

SUPPORTING INFORMATION

Computationally guided circularly polarized luminescence simulations in chiral adaptive supramolecular systems

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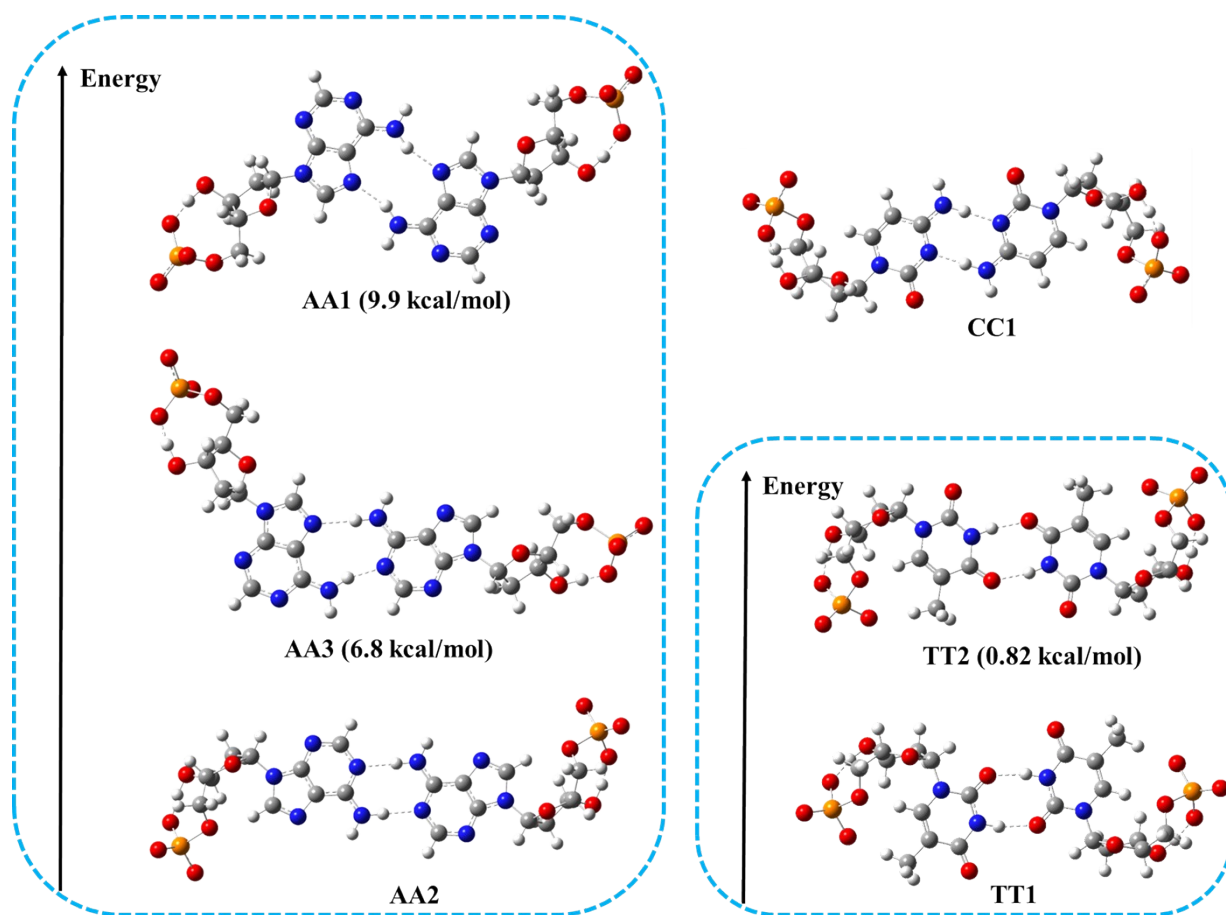


Fig. S1. DFT-optimized homo-dimers (ω B97XD/6-311G(d,p) level in gas phase), both inter- and intramolecular hydrogen bonds are illustrated with single dotted lines.

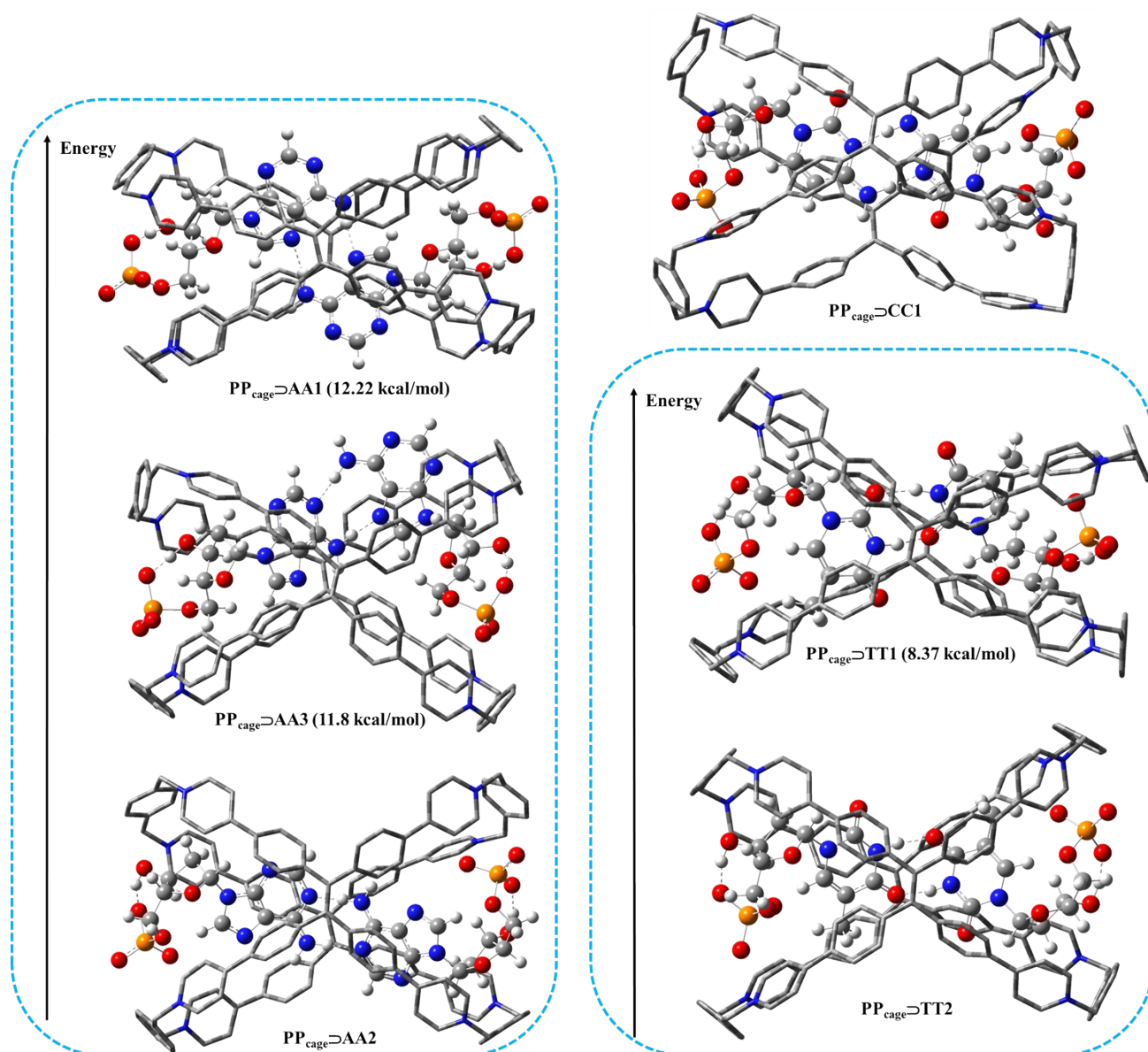


Fig. S2. DFT-optimized PP_{cage}→homo-dimers (ω B97XD/6-311G(d,p) level in gas phase), the hydrogen atoms of the cages were omitted for clarity.

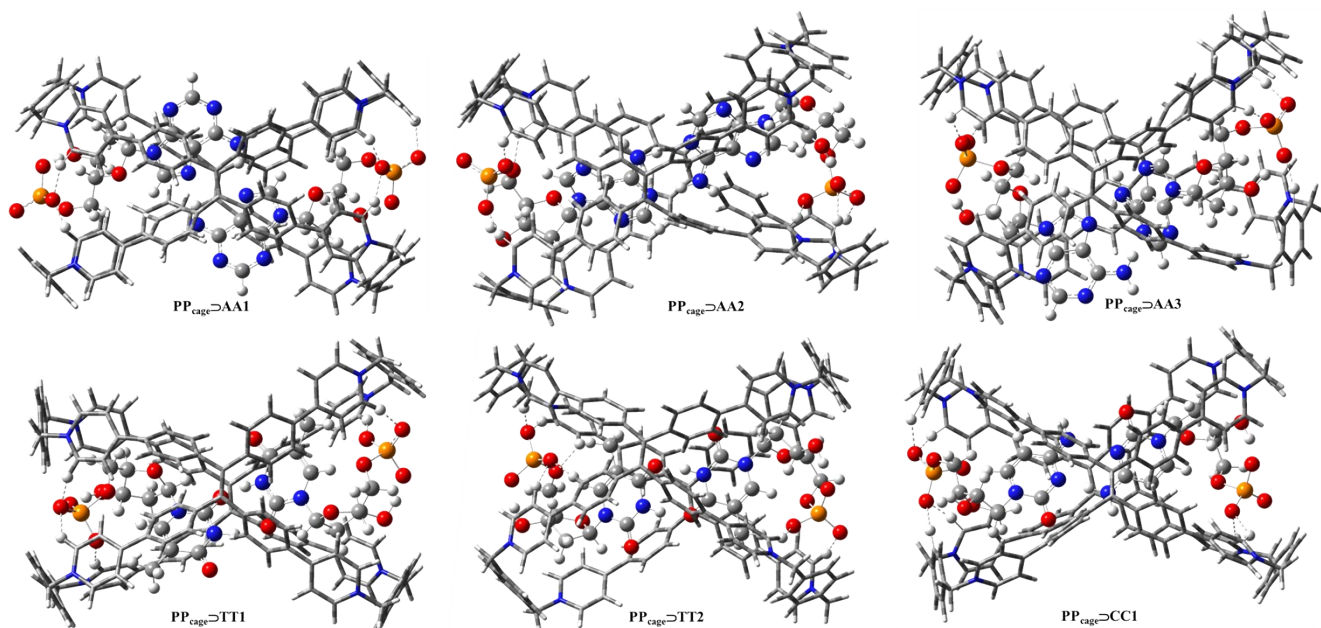


Fig. S3. DFT-optimized $PP_{cage} \rightarrow$ homo-dimers (ω B97XD/6-311G(d,p) level in gas phase), intermolecular hydrogen bonds between monophosphate and phenyl/pyridinium rings are illustrated with single dotted lines.

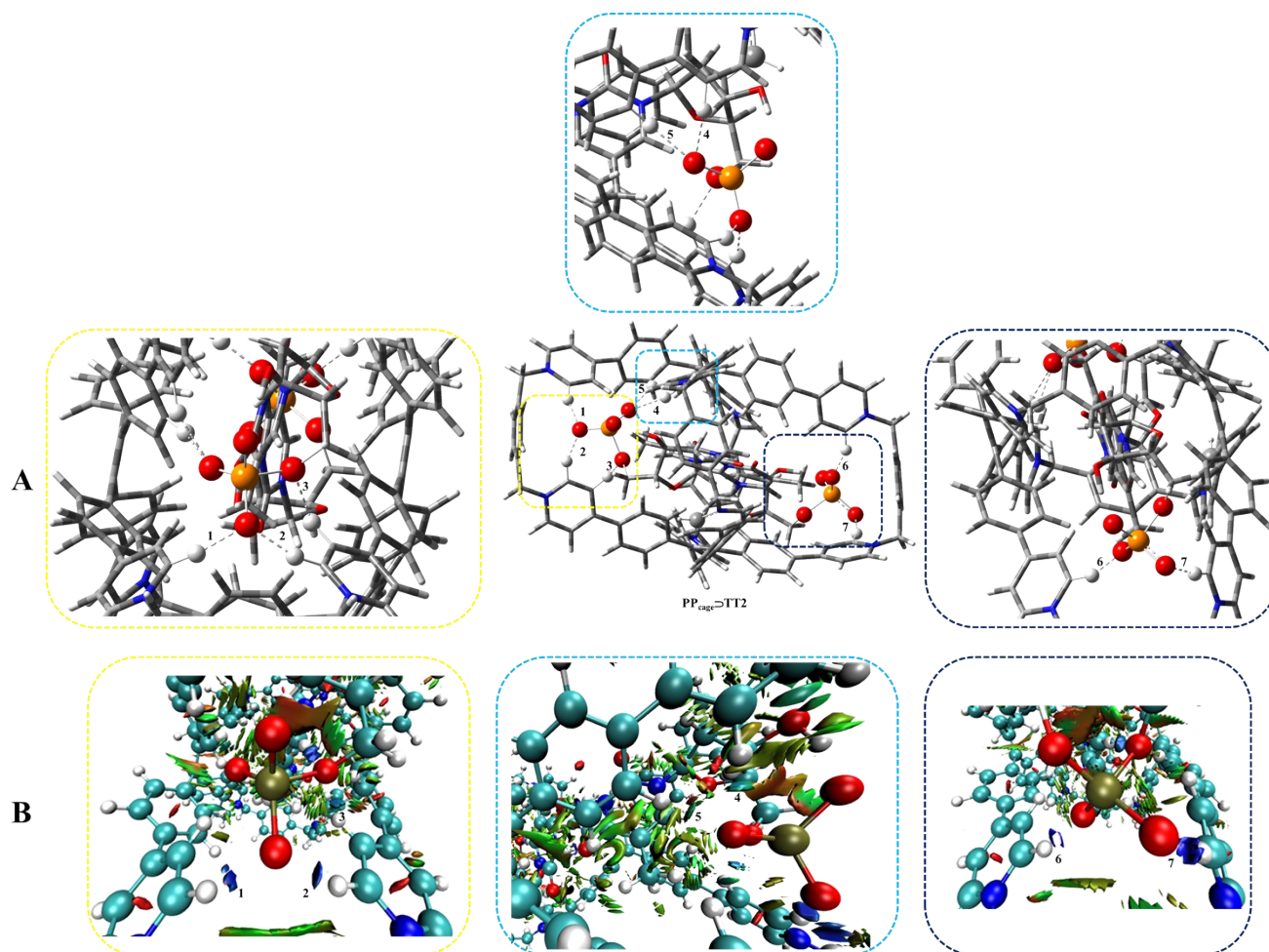


Fig. S4. (A) Partitioning of the multiple hydrogen bonds between monophosphate and phenyl/pyridinium rings in $PP_{cage} \rightarrow TT2$ complex. (B) NCI mapped surfaces related to part A.

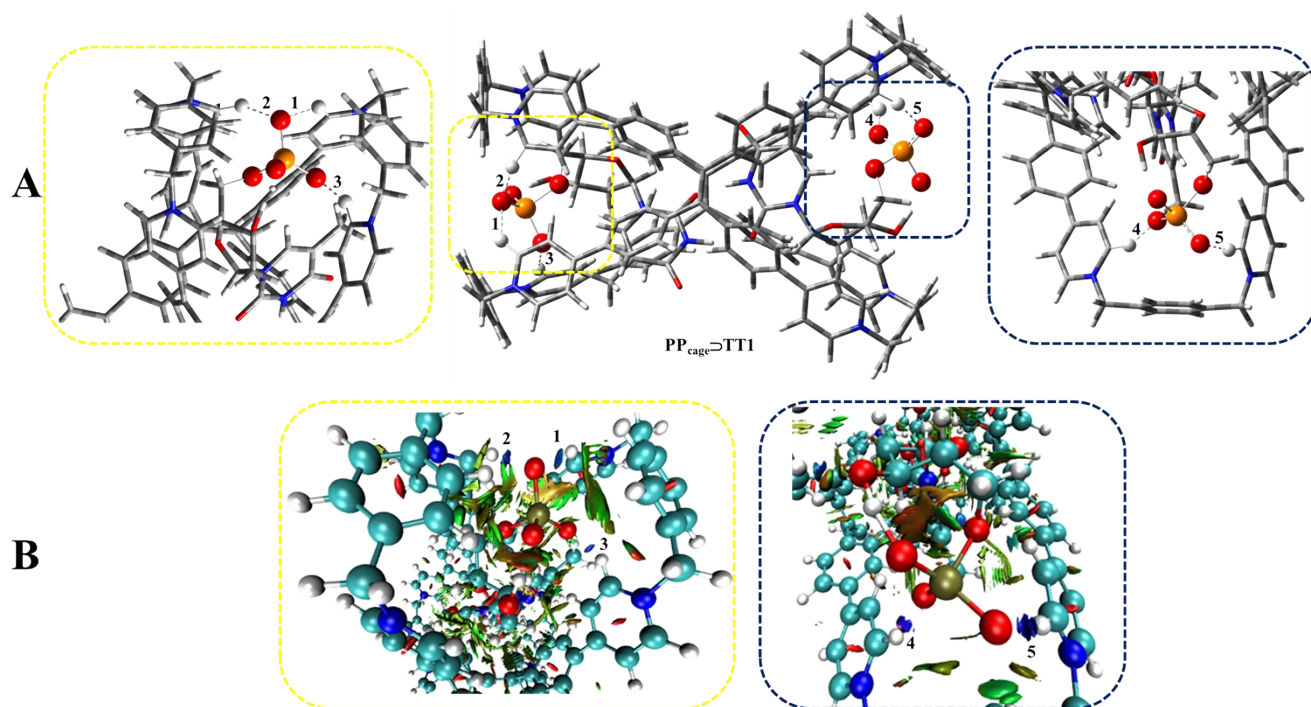


Fig. S5. (A) Partitioning of the multiple hydrogen bonds between monophosphate and phenyl/pyridinium rings in PP_{cage⇌TT1} complex. (B) NCI mapped surfaces related to part A.

