752991
H	0.3260252	-1.7462253	1.0649834
H	1.8784150	-3.0449697	-2.7646526
H	6.9451225	-0.4958780	0.9072957
H	-0.0527634	-2.7542390	-1.1927586
C	-2.6033909	1.0562073	-2.4046352
C	-2.5879701	-0.0814802	-1.9539300
C	-2.5644364	-1.4007447	-1.3994110
C	-2.4245340	-1.5797579	0.0000930
C	-2.6684260	-2.5425494	-2.2341748
C	-2.3858593	-2.8697371	0.5449955
C	-2.6288698	-3.8292218	-1.6779509
C	-2.4865823	-3.9987046	-0.2879999
H	-2.5526722	2.0704703	-2.7537832
H	-2.3397297	-0.7044889	0.6444464
H	-2.7752618	-2.4068328	-3.3141036
H	-2.2690541	-2.9919250	1.6262552
H	-2.7073242	-4.7033264	-2.3323714
H	-2.4527854	-5.0049313	0.1414776

Tetramer-06

C	1.7444543	-1.6668896	-1.8769319
C	1.1853000	-0.3672231	-1.7958974
C	1.0004001	-2.7020736	-2.4979086
C	-0.0911252	-0.1148843	-2.3130058
C	-0.2778988	-2.4387722	-3.0121162
C	-0.8292319	-1.1469523	-2.9188138
C	-1.8401586	-2.4506482	1.3839031
C	-1.9346063	-2.3966751	2.7981292
C	-0.5862926	-2.2203546	0.7654553
C	-0.7987780	-2.1076731	3.5678179
C	0.5466835	-1.9501828	1.5437612
C	0.4441190	-1.8860664	2.9445828
C	-2.9982335	-2.7142136	0.5846331
C	-3.9864977	-2.9113543	-0.1095951
C	3.0356898	-1.9178000	-1.3130596

C	4.1298151	-2.0985949	-0.7952424
H	1.7543327	0.4278470	-1.3134624
H	1.4299369	-3.7056811	-2.5590996
H	-0.5192596	0.8871510	-2.2350365
H	-0.8498520	-3.2481835	-3.4763818
H	-2.9016899	-2.5749113	3.2764313
H	-0.5127976	-2.2509739	-0.3219410
H	-0.8838385	-2.0581854	4.6582913
H	1.5061165	-1.7824956	1.0480778
H	1.3277663	-1.6632809	3.5516587
H	-4.8513920	-3.1119739	-0.7118885
H	5.1036668	-2.2317418	-0.3669337
H	-1.8324986	-0.9420283	-3.3041622
C	-2.8622047	2.0007363	-0.7444554
C	-2.5384461	0.8905187	0.0759518
C	-2.9788265	3.2863422	-0.1557873
C	-2.3443746	1.0672271	1.4523823
C	-2.7789903	3.4519064	1.2216260
C	-2.4638316	2.3435770	2.0296793
C	-3.0676994	1.8326865	-2.1515378
C	-3.2289847	1.6971209	-3.3570741
H	-2.4426107	-0.1003841	-0.3718581
H	-3.2254150	4.1429166	-0.7894787
H	-2.0935062	0.2028869	2.0717622
H	-2.8670125	4.4489110	1.6646164
H	-3.3890627	1.5778909	-4.4112564
H	-2.3063762	2.4769910	3.1045998
C	6.0494659	0.8611875	0.7835191
C	4.8774880	1.1989298	0.6807618
C	3.5105182	1.6092776	0.5706453
C	2.5076162	0.9983891	1.3647478
C	3.1392402	2.6384506	-0.3320854
C	1.1733598	1.4116766	1.2600757
C	1.8000163	3.0446498	-0.4282672
C	0.8125537	2.4359853	0.3674167
H	7.0795742	0.5748772	0.8728524
H	2.7874613	0.1930386	2.0482388
H	3.9099629	3.1075971	-0.9497862
H	0.4072537	0.9189253	1.8615725
H	1.5262601	3.8363814	-1.1327676
H	-0.2327811	2.7428358	0.2835192

Tetramer-07 (Te6)

C	-4.3681536	-2.4912781	-2.6381310
C	-4.2841450	-1.5935868	-1.8099823
C	-4.1524202	-0.5318998	-0.8579758
C	-3.3718549	-0.7114367	0.3112004
C	-4.7774266	0.7203642	-1.0878017
C	-3.2210636	0.3388477	1.2261804
C	-4.6165702	1.7661439	-0.1677826

C	-3.8384366	1.5792070	0.9895255
H	-4.4669466	-3.2854415	-3.3527220
H	-2.8713484	-1.6678233	0.4797149
H	-5.3752258	0.8619593	-1.9925115
H	-2.6054104	0.1930070	2.1169540
H	-5.0939520	2.7324715	-0.3589531
H	-3.7040659	2.4025099	1.6978790
C	-0.5165301	-3.7785671	0.5270340
C	-0.4066026	-2.7569550	1.1919424
C	-0.2949780	-1.5474585	1.9501510
C	-0.6326075	-1.5240835	3.3273583
C	0.1369714	-0.3541389	1.3219352
C	-0.5369400	-0.3284033	4.0534862
C	0.2325815	0.8346940	2.0564473
C	-0.1033804	0.8527482	3.4213519
H	-0.6172701	-4.6754956	-0.0528441
H	-0.9713298	-2.4437854	3.8123535
H	0.3911459	-0.3711391	0.2631000
H	-0.8022389	-0.3182328	5.1154206
H	0.5552241	1.7513234	1.5566898
H	-0.0326109	1.7844157	3.9915056
C	-0.3656782	4.2962443	-0.0594852
C	-0.2019877	3.2328868	-0.6439127
C	-0.0016455	1.9683231	-1.2857872
C	-1.1119084	1.1648243	-1.6483328
C	1.3116183	1.4914586	-1.5299223
C	-0.9085293	-0.0861969	-2.2463945
C	1.5033122	0.2365138	-2.1241985
C	0.3967056	-0.5529436	-2.4852528
H	-0.5104291	5.2457675	0.4184041
H	-2.1229600	1.5166191	-1.4336947
H	2.1700381	2.0970259	-1.2280034
H	-1.7707655	-0.7056968	-2.5071838
H	2.5186282	-0.1360333	-2.2795067
H	0.5524299	-1.5378228	-2.9361399
C	4.8088932	2.8164987	0.4387735
C	4.6350380	1.6290243	0.1980670
C	4.3888489	0.2525223	-0.1092256
C	3.4405146	-0.4873638	0.6394647
C	5.0611372	-0.3772275	-1.1875152
C	3.1578873	-1.8179445	0.3052807
C	4.7776890	-1.7120537	-1.5098380
C	3.8234482	-2.4341396	-0.7690425
H	4.9811940	3.8513861	0.6637997
H	2.9104125	-0.0023418	1.4617793
H	5.7922768	0.1925090	-1.7679979
H	2.4013979	-2.3698416	0.8702866
H	5.2989952	-2.1887359	-2.3463916
H	3.5968648	-3.4724744	-1.0313312

Tetramer-08 (Te7)

C	0.4189523	-2.8609589	-1.4637117
C	-0.7598468	-2.5625335	-1.3223463
C	-2.1200521	-2.1570336	-1.1384164
C	-2.5738715	-1.7604450	0.1439445
C	-3.0188395	-2.1119213	-2.2337548
C	-3.8931046	-1.3241104	0.3220310
C	-4.3389307	-1.6779877	-2.0451364
C	-4.7809379	-1.2819925	-0.7685277
H	1.4549895	-3.1321459	-1.5596074
H	-1.8800371	-1.7850925	0.9843307
H	-2.6692169	-2.4137677	-3.2251861
H	-4.2219091	-1.0005945	1.3142641
H	-5.0237757	-1.6440611	-2.8984923
H	-5.8111558	-0.9389996	-0.6273856
C	2.3441986	4.6465798	-1.2180054
C	1.3632381	3.9176458	-1.2939952
C	0.2227786	3.0560463	-1.3783287
C	0.3353371	1.7688627	-1.9628536
C	-1.0356919	3.4761823	-0.8765204
C	-0.7802361	0.9252343	-2.0335685
C	-2.1456484	2.6231281	-0.9537264
C	-2.0225619	1.3452017	-1.5268823
H	3.1953633	5.2978755	-1.1682072
H	1.3030028	1.4391241	-2.3478066
H	-1.1243640	4.4670941	-0.4229733
H	-0.6731936	-0.0732566	-2.4633855
H	-3.1051797	2.9490664	-0.5422563
H	-2.8818265	0.6713934	-1.5611819
C	-3.2331953	2.3542394	2.8304962
C	-2.3592841	1.5076408	2.6961171
C	-1.3543169	0.4989594	2.5447731
C	-1.3267587	-0.6154151	3.4213325
C	-0.3842978	0.5924917	1.5148858
C	-0.3583781	-1.6169171	3.2568518
C	0.5788546	-0.4119041	1.3614002
C	0.5941784	-1.5196899	2.2259942
H	-3.9770064	3.1144628	2.9702486
H	-2.0693167	-0.6842665	4.2214180
H	-0.4047103	1.4460658	0.8371894
H	-0.3515936	-2.4769648	3.9339810
H	1.3150078	-0.3335236	0.5597220
H	1.3434748	-2.3047012	2.0897665
C	4.0493267	-3.7044552	-1.4856611
C	3.9842278	-2.6145916	-0.9310795
C	3.9026316	-1.3393840	-0.2851262
C	3.6109236	-0.1705940	-1.0337935
C	4.1206990	-1.2271274	1.1113013
C	3.5459967	1.0771643	-0.3985304
C	4.0515691	0.0246245	1.7374159

C	3.7660605	1.1787311	0.9865538
H	4.1268542	-4.6583296	-1.9709753
H	3.4380482	-0.2573772	-2.1100394
H	4.3401003	-2.1284906	1.6904099
H	3.3106981	1.9749401	-0.9761573
H	4.2113062	0.0970642	2.8174664
H	3.7008828	2.1540703	1.4783645

Tetramer-09

C	0.2185305	-2.7953412	-1.3749194
C	-0.0355854	-1.4561605	-1.7638354
C	-0.8605108	-3.6046476	-0.9359939
C	-1.3353690	-0.9391062	-1.7008371
C	-2.1593868	-3.0780161	-0.8856142
C	-2.4015257	-1.7442937	-1.2625232
C	-1.0038091	-0.4652804	2.8529520
C	-0.3746565	0.5674592	3.5944012
C	-0.3026724	-1.0724343	1.7818127
C	0.9249600	0.9794148	3.2657320
C	0.9982416	-0.6581523	1.4694732
C	1.6177691	0.3675912	2.2040101
C	-2.3408324	-0.8706327	3.1667941
C	-3.4966896	-1.1909948	3.4121909
C	1.5499462	-3.3216403	-1.4105569
C	2.6893246	-3.7700666	-1.4242205
H	0.7892560	-0.8209829	-2.0945645
H	-0.6648084	-4.6367818	-0.6327253
H	-1.5143425	0.1028046	-1.9751819
H	-2.9837518	-3.7089561	-0.5386849
H	-0.9183437	1.0409730	4.4166346
H	-0.7892476	-1.8502435	1.1906572
H	1.3970583	1.7831594	3.8399602
H	1.5275424	-1.1318585	0.6405189
H	2.6298429	0.6893314	1.9448443
H	-4.5018292	-1.4865197	3.6422213
H	3.6798640	-4.1796132	-1.4687398
H	-3.4107811	-1.3270808	-1.1984147
C	-3.5550202	1.6398856	-0.7342447
C	-2.6587651	1.4466263	0.3463391
C	-3.1291476	2.3887007	-1.8613103
C	-1.3649977	1.9825007	0.2940029
C	-1.8336738	2.9236267	-1.9006462
C	-0.9478154	2.7218651	-0.8259847
C	-4.8641643	1.0604696	-0.7026651
C	-5.9712551	0.5378919	-0.6886400
H	-2.9782400	0.8535622	1.2059140
H	-3.8193603	2.5359875	-2.6967157
H	-0.6747102	1.8011878	1.1206397
H	-1.5131854	3.4965015	-2.7772994
H	-6.9548297	0.1102356	-0.6627345

H	0.0699340	3.1186680	-0.8738230
C	1.6421132	1.7036559	-2.9476821
C	2.4518424	1.4406845	-2.0687531
C	3.3921845	1.1274233	-1.0361784
C	3.7151935	-0.2217218	-0.7455535
C	4.0123721	2.1623705	-0.2912629
C	4.6358339	-0.5222098	0.2673428
C	4.9346485	1.8507706	0.7175031
C	5.2510057	0.5090536	1.0005250
H	0.9243022	1.9258808	-3.7127395
H	3.2342221	-1.0280511	-1.3047750
H	3.7654141	3.2039234	-0.5152687
H	4.8678432	-1.5685301	0.4891493
H	5.4062463	2.6583953	1.2865169
H	5.9688777	0.2695113	1.7912699

Tetramer-10

C	-1.0501483	4.7106825	0.2390650
C	-0.8912491	3.7188700	-0.4607987
C	-0.7300237	2.5397555	-1.2576589
C	-0.1051382	1.3923952	-0.7112755
C	-1.2131495	2.4963506	-2.5909342
C	0.0298184	0.2286856	-1.4784622
C	-1.0743574	1.3259415	-3.3504934
C	-0.4543889	0.1897755	-2.7968378
H	-1.1731628	5.5915366	0.8390695
H	0.2515916	1.4174055	0.3190726
H	-1.6997637	3.3797158	-3.0135316
H	0.5058851	-0.6501906	-1.0415837
H	-1.4570699	1.2986670	-4.3756805
H	-0.3600186	-0.7261591	-3.3876755
C	0.2299213	1.2720332	3.4005903
C	0.2816863	0.2522054	2.7256353
C	0.3375695	-0.9067756	1.8860967
C	1.5855678	-1.3997230	1.4298857
C	-0.8568302	-1.5441704	1.4672551
C	1.6325416	-2.5101367	0.5755735
C	-0.7996274	-2.6508043	0.6100949
C	0.4424635	-3.1388870	0.1644748
H	0.1821934	2.1505994	4.0139728
H	2.5045680	-0.8927389	1.7291313
H	-1.8186445	-1.1508655	1.7992309
H	2.5992129	-2.8665474	0.2090310
H	-1.7294745	-3.1139004	0.2685723
H	0.4829244	-3.9965711	-0.5147336
C	-3.7328604	-2.6944109	-2.3333522
C	-3.8120489	-1.9213922	-1.3874652
C	-3.8734994	-1.0347980	-0.2648076
C	-3.3138893	0.2643972	-0.3444264
C	-4.4720918	-1.4578197	0.9494147

C	-3.3424398	1.1137329	0.7697466
C	-4.4992459	-0.5992009	2.0574017
C	-3.9327178	0.6863159	1.9721825
H	-3.6934712	-3.3600367	-3.1738066
H	-2.8445014	0.5892079	-1.2744360
H	-4.9020528	-2.4614074	1.0131094
H	-2.8876446	2.1059253	0.7018233
H	-4.9577403	-0.9364963	2.9923357
H	-3.9414634	1.3477722	2.8440420
C	4.4563810	-2.2955307	-2.4261530
C	4.3826384	-1.4127295	-1.5814095
C	4.2693315	-0.4006329	-0.5751749
C	3.3707210	0.6818567	-0.7444775
C	5.0347888	-0.4826447	0.6155751
C	3.2342955	1.6500291	0.2588808
C	4.8929605	0.4926735	1.6128999
C	3.9910617	1.5589161	1.4401591
H	4.5442562	-3.0524244	-3.1815964
H	2.7684878	0.7423905	-1.6534841
H	5.7272483	-1.3184646	0.7497169
H	2.5230399	2.4694385	0.1224401
H	5.4831930	0.4169889	2.5315987
H	3.8711179	2.3089346	2.2277267

Tetramer-11 (Te8)

C	-0.0837048	-3.8871770	0.9816091
C	-0.9902132	-3.2621942	0.4471238
C	-2.0851992	-2.5704273	-0.1643923
C	-2.6004967	-1.3831210	0.4121596
C	-2.6771309	-3.0811737	-1.3476272
C	-3.6956718	-0.7349985	-0.1750365
C	-3.7709732	-2.4240495	-1.9281961
C	-4.2863203	-1.2528800	-1.3414533
H	0.7254942	-4.4179859	1.4444604
H	-2.1357850	-0.9762591	1.3119780
H	-2.2769831	-3.9960835	-1.7937034
H	-4.0772458	0.1873359	0.2699198
H	-4.2240246	-2.8297846	-2.8382894
H	-5.1399902	-0.7412453	-1.7976199
C	3.1882346	3.7825166	-1.7549575
C	2.2587422	2.9953461	-1.8772570
C	1.1642997	2.0826635	-2.0180688
C	1.2979346	0.7300316	-1.6152989
C	-0.0728224	2.5237363	-2.5555109
C	0.2158067	-0.1506206	-1.7394911
C	-1.1462949	1.6303041	-2.6795348
C	-1.0072112	0.2916529	-2.2710484
H	4.0022377	4.4739461	-1.6542343
H	2.2464125	0.3855440	-1.1986136
H	-0.1777746	3.5677664	-2.8631981

H	0.3212126	-1.1835557	-1.4002144
H	-2.0999593	1.9853718	-3.0822683
H	-1.8507879	-0.3980897	-2.3479298
C	-4.0807034	3.2857175	0.4335822
C	-3.1953092	2.6554573	0.9972306
C	-2.1788805	1.8918372	1.6563329
C	-2.4404012	1.2949371	2.9162464
C	-0.9087101	1.7104278	1.0549100
C	-1.4489394	0.5378681	3.5565755
C	0.0784458	0.9629904	1.7100077
C	-0.1848045	0.3752215	2.9591328
H	-4.8422240	3.8715822	-0.0437311
H	-3.4228678	1.4297265	3.3773999
H	-0.7098919	2.1449947	0.0739756
H	-1.6640297	0.0758077	4.5253024
H	1.0567100	0.8366973	1.2421898
H	0.5953417	-0.2038163	3.4617605
C	3.4295565	0.6291337	3.3714388
C	3.5062115	0.0273094	2.3087322
C	3.5908001	-0.6746391	1.0642534
C	4.6454755	-0.4025645	0.1560844
C	2.6162404	-1.6452667	0.7193648
C	4.7217782	-1.0912872	-1.0624391
C	2.7069422	-2.3340880	-0.4975267
C	3.7564494	-2.0604527	-1.3924164
H	3.3585130	1.1603926	4.3006857
H	5.3916270	0.3531303	0.4157529
H	1.7840396	-1.8396610	1.3997167
H	5.5352791	-0.8667568	-1.7592655
H	1.9405791	-3.0725130	-0.7493655
H	3.8172299	-2.5917355	-2.3473625

Tetramer-12

C	-0.0837048	-3.8871770	0.9816091
C	-0.9902132	-3.2621942	0.4471238
C	-2.0851992	-2.5704273	-0.1643923
C	-2.6004967	-1.3831210	0.4121596
C	-2.6771309	-3.0811737	-1.3476272
C	-3.6956718	-0.7349985	-0.1750365
C	-3.7709732	-2.4240495	-1.9281961
C	-4.2863203	-1.2528800	-1.3414533
H	0.7254942	-4.4179859	1.4444604
H	-2.1357850	-0.9762591	1.3119780
H	-2.2769831	-3.9960835	-1.7937034
H	-4.0772458	0.1873359	0.2699198
H	-4.2240246	-2.8297846	-2.8382894
H	-5.1399902	-0.7412453	-1.7976199
C	3.1882346	3.7825166	-1.7549575
C	2.2587422	2.9953461	-1.8772570
C	1.1642997	2.0826635	-2.0180688

C	1.2979346	0.7300316	-1.6152989
C	-0.0728224	2.5237363	-2.5555109
C	0.2158067	-0.1506206	-1.7394911
C	-1.1462949	1.6303041	-2.6795348
C	-1.0072112	0.2916529	-2.2710484
H	4.0022377	4.4739461	-1.6542343
H	2.2464125	0.3855440	-1.1986136
H	-0.1777746	3.5677664	-2.8631981
H	0.3212126	-1.1835557	-1.4002144
H	-2.0999593	1.9853718	-3.0822683
H	-1.8507879	-0.3980897	-2.3479298
C	-4.0807034	3.2857175	0.4335822
C	-3.1953092	2.6554573	0.9972306
C	-2.1788805	1.8918372	1.6563329
C	-2.4404012	1.2949371	2.9162464
C	-0.9087101	1.7104278	1.0549100
C	-1.4489394	0.5378681	3.5565755
C	0.0784458	0.9629904	1.7100077
C	-0.1848045	0.3752215	2.9591328
H	-4.8422240	3.8715822	-0.0437311
H	-3.4228678	1.4297265	3.3773999
H	-0.7098919	2.1449947	0.0739756
H	-1.6640297	0.0758077	4.5253024
H	1.0567100	0.8366973	1.2421898
H	0.5953417	-0.2038163	3.4617605
C	3.4295565	0.6291337	3.3714388
C	3.5062115	0.0273094	2.3087322
C	3.5908001	-0.6746391	1.0642534
C	4.6454755	-0.4025645	0.1560844
C	2.6162404	-1.6452667	0.7193648
C	4.7217782	-1.0912872	-1.0624391
C	2.7069422	-2.3340880	-0.4975267
C	3.7564494	-2.0604527	-1.3924164
H	3.3585130	1.1603926	4.3006857
H	5.3916270	0.3531303	0.4157529
H	1.7840396	-1.8396610	1.3997167
H	5.5352791	-0.8667568	-1.7592655
H	1.9405791	-3.0725130	-0.7493655
H	3.8172299	-2.5917355	-2.3473625

Tetramer-13

C	-4.9857239	1.3491708	2.6215490
C	-4.6259983	1.0081188	1.5022103
C	-4.1865365	0.5862739	0.2060688
C	-3.0380669	1.1678392	-0.3866134
C	-4.8819750	-0.4364831	-0.4877592
C	-2.5983474	0.7339921	-1.6443378
C	-4.4349963	-0.8615664	-1.7467445
C	-3.2940833	-0.2780206	-2.3284664
H	-5.3237505	1.6702618	3.5876919

H	-2.4859905	1.9375744	0.1572297
H	-5.7623434	-0.8916855	-0.0257917
H	-1.6981610	1.1733295	-2.0799121
H	-4.9746673	-1.6566833	-2.2709986
H	-2.9405994	-0.6218819	-3.3054889
C	-0.2269616	3.2130828	1.9859642
C	0.0922435	2.6768535	0.9333326
C	0.4330443	2.0529601	-0.3090146
C	0.5272851	2.8264449	-1.4931502
C	0.6610041	0.6576734	-0.3712782
C	0.8431712	2.2097452	-2.7118836
C	0.9822130	0.0517044	-1.5917258
C	1.0735057	0.8221220	-2.7640612
H	-0.5100212	3.6849397	2.9067740
H	0.3452541	3.9033189	-1.4441578
H	0.5862757	0.0638086	0.5386529
H	0.9051367	2.8136948	-3.6227266
H	1.1552437	-1.0259009	-1.6276599
H	1.3226862	0.3443093	-3.7168552
C	-0.3795542	-3.7387586	-2.0743950
C	-0.4233111	-3.2000774	-0.9759794
C	-0.4556188	-2.5548082	0.3016682
C	-1.5864771	-1.7966589	0.6948857
C	0.6542438	-2.6524769	1.1782074
C	-1.6070187	-1.1574786	1.9419230
C	0.6182975	-2.0162286	2.4263806
C	-0.5092169	-1.2690650	2.8134493
H	-0.3564468	-4.2421510	-3.0211814
H	-2.4296415	-1.6978916	0.0097424
H	1.5419946	-3.2054546	0.8624300
H	-2.4771590	-0.5593933	2.2249959
H	1.4775966	-2.1008139	3.0985028
H	-0.5290282	-0.7689579	3.7867711
C	4.1673651	-3.0892150	-0.3162981
C	4.0870026	-1.8933369	-0.0663051
C	3.9685390	-0.4952460	0.2166140
C	3.5646840	-0.0529062	1.5005555
C	4.2339076	0.4658994	-0.7902943
C	3.4185224	1.3151842	1.7629511
C	4.0866442	1.8319850	-0.5179391
C	3.6755305	2.2613795	0.7555649
H	4.2608507	-4.1359889	-0.5314478
H	3.3544667	-0.7922831	2.2763446
H	4.5401969	0.1267766	-1.7832974
H	3.0861784	1.6448202	2.7518052
H	4.2762419	2.5631515	-1.3095839
H	3.5386043	3.3275597	0.9591372

Tetramer-14

C	-2.7720918	-1.2493285	-1.8148923
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C	-1.4266908	-0.9893788	-1.4528231
C	-3.6808664	-0.1664371	-1.9071322
C	-1.0007944	0.3184539	-1.1881224
C	-3.2479029	1.1392530	-1.6361562
C	-1.9114414	1.3867794	-1.2758463
C	-1.9201409	-0.0011447	2.1207124
C	-0.7434005	-0.7546089	2.3594663
C	-3.0926877	-0.6727955	1.6940108
C	-0.7462306	-2.1447304	2.1786250
C	-3.0835947	-2.0609525	1.5070574
C	-1.9134459	-2.8018792	1.7493379
C	-1.9215218	1.4207203	2.2868384
C	-1.9264066	2.6375207	2.4168247
C	-3.2091549	-2.5904787	-2.0641890
C	-3.5842461	-3.7395895	-2.2580612
H	-0.7399042	-1.8334459	-1.3682797
H	-4.7200474	-0.3637441	-2.1856529
H	0.0365571	0.5115217	-0.9006468
H	-3.9594843	1.9688794	-1.7020517
H	0.1700796	-0.2442108	2.6745397
H	-3.9956717	-0.0913972	1.4924119
H	0.1723781	-2.7084441	2.3663846
H	-3.9864986	-2.5657244	1.1509629
H	-1.9107939	-3.8855112	1.5958984
H	-1.9049372	3.7084167	2.4754979
H	-3.9106032	-4.7437265	-2.4509423
H	-1.5859845	2.4043910	-1.0495518
C	0.8790895	3.5213110	-0.2802355
C	1.2855586	2.6959276	0.7984436
C	1.4571915	3.3197863	-1.5592224
C	2.2523060	1.7009292	0.5990132
C	2.4229936	2.3211680	-1.7474870
C	2.8258460	1.5109616	-0.6711800
C	-0.1095689	4.5405994	-0.0900751
C	-0.9630502	5.4068216	0.0545447
H	0.8227342	2.8333105	1.7778616
H	1.1380211	3.9498872	-2.3940379
H	2.5524603	1.0596439	1.4326892
H	2.8605629	2.1720966	-2.7398564
H	-1.6981698	6.1784350	0.1794800
H	3.5687718	0.7237001	-0.8235703
C	2.7571813	-1.5519124	3.2411779
C	2.9287364	-1.6711573	2.0350604
C	3.1313680	-1.7813952	0.6214650
C	4.4436618	-1.8687938	0.0913220
C	2.0257670	-1.7811328	-0.2655620
C	4.6400934	-1.9552643	-1.2942199
C	2.2331112	-1.8683466	-1.6485664
C	3.5369441	-1.9564370	-2.1677471
H	2.5994481	-1.4687733	4.2993931

H	5.2974376	-1.8642069	0.7745029
H	1.0173938	-1.6961462	0.1441847
H	5.6571879	-2.0216411	-1.6939114
H	1.3763342	-1.8536183	-2.3279838
H	3.6946821	-2.0220538	-3.2488267

Tetramer-15 (Te9)

C	1.0760508	-2.0041075	1.8872553
C	0.0485357	-1.4014925	2.1670994
C	-1.1431915	-0.6514916	2.4213415
C	-1.1536736	0.3784717	3.3954778
C	-2.3154809	-0.8971037	1.6639652
C	-2.3087737	1.1472950	3.5977531
C	-3.4648026	-0.1245683	1.8749225
C	-3.4680763	0.8996374	2.8390274
H	1.9786587	-2.5169560	1.6127656
H	-0.2492693	0.5701090	3.9799226
H	-2.3056602	-1.6753806	0.9001735
H	-2.3024664	1.9459929	4.3463481
H	-4.3542405	-0.3126637	1.2664326
H	-4.3645737	1.5084643	2.9932235
C	1.5393602	-2.4681696	-1.6843629
C	0.3215562	-2.3521298	-1.6514110
C	-1.1014980	-2.2096476	-1.6070681
C	-1.7035039	-0.9591265	-1.8925469
C	-1.9271164	-3.3081717	-1.2563609
C	-3.0949019	-0.8102730	-1.8206694
C	-3.3195372	-3.1524106	-1.1951318
C	-3.9081174	-1.9045423	-1.4753633
H	2.6074301	-2.5524557	-1.6271736
H	-1.0701233	-0.1121259	-2.1561608
H	-1.4643708	-4.2726700	-1.0297202
H	-3.5398144	0.1692811	-2.0200732
H	-3.9469916	-4.0076798	-0.9245458
H	-4.9954954	-1.7872281	-1.4205693
C	-4.0450494	3.3748990	-1.0784803
C	-2.8894338	2.9711175	-1.1030220
C	-1.5453381	2.4789728	-1.1493882
C	-0.9703475	1.8472095	-0.0183274
C	-0.7797916	2.6010504	-2.3370778
C	0.3347106	1.3429040	-0.0833217
C	0.5252698	2.0889652	-2.3899966
C	1.0861634	1.4565776	-1.2655122
H	-5.0441874	3.7642331	-1.0472901
H	-1.5607702	1.7399073	0.8932188
H	-1.2226779	3.0902101	-3.2091819
H	0.7638513	0.8379042	0.7838665
H	1.1020478	2.1773772	-3.3161386
H	2.0988003	1.0482369	-1.3088077
C	4.4420584	-3.0592041	0.4575280

C	4.3816664	-1.8384534	0.3823713
C	4.3210656	-0.4106024	0.2928621
C	3.6493334	0.3462537	1.2855071
C	4.9498405	0.2647125	-0.7842308
C	3.6205900	1.7445554	1.2034662
C	4.9139640	1.6642740	-0.8557030
C	4.2525866	2.4086984	0.1376776
H	4.5000218	-4.1285523	0.5255949
H	3.1465777	-0.1722616	2.1052725
H	5.4671940	-0.3181879	-1.5515134
H	3.0919524	2.3184128	1.9704452
H	5.4035336	2.1751126	-1.6909175
H	4.2218765	3.5008647	0.0757990

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C	1.4392881	-2.3961796	0.9013369
C	0.2807233	-2.1936399	1.2390857
C	-1.0723508	-1.9288990	1.6237127
C	-1.3911703	-1.6284233	2.9725441
C	-2.1072191	-1.9370553	0.6550767
C	-2.7139092	-1.3389302	3.3373199
C	-3.4250869	-1.6459745	1.0303455
C	-3.7344103	-1.3453404	2.3686448
H	2.4587027	-2.5653375	0.6059759
H	-0.5930231	-1.6171000	3.7202809
H	-1.8640891	-2.1490988	-0.3864042
H	-2.9496888	-1.1008839	4.3794518
H	-4.2104980	-1.6337224	0.2689709
H	-4.7621949	-1.1023184	2.6541653
C	2.0775075	0.0505432	-1.9317942
C	0.9393981	-0.3268955	-2.1733131
C	-0.3958256	-0.7752292	-2.4307952
C	-1.4956093	0.1054990	-2.2711884
C	-0.6372306	-2.1142198	-2.8323417
C	-2.8015946	-0.3478157	-2.5006356
C	-1.9473010	-2.5555919	-3.0672218
C	-3.0333231	-1.6757894	-2.9010464
H	3.0687807	0.3806609	-1.6858419
H	-1.3159050	1.1339633	-1.9559917
H	0.2089081	-2.7973283	-2.9461435
H	-3.6424939	0.3371250	-2.3539716
H	-2.1237384	-3.5912917	-3.3744918
H	-4.0548827	-2.0269795	-3.0783525
C	-5.1145762	2.2933046	0.9329426
C	-3.9153473	2.3568762	0.6950302
C	-2.5155439	2.4350965	0.4017082
C	-1.6108293	1.4925758	0.9521462
C	-2.0209501	3.4520146	-0.4543717
C	-0.2472363	1.5594809	0.6391817
C	-0.6517423	3.5166326	-0.7510062