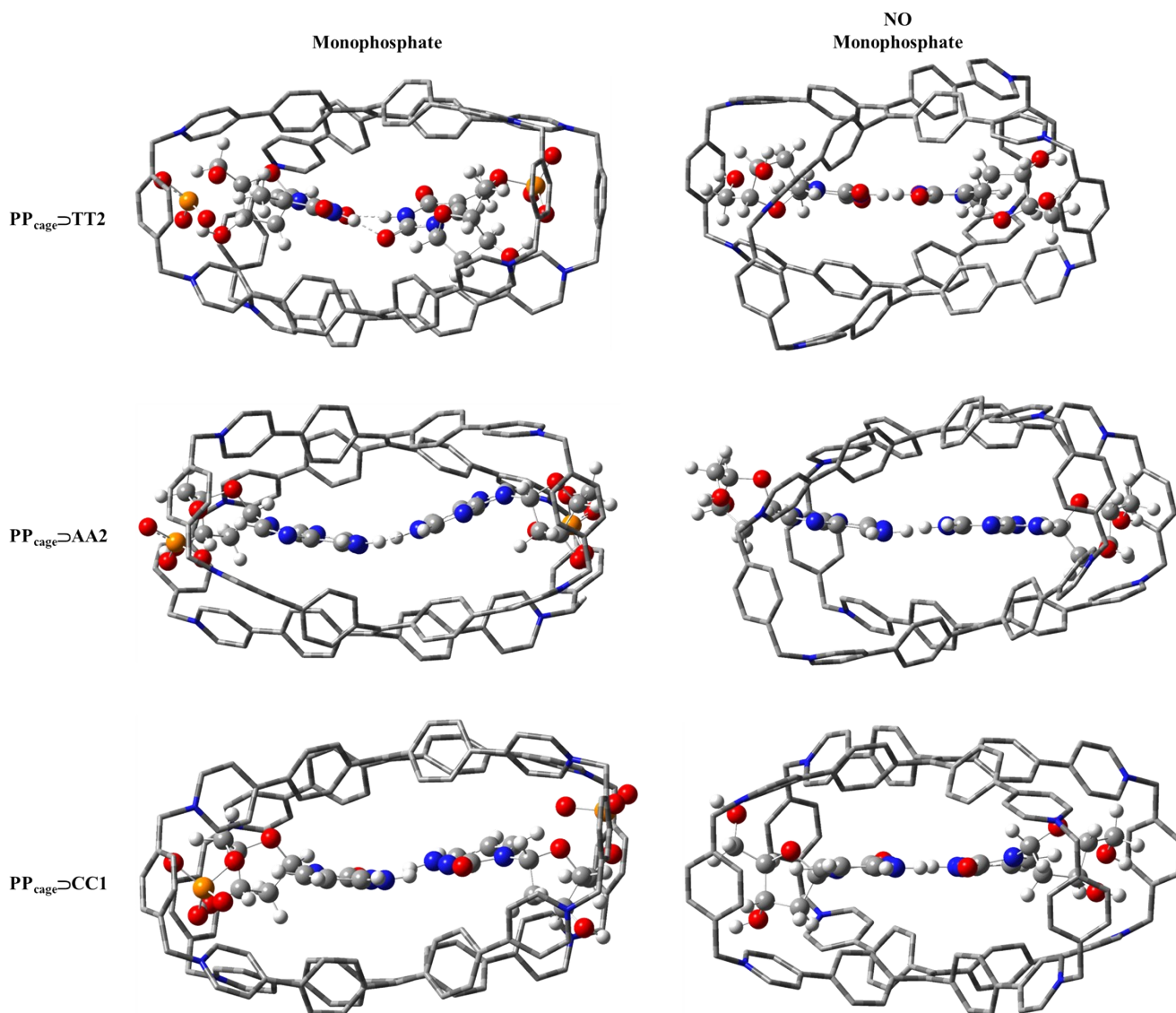


Fig. S6. DFT-optimization (ω B97XD/6-311G(d,p) level in gas phase) comparisons of PP_{cage}→AA2, PP_{cage}→TT2 and PP_{cage}→CC1 with and without the PO₄²⁻. The monophosphate groups were substituted with CH₂-OH fragments in position 3. The hydrogen atoms of the cages were omitted for clarity.

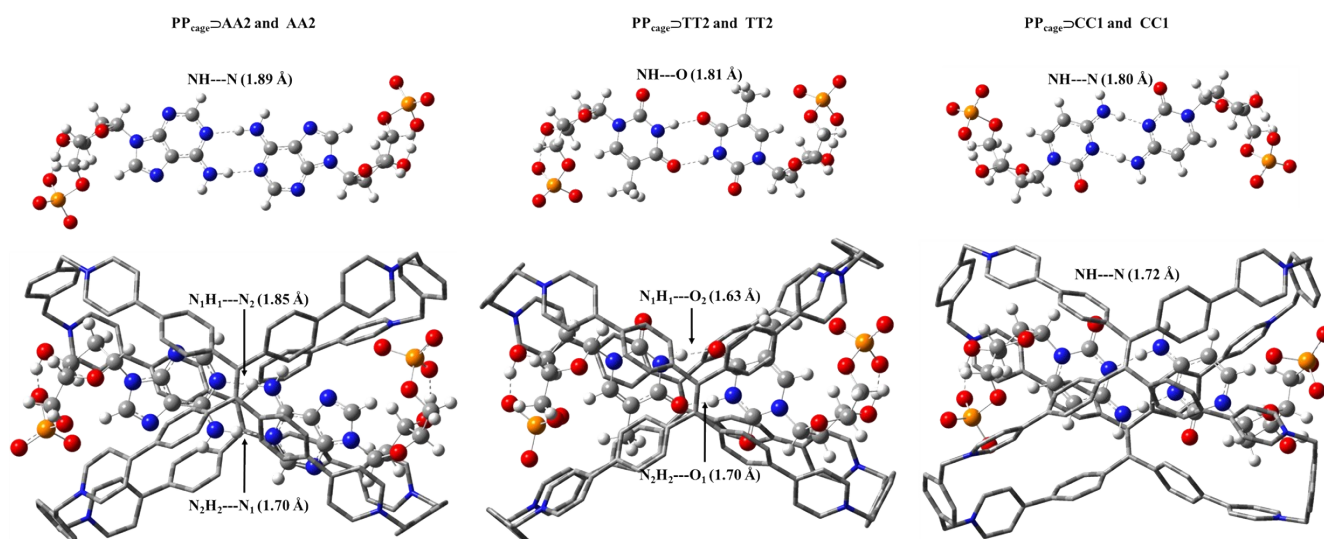


Fig. S7. H-bonded distance comparisons in the supramolecular nucleobase adducts (ω B97XD/6-311G(d,p) level in gas phase) between AA2, TT2 and CC1 and their relative more stable complexed homo-dimers (PP_{cage}→AA2, PP_{cage}→TT2 and PP_{cage}→CC1). The hydrogen atoms of the cages were omitted for clarity.

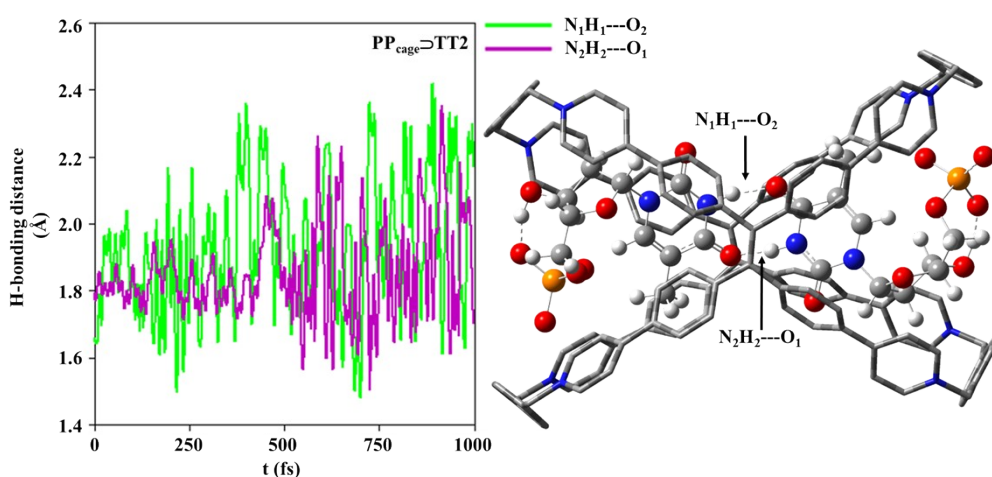


Fig. S8. H-bonding distance evolution plots of BOMD trajectories (S1) computed at ω B97XD/6-311G(d,p) level in solvent phase (H₂O) for PP_{cage}→TT2. The hydrogen atoms of the cage were omitted for clarity.

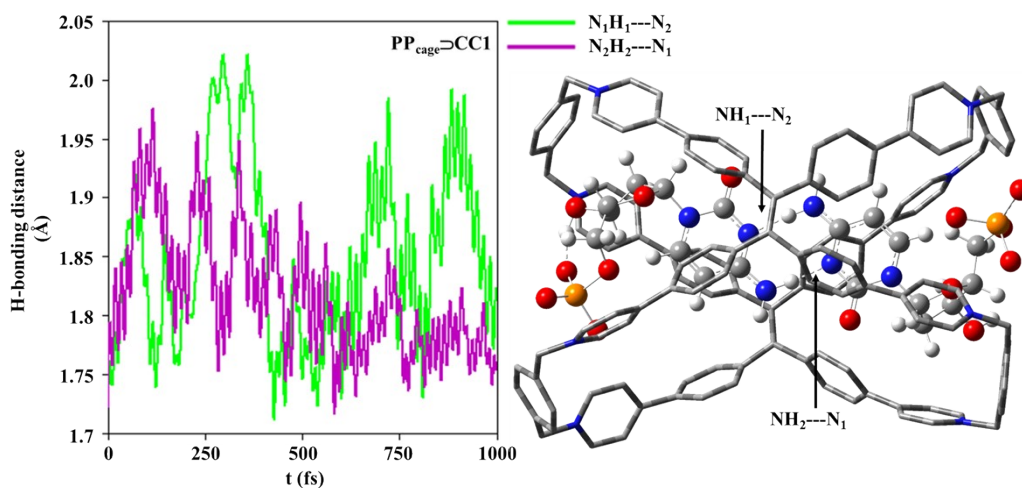


Fig. S9. H-bonding distance evolution plots of BOMD trajectories (S1) computed at ω B97XD/6-311G(d,p) level in solvent phase (H₂O) for PP_{cage}→CC1. The hydrogen atoms of the cage were omitted for clarity.

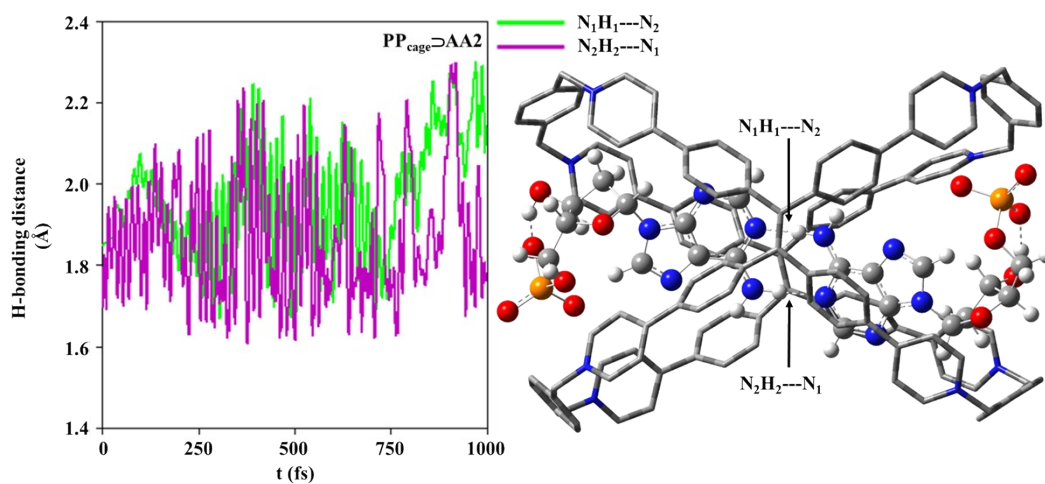


Fig. S10. H-bonding distance evolution plots of BOMD trajectories (S1) computed at ω B97XD/6-311G(d,p) level in solvent phase (H₂O) for PP_{cage}→AA2. The hydrogen atoms of the cage were omitted for clarity.

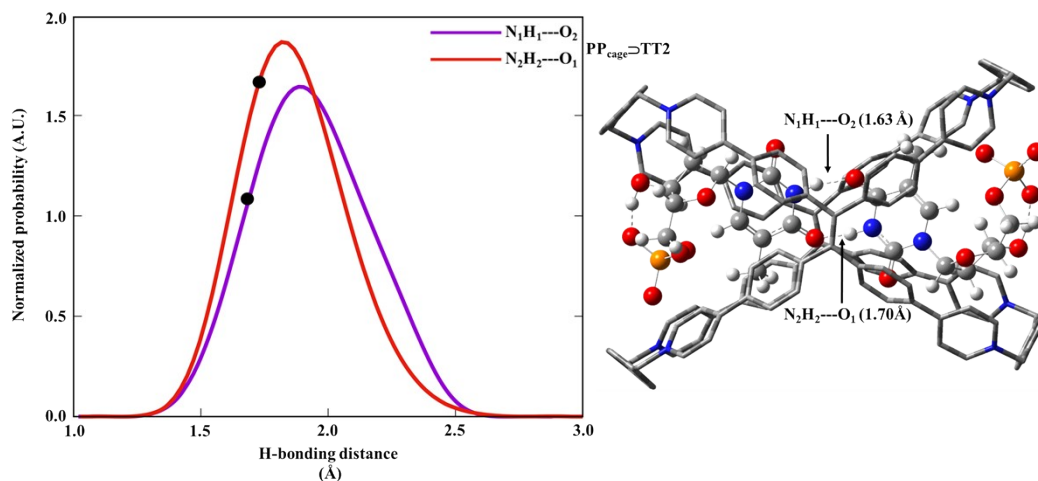


Fig. S11. Distribution functions of H-bonding distances as obtained from the first excited state molecular dynamics in H_2O for $PP_{\text{cage}} \rightarrow TT2$. Black circles and the expressed supramolecular lengths indicate the relative values for the S_0 optimization. The hydrogen atoms of the cage were omitted for clarity.

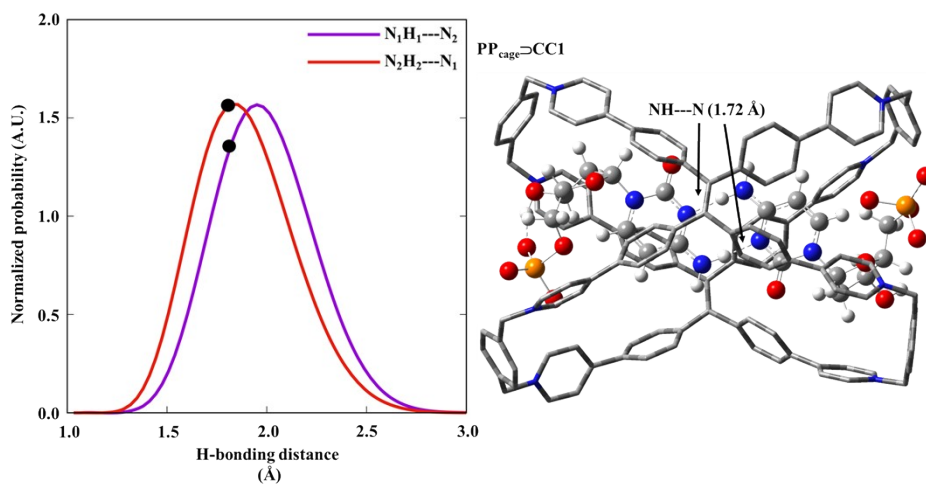


Fig. S12. Distribution functions of H-bonding distances as obtained from the first excited state molecular dynamics in H_2O for $PP_{\text{cage}} \rightarrow CC1$. Black circles and the expressed supramolecular lengths indicate the relative values for the S_0 optimization. The hydrogen atoms of the cage were omitted for clarity.

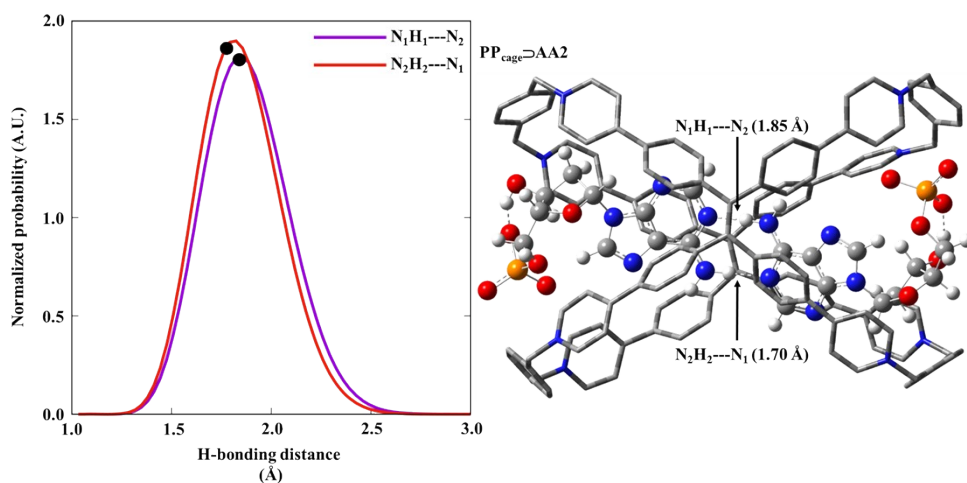


Fig. S13. Distribution functions of H-bonding distances as obtained from the first excited state molecular dynamics in H_2O for $PP_{\text{cage}} \rightarrow AA2$. Black circles and the expressed supramolecular lengths indicate the relative values for the S_0 optimization. The hydrogen atoms of the cage were omitted for clarity.

Table S1. Computed rotational strengths for $PP_{\text{cage}} \rightarrow TT2$ at M06L and MN12L/6-311G(d,p) level.

Time (fs)	Rlength (cgs units)	
	MN12L	M06L
0	-0.3412	-0.1635
40	-0.0381	0.1044
80	-0.0504	-0.0180
120	0.6926	0.4577
160	-0.0772	-0.1244
200	0.2286	0.1310
240	0.4330	0.1404
300	0.7195	0.0757
340	-0.0711	-0.0602
380	-6.6175	0.7627
420	0.0412	-0.0051
460	-0.0339	-0.0207
500	-0.0696	-0.0142
540	0.0257	0.0023
580	-0.2749	-0.1750
620	-0.3736	-0.2676
660	0.0003	0.0027
700	-0.0275	-0.0046
740	0.0328	0.0359
780	-0.5840	-0.6563
820	-0.0112	-0.0028
880	-0.6195	-0.1270
920	0.0276	0.0146
960	-0.1036	-0.0163
1000	0.0206	-0.0116

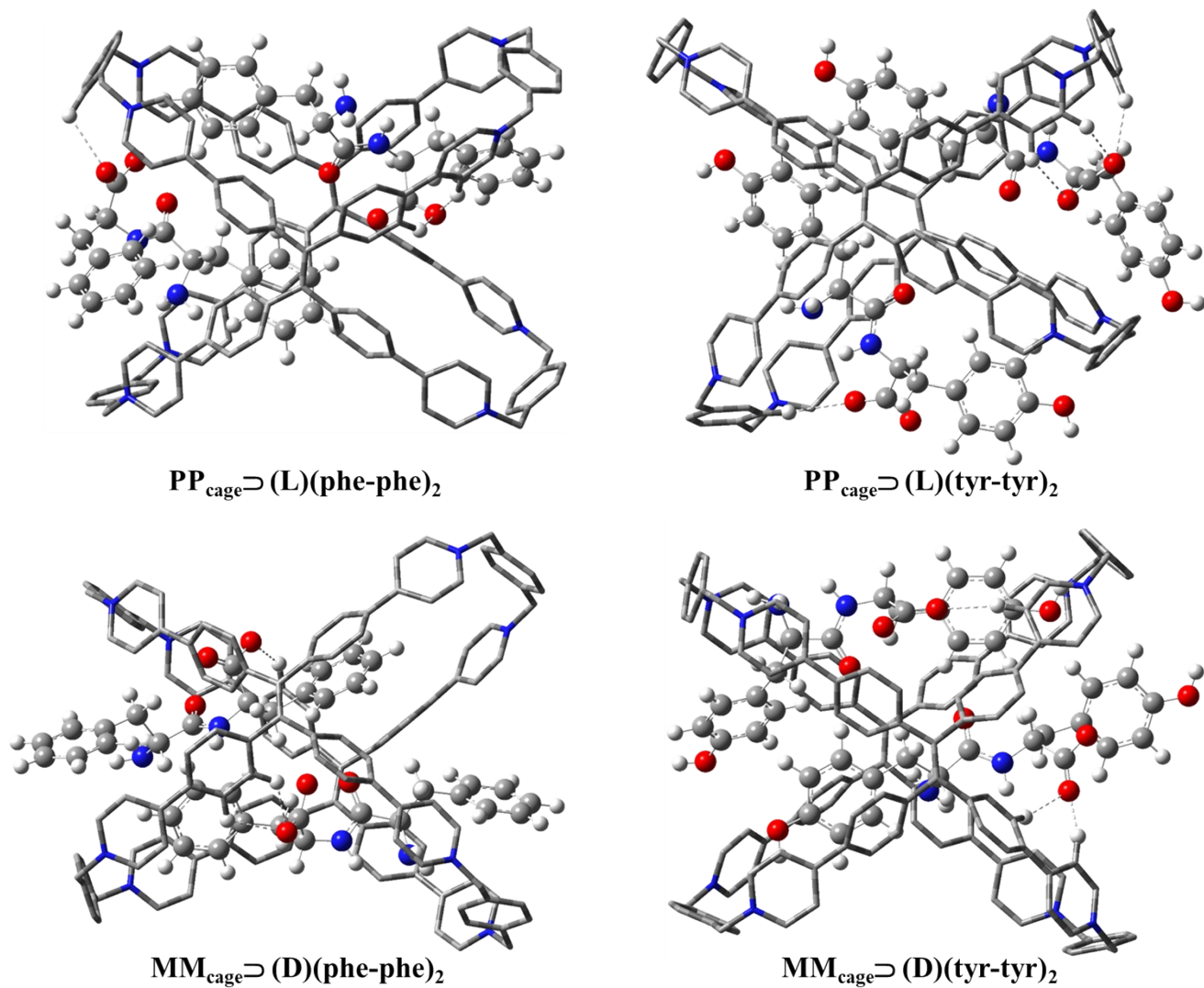


Fig. S14. DFT-optimized PP_{cage}⊃(L)(phe-phe)₂, PP_{cage}⊃(L)(tyr-tyr)₂, MM_{cage}⊃(D)(phe-phe)₂ and MM_{cage}⊃(D)(tyr-tyr)₂ (ωB97XD/6-311G(d,p) level in gas phase), intermolecular hydrogen bonds between carboxylate and phenyl/pyridinium rings are illustrated with single dotted lines. The hydrogen atoms of the cages not involved in H-bonds were omitted for clarity.

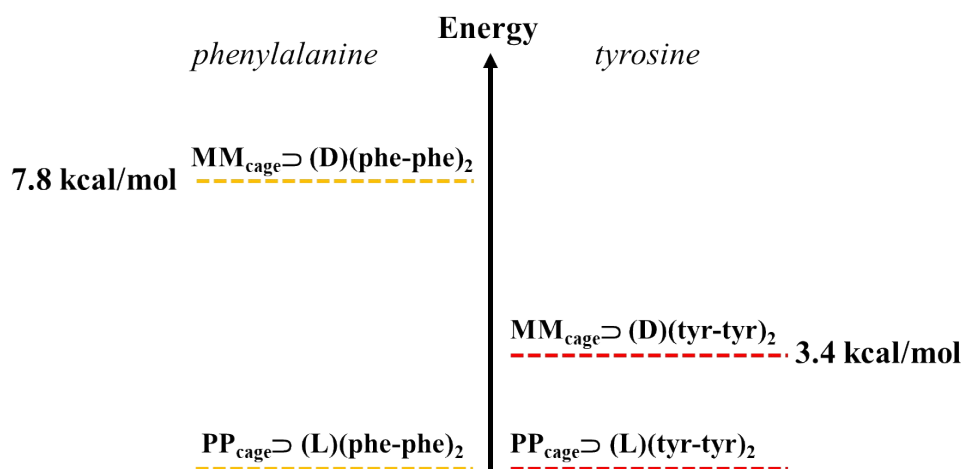


Fig. S15. DFT-optimized energy levels for PP_{cage}⊃(L)(phe-phe)₂, PP_{cage}⊃(L)(tyr-tyr)₂, MM_{cage}⊃(D)(phe-phe)₂ and MM_{cage}⊃(D)(tyr-tyr)₂ (ωB97XD/6-311G(d,p) level in gas phase).

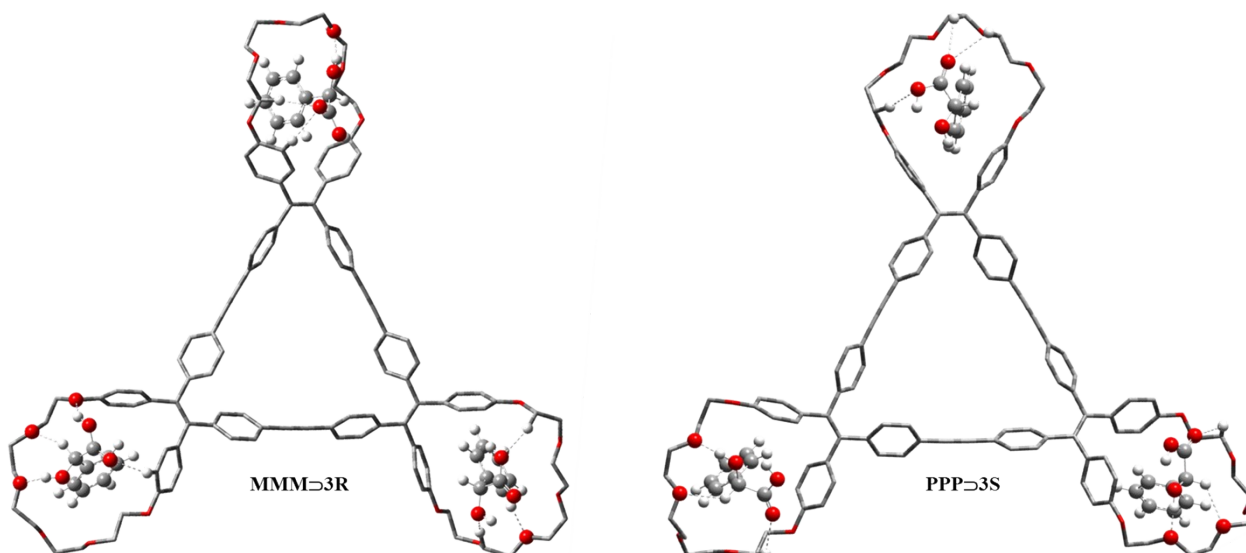


Fig. S16. DFT-optimized MMM⊃3R and PPP⊃3S (ω B97XD/6-311G(d,p) level in gas phase), intermolecular hydrogen bonds between S/R-mandelic acid and the crown ethers are illustrated with single dotted lines. The hydrogen atoms of the macrocycles not involved in H-bonds were omitted for clarity.

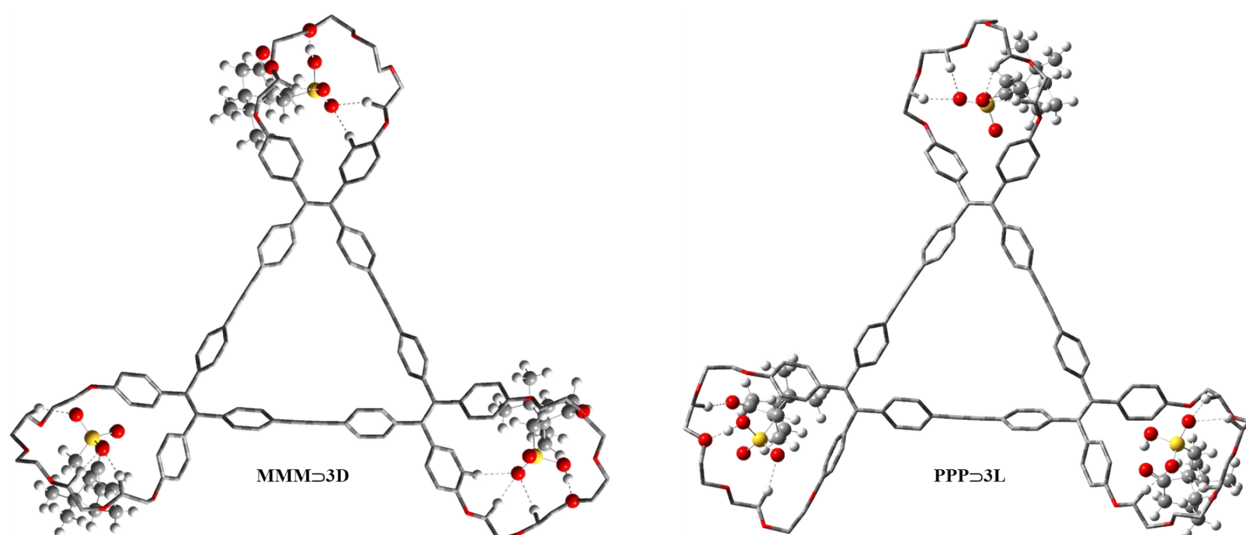


Fig. S17. DFT-optimized MMM⊃3D and PPP⊃3L (ω B97XD/6-311G(d,p) level in gas phase), intermolecular hydrogen bonds between D/L-camphorsulfonic acid and the crown ethers are illustrated with single dotted lines. The hydrogen atoms of the macrocycles not involved in H-bonds were omitted for clarity.