C	0.2366246	2.5702227	-0.2093086
H	-6.1625663	2.2537794	1.1587679
H	-1.9919080	0.7051372	1.6025687
H	-2.7188758	4.1777376	-0.8816534
H	0.4350408	0.7984969	1.0269741
H	-0.2782895	4.2998989	-1.4183316
H	1.2966081	2.5979625	-0.4714137
C	5.1945329	-2.8817067	0.6504609
C	4.9588305	-1.6818874	0.5963023
C	4.6615186	-0.2833452	0.5204835
C	3.6302791	0.2771212	1.3160647
C	5.3855252	0.5548890	-0.3659893
C	3.3355903	1.6435920	1.2243288
C	5.0795921	1.9209884	-0.4515242
C	4.0556064	2.4686714	0.3425662
H	5.4158734	-3.9302157	0.7108822
H	3.0575691	-0.3700929	1.9844276
H	6.1772100	0.1220970	-0.9839093
H	2.5299757	2.0656128	1.8313373
H	5.6414538	2.5603901	-1.1395643
H	3.8166952	3.5344108	0.2718125

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C	-1.6457869	2.9571956	0.2451016
C	-0.5743476	3.3878699	-0.5790967
C	-1.4210054	1.9227261	1.1881124
C	0.6898476	2.7939773	-0.4557733
C	-0.1515831	1.3426130	1.3054761
C	0.9056340	1.7724393	0.4860329
C	-1.1462089	-1.2044215	-2.5068782
C	-2.1142516	-2.2254557	-2.6904133
C	-1.5533144	0.0507004	-1.9893306
C	-3.4557428	-1.9937340	-2.3572872
C	-2.8997950	0.2745804	-1.6693838
C	-3.8523246	-0.7437883	-1.8478150
C	0.2287294	-1.4686004	-2.8059633
C	1.3988820	-1.7428794	-3.0369914
C	-2.9460313	3.5418087	0.1072855
C	-4.0662277	4.0165278	-0.0300107
H	-0.7501904	4.1795949	-1.3127607
H	-2.2497316	1.5692612	1.8071298
H	1.5107845	3.1222983	-1.1001978
H	0.0109107	0.5426505	2.0299461
H	-1.7981014	-3.1963622	-3.0820098
H	-0.8105804	0.8324768	-1.8154774
H	-4.1923288	-2.7924202	-2.4913179
H	-3.2054284	1.2415250	-1.2632606
H	-4.8987473	-0.5676168	-1.5802500
H	2.4292633	-1.9967433	-3.1878188
H	-5.0411311	4.4524616	-0.1329942

H	1.8889157	1.3066524	0.5737467
C	3.9732507	-0.4659334	-0.1922153
C	3.8465189	0.4423411	-1.2737302
C	4.3716558	0.0260371	1.0769646
C	4.1274716	1.8027117	-1.0891311
C	4.6418449	1.3903095	1.2527910
C	4.5249435	2.2823472	0.1715310
C	3.7082202	-1.8605581	-0.3747586
C	3.4881633	-3.0553320	-0.5203114
H	3.5148998	0.0748914	-2.2473238
H	4.4643730	-0.6701767	1.9150117
H	4.0268887	2.4936511	-1.9318332
H	4.9436343	1.7595153	2.2378341
H	3.2713442	-4.0981966	-0.6492162
H	4.7344931	3.3469568	0.3137495
C	-4.4069359	-0.9090336	2.5019121
C	-3.2348576	-1.2426614	2.3866348
C	-1.8524667	-1.5863532	2.2403796
C	-1.3121160	-1.8439192	0.9557223
C	-1.0005652	-1.6370243	3.3733130
C	0.0533634	-2.1224030	0.8078270
C	0.3627067	-1.9252430	3.2152988
C	0.8944638	-2.1626631	1.9339416
H	-5.4402405	-0.6406868	2.6074526
H	-1.9666217	-1.7954346	0.0842321
H	-1.4163768	-1.4384006	4.3651898
H	0.4710875	-2.2838860	-0.1894196
H	1.0135317	-1.9563536	4.0953067
H	1.9608650	-2.3681862	1.8055669

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C	-2.9576710	-0.1766576	2.4077892
C	-3.4469665	0.9414528	1.7098641
C	-2.8705924	-1.4212805	1.7604434
H	-3.4999923	1.9160288	2.2032565
H	-2.4895678	-2.2948148	2.2986977
C	-3.8420680	0.8220295	0.3721243
C	-3.2620934	-1.5524486	0.4210351
H	-4.1974202	1.6948736	-0.1806314
H	-3.1745730	-2.5134581	-0.0903167
C	-3.7482496	-0.4277090	-0.2899357
H	-2.6267190	-0.0730180	3.4449196
C	-4.1144776	-0.5426734	-1.6690111
C	-4.3922583	-0.6323821	-2.8587836
H	-4.6912230	-0.7158170	-3.8858206
C	-0.2116174	1.5794788	0.9908605
C	-0.5588232	2.9531672	0.9730892
C	-0.4115682	0.8013966	-0.1728884
H	-0.3859061	3.5602990	1.8652919
H	-0.1291713	-0.2488753	-0.1776665

C	-1.1038675	3.5248245	-0.1838582
C	-0.9609130	1.3793723	-1.3213082
H	-1.3634504	4.5884337	-0.1909746
H	-1.1181346	0.7585565	-2.2068302
C	-1.3118611	2.7396092	-1.3329141
H	-1.7424689	3.1893668	-2.2333283
C	0.3296044	0.9877017	2.1759506
C	0.7754458	0.4850360	3.1988912
H	1.1868996	0.0587787	4.0924696
C	2.5257423	-0.2378015	-1.8759846
C	2.9125924	-0.2654970	-0.5248482
C	2.3096594	0.9945469	-2.5166570
H	3.0687798	-1.2219865	-0.0211580
H	1.9999855	1.0208631	-3.5664061
C	3.0769477	0.9289004	0.1870351
C	2.4707024	2.1956214	-1.8126542
H	3.3489068	0.9112443	1.2448781
H	2.2871840	3.1559424	-2.3018808
C	2.8534120	2.1761889	-0.4485139
H	2.3725672	-1.1759463	-2.4169826
C	3.0007599	3.3971813	0.2840190
C	3.1224945	4.4376925	0.9172556
H	3.2420840	5.3498747	1.4687857
C	-1.1042192	-2.2661635	-2.1208164
C	-0.2332570	-2.6394127	-1.3470367
C	0.7912916	-3.0099677	-0.4194310
C	0.6945349	-2.6230709	0.9411645
C	1.9312576	-3.7326939	-0.8524314
C	1.7212067	-2.9444174	1.8383737
C	2.9520322	-4.0503084	0.0536141
C	2.8524377	-3.6561893	1.4012032
H	-1.9158881	-1.9300774	-2.7389596
H	-0.1734029	-2.0535507	1.2805520
H	2.0083463	-4.0277365	-1.9025475
H	1.6418637	-2.6232633	2.8812678
H	3.8312012	-4.6024001	-0.2931458
H	3.6562611	-3.8981156	2.1035968

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C	-3.2842542	0.6830429	1.0309203
C	-2.7034611	0.6304158	-0.2479010
C	-4.1624066	-0.3343042	1.4436516
H	-2.0214401	1.4194538	-0.5700293
H	-4.6204316	-0.2974768	2.4375417
C	-2.9889243	-0.4354491	-1.1093037
C	-4.4582576	-1.4035782	0.5864855
H	-2.5243284	-0.4902316	-2.0966932
H	-5.1437778	-2.1963611	0.9000533
C	-3.8680976	-1.4688980	-0.7001937
H	-3.0406258	1.5095855	1.7037286

C	-4.1453012	-2.5726035	-1.5688417
C	-4.3712603	-3.5241697	-2.3055975
H	-4.5967836	-4.3411357	-2.9633623
C	-0.0968505	-1.0010701	1.2436777
C	0.6578738	-0.6742750	0.0922298
C	-0.9115350	-2.1607493	1.2310624
H	1.3025447	0.2036427	0.0939294
H	-1.5082508	-2.4047220	2.1134972
C	0.5917838	-1.4840643	-1.0473324
C	-0.9676117	-2.9673268	0.0879120
H	1.1786793	-1.2098210	-1.9286746
H	-1.6183560	-3.8465042	0.0775848
C	-0.2186218	-2.6325411	-1.0549653
H	-0.2783685	-3.2611085	-1.9492732
C	-0.0404780	-0.1749094	2.4110751
C	-0.0019813	0.5279102	3.4130580
H	0.0380246	1.1284212	4.3005838
C	4.1529563	0.3500081	0.4284640
C	4.2565620	-0.8209706	-0.3641159
C	3.6968184	0.2654347	1.7504098
H	3.6064688	1.1765139	2.3497494
C	3.8977369	-2.0706790	0.1992351
C	3.3409751	-0.9780171	2.3019984
H	3.9700107	-2.9727717	-0.4142963
H	2.9614872	-1.0334580	3.3261539
C	3.4443439	-2.1430873	1.5227591
H	4.4179690	1.3163780	-0.0074325
H	3.1532117	-3.1113417	1.9409811
C	4.7086528	-0.7402371	-1.7202294
C	5.0721031	-0.6567142	-2.8870014
H	5.4357701	-0.5985592	-3.8948746
C	2.3112652	1.7567785	-2.1138582
C	1.3757304	2.3359768	-1.5782424
C	0.2781543	2.9716798	-0.9154716
C	-0.6926545	3.6986546	-1.6504323
C	0.1380893	2.8638982	0.4914338
C	-1.7741904	4.2986125	-0.9902168
C	-0.9446406	3.4698139	1.1411863
C	-1.9038104	4.1888605	0.4065318
H	3.1355379	1.2219839	-2.5497737
H	-0.5893647	3.7798057	-2.7360518
H	0.8662545	2.2866503	1.0650784
H	-2.5223103	4.8491517	-1.5693431
H	-1.0451372	3.3610231	2.2251563
H	-2.7542278	4.6531291	0.9161873

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C	-3.6836178	-2.8418500	1.1211514
C	-3.1555650	-1.5618138	1.3608094
C	-4.0311738	-3.2207461	-0.1890775

H	-2.8529584	-1.2713968	2.3707687
H	-4.4458187	-4.2155220	-0.3828871
C	-2.9775202	-0.6591394	0.3041445
C	-3.8523132	-2.3273402	-1.2533410
H	-2.5565423	0.3300893	0.4895263
H	-4.1186300	-2.6169669	-2.2736953
C	-3.3254795	-1.0321387	-1.0169003
H	-3.8200346	-3.5440723	1.9500199
C	-3.1555903	-0.1169865	-2.1048823
C	-3.0311871	0.6641201	-3.0389717
H	-2.9260268	1.3579852	-3.8502039
C	0.2220342	-1.5760529	0.9008487
C	0.5955115	-0.3747795	0.2519719
C	-0.1767524	-2.6900758	0.1221583
H	0.9083076	0.4875910	0.8424669
H	-0.4859707	-3.6096292	0.6241348
C	0.5756359	-0.2968034	-1.1456613
C	-0.2028450	-2.5977578	-1.2749639
H	0.8740478	0.6377493	-1.6263526
H	-0.5309039	-3.4580355	-1.8659475
C	0.1755082	-1.4033382	-1.9139371
H	0.1467159	-1.3330382	-3.0052108
C	0.2390816	-1.6645010	2.3287637
C	0.2549011	-1.7460420	3.5501679
H	0.2603463	-1.8169747	4.6204520
C	4.3077227	0.0200335	0.9785871
C	4.4671135	-0.0759489	-0.4272357
C	3.7914034	-1.0615813	1.7037313
H	3.6584081	-0.9747122	2.7860640
C	4.0948566	-1.2751312	-1.0844240
C	3.4240571	-2.2473472	1.0437813
H	4.2117970	-1.3481251	-2.1689571
H	2.9926943	-3.0758501	1.6124160
C	3.5769807	-2.3493946	-0.3492562
H	4.5874323	0.9474119	1.4857689
H	3.2736106	-3.2626360	-0.8693756
C	4.9916153	1.0294166	-1.1708641
C	5.4138259	1.9943956	-1.7962757
H	5.8123291	2.8257438	-2.3451003
C	2.0759249	2.8953327	-0.3794797
C	0.9118294	3.1298611	-0.0813852
C	-0.4583477	3.3823207	0.2478882
C	-0.7992126	4.3066559	1.2678161
C	-1.4956667	2.7111051	-0.4474111
C	-2.1443576	4.5555625	1.5742289
C	-2.8375898	2.9699883	-0.1365661
C	-3.1683200	3.8921613	0.8728249
H	3.0887177	2.6714995	-0.6643813
H	-0.0010885	4.8226200	1.8090787
H	-1.2476271	1.9799865	-1.2198211

H	-2.3938452	5.2721885	2.3639015
H	-3.6204804	2.4370869	-0.6843651
H	-4.2174226	4.0925903	1.1135681

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C	-3.9214756	-1.9482723	-0.3478072
C	-3.7125543	-1.5298003	0.9767654
C	-4.4120560	-1.0369530	-1.3002071
H	-3.3092664	-2.2294318	1.7141359
H	-4.5710554	-1.3572749	-2.3349977
C	-3.9890084	-0.2092010	1.3530292
C	-4.6914704	0.2867095	-0.9355266
H	-3.8172039	0.1223373	2.3806198
H	-5.0724672	0.9990978	-1.6728536
C	-4.4847554	0.7159730	0.4005851
H	-3.6809786	-2.9742604	-0.6411907
C	-4.7771707	2.0653192	0.7814594
C	-5.0197462	3.2226026	1.1013683
H	-5.2563769	4.2287678	1.3897793
C	-0.3901596	-2.5699786	-0.4385355
C	-0.0758746	-2.4340508	0.9361925
C	-0.7767214	-1.4224087	-1.1748428
H	0.2411114	-3.3145149	1.5007593
H	-1.0251090	-1.5282821	-2.2338884
C	-0.1455070	-1.1781810	1.5518065
C	-0.8461013	-0.1729366	-0.5487979
H	0.1270251	-1.0766315	2.6061933
H	-1.1500224	0.7088468	-1.1167550
C	-0.5315484	-0.0461888	0.8137432
H	-0.5783096	0.9361593	1.2885609
C	-0.3147634	-3.8477303	-1.0790616
C	-0.2495981	-4.9386025	-1.6317833
H	-0.1973773	-5.8969009	-2.1109935
C	3.2140251	-2.6585784	-0.7584046
C	3.6997783	-2.9410256	0.5308890
C	2.7101147	-1.3789334	-1.0493004
H	4.0904826	-3.9369966	0.7643088
H	2.3137670	-1.1571283	-2.0440359
C	3.6790610	-1.9539814	1.5262368
C	2.6805373	-0.3871077	-0.0625592
H	4.0492436	-2.1712327	2.5325005
H	2.2633714	0.5947411	-0.2827321
C	3.1616257	-0.6656785	1.2404462
H	3.2111779	-3.4381614	-1.5261612
C	3.0883887	0.3286061	2.2681984
C	2.9932430	1.1633768	3.1587592
H	2.9320601	1.9014778	3.9346679
C	-1.4907959	3.3440825	-0.0369541
C	-0.3143680	3.2420640	-0.3590257
C	1.0565169	3.0725461	-0.7334126

C	2.0949922	3.3026578	0.2034908
C	1.3949169	2.6503054	-2.0451627
C	3.4346186	3.1220026	-0.1664855
C	2.7375664	2.4735701	-2.4058446
C	3.7613952	2.7105128	-1.4702789
H	-2.5263874	3.3967070	0.2506951
H	1.8376233	3.6027931	1.2221078
H	0.5960655	2.4617572	-2.7675708
H	4.2239942	3.2820016	0.5735152
H	2.9872073	2.1433826	-3.4192011
H	4.8079454	2.5598716	-1.7521868

Tetramer-22 (Tel1)

C	-1.3192254	2.8561467	-0.6889051
C	-0.7333878	2.6925142	-1.9700094
C	-0.5868599	2.4593331	0.4582397
C	0.5539833	2.1512544	-2.0908182
C	0.6978220	1.9177343	0.3249274
C	1.2736001	1.7627744	-0.9473699
C	1.0914398	-2.7163013	-0.4757669
C	0.8625389	-2.3744812	-1.8324889
C	0.2824513	-2.1281271	0.5295170
C	-0.1527940	-1.4684163	-2.1675662
C	-0.7294405	-1.2242043	0.1821199
C	-0.9504914	-0.8932009	-1.1644809
C	2.1366126	-3.6286683	-0.1227376
C	3.0603629	-4.3701249	0.1879346
C	-2.6281560	3.4209769	-0.5544500
C	-3.7516986	3.8918304	-0.4316090
H	-1.2966548	2.9967072	-2.8568948
H	-1.0372902	2.5773971	1.4469352
H	0.9955964	2.0252096	-3.0845949
H	1.2496259	1.6100338	1.2161646
H	1.4863746	-2.8255835	-2.6095179
H	0.4609343	-2.3865622	1.5771891
H	-0.3206968	-1.2074897	-3.2171767
H	-1.3467771	-0.7748372	0.9619787
H	-1.7337553	-0.1797532	-1.4275363
H	3.8467466	-5.0476764	0.4594010
H	-4.7321797	4.3147943	-0.3268507
H	2.2706992	1.3288202	-1.0457677
C	3.9363520	0.6670590	1.2442417
C	3.6976103	-0.5673916	0.5908757
C	4.6406440	1.6888268	0.5575789
C	4.1520180	-0.7718556	-0.7186136
C	5.0932700	1.4737084	-0.7513734
C	4.8507587	0.2448755	-1.3935189
C	3.4514457	0.8849622	2.5740331
C	3.0047261	1.0794720	3.6970121
H	3.1502490	-1.3573271	1.1085034

H	4.8179478	2.6452019	1.0572190
H	3.9516139	-1.7293303	-1.2069240
H	5.6333982	2.2695854	-1.2740878
H	2.6388560	1.2432859	4.6922522
H	5.2026048	0.0834230	-2.4175267
C	-4.7681390	-1.9692969	-2.2936800
C	-4.5081588	-1.5690283	-1.1668193
C	-4.1777812	-1.0907297	0.1411016
C	-3.9579289	0.2919196	0.3596641
C	-4.0426326	-1.9916553	1.2271981
C	-3.6069870	0.7581913	1.6333877
C	-3.6924732	-1.5154768	2.4981355
C	-3.4719311	-0.1411773	2.7064812
H	-5.0108752	-2.3240244	-3.2767143
H	-4.0489559	0.9944043	-0.4717845
H	-4.2038625	-3.0599120	1.0589908
H	-3.4348484	1.8284516	1.7757962
H	-3.5857780	-2.2206757	3.3286998
H	-3.1940380	0.2246469	3.7001195

Tetramer-23

C	-4.2125299	-1.6998976	-0.7158063
C	-3.9434593	-1.5342695	0.6534640
C	-4.5748090	-0.5880897	-1.4972263
H	-3.6417020	-2.3931330	1.2598747
H	-4.7829002	-0.7123626	-2.5651354
C	-4.0346048	-0.2673375	1.2429802
C	-4.6687142	0.6844159	-0.9172655
H	-3.8162146	-0.1328361	2.3055031
H	-4.9508848	1.5518437	-1.5207368
C	-4.4020133	0.8592164	0.4644196
H	-4.1256569	-2.6896201	-1.1744080
C	-4.5071802	2.1553353	1.0663446
C	-4.5973996	3.2640849	1.5790833
H	-4.6994160	4.2279386	2.0404183
C	-0.5510494	-2.5408495	-0.3940949
C	-0.2609017	-2.4124821	0.9868737
C	-0.8641062	-1.3788143	-1.1427048
H	-0.0055978	-3.3054531	1.5630804
H	-1.0940795	-1.4780925	-2.2065247
C	-0.2800905	-1.1511348	1.5959284
C	-0.8826293	-0.1237049	-0.5238556
H	-0.0333804	-1.0593803	2.6577322
H	-1.1283076	0.7700517	-1.1017178
C	-0.5906651	-0.0045859	0.8448042
H	-0.5970059	0.9823140	1.3130149
C	-0.5265527	-3.8254705	-1.0263918
C	-0.5054233	-4.9233431	-1.5696779
H	-0.4892389	-5.8868061	-2.0411766
C	3.5595473	-3.1192085	0.6548071

C	3.5478325	-2.1132794	1.6311889
C	3.1427692	-2.8369970	-0.6585074
H	3.8665851	-2.3293437	2.6550959
H	3.1378104	-3.6286265	-1.4140062
C	3.1115826	-0.8050132	1.3020054
C	2.7153788	-1.5396222	-0.9915522
H	2.3791821	-1.3166572	-2.0082519
C	2.6974923	-0.5275221	-0.0243818
H	3.8914788	-4.1286452	0.9202592
H	2.3491203	0.4738282	-0.2798432
C	3.0642472	0.2158020	2.3058824
C	3.0004070	1.0778096	3.1728635
H	2.9601233	1.8358586	3.9311194
C	-1.2577896	3.4576770	-0.0402381
C	-0.0978915	3.2901803	-0.3948592
C	1.2527842	3.0482565	-0.8043499
C	2.3290243	3.2586033	0.0942959
C	1.5329115	2.5748352	-2.1122705
C	3.6475569	3.0066337	-0.3087827
C	2.8548211	2.3262601	-2.5063731
C	3.9162013	2.5424591	-1.6084146
H	-2.2772894	3.5605400	0.2881637
H	2.1165162	3.6035038	1.1090616
H	0.7046860	2.4053465	-2.8056813
H	4.4668834	3.1573050	0.4004883
H	3.0592520	1.9590146	-3.5172805
H	4.9463837	2.3397000	-1.9171461

Tetramer-24 (Te12)

C	-2.1234753	-1.4828511	-1.4259205
C	-1.8019679	-0.9227952	-0.1779214
C	-2.3415374	-0.6441702	-2.5329803
H	-1.6320192	-1.5729620	0.6836064
H	-2.5919969	-1.0751028	-3.5080024
C	-1.6981598	0.4641196	-0.0309080
C	-2.2399309	0.7474978	-2.3960698
H	-1.4485751	0.9023731	0.9369654
H	-2.4086286	1.4051798	-3.2534949
C	-1.9162406	1.3167721	-1.1397406
H	-2.2019711	-2.5681216	-1.5333132
C	-1.8101651	2.7365587	-0.9933255
C	-1.7185931	3.9513417	-0.8700049
H	-1.6377470	5.0157522	-0.7642200
C	1.5666329	-1.2053652	-0.5067348
C	1.8291967	-0.6238679	0.7576867
C	1.3844001	-0.3623533	-1.6300039
H	1.9848161	-1.2742077	1.6218394
H	1.1665802	-0.8097321	-2.6028487
C	1.9097235	0.7678056	0.8894787
C	1.4626819	1.0284047	-1.4865692

H	2.1298924	1.2077446	1.8664590
H	1.3024625	1.6723265	-2.3561901
C	1.7264711	1.5984017	-0.2292690
H	1.7879758	2.6844899	-0.1213878
C	1.4865630	-2.6274190	-0.6473099
C	1.4188660	-3.8441171	-0.7674833
H	1.3557377	-4.9098183	-0.8723559
C	5.4441422	-1.5309888	1.5726817
C	5.5182706	-0.1388467	1.7201547
C	5.1582282	-2.0970279	0.3175070
H	5.7359992	0.3066637	2.6951573
H	5.0842665	-3.1831866	0.2079047
C	5.3046061	0.7089922	0.6046440
C	4.9496786	-1.2619968	-0.7941821
H	4.7098252	-1.6987838	-1.7680984
C	5.0238330	0.1295581	-0.6576208
H	5.6078964	-2.1769809	2.4417831
H	4.8419065	0.7824244	-1.5147836
C	5.3540804	2.1323373	0.7546911
C	5.3770586	3.3490910	0.8863597
H	5.4198461	4.4156620	0.9970885
C	-5.0583687	-3.4753645	0.9797781
C	-5.0213876	-2.2527091	1.0311313
C	-4.9538266	-0.8234180	1.0856304
C	-5.2232199	-0.0470837	-0.0687651
C	-4.5975676	-0.1668597	2.2900779
C	-5.1293349	1.3490518	-0.0175218
C	-4.5075980	1.2315079	2.3314187
C	-4.7709545	1.9936044	1.1795105
H	-5.1124126	-4.5462542	0.9412723
H	-5.4822414	-0.5530804	-1.0021488
H	-4.3894631	-0.7646843	3.1820732
H	-5.3182308	1.9381534	-0.9198679
H	-4.2274632	1.7284422	3.2662101
H	-4.6829590	3.0836737	1.2091368

Tetramer-25 (Tel3)

C	-1.0315436	3.0695773	-0.1838663
C	-1.4893618	3.4993447	1.0882409
C	-1.5354049	3.7102187	-1.3447729
C	-2.4229798	4.5400381	1.1921056
C	-2.4705832	4.7490688	-1.2317658
C	-2.9188315	5.1691183	0.0348708
C	-0.0847534	2.0019472	-0.2903998
C	0.7317555	1.0943199	-0.3700460
H	-1.1129237	2.9992557	1.9848063
H	-1.1910300	3.3772594	-2.3276790
H	-2.7706112	4.8570380	2.1804827
H	-2.8548920	5.2305452	-2.1367005
H	-3.6506768	5.9787512	0.1189648

H	1.4271900	0.2788013	-0.4311034
C	0.4129373	-2.4537336	-0.2121002
C	1.0086228	-2.3899164	-1.4977057
C	1.2246055	-2.2325981	0.9300735
C	2.3762123	-2.1092645	-1.6319388
C	2.5897649	-1.9483543	0.7841870
C	3.1732786	-1.8856399	-0.4942439
C	-0.9878843	-2.7148613	-0.0733872
C	-2.1879315	-2.9265737	0.0379655
H	0.3846816	-2.5536661	-2.3805900
H	0.7673335	-2.2740857	1.9223229
H	2.8214126	-2.0596780	-2.6308449
H	3.2050983	-1.7642828	1.6696313
H	4.2363055	-1.6558182	-0.5997276
H	-3.2480569	-3.0683028	0.1320350
C	-5.1418436	-0.8593848	0.0801408
C	-5.2724154	-1.4599021	1.3584167
C	-5.4286495	-1.6333485	-1.0730754
C	-5.6723258	-2.7986592	1.4752597
C	-5.8283777	-2.9714117	-0.9470496
C	-5.9503028	-3.5608800	0.3251998
C	-4.7054120	0.4982537	-0.0417704
C	-4.3164906	1.6540444	-0.1396810
H	-5.0461452	-0.8677850	2.2492692
H	-5.3232427	-1.1759390	-2.0605673
H	-5.7611187	-3.2511505	2.4680600
H	-6.0392865	-3.5590964	-1.8461988
H	-6.2579349	-4.6071737	0.4194996
H	-3.9380766	2.6556931	-0.2217279
C	3.5311532	2.6017693	0.6538144
C	4.4005204	1.7498845	0.5313319
C	5.3700588	0.7120890	0.3627902
C	5.6902450	-0.1574284	1.4358622
C	5.9955206	0.5108975	-0.8940556
C	6.5969976	-1.2095990	1.2478926
C	6.9017130	-0.5437367	-1.0725088
C	7.2035534	-1.4102039	-0.0057402
H	2.7463981	3.3273536	0.7464088
H	5.2110487	-0.0027633	2.4065252
H	5.7513868	1.1809733	-1.7229939
H	6.8299538	-1.8784874	2.0826518
H	7.3710525	-0.6931085	-2.0503504
H	7.9088154	-2.2350108	-0.1495847

Tetramer-26 (Te15)

C	-1.6730651	-4.1359800	-0.1897710
C	-1.2014978	-4.8881243	0.9168891
C	-1.3063010	-4.5414669	-1.4991536
C	-0.3869585	-6.0115834	0.7152675
C	-0.4911655	-5.6664125	-1.6909636

C	-0.0284319	-6.4056775	-0.5868697
C	-2.4977042	-2.9823258	0.0103726
C	-3.1950267	-1.9912665	0.1808460
C	4.1393094	-1.6713004	0.1898925
C	4.8937080	-1.2029227	-0.9165495
C	4.5453973	-1.3055605	1.4993403
C	6.0203542	-0.3928644	-0.7146601
C	5.6735544	-0.4949231	1.6914537
C	6.4153462	-0.0356688	0.5875841
C	2.9829752	-2.4922431	-0.0107931
C	1.9904198	-3.1868910	-0.1821626
H	-1.4768106	-4.5758083	1.9279455
H	-1.6633356	-3.9615851	-2.3546453
H	-0.0245357	-6.5790448	1.5783567
H	-0.2115266	-5.9650344	-2.7063093
H	0.6122374	-7.2796902	-0.7399847
H	-3.8038740	-1.1178433	0.3251002
H	4.5807032	-1.4772192	-1.9276803
H	3.9635719	-1.6598258	2.3546809
H	6.5897048	-0.0330464	-1.5775802
H	5.9728391	-0.2161978	2.7068489
H	7.2921145	0.6011622	0.7409520
H	1.1155822	-3.7936746	-0.3271748
C	-4.1444648	1.6749668	0.2059895
C	-4.8835233	1.2116007	-0.9128670
C	-4.5635785	1.2962054	1.5076040
C	-6.0078597	0.3936755	-0.7306373
C	-5.6892825	0.4777531	1.6800525
C	-6.4157500	0.0235073	0.5639779
C	-2.9906793	2.5042061	0.0254462
C	-2.0009390	3.2071632	-0.1277858
H	-4.5606481	1.4961318	-1.9180559
H	-3.9937935	1.6467656	2.3725278
H	-6.5651976	0.0378192	-1.6029882
H	-5.9985945	0.1889299	2.6895968
H	-7.2904877	-0.6195775	0.7020231
H	-1.1277662	3.8196382	-0.2585867
H	3.8101367	1.1204394	0.3266990
C	3.1998349	1.9924588	0.1798750
C	2.5006040	2.9815250	0.0062686
C	1.6758800	4.1346716	-0.1967672
C	1.2896504	4.5234150	-1.5055955
H	1.6304921	3.9301677	-2.3585195
C	0.4763166	5.6491788	-1.6999756
H	0.1816328	5.9349094	-2.7147726
H	-0.6046233	7.2805723	-0.7541197
C	0.0344971	6.4057695	-0.5990691
C	0.4120175	6.0280959	0.7026098
H	0.0660763	6.6092029	1.5633701
C	1.2250651	4.9039580	0.9067844

H 1.5156184 4.6046460 1.9175093

Tetramer-27 (Tel4)