Cartesian coordinates in gas phase ω B97XD/6-311G(d,p)

*PP*_{cage} \Rightarrow *TT2*

	X	Y	Z
C	3.0005020	-4.6640880	3.1424250
N	6.4930770	-6.6537660	1.6708220
C	0.7825840	-3.0400730	3.8181140
C	7.7209250	-7.2325440	1.0181950
H	8.5080460	-7.2683860	1.7739410
H	7.4793810	-8.2592770	0.7350330
C	2.9480420	-4.0034720	4.3872540
H	3.7564480	-4.1137210	5.1032040
C	9.5153720	-4.6608690	-1.1732970
H	10.3043500	-3.9266250	-1.0639480
C	8.1350350	-6.4006170	-0.1812890
C	0.5440200	1.3605080	-4.4552180
N	7.9915070	-2.9166150	-3.8636630
C	5.5026020	-4.9815030	3.0664600
H	5.6442640	-4.1271780	3.7126180
C	2.7899270	0.9280540	-3.3657420
H	2.5347590	1.6390970	-2.5912740
C	5.8187440	-2.6662280	-4.8270450
H	5.0384480	-3.1016970	-5.4357520
C	1.8453060	-3.2150170	4.7255930
H	1.8188010	-2.7115790	5.6855300
C	7.4533980	-6.5335630	-1.4038010
H	6.6717380	-7.2792860	-1.5207750
C	4.2017140	-5.3981600	2.6971840
C	4.0231160	0.2786500	-3.3029740
H	4.7045060	0.5220440	-2.4862750
C	5.6458980	-1.4107140	-4.1880620
C	8.8090110	-4.7589330	-2.3785830
C	1.8745540	0.6780640	-4.4066990

C	2.2218040	-0.2745800	-5.3831710
H	1.5330520	-0.4912990	-6.1931170
C	1.9023180	-4.5469100	2.2661550
H	1.9148650	-5.0037250	1.2828980
C	0.8137150	-3.7415820	2.5978170
H	0.0055750	-3.6273570	1.8829860
C	6.7378320	-0.9163430	-3.4416370
H	6.6944500	0.0369480	-2.9134020
C	7.8897270	-1.6818910	-3.2968510
H	8.7293330	-1.3161040	-2.7257520
C	6.6174630	-5.6145930	2.5434490
H	7.6245840	-5.3009030	2.7827210
C	4.1119040	-6.5016270	1.8166180
H	3.1507350	-6.8999190	1.5206600
C	5.2572140	-7.1035410	1.3213940
H	5.2160310	-7.9475100	0.6465010
C	6.9810240	-3.3864520	-4.6526020
H	7.1372520	-4.3442410	-5.1290630
C	3.4493980	-0.9367360	-5.3255110
H	3.6923820	-1.6375100	-6.1173730
C	7.7931250	-5.7248040	-2.4919330
H	7.2594010	-5.8643350	-3.4263600
C	9.1372180	-3.8221920	-3.5363970
H	9.9967520	-3.1962320	-3.2936490
H	9.3750360	-4.3840550	-4.4441500
C	4.3667970	-0.6745170	-4.2846550
C	9.1857590	-5.4773270	-0.0840060
H	9.7498590	-5.3804660	0.8390090
C	-3.4444820	1.9749490	4.7459700
N	-6.8538220	4.5466710	4.4977740
C	-1.2616340	0.1811270	4.5852110
C	-8.0450070	5.4290130	4.2395200
H	-8.9007120	4.9798990	4.7468160

H	-7.8444020	6.3953390	4.7073160
C	-3.3758270	0.8502650	5.5939690
H	-4.1567730	0.6629450	6.3241330
C	-9.2018980	4.6742030	0.6756720
H	-9.7409630	3.8868030	0.1642610
C	-8.2882970	5.5666970	2.7478890
C	0.3681170	2.6896920	-4.2080550
N	-7.5297510	5.3799560	-2.2318970
C	-5.9251840	2.3950030	4.9774090
H	-6.1022530	1.3535630	5.2044310
C	-1.7675650	2.6919970	-2.9155960
H	-1.3307410	1.9303200	-2.2803170
C	-5.4248500	5.9310130	-3.2298110
H	-4.7516070	6.7004460	-3.5850140
C	-2.2901630	-0.0273680	5.5232140
H	-2.2540430	-0.8926560	6.1755000
C	-7.7558150	6.6551120	2.0331460
H	-7.2281240	7.4493390	2.5538060
C	-4.6176710	2.8704380	4.7294400
C	-3.0703580	3.1247310	-2.6890260
H	-3.6229220	2.7023130	-1.8568130
C	-5.0225030	4.5746420	-3.1815110
C	-8.6447520	5.7437260	-0.0417510
C	-1.0007780	3.2413180	-3.9607240
C	-1.5467240	4.2905130	-4.7225520
H	-0.9583480	4.7424400	-5.5142020
C	-2.3812570	2.2154750	3.8514170
H	-2.4053760	3.0465370	3.1545960
C	-1.3088540	1.3298980	3.7725120
H	-0.5257290	1.5134990	3.0444700
C	-5.9848150	3.6425800	-2.7380470
H	-5.7768010	2.5806710	-2.7479300
C	-7.2095860	4.0574410	-2.2365160

H	-7.8875020	3.3455710	-1.7514130
C	-7.0149460	3.2425270	4.8579210
H	-8.0282200	2.9008310	5.0201330
C	-4.4873720	4.2394630	4.3963970
H	-3.5136600	4.6821180	4.2355330
C	-5.6057730	5.0446090	4.2814300
H	-5.5369000	6.0908040	4.0170390
C	-6.6732500	6.3033620	-2.7582140
H	-7.0033710	7.3336600	-2.7597700
C	-2.8543070	4.7366060	-4.4892210
H	-3.2670040	5.5197900	-5.1181500
C	-7.9343350	6.7423220	0.6479790
H	-7.5329160	7.5986800	0.1133640
C	-8.7975430	5.8101270	-1.5520730
H	-9.5955390	5.1497510	-1.8950990
H	-9.0242190	6.8238210	-1.8893130
C	-3.6416050	4.1400640	-3.4838290
C	-9.0256980	4.5902870	2.0618390
H	-9.4784270	3.7619580	2.5991220
C	4.0027940	4.7603840	-3.2904780
N	7.7971640	5.9021900	-1.6936550
C	1.5405720	3.5882640	-3.9883770
C	9.0992120	6.3153350	-1.0522780
H	9.9089080	5.8465160	-1.6159760
H	9.1798810	7.3994930	-1.1612730
C	3.7916160	4.2964670	-4.5989800
H	4.5953990	4.3314530	-5.3268860
C	9.8536340	4.3515510	2.1255880
H	10.4671510	3.5067040	2.4181660
C	9.1249040	5.8929210	0.3999670
C	-0.1364690	-0.7858380	4.3750860
N	7.3689670	3.4860520	4.3806390
C	6.0512200	4.2944700	-1.9499640

H	5.7026050	3.2899510	-1.7092150
C	2.1998930	-0.3474440	3.4302780
H	2.0162700	-1.0363450	2.6133350
C	5.5067620	2.6511070	5.6385340
H	5.0260280	2.5691620	6.6044390
C	2.5688840	3.7038700	-4.9394490
H	2.4371960	3.2701060	-5.9248940
C	8.2279480	6.4805280	1.3132610
H	7.6003780	7.3114340	1.0032630
C	5.3544350	5.1632950	-2.8088460
C	3.4192090	0.3303680	3.4751140
H	4.1530020	0.1152210	2.7063540
C	4.9677920	2.0318370	4.4827680
C	8.9138090	4.8867980	3.0115000
C	1.2189370	-0.1413480	4.4203420
C	1.5068210	0.7764350	5.4520100
H	0.7655070	0.9657240	6.2213680
C	2.9387080	4.7406240	-2.3693980
H	3.0879090	5.1242870	-1.3649220
C	1.7067230	4.1858600	-2.7252510
H	0.9071460	4.1297930	-1.9934960
C	5.6988540	2.1847270	3.2911440
H	5.3980960	1.7253790	2.3602350
C	6.8951890	2.8917530	3.2508630
H	7.4501180	2.9563500	2.3010250
C	7.2633960	4.6870170	-1.3886320
H	7.7644010	4.0231430	-0.6686010
C	5.9579000	6.3948310	-3.1413790
H	5.4718140	7.0899770	-3.8137850
C	7.1758290	6.7398920	-2.5730750
H	7.6652360	7.6806420	-2.7883700
C	6.6881290	3.3680290	5.5592220
H	7.1216490	3.8507400	6.4254190

C	2.7216680	1.4651570	5.4926920
H	2.8821790	2.1849790	6.2885980
C	8.1226000	5.9807760	2.6100850
H	7.4146860	6.4253570	3.3039560
C	8.6775300	4.2421820	4.3566790
H	9.4694300	3.5284340	4.5967240
H	8.6248900	4.9864580	5.1552750
C	3.6978790	1.2625060	4.4963020
C	9.9591870	4.8536930	0.8213880
H	10.6494370	4.3863820	0.1280850
C	-3.0123830	-1.0512400	-4.8681100
N	-6.6493450	-3.2985350	-4.8224370
C	-0.6435200	0.4730340	-4.6731950
C	-7.9218120	-4.1082300	-4.8027980
H	-8.7473740	-3.4223410	-5.0077490
H	-7.8506420	-4.8231840	-5.6270900
C	-2.7002010	-0.0956270	-5.8525640
H	-3.3861810	0.0862000	-6.6744270
C	-9.3893640	-5.0832700	-1.4205920
H	-10.2119650	-4.7664200	-0.7928250
C	-8.1279680	-4.8120880	-3.4802080
C	-0.3570120	-2.0995790	4.0723150
N	-7.4875830	-5.9435620	1.3187340
C	-5.0593660	-1.9188410	-3.7181960
H	-4.7742890	-1.4220040	-2.7996160
C	-2.7359120	-2.0227660	3.1495210
H	-2.5843290	-1.0092540	2.7973940
C	-5.3898170	-6.0911260	2.4519330
H	-4.5653990	-6.7187040	2.7631570
C	-1.5328130	0.6710420	-5.7443590
H	-1.3222740	1.4404510	-6.4799540
C	-7.2049530	-5.7785070	-3.0351090
H	-6.3621140	-6.0592070	-3.6611450

C	-4.2905760	-1.8038050	-4.8875500
C	-3.9464360	-2.6513520	2.8635790
H	-4.6965580	-2.0979090	2.3153420
C	-5.3721960	-4.6890380	2.6561880
C	-8.4495470	-6.0109480	-0.9594030
C	-1.7139630	-2.6993860	3.8426470
C	-1.9719750	-4.0242100	4.2563670
H	-1.2162910	-4.5686470	4.8130980
C	-2.1016120	-1.2759540	-3.8173300
H	-2.3014740	-2.0302440	-3.0633040
C	-0.9189060	-0.5402460	-3.7385280
H	-0.2322890	-0.7202880	-2.9189690
C	-6.4962670	-3.9688160	2.2112740
H	-6.5925570	-2.8917680	2.2953600
C	-7.5378690	-4.6035540	1.5420880
H	-8.3826110	-4.0190750	1.1246500
C	-6.2345360	-2.6667650	-3.6918960
H	-6.8120940	-2.7095620	-2.7418460
C	-4.7817720	-2.4406640	-6.0517680
H	-4.2382920	-2.3913210	-6.9867660
C	-5.9499600	-3.1809430	-5.9903690
H	-6.3453990	-3.7009370	-6.8531440
C	-6.4460180	-6.6881980	1.7844910
H	-6.4739710	-7.7517270	1.5882900
C	-3.1721350	-4.6670850	3.9353650
H	-3.3176850	-5.6903620	4.2657800
C	-7.3633660	-6.3692670	-1.7814160
H	-6.6397170	-7.1059960	-1.4414590
C	-8.5526090	-6.5578190	0.4523500
H	-9.5193650	-6.3137510	0.8959910
H	-8.4151910	-7.6412640	0.4856510
C	-4.1712170	-3.9989850	3.1993520
C	-9.2235900	-4.4834290	-2.6769380

H	-9.9336340	-3.7266510	-2.9938270
C	4.5013540	-2.8799010	0.4167120
O	5.1644540	-2.3909340	1.6115040
C	5.6218260	-3.1817020	-0.5985400
C	6.5727200	-2.0821930	1.2994050
C	6.6548790	-2.1179690	-0.2348150
H	5.2677320	-3.1181130	-1.6288350
H	6.0260500	-4.1857230	-0.4204390
C	7.0198680	-0.7585050	1.9140790
H	7.1973100	-2.8961740	1.6943980
O	7.9966380	-2.3531220	-0.6503760
H	6.3062630	-1.1641230	-0.6488240
O	6.4868820	0.3652620	1.1888890
H	6.6613820	-0.6832930	2.9467430
H	8.1163360	-0.7327010	1.9078620
H	8.4262340	-1.4192630	-0.5885960
P	7.3945520	1.1597740	-0.1362730
O	7.8482970	2.5663150	0.5075250
O	8.5668870	0.1000310	-0.4959220
O	6.2328950	1.2758830	-1.2641850
H	3.9166240	-3.7648850	0.6554680
C	-5.0067350	1.8192960	1.4540510
O	-5.8996820	1.1190500	2.3376060
C	-5.9016760	2.5539500	0.4448720
C	-7.2750840	1.1608210	1.7798100
C	-7.0532820	1.5525780	0.3007990
H	-5.3592150	2.7636980	-0.4735940
H	-6.2629300	3.4998080	0.8675870
C	-7.9551130	-0.1750560	2.0272030
H	-7.8244700	1.9689770	2.2860480
O	-8.2309480	2.0084880	-0.3583320
H	-6.6858450	0.6700060	-0.2364080
O	-7.3700190	-1.1851320	1.1887180

H	-7.8171930	-0.4716790	3.0728850
H	-9.0294500	-0.0723680	1.8290550
H	-8.7002740	1.0977550	-0.6276930
P	-8.3177770	-1.6849680	-0.2691610
O	-9.3450130	-2.7714130	0.3127160
O	-8.9561060	-0.2965080	-0.7986970
O	-7.0967090	-2.2547780	-1.1612240
H	-4.3709790	2.4952450	2.0214560
N	-4.0872840	0.8484800	0.7994760
C	-4.4921970	-0.4366090	0.4486600
C	-2.8094690	1.3148530	0.5064310
H	-5.5170340	-0.7161870	0.6997150
C	-3.6494650	-1.3430960	-0.1270140
N	-1.9531020	0.3732990	-0.0280080
O	-2.4649550	2.5043460	0.7116850
C	-4.0754650	-2.7476760	-0.4578270
C	-2.2670900	-0.9507550	-0.3240610
H	-0.9776660	0.6781600	-0.2430760
H	-5.1687030	-2.8001740	-0.5525600
H	-3.6192340	-3.0785860	-1.3966630
H	-3.7297720	-3.4476950	0.3124700
O	-1.3615450	-1.7335670	-0.7339630
N	3.5182050	-1.8542780	-0.0055620
C	3.7996080	-0.5071180	0.1495480
C	2.2608210	-2.2930230	-0.4184510
H	4.8010980	-0.2404710	0.4700450
C	2.8797470	0.4732570	-0.0468390
N	1.3195330	-1.2879390	-0.5768830
O	2.0013320	-3.5011920	-0.6088850
C	3.2149180	1.9240630	0.1609980
C	1.5434930	0.0775730	-0.4281730
H	0.3355640	-1.5790740	-0.7529360
H	4.2743040	2.0909030	-0.0607580

H	2.6067700	2.5545190	-0.4929460
H	3.0029600	2.2332220	1.1928930
O	0.5954990	0.8977160	-0.6186440

$PP_{cage} \rightarrow AA2$

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C	-3.2146390	5.2317510	2.1456620
N	-6.8039210	6.8278950	0.4400730
C	-0.8383660	3.9595960	3.0434960
C	-8.0390590	7.2355600	-0.3189420
H	-8.8382890	7.4096990	0.4045580
H	-7.8131960	8.1869320	-0.8065940
C	-3.1234610	4.7203080	3.4565040
H	-3.9569830	4.8220260	4.1445400
C	-9.9847650	4.4791760	-2.1216130
H	-10.9376920	3.9750300	-2.0154590
C	-8.4205890	6.1580780	-1.3193870
C	-0.5077060	-1.9243290	-4.2339390
N	-8.2396350	1.8896610	-4.1303900
C	-5.7405160	5.3308800	1.9774410
H	-5.8525330	4.5111100	2.6769820
C	-2.8073940	-1.5381430	-3.2245190
H	-2.5200220	-2.1267320	-2.3636250
C	-6.1298220	1.5406950	-5.2030160
H	-5.4252540	1.8814780	-5.9487550
C	-1.9482180	4.1066890	3.9002520
H	-1.8970060	3.7317350	4.9155300
C	-7.5065390	5.7471240	-2.3021580
H	-6.5401550	6.2352330	-2.4000910
C	-4.4627170	5.8259430	1.6211720
C	-4.0805930	-0.9746680	-3.2612280
H	-4.7299540	-1.1275410	-2.4063440
C	-5.8335700	0.4528930	-4.3421270

C	-9.0481770	4.0191960	-3.0592180
C	-1.8929220	-1.3529840	-4.2793000
C	-2.3068340	-0.5743990	-5.3773840
H	-1.6262510	-0.4104630	-6.2065700
C	-2.0851960	5.1384660	1.3075430
H	-2.1335300	5.4911830	0.2826850
C	-0.9182380	4.5194470	1.7527680
H	-0.0659600	4.4432050	1.0862330
C	-6.8591980	0.0595210	-3.4555110
H	-6.7847540	-0.8065660	-2.8062840
C	-8.0454070	0.7850740	-3.3565430
H	-8.8063940	0.4572060	-2.6325430
C	-6.8805840	5.8349910	1.3698720
H	-7.8668140	5.4412320	1.5775620
C	-4.4283300	6.8915710	0.6916430
H	-3.4922060	7.3604550	0.4192750
C	-5.5966740	7.3691070	0.1212130
H	-5.5974680	8.1790690	-0.5957610
C	-7.3224250	2.2250250	-5.0855730
H	-7.5731070	3.0558630	-5.7316680
C	-3.5902270	-0.0193880	-5.4239490
H	-3.8715500	0.5401780	-6.3093700
C	-7.8183680	4.6887990	-3.1621920
H	-7.0690460	4.3869430	-3.8853030
C	-9.4053390	2.7947640	-3.9029590
H	-10.1752250	2.2143160	-3.3946040
H	-9.7894980	3.0895280	-4.8848010
C	-4.5004560	-0.2003270	-4.3603060
C	-9.6758750	5.5350130	-1.2569120
H	-10.4092800	5.8448610	-0.5187330
C	3.6240920	-0.7533220	4.6966990
N	6.9320690	-3.4809210	4.8045720
C	1.4531740	1.0349900	4.2605900

C	8.0725120	-4.4451210	4.6323760
H	8.9574560	-3.9850250	5.0745490
H	7.8291820	-5.3315840	5.2241310
C	3.6675890	0.5724600	5.1792050
H	4.5272240	0.9264320	5.7391010
C	9.7041700	-4.6861770	1.1635960
H	10.5796210	-4.2845600	0.6636320
C	8.3298570	-4.8225700	3.1770550
C	-0.2137320	-3.1973860	-3.8265670
N	7.8156420	-5.5008580	-1.8159740
C	6.1003440	-1.2373280	4.9127830
H	6.3423090	-0.1836580	4.9119910
C	2.0539610	-2.8667020	-2.7603570
H	1.6794850	-1.9680070	-2.2872040
C	5.6334910	-6.1684560	-2.5447420
H	4.9093880	-6.9647940	-2.6586090
C	2.5966040	1.4485570	4.9735700
H	2.6550250	2.4610590	5.3561520
C	7.4631400	-5.6943800	2.4907980
H	6.6042510	-6.1284840	2.9935660
C	4.7661490	-1.6844340	4.8308390
C	3.3804920	-3.2402330	-2.5514950
H	4.0050110	-2.6237410	-1.9112100
C	5.2873130	-4.8224730	-2.8177040
C	8.8134650	-5.5161500	0.4678600
C	1.1967560	-3.6413370	-3.5672060
C	1.6969030	-4.8433620	-4.1050140
H	1.0512820	-5.4682370	-4.7132840
C	2.4597410	-1.1766490	4.0239520
H	2.3911290	-2.1793050	3.6157210
C	1.3977940	-0.3009080	3.8128940
H	0.5287090	-0.6506000	3.2662170
C	6.3195160	-3.8672200	-2.7012270

H	6.1583650	-2.8290340	-2.9610830
C	7.5641770	-4.2143000	-2.1884110
H	8.3189000	-3.4459300	-2.0038880
C	7.1550960	-2.1415300	4.8854260
H	8.1823280	-1.8118990	4.8752750
C	4.5710850	-3.0909090	4.8246160
H	3.5778180	-3.5170240	4.8363980
C	5.6485360	-3.9524530	4.8141350
H	5.5226260	-5.0259670	4.8168200
C	6.8869400	-6.4772940	-2.0472750
H	7.1688890	-7.4898290	-1.7902750
C	3.0247090	-5.2329260	-3.8842660
H	3.3879990	-6.1478050	-4.3428020
C	7.7006270	-6.0357840	1.1557000
H	7.0067120	-6.7085840	0.6616430
C	9.0399210	-5.8225890	-1.0115760
H	9.8695770	-5.2346350	-1.4075140
H	9.2693920	-6.8795590	-1.1694510
C	3.8918630	-4.4262690	-3.1188740
C	9.4635730	-4.3443640	2.5046890
H	10.1646290	-3.6922170	3.0155850
C	-3.6635430	-5.3690790	-2.5340080
N	-7.3920850	-6.2599910	-0.6596140
C	-1.3098450	-4.1521610	-3.4861480
C	-8.6624280	-6.5270570	0.1019660
H	-9.4969340	-6.1969860	-0.5190530
H	-8.7370730	-7.6078060	0.2423180
C	-3.5879440	-4.9228510	-3.8640940
H	-4.4567670	-4.9927980	-4.5098030
C	-9.3680390	-3.8931800	2.7556930
H	-9.9960730	-3.0099290	2.8122590
C	-8.6384230	-5.7785730	1.4169880
C	0.2911070	1.9282150	3.9424290

N	-7.0528360	-2.4897000	4.8565000
C	-5.8885910	-4.7045910	-1.6405440
H	-5.6715760	-3.6697770	-1.8698880
C	-1.8657880	0.9596500	3.0393150
H	-1.5542790	1.2603420	2.0441590
C	-4.9300620	-1.8129450	5.7235930
H	-4.1721970	-1.9502830	6.4832250
C	-2.4113620	-4.3372530	-4.3406170
H	-2.3764980	-3.9503670	-5.3528800
C	-7.7343950	-6.1476000	2.4349430
H	-7.1084300	-7.0289350	2.3198290
C	-4.9751760	-5.7316510	-1.9275420
C	-3.0689490	0.2750710	3.2179230
H	-3.6634410	0.0145920	2.3524980
C	-4.7444020	-0.9110690	4.6504020
C	-8.4482690	-4.2347920	3.7501720
C	-1.0382040	1.2539970	4.1369890
C	-1.4500870	0.8422840	5.4181850
H	-0.8221620	1.0566160	6.2768850
C	-2.5109370	-5.3352690	-1.7279050
H	-2.5505590	-5.7199050	-0.7134450
C	-1.3415070	-4.7322110	-2.2038260
H	-0.4743770	-4.6464540	-1.5557100
C	-5.7892280	-0.8243650	3.7048820
H	-5.7670780	-0.1144920	2.8873770
C	-6.9092320	-1.6402100	3.8020500
H	-7.6680210	-1.6228170	3.0172800
C	-7.0922900	-4.9747300	-0.9930290
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C	-5.3257320	-7.0498530	-1.5704150
H	-4.6659960	-7.8813190	-1.7817240
C	-6.5415070	-7.2861660	-0.9466300
H	-6.8579100	-8.2807360	-0.6619970

C	-6.0868460	-2.5698530	5.8116120
H	-6.2591350	-3.2586120	6.6276730
C	-2.6633840	0.1709220	5.6005370
H	-2.9641830	-0.0957020	6.6086020
C	-7.6391620	-5.3799240	3.5955120
H	-6.9429710	-5.6698530	4.3785100
C	-8.2943420	-3.3427070	4.9596420
H	-9.1449370	-2.6643540	5.0539400
H	-8.2063640	-3.9177230	5.8840270
C	-3.4897040	-0.1324670	4.4987000
C	-9.4627480	-4.6657130	1.5892580
H	-10.1525250	-4.3257390	0.8249820
C	3.0266800	0.4796830	-4.6501940
N	6.9819530	2.0610850	-4.2771260
C	0.6138470	-0.9816350	-4.5398490
C	8.4072380	2.4884970	-4.1142460
H	8.8819430	1.7542140	-3.4478350
H	8.8732680	2.4591200	-5.1030030
C	2.7836380	-0.5677150	-5.5597310
H	3.5505570	-0.8718530	-6.2647420
C	9.7490510	5.2461780	-1.8948690
H	10.5793080	5.3493520	-1.2069420
C	8.5371580	3.8535910	-3.4672280
C	0.3943150	3.1833060	3.4131170
N	7.4991330	6.7412050	0.1555500
C	4.8917820	1.4815430	-3.3015170
H	4.3166180	1.3773400	-2.3897370
C	2.6642890	3.0977680	2.2969690
H	2.5270770	2.0421040	2.1058940
C	5.2982250	7.0308950	1.0397880
H	4.4285420	7.6673660	1.1419530
C	1.5901260	-1.2928150	-5.5011950
H	1.4444940	-2.1450000	-6.1563880

C	7.5396800	4.8424750	-3.5673280
H	6.6792970	4.7009810	-4.2152260
C	4.3741320	1.0907610	-4.5499210
C	3.8342350	3.7037910	1.8355010
H	4.5323120	3.0988890	1.2625410
C	5.2949950	5.6978900	1.5163340
C	8.6977510	6.1662960	-1.8903870
C	1.6903390	3.8216830	3.0074850
C	1.9348650	5.1874190	3.2596950
H	1.2072640	5.7736550	3.8122060
C	1.9956850	0.8623940	-3.7681100
H	2.1404570	1.7010760	-3.0948290
C	0.7938870	0.1536310	-3.7272650
H	0.0325930	0.4231200	-3.0011010
C	6.4744960	4.9534780	1.3514670
H	6.5604210	3.9284250	1.6834910
C	7.5642350	5.4817370	0.6657740
H	8.4435370	4.8423540	0.4688340
C	6.1889080	1.9712590	-3.1729600
H	6.5728950	2.2670770	-2.1671580
C	5.2184220	1.2448040	-5.6740840
H	4.8759360	1.0074190	-6.6730250
C	6.5075000	1.7226400	-5.5092510
H	7.1837720	1.8458140	-6.3445420
C	6.4010290	7.5231070	0.3623210
H	6.4231180	8.5217770	-0.0526550
C	3.1099080	5.8017440	2.8075330
H	3.2803450	6.8477770	3.0434420
C	7.6177030	5.9890970	-2.7769060
H	6.8137460	6.7201320	-2.8113760
C	8.5960600	7.1931490	-0.7808490
H	9.5237650	7.2610220	-0.2098190
H	8.3261440	8.1888860	-1.1398330

C	4.0704310	5.0709560	2.0789870
C	9.6658300	4.0894060	-2.6794620
H	10.4304110	3.3292960	-2.5725430
C	-5.7004280	2.2830160	0.5821350
O	-6.5147960	1.9585780	1.7353610
C	-6.6641860	2.7572060	-0.5135220
C	-7.9340790	1.8453570	1.3011680
C	-7.8519260	1.8467640	-0.2288100
H	-6.2402870	2.6322040	-1.5115980
H	-6.9285160	3.8090120	-0.3715520
C	-8.6179170	0.6029340	1.8617910
H	-8.4634690	2.7422170	1.6483200
O	-9.0982290	2.1866500	-0.8145670
H	-7.5765100	0.8348460	-0.5459300
O	-8.1125850	-0.6007920	1.2525890
H	-8.4525460	0.5526750	2.9453980
H	-9.6988460	0.7000900	1.6930950
H	-9.5547280	1.2652030	-0.8967920
P	-9.1301920	-1.4360460	-0.0381500
O	-10.3647270	-2.0304230	0.7721750
O	-9.4870360	-0.2284730	-1.0756310
O	-7.9940630	-2.4261360	-0.6261460
N	-4.9256580	1.0913390	0.1955970
C	-3.5991980	1.1556180	-0.1660460
C	-5.2493560	-0.2643340	0.3198300
N	-2.8580290	2.2659740	-0.4169720
C	-3.1508630	-0.1691790	-0.1966510
N	-4.1920780	-1.0484480	0.0996960
H	-6.2472400	-0.6060590	0.5913380
C	-1.5845360	1.9614630	-0.6891910
C	-1.7668810	-0.3769890	-0.3911320
N	-1.0166020	0.7261110	-0.6803370
H	-0.9230050	2.7842390	-0.9335980

N	-1.1822190	-1.5865510	-0.2698240
H	-0.1526890	-1.6773230	-0.1900890
H	-1.7737530	-2.3676780	-0.0229340
H	-4.9583430	3.0318120	0.8659050
C	6.5301520	-2.2165200	1.7096630
O	7.6948800	-1.6275580	2.3078870
C	6.9219960	-2.5409780	0.2693690
C	8.6618410	-1.2340870	1.2402660
C	7.8380220	-1.3595580	-0.0586780
H	6.0457640	-2.6206230	-0.3730820
H	7.4722430	-3.4797200	0.2561030
C	9.2183030	0.1488210	1.5407920
H	9.4693440	-1.9741760	1.2332610
O	8.6438080	-1.5239950	-1.2262890
H	7.2278910	-0.4566790	-0.1747920
O	8.2222560	1.1426920	1.2627730
H	9.4971710	0.2228650	2.5963080
H	10.1167470	0.3058480	0.9312100
H	8.9125270	-0.5552780	-1.4533910
P	8.3957640	2.0986290	-0.2204080
O	9.3810160	3.2951860	0.1839740
O	8.9335200	1.0220070	-1.3359260
O	6.8535900	2.5165410	-0.5090240
N	5.4156630	-1.2563250	1.6971050
C	4.1423330	-1.6017490	1.2872890
C	5.5077750	0.1366740	1.6148000
N	3.5718850	-2.8353090	1.1778270
C	3.5223690	-0.3944270	0.9732140
N	4.3723270	0.6804580	1.1917620
H	6.4404290	0.6681580	1.7892560
C	2.3141950	-2.7705960	0.7082220
C	2.2301140	-0.4367640	0.4119560
N	1.6262990	-1.6609610	0.3172880

H	1.7881340	-3.7121910	0.6041970
N	1.6350260	0.6806090	-0.0416420
H	0.6543540	0.6788660	-0.3927090
H	2.1494010	1.5468060	0.0407030
H	6.2135340	-3.0929630	2.2763480

PP_{cage} ⇒ CCI

	X	Y	Z
C	4.2426700	-2.8788350	-0.4764000
O	4.9098040	-2.9066320	0.8094110
C	5.3681130	-2.8438970	-1.5286050
C	6.3276270	-2.5301780	0.6411260
C	6.4269910	-2.0130680	-0.8043570
H	5.0305490	-2.4100790	-2.4713670
H	5.7360850	-3.8610560	-1.7131470
C	6.7517810	-1.5202640	1.7046830
H	6.9338140	-3.4426820	0.7242990
O	7.7630080	-2.0849730	-1.2844230
H	6.1175700	-0.9632270	-0.8278810
O	6.3955330	-0.1786330	1.3038910
H	6.2430770	-1.7501440	2.6480970
H	7.8335560	-1.5805510	1.8760590
H	8.1560340	-1.1645320	-0.9914580
P	7.7645800	0.8841520	0.8081180
O	8.8055680	0.6849200	2.0180290
O	8.2047220	0.2729950	-0.6376380
O	7.0174960	2.3166350	0.7289700
H	3.6025370	-3.7509160	-0.5799560
C	-5.4536160	1.8526140	0.3471410
O	-6.7566050	1.2871110	0.3604770
C	-5.4637260	2.8819210	-0.7934170
C	-7.4395640	1.4375140	-0.9322340
C	-6.5516680	2.3993520	-1.7590770

H	-4.4924650	3.0078580	-1.2688900
H	-5.7891210	3.8410790	-0.3846770
C	-7.6592100	0.0977670	-1.6505450
H	-8.4164070	1.8760240	-0.7151110
O	-7.2733400	3.5695910	-2.2385050
H	-6.1110860	1.8702160	-2.6162650
O	-8.7068350	-0.7116450	-1.1358660
H	-7.9512750	0.3337400	-2.6858900
H	-6.7052810	-0.4513730	-1.6842390
H	-7.9624400	3.3162750	-2.8798850
P	-8.7061410	-1.2471950	0.5672660
O	-9.6405120	-2.5497930	0.5476860
O	-7.1318930	-1.6221360	0.8429690
O	-9.1869890	0.0558870	1.3965500
H	-5.2619810	2.3078460	1.3199000
N	3.3261480	-1.7127150	-0.4937490
C	3.6964730	-0.5112430	0.0652680
C	2.0013460	-1.9153680	-0.9588090
H	4.7164070	-0.3943930	0.4326770
C	2.8028270	0.5031770	0.2225590
N	1.0939190	-0.9044870	-0.7486120
O	1.6872370	-3.0019150	-1.5104460
H	3.1091110	1.4327330	0.6820100
C	1.4392280	0.2572970	-0.1554780
N	0.4668750	1.1597510	0.0822610
H	-0.5352750	0.8717130	-0.0331190
H	0.6820560	2.0036190	0.5916990
N	-4.4320390	0.7779100	0.1451030
C	-4.7945450	-0.5359850	-0.0254340
C	-3.0753470	1.1444600	0.2523190
H	-5.8481750	-0.8442780	0.2057630
C	-3.8399130	-1.4654670	-0.3405180
N	-2.1289620	0.2219420	-0.0959450