C	-4.8752230	2.0281940	0.0000209
C	-4.9806056	1.3303349	-1.2151974
C	-4.9805693	1.3303384	1.2152240
H	-4.8835594	1.8667839	-2.1642265
H	-4.8834318	1.8667796	2.1642703
C	-5.1940043	-0.0545344	-1.2212342
C	-5.1940308	-0.0545224	1.2212586
H	-5.2683618	-0.6022998	-2.1647653
H	-5.2684506	-0.6022929	2.1647517
C	-5.3038411	-0.7646531	0.0000074
H	-4.6877893	3.1059400	0.0000269
C	-5.5151962	-2.1803112	0.0000397
C	-5.6930343	-3.3914797	-0.0000026
H	-5.8635657	-4.4506952	-0.0000617
C	-1.2934732	3.2319466	-0.0000049
C	-1.3845714	2.5315489	-1.2160292
C	-1.3845334	2.5315388	1.2160044
H	-1.3141662	3.0712231	-2.1660244
H	-1.3140224	3.0711956	2.1660071
C	-1.5647803	1.1426640	-1.2194722
C	-1.5648337	1.1426622	1.2194895
H	-1.6379497	0.5936021	-2.1613338
H	-1.6381254	0.5936077	2.1612964
C	-1.6577536	0.4291179	-0.0000500
C	-1.8442679	-0.9873537	-0.0000367
C	-2.0055009	-2.1990541	0.0000081
H	-2.1434459	-3.2616230	0.0000440
H	-1.1520731	4.3175646	-0.0000038
C	1.8637094	1.1592406	0.0000388
C	1.7841627	0.4580744	-1.2136207
C	1.7841258	0.4580653	1.2136573
H	1.8455245	0.9994014	-2.1619374
H	1.8454396	0.9993805	2.1620024
C	1.6269893	-0.9337088	-1.2203959
C	1.6269703	-0.9337282	1.2204489
H	1.5634373	-1.4828010	-2.1632579
H	1.5634228	-1.4828365	2.1632591
C	1.5464526	-1.6467081	-0.0000169
H	1.9865496	2.2448201	0.0000414
C	1.3876008	-3.0683006	-0.0000178
C	1.2565800	-4.2855374	-0.0000231
H	1.1321101	-5.3508718	-0.0000964
C	5.1491596	-0.3064757	0.0000100
C	5.2092239	0.4105016	1.2208496
C	5.2092589	0.4104638	-1.2208648
H	5.1530365	-0.1399890	2.1637890
H	5.1530924	-0.1400504	-2.1637755

C	5.3236033	1.8069829	1.2163177
C	5.3236468	1.8069522	-1.2163672
H	5.3659377	2.3497479	2.1664411
H	5.3660217	2.3496855	-2.1665033
C	5.3797001	2.5108160	-0.0000337
H	5.4685291	3.6021891	-0.0000515
C	5.0069085	-1.7299221	0.0000152
C	4.8661501	-2.9450965	0.0000313
H	4.6856199	-4.0022949	0.0000536

Pentamer

Pentamer-01 (P1)

C	3.9827469	3.5796483	0.5145860
C	3.8408701	2.3879528	0.7542307
C	3.6292856	0.9974613	1.0201930
C	3.6530657	0.5020880	2.3479682
C	3.3563209	0.1050768	-0.0464522
C	3.4108039	-0.8557047	2.5975541
C	3.1148468	-1.2503510	0.2143236
C	3.1431171	-1.7360915	1.5333997
H	4.1288027	4.6212544	0.3042410
H	3.8453315	1.1935446	3.1728056
H	3.3186885	0.4875282	-1.0681554
H	3.4170477	-1.2250393	3.6275833
H	2.8859156	-1.9297693	-0.6101385
H	2.9391272	-2.7935258	1.7236249
C	0.0911255	4.2884957	-1.6396591
C	0.5432639	3.2136503	-2.0115307
C	1.0689585	1.9565799	-2.4527420
C	0.4728756	0.7375206	-2.0422170
C	2.1946148	1.9207359	-3.3151874
C	0.9821026	-0.4835206	-2.5016714
C	2.6984721	0.6925996	-3.7653550
C	2.0903070	-0.5119372	-3.3650525
H	-0.3060503	5.2310527	-1.3168727
H	-0.3803521	0.7524319	-1.3624713
H	2.6633344	2.8600415	-3.6209321
H	0.5166602	-1.4137188	-2.1759622
H	3.5681327	0.6765995	-4.4296413
H	2.4861627	-1.4702934	-3.7157445
C	-0.7322567	-2.0682528	3.8015797
C	-0.6717229	-0.9266874	3.3648339
C	-0.5942030	0.4047387	2.8449781
C	0.2770071	0.7023168	1.7671671
C	-1.3863701	1.4404880	3.4021163
C	0.3604418	2.0087765	1.2707130

C	-1.2978063	2.7441149	2.8945189
C	-0.4230489	3.0317188	1.8304732
H	-0.7868853	-3.0732879	4.1722942
H	0.8807121	-0.0920101	1.3281792
H	-2.0704290	1.2088385	4.2220156
H	1.0371672	2.2345184	0.4463611
H	-1.9186449	3.5351137	3.3264379
H	-0.3564773	4.0464378	1.4276020
C	2.5142492	-5.0331101	-0.1710863
C	1.4769159	-4.4229258	-0.3953161
C	0.2839535	-3.6798065	-0.6704481
C	-0.1723975	-2.6931772	0.2395452
C	-0.4461926	-3.9092393	-1.8653305
C	-1.3224009	-1.9472714	-0.0484695
C	-1.5935281	-3.1526339	-2.1446010
C	-2.0315434	-2.1652680	-1.2425524
H	3.4128277	-5.5827276	0.0327529
H	0.3762528	-2.5139245	1.1657742
H	-0.0988941	-4.6733391	-2.5662063
H	-1.6675520	-1.1949897	0.6625463
H	-2.1436249	-3.3297715	-3.0741181
H	-2.9177653	-1.5665365	-1.4669161
C	-4.1576638	-0.8936200	2.6191219
C	-4.1608958	-0.3330684	1.5319689
C	-4.0999992	0.2958543	0.2479475
C	-3.0464527	1.1967071	-0.0509307
C	-5.0621241	0.0018624	-0.7513429
C	-2.9570290	1.7829391	-1.3205212
C	-4.9596992	0.5877918	-2.0212839
C	-3.9079457	1.4766491	-2.3106809
H	-4.1330601	-1.3815043	3.5737669
H	-2.3032994	1.4197759	0.7157938
H	-5.8747915	-0.6934078	-0.5232774
H	-2.1395220	2.4764618	-1.5387530
H	-5.7036641	0.3488710	-2.7883711
H	-3.8300092	1.9291317	-3.3043709

Pentamer-02 (P2)

C	-1.2990416	-4.0386925	1.6410690
C	-0.9592471	-2.8979232	1.9251019
C	-0.5442374	-1.5574326	2.2092589
C	-0.0106925	-1.2067954	3.4757579
C	-0.6488700	-0.5640283	1.2047777
C	0.4128755	0.1082989	3.7188692
C	-0.2247058	0.7455468	1.4580186
C	0.3102326	1.0866887	2.7118119
H	-1.5911511	-5.0393412	1.3883421
H	0.0755213	-1.9721149	4.2517601
H	-1.0693423	-0.8300053	0.2374141
H	0.8339877	0.3673905	4.6951240

H	-0.3178603	1.4994038	0.6755161
H	0.6515617	2.1090804	2.8953208
C	0.4932339	-4.5665157	-2.1888711
C	-0.0500188	-3.4696848	-2.1772550
C	-0.6904571	-2.1895214	-2.1437114
C	0.0620558	-0.9994353	-2.3115523
C	-2.0886676	-2.0973455	-1.9213614
C	-0.5740284	0.2484865	-2.2636776
C	-2.7147769	-0.8445246	-1.8754277
C	-1.9608583	0.3298854	-2.0513476
H	0.9689793	-5.5277667	-2.2087808
H	1.1425623	-1.0622967	-2.4555800
H	-2.6655840	-3.0130064	-1.7678269
H	0.0204662	1.1575845	-2.3755267
H	-3.7872843	-0.7817670	-1.6753600
H	-2.4468690	1.3063267	-1.9893341
C	4.8983011	1.0675856	2.8401451
C	4.5703754	0.2199660	2.0202905
C	4.1602304	-0.7401384	1.0402016
C	2.8268925	-1.2213459	1.0315177
C	5.0687373	-1.1988003	0.0522401
C	2.4105008	-2.1292337	0.0497885
C	4.6414849	-2.1083343	-0.9262886
C	3.3125037	-2.5722693	-0.9336395
H	5.1979126	1.7937693	3.5708259
H	2.1253697	-0.8663244	1.7869116
H	6.0973378	-0.8277848	0.0571142
H	1.3785068	-2.4869223	0.0467708
H	5.3481351	-2.4520747	-1.6885602
H	2.9709688	-3.2706964	-1.7028747
C	0.7628586	4.5804954	1.3756175
C	1.1729727	3.9435104	0.4138357
C	1.6572577	3.1949903	-0.7072450
C	2.3459779	1.9721714	-0.5068922
C	1.4606560	3.6721544	-2.0286842
C	2.8298052	1.2492312	-1.6049351
C	1.9528414	2.9430043	-3.1202623
C	2.6399326	1.7325899	-2.9115367
H	0.4091389	5.1365476	2.2222079
H	2.4955220	1.5976384	0.5068598
H	0.9257584	4.6132006	-2.1848760
H	3.3526099	0.3055078	-1.4373696
H	1.7968432	3.3189361	-4.1362283
H	3.0166398	1.1627957	-3.7666752
C	-2.4520221	3.3872205	0.3074593
C	-3.2704200	2.4796917	0.3735568
C	-4.1785929	1.3737647	0.4003162
C	-3.9538686	0.2865165	1.2815532
C	-5.2849490	1.3279226	-0.4849597
C	-4.8050983	-0.8261750	1.2605266

C	-6.1360936	0.2137175	-0.4928997
C	-5.8972125	-0.8680927	0.3749720
H	-1.6964087	4.1498765	0.2817175
H	-3.0968816	0.3153595	1.9574109
H	-5.4594830	2.1654367	-1.1663875
H	-4.6074256	-1.6677581	1.9315345
H	-6.9863446	0.1869879	-1.1819807
H	-6.5596315	-1.7396299	0.3594256

Pentamer-03 (P4)

C	-1.3008449	4.0406649	-1.6550008
C	-0.9577466	2.8963566	-1.9199927
C	-0.5419957	1.5557651	-2.2023649
C	-0.0170318	1.2085607	-3.4734908
C	-0.6381011	0.5605771	-1.1989169
C	0.4041074	-0.1058794	-3.7234560
C	-0.2168248	-0.7487601	-1.4593059
C	0.3077836	-1.0866171	-2.7182521
H	-1.5940284	5.0448551	-1.4182242
H	0.0637663	1.9765115	-4.2474939
H	-1.0482926	0.8248969	-0.2268141
H	0.8161046	-0.3640771	-4.7037686
H	-0.3035114	-1.5060739	-0.6793612
H	0.6464947	-2.1088359	-2.9074637
C	0.4969981	4.5674796	2.1988037
C	-0.0463816	3.4708756	2.1811854
C	-0.6886602	2.1916657	2.1452444
C	0.0618639	0.9999669	2.3114606
C	-2.0873108	2.1029084	1.9234224
C	-0.5772411	-0.2465606	2.2661906
C	-2.7160995	0.8512370	1.8780732
C	-1.9644798	-0.3244249	2.0555206
H	0.9722976	5.5289409	2.2203275
H	1.1432771	1.0605427	2.4504383
H	-2.6619934	3.0200565	1.7700971
H	0.0142265	-1.1578756	2.3783937
H	-3.7886301	0.7888949	1.6780089
H	-2.4529851	-1.2996227	1.9947020
C	4.9043041	-1.0551343	-2.8522173
C	4.5651878	-0.2180705	-2.0260452
C	4.1566360	0.7383290	-1.0416990
C	2.8250163	1.2239925	-1.0273830
C	5.0708907	1.1923384	-0.0566454
C	2.4173996	2.1362605	-0.0458817
C	4.6523027	2.1059510	0.9218126
C	3.3261384	2.5775828	0.9319809
H	5.2128171	-1.7747874	-3.5855521
H	2.1180926	0.8702928	-1.7785367
H	6.0970838	0.8146095	-0.0648329
H	1.3878204	2.5008991	-0.0382943

H	5.3626453	2.4484493	1.6812158
H	2.9917561	3.2811946	1.6996546
C	0.7583978	-4.5895009	-1.3661264
C	1.1698215	-3.9434782	-0.4109780
C	1.6564396	-3.1936860	0.7081858
C	2.3489504	-1.9728044	0.5083029
C	1.4596058	-3.6720931	2.0292889
C	2.8388737	-1.2545187	1.6068730
C	1.9576587	-2.9474484	3.1211410
C	2.6506445	-1.7405180	2.9125627
H	0.4050087	-5.1547868	-2.2067409
H	2.4964068	-1.5960637	-0.5050451
H	0.9207416	-4.6111691	2.1841218
H	3.3655253	-0.3123705	1.4417789
H	1.8029807	-3.3233208	4.1372767
H	3.0346227	-1.1755477	3.7676863
C	-2.4602450	-3.3895444	-0.3084167
C	-3.2759529	-2.4789510	-0.3652952
C	-4.1838757	-1.3728109	-0.3920482
C	-3.9583861	-0.2873469	-1.2757518
C	-5.2919670	-1.3260956	0.4912803
C	-4.8147805	0.8215119	-1.2637059
C	-6.1472580	-0.2149567	0.4911025
C	-5.9106138	0.8623711	-0.3828519
H	-1.7056621	-4.1534254	-0.2883010
H	-3.0972586	-0.3152459	-1.9464933
H	-5.4652286	-2.1607129	1.1768242
H	-4.6204490	1.6608844	-1.9384453
H	-7.0003748	-0.1863189	1.1765796
H	-6.5781164	1.7300546	-0.3757631

Pentamer-04 (P3)

C	-0.3095383	-4.9211252	1.2706594
C	-0.1618194	-3.7494314	1.5929444
C	-0.0046139	-2.3784721	1.9748166
C	0.5270922	-2.0422505	3.2464478
C	-0.3888902	-1.3427217	1.0883714
C	0.6674848	-0.6970732	3.6172609
C	-0.2394455	-0.0044831	1.4684937
C	0.2839255	0.3251043	2.7303612
H	-0.4172277	-5.9477094	0.9783475
H	0.8277478	-2.8421911	3.9286057
H	-0.8048643	-1.5981016	0.1148985
H	1.0874826	-0.4460183	4.5959222
H	-0.5278265	0.7851751	0.7737726
H	0.4043091	1.3752935	3.0079041
C	1.8522867	-3.7648253	-3.1524872
C	0.9817415	-2.9442787	-2.8930521
C	-0.0401467	-1.9944673	-2.5706253
C	0.2766188	-0.6245407	-2.3851675

C	-1.3847888	-2.4206242	-2.4155098
C	-0.7321593	0.2935206	-2.0646008
C	-2.3832356	-1.4936565	-2.0888326
C	-2.0623287	-0.1349099	-1.9185648
H	2.6113515	-4.4862812	-3.3852401
H	1.3135536	-0.2947006	-2.4758749
H	-1.6260867	-3.4795417	-2.5398102
H	-0.4759955	1.3435776	-1.9121855
H	-3.4128029	-1.8300796	-1.9419082
H	-2.8440325	0.5803423	-1.6535679
C	4.2151243	1.6920451	3.1346612
C	4.1987342	1.0008296	2.1246751
C	4.1563256	0.2176438	0.9263643
C	3.1411656	-0.7544195	0.7424179
C	5.1142447	0.4216463	-0.1001376
C	3.0769815	-1.4898291	-0.4476922
C	5.0434008	-0.3237745	-1.2860212
C	4.0220266	-1.2754497	-1.4659320
H	4.2478417	2.2856669	4.0277703
H	2.4055838	-0.9168906	1.5302450
H	5.8973087	1.1719015	0.0406178
H	2.2843264	-2.2279809	-0.5898553
H	5.7845339	-0.1579044	-2.0746050
H	3.9532991	-1.8471393	-2.3960303
C	-0.9552355	3.7625105	2.2282144
C	-0.3326051	3.5879195	1.1890091
C	0.3787094	3.3723894	-0.0352714
C	1.5055006	2.5120071	-0.0743604
C	-0.0459268	4.0139227	-1.2272546
C	2.1830119	2.2956205	-1.2815236
C	0.6455054	3.7980463	-2.4273601
C	1.7589603	2.9382929	-2.4578990
H	-1.4889273	3.9203339	3.1454498
H	1.8370630	2.0117270	0.8372147
H	-0.9171329	4.6741773	-1.1977699
H	3.0401501	1.6189345	-1.3017829
H	0.3116598	4.2967838	-3.3424709
H	2.2891519	2.7634860	-3.3991287
C	-3.5523814	-2.6860078	1.6314240
C	-3.9089154	-1.5925984	1.2151058
C	-4.2635645	-0.3109768	0.6872479
C	-3.5775773	0.8536058	1.1160551
C	-5.2664373	-0.1916713	-0.3080726
C	-3.8726472	2.0992075	0.5451168
C	-5.5603344	1.0592433	-0.8687787
C	-4.8623147	2.2069162	-0.4487682
H	-3.1886177	-3.6301494	1.9901033
H	-2.7978582	0.7630189	1.8750201
H	-5.7965656	-1.0882648	-0.6419433
H	-3.3131706	2.9826867	0.8669530

H -6.3336321 1.1399163 -1.6393689
H -5.0886367 3.1797912 -0.8965079

Pentamer-05 (P5)

C -0.0775430 4.3088037 -2.1650795
C -0.3857883 3.1277964 -2.0737488
C -0.7337059 1.7442600 -1.9568896
C -1.0381506 0.9737996 -3.1079426
C -0.7726933 1.1270927 -0.6825884
C -1.3690163 -0.3828345 -2.9777748
C -1.0987368 -0.2277634 -0.5654869
C -1.3967126 -0.9876427 -1.7080449
H 0.2033400 5.3406330 -2.2481678
H -1.0033537 1.4471968 -4.0929591
H -0.5578108 1.7200944 0.2048882
H -1.5996285 -0.9718565 -3.8704087
H -1.1327855 -0.6912714 0.4200116
H -1.6520575 -2.0447280 -1.6046111
C 3.3296771 4.2401536 0.4981464
C 2.4756789 3.5790350 1.0732492
C 1.4668072 2.8042345 1.7305660
C 1.6545469 1.4173395 1.9571870
C 0.2568173 3.4158097 2.1493584
C 0.6567113 0.6650430 2.5909808
C -0.7366149 2.6524572 2.7779102
C -0.5391944 1.2776278 3.0010190
H 4.0799006 4.8218177 -0.0018406
H 2.5717317 0.9342062 1.6146417
H 0.1067335 4.4827735 1.9641644
H 0.8101865 -0.4028018 2.7546106
H -1.6703957 3.1307465 3.0892881
H -1.3197843 0.6811747 3.4816702
C 2.0701161 -3.5080289 -3.3279099
C 2.5521321 -2.5070260 -2.8146554
C 3.1116087 -1.3465197 -2.1895035
C 2.2952413 -0.2231467 -1.9053061
C 4.4828112 -1.3164165 -1.8265440
C 2.8377115 0.8988630 -1.2662176
C 5.0148664 -0.1891502 -1.1841316
C 4.1946666 0.9187077 -0.8994647
H 1.6553771 -4.3826535 -3.7906412
H 1.2400512 -0.2443938 -2.1781124
H 5.1122458 -2.1840916 -2.0432338
H 2.2007279 1.7585327 -1.0465033
H 6.0728726 -0.1754498 -0.9025109
H 4.6038201 1.7951595 -0.3886186
C -2.1393518 -3.3702381 0.8478019
C -0.9933573 -3.2030411 1.2434266
C 0.3368104 -2.9283924 1.6968156
C 1.2989898 -2.3901175 0.8041626

C	0.6975609	-3.1501898	3.0508419
C	2.5832608	-2.0681235	1.2630731
C	1.9873362	-2.8303633	3.4981495
C	2.9312402	-2.2852640	2.6079359
H	-3.1365678	-3.4748146	0.4596519
H	1.0288830	-2.2121631	-0.2381172
H	-0.0436927	-3.5642391	3.7403658
H	3.3093155	-1.6391744	0.5688212
H	2.2557174	-3.0015723	4.5454262
H	3.9334009	-2.0261771	2.9635287
C	-5.2486819	-2.9620571	-1.1423529
C	-4.9391747	-1.8470249	-0.7404843
C	-4.5580749	-0.5498390	-0.2695515
C	-4.4529683	0.5368054	-1.1737144
C	-4.2695497	-0.3403529	1.1021811
C	-4.0677601	1.8013433	-0.7124683
C	-3.8879888	0.9305640	1.5525882
C	-3.7846970	2.0021435	0.6497725
H	-5.5509485	-3.9276616	-1.4993268
H	-4.6549855	0.3703530	-2.2347560
H	-4.3373481	-1.1806946	1.7982079
H	-3.9669469	2.6291550	-1.4200526
H	-3.6621703	1.0843371	2.6117972
H	-3.4642112	2.9868816	1.0019529

Pentamer-06 (P6)

C	2.4107658	4.7116413	1.2488533
C	2.8089806	3.5588294	1.1489913
C	3.2581581	2.2043102	1.0311355
C	3.9851282	1.5899416	2.0834044
C	2.9678326	1.4558319	-0.1369867
C	4.3993834	0.2552572	1.9673483
C	3.3849026	0.1226921	-0.2408625
C	4.0973213	-0.4833084	0.8082935
H	2.0623218	5.7226644	1.3319694
H	4.2051866	2.1651868	2.9869800
H	2.4084029	1.9239189	-0.9477410
H	4.9472314	-0.2147709	2.7897060
H	3.1442775	-0.4519041	-1.1378640
H	4.3981741	-1.5310488	0.7243670
C	-1.5021676	4.0537590	0.2191571
C	-0.8974350	3.3918323	-0.6130738
C	-0.1833132	2.6183090	-1.5828178
C	-0.2631006	1.2021791	-1.5823383
C	0.6297241	3.2651153	-2.5487513
C	0.4511708	0.4562057	-2.5292771
C	1.3451736	2.5087475	-3.4873468
C	1.2569243	1.1041304	-3.4813409
H	-2.0249308	4.6230652	0.9625660
H	-0.8636252	0.6971083	-0.8250490

H	0.7018808	4.3559145	-2.5410772
H	0.3883074	-0.6333016	-2.5163015
H	1.9767244	3.0161723	-4.2231010
H	1.8215220	0.5156993	-4.2112068
C	2.1286485	-3.0889043	3.4704451
C	1.2691358	-2.2639989	3.1899222
C	0.2675205	-1.3099502	2.8189882
C	0.6420077	-0.0672955	2.2497855
C	-1.1093677	-1.6057734	2.9904830
C	-0.3391942	0.8510992	1.8546049
C	-2.0819054	-0.6828346	2.5830543
C	-1.7027784	0.5439320	2.0081721
H	2.8792986	-3.8077238	3.7364300
H	1.6988539	0.1621840	2.1136595
H	-1.4006163	-2.5661825	3.4245527
H	-0.0401819	1.8060940	1.4162951
H	-3.1405844	-0.9294418	2.6945118
H	-2.4662292	1.2480325	1.6662885
C	4.2638571	-3.2149012	-1.6124926
C	3.0435345	-3.1217148	-1.6163403
C	1.6161025	-3.0077340	-1.6384982
C	0.9094392	-2.5235158	-0.5077028
C	0.8944029	-3.3808394	-2.8017840
C	-0.4894396	-2.4309353	-0.5403811
C	-0.5037605	-3.2859028	-2.8221621
C	-1.1986306	-2.8191199	-1.6911885
H	5.3333226	-3.2988451	-1.6018927
H	1.4627738	-2.2252854	0.3845996
H	1.4415457	-3.7464128	-3.6752632
H	-1.0281515	-2.0606916	0.3348302
H	-1.0535852	-3.5821201	-3.7210277
H	-2.2901913	-2.7680481	-1.6981130
C	-4.1943220	-3.2664500	0.3492542
C	-4.2946559	-2.0553038	0.2058915
C	-4.3993914	-0.6350773	0.0622563
C	-5.2429734	0.1072869	0.9260213
C	-3.6459605	0.0498490	-0.9240886
C	-5.3276385	1.5012122	0.8016451
C	-3.7387088	1.4420335	-1.0411027
C	-4.5779033	2.1716318	-0.1813302
H	-4.1031386	-4.3298906	0.4590148
H	-5.8190248	-0.4192362	1.6922019
H	-2.9788349	-0.5140491	-1.5796952
H	-5.9811768	2.0661697	1.4739602
H	-3.1370233	1.9645557	-1.7885350
H	-4.6346019	3.2603888	-0.2712855

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C	2.4113715	4.7125654	1.2507174
C	2.8076370	3.5590021	1.1523160

C	3.2564620	2.2045408	1.0349803
C	3.9824781	1.5900681	2.0875715
C	2.9699589	1.4564287	-0.1340948
C	4.3971414	0.2555431	1.9724831
C	3.3875339	0.1234278	-0.2376027
C	4.0973066	-0.4836205	0.8130575
H	2.0665538	5.7246763	1.3338112
H	4.2047732	2.1663346	2.9898315
H	2.4160271	1.9257388	-0.9478732
H	4.9452943	-0.2121518	2.7961927
H	3.1507028	-0.4487334	-1.1372571
H	4.4002649	-1.5308649	0.7286033
C	-1.5017492	4.0550244	0.2141423
C	-0.8949976	3.3930822	-0.6165396
C	-0.1796625	2.6195129	-1.5851096
C	-0.2591279	1.2036883	-1.5838211
C	0.6330323	3.2651239	-2.5519536
C	0.4551515	0.4565988	-2.5297737
C	1.3481357	2.5080331	-3.4901564
C	1.2611270	1.1033099	-3.4828165
H	-2.0260416	4.6272706	0.9540249
H	-0.8604510	0.6994420	-0.8267739
H	0.7043346	4.3559486	-2.5463409
H	0.3910162	-0.6328153	-2.5141038
H	1.9779689	3.0165080	-4.2269995
H	1.8258885	0.5138610	-4.2119967
C	2.1238832	-3.0870889	3.4676622
C	1.2644306	-2.2608425	3.1894168
C	0.2632896	-1.3064060	2.8199233
C	0.6371850	-0.0634833	2.2513677
C	-1.1134180	-1.6009047	2.9931586
C	-0.3439063	0.8554814	1.8574605
C	-2.0862846	-0.6786378	2.5853123
C	-1.7078239	0.5488423	2.0109398
H	2.8740067	-3.8018736	3.7441635
H	1.6939323	0.1664755	2.1160925
H	-1.4044173	-2.5596158	3.4309358
H	-0.0430535	1.8098856	1.4187399
H	-3.1446001	-0.9282419	2.6949147
H	-2.4715644	1.2533231	1.6699864
C	4.2683581	-3.2108151	-1.6124906
C	3.0479907	-3.1200573	-1.6151457
C	1.6204197	-3.0086594	-1.6374183
C	0.9122921	-2.5266852	-0.5068529
C	0.8990541	-3.3841841	-2.7999247
C	-0.4865985	-2.4353628	-0.5397941
C	-0.4992380	-3.2910179	-2.8209377
C	-1.1956377	-2.8243858	-1.6906346
H	5.3372046	-3.3014084	-1.5991861
H	1.4642756	-2.2314273	0.3871328

H	1.4464789	-3.7519927	-3.6721955
H	-1.0242958	-2.0664341	0.3367913
H	-1.0469646	-3.5898486	-3.7204368
H	-2.2875829	-2.7764311	-1.6968510
C	-4.1920083	-3.2676082	0.3505115
C	-4.2941175	-2.0565767	0.2056647
C	-4.4004421	-0.6370045	0.0603730
C	-5.2474589	0.1055380	0.9203156
C	-3.6465503	0.0477703	-0.9254048
C	-5.3347726	1.4989728	0.7932921
C	-3.7402149	1.4396190	-1.0443622
C	-4.5830984	2.1698021	-0.1883008
H	-4.1062471	-4.3315861	0.4562867
H	-5.8254756	-0.4206752	1.6851072
H	-2.9798483	-0.5169317	-1.5807254
H	-5.9921426	2.0622014	1.4635564
H	-3.1358571	1.9604906	-1.7910706
H	-4.6418255	3.2584272	-0.2803501

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C	0.3492104	2.9114337	-1.5919350
C	0.2551170	1.5299444	-1.2909005
C	1.6232769	3.4759545	-1.8498997
C	1.4076062	0.7356010	-1.2421263
C	2.7705016	2.6732964	-1.7971946
C	2.6682298	1.3046823	-1.4920126
C	-0.8217155	3.7346691	-1.6093177
C	-1.8184140	4.4458515	-1.6045723
H	-0.7263617	1.1042987	-1.0807352
H	1.6984060	4.5427888	-2.0790181
H	1.3309723	-0.3256973	-0.9914197
H	3.7520450	3.1199073	-1.9852617
H	-2.6993109	5.0579129	-1.6180568
H	3.5686166	0.6908629	-1.4276059
C	1.8428776	1.8115450	1.9726971
C	0.8726997	0.8420296	2.3315250
C	1.4210728	3.1329925	1.6829048
C	-0.4815420	1.1934799	2.4032927
C	0.0635603	3.4729349	1.7516416
C	-0.8909560	2.5068083	2.1137199
C	3.2263608	1.4583239	1.8811555
C	4.4100107	1.1596485	1.7956547
H	1.1837110	-0.1844808	2.5407435
H	2.1649156	3.8759449	1.3848587
H	-1.2218739	0.4378248	2.6734374
H	-0.2518097	4.4893956	1.4998238
H	-1.9517338	2.7670245	2.1686943
H	5.4262148	0.8528078	1.6420168
C	4.0697471	-1.8988205	-0.6138266
C	3.3249649	-1.9960760	0.5887439

C	3.5336733	-2.4496011	-1.8054931
C	2.0843365	-2.6469474	0.5966143
C	2.2908028	-3.0973901	-1.7851620
C	1.5661176	-3.2052906	-0.5856094
C	5.3458965	-1.2488305	-0.6366047
C	6.4358441	-0.6925609	-0.6771037
H	3.7205011	-1.5412144	1.4991840
H	4.1004957	-2.3612833	-2.7365475
H	1.5087383	-2.7103254	1.5242801
H	1.8843998	-3.5166555	-2.7110574
H	7.3994075	-0.2219816	-0.7132426
H	0.5929854	-3.7021253	-0.5747837
C	-0.7506079	-2.2480897	3.6180504
C	-1.1018704	-2.3793603	2.4531565
C	-1.4580578	-2.5546782	1.0779222
C	-2.0297443	-3.7752918	0.6381898
C	-1.2074183	-1.5291654	0.1333710
C	-2.3305969	-3.9631557	-0.7183995
C	-1.5105382	-1.7276644	-1.2178258
C	-2.0704135	-2.9409088	-1.6493562
H	-0.4670826	-2.1135781	4.6439572
H	-2.2233664	-4.5678874	1.3661056
H	-0.7629059	-0.5939981	0.4725705
H	-2.7667238	-4.9111158	-1.0492109
H	-1.3163677	-0.9321821	-1.9389324
H	-2.3097458	-3.0888017	-2.7066127
C	-3.9635106	0.4310965	2.9350603
C	-3.9990868	0.3839390	1.7129965
C	-4.0528820	0.3208642	0.2840820
C	-3.3728528	1.2792705	-0.5087359
C	-4.7897224	-0.7068327	-0.3560724
C	-3.4352026	1.2099683	-1.9069773
C	-4.8461679	-0.7669715	-1.7543725
C	-4.1726108	0.1903551	-2.5342989
H	-3.9200244	0.4703667	4.0060328
H	-2.7894460	2.0679800	-0.0284708
H	-5.3024662	-1.4555347	0.2536206
H	-2.8960875	1.9546797	-2.4989386
H	-5.4126590	-1.5693386	-2.2376282
H	-4.2189897	0.1391599	-3.6269039

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C	-3.6978669	-4.3668966	0.3996760
C	-3.7661367	-3.1554761	0.5633986
C	-3.8104038	-1.7390000	0.7656772
C	-4.4264002	-1.1963400	1.9222189
C	-3.2187198	-0.8633254	-0.1780526
C	-4.4470669	0.1912386	2.1242555
C	-3.2450373	0.5205819	0.0344004
C	-3.8579692	1.0542092	1.1810385

H	-3.6612272	-5.4268082	0.2410404
H	-4.8786948	-1.8731272	2.6524362
H	-2.7357741	-1.2770272	-1.0650179
H	-4.9203848	0.5982959	3.0234479
H	-2.7809252	1.1864213	-0.6947672
H	-3.8732375	2.1374722	1.3340533
C	0.5534951	-4.5933307	-1.4088912
C	0.1513037	-3.4846939	-1.7354398
C	-0.3104055	-2.1975310	-2.1596922
C	0.1011858	-1.0192133	-1.4879354
C	-1.1854081	-2.0891565	-3.2708683
C	-0.3376909	0.2333759	-1.9331051
C	-1.6305754	-0.8298253	-3.6982553
C	-1.2054225	0.3353709	-3.0336924
H	0.8926993	-5.5652365	-1.1078017
H	0.7514454	-1.0994753	-0.6169656
H	-1.5100461	-2.9984415	-3.7839740
H	-0.0154205	1.1324101	-1.4074523
H	-2.3102296	-0.7598477	-4.5533052
H	-1.5556740	1.3184950	-3.3622728
C	-0.2817731	2.4240713	3.6874585
C	-0.0255646	1.3291186	3.2034597
C	0.2873479	0.0455096	2.6509192
C	-0.7459887	-0.8705248	2.3290437
C	1.6381068	-0.3268474	2.4331711
C	-0.4280497	-2.1407463	1.8306675
C	1.9436797	-1.5959552	1.9231602
C	0.9149416	-2.5101302	1.6352393
H	-0.5094694	3.3799566	4.1172761
H	-1.7874592	-0.5729468	2.4646400
H	2.4348349	0.3856881	2.6601768
H	-1.2310363	-2.8368953	1.5755063
H	2.9867251	-1.8630889	1.7341263
H	1.1541866	-3.4933553	1.2219961
C	-3.7404224	3.9939339	-1.0881094
C	-2.5255966	3.8529337	-1.0417124
C	-1.1067028	3.6702658	-0.9923137
C	-0.4826362	3.1899221	0.1870695
C	-0.3088481	3.9606440	-2.1283770
C	0.9074774	3.0104506	0.2252402
C	1.0799385	3.7785185	-2.0789661
C	1.6928768	3.3056191	-0.9036906
H	-4.8045156	4.1254350	-1.1212150
H	-1.0878801	2.9466492	1.0627120
H	-0.7903687	4.3310990	-3.0377037
H	1.3750066	2.6263112	1.1349587
H	1.6859679	4.0102127	-2.9604284
H	2.7759760	3.1619315	-0.8617297
C	4.2894492	2.6095805	1.5217785
C	4.3404696	1.5375630	0.9331566

C	4.3894765	0.2657043	0.2781618
C	5.3488305	-0.6998800	0.6755748
C	3.4676597	-0.0579583	-0.7485076
C	5.3821521	-1.9567976	0.0556035
C	3.5100284	-1.3167522	-1.3621761
C	4.4652354	-2.2688008	-0.9653384
H	4.2429308	3.5585746	2.0194376
H	6.0537412	-0.4540117	1.4746861
H	2.7110762	0.6734749	-1.0418998
H	6.1254069	-2.6956447	0.3723924
H	2.7794460	-1.5629264	-2.1371242
H	4.4909320	-3.2516616	-1.4463969

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C	0.0701526	-0.7355325	2.7603497
C	-0.2470441	-0.7872459	1.3809132
C	-0.4660857	0.3113134	3.5529162
C	-1.0692094	0.1878819	0.8093264
C	-1.2983892	1.2784348	2.9697001
C	-1.6002305	1.2220240	1.5970475
C	2.0510563	3.3919799	0.5688074
C	3.0638061	3.6086876	-0.4006391
C	1.8774199	2.0931320	1.1074420
C	3.8672333	2.5425324	-0.8302070
C	2.6903912	1.0379269	0.6751859
C	3.6817080	1.2524664	-0.2976304
C	1.1979101	4.4670333	0.9772035
C	0.4483921	5.3802123	1.2983811
C	0.9195754	-1.7287314	3.3454474
C	1.6534151	-2.5739627	3.8425705
H	0.1494057	-1.5907329	0.7592399
H	-0.2172759	0.3565596	4.6166738
H	-1.2971057	0.1325123	-0.2537648
H	-1.7022820	2.0847453	3.5895955
H	3.2005175	4.6118605	-0.8142105
H	1.0936460	1.9166625	1.8451359
H	4.6380602	2.7201012	-1.5872595
H	2.5398977	0.0400309	1.0915441
H	4.2998890	0.4173035	-0.6390360
H	-0.1849219	6.1905106	1.6035482
H	2.2796690	-3.3201619	4.2914335
H	-2.2403796	1.9811916	1.1403549
C	-2.1589296	2.1585651	-1.8169935
C	-0.8342631	2.5994399	-1.5685393
C	-2.3641361	0.9611310	-2.5490621
C	0.2547047	1.8493813	-2.0335924
C	-1.2672214	0.2220221	-3.0099181
C	0.0434981	0.6611393	-2.7527869
C	-3.2770495	2.8881154	-1.3002656
C	-4.2319737	3.4885180	-0.8233273

H	-0.6687224	3.5070454	-0.9823378
H	-3.3811197	0.6046792	-2.7287666
H	1.2707318	2.1785728	-1.8086526
H	-1.4413039	-0.7135035	-3.5471527
H	-5.0680975	4.0491095	-0.4526983
H	0.8952257	0.0624984	-3.0876609
C	0.0800613	-2.7435926	-1.7640844
C	1.2611991	-2.6349715	-1.4624061
C	2.6379596	-2.4832034	-1.1009697
C	3.0349298	-2.5198357	0.2596349
C	3.6245616	-2.2868992	-2.1006325
C	4.3837862	-2.3599952	0.6053704
C	4.9718521	-2.1343991	-1.7447805
C	5.3576773	-2.1698643	-0.3918313
H	-0.9591050	-2.8042639	-2.0316271
H	2.2856204	-2.6629706	1.0422666
H	3.3212769	-2.2606665	-3.1511451
H	4.6725145	-2.3793794	1.6609059
H	5.7231731	-1.9843469	-2.5268067
H	6.4103707	-2.0472571	-0.1175416
C	-3.4529514	-2.7386336	-3.1134895
C	-3.5245221	-2.4614761	-1.9227056
C	-3.5917174	-2.1505088	-0.5269535
C	-2.9498933	-2.9858369	0.4216045
C	-4.3070500	-1.0129475	-0.0759810
C	-3.0326387	-2.6911357	1.7891392
C	-4.3865525	-0.7316618	1.2937331
C	-3.7552376	-1.5694275	2.2299143
H	-3.4215464	-2.9950255	-4.1546978
H	-2.3882249	-3.8571629	0.0743298
H	-4.7881841	-0.3566890	-0.8054129
H	-2.5217731	-3.3341904	2.5118948
H	-4.9336328	0.1542053	1.6295485
H	-3.8066007	-1.3356968	3.2975525

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C	-0.1614003	-3.1653470	0.1300393
C	-0.3525014	-1.7720652	0.2971541
C	-0.0567121	-3.6970102	-1.1793338
C	-0.4324025	-0.9285072	-0.8162773
C	-0.1501623	-2.8458132	-2.2902397
C	-0.3389267	-1.4637509	-2.1126674
C	-3.6533174	-0.7931293	0.0793853
C	-3.3848110	0.1088795	1.1388402
C	-3.6922739	-2.1836873	0.3510873
C	-3.1605586	-0.3731100	2.4361136
C	-3.4594092	-2.6563954	1.6488589
C	-3.1928905	-1.7549519	2.6953441
C	-3.8332359	-0.3112962	-1.2550894
C	-3.9533966	0.0963247	-2.4023334

C	-0.0668453	-4.0203278	1.2742785
C	0.0404822	-4.7388617	2.2597997
H	-0.4539000	-1.3798597	1.3089061
H	0.0944039	-4.7718713	-1.3110558
H	-0.5800131	0.1456560	-0.6857291
H	-0.0748624	-3.2639391	-3.2988792
H	-3.3309091	1.1815860	0.9373988
H	-3.8764909	-2.8816271	-0.4698441
H	-2.9449270	0.3382689	3.2388387
H	-3.4640379	-3.7333542	1.8415491
H	-3.0022349	-2.1296797	3.7058208
H	-3.9695660	0.4615235	-3.4110710
H	0.1175209	-5.3768281	3.1187520
H	-0.4233624	-0.8059256	-2.9796296
C	-0.7545357	1.9771260	-3.0530483
C	-1.5260017	2.5850797	-2.0301515
C	0.6440083	1.8343054	-2.8709649
C	-0.9029069	3.0546025	-0.8659483
C	1.2564549	2.3049916	-1.7028552
C	0.4883350	2.9252401	-0.7029653
C	-1.3728729	1.4972195	-4.2520817
C	-1.8850952	1.0712364	-5.2797365
H	-2.6079398	2.6685406	-2.1529240
H	1.2389576	1.3347167	-3.6389535
H	-1.5044824	3.5068478	-0.0719988
H	2.3329084	2.1669552	-1.5711432
H	-2.3293750	0.7207505	-6.1912285
H	0.9670547	3.2866043	0.2098167
C	-2.8803399	3.3405368	2.8677158
C	-1.7036196	3.0122658	2.7901533
C	-0.3299962	2.6283061	2.6618327
C	0.7066745	3.5292220	3.0135735
C	0.0095345	1.3520399	2.1485456
C	2.0483226	3.1545003	2.8492375
C	1.3515692	0.9855599	1.9901741
C	2.3745216	1.8841935	2.3390081
H	-3.9127158	3.6188423	2.9569540
H	0.4482001	4.5173788	3.4040307
H	-0.7917646	0.6735330	1.8555345
H	2.8415903	3.8595252	3.1178439
H	1.6044237	0.0075296	1.5744651
H	3.4195939	1.5943074	2.2016712
C	3.8242898	0.2205304	-3.3809460
C	3.8533251	-0.1746805	-2.2230001
C	3.9168504	-0.6414348	-0.8704879
C	4.8670533	-0.0916343	0.0284568
C	3.0463556	-1.6638958	-0.4162635
C	4.9471337	-0.5634893	1.3456126
C	3.1371735	-2.1303011	0.9029093
C	4.0850701	-1.5843276	1.7865356

H	3.7930665	0.5660345	-4.3959852
H	5.5380558	0.6984691	-0.3207075
H	2.2988919	-2.0782830	-1.0960294
H	5.6853423	-0.1335921	2.0305305
H	2.4562222	-2.9142457	1.2445976
H	4.1484782	-1.9486204	2.8166946

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C	2.7715512	4.5292815	0.0515889
C	3.0752084	3.4212524	-0.3698941
C	3.3839028	2.1030823	-0.8356495
C	4.6614679	1.5293732	-0.6113748
C	2.3918808	1.3418325	-1.5031199
C	4.9274535	0.2184035	-1.0333025
C	2.6674491	0.0330018	-1.9175727
C	3.9310676	-0.5355667	-1.6810434
H	2.5059828	5.5033713	0.4134366
H	5.4267521	2.1132341	-0.0927338
H	1.4100259	1.7816851	-1.6770757
H	5.9111505	-0.2214483	-0.8416758
H	1.8905881	-0.5547067	-2.4120469
H	4.1268622	-1.5669153	-1.9884186
C	-0.8915059	3.8756275	1.9338099
C	-0.9027598	3.2566020	0.8781254
C	-0.9422590	2.5419086	-0.3608335
C	-1.0115944	1.1271032	-0.3759070
C	-0.9316899	3.2491720	-1.5894443
C	-1.0741347	0.4389163	-1.5928468
C	-0.9947655	2.5508035	-2.8033945
C	-1.0676152	1.1453303	-2.8079574
H	-0.8470887	4.4172309	2.8585566
H	-1.0224870	0.5776305	0.5648694
H	-0.8685734	4.3403167	-1.5776975
H	-1.1270697	-0.6499077	-1.5932464
H	-0.9802377	3.1045496	-3.7472100
H	-1.1112005	0.6022503	-3.7570027
C	4.2943197	-3.1516285	2.0966038
C	3.4830238	-2.2752852	2.3647560
C	2.5133464	-1.2589345	2.6411898
C	2.4258445	-0.1156487	1.8075880
C	1.6124124	-1.3928296	3.7284503
C	1.4541685	0.8630414	2.0502973
C	0.6397582	-0.4092793	3.9598207
C	0.5544022	0.7171597	3.1205759
H	5.0156210	-3.9148063	1.8771197
H	3.1127111	-0.0139392	0.9670305
H	1.6776483	-2.2740926	4.3724436
H	1.3933650	1.7372842	1.3983491
H	-0.0566514	-0.5258381	4.7965187
H	-0.2134805	1.4778377	3.2875802

C	2.3327675	-3.4482887	-3.3769933
C	1.4636888	-3.2749900	-2.5324335
C	0.4416820	-3.0391569	-1.5572486
C	0.7629011	-2.4533366	-0.3066676
C	-0.9087834	-3.3736591	-1.8395474
C	-0.2468143	-2.2050534	0.6328630
C	-1.9098199	-3.1221249	-0.8910767
C	-1.5816574	-2.5374557	0.3458598
H	3.0966388	-3.6191078	-4.1106209
H	1.7982860	-2.1909433	-0.0829565
H	-1.1562757	-3.8230785	-2.8054260
H	0.0108675	-1.7407627	1.5863716
H	-2.9527792	-3.3663512	-1.1115391
H	-2.3729754	-2.3311543	1.0704220
C	-5.2947046	-3.1857450	0.5953627
C	-5.0435192	-1.9928318	0.4835865
C	-4.7301080	-0.6013714	0.3607090
C	-4.3217246	0.1442679	1.4964684
C	-4.8240476	0.0509217	-0.8943228
C	-4.0297413	1.5089962	1.3757875
C	-4.5302858	1.4168591	-1.0031597
C	-4.1383682	2.1499704	0.1292489
H	-5.5275802	-4.2282055	0.6963296
H	-4.2413002	-0.3587828	2.4643912
H	-5.1262727	-0.5245239	-1.7736760
H	-3.6986306	2.0756734	2.2508883
H	-4.5914297	1.9075853	-1.9790584
H	-3.8848580	3.2094524	0.0390972

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C	-0.6965678	0.4420984	3.0019339
C	-0.0074694	0.3704416	1.7665601
C	-0.8372338	-0.7341251	3.7834165
C	0.5118697	-0.8499661	1.3195728
C	-0.3058585	-1.9495083	3.3276052
C	0.3655667	-2.0142740	2.0919937
C	-3.4458744	-2.3457699	-0.0765067
C	-4.1346814	-2.1013946	-1.2919609
C	-2.9353522	-1.2492696	0.6611767
C	-4.2973446	-0.7886359	-1.7575811
C	-3.1116530	0.0579330	0.1904357
C	-3.7868573	0.2958365	-1.0193000
C	-3.2476089	-3.6868150	0.3848119
C	-3.0496200	-4.8363838	0.7561216
C	-1.2484711	1.6851094	3.4510515
C	-1.7282200	2.7472555	3.8266744
H	0.1144076	1.2675205	1.1575877
H	-1.3669448	-0.6807086	4.7384475
H	1.0244076	-0.8880291	0.3588359
H	-0.4278740	-2.8518205	3.9346852

H	-4.5262228	-2.9480638	-1.8627487
H	-2.3861719	-1.4333662	1.5856023
H	-4.8198131	-0.6132233	-2.7033849
H	-2.7078026	0.8945923	0.7641723
H	-3.9030265	1.3193506	-1.3855160
H	-2.8971434	-5.8434890	1.0926000
H	-2.1291127	3.6784207	4.1775139
H	0.7567854	-2.9666185	1.7226859
C	1.1924664	-3.1080892	-1.2681800
C	-0.1761004	-2.7724803	-1.4226629
C	2.1837839	-2.1839347	-1.6872343
C	-0.5393719	-1.5347810	-1.9707894
C	1.8085099	-0.9509195	-2.2382772
C	0.4480883	-0.6216559	-2.3792809
C	1.5701201	-4.3505889	-0.6641280
C	1.8927300	-5.3969963	-0.1166457
H	-0.9414322	-3.4733543	-1.0814745
H	3.2414051	-2.4283805	-1.5606465
H	-1.5966116	-1.2729230	-2.0514671
H	2.5853230	-0.2431729	-2.5389805
H	2.1769514	-6.3327304	0.3248033
H	0.1622829	0.3557247	-2.7775366
C	1.4871716	2.4720285	-0.9033640
C	0.3192146	2.8155417	-1.0219216
C	-1.0506134	3.2165606	-1.1335246
C	-1.8348648	3.4151821	0.0313345
C	-1.6407172	3.4305422	-2.4052153
C	-3.1704193	3.8245824	-0.0790406
C	-2.9766420	3.8438889	-2.5044358
C	-3.7460937	4.0457600	-1.3437459
H	2.5070801	2.1637030	-0.7715811
H	-1.3950254	3.2409478	1.0169937
H	-1.0382231	3.2781282	-3.3052838
H	-3.7655846	3.9673479	0.8284168
H	-3.4189282	4.0100439	-3.4921257
H	-4.7888994	4.3688143	-1.4248426
C	5.5827193	-0.8302611	-2.3292206
C	5.1986160	-0.1281437	-1.4033515
C	4.7503316	0.6949113	-0.3210260
C	5.1644254	2.0494517	-0.2320091
C	3.8886261	0.1699332	0.6755202
C	4.7296294	2.8512854	0.8331487
C	3.4631314	0.9792905	1.7380494
C	3.8815668	2.3191549	1.8220057
H	5.9254351	-1.4521647	-3.1335819
H	5.8243980	2.4574145	-1.0025748
H	3.5498016	-0.8656205	0.5996125
H	5.0502772	3.8961967	0.8879716
H	2.7867561	0.5651827	2.4898609
H	3.5393803	2.9499736	2.6482425

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C	-0.6965872	0.4420878	3.0018906
C	-0.0074780	0.3704428	1.7665075
C	-0.8372259	-0.7341277	3.7833623
C	0.5118636	-0.8499760	1.3195313
C	-0.3058668	-1.9494904	3.3275772
C	0.3655536	-2.0142812	2.0919607
C	-3.4458294	-2.3457485	-0.0765057
C	-4.1346553	-2.1013656	-1.2919463
C	-2.9353018	-1.2492437	0.6611657
C	-4.2973153	-0.7886251	-1.7575666
C	-3.1116148	0.0579460	0.1904383
C	-3.7868333	0.2958564	-1.0192931
C	-3.2475670	-3.6868013	0.3848177
C	-3.0495963	-4.8363729	0.7561045
C	-1.2484877	1.6851048	3.4510024
C	-1.7282374	2.7472439	3.8266509
H	0.1144049	1.2675053	1.1575471
H	-1.3669340	-0.6806860	4.7384184
H	1.0244018	-0.8880158	0.3587975
H	-0.4278785	-2.8518135	3.9346809
H	-4.5262086	-2.9480480	-1.8627128
H	-2.3860872	-1.4333527	1.5855722
H	-4.8197738	-0.6132285	-2.7033932
H	-2.7077545	0.8946108	0.7641843
H	-3.9030038	1.3193617	-1.3855118
H	-2.8971636	-5.8434824	1.0925890
H	-2.1291035	3.6784032	4.1775242
H	0.7567595	-2.9666228	1.7226453
C	1.1924599	-3.1080773	-1.2681441
C	-0.1761111	-2.7724550	-1.4226395
C	2.1837750	-2.1839038	-1.6871999
C	-0.5393741	-1.5347670	-1.9707402
C	1.8084968	-0.9509076	-2.2382416
C	0.4480781	-0.6216370	-2.3792455
C	1.5701121	-4.3505753	-0.6641052
C	1.8927269	-5.3969713	-0.1166089
H	-0.9414310	-3.4733535	-1.0814628
H	3.2413851	-2.4283561	-1.5605970
H	-1.5966322	-1.2728992	-2.0513849
H	2.5853251	-0.2431559	-2.5389402
H	2.1769497	-6.3327308	0.3247868
H	0.1622711	0.3557354	-2.7775030
C	1.4871689	2.4719924	-0.9033413
C	0.3192103	2.8154933	-1.0219162
C	-1.0506163	3.2165163	-1.1335276
C	-1.8348702	3.4151388	0.0313404
C	-1.6407315	3.4305224	-2.4052052
C	-3.1704031	3.8245546	-0.0790244

C	-2.9766150	3.8438689	-2.5044324
C	-3.7460982	4.0457486	-1.3437431
H	2.5070796	2.1637032	-0.7715166
H	-1.3950219	3.2408875	1.0169893
H	-1.0382088	3.2781145	-3.3052771
H	-3.7655636	3.9673285	0.8284387
H	-3.4189079	4.0100357	-3.4921366
H	-4.7888773	4.3688062	-1.4248335
C	5.5826987	-0.8302628	-2.3292368
C	5.1985783	-0.1281415	-1.4033728
C	4.7502898	0.6949170	-0.3210415
C	5.1643981	2.0494504	-0.2320167
C	3.8885814	0.1699426	0.6754972
C	4.7296120	2.8512765	0.8331477
C	3.4631041	0.9792905	1.7380265
C	3.8815518	2.3191400	1.8219980
H	5.9254510	-1.4521685	-3.1335687
H	5.8243783	2.4574026	-1.0025767
H	3.5497471	-0.8656096	0.5995717
H	5.0502734	3.8961950	0.8879587
H	2.7867120	0.5651632	2.4898391
H	3.5393749	2.9499583	2.6482452

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C	0.5799105	2.6251027	1.7902397
C	0.1053059	1.3487228	1.3969160
C	-0.3490082	3.6780054	1.9802679
C	-1.2637342	1.1375608	1.1877163
C	-1.7161994	3.4575272	1.7628609
C	-2.1779456	2.1910667	1.3640936
C	-0.7686401	2.0473055	-2.0790578
C	-0.1649196	0.7734202	-2.2281891
C	0.0322939	3.1480279	-1.6837804
C	1.2062220	0.6102609	-1.9846806
C	1.4005266	2.9734642	-1.4441880
C	1.9922591	1.7074439	-1.5927356
C	-2.1707818	2.2270360	-2.3006806
C	-3.3684458	2.4045563	-2.4796767
C	1.9842050	2.8547513	1.9452833
C	3.1889475	3.0528709	2.0315183
H	0.8327112	0.5524986	1.2254235
H	0.0155021	4.6638111	2.2833047
H	-1.6308981	0.1585382	0.8700846
H	-2.4250293	4.2809407	1.8988786
H	-0.7757160	-0.0850214	-2.5188810
H	-0.4371621	4.1258453	-1.5491178
H	1.6570577	-0.3809979	-2.0850362
H	2.0062305	3.8205399	-1.1102643
H	3.0559967	1.5784530	-1.3845154
H	-4.4288349	2.5301891	-2.5779438

H	4.2506816	3.1986605	2.0707324
H	-3.2411394	2.0314511	1.1717721
C	-4.6699703	-0.2352100	0.2157904
C	-3.9231486	-0.7175550	-0.8888953
C	-4.6242766	-0.9443918	1.4426658
C	-3.1617999	-1.8868788	-0.7667425
C	-3.8584973	-2.1135972	1.5526737
C	-3.1303241	-2.5913456	0.4496162
C	-5.4553201	0.9570075	0.1031961
C	-6.1204760	1.9818193	0.0269571
H	-3.9301783	-0.1562866	-1.8250659
H	-5.1913678	-0.5680470	2.2986827
H	-2.5769706	-2.2444015	-1.6189720
H	-3.8266023	-2.6516616	2.5055102
H	-6.7114313	2.8746890	-0.0405008
H	-2.5202018	-3.4935690	0.5430504
C	0.1986197	-2.7325396	-3.3185530
C	0.1762761	-2.9461987	-2.1138262
C	0.1413781	-3.1731816	-0.7013808
C	0.1653387	-4.4908460	-0.1786815
C	0.0774844	-2.0772642	0.1917154
C	0.1326576	-4.6968304	1.2080134
C	0.0362934	-2.2928365	1.5737977
C	0.0686099	-3.5992896	2.0880651
H	0.2261176	-2.5360582	-4.3730491
H	0.2107155	-5.3401233	-0.8658942
H	0.0556045	-1.0672340	-0.2147249
H	0.1537992	-5.7169987	1.6038219
H	-0.0276414	-1.4359516	2.2487153
H	0.0388483	-3.7667509	3.1690546
C	6.0050802	2.2695326	-0.3303717
C	5.4211936	1.2101435	-0.1424817
C	4.7139471	-0.0189748	0.0556756
C	4.5771355	-0.9448695	-1.0097172
C	4.1241316	-0.3173078	1.3097430
C	3.8743345	-2.1429292	-0.8181811
C	3.4286531	-1.5194177	1.4899985
C	3.3030135	-2.4366594	0.4319533
H	6.5362455	3.1868710	-0.4960362
H	5.0209316	-0.7097254	-1.9811507
H	4.2016357	0.4059688	2.1242512
H	3.7632655	-2.8450542	-1.6501635
H	2.9652878	-1.7375958	2.4566853
H	2.7421730	-3.3635213	0.5768205

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C	-3.0316773	-1.5365306	2.0097037
C	-2.2334122	-0.7402237	1.1717827
C	-3.4692434	-2.7983662	1.5675110
H	-1.8975373	0.2410651	1.5118242

H	-4.0921653	-3.4230186	2.2163123
C	-1.8709972	-1.1955151	-0.1002439
C	-3.1129415	-3.2630708	0.2934243
H	-1.2546552	-0.5841834	-0.7576897
H	-3.4511641	-4.2428051	-0.0557751
C	-2.3072760	-2.4626917	-0.5546391
H	-3.3130404	-1.1748234	3.0033220
C	-1.9413306	-2.9299034	-1.8577836
C	-1.6313888	-3.3344365	-2.9711685
H	-1.3775660	-3.6937386	-3.9495241
C	1.0756312	-1.5901088	2.0675487
C	1.9772078	-1.3810610	0.9940429
C	0.3000829	-2.7761068	2.1025751
H	2.5722194	-0.4672821	0.9636682
H	-0.4117868	-2.9272121	2.9171384
C	2.0842148	-2.3311831	-0.0298642
C	0.4165017	-3.7198084	1.0754115
H	2.7734629	-2.1503324	-0.8586256
H	-0.2032031	-4.6208925	1.0976054
C	1.3029896	-3.4991223	0.0054400
H	1.3720791	-4.2306932	-0.8054346
C	0.9228814	-0.5923579	3.0832960
C	0.7601268	0.2887197	3.9180872
H	0.6540879	1.0311172	4.6848555
C	3.6910220	1.9879376	0.1674046
C	3.9218205	1.1490741	-0.9313418
C	4.2975564	1.7148315	1.4060843
H	3.4316858	1.3420442	-1.8877421
H	4.1007093	2.3609033	2.2669910
C	4.7667575	0.0186138	-0.8017146
C	5.1426931	0.5981508	1.5421406
H	5.6095565	0.3774474	2.5070484
C	5.3792680	-0.2469140	0.4493804
H	3.0178853	2.8422305	0.0604013
H	6.0238017	-1.1239211	0.5539374
C	4.9783144	-0.8585515	-1.9134719
C	5.1346998	-1.6263649	-2.8539975
H	5.2968341	-2.2846810	-3.6854879
C	-3.7775667	3.1906730	2.3387203
C	-3.8157598	2.6274247	1.2521242
C	-3.8210628	1.9336629	-0.0001437
C	-4.7966051	0.9408452	-0.2695791
C	-2.8218880	2.2026518	-0.9677040
C	-4.7588146	0.2254732	-1.4728266
C	-2.7912100	1.4778726	-2.1661842
C	-3.7539913	0.4861624	-2.4215918
H	-3.7728536	3.7109810	3.2767701
H	-5.5610502	0.7247589	0.4816267
H	-2.0650459	2.9613110	-0.7591402
H	-5.5035846	-0.5536662	-1.6621943

H	-1.9939218	1.6684455	-2.8896562
H	-3.7089439	-0.0977426	-3.3457886
C	0.7347766	-0.3180025	-2.7222144
C	0.6673753	0.6767262	-2.0148672
C	0.5539557	1.8086868	-1.1492494
C	0.3329357	1.6169554	0.2365257
C	0.6520716	3.1271773	-1.6570664
C	0.1982043	2.7172413	1.0900663
C	0.5214474	4.2248534	-0.7934625
C	0.2897125	4.0246660	0.5807521
H	0.7730578	-1.2140202	-3.3094549
H	0.2768059	0.6052849	0.6339750
H	0.8249613	3.2788260	-2.7260064
H	0.0227124	2.5453948	2.1550334
H	0.5944212	5.2401544	-1.1950951
H	0.1772907	4.8849509	1.2473051

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C	-0.7189865	-3.4700739	0.3263866
C	-1.6872862	-3.6060666	1.3373774
C	-1.0292352	-2.7735080	-0.8541263
H	-1.4429315	-4.1339846	2.2643174
H	-0.2705704	-2.6295716	-1.6286442
C	-2.9653854	-3.0580405	1.1701527
C	-2.3095386	-2.2320387	-1.0365017
H	-3.7138925	-3.1424532	1.9611621
H	-2.5545196	-1.6868704	-1.9483376
C	-3.2930788	-2.3697296	-0.0251927
H	0.2757283	-3.9013977	0.4668211
C	-4.5988766	-1.8108270	-0.2046653
C	-5.7152213	-1.3329942	-0.3572914
H	-6.6957199	-0.9216267	-0.4990242
C	-0.7110230	0.4679960	-2.4735834
C	-1.5312178	1.0892298	-1.4997443
C	-1.2944837	0.0245740	-3.6873000
H	-1.0831381	1.4489723	-0.5736270
H	-0.6622745	-0.4536390	-4.4408104
C	-2.9054546	1.2342149	-1.7244817
C	-2.6699233	0.1865796	-3.9087094
H	-3.5305845	1.6930827	-0.9534621
H	-3.1119560	-0.1645008	-4.8466332
C	-3.4810360	0.7829662	-2.9252343
H	-4.5575793	0.8848942	-3.0912063
C	0.6821000	0.2670343	-2.2169800
C	1.8624908	0.0671142	-1.9669942
H	2.8922501	-0.1028254	-1.7216171
C	0.6883488	3.7715686	-1.1903751
C	1.0360015	3.2543347	0.0836684
C	-0.5786566	4.3298190	-1.4038203
H	-0.8390651	4.7160445	-2.3940412

C	0.0812008	3.3024215	1.1308352
C	-1.5191511	4.3772520	-0.3591677
H	0.3352896	2.8890683	2.1085574
H	-2.5118615	4.8039836	-0.5340970
C	-1.1857760	3.8587739	0.9045303
H	1.4167608	3.7166545	-2.0034450
H	-1.9174044	3.8779549	1.7181651
C	2.3338062	2.6878273	0.2933315
C	3.4473408	2.2009912	0.4373398
H	4.4262803	1.7714627	0.5492191
C	-4.1767048	-0.1142606	2.9458971
C	-2.9583336	-0.0016243	2.9383528
C	-1.5337012	0.1340347	2.8945976
C	-0.8096464	0.5826903	4.0283021
C	-0.8296257	-0.1732726	1.7035386
C	0.5849193	0.7183273	3.9641809
C	0.5596092	-0.0132636	1.6418544
C	1.2711215	0.4267502	2.7712572
H	-5.2419652	-0.2353393	2.9288840
H	-1.3501694	0.8215990	4.9486156
H	-1.3825595	-0.5275675	0.8336680
H	1.1352564	1.0672333	4.8440458
H	1.0813409	-0.2018125	0.7013483
H	2.3510331	0.5824849	2.7108763
C	6.8434343	0.5010836	0.4514376
C	5.9776261	-0.3112937	0.1529228
C	4.9387290	-1.2349629	-0.1896506
C	3.8597513	-1.4583575	0.7023678
C	4.9697546	-1.9346027	-1.4235897
C	2.8392592	-2.3563004	0.3659671
C	3.9439201	-2.8330296	-1.7491186
C	2.8766788	-3.0451305	-0.8582635
H	7.6187255	1.1949136	0.7145977
H	3.8271854	-0.9169415	1.6502066
H	5.7989538	-1.7624801	-2.1152287
H	2.0048720	-2.4985306	1.0563666
H	3.9733829	-3.3621996	-2.7065998
H	2.0713145	-3.7350171	-1.1258831