O	-2.7782510	2.2992610	0.6747310
H	-4.1170760	-2.5040560	-0.4543930
C	-2.4701580	-1.0457370	-0.4212600
N	-1.4911990	-1.8875240	-0.8010150
H	-0.5013030	-1.5488420	-0.8371390
H	-1.6976950	-2.8556230	-0.9931870
C	-2.9440160	0.4474680	-4.4854650
N	-6.4627090	-1.9392090	-5.0819030
C	-0.5954150	1.9646510	-3.9989700
C	-7.6997070	-2.7932100	-5.3429460
H	-8.5032170	-2.0930590	-5.5853970
H	-7.4713010	-3.3902700	-6.2294860
C	-2.7777020	1.7202060	-5.0696690
H	-3.5558000	2.1449950	-5.6970240
C	-9.2016860	-3.9272680	-2.0265020
H	-9.7623820	-3.4729290	-1.2081240
C	-8.0809850	-3.6662880	-4.1741470
C	-0.3578660	-3.2451380	3.3673740
N	-7.8944080	-5.8816240	0.2919070
C	-4.8943010	-0.3301300	-5.9222840
H	-4.5669130	0.2769040	-6.7564950
C	-2.7345030	-2.9244920	2.5073800
H	-2.5385020	-1.8732400	2.3476680
C	-5.7175160	-6.5025130	1.0595120
H	-4.9082060	-7.2213270	1.0405090
C	-1.6224630	2.4687830	-4.8224150
H	-1.5134670	3.4490980	-5.2730300
C	-7.6405710	-5.0020240	-4.1014680
H	-7.0562410	-5.4312510	-4.9105210
C	-4.1683320	-0.3554930	-4.7058850
C	-3.9927110	-3.4212500	2.1777440
H	-4.7439700	-2.7406700	1.7926080
C	-5.5844490	-5.2613060	1.7318060

C	-8.7372850	-5.2501490	-1.9414760
C	-1.7269830	-3.7646450	3.0193870
C	-2.0288370	-5.1376880	3.1498170
H	-1.2785060	-5.8161800	3.5432880
C	-1.9097900	-0.0594740	-3.6722240
H	-1.9840880	-1.0481150	-3.2318830
C	-0.7492520	0.6800410	-3.4413340
H	0.0261980	0.2564840	-2.8093320
C	-6.7029000	-4.4104410	1.7340800
H	-6.7032300	-3.4381680	2.2081390
C	-7.8452130	-4.7250560	1.0043540
H	-8.6790690	-4.0004460	0.9121790
C	-6.0193020	-1.1234470	-6.0822650
C	-4.6680040	-1.1999690	-3.6925340
H	-4.1986330	-1.2400730	-2.7181140
C	-5.8026460	-1.9725300	-3.8957780
H	-6.2123330	-2.6110120	-3.1248670
C	-6.8703160	-6.7833890	0.3460940
H	-6.9925820	-7.6996220	-0.2158980
C	-3.2791540	-5.6498150	2.7735170
H	-3.4703380	-6.7119820	2.8927520
C	-7.9712090	-5.7898960	-2.9916360
H	-7.6397640	-6.8240350	-2.9545260
C	-9.0211370	-6.0614350	-0.6844700
H	-9.9336650	-5.7155430	-0.1970710
H	-9.1161010	-7.1284380	-0.8973770
C	-4.2821350	-4.7950080	2.2756100
C	-8.8724340	-3.1433900	-3.1389530
H	-9.2254050	-2.1165410	-3.1569200
C	4.3340720	5.6636870	-1.9235920
N	8.1193890	6.1751790	-0.0021680
C	1.8238370	4.7701270	-2.8389730
C	9.4097470	6.3764810	0.7758400

H	10.2353890	6.2264030	0.0762510
H	9.4121390	7.4169270	1.1092390
C	4.1211650	5.4483020	-3.2946760
H	4.9366390	5.5709880	-3.9997180
C	10.0309430	3.1897560	2.7499340
H	10.4800870	2.2205750	2.5791380
C	9.4765480	5.4105050	1.9330050
C	-0.1376340	-2.0542740	4.0026490
N	7.5294840	1.7849720	4.8280560
C	6.2522040	4.8217800	-0.6073780
H	5.7948200	3.8452790	-0.5032150
C	2.1673900	-1.3679270	3.1692910
H	1.9602180	-1.8191360	2.2050650
C	5.8076330	0.5047230	5.8946680
H	5.4833250	-0.0528580	6.7642660
C	2.8742340	4.9915440	-3.7455140
H	2.7364330	4.7549420	-4.7950080
C	8.7194700	5.6447970	3.0955850
H	8.2101110	6.5941670	3.2337050
C	5.6898880	5.8746330	-1.3440630
C	3.3915630	-0.7299100	3.3699870
H	4.1225450	-0.7189750	2.5708520
C	5.0008480	0.5856640	4.7338270
C	9.2110930	3.3925090	3.8686140
C	1.2091510	-1.4279260	4.1998180
C	1.5219400	-0.8192770	5.4340160
H	0.7911330	-0.8340560	6.2361820
C	3.2547050	5.5385490	-1.0288900
H	3.4041050	5.7421080	0.0267720
C	2.0040470	5.1268060	-1.4885680
H	1.1830770	5.0211060	-0.7872610
C	5.5000330	1.3422920	3.6623270
H	4.9524490	1.4561900	2.7388790

C	6.7619220	1.9229530	3.7206760
C	7.4645510	4.9863750	0.0505860
C	6.4239500	7.0774830	-1.4379960
H	6.0482490	7.9196280	-2.0047430
C	7.6247790	7.2040320	-0.7528470
H	8.2027790	8.1189110	-0.7706860
C	7.0585450	1.0998360	5.9115140
H	7.7182970	1.0247610	6.7659060
C	2.7543790	-0.1865990	5.6405620
H	2.9562180	0.2855200	6.5973010
C	8.5957850	4.6429890	4.0632620
H	7.9960390	4.8254890	4.9506240
C	8.9672430	2.2418210	4.8182790
H	9.5495970	1.3749360	4.4987940
H	9.2219160	2.5066020	5.8485220
C	3.7010130	-0.1213700	4.6004610
C	10.1702320	4.2010820	1.7920330
H	10.7676690	4.0134990	0.9053660
C	-3.8064050	0.0436950	4.6854640
N	-7.8231900	1.4189650	4.2734980
C	-1.3077590	-1.2197210	4.4285740
C	-9.1836760	1.9962720	3.9902890
H	-9.7398620	1.2336900	3.4365330
H	-9.6734500	2.1964610	4.9452210
C	-3.4731330	-1.0334290	5.5231050
H	-4.2048360	-1.4271050	6.2209360
C	-8.6864380	4.2525770	0.9643540
H	-8.6110020	4.1511640	-0.1163740
C	-9.0179080	3.2533120	3.1511740
C	0.5798060	4.0235140	-3.2065540
N	-6.8639340	6.6263650	0.0625800
C	-5.9367230	0.2479010	3.4301240
H	-5.5239240	-0.3508370	2.6288810

C	-1.2934400	4.0827430	-1.5816700
H	-0.8743280	3.1913180	-1.1266910
C	-4.5259610	6.2340340	0.3415610
H	-3.6938180	6.0705470	1.0131050
C	-2.2333250	-1.6712980	5.3815580
H	-2.0196000	-2.5662090	5.9562270
C	-8.8824440	4.5175610	3.7449170
H	-8.9770830	4.6315740	4.8210490
C	-5.2104950	0.5315420	4.5968400
C	-2.4282030	4.6610790	-1.0180270
H	-2.8427990	4.1867930	-0.1355930
C	-4.3352420	6.2140790	-1.0619060
C	-8.5242530	5.5176790	1.5580390
C	-0.7020990	4.6345500	-2.7303400
C	-1.2840010	5.7757090	-3.3142040
H	-0.8201040	6.2341480	-4.1813770
C	-2.8363980	0.5678880	3.8086270
H	-3.0673160	1.4226080	3.1788120
C	-1.5822510	-0.0403330	3.7088680
H	-0.8595060	0.3371570	2.9919560
C	-5.4558300	6.4970750	-1.8666970
H	-5.3824420	6.4934600	-2.9456770
C	-6.7042020	6.6828110	-1.2851840
H	-7.5936750	6.8369460	-1.8794750
C	-7.2446400	0.6947890	3.2800180
H	-7.8778680	0.4719450	2.3975570
C	-5.8633410	1.2442510	5.6273420
H	-5.3567900	1.4676620	6.5574100
C	-7.1656720	1.6844980	5.4371140
H	-7.7015120	2.2501350	6.1878690
C	-5.7849440	6.4343690	0.8735880
H	-5.9770550	6.4172690	1.9378470
C	-2.4686990	6.3160550	-2.7946540

H	-2.9137890	7.1840280	-3.2719510
C	-8.6393600	5.6491380	2.9510550
H	-8.5571420	6.6258700	3.4197880
C	-8.2314190	6.7280770	0.6919070
H	-8.9499040	6.8156740	-0.1255940
H	-8.2592660	7.6527750	1.2735960
C	-3.0468380	5.7645830	-1.6335410
C	-8.9451280	3.1256470	1.7509900
H	-9.0900370	2.1351540	1.3147830
C	3.0036280	-5.4191490	1.7367460
N	6.5331890	-6.8954610	-0.1853670
C	0.7768270	-4.0777700	2.8582070
C	7.7775410	-7.2623210	-0.9482910
H	8.5564580	-7.4840080	-0.2162290
H	7.5611570	-8.1808410	-1.4978890
C	2.9446680	-5.1550870	3.1211080
H	3.7516030	-5.4670980	3.7764030
C	9.4208640	-4.0779680	-2.2800760
H	10.1073700	-3.3213990	-1.9205280
C	8.1857530	-6.1332900	-1.8762100
C	0.6407200	2.7543570	-3.6970550
N	7.9519520	-1.7658240	-4.4073820
C	5.5014870	-5.7509790	1.6439100
H	5.6284620	-5.1653000	2.5432370
C	2.8435160	1.9124320	-2.7829580
H	2.5995500	2.3710850	-1.8325500
C	5.7404130	-1.2611370	-5.1626300
H	4.9132270	-1.5295660	-5.8056080
C	1.8411180	-4.5030120	3.6752980
H	1.8146560	-4.2964430	4.7393020
C	7.6227320	-6.0314830	-3.1605450
H	6.9544860	-6.8038320	-3.5313170
C	4.2124160	-5.9808920	1.1077810

C	4.0475110	1.2206510	-2.9152620
H	4.7068770	1.1466460	-2.0558030
C	5.6443410	-0.1759740	-4.2529330
C	8.8244130	-3.9467700	-3.5407990
C	1.9400060	2.0196120	-3.8566150
C	2.2723630	1.3897510	-5.0696830
H	1.5916550	1.4525740	-5.9123570
C	1.9028400	-5.0578850	0.9329410
H	1.9113360	-5.2081590	-0.1412730
C	0.8097410	-4.3967580	1.4879240
H	0.0007060	-4.0755390	0.8415500
C	6.7769550	0.0953500	-3.4638770
H	6.8213410	0.8985290	-2.7390020
C	7.9079240	-0.7150710	-3.5477500
H	8.7759750	-0.5058770	-2.9400890
C	6.6301900	-6.2105450	0.9889840
H	7.6278120	-6.0286120	1.3651220
C	4.1503440	-6.7242160	-0.0951790
H	3.1999190	-6.9783020	-0.5445350
C	5.3084110	-7.1598720	-0.7162920
H	5.2876130	-7.7267210	-1.6370330
C	6.8863400	-2.0252490	-5.2209790
H	6.9856300	-2.8541040	-5.9072570
C	3.4790260	0.6973070	-5.2088280
H	3.7174120	0.2601300	-6.1729390
C	7.9476930	-4.9513310	-3.9874070
H	7.5243560	-4.9137010	-4.9866830
C	9.1088200	-2.7226510	-4.3992440
H	9.9795930	-2.1798510	-4.0294110
H	9.2999450	-3.0015200	-5.4390550
C	4.3865580	0.5997250	-4.1329010
C	9.1093620	-5.1652510	-1.4559600
H	9.5867980	-5.2442640	-0.4837740

H	-6.5826240	-1.1407320	-7.0066080
H	7.8486120	4.1331030	0.6056180
H	7.1513210	2.4689670	2.8694940

PP_{cage}⇒(L)(phe-phe)₂

	X	Y	Z
C	6.0056300	-1.3975830	2.1428010
H	4.9776040	-1.2354670	2.4523770
C	7.0331150	-0.8828600	2.9481110
H	6.7816150	-0.3406620	3.8544020
C	8.3776440	-1.0818990	2.5974930
H	9.1724050	-0.6901860	3.2225070
C	8.6852690	-1.8016200	1.4300410
H	9.7212320	-1.9600970	1.1487930
C	7.6547590	-2.3115480	0.6282730
H	7.9055550	-2.8910850	-0.2587450
C	6.3057450	-2.1111350	0.9714190
C	5.2326140	-2.7254870	0.0923100
H	5.0715610	-3.7683760	0.4018540
H	5.5935050	-2.7582280	-0.9424640
C	3.8608780	-2.0414770	0.1189100
H	3.4437550	-2.0766720	1.1348340
C	3.9053330	-0.5471330	-0.2728890
C	1.6125720	-2.6996790	-0.7495990
C	0.8696530	-3.7670750	-1.5561830
H	0.0265260	-3.2593150	-2.0382520
C	0.3033500	-4.8414140	-0.5649280
H	0.7221260	-5.8177810	-0.8297330
H	0.6551790	-4.6253990	0.4508540
C	-1.2143970	-4.9112800	-0.5483550
C	-1.9630880	-3.7657860	-0.2167670
H	-1.4433170	-2.8421880	0.0303260
C	-3.3620810	-3.8104960	-0.2027790

H	-3.9315080	-2.9188620	0.0334640
C	-4.0405000	-5.0028850	-0.5020720
H	-5.1267570	-5.0173560	-0.5031580
C	-3.2996760	-6.1533010	-0.8105290
H	-3.8102510	-7.0848100	-1.0331350
C	-1.8947520	-6.1062120	-0.8393020
H	-1.3360010	-7.0045970	-1.0856860
N	2.9542920	-2.7964590	-0.7581620
H	3.3039580	-3.5143670	-1.3984160
N	1.7871450	-4.3624820	-2.5368520
H	1.8364660	-3.8601940	-3.4182730
H	1.6628180	-5.3572180	-2.6875890
O	4.9274110	0.0552170	-0.6184970
O	2.7164020	0.0931320	-0.1754920
O	0.9896350	-1.7989530	-0.0943960
C	-6.7277040	0.5971900	-2.8908700
H	-6.0628780	-0.1325870	-2.4381240
C	-6.2858170	1.2865800	-4.0332830
H	-5.2852020	1.1048680	-4.4141840
C	-7.1288380	2.1984070	-4.6837130
H	-6.7989210	2.7104580	-5.5803450
C	-8.4198610	2.4238630	-4.1774120
H	-9.0936960	3.1018350	-4.6886090
C	-8.8496020	1.7518470	-3.0249190
H	-9.8595210	1.9190380	-2.6603270
C	-8.0153200	0.8254330	-2.3653500
C	-8.6031330	0.0850320	-1.1647510
H	-9.1948020	0.7892100	-0.5691310
H	-9.3059100	-0.6678600	-1.5350990
C	-7.6196240	-0.6272340	-0.2195550
H	-8.1506110	-0.8700530	0.7110520
C	-7.1544020	-1.9970740	-0.7904950
C	-5.4608810	0.0701360	0.9259970