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C	4.3247198	0.5023996	-0.5057926
C	3.9169637	1.3376301	-1.5597040
C	4.0716069	0.8800592	0.8243405
H	4.0861541	1.0339185	-2.5962196
H	4.3839303	0.2284972	1.6464664
C	3.2607376	2.5446542	-1.2903378
C	3.4133539	2.0840182	1.1066429
H	2.9307523	3.1903267	-2.1085938
H	3.1966305	2.3734006	2.1376741
C	3.0036291	2.9334222	0.0483149

H	4.8072457	-0.4547372	-0.7205346
C	2.3355675	4.1672128	0.3335523
C	1.7560581	5.2144305	0.5947481
H	1.2696598	6.1420909	0.8273836
C	1.7488790	-1.3517873	-1.5660754
C	1.7033315	-1.1653817	-2.9693817
C	1.0505130	-0.4523342	-0.7266784
H	2.2260080	-1.8708188	-3.6200968
H	1.0670523	-0.6025833	0.3505576
C	0.9791011	-0.0941426	-3.5116190
C	0.3321046	0.6120520	-1.2758360
H	0.9447172	0.0385467	-4.5978711
H	-0.2038210	1.2938083	-0.6158512
C	0.2945502	0.7991060	-2.6674909
H	-0.2746276	1.6342384	-3.0869492
C	2.4984063	-2.4295003	-0.9971228
C	3.1574916	-3.3336793	-0.5000966
H	3.7129189	-4.1499472	-0.0811099
C	-2.0533818	-1.5321580	0.5385102
C	-1.1839463	-2.6088886	0.7826584
C	-2.4626043	-1.2424701	-0.7737800
H	-0.8487019	-2.8199655	1.8004582
H	-3.1268078	-0.3962501	-0.9644698
C	-0.7210837	-3.3957772	-0.2791132
C	-2.0032419	-2.0222560	-1.8427800
H	-0.0218314	-4.2162089	-0.1009659
H	-2.3003360	-1.7895938	-2.8687559
C	-1.1237760	-3.1082652	-1.6078219
H	-2.3923544	-0.9048485	1.3663098
C	-0.6306225	-3.8933121	-2.6983794
C	-0.1942665	-4.5564177	-3.6302668
H	0.1755669	-5.1498038	-4.4436605
C	0.1005917	2.0874673	2.0186830
C	0.1408456	0.9837284	2.5444301
C	0.2191748	-0.3140597	3.1424413
C	1.3727000	-1.1173030	2.9555510
C	-0.8557126	-0.8215469	3.9143862
C	1.4405392	-2.3974607	3.5208528
C	-0.7772407	-2.1015075	4.4799878
C	0.3690788	-2.8943832	4.2849865
H	0.0866350	3.0381701	1.5184611
H	2.2003135	-0.7321459	2.3549641
H	-1.7470671	-0.2044739	4.0582802
H	2.3300421	-3.0132617	3.3565411
H	-1.6151716	-2.4848860	5.0705583
H	0.4226999	-3.8966555	4.7211298
C	-1.0500503	3.9130470	-1.0486122
C	-2.0461099	3.2526246	-0.7848397
C	-3.1967952	2.4558882	-0.4840251
C	-4.1976078	2.2382877	-1.4648541

C	-3.3437316	1.8633840	0.7959540
C	-5.3163555	1.4474655	-1.1680153
C	-4.4688203	1.0789427	1.0827877
C	-5.4572082	0.8663753	0.1056082
H	-0.1415924	4.4547439	-1.2325398
H	-4.0834663	2.6905323	-2.4539241
H	-2.5599370	2.0059638	1.5438359
H	-6.0797720	1.2801147	-1.9343390
H	-4.5682224	0.6179542	2.0705312
H	-6.3288598	0.2443873	0.3310813

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C	-0.3241154	2.4884455	2.4908299
C	0.5068792	3.4738659	1.9292448
C	-1.3742683	1.9446984	1.7316728
H	1.3354502	3.8895601	2.5097964
H	-2.0248042	1.1763238	2.1592036
C	0.2990166	3.9081383	0.6146124
C	-1.5926899	2.3713901	0.4151605
H	0.9597446	4.6542018	0.1661109
H	-2.3965207	1.9407805	-0.1823413
C	-0.7510810	3.3546036	-0.1603257
H	-0.1376169	2.1302129	3.5070489
C	-0.9355147	3.7598995	-1.5212821
C	-1.0625759	4.0729588	-2.6988792
H	-1.1970594	4.3967217	-3.7128345
C	2.4125154	0.7914928	1.1198233
C	3.5371889	1.6428689	1.2530588
C	1.6895693	0.7878888	-0.0957347
H	4.1083087	1.6333375	2.1847817
H	0.8354930	0.1253282	-0.2175857
C	3.9167512	2.4761392	0.1929677
C	2.0728741	1.6267611	-1.1464496
H	4.7907297	3.1263094	0.3028079
H	1.4929139	1.6176977	-2.0725707
C	3.1837599	2.4751038	-1.0081116
H	3.4808374	3.1321602	-1.8316378
C	2.0125032	-0.0510648	2.2051034
C	1.6700177	-0.7592583	3.1427091
H	1.3889404	-1.3933718	3.9602215
C	2.0721666	-2.1379669	-2.0468362
C	2.1231378	-2.6346151	-0.7326738
C	3.1459009	-1.3847105	-2.5523949
H	1.2841610	-3.2079928	-0.3319430
H	3.1069386	-0.9885258	-3.5721499
C	3.2360747	-2.3760778	0.0766413
C	4.2644588	-1.1206517	-1.7504156
H	3.2658899	-2.7321159	1.1089067
H	5.0942807	-0.5204676	-2.1329556
C	4.3203022	-1.6111941	-0.4223305

H	1.1866191	-2.3190344	-2.6624642
C	5.4500520	-1.3292502	0.4105918
C	6.4111079	-1.0861754	1.1288690
H	7.2596370	-0.8853573	1.7536587
C	-1.2858442	0.3517776	-2.3021353
C	-1.2760009	-0.6616871	-1.6186247
C	-1.2418641	-1.8271112	-0.7915797
C	-1.0360403	-1.7054323	0.6040570
C	-1.4060415	-3.1166697	-1.3556173
C	-0.9924566	-2.8488929	1.4104025
C	-1.3620941	-4.2550802	-0.5403204
C	-1.1545686	-4.1262570	0.8461927
H	-1.3178172	1.2839614	-2.8333819
H	-0.9089673	-0.7169848	1.0480256
H	-1.5623916	-3.2103736	-2.4336484
H	-0.8245714	-2.7406080	2.4855701
H	-1.4834082	-5.2465526	-0.9876479
H	-1.1137001	-5.0180650	1.4790042
C	-4.6552583	2.1067499	-2.0750726
C	-4.6510106	1.1948917	-1.2592444
C	-4.6014383	0.1517569	-0.2810350
C	-4.5394740	-1.2083714	-0.6729767
C	-4.5910430	0.4727390	1.1002017
C	-4.4715402	-2.2189107	0.2940854
C	-4.5215838	-0.5460772	2.0601775
C	-4.4624302	-1.8935482	1.6613019
H	-4.6572647	2.9114499	-2.7841831
H	-4.5211004	-1.4549795	-1.7372804
H	-4.6262719	1.5223190	1.4039089
H	-4.3960479	-3.2634958	-0.0204284
H	-4.5121299	-0.2870346	3.1239463
H	-4.3970312	-2.6866696	2.4124203

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C	-2.9496435	1.2565522	-2.3081696
C	-2.1375283	0.5319240	-1.4203453
C	-3.6735446	2.3703131	-1.8437759
H	-1.5554776	-0.3193436	-1.7800626
H	-4.3053753	2.9414077	-2.5321101
C	-2.0491017	0.9088119	-0.0764759
C	-3.5872111	2.7580878	-0.4996842
H	-1.4055413	0.3572716	0.6063580
H	-4.1474837	3.6229831	-0.1331984
C	-2.7719782	2.0268743	0.4002282
H	-3.0149389	0.9580124	-3.3589196
C	-2.6796905	2.4141585	1.7748406
C	-2.6050865	2.7413988	2.9520669
H	-2.5339465	3.0360544	3.9810277
C	1.0995419	1.3215874	-1.4824941
C	1.3833402	0.8125501	-0.1936937

C	0.6179465	2.6475837	-1.6133382
H	1.7556545	-0.2045896	-0.0916842
H	0.3832708	3.0368007	-2.6075515
C	1.1878809	1.6114385	0.9378414
C	0.4219799	3.4383168	-0.4737348
H	1.4091563	1.1995038	1.9260577
H	0.0306768	4.4545816	-0.5809096
C	0.7045279	2.9239191	0.8049075
H	0.5288508	3.5380558	1.6927099
C	1.2833710	0.4928052	-2.6343245
C	1.4312399	-0.2327165	-3.6091356
H	1.5779749	-0.8668638	-4.4614124
C	4.5782905	0.3176088	-1.3064729
C	4.6912842	-0.3279068	-0.0691781
C	4.4893606	1.7193567	-1.3691902
H	4.7486835	-1.4172397	-0.0253335
H	4.3746687	2.2174313	-2.3365019
C	4.7036623	0.4267245	1.1305859
C	4.5178039	2.4764518	-0.1853615
H	4.4358860	3.5668297	-0.2291060
C	4.6211298	1.8397913	1.0584989
H	4.5270397	-0.2790356	-2.2212772
H	4.6243293	2.4238657	1.9828797
C	4.7748793	-0.2350068	2.3984858
C	4.8023507	-0.8134465	3.4776541
H	4.8677519	-1.3157212	4.4234072
C	-3.4821412	-3.4424112	-2.1459457
C	-3.8578033	-2.7598284	-1.2015877
C	-4.2416927	-1.9334113	-0.0979233
C	-5.0848288	-0.8123743	-0.2979430
C	-3.7521991	-2.2055845	1.2042012
C	-5.4172476	0.0192861	0.7780096
C	-4.0860888	-1.3624112	2.2727299
C	-4.9165309	-0.2477299	2.0641996
H	-3.1890553	-4.0676851	-2.9669790
H	-5.4468106	-0.5889765	-1.3042140
H	-3.1002087	-3.0686266	1.3613455
H	-6.0497658	0.8949183	0.6071604
H	-3.6930836	-1.5740501	3.2722596
H	-5.1552881	0.4218961	2.8950660
C	3.9819085	-3.7304877	-1.6282266
C	3.0475569	-3.3464750	-0.9369248
C	1.9694581	-2.8678711	-0.1261827
C	2.2024149	-2.4696410	1.2152684
C	0.6590869	-2.7686209	-0.6580942
C	1.1464547	-1.9846930	1.9990842
C	-0.3899154	-2.2907227	0.1369505
C	-0.1515511	-1.8984378	1.4658788
H	4.7977140	-4.0889502	-2.2255328
H	3.2121614	-2.5182053	1.6280026

H 0.4787460 -3.0569432 -1.6964275
H 1.3468219 -1.6623229 3.0253837
H -1.3931749 -2.2173517 -0.2867245
H -0.9747939 -1.5155712 2.0758404

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C -1.2157752 2.2635007 -1.8104485
C -1.9269570 2.6314070 -0.6561015
C 0.1007453 2.7174666 -1.9993787
H -2.9459268 2.2740132 -0.4915301
H 0.6600652 2.4214202 -2.8921713
C -1.3231923 3.4424056 0.3126172
C 0.7126361 3.5334484 -1.0387984
H -1.8630663 3.7089447 1.2247471
H 1.7420193 3.8729827 -1.1736222
C 0.0065644 3.8993091 0.1343778
H -1.6701296 1.5952552 -2.5464381
C 0.6376647 4.6953407 1.1434149
C 1.1928196 5.3401083 2.0249335
H 1.6541841 5.9520737 2.7759403
C -0.4587976 -0.3958427 0.0605899
C -1.6898783 -0.6995016 0.6904792
C 0.4812589 0.4197914 0.7324118
H -2.4036369 -1.3455861 0.1832787
H 1.4318421 0.6594280 0.2605741
C -1.9747491 -0.1814781 1.9587352
C 0.1876581 0.9313159 2.0008293
H -2.9343544 -0.4134559 2.4306135
H 0.9201707 1.5700138 2.5015899
C -1.0398220 0.6370483 2.6182487
H -1.2686706 1.0435275 3.6086656
C -0.1822299 -0.8960334 -1.2514286
C 0.0306647 -1.3047191 -2.3852222
H 0.2276250 -1.6916772 -3.3649885
C 2.9905885 -1.7485817 2.0665551
C 2.9149656 -2.3164846 0.7833878
C 1.9283889 -1.9200676 2.9715474
H 3.7320135 -2.1745101 0.0731162
H 1.9763461 -1.4683007 3.9673741
C 1.7837351 -3.0474153 0.4005323
C 0.7919594 -2.6489316 2.5979324
H 1.7076824 -3.4638331 -0.6065374
H -0.0466811 -2.7641995 3.2892905
C 0.7048262 -3.2184832 1.3033356
H 3.8673936 -1.1587910 2.3511847
C -0.4696185 -3.9319054 0.9027687
C -1.4846214 -4.5183325 0.5500167
H -2.3668688 -5.0472873 0.2489086
C 3.4425274 2.6056935 0.8198022
C 3.8369464 1.6942069 0.1051811

C	4.2409197	0.6021827	-0.7274855
C	3.3680411	0.1097747	-1.7304179
C	5.5025832	-0.0183229	-0.5450408
C	3.7507893	-0.9807886	-2.5218972
C	5.8768709	-1.1066675	-1.3449437
C	5.0029684	-1.5929925	-2.3354731
H	3.0458904	3.4178518	1.4015860
H	2.3854651	0.5670438	-1.8668188
H	6.1747783	0.3582772	0.2309831
H	3.0586787	-1.3636342	-3.2777982
H	6.8512939	-1.5810081	-1.1915421
H	5.2953043	-2.4486224	-2.9520604
C	-5.6976766	2.2474274	0.5158211
C	-5.3623551	1.1694741	0.0428928
C	-4.9344976	-0.0814436	-0.5057648
C	-5.2241216	-1.2973638	0.1628122
C	-4.1979700	-0.1187568	-1.7161459
C	-4.7793725	-2.5162818	-0.3674999
C	-3.7530837	-1.3414160	-2.2351504
C	-4.0406613	-2.5431670	-1.5643630
H	-6.0091925	3.1921036	0.9180609
H	-5.7884219	-1.2709518	1.0989443
H	-3.9705278	0.8178380	-2.2306430
H	-5.0001584	-3.4475291	0.1631334
H	-3.1605292	-1.3552890	-3.1538213
H	-3.6751536	-3.4933870	-1.9643094

Pentamer-22 (P11)

C	5.4075701	-1.4403138	0.0445505
C	5.7505156	-0.6629630	-1.0742767
C	5.1953795	-0.8224052	1.2891224
H	5.8958082	-1.1393965	-2.0487170
H	4.8894057	-1.4210896	2.1514857
C	5.8913903	0.7262412	-0.9542891
C	5.3321005	0.5651802	1.4209781
H	6.1558068	1.3364184	-1.8226482
H	5.1588694	1.0517967	2.3848973
C	5.6873084	1.3567671	0.2989397
H	5.2720980	-2.5202741	-0.0593754
C	5.8366114	2.7751688	0.4296333
C	5.9418286	3.9907993	0.5365218
H	6.0597041	5.0525801	0.6377975
C	2.3320855	-1.3827022	-2.2964989
C	2.2467146	-0.2834752	-1.4244620
C	2.2735422	-2.6904883	-1.7829032
H	2.2934244	0.7381713	-1.8081862
H	2.3323410	-3.5500453	-2.4584779
C	2.1045705	-0.4838756	-0.0471340
C	2.1347841	-2.9016096	-0.4045699
H	2.0385266	0.3732748	0.6247223

H	2.0808681	-3.9153834	0.0005715
C	2.0511211	-1.7982538	0.4790627
C	1.9302599	-2.0101060	1.8883186
C	1.8474988	-2.1896743	3.0956576
H	1.7335481	-2.3400505	4.1514438
H	2.4453881	-1.2225029	-3.3734999
C	-1.4317380	-3.2602834	-1.1690117
C	-1.1298517	-1.8995396	-1.3467779
C	-1.7226473	-3.7499315	0.1182175
H	-0.8888643	-1.5122378	-2.3397716
H	-1.9568118	-4.8091485	0.2633939
C	-1.1170802	-1.0293734	-0.2512725
C	-1.7148744	-2.8849295	1.2215354
H	-0.8768082	0.0225901	-0.3882986
H	-1.9403127	-3.2598792	2.2232035
C	-1.4144028	-1.5114295	1.0460696
H	-1.4336488	-3.9409203	-2.0262116
C	-1.4280909	-0.6170359	2.1629632
C	-1.4846345	0.1548324	3.1104353
H	-1.5059304	0.8297318	3.9436317
C	-5.6373024	0.7639533	0.6444715
C	-4.7350177	-0.3277618	0.6981943
C	-6.4257498	0.9546942	-0.5189387
H	-4.1096072	-0.4624648	1.5834918
H	-7.1186311	1.7995816	-0.5629669
C	-4.6217337	-1.2034600	-0.3897941
C	-6.3066817	0.0716824	-1.6015501
H	-3.9084787	-2.0294826	-0.3439971
H	-6.9161186	0.2298421	-2.4972608
C	-5.4053351	-1.0076029	-1.5404751
H	-5.3085894	-1.6897673	-2.3912093
C	-5.7298814	1.6798004	1.7415579
C	-5.7825663	2.4783515	2.6678568
H	-5.8518878	3.1660229	3.4885612
C	2.3641494	3.2110549	-0.2748296
C	1.1912689	2.9510545	-0.5102205
C	-0.1705946	2.6027400	-0.7798478
C	-1.1444674	2.6566463	0.2496524
C	-0.5622775	2.1769725	-2.0753873
C	-2.4713339	2.2901607	-0.0113202
C	-1.8924177	1.8114907	-2.3250742
C	-2.8497715	1.8636212	-1.2960916
H	3.3942327	3.4404849	-0.0650047
H	-0.8419026	2.9685458	1.2523817
H	0.1862498	2.1324672	-2.8711880
H	-3.2094064	2.3166408	0.7938932
H	-2.1817936	1.4736408	-3.3252582
H	-3.8798747	1.5533585	-1.4860022

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C	0.5663573	2.9875978	-2.4085984
C	1.1926988	1.8476749	-1.8460072
C	0.2479414	4.0834637	-1.5687483
C	1.4904859	1.8038549	-0.4782108
C	0.5470992	4.0296861	-0.2007183
C	1.1670886	2.8942207	0.3484828
C	-1.6303203	0.7130833	0.1757017
C	-1.1880173	-0.5755917	-0.2106077
C	-2.1844087	1.5752203	-0.8005639
C	-1.3080735	-0.9895394	-1.5425491
C	-2.2895618	1.1568380	-2.1322043
C	-1.8538867	-0.1253148	-2.5077638
C	-1.5215864	1.1411568	1.5353187
C	-1.4453452	1.5065833	2.7004941
C	0.2396331	3.0216569	-3.8019566
C	-0.0562582	3.0436138	-4.9899125
H	1.4144196	1.0000536	-2.4976156
H	-0.2388172	4.9629174	-1.9999903
H	1.9587297	0.9160665	-0.0451837
H	0.2877452	4.8758991	0.4435089
H	-0.7602565	-1.2473680	0.5353752
H	-2.5228147	2.5688822	-0.5019215
H	-0.9732638	-1.9915881	-1.8211342
H	-2.6968172	1.8389000	-2.8836135
H	-1.9347188	-0.4466776	-3.5506284
H	-1.2733656	1.8502602	3.7015497
H	-0.2942557	3.0747325	-6.0355552
H	1.3773846	2.8518603	1.4185247
C	2.3895873	1.0001190	3.1617288
C	1.6546621	-0.1597861	2.8091665
C	3.7049341	1.1643872	2.6584114
C	2.2320249	-1.1351717	1.9855589
C	4.2712656	0.1828166	1.8336415
C	3.5413850	-0.9711733	1.4991059
C	1.8149415	2.0041302	4.0063181
C	1.3370206	2.8769257	4.7195436
H	0.6295279	-0.2725142	3.1671509
H	4.2679748	2.0650238	2.9186780
H	1.6553733	-2.0223895	1.7104492
H	5.2857801	0.3213486	1.4466516
H	0.9291829	3.6364263	5.3583095
H	3.9830363	-1.7290011	0.8476454
C	-0.0077271	-3.9609756	-0.0123220
C	1.0372701	-3.5449797	-0.4937194
C	2.2487232	-3.0069259	-1.0346681
C	3.4425085	-3.7711051	-1.0453389
C	2.2702567	-1.6813535	-1.5369115
C	4.6286974	-3.2158009	-1.5463492
C	3.4605591	-1.1364729	-2.0346798
C	4.6420244	-1.8988358	-2.0420529

H	-0.9514349	-4.2815746	0.3837451
H	3.4280853	-4.7919423	-0.6534242
H	1.3537583	-1.0893749	-1.5090048
H	5.5470174	-3.8116241	-1.5466022
H	3.4732133	-0.1063733	-2.4015978
H	5.5712225	-1.4679223	-2.4280050
C	-5.5570620	1.7072097	0.5960400
C	-5.1087247	0.5690245	0.6071272
C	-4.5952427	-0.7666106	0.6274262
C	-3.9865448	-1.2823113	1.7993446
C	-4.6901086	-1.5905699	-0.5210527
C	-3.5102086	-2.5994921	1.8242193
C	-4.2110505	-2.9067547	-0.4867778
C	-3.6318334	-3.4192039	0.6874935
H	-5.9405576	2.7088918	0.5848253
H	-3.8793814	-0.6340843	2.6719437
H	-5.1362248	-1.1850023	-1.4326304
H	-3.0474036	-2.9890711	2.7367086
H	-4.2936106	-3.5359826	-1.3785132
H	-3.2872951	-4.4584325	0.7191908

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C	1.3087511	2.7803529	-2.3807087
C	0.8070232	3.5547829	-1.3198581
C	2.6164706	2.2691877	-2.3153748
H	-0.2186258	3.9320931	-1.3539310
H	3.0108357	1.6617042	-3.1359235
C	1.6029527	3.8174855	-0.1985257
C	3.4223967	2.5259063	-1.1977229
H	1.2055976	4.3925452	0.6409612
H	4.4320207	2.1141414	-1.1358975
C	2.9209996	3.3021081	-0.1240307
H	0.6749479	2.5585679	-3.2438140
C	3.7259499	3.5408132	1.0356270
C	4.4044862	3.7150338	2.0405769
H	5.0127710	3.9199906	2.9003685
C	-0.3644279	0.6895940	-0.0740123
C	-1.3813001	1.5085647	0.4741242
C	0.8496029	0.5276912	0.6329827
H	-2.3255453	1.6360528	-0.0564506
H	1.6309500	-0.1151261	0.2347678
C	-1.1782972	2.1522843	1.7009231
C	1.0460098	1.1801773	1.8537556
H	-1.9756674	2.7747687	2.1186734
H	1.9954429	1.0500792	2.3783397
C	0.0361295	1.9947638	2.3931228
H	0.1929027	2.5042371	3.3490177
C	-0.5627682	0.0372249	-1.3324042
C	-0.7327616	-0.5064892	-2.4160664
H	-0.8911837	-0.9879767	-3.3606069

C	1.6391493	-2.6874600	2.0710888
C	0.8997058	-2.9604652	0.9070243
C	1.0081454	-2.0905794	3.1765259
H	1.3893367	-3.4132452	0.0416368
H	1.5817984	-1.8700712	4.0825357
C	-0.4594946	-2.6303495	0.8416159
C	-0.3518811	-1.7558080	3.1197603
H	-1.0296309	-2.8092148	-0.0731094
H	-0.8424768	-1.2709191	3.9680467
C	-1.1012946	-2.0144878	1.9458998
H	2.7071869	-2.9208069	2.1034974
C	-2.4762704	-1.6295140	1.8517485
C	-3.6413203	-1.2770398	1.7294113
H	-4.6532664	-0.9593168	1.5669522
C	4.5225520	0.1202981	0.9628575
C	4.2142451	-0.7933735	0.2100794
C	3.7811324	-1.8368001	-0.6682382
C	2.8707603	-1.5485742	-1.7164742
C	4.2231271	-3.1711362	-0.4845350
C	2.4111769	-2.5754903	-2.5506986
C	3.7595957	-4.1905078	-1.3272433
C	2.8523995	-3.8973218	-2.3627352
H	4.7676120	0.9723955	1.5694342
H	2.5121569	-0.5260809	-1.8542903
H	4.9195062	-3.3962448	0.3280795
H	1.6942508	-2.3417881	-3.3434494
H	4.1023972	-5.2185266	-1.1734861
H	2.4887777	-4.6970603	-3.0155913
C	-4.6214940	3.4091112	-0.3878443
C	-4.9047948	2.2293185	-0.5495987
C	-5.2151457	0.8421431	-0.7229787
C	-6.4178759	0.3036377	-0.1973740
C	-4.3178470	-0.0130773	-1.4098968
C	-6.7119719	-1.0574985	-0.3628429
C	-4.6198271	-1.3723033	-1.5641422
C	-5.8154590	-1.8995458	-1.0465965
H	-4.3839220	4.4477292	-0.2611265
H	-7.1101601	0.9611423	0.3359811
H	-3.3788943	0.3850946	-1.8009963
H	-7.6421041	-1.4636718	0.0473991
H	-3.9062422	-2.0252748	-2.0758817
H	-6.0440385	-2.9635742	-1.1633131

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C	4.6976901	1.3705831	-1.5419497
C	5.1525628	1.6929208	-0.2502369
C	4.2603175	0.0646585	-1.8238917
H	5.4727283	2.7138450	-0.0204154
H	3.8723201	-0.1858674	-2.8154148
C	5.1802049	0.7168339	0.7544302

C	4.2901003	-0.9208558	-0.8274708
H	5.5173311	0.9664925	1.7636496
H	3.9400643	-1.9318679	-1.0403278
C	4.7570052	-0.6067399	0.4727452
H	4.6648484	2.1407327	-2.3188941
C	4.8062017	-1.6168832	1.4860735
C	4.8654952	-2.4863742	2.3456311
H	4.9334339	-3.2540111	3.0918599
C	1.1251275	-1.7509330	-1.8686910
C	0.9663781	-1.5721316	-0.4725913
C	1.7111277	-2.9482786	-2.3508143
H	0.4986630	-0.6616351	-0.0997731
H	1.8309290	-3.0903039	-3.4286223
C	1.4115931	-2.5543118	0.4196109
C	2.1419880	-3.9326990	-1.4493516
H	1.3096816	-2.3841271	1.4945298
H	2.5983592	-4.8522979	-1.8293634
C	2.0016492	-3.7353093	-0.0627392
H	2.3622145	-4.4945595	0.6375845
C	0.7118951	-0.7199568	-2.7705478
C	0.3787189	0.1890258	-3.5186824
H	0.0188140	0.9808975	-4.1449548
C	-2.3890402	-0.5207415	-0.9731980
C	-1.9653346	0.8013423	-0.6915736
C	-2.3821699	-1.4894417	0.0365067
H	-2.7256050	-2.5032324	-0.1843710
C	-1.5092596	1.1197503	0.6103661
C	-1.9428529	-1.1637380	1.3317839
H	-1.1613734	2.1311103	0.8232907
H	-1.9464905	-1.9253174	2.1161841
C	-1.4974578	0.1392120	1.6117617
H	-2.7313707	-0.7687917	-1.9797049
H	-1.1254505	0.3933276	2.6081913
C	-2.0263812	1.8136511	-1.7006839
C	-2.1219600	2.6912891	-2.5487323
H	-2.1912893	3.4595302	-3.2938510
C	2.4102376	0.0517191	3.2968094
C	2.0688465	0.9557463	2.5464463
C	1.6465128	1.9787062	1.6399028
C	1.0594261	3.1778122	2.1161405
C	1.7954842	1.7888772	0.2441714
C	0.6180831	4.1528662	1.2095445
C	1.3403383	2.7618308	-0.6531275
C	0.7489396	3.9444917	-0.1764149
H	2.7733099	-0.7375859	3.9245461
H	0.9471555	3.3284600	3.1935323
H	2.2619398	0.8757007	-0.1240160
H	0.1614480	5.0739156	1.5855849
H	1.4333726	2.5817500	-1.7271653
H	0.3795649	4.6959839	-0.8805360

C	-5.4425865	-2.7217097	2.7470177
C	-5.5073994	-1.8503948	1.8893914
C	-5.5504436	-0.8391939	0.8770581
C	-5.0784198	0.4687683	1.1497251
C	-6.0399353	-1.1396077	-0.4185698
C	-5.0848368	1.4438143	0.1453091
C	-6.0450702	-0.1547012	-1.4159651
C	-5.5656496	1.1376897	-1.1396150
H	-5.4150722	-3.4785110	3.5069928
H	-4.6818320	0.6966061	2.1419778
H	-6.4030730	-2.1491069	-0.6318171
H	-4.6873149	2.4407046	0.3562819
H	-6.4183953	-0.3995546	-2.4157938
H	-5.5460869	1.8979426	-1.9261208

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C	0.3917098	2.8905035	-0.6388685
C	0.9035237	3.7243498	-1.6657109
C	0.4815450	3.3254501	0.7088978
C	1.4934048	4.9565927	-1.3496172
C	1.0708826	4.5604026	1.0145881
C	1.5802616	5.3798059	-0.0101057
C	-0.1860378	1.6201364	-0.9497466
C	-0.6676000	0.5226890	-1.1887000
H	0.8440186	3.3876457	-2.7043021
H	0.1190911	2.6715243	1.5044014
H	1.8929640	5.5885062	-2.1492793
H	1.1433470	4.8816579	2.0585341
H	2.0431720	6.3412197	0.2331274
H	-1.0933304	-0.4451179	-1.3685776
C	0.3703331	-2.8446182	-0.8805350
C	-0.2961889	-2.6754052	0.3591355
C	-0.4006169	-2.9603469	-2.0660428
C	-1.6945551	-2.5983563	0.4085243
C	-1.7996712	-2.8761193	-2.0067963
C	-2.4508394	-2.6869691	-0.7734147
C	1.8013836	-2.8533846	-0.9280828
C	3.0242215	-2.8151006	-0.9459341
H	0.2972480	-2.5685324	1.2689332
H	0.1099612	-3.0919415	-3.0240983
H	-2.1920136	-2.4420773	1.3688845
H	-2.3884583	-2.9385715	-2.9269165
H	-3.5385506	-2.5839239	-0.7411979
H	4.0964098	-2.7555744	-0.9495930
C	5.2446646	-0.0039648	-0.2181087
C	5.8018757	-0.4348692	-1.4488820
C	5.4357809	-0.8002963	0.9397020
C	6.5286716	-1.6317850	-1.5156892
C	6.1627846	-1.9965297	0.8631526
C	6.7117772	-2.4169534	-0.3620584

C	4.4859475	1.2089526	-0.1530562
C	3.8220613	2.2357285	-0.1064094
H	5.6498969	0.1740717	-2.3442408
H	5.0031416	-0.4772565	1.8906936
H	6.9479289	-1.9587708	-2.4724959
H	6.2959271	-2.6083582	1.7609222
H	7.2746363	-3.3537037	-0.4191848
H	3.2112308	3.1189225	-0.0700797
C	-3.6002250	2.9052232	0.4185351
C	-3.9743917	1.9473798	-0.2443105
C	-4.4133317	0.8372463	-1.0336859
C	-3.8288680	0.5880403	-2.3013167
C	-5.4452326	-0.0181107	-0.5708335
C	-4.2759998	-0.4840415	-3.0849518
C	-5.8853941	-1.0878861	-1.3628076
C	-5.3055423	-1.3228295	-2.6227513
H	-3.2446016	3.7359345	0.9964268
H	-3.0219195	1.2369056	-2.6492361
H	-5.8987385	0.1704661	0.4062315
H	-3.8183610	-0.6668740	-4.0623534
H	-6.6869632	-1.7386410	-0.9987842
H	-5.6531392	-2.1579105	-3.2392551
C	1.6276485	0.2535796	1.9611245
C	0.5189481	-0.0126975	2.4036713
C	-0.8030666	-0.3392016	2.8416252
C	-1.9227587	0.2866634	2.2372434
C	-1.0169569	-1.3169708	3.8456883
C	-3.2212239	-0.0546427	2.6369086
C	-2.3211908	-1.6597613	4.2303448
C	-3.4270750	-1.0292287	3.6299172
H	2.5686934	0.5275642	1.5205858
H	-1.7703268	1.0079966	1.4322299
H	-0.1546257	-1.8059246	4.3078951
H	-4.0709030	0.4404846	2.1594673
H	-2.4765525	-2.4196824	5.0030914
H	-4.4431163	-1.2994695	3.9352077

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C	2.7614975	1.1069793	-1.7481838
C	2.5637841	1.2345759	-0.3627723
C	2.5800227	-0.1416861	-2.3677345
H	2.7040511	2.2043469	0.1205891
H	2.7327977	-0.2460052	-3.4468260
C	2.1891706	0.1266556	0.4027076
C	2.2034401	-1.2588382	-1.6091997
H	2.0276007	0.2241286	1.4770132
H	2.0570495	-2.2321479	-2.0855973
C	2.0022875	-1.1343420	-0.2130938
H	3.0584218	1.9776958	-2.3394708
C	1.5910501	-2.2613675	0.5648892

C	1.2189826	-3.2163752	1.2337545
H	0.8314466	-4.0367902	1.8048397
C	-0.7084663	2.3715778	-0.4782026
C	-0.9179780	2.3261611	0.9221820
C	-0.7590668	1.1672996	-1.2224395
H	-0.8927471	3.2559285	1.4962064
H	-0.5848700	1.1967859	-2.3004497
C	-1.1736042	1.1026242	1.5555970
C	-1.0110154	-0.0474944	-0.5779026
H	-1.3519185	1.0789008	2.6346672
H	-1.0275028	-0.9689897	-1.1577658
C	-1.2210089	-0.0872882	0.8102715
H	-1.4197017	-1.0402446	1.3048301
C	-0.4507440	3.6160710	-1.1357270
C	-0.2331121	4.6771670	-1.7070302
H	-0.0350496	5.6074998	-2.2027498
C	-4.7005467	3.6391984	1.2110524
C	-4.8327312	2.4003920	1.8544462
C	-4.2985301	3.7004373	-0.1352871
H	-5.1349641	2.3485556	2.9044127
H	-4.1765097	4.6694382	-0.6292677
C	-4.5594869	1.2005846	1.1517140
C	-4.0329019	2.5129511	-0.8394072
H	-3.6927252	2.5571226	-1.8779881
C	-4.1645619	1.2711629	-0.2072526
H	-4.9066663	4.5615182	1.7644181
H	-3.9185902	0.3511139	-0.7408204
C	-4.6403656	-0.0675914	1.8109418
C	-4.6691363	-1.1560893	2.3700854
H	-4.6743233	-2.1231559	2.8335927
C	6.4019349	2.9142709	-0.7981633
C	6.1006748	1.8916769	-0.1961888
C	5.7190401	0.7019454	0.5024086
C	5.6222745	-0.5339685	-0.1840189
C	5.4083219	0.7489274	1.8843331
C	5.2139351	-1.6877146	0.4961086
C	5.0026091	-0.4124559	2.5561047
C	4.9017151	-1.6330779	1.8657144
H	6.6924792	3.8060451	-1.3191663
H	5.8456590	-0.5688130	-1.2532754
H	5.4794249	1.7027581	2.4147304
H	5.1153906	-2.6313859	-0.0486392
H	4.7564394	-0.3633693	3.6218646
H	4.5614599	-2.5333265	2.3857488
C	-2.2951690	-4.0811002	2.1933424
C	-2.3345695	-3.7322274	1.0208481
C	-2.3773954	-3.3163483	-0.3486060
C	-1.3309497	-3.6690632	-1.2377828
C	-3.4603826	-2.5366868	-0.8265161
C	-1.3744063	-3.2518162	-2.5752225

C -3.4931391 -2.1265306 -2.1661862
C -2.4541034 -2.4819738 -3.0449907
H -2.2646506 -4.3938689 3.2190577
H -0.4823199 -4.2452442 -0.8632624
H -4.2506661 -2.2377457 -0.1341710
H -0.5580313 -3.5221414 -3.2521295
H -4.3295132 -1.5182563 -2.5244955
H -2.4818792 -2.1551439 -4.0890710

Pentamer-28 (P13)

C -0.1103030 -3.8418663 -0.4110093
C 0.4094398 -3.2032375 0.7433523
C 0.5708139 -4.9672381 -0.9412249
C 1.5774803 -3.6803903 1.3533425
C 1.7386851 -5.4395499 -0.3229395
C 2.2447892 -4.8007778 0.8257677
C -1.3078717 -3.3448263 -1.0186708
C -2.3431495 -2.8987066 -1.4938133
C 3.5026476 0.3799658 -2.3396927
C 2.6842793 1.1230327 -3.2285490
C 4.6766838 0.9851686 -1.8214416
C 3.0352136 2.4317339 -3.5866895
C 5.0192728 2.2955895 -2.1856886
C 4.2016182 3.0235622 -3.0693261
C 3.1385951 -0.9502838 -1.9582885
C 2.8086044 -2.0760460 -1.6117705
H -0.1052566 -2.3258876 1.1401402
H 0.1772312 -5.4593958 -1.8350850
H 1.9748771 -3.1611328 2.2298890
H 2.2573810 -6.3083030 -0.7412139
H 3.1590760 -5.1707038 1.3009182
H -3.2649453 -2.5054958 -1.8783060
H 1.7727015 0.6644490 -3.6206886
H 5.3114730 0.4172640 -1.1358467
H 2.3875704 2.9977468 -4.2635408
H 5.9264537 2.7507857 -1.7759662
H 4.4679977 4.0483669 -3.3465939
H 2.4950306 -3.0493141 -1.2830321
C -4.7225290 -0.2795997 -0.6105130
C -5.2916021 -0.5832046 -1.8738791
C -4.7764434 -1.2532688 0.4184465
C -5.9023487 -1.8265878 -2.0940802
C -5.3906426 -2.4921000 0.1894802
C -5.9571291 -2.7841362 -1.0640622
C -4.0999445 0.9895816 -0.3811567
C -3.5756060 2.0795085 -0.1910443
H -5.2470345 0.1631175 -2.6718521
H -4.3238829 -1.0323404 1.3889230
H -6.3362873 -2.0493682 -3.0741661
H -5.4163394 -3.2379708 0.9898828

H	-6.4307472	-3.7550348	-1.2409372
H	-3.0854628	3.0191912	-0.0128946
H	2.7104550	2.4920516	-0.6778722
C	1.8142126	2.9493315	-0.3043247
C	0.7791491	3.4590819	0.1006172
C	-0.4256532	4.0772229	0.5657073
C	-1.1335318	4.9816053	-0.2675426
H	-0.7490789	5.1939851	-1.2691024
C	-2.3113567	5.5924164	0.1874069
H	-2.8484499	6.2860664	-0.4673653
H	-3.7246343	5.7894125	1.8275220
C	-2.8031470	5.3141499	1.4765680
C	-2.1081525	4.4162630	2.3078176
H	-2.4896531	4.1900009	3.3086009
C	-0.9302337	3.7998896	1.8618051
H	-0.3990358	3.0882886	2.4976482
C	-1.1696152	0.3826458	1.8308426
C	-0.0234040	0.1156908	2.1661474
C	1.3234671	-0.2534264	2.4784723
C	2.3020508	-0.2573100	1.4532276
C	1.6917531	-0.6549868	3.7872666
C	3.6141757	-0.6581693	1.7336284
C	3.0098540	-1.0500253	4.0584426
C	3.9755112	-1.0523996	3.0342970
H	-2.1467585	0.6753546	1.4920857
H	2.0153751	0.0300089	0.4405147
H	0.9365583	-0.6587566	4.5783756
H	4.3486906	-0.6803354	0.9239796
H	3.2836388	-1.3607276	5.0720427
H	5.0024586	-1.3649927	3.2507919

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C	-1.1278096	-2.5461344	1.7914595
C	-1.4327360	-3.2390263	0.5920556
C	-1.8027525	-2.9080789	2.9855403
C	-2.3894538	-4.2634315	0.5914572
C	-2.7566276	-3.9354481	2.9753452
C	-3.0548556	-4.6168439	1.7796318
C	-0.1591350	-1.4918998	1.7952769
C	0.6804805	-0.6025488	1.7877172
H	-0.9306058	-2.9566917	-0.3354001
H	-1.5763821	-2.3696753	3.9098592
H	-2.6234350	-4.7792337	-0.3449322
H	-3.2744590	-4.2019885	3.9022502
H	-3.8039043	-5.4149187	1.7748692
H	1.4090286	0.1851355	1.7582039
C	0.4921920	2.7949645	1.0122214
C	1.2576794	2.9226423	2.1996897
C	1.1378800	2.3694405	-0.1767811
C	2.6298015	2.6309433	2.1933808

C	2.5110078	2.0895947	-0.1729888
C	3.2641495	2.2169163	1.0075346
C	-0.9110446	3.0759579	1.0149928
C	-2.1110348	3.3130349	1.0068799
H	0.7607930	3.2401815	3.1203756
H	0.5508732	2.2470284	-1.0905835
H	3.2065364	2.7255191	3.1191054
H	2.9991422	1.7606684	-1.0940027
H	4.3320110	1.9855798	1.0018337
H	-3.1688278	3.4940778	0.9817833
C	-4.7807385	1.2736043	0.0659874
C	-4.1957848	1.6919698	-1.1565288
C	-5.6030980	2.1811302	0.7815953
C	-4.4327955	2.9835747	-1.6462041
C	-5.8284963	3.4736574	0.2857476
C	-5.2465450	3.8796329	-0.9299700
C	-4.5263684	-0.0373503	0.5819016
C	-4.2954139	-1.1554410	1.0209681
H	-3.5502650	0.9991908	-1.7019677
H	-6.0501065	1.8632650	1.7277305
H	-3.9681382	3.2974252	-2.5864386
H	-6.4603418	4.1672489	0.8499891
H	-5.4228575	4.8898599	-1.3128529
H	-4.0476541	-2.1295244	1.3986164
C	3.2508954	-2.4048981	0.8658279
C	4.1536346	-1.6171368	0.6201452
C	5.1551462	-0.6373133	0.3348901
C	5.2291592	-0.0435453	-0.9501944
C	6.0581001	-0.2094922	1.3409625
C	6.1649832	0.9655141	-1.2126283
C	6.9939833	0.7983243	1.0689007
C	7.0478823	1.3940027	-0.2047479
H	2.4335731	-3.0640436	1.0852936
H	4.5351300	-0.3708555	-1.7275812
H	6.0045799	-0.6643695	2.3338491
H	6.2036040	1.4238528	-2.2060056
H	7.6814494	1.1250368	1.8558097
H	7.7754418	2.1851384	-0.4113071
C	-3.4106661	-1.5944978	-2.3822418
C	-2.2170476	-1.4545901	-2.6120553
C	-0.8062626	-1.3376225	-2.8250831
C	0.0321484	-0.8741305	-1.7786285
C	-0.2243005	-1.7121081	-4.0630769
C	1.4212202	-0.8248461	-1.9573591
C	1.1643542	-1.6400060	-4.2385377
C	1.9903604	-1.2068944	-3.1846190
H	-4.4524629	-1.6691049	-2.1389008
H	-0.4072227	-0.5754734	-0.8244387
H	-0.8699398	-2.0625352	-4.8733618
H	2.0536067	-0.5046394	-1.1262796

H 1.6045517 -1.9325408 -5.1974471
H 3.0752009 -1.1761034 -3.3259257

Pentamer-30 (P14)

C 3.3895304 1.3284040 1.3404378
C 3.3942529 0.3472408 2.3469745
C 3.3718172 0.9428072 -0.0107350
H 3.4073421 0.6416485 3.4014495
H 3.3667856 1.7043423 -0.7942198
C 3.3817855 -1.0131170 2.0078149
C 3.3589562 -0.4113958 -0.3595996
H 3.3841897 -1.7812693 2.7861716
H 3.3437898 -0.7147872 -1.4079314
C 3.3637751 -1.4067019 0.6471634
H 3.3979148 2.3891473 1.6047923
C 3.3505617 -2.7937212 0.2946061
C 3.3387426 -3.9808279 -0.0042411
H 3.3255296 -5.0217108 -0.2639246
C -0.0019214 1.1785355 -0.3098406
C 0.0002136 0.1854316 0.6990374
C -0.0162742 0.7821368 -1.6696410
H 0.0109209 0.4912458 1.7466550
H -0.0179486 1.5488375 -2.4493243
C -0.0113650 -1.1694684 0.3529490
C -0.0277180 -0.5788718 -2.0060535
H -0.0096953 -1.9292653 1.1381123
H -0.0382732 -0.8753476 -3.0598738
C -0.0252463 -1.5579272 -0.9974668
H -0.0332688 -2.6191573 -1.2596515
C 0.0111611 2.5661300 0.0396500
C 0.0233960 3.7540276 0.3362242
H 0.0340850 4.7951324 0.5941663
C -3.3728280 1.4446562 1.3690217
C -3.3752086 0.4944358 2.4052046
C -3.3759125 1.0185545 0.0300478
H -3.3720889 0.8208220 3.4503606
H -3.3748992 1.7562882 -0.7759142
C -3.3809070 -0.8753887 2.1073106
C -3.3810655 -0.3459164 -0.2775232
H -3.3814765 -1.6198137 2.9083791
H -3.3809692 -0.6814689 -1.3161085
C -3.3831909 -1.3100514 0.7589694
H -3.3641318 2.5129366 1.6019125
C -3.3835121 -2.7072832 0.4494355
C -3.3784717 -3.9035130 0.1886613
H -3.3736603 -4.9519785 -0.0382533
C 6.7434962 1.0748460 -0.4606959
C 6.7601332 0.1094512 0.5763085
C 6.7115427 0.6380800 -1.8086257
H 6.7687448 0.4450432 1.6162743

H	6.6991122	1.3821376	-2.6101914
C	6.7363379	-1.2564344	0.2689724
C	6.6896313	-0.7317160	-2.1060246
H	6.7270065	-1.9934230	1.0774340
H	6.6614113	-1.0581816	-3.1509481
C	6.7000072	-1.6826636	-1.0703044
H	6.6656661	-2.7509721	-1.3039567
C	6.7398426	2.4727771	-0.1513745
C	6.7162964	3.6682988	0.1115542
H	6.7174164	4.7164568	0.3407487
C	-6.7121094	1.0644502	-0.6389941
C	-6.7694973	0.3489707	0.5827153
C	-6.6810828	0.3439627	-1.8589470
H	-6.7773668	0.9029494	1.5246437
H	-6.6362145	0.8948510	-2.8027918
C	-6.7870764	-1.0511705	0.5798930
C	-6.6995267	-1.0578159	-1.8510720
H	-6.8118068	-1.5938460	1.5295571
H	-6.6693969	-1.6048371	-2.7991826
C	-6.7510504	-1.7597816	-0.6339575
H	-6.7458639	-2.8536333	-0.6296797
C	-6.6631488	2.4954413	-0.6401010
C	-6.5980110	3.7179056	-0.6407401
H	-6.5634055	4.7903854	-0.6433344

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C	0.2858478	-1.0507587	-2.2032872
C	0.3628146	-0.7042128	-0.8435186
C	0.3016015	-0.0429348	-3.1833614
H	0.3528019	-1.4865661	-0.0807601
H	0.2438175	-0.3071295	-4.2444806
C	0.4552688	0.6375408	-0.4599646
C	0.3931803	1.3050264	-2.8092055
H	0.5190004	0.9105594	0.5947897
H	0.4071166	2.0935603	-3.5668978
C	0.4715588	1.6593435	-1.4396618
H	0.2191030	-2.1021718	-2.4958876
C	0.5696350	3.0332183	-1.0510694
C	0.6553243	4.2087480	-0.7191386
H	0.7336637	5.2389443	-0.4305130
C	3.7160344	-1.1495694	-0.6186413
C	3.7407090	-0.8053180	0.7548846
C	3.7676730	-0.1198800	-1.5896889
H	3.7180676	-1.6001195	1.5043123
H	3.7342089	-0.3839826	-2.6494759
C	3.8159490	0.5380216	1.1427492
C	3.8391842	1.2205225	-1.1911763
H	3.8520360	0.7937025	2.2057324
H	3.8597616	2.0102831	-1.9478542
C	3.8642317	1.5547841	0.1738317

H	3.9205091	2.6025453	0.4806067
C	3.6391426	-2.5208979	-1.0206639
C	3.5711251	-3.6937179	-1.3662487
H	3.5106950	-4.7211168	-1.6687577
C	7.0871832	-2.0889088	2.0397691
C	7.1552850	-0.7513424	2.4535891
C	7.0529273	-2.4069488	0.6703330
H	7.1784533	-0.4983845	3.5175551
H	6.9840019	-3.4508793	0.3498181
C	7.1888330	0.2913600	1.4940615
C	7.0897055	-1.3778354	-0.2868081
H	7.0454625	-1.6210747	-1.3526400
C	7.1592470	-0.0387360	0.1163479
H	7.0589507	-2.8868896	2.7894951
H	7.1674815	0.7648148	-0.6242154
C	7.2347094	1.6602859	1.9116410
C	7.2556030	2.8306992	2.2697702
H	7.2974537	3.8560822	2.5834610
C	-3.1333554	-3.1816640	-0.5072550
C	-3.0570695	-1.9704284	-0.3498149
C	-2.9717450	-0.5536486	-0.1627502
C	-3.0013067	0.3201693	-1.2774549
C	-2.8512739	-0.0083582	1.1393371
C	-2.9028376	1.7042375	-1.0899075
C	-2.7544913	1.3783801	1.3165981
C	-2.7781643	2.2388051	0.2047648
H	-3.2009096	-4.2435456	-0.6461659
H	-3.0844290	-0.1004721	-2.2821517
H	-2.8353870	-0.6819592	2.0002698
H	-2.9086683	2.3700992	-1.9573948
H	-2.6604112	1.7895069	2.3266069
H	-2.6857786	3.3194103	0.3439457
C	-11.3262495	-1.5297800	1.5060384
C	-10.2280785	-1.0547398	1.2471845
C	-8.9424791	-0.4987856	0.9442414
C	-7.8363671	-1.3452038	0.6751692
C	-8.7565194	0.9066333	0.9089624
C	-6.5801115	-0.7973429	0.3800966
C	-7.4962013	1.4445808	0.6120875
C	-6.4041248	0.5979685	0.3476874
H	-12.2894048	-1.9455327	1.7329966
H	-7.9783768	-2.4295413	0.7015177
H	-9.6079755	1.5617621	1.1155290
H	-5.7331814	-1.4588628	0.1744795
H	-7.3653348	2.5318730	0.5878275
H	-5.4220079	1.0201500	0.1183878

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C	-0.2856970	-1.0557049	2.1907204
C	-0.3624907	-0.7037034	0.8323399

C	-0.3025000	-0.0518634	3.1748306
H	-0.3517203	-1.4829419	0.0664051
H	-0.2448672	-0.3202886	4.2348867
C	-0.4558415	0.6395107	0.4541803
C	-0.3948960	1.2975404	2.8061010
H	-0.5195199	0.9167694	-0.5994789
H	-0.4095602	2.0830100	3.5669536
C	-0.4731037	1.6573413	1.4380011
H	-0.2181758	-2.1082327	2.4790503
C	-0.5717931	3.0327236	1.0549275
C	-0.6577799	4.2095797	0.7277596
H	-0.7365239	5.2409124	0.4433440
C	-3.7163451	-1.1483150	0.6117221
C	-3.7420518	-0.8015656	-0.7611551
C	-3.7679947	-0.1204386	1.5846743
H	-3.7191171	-1.5949747	-1.5120510
H	-3.7337154	-0.3864629	2.6439516
C	-3.8183843	0.5424417	-1.1465116
C	-3.8406231	1.2206429	1.1886679
H	-3.8551412	0.8000643	-2.2090050
H	-3.8612411	2.0089937	1.9468123
C	-3.8667780	1.5573926	-0.1757026
H	-3.9240522	2.6056728	-0.4805152
C	-3.6384586	-2.5203336	1.0111957
C	-3.5697081	-3.6937572	1.3545497
H	-3.5085769	-4.7216962	1.6550852
C	-7.0942548	-2.0865602	-2.0376012
C	-7.1626800	-0.7484511	-2.4496018
C	-7.0566622	-2.4063058	-0.6686427
H	-7.1884547	-0.4941796	-3.5131959
H	-6.9875224	-3.4506688	-0.3495917
C	-7.1931917	0.2930936	-1.4887170
C	-7.0903820	-1.3783419	0.2898409
H	-7.0435073	-1.6229047	1.3552580
C	-7.1602206	-0.0387109	-0.1114974
H	-7.0683605	-2.8836352	-2.7883745
H	-7.1660831	0.7639284	0.6300752
C	-7.2394594	1.6625603	-1.9044908
C	-7.2607509	2.8334212	-2.2611131
H	-7.3028900	3.8592123	-2.5734352
C	3.1418181	-3.1845500	0.5219314
C	3.0634864	-1.9739525	0.3606314
C	2.9760864	-0.5579022	0.1689773
C	3.0002469	0.3193536	1.2811097
C	2.8591990	-0.0167826	-1.1351675
C	2.9000984	1.7026805	1.0890196
C	2.7608453	1.3692427	-1.3169924
C	2.7791844	2.2330926	-0.2077156
H	3.2111088	-4.2458783	0.6641980
H	3.0805317	-0.0980885	2.2873712

H	2.8474104	-0.6930374	-1.9940855
H	2.9015882	2.3711730	1.9544913
H	2.6696705	1.7771345	-2.3285804
H	2.6856799	3.3131398	-0.3505351
C	11.3266121	-1.5218856	-1.5202918
C	10.2291897	-1.0482902	-1.2556609
C	8.9444938	-0.4939686	-0.9459775
C	8.7571668	0.9112195	-0.9088673
C	7.8406641	-1.3417798	-0.6719696
C	7.4977435	1.4475939	-0.6054168
C	6.5852699	-0.7954957	-0.3703998
C	6.4079093	0.5995991	-0.3362195
H	12.2891057	-1.9364000	-1.7522634
H	9.6068751	1.5674125	-1.1192282
H	7.9837210	-2.4259447	-0.6997262
H	7.3658142	2.5347257	-0.5798148
H	5.7400428	-1.4580751	-0.1612109
H	5.4264419	1.0205033	-0.1018972

Pentamer-33

C	-0.5811794	-2.2994093	0.2101837
C	-0.7230043	-2.8079490	-1.1068468
C	-0.5415116	-3.2113733	1.2962869
C	-0.8178723	-4.1891061	-1.3278398
C	-0.6397359	-4.5916430	1.0664590
C	-0.7767594	-5.0869415	-0.2443214
C	-0.4709243	-0.8913229	0.4306080
C	-0.3446025	0.3132202	0.5957859
H	-0.7594480	-2.1071052	-1.9446800
H	-0.4321911	-2.8244380	2.3127217
H	-0.9289323	-4.5683844	-2.3479970
H	-0.6085722	-5.2855282	1.9119597
H	-0.8514475	-6.1639962	-0.4200807
H	-0.2431557	1.3734690	0.7284829
C	-2.5951485	2.9964058	0.2390280
C	-2.0654474	3.3946156	1.4931848
C	-1.7995966	3.1611559	-0.9240927
C	-0.7728013	3.9331282	1.5770949
C	-0.5086119	3.6983412	-0.8282521
C	0.0119926	4.0858483	0.4194376
C	-3.8987964	2.4104329	0.1507492
C	-5.0041124	1.8910879	0.0748448
H	-2.6733100	3.2645706	2.3929139
H	-2.2015499	2.8470767	-1.8913513
H	-0.3709992	4.2276644	2.5518243
H	0.1068924	3.8050984	-1.7260193
H	1.0240394	4.4916889	0.4868790
H	-5.9567164	1.3992904	0.0093557
C	-6.1511800	-1.5418669	-0.0678571
C	-6.5698872	-1.0933088	-1.3467307

C	-6.8713395	-1.1168968	1.0777516
C	-7.6751357	-0.2399350	-1.4716499
C	-7.9753101	-0.2627147	0.9434690
C	-8.3808477	0.1804014	-0.3291285
C	-5.0082155	-2.3942989	0.0620580
C	-4.0232885	-3.1125708	0.1656413
H	-6.0128834	-1.4134444	-2.2316263
H	-6.5486980	-1.4557410	2.0660992
H	-7.9839386	0.1054380	-2.4633986
H	-8.5186317	0.0652237	1.8353573
H	-9.2394767	0.8515767	-0.4296089
H	-3.1358263	-3.7116056	0.2493949
C	3.0209363	0.2601896	0.0123436
C	3.1764309	1.4713962	-0.0617130
C	3.3157542	2.8920346	-0.1535485
C	3.0602625	3.5587574	-1.3790900
C	3.6922739	3.6593418	0.9785686
C	3.1698647	4.9533057	-1.4640808
C	3.8009029	5.0541940	0.8837549
C	3.5381359	5.7069838	-0.3346438
H	2.8880633	-0.8056494	0.0706215
H	2.7672758	2.9692512	-2.2523630
H	3.8887506	3.1496185	1.9260246
H	2.9657876	5.4565944	-2.4146557
H	4.0901889	5.6366240	1.7645749
H	3.6208355	6.7961253	-0.4037828
C	2.7857390	-3.5276102	-0.2510741
C	3.9654939	-3.2059733	-0.1900912
C	5.3417051	-2.8150169	-0.1088731
C	6.2516728	-3.5522162	0.6913961
C	5.8104681	-1.6798505	-0.8178832
C	7.5945840	-3.1600246	0.7774358
C	7.1551892	-1.2955263	-0.7237131
C	8.0510622	-2.0320421	0.0715529
H	1.7488874	-3.8042353	-0.2989257
H	5.8924757	-4.4279656	1.2398769
H	5.1115252	-1.1007068	-1.4268074
H	8.2885511	-3.7343185	1.4002288
H	7.5051682	-0.4139396	-1.2707201
H	9.1004522	-1.7276238	0.1427970

Pentamer-34 (P15)

C	-7.0382537	-1.5559366	0.0182706
C	-7.0430055	-0.8478012	1.2324815
C	-7.0548954	-0.8525514	-1.1985808
H	-7.0203444	-1.3905673	2.1827876
H	-7.0416006	-1.3990176	-2.1469336
C	-7.0657926	0.5534092	1.2354138
C	-7.0777477	0.5486446	-1.2067465
H	-7.0626103	1.1083913	2.1775309

H	-7.0838817	1.0999556	-2.1509994
C	-7.0829046	1.2698320	0.0129781
H	-7.0032776	-2.6492655	0.0202247
C	-7.1009584	2.7014566	0.0102632
C	-7.1159269	3.9257297	0.0078782
H	-7.1402111	4.9983721	0.0058089
C	-3.5103470	-3.2435488	-0.0034477
C	-3.5100209	-2.5364130	1.2125479
C	-3.5191745	-2.5375913	-1.2201077
H	-3.5021164	-3.0804470	2.1627508
H	-3.5184747	-3.0825480	-2.1698167
C	-3.5191505	-1.1356138	1.2152301
C	-3.5283721	-1.1367822	-1.2240916
H	-3.5185320	-0.5812973	2.1568615
H	-3.5350116	-0.5833923	-2.1662557
C	-3.5289845	-0.4165526	-0.0047533
C	-3.5402386	1.0128177	-0.0053695
C	-3.5484367	2.2352678	-0.0059254
H	-3.5530501	3.3070279	-0.0064528
H	-3.5027255	-4.3382480	-0.0029621
C	0.0000581	-1.5317333	-0.0173840
C	-0.0000075	-0.8264056	1.1970648
C	0.0000598	-0.8255749	-1.2313474
H	0.0000129	-1.3712910	2.1455163
H	0.0000854	-1.3697483	-2.1802286
C	-0.0000719	0.5744193	1.2036477
C	-0.0000189	0.5753018	-1.2369166
H	-0.0001387	1.1273873	2.1462992
H	-0.0000198	1.1289254	-2.1791965
C	-0.0000877	1.2930633	-0.0163721
H	0.0000984	-2.6242628	-0.0177508
C	-0.0002167	2.7239155	-0.0158503
C	-0.0003771	3.9482410	-0.0154089
H	-0.0005520	5.0208648	-0.0150441
C	3.5290335	-0.4154376	-0.0115551
C	3.5308660	-1.1351155	-1.2312414
C	3.5168791	-1.1350616	1.2080575
H	3.5393586	-0.5812876	-2.1731460
H	3.5143200	-0.5811756	2.1499265
C	3.5217402	-2.5359295	-1.2279227
C	3.5078963	-2.5358574	1.2047095
H	3.5229550	-3.0804458	-2.1778852
H	3.4981882	-3.0803248	2.1546436
C	3.5106212	-3.2424377	-0.0115873
H	3.5030965	-4.3371370	-0.0116379
C	3.5401292	1.0138828	-0.0115180
C	3.5481652	2.2364278	-0.0116246
H	3.5525934	3.3081310	-0.0117870
H	7.1404739	4.9977784	-0.0194937
C	7.1161384	3.9250281	-0.0098215

C	7.1010099	2.7010473	0.0011217
C	7.0828645	1.2693406	0.0135119
C	7.0832828	0.5399215	-1.2012950
H	7.0938273	1.0848460	-2.1492113
C	7.0603811	-0.8611976	-1.1837605
H	7.0514207	-1.4140908	-2.1284243
C	7.0382374	-1.5563186	0.0377238
H	7.0033302	-2.6496130	0.0468945
C	7.0374360	-0.8399619	1.2471326
H	7.0104569	-1.3762756	2.2009928
C	7.0601474	0.5612189	1.2406965
H	7.0525417	1.1225478	2.1790196

Hexamers

Hexamer-01 (H1)

C	4.1560784	3.4650044	2.3990419
C	4.2185898	2.7624566	1.3989000
C	4.2399622	1.9164189	0.2443329
C	5.2146358	0.8958447	0.1095730
C	3.2553097	2.0696517	-0.7632477
C	5.1974394	0.0484499	-1.0069250
C	3.2472407	1.2171809	-1.8750121
C	4.2155438	0.2056891	-2.0019268
H	4.1147550	4.0946635	3.2663992
H	5.9662856	0.7674735	0.8932080
H	2.4939208	2.8442872	-0.6538775
H	5.9440497	-0.7468510	-1.0932768
H	2.4747235	1.3265072	-2.6394794
H	4.1866493	-0.4619444	-2.8674955
C	0.0878515	2.4629393	3.7104180
C	0.0779741	2.5936818	2.4939252
C	0.0414641	2.7487987	1.0713497
C	-0.0685990	1.6195485	0.2219713
C	0.0932828	4.0450394	0.4967601
C	-0.1423151	1.7894855	-1.1657809
C	0.0192442	4.2029501	-0.8942915
C	-0.1055558	3.0759015	-1.7283500
H	0.1029250	2.3412098	4.7759552
H	-0.1034889	0.6199845	0.6550764
H	0.1887252	4.9155424	1.1510875
H	-0.2357778	0.9171511	-1.8098325
H	0.0565484	5.2069353	-1.3276405
H	-0.1673230	3.2000280	-2.8135464
C	3.0322683	-3.9693073	-0.7850839
C	2.8170926	-3.2437916	0.1765888
C	2.5722815	-2.3841640	1.2947501