C	-4.4268720	1.2037760	0.9266620
H	-3.8197430	1.0109190	0.0296910
C	-3.4551910	1.1665350	2.1300060
H	-3.9623290	1.5592750	3.0196420
H	-3.1891750	0.1278630	2.3428310
C	-2.2273450	1.9888970	1.7903640
C	-1.1259690	1.3933480	1.1456010
H	-1.1339670	0.3264270	0.9330400
C	-0.0148210	2.1614390	0.7683610
H	0.8347670	1.6944860	0.2805610
C	0.0032720	3.5423900	1.0215830
H	0.8650630	4.1364260	0.7359110
C	-1.0942910	4.1495240	1.6501940
H	-1.0851480	5.2164680	1.8480130
C	-2.1993200	3.3736350	2.0307850
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N	-6.5033750	0.2818360	0.1052850
H	-6.5102190	1.2042870	-0.3282390
N	-5.1079570	2.4863040	0.7034890
H	-4.4854340	3.2190490	0.3775860
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O	-7.5150270	-2.4391570	-1.8792850
O	-6.3811500	-2.7385050	0.0468800
O	-5.2753930	-1.0129070	1.5701650
C	-3.3760200	-1.8587520	-4.3028970
N	-6.4247500	-4.8566020	-4.0642190
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C	-7.4748480	-5.9175210	-3.8184190
H	-8.4358970	-5.5064540	-4.1303020
H	-7.2416330	-6.7660960	-4.4657230
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C	1.0631520	-1.6941340	4.3539860
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C	-2.2947830	0.1103140	-5.2577720
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C	-6.7498680	-7.4209720	-1.8988750
H	-6.2825890	-8.0959610	-2.6107170
C	-4.4426120	-2.8938920	-4.2859120
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C	-0.2360500	-2.4264570	4.1834750
C	-0.4417990	-3.6854500	4.7795210
H	0.2971110	-4.0870220	5.4649730
C	-2.3579720	-1.9110500	-3.3271400
H	-2.3905260	-2.6721490	-2.5532080
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H	-0.5597680	-1.0171650	-2.5514280
C	-4.9862310	-4.1684620	2.9254330
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H	-3.1106420	-4.5212630	-3.7056350
C	-5.1243980	-5.1719230	-3.8140820
H	-4.9143740	-6.1912580	-3.5241970
C	-4.7677080	-6.9099440	2.7153480
H	-4.7324620	-7.9873560	2.6231440
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H	-1.7222580	-5.3938470	4.9860810
C	-6.6554440	-7.6969080	-0.5283150
H	-6.1065030	-8.5735930	-0.1971610
C	-7.1218920	-7.0964960	1.8951980
H	-8.0007700	-6.7798310	2.4611660
H	-6.9353260	-8.1460440	2.1282170
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C	-8.1779830	-5.5219010	-1.4210990
H	-8.7891950	-4.6939920	-1.7611270
C	2.9133240	5.2314970	-4.0920910
N	6.3690120	7.6409690	-3.3621620
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C	7.5957740	8.3091040	-2.7945630
H	8.3940050	8.2423680	-3.5359710
H	7.3618880	9.3660420	-2.6505920
C	2.7489510	4.3477300	-5.1774900
H	3.4322250	4.3800310	-6.0203930
C	9.4179810	6.1452820	-0.2000080
H	10.3145350	5.5346850	-0.1497990
C	7.9740430	7.6280740	-1.4849180
C	1.1642110	-0.3611760	4.6383800
N	7.8928170	4.6678740	2.6862050
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H	5.5357160	4.7378490	-4.8272070
C	2.8432710	0.5961970	3.0572320
H	2.2441010	0.1746070	2.2580980
C	6.2201570	3.9720850	4.2504250

H	5.7105730	4.1746950	5.1832460
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H	1.5610330	2.7839750	-6.0562600
C	7.1830680	7.8229210	-0.3356260
H	6.3422750	8.5104640	-0.3582250
C	4.0929920	6.1239300	-3.9648790
C	3.9494690	1.3902780	2.7445690
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C	8.6098500	6.3154680	0.9340800
C	2.4492060	0.3844400	4.3912680
C	3.2036610	0.9851760	5.4149560
H	2.9163970	0.8475320	6.4521220
C	1.9565350	5.2129050	-3.0556640
H	2.0591230	5.8819600	-2.2068100
C	0.8955320	4.3064520	-3.0821100
H	0.1808730	4.2954590	-2.2649870
C	6.5781180	2.7197450	2.2240060
H	6.3861640	1.8831080	1.5633300
C	7.5770390	3.6153130	1.8797290
H	8.1443110	3.5240820	0.9630550
C	6.4986560	6.4543120	-4.0166740
H	7.5056670	6.1295580	-4.2426320
C	3.9900170	7.4102940	-3.3888540
H	3.0253220	7.8490620	-3.1697240
C	5.1319210	8.1433130	-3.0979790
H	5.0858930	9.1262490	-2.6481200
C	7.2393890	4.8366200	3.8675490
H	7.5391430	5.6737650	4.4848250
C	4.3233190	1.7697540	5.1091220
H	4.8968010	2.1929520	5.9277640
C	7.4957240	7.1732710	0.8602290
H	6.8921610	7.3660170	1.7428270

C	8.9658040	5.6363950	2.2464300
H	9.9014980	5.0782670	2.1658030
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C	4.7076330	1.9958170	3.7686600
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C	-2.1741740	2.2074160	5.7050150
N	-5.5927700	4.7783260	5.9072820
C	0.0180590	0.5098710	5.0553250
C	-6.7697700	5.6834950	5.7258580
H	-7.6128440	5.2675290	6.2825860
H	-6.5240500	6.6444300	6.1864600
C	-2.1465580	0.8654550	6.1427440
H	-2.9486860	0.4711600	6.7589900
C	-8.7848680	6.4599410	2.5649210
H	-9.8136930	6.7122160	2.3273380
C	-7.1210080	5.8739980	4.2506080
C	-0.3596570	2.3839450	-4.0942900
N	-7.2724460	6.2229690	-0.8750220
C	-4.6725110	2.5715690	5.8062320
H	-4.8514130	1.5083120	5.7091850
C	-2.5433800	2.3875260	-2.7994320
H	-2.2466790	1.4661090	-2.3125810
C	-5.3022250	6.3516300	-2.2255320
H	-4.5180000	6.9738050	-2.6368300
C	-1.0581370	0.0412490	5.8442150
H	-1.0453680	-0.9697910	6.2330890
C	-6.1454060	5.8351180	3.2398600
H	-5.1060600	5.6244090	3.4783970
C	-3.3541050	3.0819820	5.8899270
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H	-1.0384530	3.7292460	4.6561320
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H	0.8203430	2.2752690	4.0833030
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H	-6.4929200	3.1673290	-2.0269330
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C	-5.7614290	3.4292220	5.8073630
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C	-3.2248550	4.4781610	6.0801330
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H	-3.5864890	5.7463900	-4.4461110
C	-6.4836290	6.1132810	1.9080980
H	-5.6949990	6.1085610	1.1599330
C	-8.1915850	6.8353170	0.1321720
H	-9.2147120	6.5297590	-0.1006540
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C	-4.1202190	4.2433570	-2.9707010
C	-8.4462820	6.1824040	3.8971160
H	-9.2219510	6.2279330	4.6552770
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N	7.8923500	-6.2491970	1.9068850
C	2.2687160	-2.5430460	4.0712120

C	8.9941680	-6.7288430	1.0032780
H	9.9461170	-6.6009970	1.5214440
H	8.8490640	-7.7986560	0.8359030
C	4.5162200	-3.3457980	4.6101940
H	5.3724040	-3.3219850	5.2764240
C	9.9446490	-4.3873190	-1.8943080
H	10.7882820	-3.7671880	-2.1814860
C	8.9475640	-5.9445030	-0.3047390
C	-0.1485020	1.0420360	-4.2462280
N	7.5191710	-2.9853450	-4.2311010
C	6.9910530	-4.4754540	3.2307890
H	7.1703910	-3.5362400	3.7365060
C	2.2555810	0.8064780	-3.4507140
H	2.0939380	1.5945320	-2.7254240
C	5.4854330	-2.4734420	-5.3894890
H	4.8808370	-2.6536880	-6.2679090
C	3.4148810	-2.5294010	4.8928320
H	3.4391410	-1.8964250	5.7720560
C	7.8371310	-6.0726130	-1.1627660
H	7.0325090	-6.7608950	-0.9203270
C	5.6899320	-5.0041130	3.0986550
C	3.5064840	0.1912870	-3.5008560
H	4.2717460	0.5644380	-2.8318510
C	5.0844370	-1.5647100	-4.3804190
C	8.8304490	-4.5055800	-2.7380800
C	1.2139870	0.4149320	-4.3152230
C	1.4732860	-0.6424320	-5.2140720
H	0.6955490	-0.9721430	-5.8949870
C	3.3344960	-4.2718910	2.7124220
H	3.2865220	-4.9380510	1.8550680
C	2.2426130	-3.4474080	2.9893370
H	1.3577680	-3.4969060	2.3626480
C	6.0096130	-1.3647270	-3.3217250

H	5.8121080	-0.6811360	-2.5058640
C	7.1954910	-2.0727420	-3.2729430
H	7.9046430	-1.9436720	-2.4661210
C	8.0650960	-5.1028440	2.6181400
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H	2.8600650	-2.0790660	-5.9668900
C	7.7773410	-5.3621560	-2.3629740
H	6.9297180	-5.5111680	-3.0264910
C	8.7883750	-3.7822780	-4.0765530
H	9.6326790	-3.0975130	-4.1872380
H	8.8268400	-4.4956920	-4.9035010
C	3.7685650	-0.8728200	-4.3918940
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PP_{cage}⇒(L)(tyr-tyr)₂

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H	4.5858040	-1.5630820	-2.3806420
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C	7.2475590	-4.5144290	-2.1498720
H	7.5977580	-4.6191280	-1.1342490
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H	9.6091170	-4.0321420	4.0623060
C	6.1054620	-5.5513440	3.6888850

H	5.1491530	-6.0509010	3.6145390
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H	3.8249720	-4.0907530	-5.8119690
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C	9.2684760	-5.8573140	-2.8297110
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H	-7.4481410	6.1560100	5.3347060
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C	-8.9412180	3.5654300	1.8932010
H	-9.6612350	2.8018330	1.6143390
C	-7.8126000	4.8353530	3.6373130
C	0.1228060	0.1627720	-4.3473960
N	-7.2492280	3.4142760	-1.2007250
C	-4.8456000	2.5178650	5.7958850
H	-4.8250450	1.4567560	6.0072440
C	-1.6797660	0.3282230	-2.6169890
H	-1.0490690	-0.2740280	-1.9722090
C	-5.6399460	3.3307540	-2.9691430

H	-5.3119010	3.7612280	-3.9048070
C	-0.7803600	0.7880780	6.0646710
H	-0.5147480	-0.0226910	6.7342280
C	-7.1677560	5.5947880	2.6421570
H	-6.5132630	6.4172510	2.9173350
C	-3.6553030	3.2327030	5.5355230
C	-2.8701560	0.8536790	-2.1111930
H	-3.1178900	0.6225030	-1.0811910
C	-4.9309700	2.2865960	-2.3379660
C	-8.2651170	4.2972150	0.9051780
C	-1.2465020	0.6232950	-3.9219730
C	-2.0556550	1.4577270	-4.7152480
H	-1.7430440	1.7146410	-5.7221200
C	-1.4508850	2.9306090	4.3984040
H	-1.7079930	3.7469470	3.7299400
C	-0.2494360	2.2453020	4.2074670
H	0.4153830	2.5504630	3.4052390
C	-5.4642800	1.8318950	-1.1065430
H	-4.9859180	1.0415660	-0.5457340
C	-6.6071770	2.3928120	-0.5708490
H	-7.0271760	2.0600120	0.3687010
C	-6.0755120	3.1569490	5.7279350
H	-7.0083500	2.6295090	5.8764970
C	-3.7756930	4.6248850	5.3274530
H	-2.8999500	5.2498660	5.2115270
C	-5.0270330	5.2219390	5.2815140
H	-5.1523500	6.2840430	5.1200380
C	-6.7855180	3.8713790	-2.3914720
H	-7.3390190	4.6713420	-2.8615110
C	-3.2604560	1.9697310	-4.2193610
H	-3.8573950	2.5891370	-4.8795640
C	-7.3882670	5.3290150	1.2893530
H	-6.9051460	5.9364340	0.5286420

C	-8.4842390	4.0067670	-0.5679820
H	-9.2973160	3.2962610	-0.7307600
H	-8.7163110	4.9169260	-1.1227540
C	-3.6867510	1.6927170	-2.9005400
C	-8.7165810	3.8332500	3.2540840
H	-9.2690090	3.2744850	4.0035410
C	2.8797530	3.4872340	-4.7860140
N	5.5185300	6.8173260	-4.4114330
C	1.1069250	1.2810010	-4.5082550
C	6.4300420	7.9097920	-3.9383330
H	7.3193370	7.9177900	-4.5720070
H	5.9118220	8.8601990	-4.0885070
C	3.0169720	2.3510840	-5.6074020
H	3.7770530	2.3229700	-6.3818560
C	8.4553940	7.7345210	-0.6882010
H	9.4885240	7.8751190	-0.3857120
C	6.7907610	7.7098680	-2.4688830
C	1.3724420	0.3960410	4.7672480
N	7.0897420	6.3320200	2.4654750
C	5.2048540	4.4965480	-4.8972080
H	5.6514630	3.5269800	-5.0768250
C	3.4980750	1.0595840	3.5561470
H	3.4137580	0.1758610	2.9359940
C	5.2968610	5.6163430	3.8785670
H	4.4799930	5.9112680	4.5231750
C	2.1340350	1.2700010	-5.4772240
H	2.2322300	0.4261380	-6.1509710
C	5.7940980	7.4337460	-1.5125250
H	4.7498610	7.3386740	-1.7989340
C	3.8017040	4.6518850	-4.8228430
C	4.4965580	1.9899400	3.2677740
H	5.1389110	1.7920560	2.4148480
C	5.5398270	4.2586300	3.5679860

C	7.4626950	7.4631190	0.2651920
C	2.5804570	1.2716930	4.6042440
C	2.7595790	2.4172720	5.4081640
H	2.1011460	2.5927560	6.2520230
C	1.8397790	3.5081450	-3.8363850
H	1.7326000	4.3683320	-3.1831610
C	0.9710230	2.4265980	-3.6977180
H	0.1958360	2.4690700	-2.9410900
C	6.6573010	3.9946920	2.7372500
H	6.9641000	2.9813900	2.5148370
C	7.3985450	5.0328240	2.1973610
H	8.2422720	4.8636710	1.5413900
C	6.0362450	5.5845790	-4.6796880
H	7.1149520	5.5000100	-4.6798820
C	3.3057220	5.9610670	-4.6668990
H	2.2447720	6.1684710	-4.6798130
C	4.1755520	7.0210910	-4.4524280
H	3.8163820	8.0252440	-4.2731380
C	6.0765860	6.6237770	3.3247600
H	5.8957090	7.6695830	3.5368430
C	3.7586820	3.3536580	5.1223100
H	3.8625140	4.2121160	5.7775170
C	6.1296150	7.3110050	-0.1606450
H	5.3345930	7.1252130	0.5569180
C	7.8274310	7.4242600	1.7452340
H	8.8988240	7.2644500	1.8882560
H	7.5699070	8.3681900	2.2327730
C	4.6181430	3.1825630	4.0154190
C	8.1205680	7.8572460	-2.0467440
H	8.9035030	8.0889070	-2.7621090
C	-2.6639290	-4.2234270	-4.4456220
N	-5.8932920	-6.8861390	-3.5498330
C	-0.6231660	-2.2257880	-4.4812590

C	-6.9926530	-7.6699650	-2.8804120
H	-7.9316680	-7.4202650	-3.3790450
H	-6.8018770	-8.7321680	-3.0429910
C	-2.8183270	-3.0387650	-5.1971580
H	-3.7026700	-2.8793850	-5.8050040
C	-7.5642140	-5.7214940	0.3692860
H	-8.0149810	-4.7789270	0.6698050
C	-7.0224580	-7.3132340	-1.3990480
C	1.3722170	-0.9625350	4.5989100
N	-5.8873730	-5.4446970	3.2238330
C	-5.1241780	-4.8009330	-4.4281160
H	-5.3875500	-3.8201590	-4.8006980
C	-0.8659570	-1.3213830	3.4782060
H	-0.6827760	-0.4362260	2.8785150
C	-3.6105790	-5.3824760	3.9602120
H	-2.7494430	-5.9412140	4.3032080
C	-1.8147350	-2.0676100	-5.2215750
H	-1.9523980	-1.1869510	-5.8369170
C	-6.5318360	-8.2040690	-0.4321800
H	-6.1752300	-9.1880800	-0.7211110
C	-3.7733920	-5.1932650	-4.2752980
C	-2.0497710	-2.0359570	3.2911270
H	-2.7477720	-1.6815920	2.5379930
C	-3.5577060	-3.9775230	3.7970670
C	-7.0523790	-6.6072250	1.3368640
C	0.0904280	-1.7294910	4.4293940
C	-0.1685060	-2.8999040	5.1698210
H	0.5475600	-3.2379790	5.9114580
C	-1.4340320	-4.4232280	-3.7817490
H	-1.2355590	-5.3402770	-3.2344260
C	-0.4374820	-3.4465450	-3.7996250
H	0.4879170	-3.6378130	-3.2681750
C	-4.7500120	-3.3456310	3.3702580