C	2.4719388	-0.9822803	1.1103231
C	2.4345733	-2.9219961	2.5994648
C	2.2517529	-0.1418175	2.2087193
C	2.2125954	-2.0718314	3.6916492
C	2.1222569	-0.6807947	3.4993997
H	3.2036212	-4.5972864	-1.6376409
H	2.5730860	-0.5621674	0.1094862
H	2.4939567	-4.0037174	2.7408250
H	2.1853918	0.9366781	2.0603956
H	2.1036109	-2.4980574	4.6937172
H	1.9423562	-0.0165054	4.3496608
C	2.5499835	-0.2378214	-5.3126166
C	1.6581141	-0.5652520	-4.5406241
C	0.6200332	-0.9169883	-3.6193526
C	0.9390915	-1.4982180	-2.3658985
C	-0.7401020	-0.6737406	-3.9419143
C	-0.0776980	-1.8171302	-1.4559465
C	-1.7488153	-0.9948208	-3.0230111
C	-1.4227889	-1.5600457	-1.7756948
H	3.3311964	0.0340261	-5.9957731
H	1.9817633	-1.6914533	-2.1085689
H	-0.9883422	-0.2291986	-4.9097105
H	0.1827585	-2.2680319	-0.4965425
H	-2.7955178	-0.7982036	-3.2694907
H	-2.2131259	-1.7928460	-1.0582191
C	-0.2004988	-5.0133185	1.0485382
C	-0.9262619	-4.0608855	1.2994516
C	-1.7432521	-2.9124722	1.5493302
C	-1.1657282	-1.7289870	2.0750400
C	-3.1282798	-2.9284009	1.2447598
C	-1.9571502	-0.5908105	2.2821447
C	-3.9069080	-1.7808021	1.4466686
C	-3.3252962	-0.6088807	1.9610866
H	0.4502507	-5.8368291	0.8293964
H	-0.1000668	-1.7119912	2.3076990
H	-3.5747617	-3.8376054	0.8328562
H	-1.4991897	0.3182471	2.6816356
H	-4.9665015	-1.7919733	1.1771161
H	-3.9319300	0.2915879	2.0889376
C	-5.2727917	-1.5624711	-2.2090372
C	-5.1056838	-0.5361730	-1.5635484
C	-4.9041154	0.6389671	-0.7713027
C	-5.9257158	1.0934754	0.1005626
C	-3.6749661	1.3421894	-0.8206770
C	-5.7133816	2.2196887	0.9077343
C	-3.4746760	2.4714220	-0.0162849
C	-4.4885009	2.9111229	0.8527323
H	-5.4140737	-2.4520554	-2.7918775
H	-6.8746275	0.5510383	0.1419542
H	-2.8764135	0.9870609	-1.4743071

H	-6.5063236	2.5582631	1.5823760
H	-2.5185076	2.9982362	-0.0601614
H	-4.3245888	3.7871603	1.4882347

Hexamer-02 (H5)

C	-4.4154072	1.4755404	3.5277239
C	-4.4186472	0.8499510	2.4758282
C	-4.3929163	0.1270640	1.2403687
C	-5.1911770	0.5414803	0.1443338
C	-3.5478773	-1.0009312	1.0940460
C	-5.1444897	-0.1634465	-1.0666275
C	-3.5117052	-1.6999389	-0.1194022
C	-4.3094176	-1.2874915	-1.2009182
H	-4.4230888	2.0142548	4.4551430
H	-5.8315831	1.4210590	0.2529382
H	-2.9176258	-1.3100174	1.9291105
H	-5.7556555	0.1695656	-1.9110315
H	-2.8526600	-2.5632499	-0.2306488
H	-4.2654854	-1.8393363	-2.1439770
C	-0.2943845	2.1931323	3.9936920
C	-0.3565528	1.0733782	3.5035332
C	-0.4265240	-0.2445572	2.9487236
C	-0.0737178	-0.4848653	1.5980022
C	-0.8389346	-1.3316419	3.7608842
C	-0.1265272	-1.7826530	1.0777675
C	-0.8889760	-2.6278157	3.2291729
C	-0.5308866	-2.8554781	1.8878890
H	-0.2511869	3.1751442	4.4231591
H	0.2488585	0.3435395	0.9687665
H	-1.1218823	-1.1440526	4.8000107
H	0.1553163	-1.9608429	0.0423280
H	-1.2115051	-3.4607941	3.8611629
H	-0.5699688	-3.8664734	1.4721649
C	-2.1663470	1.2867935	-4.3112191
C	-1.9803495	1.8133731	-3.2222456
C	-1.7530991	2.4279514	-1.9495249
C	-1.9979515	1.7119526	-0.7505091
C	-1.2839077	3.7647569	-1.8753289
C	-1.7951288	2.3301217	0.4910016
C	-1.0818160	4.3709259	-0.6283387
C	-1.3412074	3.6575676	0.5555904
H	-2.3296383	0.8180847	-5.2620928
H	-2.3467869	0.6800060	-0.8006722
H	-1.0788481	4.3102664	-2.8002906
H	-1.9920994	1.7776395	1.4105568
H	-0.7125824	5.3999265	-0.5804342
H	-1.1762752	4.1283368	1.5289878
C	-2.8994218	-4.5070848	-2.5172922
C	-1.9035830	-3.7969593	-2.4646430
C	-0.7397843	-2.9666564	-2.3772879

C	-0.8448693	-1.5592988	-2.5164663
C	0.5346673	-3.5460441	-2.1425899
C	0.3006780	-0.7566778	-2.4258080
C	1.6716482	-2.7317315	-2.0482731
C	1.5586313	-1.3365925	-2.1895350
H	-3.7724523	-5.1283554	-2.5736244
H	-1.8202704	-1.1013534	-2.6904589
H	0.6138955	-4.6314890	-2.0336630
H	0.2150731	0.3247898	-2.5465739
H	2.6526791	-3.1752064	-1.8603237
H	2.4481381	-0.7079593	-2.1140576
C	2.2928551	1.8510626	-3.8541676
C	2.5300408	2.1251855	-2.6860317
C	2.7948773	2.4414319	-1.3153602
C	4.0913226	2.8460184	-0.9057542
C	1.7588639	2.3630474	-0.3518015
C	4.3371733	3.1689945	0.4361865
C	2.0154130	2.6852396	0.9871313
C	3.3010621	3.0898883	1.3854087
H	2.0695291	1.5959119	-4.8718420
H	4.8928491	2.8993944	-1.6475006
H	0.7581281	2.0609736	-0.6646339
H	5.3407414	3.4779429	0.7440710
H	1.2094422	2.6144404	1.7212539
H	3.4996964	3.3334526	2.4336715
C	5.2745842	-1.6763909	-1.8778459
C	4.7458257	-1.6746841	-0.7738718
C	4.1007910	-1.6768394	0.5043655
C	3.7230215	-0.4560063	1.1175926
C	3.8292046	-2.8989773	1.1701212
C	3.1014056	-0.4637173	2.3727285
C	3.2054092	-2.8929554	2.4254654
C	2.8441709	-1.6775772	3.0318250
H	5.7438822	-1.6730966	-2.8425530
H	3.9140644	0.4856195	0.6004480
H	4.1125028	-3.8418632	0.6935320
H	2.7950817	0.4819148	2.8271116
H	2.9936367	-3.8403201	2.9310513
H	2.3364887	-1.6774467	4.0003468

Hexamer-03 (H2)

C	5.6263464	-0.9601609	2.5878022
C	4.6154288	-1.5790042	2.2832312
C	3.4145691	-2.2595084	1.9034948
C	2.5108150	-2.7399107	2.8841620
C	3.1005016	-2.4280093	0.5319109
C	1.3212291	-3.3717309	2.4963626
C	1.9097633	-3.0627969	0.1552779
C	1.0175290	-3.5372168	1.1330090
H	6.5223046	-0.4351429	2.8563982

H	2.7445123	-2.5961781	3.9424667
H	3.7855677	-2.0422554	-0.2244045
H	0.6223255	-3.7233844	3.2612878
H	1.6648991	-3.1716188	-0.9038981
H	0.0832156	-4.0158090	0.8263882
C	4.7571105	2.8143995	0.4330407
C	4.4669245	1.8714369	-0.2911611
C	4.1305887	0.7773423	-1.1520201
C	2.7790260	0.5013105	-1.4797837
C	5.1555843	-0.0384131	-1.6965387
C	2.4685753	-0.5505189	-2.3517115
C	4.8325024	-1.0942415	-2.5600371
C	3.4895918	-1.3485352	-2.8956157
H	5.0069493	3.6402886	1.0701266
H	1.9807558	1.1090244	-1.0499143
H	6.1968570	0.1651358	-1.4325588
H	1.4258664	-0.7495078	-2.6013109
H	5.6312257	-1.7197409	-2.9709170
H	3.2391710	-2.1742081	-3.5689594
C	-2.4659291	-0.9612249	2.0143412
C	-1.4699691	-0.2971970	2.2657234
C	-0.3046950	0.4976312	2.5068711
C	0.9310653	0.1575303	1.9002925
C	-0.3735801	1.6447613	3.3375894
C	2.0670817	0.9451502	2.1226979
C	0.7699714	2.4263016	3.5552032
C	1.9917110	2.0795298	2.9490287
H	-3.3422011	-1.5246536	1.7560003
H	0.9923099	-0.7199546	1.2567362
H	-1.3292912	1.9172878	3.7917966
H	3.0157898	0.6720569	1.6586980
H	0.7043320	3.3122529	4.1944670
H	2.8827949	2.6926021	3.1136195
C	-0.8812405	-4.7698677	-1.9503183
C	-0.9096800	-3.5526949	-2.0766517
C	-0.9361252	-2.1274377	-2.2070667
C	-0.8485694	-1.3063757	-1.0564605
C	-1.0593965	-1.5199353	-3.4831147
C	-0.8751618	0.0870032	-1.1798593
C	-1.0804991	-0.1217246	-3.5949398
C	-0.9824436	0.6860711	-2.4459372
H	-0.8464197	-5.8369191	-1.8436316
H	-0.7799977	-1.7658217	-0.0716068
H	-1.1362336	-2.1512127	-4.3723822
H	-0.8262431	0.7054119	-0.2838386
H	-1.1698345	0.3388103	-4.5834861
H	-0.9905461	1.7748925	-2.5343826
C	-3.2912190	2.6244347	0.9773177
C	-2.3531349	3.0852902	0.3410909
C	-1.2501459	3.5758999	-0.4279789

C	0.0824134	3.3037604	-0.0269047
C	-1.4739858	4.3090692	-1.6217408
C	1.1596336	3.7451219	-0.8068469
C	-0.3895095	4.7420988	-2.3980752
C	0.9291161	4.4593372	-1.9963487
H	-4.1216742	2.2039115	1.5143718
H	0.2604400	2.7402159	0.8892294
H	-2.5005061	4.5222514	-1.9329942
H	2.1823713	3.5242576	-0.4882371
H	-0.5742079	5.3022551	-3.3206928
H	1.7731800	4.7953976	-2.6069842
C	-6.7874308	1.4853841	1.9550157
C	-6.2811454	0.5921769	1.2879247
C	-5.6458405	-0.4431490	0.5297877
C	-4.8050332	-0.1178935	-0.5644042
C	-5.8258820	-1.8053189	0.8831718
C	-4.1504987	-1.1315315	-1.2756767
C	-5.1620570	-2.8116251	0.1655256
C	-4.3190063	-2.4786919	-0.9111931
H	-7.2581003	2.2654771	2.5219709
H	-4.6488203	0.9306539	-0.8280409
H	-6.4752094	-2.0578391	1.7260597
H	-3.4883351	-0.8677377	-2.1032655
H	-5.2988782	-3.8591246	0.4522865
H	-3.7815884	-3.2623944	-1.4532691

Hexamer-04 (H4)

C	-0.9459687	-4.3728134	2.3005748
C	-0.0100018	-4.0296395	1.5909833
C	1.0783252	-3.6121789	0.7599777
C	1.3164815	-4.2366628	-0.4916002
C	1.9318897	-2.5616649	1.1809192
C	2.3812546	-3.8124794	-1.2997029
C	2.9934858	-2.1476496	0.3664285
C	3.2217610	-2.7669731	-0.8745692
H	-1.7598993	-4.6714884	2.9319241
H	0.6582777	-5.0458883	-0.8196132
H	1.7520325	-2.0768219	2.1409629
H	2.5465735	-4.2886557	-2.2706008
H	3.6394196	-1.3308942	0.6954237
H	4.0405779	-2.4191039	-1.5100725
C	-2.5025033	-0.5754147	2.7110650
C	-1.3181520	-0.3744457	2.9419120
C	0.0766806	-0.1362244	3.1538466
C	0.8067681	0.6747758	2.2470705
C	0.7538438	-0.7295263	4.2498283
C	2.1809566	0.8761826	2.4301469
C	2.1300919	-0.5243016	4.4217947
C	2.8474144	0.2755742	3.5124157
H	-3.5367115	-0.7282464	2.4630145

H	0.2946910	1.1196098	1.3922342
H	0.1940920	-1.3601073	4.9457057
H	2.7336529	1.4929346	1.7190372
H	2.6456412	-0.9955194	5.2644279
H	3.9236402	0.4254363	3.6434858
C	2.0277656	-1.2825439	-4.5764728
C	1.1990028	-0.8375440	-3.7928858
C	0.2481686	-0.3079252	-2.8626857
C	0.1133189	-0.8822779	-1.5756409
C	-0.5606120	0.8051150	-3.2108842
C	-0.8073238	-0.3591268	-0.6619798
C	-1.4720943	1.3265288	-2.2836743
C	-1.5998675	0.7458454	-1.0085629
H	2.7474839	-1.6692780	-5.2714563
H	0.7242180	-1.7420933	-1.3059760
H	-0.4528049	1.2554714	-4.2012465
H	-0.9282284	-0.8267650	0.3153483
H	-2.0762149	2.1975404	-2.5499153
H	-2.3170819	1.1480354	-0.2927925
C	6.1858964	-0.5572405	-0.7305423
C	5.3361509	0.3219894	-0.6746597
C	4.3356152	1.3426257	-0.5839176
C	3.0273456	1.1158241	-1.0816905
C	4.6426784	2.5908581	0.0168058
C	2.0529367	2.1187116	-0.9824355
C	3.6610844	3.5874940	0.1081989
C	2.3666618	3.3565263	-0.3937221
H	6.9331428	-1.3244449	-0.7928211
H	2.7839686	0.1555449	-1.5391102
H	5.6504534	2.7641974	0.4044632
H	1.0481806	1.9338442	-1.3658958
H	3.9080024	4.5481733	0.5710071
H	1.6057797	4.1395745	-0.3417721
C	-0.3828913	5.2945928	-1.9874552
C	-1.0572984	4.7457459	-1.1261200
C	-1.8437675	4.0679100	-0.1412460
C	-3.2238224	3.8355583	-0.3661452
C	-1.2494126	3.5908046	1.0542847
C	-3.9834213	3.1301074	0.5777540
C	-2.0178302	2.8907453	1.9926926
C	-3.3831401	2.6542773	1.7568165
H	0.2135251	5.7871072	-2.7309124
H	-3.6822240	4.1984929	-1.2901849
H	-0.1834269	3.7554295	1.2284333
H	-5.0428269	2.9359582	0.3857017
H	-1.5453049	2.4990757	2.8966036
H	-3.9683734	2.0797443	2.4795772
C	-5.8891715	-0.5289496	1.1943591
C	-5.1185208	-1.0669181	0.4083382
C	-4.2005166	-1.6911701	-0.4961591

C	-3.3325464	-2.7173645	-0.0451451
C	-4.1437334	-1.2853240	-1.8532699
C	-2.4403073	-3.3257325	-0.9360366
C	-3.2449932	-1.8985563	-2.7352150
C	-2.3934525	-2.9200484	-2.2809831
H	-6.5969529	-0.0843327	1.8669022
H	-3.3451318	-3.0156060	1.0058807
H	-4.7989347	-0.4811078	-2.1985624
H	-1.7629955	-4.0982523	-0.5644195
H	-3.1928724	-1.5627631	-3.7748693
H	-1.6754752	-3.3783561	-2.9674099

Hexamer-05 (H3)

C	-1.0330820	-5.2274835	0.1393252
C	-1.7753293	-4.3527048	0.5651688
C	-2.6093127	-3.2936715	1.0476210
C	-2.8042552	-3.1025747	2.4388534
C	-3.2235600	-2.4016204	0.1334042
C	-3.5965379	-2.0419735	2.8999420
C	-4.0113282	-1.3434825	0.6054458
C	-4.2030333	-1.1604077	1.9864303
H	-0.3950813	-6.0047373	-0.2337588
H	-2.3175552	-3.7810630	3.1445184
H	-3.0617926	-2.5374631	-0.9375732
H	-3.7290456	-1.8948127	3.9762067
H	-4.4664032	-0.6464408	-0.1018711
H	-4.8117872	-0.3233533	2.3399187
C	1.6824663	-2.6194528	-2.1407957
C	0.5422831	-2.2406679	-2.3744921
C	-0.7864892	-1.7741532	-2.6341260
C	-1.2482282	-0.5636403	-2.0581373
C	-1.6586420	-2.5156320	-3.4715733
C	-2.5394772	-0.0974723	-2.3342703
C	-2.9544160	-2.0474625	-3.7308416
C	-3.3962046	-0.8345139	-3.1691944
H	2.6752637	-2.9458731	-1.8881623
H	-0.5993429	0.0007733	-1.3877961
H	-1.3098460	-3.4561420	-3.9068155
H	-2.8787291	0.8364517	-1.8845795
H	-3.6207083	-2.6303421	-4.3745669
H	-4.4082759	-0.4710717	-3.3736231
C	-1.4155490	1.9290146	4.0243266
C	-0.6856543	1.1745852	3.3946400
C	0.1601005	0.2921540	2.6495368
C	-0.4012661	-0.6269968	1.7270349
C	1.5673672	0.3281314	2.8232247
C	0.4297499	-1.5003356	1.0132031
C	2.3889486	-0.5441956	2.0978096
C	1.8220004	-1.4640692	1.1979254
H	-2.0615036	2.5867515	4.5726221

H	-1.4817798	-0.6513553	1.5803854
H	2.0006500	1.0559830	3.5128019
H	-0.0051651	-2.2089272	0.3072814
H	3.4737795	-0.4959549	2.2186433
H	2.4653479	-2.1407377	0.6312704
C	-6.4871365	1.6039174	0.7857245
C	-5.3899151	1.9954310	0.4098841
C	-4.1022730	2.4264474	-0.0443543
C	-2.9318057	2.0704439	0.6722867
C	-3.9809358	3.2038859	-1.2252256
C	-1.6737979	2.4791314	0.2124041
C	-2.7147492	3.5991633	-1.6800062
C	-1.5579574	3.2358886	-0.9661647
H	-7.4513728	1.2761306	1.1228912
H	-3.0111085	1.4739794	1.5830535
H	-4.8828270	3.4822630	-1.7774056
H	-0.7846406	2.2117388	0.7849251
H	-2.6301351	4.1893435	-2.5978075
H	-0.5702777	3.5360848	-1.3253344
C	1.4179400	3.8042296	2.2164121
C	1.6715274	3.4345874	1.0786901
C	1.9302302	2.9973937	-0.2584736
C	1.6149278	1.6734558	-0.6536694
C	2.4952598	3.8853450	-1.2093586
C	1.8548333	1.2531296	-1.9683947
C	2.7331578	3.4549394	-2.5225595
C	2.4123006	2.1388919	-2.9063129
H	1.1684189	4.0978255	3.2172033
H	1.1988895	0.9816004	0.0780723
H	2.7416872	4.9065913	-0.9060584
H	1.6252977	0.2237325	-2.2539416
H	3.1708894	4.1477596	-3.2482075
H	2.6002137	1.8055842	-3.9314887
C	4.8005664	-3.9975606	-0.7134349
C	4.9992675	-2.8365344	-0.3788044
C	5.2187505	-1.4828893	0.0345210
C	5.9695966	-1.2076600	1.2060609
C	4.6760103	-0.4049758	-0.7078373
C	6.1667829	0.1173930	1.6189388
C	4.8795021	0.9156297	-0.2871452
C	5.6221859	1.1810781	0.8758108
H	4.6466692	-5.0171190	-1.0102590
H	6.3837470	-2.0384135	1.7838831
H	4.0813857	-0.6108959	-1.6007429
H	6.7438836	0.3199598	2.5268077
H	4.4430523	1.7365512	-0.8612243
H	5.7689499	2.2136971	1.2071772

Hexamer-06 (H7)

C	-5.1795750	0.2441908	3.1564941
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C	-4.9056566	-0.3624162	2.1294659
C	-4.5364272	-1.0470638	0.9276135
C	-5.2808542	-0.8719001	-0.2661128
C	-3.3950807	-1.8871699	0.9141286
C	-4.8873569	-1.5236532	-1.4435270
C	-3.0107574	-2.5335994	-0.2678139
C	-3.7538387	-2.3568498	-1.4482405
H	-5.4317847	0.7605813	4.0621410
H	-6.1542176	-0.2142824	-0.2603060
H	-2.8101815	-2.0103019	1.8272569
H	-5.4615384	-1.3714239	-2.3624968
H	-2.1210368	-3.1665160	-0.2768071
H	-3.4354970	-2.8599824	-2.3656271
C	-1.4203307	2.0965206	4.0165563
C	-1.1289348	0.9867006	3.5909562
C	-0.7870410	-0.3071707	3.0818371
C	-0.2803366	-0.4507788	1.7667803
C	-0.9526378	-1.4628391	3.8878257
C	0.0612358	-1.7147971	1.2746648
C	-0.6157091	-2.7266236	3.3819623
C	-0.1066973	-2.8557078	2.0761111
H	-1.6776969	3.0676911	4.3921741
H	-0.1560531	0.4324212	1.1410140
H	-1.3506096	-1.3561965	4.9002907
H	0.4638489	-1.8071737	0.2678251
H	-0.7528739	-3.6126822	4.0094711
H	0.1553923	-3.8422826	1.6819863
C	-2.2194098	0.7955102	-4.3677677
C	-2.2677490	1.3509856	-3.2783965
C	-2.3112558	1.9793639	-1.9927984
C	-2.4977282	1.1976634	-0.8244610
C	-2.1696718	3.3849774	-1.8716307
C	-2.5600813	1.8148872	0.4319729
C	-2.2275455	3.9903356	-0.6090933
C	-2.4263735	3.2087645	0.5432710
H	-2.1846402	0.3027805	-5.3199381
H	-2.5927995	0.1155611	-0.9137650
H	-2.0056024	3.9851908	-2.7699739
H	-2.7139858	1.2090278	1.3259272
H	-2.1070786	5.0746633	-0.5247127
H	-2.4603184	3.6792651	1.5301584
C	-1.2850326	-4.9946348	-2.5382157
C	-0.5615217	-4.0158620	-2.4055740
C	0.2664527	-2.8632394	-2.2144498
C	-0.2665265	-1.5613226	-2.3924578
C	1.6239424	-3.0072591	-1.8256806
C	0.5410659	-0.4361818	-2.1823094
C	2.4198922	-1.8732701	-1.6096230
C	1.8805657	-0.5864490	-1.7867793
H	-1.9134811	-5.8534097	-2.6740356

H	-1.3098278	-1.4356558	-2.6877733
H	2.0365758	-4.0104416	-1.6874697
H	0.1257210	0.5603928	-2.3352966
H	3.4571481	-1.9907305	-1.2882866
H	2.4987837	0.2960275	-1.6093573
C	1.2624588	2.7909124	-3.6695325
C	1.5227740	3.0295197	-2.4982792
C	1.7945459	3.2895244	-1.1175742
C	0.9371213	2.7651783	-0.1186470
C	2.9060172	4.0801498	-0.7281938
C	1.1852668	3.0275000	1.2346517
C	3.1485064	4.3342733	0.6292481
C	2.2908960	3.8085798	1.6138545
H	1.0185364	2.5604024	-4.6880233
H	0.0728857	2.1715738	-0.4180235
H	3.5681261	4.4875981	-1.4972041
H	0.5084085	2.6287237	1.9958348
H	4.0106640	4.9425743	0.9201228
H	2.4866543	4.0050834	2.6725569
C	7.2997988	-2.7836451	-0.4952405
C	6.3854323	-2.1453972	0.0102358
C	5.3052585	-1.4014145	0.5851378
C	5.0718246	-0.0575847	0.1952295
C	4.4399497	-2.0046467	1.5340177
C	4.0012033	0.6607662	0.7451507
C	3.3702660	-1.2782323	2.0738515
C	3.1500741	0.0535947	1.6832715
H	8.1090787	-3.3385088	-0.9294685
H	5.7324598	0.4053487	-0.5432496
H	4.6148771	-3.0429936	1.8296336
H	3.8216446	1.6927581	0.4350472
H	2.6933267	-1.7552846	2.7879426
H	2.3086447	0.6133175	2.0966380

Hexamer-07 (H6)

C	6.0187572	-0.0325758	1.5355884
C	5.1957494	-0.9130358	1.3247453
C	4.2092382	-1.9170313	1.0638885
C	3.9175406	-2.9183430	2.0256850
C	3.4951722	-1.9074328	-0.1604902
C	2.9247613	-3.8749418	1.7681755
C	2.5071363	-2.8681266	-0.4074819
C	2.2133397	-3.8502963	0.5542237
H	6.7387082	0.7418745	1.7144126
H	4.4648832	-2.9258304	2.9722373
H	3.7140791	-1.1399592	-0.9033069
H	2.6963936	-4.6330033	2.5237167
H	1.9529200	-2.8458124	-1.3481335
H	1.4237991	-4.5814036	0.3582452
C	4.0040788	3.1379733	0.5988709

C	3.7115180	2.4110266	-0.3402202
C	3.3701051	1.5296088	-1.4146399
C	2.0383164	1.0686734	-1.5758767
C	4.3708020	1.0802660	-2.3139977
C	1.7204611	0.1783948	-2.6102589
C	4.0432712	0.1851393	-3.3417801
C	2.7193884	-0.2689610	-3.4922104
H	4.2448204	3.7697063	1.4311043
H	1.2676449	1.3944331	-0.8763971
H	5.3998497	1.4252744	-2.1835577
H	0.6934408	-0.1773708	-2.7159421
H	4.8253463	-0.1646177	-4.0227963
H	2.4692154	-0.9749597	-4.2902099
C	-1.1616820	-3.1761359	3.5099938
C	-0.7647506	-2.0663144	3.1793540
C	-0.2907960	-0.7766964	2.7764309
C	1.0016286	-0.6445513	2.2098771
C	-1.0994545	0.3782995	2.9302175
C	1.4709746	0.6123105	1.8078209
C	-0.6241171	1.6290586	2.5134172
C	0.6590961	1.7519761	1.9495334
H	-1.5071862	-4.1429390	3.8204444
H	1.6241531	-1.5309513	2.0867325
H	-2.1001414	0.2829200	3.3580460
H	2.4712686	0.7013067	1.3790562
H	-1.2646476	2.5090962	2.6089715
H	1.0157750	2.7269931	1.6063808
C	-0.1013820	-4.8717352	-2.1450222
C	-0.4921402	-3.7143699	-2.0648624
C	-0.9578806	-2.3639759	-1.9725289
C	-0.7704193	-1.6156551	-0.7840327
C	-1.6339694	-1.7679712	-3.0679305
C	-1.2644519	-0.3082458	-0.6893598
C	-2.1264768	-0.4607888	-2.9609401
C	-1.9511133	0.2687249	-1.7703525
H	0.2524726	-5.8817688	-2.2184095
H	-0.2495235	-2.0683352	0.0604727
H	-1.7752614	-2.3435397	-3.9867661
H	-1.1258342	0.2521583	0.2355660
H	-2.6581847	-0.0121667	-3.8055472
H	-2.3621869	1.2758653	-1.6759098
C	-3.7365558	2.8655639	0.0675470
C	-2.6406238	3.4102843	0.0752579
C	-1.3496516	4.0271773	0.0889267
C	-1.0065667	4.9513450	1.1070335
C	-0.3887217	3.7104684	-0.9045510
C	0.2670493	5.5373532	1.1300978
C	0.8798485	4.3026571	-0.8743925
C	1.2133583	5.2154777	0.1411029
H	-4.6966573	2.3831243	0.0133698

H	-1.7447775	5.1955351	1.8760123
H	-0.6396434	2.9893134	-1.6862523
H	0.5210418	6.2463953	1.9245156
H	1.6209688	4.0317632	-1.6304228
H	2.2133934	5.6576996	0.1677218
C	-7.0171319	1.2991374	-0.8192718
C	-6.2549806	0.4060177	-0.4699611
C	-5.3387346	-0.6129704	-0.0551986
C	-4.9403881	-1.6328395	-0.9563534
C	-4.8131306	-0.6094657	1.2616314
C	-4.0416808	-2.6244704	-0.5445485
C	-3.9137774	-1.6059691	1.6618163
C	-3.5246065	-2.6123924	0.7620965
H	-7.7071348	2.0622177	-1.1240695
H	-5.3340677	-1.6281034	-1.9762433
H	-5.1138011	0.1806688	1.9554027
H	-3.7207256	-3.3931697	-1.2527519
H	-3.4985144	-1.5999329	2.6724765
H	-2.7969668	-3.3651513	1.0767617

Hexamer-08 (H8)

C	-6.3177964	1.1374075	-0.3451584
C	-5.5693394	0.2179106	-0.6488046
C	-4.6538099	-0.8308591	-0.9821778
C	-4.4330591	-1.2005676	-2.3325494
C	-3.9282596	-1.4876813	0.0426746
C	-3.5063387	-2.2050373	-2.6448746
C	-3.0063785	-2.4921405	-0.2801618
C	-2.7928374	-2.8553810	-1.6217223
H	-6.9917784	1.9285028	-0.0796385
H	-4.9795053	-0.6823320	-3.1250598
H	-4.0819605	-1.1900327	1.0811901
H	-3.3316111	-2.4720997	-3.6916244
H	-2.4373481	-2.9827282	0.5129090
H	-2.0594831	-3.6307184	-1.8606617
C	-3.1540760	3.7157801	1.8798179
C	-3.0449213	2.5385210	2.1959037
C	-2.9027889	1.1646699	2.5749020
C	-1.7692852	0.4166511	2.1674637
C	-3.8932759	0.5404790	3.3758885
C	-1.6206144	-0.9143319	2.5776295
C	-3.7388865	-0.7950163	3.7729101
C	-2.5991050	-1.5228497	3.3824225
H	-3.2454460	4.7482366	1.6040736
H	-1.0146812	0.8796347	1.5296184
H	-4.7755563	1.1118904	3.6765353
H	-0.7415216	-1.4769390	2.2612493
H	-4.5104404	-1.2680906	4.3884649
H	-2.4807771	-2.5653161	3.6940749
C	0.6942175	-1.0231802	-3.7431842

C	0.0205125	-0.1048918	-3.2950291
C	-0.7658136	0.9629549	-2.7551668
C	-1.6511072	0.7236770	-1.6741186
C	-0.6710454	2.2704839	-3.2945899
C	-2.4191748	1.7690551	-1.1480953
C	-1.4478844	3.3095021	-2.7637527
C	-2.3219619	3.0619061	-1.6889277
H	1.2751762	-1.8355266	-4.1339369
H	-1.7347203	-0.2787174	-1.2553703
H	0.0231652	2.4602993	-4.1161549
H	-3.0987738	1.5759863	-0.3175279
H	-1.3635567	4.3159021	-3.1852858
H	-2.9217849	3.8732553	-1.2665272
C	-0.4621188	-5.4158870	-0.0669525
C	0.0706191	-4.3518538	0.2211551
C	0.6641213	-3.0957081	0.5665233
C	0.4676333	-1.9619591	-0.2607206
C	1.4447977	-2.9659079	1.7431706
C	1.0301481	-0.7298117	0.0895893
C	2.0023623	-1.7253057	2.0823227
C	1.7928564	-0.6033262	1.2616826
H	-0.9236719	-6.3509217	-0.3190246
H	-0.1152312	-2.0577149	-1.1768135
H	1.6038187	-3.8415279	2.3779849
H	0.8861533	0.1338558	-0.5602029
H	2.6062080	-1.6338564	2.9895413
H	2.2278940	0.3609636	1.5272532
C	2.8577357	2.2920815	-2.8965401
C	2.6112266	2.4823879	-1.7135311
C	2.3240240	2.6846749	-0.3258766
C	0.9849184	2.8596230	0.1071753
C	3.3699726	2.7020157	0.6314645
C	0.7038551	3.0526530	1.4662951
C	3.0762764	2.8877560	1.9895936
C	1.7459030	3.0643880	2.4115805
H	3.0628748	2.1139374	-3.9337290
H	0.1774615	2.8375308	-0.6264970
H	4.4035182	2.5518987	0.3125469
H	-0.3325073	3.1939184	1.7860832
H	3.8916191	2.8841227	2.7194196
H	1.5197666	3.2043117	3.4733024
C	6.9175249	1.2619834	1.4287320
C	6.2539902	0.4119413	0.8483408
C	5.4437657	-0.5596523	0.1770740
C	4.6949242	-0.1928045	-0.9686187
C	5.3621381	-1.8908946	0.6569790
C	3.8697163	-1.1290413	-1.6024642
C	4.5424052	-2.8237743	0.0067684
C	3.7913834	-2.4464642	-1.1197082
H	7.5292253	1.9933005	1.9206689

H	4.7442082	0.8302971	-1.3444368
H	5.9365746	-2.1772615	1.5425289
H	3.2589923	-0.8138737	-2.4530571
H	4.4727058	-3.8450929	0.3933410
H	3.1248134	-3.1691968	-1.5987646

Hexamer-09 (H9)

C	1.8947846	-0.2749943	3.4601580
C	1.8323141	0.1884720	2.1225319
C	2.7921757	-1.3214908	3.7872920
C	2.6406422	-0.3876099	1.1351324
C	3.5956488	-1.8932109	2.7906417
C	3.5217942	-1.4327452	1.4641403
C	0.4423130	-2.9014341	0.4319180
C	-0.2061765	-1.8628676	-0.2844877
C	0.1797017	-3.0529616	1.8161865
C	-1.1046799	-1.0109750	0.3691270
C	-0.7179706	-2.1922819	2.4613803
C	-1.3672300	-1.1772294	1.7395208
C	1.3612673	-3.7798168	-0.2238136
C	2.1526390	-4.5313883	-0.7772997
C	1.0359557	0.2933902	4.4549212
C	0.2732014	0.7713167	5.2851582
H	1.1270763	0.9842552	1.8798475
H	2.8432852	-1.6809644	4.8190015
H	2.5767445	-0.0390126	0.1014889
H	4.2787446	-2.7088657	3.0487597
H	0.0031778	-1.7327427	-1.3486718
H	0.6958257	-3.8393377	2.3723732
H	-1.6152559	-0.2247388	-0.1893141
H	-0.9014563	-2.3064688	3.5335782
H	-2.0902838	-0.5232090	2.2296278
H	2.8785153	-5.1479907	-1.2696738
H	-0.3747496	1.2090502	6.0194896
H	4.1347772	-1.8965493	0.6881838
C	4.3885640	-1.3855044	-2.1046048
C	3.0067540	-1.4050071	-2.4233873
C	5.0918404	-0.1549873	-2.1508731
C	2.3528449	-0.2204389	-2.7878991
C	4.4261860	1.0226275	-2.5178064
C	3.0586880	0.9941626	-2.8410370
C	5.0724853	-2.5870658	-1.7299482
C	5.6720003	-3.5996518	-1.3926344
H	2.4601431	-2.3475557	-2.3592814
H	6.1554567	-0.1379283	-1.8968805
H	1.2834072	-0.2355642	-3.0184947
H	4.9748470	1.9694540	-2.5460146
H	6.2000492	-4.4883374	-1.1058517
H	2.5398418	1.9169480	-3.1099310
C	-2.0486268	0.9232414	-2.6979490

C	-1.1089158	1.6200416	-2.3399235
C	-0.0123599	2.4303790	-1.9051053
C	0.3591425	3.5926849	-2.6260465
C	0.7164191	2.0757696	-0.7444689
C	1.4376831	4.3758193	-2.1897820
C	1.7919003	2.8618977	-0.3187205
C	2.1578147	4.0122576	-1.0374675
H	-2.8909698	0.3241225	-2.9950475
H	-0.2022595	3.8684213	-3.5228525
H	0.4232485	1.1809667	-0.1955211
H	1.7189716	5.2707928	-2.7538880
H	2.3494356	2.5737164	0.5749311
H	3.0001282	4.6248177	-0.7016973
C	-4.0965390	0.9302850	0.7278062
C	-3.2113550	1.7324535	0.9921456
C	-2.1647389	2.6652836	1.2830512
C	-1.2554643	2.4316301	2.3458675
C	-2.0189700	3.8391475	0.5008413
C	-0.2370765	3.3540004	2.6212047
C	-1.0003510	4.7567265	0.7860502
C	-0.1081359	4.5198403	1.8464052
H	-4.8410869	0.1970404	0.4802275
H	-1.3387282	1.5259691	2.9497134
H	-2.7035444	4.0094901	-0.3339683
H	0.4605510	3.1468776	3.4380834
H	-0.8902420	5.6507661	0.1650648
H	0.6946777	5.2335246	2.0555709
C	-4.8674899	-0.8867298	-4.2536314
C	-4.9669086	-1.2664401	-3.0939793
C	-5.0768685	-1.7034183	-1.7347755
C	-6.3044721	-1.5689963	-1.0357812
C	-3.9615240	-2.2708000	-1.0698155
C	-6.4078351	-2.0023705	0.2937293
C	-4.0753027	-2.7022114	0.2587063
C	-5.2960694	-2.5722492	0.9432845
H	-4.7841393	-0.5638488	-5.2735824
H	-7.1639107	-1.1241249	-1.5446098
H	-3.0075286	-2.3600360	-1.5944077
H	-7.3581363	-1.8921827	0.8254935
H	-3.2002803	-3.1198106	0.7631256
H	-5.3801327	-2.9039743	1.9827635

Hexamer-10 (H10)

C	-2.8825229	-0.2713914	-2.6202086
C	-3.5865132	-1.4870810	-2.5798828
C	-2.9663277	0.6259730	-1.5424731
H	-3.5043632	-2.1982451	-3.4072344
H	-2.4053561	1.5628536	-1.5624087
C	-4.3736780	-1.8096373	-1.4673528
C	-3.7578623	0.3186200	-0.4286387

H	-4.9081964	-2.7623069	-1.4224500
H	-3.8245955	1.0150252	0.4094188
C	-4.4691137	-0.9069326	-0.3786885
H	-2.2407522	-0.0371614	-3.4740711
C	-5.2624829	-1.2354579	0.7673619
C	-5.9077846	-1.5206929	1.7692224
H	-6.5147231	-1.7583893	2.6213957
C	-0.3437783	-1.9654011	-1.3667522
C	-0.3080069	-3.0475939	-2.2804397
C	-1.0351868	-2.1165658	-0.1419908
H	0.2397402	-2.9341638	-3.2190330
H	-1.0773223	-1.2898676	0.5662971
C	-0.9617947	-4.2479113	-1.9740124
C	-1.6871009	-3.3187370	0.1538244
H	-0.9292912	-5.0791771	-2.6856658
H	-2.2261904	-3.4154419	1.1003224
C	-1.6567852	-4.3867180	-0.7588109
H	-2.1706640	-5.3245559	-0.5249756
C	0.2903083	-0.7260460	-1.6952143
C	0.7969853	0.3455582	-1.9968824
H	1.2409417	1.2836191	-2.2694680
C	1.2918229	-3.5225569	2.4698564
C	1.8893900	-2.2903760	2.1548675
C	1.2859860	-4.5607230	1.5207853
H	1.8815379	-1.4712320	2.8781731
H	0.8042218	-5.5155074	1.7537380
C	2.4784257	-2.0936732	0.8996698
C	1.8823300	-4.3770518	0.2670218
H	2.9172938	-1.1289633	0.6458166
H	1.8689551	-5.1770195	-0.4773595
C	2.4896511	-3.1384169	-0.0565104
H	0.8187103	-3.6690575	3.4460066
C	3.0922038	-2.9405821	-1.3400062
C	3.6056606	-2.7713049	-2.4383545
H	4.0524652	-2.6243314	-3.4022118
C	-2.5292210	-0.2550603	2.7468395
C	-1.3765397	0.1479070	2.8224967
C	-0.0214288	0.6054897	2.8593388
C	0.6751985	0.8459821	1.6486733
C	0.6467347	0.8100350	4.0929036
C	2.0058136	1.2794294	1.6735339
C	1.9820056	1.2379214	4.1071087
C	2.6651295	1.4736682	2.8994769
H	-3.5428019	-0.5967774	2.6364372
H	0.1711760	0.6817821	0.6954684
H	0.1113319	0.6240418	5.0279375
H	2.5364208	1.4514658	0.7345997
H	2.4912436	1.3877076	5.0645499
H	3.7073280	1.8039088	2.9099717
C	-4.6961174	3.4676857	2.0588991

C	-3.8061488	3.6096624	1.2313133
C	-2.7672225	3.7316132	0.2537667
C	-1.4571491	3.2729041	0.5424517
C	-3.0399791	4.2879232	-1.0215728
C	-0.4477052	3.3727127	-0.4242286
C	-2.0227612	4.3810670	-1.9818753
C	-0.7248974	3.9254350	-1.6866888
H	-5.4724268	3.3545513	2.7906503
H	-1.2495444	2.8257150	1.5167199
H	-4.0527893	4.6312479	-1.2491467
H	0.5564412	3.0083246	-0.1935997
H	-2.2465257	4.8057728	-2.9656860
H	0.0702041	3.9924358	-2.4348033
C	2.5915160	3.3850197	-3.4149703
C	3.2513919	2.8487118	-2.5341160
C	4.0036057	2.2000977	-1.5029712
C	4.5792954	2.9575021	-0.4507312
C	4.1782679	0.7926167	-1.5212184
C	5.3176387	2.3163051	0.5531336
C	4.9240099	0.1638918	-0.5151583
C	5.4937035	0.9209305	0.5235279
H	2.0513936	3.8604395	-4.2106303
H	4.4377211	4.0415283	-0.4312927
H	3.7146910	0.1966111	-2.3102586
H	5.7542820	2.9081448	1.3635466
H	5.0447187	-0.9221833	-0.5442851
H	6.0661739	0.4238132	1.3126304

Hexamer-11 (H11)

C	-0.2643635	5.2422612	-0.6855339
C	-0.8770975	4.2209955	-0.4033461
C	-1.5747206	3.0161658	-0.0688287
C	-2.6711368	2.5707281	-0.8521154
C	-1.1665712	2.2442146	1.0476320
C	-3.3335683	1.3790592	-0.5261099
C	-1.8331733	1.0522103	1.3611250
C	-2.9147820	0.6137680	0.5777305
H	0.2802383	6.1329921	-0.9303172
H	-2.9846992	3.1621562	-1.7169693
H	-0.3226405	2.5807282	1.6517785
H	-4.1708639	1.0408153	-1.1404169
H	-1.5033160	0.4571694	2.2155631
H	-3.4168392	-0.3269086	0.8175569
C	3.3882869	3.7085451	-1.0285520
C	2.9540632	3.2475919	0.0180969
C	2.4579915	2.7052319	1.2463778
C	2.2196840	1.3136504	1.3820537
C	2.1913362	3.5628484	2.3440725
C	1.7347555	0.7965374	2.5908160
C	1.7029598	3.0357904	3.5474009

C	1.4754584	1.6527075	3.6748204
H	3.7441453	4.1051016	-1.9592141
H	2.3984746	0.6539372	0.5322695
H	2.3602327	4.6373514	2.2346914
H	1.5466893	-0.2745093	2.6825875
H	1.4958773	3.7065068	4.3871577
H	1.0881435	1.2445935	4.6134905
C	-2.5049508	-2.4541438	-1.7606943
C	-1.4419707	-1.9007158	-2.0092575
C	-0.1846355	-1.2451823	-2.2077026
C	-0.0121404	0.0937173	-1.7751440
C	0.9140102	-1.9342808	-2.7822964
C	1.2319601	0.7231053	-1.9109291
C	2.1573507	-1.2985788	-2.9004858
C	2.3228229	0.0279787	-2.4622375
H	-3.4341518	-2.9165684	-1.4897978
H	-0.8512595	0.6207667	-1.3207345
H	0.7857922	-2.9709196	-3.1061209
H	1.3566494	1.7535915	-1.5700561
H	3.0090408	-1.8473699	-3.3112005
H	3.3037427	0.5064313	-2.5310720
C	-2.8866517	-1.9086220	3.3052834
C	-1.7238945	-2.1126825	2.9826615
C	-0.3661563	-2.3429593	2.5895865
C	0.0380318	-2.1137009	1.2491897
C	0.5866997	-2.8054019	3.5330469
C	1.3629023	-2.3608306	0.8613925
C	1.9082885	-3.0498096	3.1342876
C	2.2970657	-2.8372191	1.7984243
H	-3.9108248	-1.7240254	3.5633330
H	-0.6919548	-1.7472939	0.5260675
H	0.2766535	-2.9731987	4.5683517
H	1.6640210	-2.1875112	-0.1745835
H	2.6363206	-3.4135937	3.8663016
H	3.3213237	-3.0512766	1.4826935
C	4.2700131	-4.1163874	-0.9926615
C	4.6632184	-2.9597932	-1.0631936
C	5.1055650	-1.6022779	-1.1625167
C	5.7944255	-1.1593405	-2.3192838
C	4.8404282	-0.6779848	-0.1209754
C	6.2059835	0.1767535	-2.4263719
C	5.2570528	0.6536666	-0.2366416
C	5.9396633	1.0857483	-1.3867652
H	3.9267059	-5.1298930	-0.9146598
H	5.9932952	-1.8689824	-3.1274007
H	4.2906765	-1.0069689	0.7636736
H	6.7352819	0.5097738	-3.3249325
H	5.0274220	1.3645486	0.5604560
H	6.2503403	2.1310977	-1.4746315
C	-4.9861066	-3.0567204	0.8323344

C	-5.4823216	-2.1279552	0.2083376
C	-6.0204016	-1.0141175	-0.5116174
C	-6.5995605	0.0745194	0.1878956
C	-5.9555471	-0.9684587	-1.9273322
C	-7.0983892	1.1795945	-0.5140290
C	-6.4573560	0.1419561	-2.6203855
C	-7.0297684	1.2179272	-1.9181802
H	-4.5278169	-3.8551612	1.3834415
H	-6.6392051	0.0469171	1.2801870
H	-5.4987310	-1.7984217	-2.4722342
H	-7.5362833	2.0183971	0.0359707
H	-6.3980469	0.1702240	-3.7128539
H	-7.4167513	2.0850622	-2.4626574

Hexamer-12 (H12)

C	-1.3533476	-0.7961901	-3.3626021
C	-1.5528000	-0.0594081	-2.1688724
C	-2.2437304	-1.8524809	-3.6786160
C	-2.6128236	-0.3766973	-1.3096324
C	-3.3004060	-2.1628444	-2.8124860
C	-3.4879209	-1.4299535	-1.6272654
C	-0.6104247	-2.8522731	-0.0256042
C	-0.0225098	-1.7953607	0.7158594
C	-0.0436350	-3.2162486	-1.2720819
C	1.1046078	-1.1298713	0.2201476
C	1.0809498	-2.5379373	-1.7621388
C	1.6584098	-1.4955492	-1.0187236
C	-1.7713174	-3.5265443	0.4686075
C	-2.7674886	-4.0985718	0.8903937
C	-0.2520023	-0.4963666	-4.2265393
C	0.7016016	-0.2544075	-4.9553101
H	-0.8590120	0.7455331	-1.9245904
H	-2.0889066	-2.4245570	-4.5977943
H	-2.7520198	0.1833417	-0.3812305
H	-3.9763615	-2.9880590	-3.0581310
H	-0.4622472	-1.4968586	1.6704919
H	-0.5042270	-4.0191259	-1.8526696
H	1.5571774	-0.3249541	0.8009397
H	1.4960509	-2.8123200	-2.7356340
H	2.5452090	-0.9738434	-1.3866707
H	-3.6877641	-4.5245349	1.2393963
H	1.5295185	-0.0237939	-5.5972385
H	-4.2996650	-1.6923342	-0.9463651
C	-4.9647913	-0.9305212	1.6152818
C	-3.7184078	-0.9607195	2.2903635
C	-5.4819762	0.3140303	1.1747074
C	-3.0212375	0.2300769	2.5336401
C	-4.7749176	1.4986876	1.4231021
C	-3.5482302	1.4628726	2.1085089
C	-5.6962482	-2.1372233	1.3696387

C	-6.3329027	-3.1586324	1.1452119
H	-3.3030874	-1.9220547	2.5999606
H	-6.4357924	0.3369474	0.6401990
H	-2.0550979	0.2000281	3.0451174
H	-5.1814145	2.4538570	1.0759366
H	-6.9029939	-4.0490086	0.9625605
H	-2.9946810	2.3867287	2.2926401
C	1.0439170	0.4253873	3.5308713
C	0.5240227	1.2843246	2.8316004
C	-0.1341424	2.2829672	2.0454232
C	-0.3808699	3.5677688	2.5923682
C	-0.5767712	1.9963424	0.7308526
C	-1.0615497	4.5352704	1.8397652
C	-1.2546284	2.9694598	-0.0113700
C	-1.5002746	4.2384810	0.5364103
H	1.5452143	-0.3158509	4.1201722
H	-0.0418700	3.7905829	3.6077015
H	-0.3952152	1.0081116	0.3099408
H	-1.2510565	5.5223544	2.2732322
H	-1.5862029	2.7417143	-1.0258632
H	-2.0262909	4.9968710	-0.0510095
C	3.7311194	1.2514034	0.4555693
C	3.0083880	1.9158925	-0.2740617
C	2.1638329	2.6945340	-1.1282299
C	1.4878968	2.0891344	-2.2176639
C	1.9885676	4.0815455	-0.8948070
C	0.6625597	2.8554925	-3.0516064
C	1.1612917	4.8392733	-1.7340056
C	0.4972634	4.2317500	-2.8151392
H	4.3432923	0.6434220	1.0941508
H	1.6026743	1.0187439	-2.4014972
H	2.4964751	4.5483598	-0.0467629
H	0.1471466	2.3654738	-3.8824848
H	1.0282979	5.9082089	-1.5388445
H	-0.1482534	4.8280185	-3.4681739
C	6.2695720	-2.7727801	-1.6684959
C	5.8949674	-2.4180382	-0.5589063
C	5.4423928	-1.9938947	0.7315123
C	4.1441078	-2.3394172	1.1817882
C	6.2766199	-1.2082542	1.5681155
C	3.6889215	-1.8978838	2.4312769
C	5.8142434	-0.7768332	2.8198239
C	4.5190358	-1.1173149	3.2545377
H	6.6039929	-3.0916050	-2.6369252
H	3.4915390	-2.9296405	0.5355528
H	7.2775731	-0.9364525	1.2221339
H	2.6733120	-2.1535276	2.7459873
H	6.4634792	-0.1659898	3.4547456
H	4.1613051	-0.7641805	4.2266745

Hexamer-13 (H13)

C	-0.6987361	-0.7280262	-2.4710121
C	-0.4116205	-2.0912886	-2.2731481
C	-1.1666702	0.0529806	-1.3999258
H	-0.0336170	-2.6988865	-3.1000396
H	-1.3978885	1.1096149	-1.5458050
C	-0.5828098	-2.6734785	-1.0108651
C	-1.3425034	-0.5211116	-0.1350694
H	-0.3330107	-3.7232842	-0.8458474
H	-1.7108162	0.0765761	0.6959507
C	-1.0460578	-1.8889530	0.0737158
H	-0.5477104	-0.2758189	-3.4557627
C	-1.2215258	-2.4694522	1.3703397
C	-1.3830057	-2.9516713	2.4842013
H	-1.5525649	-3.3928132	3.4471747
C	2.8678727	-1.6555608	-1.3164283
C	2.9568521	-3.0075726	-1.7340905
C	2.5584009	-1.3695411	0.0341475
H	3.2034442	-3.2291438	-2.7759965
H	2.5149890	-0.3372378	0.3776687
C	2.7316856	-4.0436092	-0.8190080
C	2.3246994	-2.4116717	0.9383551
H	2.8062582	-5.0844539	-1.1500908
H	2.0690725	-2.1713482	1.9732851
C	2.4088080	-3.7494252	0.5191043
H	2.2201865	-4.5611442	1.2283659
C	3.0871502	-0.6007502	-2.2584888
C	3.2575952	0.2841068	-3.0865101
H	3.4483521	1.0582905	-3.8030382
C	4.3070824	1.1007216	2.2059799
C	4.5982304	1.5350282	0.9008463
C	4.7743009	-0.1494726	2.6486452
H	4.2216345	2.4992433	0.5504075
H	4.5449342	-0.4929716	3.6624403
C	5.3428400	0.7222805	0.0361349
C	5.5230727	-0.9676878	1.7924166
H	5.5441095	1.0397134	-0.9894678
H	5.8761941	-1.9472251	2.1258789
C	5.8113102	-0.5426156	0.4715684
H	3.6987914	1.7250712	2.8659805
C	6.5479408	-1.3892681	-0.4170347
C	7.1704949	-2.1184603	-1.1777076
H	7.7236565	-2.7538296	-1.8417690
C	0.3962964	0.4144094	2.5392017
C	0.8154871	1.3220567	1.8354997
C	1.3147096	2.3590081	0.9874652
C	1.4810685	2.1253042	-0.3996738
C	1.6547585	3.6272701	1.5203970
C	1.9858683	3.1352215	-1.2273046
C	2.1564004	4.6333743	0.6829559

C	2.3267944	4.3906563	-0.6937612
H	-0.0304944	-0.4118680	3.0754344
H	1.2159137	1.1561528	-0.8213596
H	1.5243037	3.8097306	2.5905168
H	2.1192528	2.9332401	-2.2934444
H	2.4178427	5.6086178	1.1048089
H	2.7233345	5.1773577	-1.3428901
C	-4.2570720	0.8008893	2.3630711
C	-3.8167670	1.5189016	1.4762900
C	-3.2837763	2.3065171	0.4075647
C	-2.0773217	3.0302106	0.5781502
C	-3.9356361	2.3339315	-0.8514957
C	-1.5362242	3.7647611	-0.4854508
C	-3.3919404	3.0793531	-1.9066246
C	-2.1927745	3.7953873	-1.7291625
H	-4.6813469	0.1356471	3.0907227
H	-1.5606525	2.9852008	1.5393713
H	-4.8476004	1.7481982	-0.9920345
H	-0.5916037	4.2970617	-0.3460129
H	-3.8991782	3.0916112	-2.8768295
H	-1.7664624	4.3668440	-2.5598539
C	-6.4784570	-2.1817938	3.0804504
C	-6.2204035	-1.9176996	1.9128270
C	-5.9039513	-1.5864224	0.5559153
C	-4.6378697	-1.9204050	0.0139926
C	-6.8481112	-0.9084198	-0.2557477
C	-4.3289730	-1.5897900	-1.3120056
C	-6.5291983	-0.5806104	-1.5808739
C	-5.2718831	-0.9220714	-2.1130174
H	-6.7228572	-2.4394182	4.0929111
H	-3.8990812	-2.4204193	0.6443531
H	-7.8224073	-0.6428756	0.1640893
H	-3.3447409	-1.8424846	-1.7142286
H	-7.2648857	-0.0560899	-2.1995770
H	-5.0239880	-0.6589709	-3.1464157

Hexamer-14 (H14)

C	3.2727912	2.3468754	-2.0446729
C	3.2357769	3.5399309	-1.3014327
C	3.5505443	1.1298188	-1.3994228
H	3.0032032	4.4872803	-1.7962061
H	3.5778133	0.1966285	-1.9688563
C	3.4674891	3.5190423	0.0792238
C	3.7842655	1.0955952	-0.0183146
H	3.4110650	4.4398048	0.6648665
H	3.9813051	0.1511341	0.4898028
C	3.7384727	2.2929433	0.7369164
H	3.0625055	2.3646042	-3.1176765
C	3.9281104	2.2621194	2.1559456
C	4.0470222	2.2323922	3.3748174

H	4.1982291	2.2274959	4.4368576
C	-0.0739434	2.7948605	-1.0867159
C	-0.3395673	4.1859021	-1.0517194
C	0.2901097	2.1305177	0.1075798
H	-0.6376675	4.6969835	-1.9705780
H	0.4857726	1.0606985	0.0967488
C	-0.2340098	4.8909713	0.1543650
C	0.3951432	2.8426047	1.3059815
H	-0.4472793	5.9645027	0.1735610
H	0.6874707	2.3125476	2.2157138
C	0.1370246	4.2232453	1.3359741
H	0.2222864	4.7784422	2.2753821
C	-0.1741920	2.0712925	-2.3171196
C	-0.2548215	1.4604394	-3.3746377
H	-0.3456678	0.9260977	-4.2995554
C	-2.1736961	0.0301145	1.4633776
C	-2.3389530	-0.0537549	0.0716533
C	-2.5723695	1.1913597	2.1467169
H	-2.0387197	-0.9558929	-0.4606050
H	-2.4384666	1.2642966	3.2304540
C	-2.8978649	1.0126517	-0.6378116
C	-3.1331925	2.2672238	1.4448665
H	-3.0101086	0.9558089	-1.7217957
H	-3.4327021	3.1790536	1.9682596
C	-3.2998715	2.1899619	0.0400623
H	-1.7278959	-0.8046468	2.0086015
C	-3.8632700	3.2859939	-0.6877138
C	-4.3432097	4.2205631	-1.3165364
H	-4.7620233	5.0426636	-1.8635298
C	1.7933067	-0.5611661	2.1988753
C	1.2052389	-1.1791966	1.3233059
C	0.5195776	-1.8520097	0.2648789
C	0.7044515	-1.4324137	-1.0747571
C	-0.3666262	-2.9230259	0.5379543
C	0.0200218	-2.0750635	-2.1131577
C	-1.0472445	-3.5591933	-0.5073123
C	-0.8545640	-3.1408158	-1.8369617
H	2.3665293	0.0010854	2.9111212
H	1.3726018	-0.5979264	-1.2911106
H	-0.5383991	-3.2314122	1.5715403
H	0.1644682	-1.7337237	-3.1419122
H	-1.7482965	-4.3643779	-0.2734218
H	-1.3933211	-3.6355458	-2.6509672
C	5.4037651	-1.5698312	2.4607256
C	4.9103468	-2.1056875	1.4775679
C	4.3245035	-2.6855113	0.3079113
C	3.3319114	-3.6909541	0.4145908
C	4.7195867	-2.2406181	-0.9791704
C	2.7535255	-4.2366113	-0.7382217
C	4.1341273	-2.7925408	-2.1265816

C	3.1515055	-3.7919023	-2.0104923
H	5.8404474	-1.0976401	3.3190970
H	3.0076143	-4.0156410	1.4061711
H	5.4761425	-1.4560405	-1.0621828
H	1.9676546	-4.9910796	-0.6436344
H	4.4447811	-2.4392109	-3.1152855
H	2.6870375	-4.2127394	-2.9073366
C	-3.3201607	-4.2865321	2.3786849
C	-3.9024491	-3.4894913	1.6541472
C	-4.5639001	-2.5406789	0.8106666
C	-5.1917763	-1.4001415	1.3721876
C	-4.5837788	-2.7161015	-0.5952114
C	-5.8155653	-0.4585948	0.5450995
C	-5.2122671	-1.7689155	-1.4146722
C	-5.8267380	-0.6378008	-0.8490951
H	-2.8374402	-4.9985192	3.0197836
H	-5.1614646	-1.2534333	2.4546566
H	-4.0936967	-3.5897241	-1.0320425
H	-6.2725703	0.4315120	0.9871062
H	-5.2150879	-1.9092177	-2.5004339
H	-6.2981623	0.1109952	-1.4928043

Hexamer-15 (H15)

C	5.2012912	-1.5791032	-0.3013952
C	5.3411899	-0.7558575	-1.4319838
C	4.9860031	-1.0007165	0.9611760
H	5.4906128	-1.2034151	-2.4188233
H	4.8913320	-1.6381445	1.8449740
C	5.2695585	0.6368410	-1.3060117
C	4.9084348	0.3908604	1.0976662
H	5.3633702	1.2800049	-2.1843856
H	4.7533138	0.8457815	2.0790153
C	5.0508654	1.2263990	-0.0368408
H	5.2555359	-2.6664255	-0.4043597
C	4.9705943	2.6490861	0.0968595
C	4.8988819	3.8659313	0.2109717
H	4.8333251	4.9321577	0.3104838
C	2.0420425	-0.9649552	-2.2631604
C	2.1517066	-0.1566539	-3.4214220
C	1.8570953	-0.3455528	-1.0034422
H	2.2932599	-0.6341367	-4.3952562
H	1.7726513	-0.9679962	-0.1109057
C	2.0770831	1.2394051	-3.3148943
C	1.7838723	1.0478742	-0.9088118
H	2.1627500	1.8559154	-4.2156633
H	1.6422480	1.5179038	0.0672293
C	1.8934761	1.8458120	-2.0601718
H	1.8340235	2.9344147	-1.9779508
C	2.1170685	-2.3905717	-2.3648483
C	2.1811175	-3.6102746	-2.4531684

H	2.2371238	-4.6785975	-2.5316327
C	-1.4843578	-1.8088274	-1.0453720
C	-1.3705263	-1.0915908	-2.2487985
C	-1.6568768	-1.1173239	0.1659402
H	-1.2184800	-1.6257705	-3.1911636
H	-1.7637539	-1.6726023	1.1020837
C	-1.4304925	0.3075108	-2.2466481
C	-1.7140956	0.2818069	0.1796082
H	-1.3273434	0.8696799	-3.1779121
H	-1.8624499	0.8228169	1.1172027
C	-1.6023368	1.0107016	-1.0294604
H	-1.4385609	-2.9014234	-1.0518063
C	-1.6624921	2.4404698	-1.0209845
C	-1.7146374	3.6638472	-1.0131574
H	-1.7584106	4.7355710	-1.0056031
C	8.2576898	-0.8620101	1.9554882
C	8.4199488	-0.2061037	0.7097965
C	8.0649841	-0.0835765	3.1241873
H	8.5531947	-0.8049096	-0.1946392
H	7.9401815	-0.5877649	4.0869704
C	8.3818526	1.1918491	0.6386867
C	8.0296135	1.3154973	3.0419305
H	8.4876889	1.6872228	-0.3309641
H	7.8759933	1.9073602	3.9503996
C	8.1862382	1.9578840	1.8010819
H	8.1403378	3.0492405	1.7370752
C	8.2690301	-2.2922582	2.0293971
C	8.2586743	-3.5146337	2.0899280
H	8.2728867	-4.5863498	2.1466822
C	-5.0597090	-1.2829980	0.2162691
C	-4.9329358	-0.6370056	-1.0378390
C	-5.2365586	-0.4986650	1.3822242
H	-4.7781712	-1.2397877	-1.9359524
H	-5.3489357	-0.9963962	2.3486419
C	-4.9809122	0.7602329	-1.1176519
C	-5.2866406	0.8977568	1.2902386
H	-4.8626754	1.2511696	-2.0878838
H	-5.4413828	1.4947820	2.1936535
C	-5.1589168	1.5323590	0.0429036
H	-5.1962009	2.6230349	-0.0235954
C	-5.0095505	-2.7106150	0.3044050
C	-4.9666032	-3.9321018	0.3798342
H	-4.9269985	-5.0021113	0.4452421
H	-8.7340023	4.5939523	0.9731054
C	-8.7128607	3.5229975	1.0416868
C	-8.7136683	2.3014343	1.1160857
C	-8.6931799	0.8721913	1.2056386
C	-8.4993983	0.0828567	0.0449145
H	-8.3632139	0.5779371	-0.9197732
C	-8.4544029	-1.3133981	0.1409502

H	-8.2814547	-1.9126278	-0.7578007
C	-8.6055755	-1.9454665	1.3875712
H	-8.5548243	-3.0364074	1.4583423
C	-8.8044195	-1.1702654	2.5436972
H	-8.9230769	-1.6573346	3.5173886
C	-8.8490668	0.2283929	2.4588653
H	-8.9998518	0.8355864	3.3562443