H	-4.8208880	-2.2698240	3.2774150
C	-5.8894770	-4.0892220	3.0943780
H	-6.8146270	-3.6207890	2.7771250
C	-6.1545460	-5.6545970	-4.0666350
H	-7.1946830	-5.3720080	-4.1614330
C	-3.5502760	-6.5305890	-3.8680790
H	-2.5551720	-6.9535580	-3.8363550
C	-4.6120560	-7.3422120	-3.4995300
H	-4.4673270	-8.3557740	-3.1493240
C	-4.7721540	-6.0851640	3.6705260
H	-4.8358180	-7.1592810	3.7860290
C	-1.3494100	-3.6272530	4.9790710
H	-1.5291400	-4.4973350	5.6026670
C	-6.5524870	-7.8542570	0.9275530
H	-6.2177260	-8.5808370	1.6622010
C	-7.1030620	-6.2386510	2.8120950
H	-7.9790440	-5.6276900	3.0384420
H	-7.1449880	-7.1265330	3.4458660
C	-2.3111710	-3.2067050	4.0355860
C	-7.5516990	-6.0770470	-0.9833650
H	-8.0109160	-5.4112680	-1.7092160
O	-3.6908290	-1.2350650	0.4956040
O	-6.0579320	-0.8839380	1.5081300
O	-7.7231650	-2.3503410	1.0551220
O	-9.6511980	2.5775330	-3.2264890
O	3.5458210	-5.5794850	0.6493090
N	-4.9522830	-2.8229300	-0.5720960
N	-2.9933710	-4.6115110	-0.7032150
C	-6.0869900	-1.9009150	-0.7225180
C	-2.6747570	-3.4274700	0.0972630
C	-7.1139800	-2.3309000	-1.7803960
C	-1.3474730	-2.7268530	-0.2554750
C	-3.8110280	-2.4101010	0.0049810

C	-7.8871090	-1.1014980	-2.2289280
C	-0.0907810	-3.5326330	0.0212880
C	-6.7308340	-1.7315530	0.6741440
C	-7.3615990	-0.2837870	-3.2469050
C	-9.0757850	-0.7105550	-1.5896500
C	1.1080830	-3.1358810	-0.6026560
C	-0.0464080	-4.6371610	0.8878460
C	-7.9899830	0.9114150	-3.6036220
C	-9.7068620	0.4968980	-1.9264050
C	2.3038150	-3.8261620	-0.3944880
C	1.1475850	-5.3390790	1.1136280
C	-9.1476130	1.3128900	-2.9222380
C	2.3185150	-4.9372620	0.4574120
H	-5.6684640	-0.9375080	-1.0288490
H	-2.6448120	-3.7191300	1.1548180
H	-6.5734580	-2.7717460	-2.6260840
H	-7.7838190	-3.0853210	-1.3590560
H	-1.3094720	-1.7825510	0.2993150
H	-1.3743500	-2.4649670	-1.3223790
H	-4.9622950	-3.7869470	-0.9057910
H	-2.5828990	-4.5946850	-1.6311120
H	-2.8517140	-5.5001740	-0.2400130
H	-6.4629190	-0.5879260	-3.7793150
H	-9.5161170	-1.3438160	-0.8257280
H	1.1076540	-2.2783100	-1.2712910
H	-0.9379160	-4.9694890	1.4107080
H	-7.6252310	1.5259720	-4.4181300
H	-10.6325270	0.7833330	-1.4363610
H	3.2138860	-3.5257830	-0.8990770
H	1.1588580	-6.1895950	1.7890680
H	-10.6185830	2.6166800	-3.3435330
H	3.4485580	-6.5226250	0.8712810
O	0.3386130	2.7606690	-0.5348300

O	0.1381120	7.4854250	-2.4180320
O	2.2336620	6.8388620	-1.9358400
O	-5.8649170	6.8252050	-1.2379180
O	7.3385160	-2.1095520	0.0523450
N	1.5329450	4.7302180	-0.4710560
N	3.7366350	3.4854230	0.3757980
C	0.4345540	5.5820570	-0.8791120
C	2.8008840	2.6659920	-0.4029680
C	-0.3917480	6.1789360	0.3076380
C	2.6395980	1.1957550	0.0245780
C	1.4330420	3.3758980	-0.4456500
C	-1.8430600	6.4120410	-0.0734730
C	3.9088820	0.3580520	-0.0342410
C	1.0190090	6.6827790	-1.7756580
C	-2.7115700	5.3043940	-0.1648200
C	-2.3546280	7.6910210	-0.3596360
C	3.9270240	-0.8924440	0.6179940
C	5.0785360	0.7505020	-0.7096710
C	-4.0459600	5.4690260	-0.5355290
C	-3.6907680	7.8670790	-0.7581130
C	5.0661840	-1.7009070	0.6346300
C	6.2362180	-0.0457450	-0.7018400
C	-4.5302610	6.7487580	-0.8523560
C	6.2320540	-1.2645710	-0.0094630
H	-0.2539270	4.9672610	-1.4741680
H	3.1424300	2.6892330	-1.4477910
H	-0.3355000	5.4397220	1.1121480
H	0.0766600	7.0986300	0.6726990
H	1.8610220	0.7511130	-0.6079790
H	2.2385560	1.1673730	1.0462840
H	2.4678850	5.1161510	-0.3611790
H	3.6052950	3.4243740	1.3800310
H	4.7106020	3.4118850	0.1123430

H	-2.3334060	4.3089330	0.0561230
H	-1.7243180	8.5698150	-0.2519490
H	3.0315320	-1.2473690	1.1220930
H	5.1082570	1.6761040	-1.2751640
H	-4.7207220	4.6229080	-0.5777120
H	-4.0606170	8.8639100	-0.9787460
H	5.0675980	-2.6531820	1.1520630
H	7.1248580	0.2855990	-1.2322580
H	-6.1503990	7.7205080	-1.4974450
H	8.1542410	-1.6980250	-0.2832420

MM_{cage}⇒(D)(phe-phe)₂

	X	Y	Z
C	-0.5307050	3.2194670	1.0008750
H	0.1605490	3.5452020	1.7679900
C	-1.7681270	3.8708140	0.8807630
H	-2.0198010	4.6692730	1.5709350
C	-2.6685540	3.5024020	-0.1275780
H	-3.6199510	4.0159610	-0.2261430
C	-2.3195130	2.4800640	-1.0248420
H	-2.9984460	2.2062690	-1.8263470
C	-1.0831880	1.8373870	-0.9061730
H	-0.8089500	1.0587360	-1.6151510
C	-0.1772800	2.1925650	0.1115900
C	1.1085290	1.3872520	0.1999950
H	1.5213430	1.2768080	-0.8116880
H	0.8459760	0.3785120	0.5501570
C	2.2452370	1.8718960	1.1258870
C	4.4593660	1.0125800	1.7730250
C	5.6345390	0.1675510	1.2969590
C	6.3703750	1.0601540	0.2423230
H	5.6207580	1.4661560	-0.4487440
H	6.8040700	1.9077310	0.7860450

C	7.4397720	0.3138100	-0.5234670
C	8.7830400	0.3289780	-0.0999860
H	9.0672130	0.9075650	0.7755370
C	9.7713280	-0.3649600	-0.8176500
H	10.8040250	-0.3339270	-0.4891900
C	9.4287180	-1.0747990	-1.9791640
H	10.2008470	-1.5799960	-2.5487440
C	8.0923160	-1.0910520	-2.4115590
H	7.8265370	-1.6058870	-3.3301040
C	7.1063310	-0.4086410	-1.6860330
H	6.0743590	-0.4192510	-2.0327490
N	3.2972030	0.8593590	1.0740600
H	3.2378660	0.1323270	0.3697240
O	4.5904410	1.8892840	2.6620430
C	-0.5619540	-3.5633950	-0.1199110
C	-0.5515080	-2.9815700	-1.5436830
C	-2.5383400	-2.2890210	0.7588030
C	-3.9631870	-2.4392410	1.2978900
C	-4.8746250	-1.3046060	0.7694600
H	-4.3451740	-0.3568670	0.8995290
H	-5.0249740	-1.4467360	-0.3096720
C	-6.2047420	-1.2922220	1.4975290
C	-7.3493070	-1.8881770	0.9386050
H	-7.2917220	-2.3447180	-0.0470210
C	-8.5737210	-1.8849590	1.6279410
H	-9.4554270	-2.3247950	1.1733590
C	-8.6671350	-1.2862320	2.8946930
H	-9.6150300	-1.2637040	3.4207130
C	-7.5259690	-0.6971830	3.4675790
H	-7.5944930	-0.2304310	4.4445780
C	-6.3053050	-0.7060010	2.7756570
H	-5.4267730	-0.2550980	3.2309460
N	-1.9052170	-3.4422140	0.4691940

H	-2.4912890	-4.2669650	0.6096760
O	-0.3077390	-3.6715960	-2.5306600
O	-0.7930800	-1.6405000	-1.6437260
O	-2.0156340	-1.1409370	0.5729150
C	0.5550490	-2.9287730	0.7545420
H	0.2786350	-1.9010000	1.0051490
H	-0.3594760	-4.6293870	-0.2371730
N	-4.4590270	-3.7910580	1.0059950
H	-4.9173250	-3.8700040	0.1011140
H	-5.0507490	-4.1709250	1.7344140
H	-3.8894370	-2.3262790	2.3853950
N	6.4547350	-0.2137320	2.4443810
H	6.4573670	0.4987780	3.1708300
H	7.3976220	-0.4949710	2.1901010
H	5.2676240	-0.7359740	0.7890630
H	1.8948450	1.9961720	2.1531240
C	2.8558070	3.2088410	0.6784020
O	3.7105980	3.3337470	-0.2043230
O	2.3646840	4.2697390	1.3788020
C	-3.9094230	-1.9237970	-4.8999060
N	6.5853570	-5.2382110	2.5121980
C	-3.1077050	-2.0545450	-6.0547230
H	-3.3679170	-2.7651430	-6.8325410
C	-1.9655540	-1.2645190	-6.2269840
H	-1.3497390	-1.4101920	-7.1079530
C	0.6296770	-1.9023120	4.5265540
C	1.0212910	-3.0625420	5.2233940
H	0.3768810	-3.4739610	5.9933840
C	2.2318150	-3.7069380	4.9335440
H	2.5040090	-4.5891760	5.5044620
C	3.0974420	-3.1990400	3.9436120
C	2.7330120	-2.0063570	3.2856310
H	3.3725400	-1.5942260	2.5120950

C	1.5198300	-1.3797460	3.5648430
H	1.2479670	-0.4837400	3.0161140
N	6.3199860	-5.1340160	-4.5152370
N	-7.0909980	-4.6501630	-3.9429230
C	7.9354630	-4.8387150	-1.8168750
H	8.2831400	-3.9750440	-2.3765620
C	-1.5889670	-0.3132660	-5.2586430
C	2.0468340	-0.4199650	-6.1815770
H	2.1078710	0.4367650	-6.8437430
C	7.7524950	-5.9279600	1.8523210
H	8.6569100	-5.4032060	2.1686150
H	7.8058380	-6.9419950	2.2520090
C	6.5742150	-3.8977380	-5.0253690
H	7.6130250	-3.6348420	-5.1777560
C	0.8279390	-1.7777750	-4.5960630
H	-0.0491410	-1.9765470	-3.9972640
C	7.6205680	-5.9354750	0.3358750
C	3.9713080	-4.7296120	-4.6825680
H	2.9709670	-5.1276690	-4.5858610
C	4.1923500	-3.3997860	-5.1210150
C	3.1132830	-1.3276250	-6.1315210
H	3.9649220	-1.1622640	-6.7840370
C	4.3341000	-3.9070000	3.5301230
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C	-9.4441630	-5.8893310	-1.3566590
H	-10.3681730	-5.6964630	-1.8931040
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H	-6.0713620	-6.1363190	-1.8042680
C	-7.0994940	-6.4644030	0.0541410
H	-6.1799150	-6.7259610	0.5721120
C	-8.3393140	-6.5293530	0.7206860

C	1.8893070	-2.6738400	-4.5321880
H	1.7924210	-3.5168430	-3.8578200
C	-3.5616360	-0.9302830	-3.9588030
H	-4.1353050	-0.8102660	-3.0442510
C	-0.7252660	-1.2687920	4.7066960
C	7.1712040	-7.0841160	-0.3352900
H	6.9166310	-7.9811310	0.2212110
C	-0.2417700	0.3526470	-5.2903320
C	-8.1745560	-5.6057600	-3.5291190
H	-7.9935260	-6.5472320	-4.0542810
H	-9.1275670	-5.2100640	-3.8891520
C	5.0333890	-5.5603600	-4.3791400
H	4.8901200	-6.5716270	-4.0225890
C	-2.4257530	-0.1418570	-4.1383530
H	-2.1454290	0.5732650	-3.3744550
C	-7.1314660	-3.3646260	-3.4902660
H	-7.9844760	-3.0965110	-2.8806430
C	-5.0367320	-2.8456400	-4.6249490
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C	-6.1370760	-2.4592690	-3.8158910
H	-6.2376830	-1.4408910	-3.4644460
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C	5.5400070	-3.0227010	-5.3297590
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C	-7.5716880	-4.9725690	3.2897200
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H	-9.4157280	-6.7987740	2.5960130
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H	-2.7655440	-5.2290060	3.3047120
C	-1.8005890	-3.4296390	3.9525400
H	-0.8730380	-3.7013280	3.4642850

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C	1.8573400	3.3613560	-5.2354430
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C	-2.1178630	0.8554100	4.5656560
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H	-2.2836600	1.7111600	6.5459970
C	-3.7525390	2.5486340	5.2187900
H	-4.1812740	3.1625620	6.0043750
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H	-4.0380040	1.7779150	1.9057290
C	-2.6513930	0.8733020	3.2616270
H	-2.2145980	0.2553110	2.4814070
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C	-8.9087060	6.9287830	-1.4906720
H	-9.6787520	6.7241370	-2.2282140
C	1.3132830	2.2046290	-4.6476700
C	-2.2079050	2.6964520	-5.9237580
H	-2.2178810	1.9790860	-6.7365990
C	-8.3672590	6.3677310	2.2626450
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C	-1.1289150	3.6894180	-3.9999870
H	-0.3221920	3.7186650	-3.2759440
C	-8.1423290	6.7881870	0.8192610
C	-4.0950210	6.9046180	-4.1968240

H	-3.0869590	7.2947490	-4.1451960
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C	-5.3477980	3.5420800	3.5293650
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H	9.7683500	6.7986090	0.8538800
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C	7.0173460	4.7863740	0.9616220
H	6.3136210	4.2397410	0.3394560
C	6.8193050	4.7651300	2.3528580
H	5.9942540	4.1712910	2.7373510
C	7.6726740	5.4836420	3.2040230
C	-2.1507450	4.6340300	-3.9100650
H	-2.1203430	5.3640150	-3.1070860
C	3.2371090	2.1155390	-3.1449590
H	3.7422150	1.6595990	-2.2981160
C	-0.8521510	0.0892830	4.8334050
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H	-4.9889570	8.7558590	-3.5159760
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H	2.9523550	5.3520600	5.1774430
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H	4.3727350	5.9547470	-3.3061530
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H	-7.9267910	3.9854740	1.3109080
C	-6.8148500	7.9643020	-0.8474060
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C	-6.4889950	5.6827560	3.7658620
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C	-5.5032000	4.7906200	4.1732310
H	-4.8500230	5.0934940	4.9810940

C	-3.2335510	4.6118240	-4.8119730
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H	-10.0131500	5.9733640	0.0925780
C	7.5081700	5.5091850	4.7244820
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H	7.4707580	6.5377380	5.0933690
C	1.3086970	0.6478260	6.0653630
H	1.1909220	-0.2357490	6.6822660
C	2.4437580	1.4481300	6.2260010
H	3.1767200	1.1737440	6.9779230
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H	1.7007190	3.8718860	3.9422020
C	0.4616210	2.1841600	4.4017160
H	-0.3107310	2.4827790	3.7014100
C	0.3227460	0.9764930	5.1126100
C	1.9204020	-2.9639170	0.0843310
C	2.2970950	-1.9802630	-0.8531670
C	2.8344320	-3.9911960	0.3766240
C	3.5561370	-2.0172160	-1.4698260
H	1.5860050	-1.2114820	-1.1411750
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H	2.5567740	-4.7672670	1.0846630
C	4.4677570	-3.0375870	-1.1544390
H	3.8061610	-1.2717010	-2.2195030
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MM_{cage}⇒(D)(tyr-tyr)₂

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C	-2.1844500	-0.6392860	-0.2091610
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C	2.8066750	-0.6928700	-0.2816170
C	1.7909490	-2.8784200	-0.1536420
C	4.0824530	-1.2717060	-0.2721220
C	3.0616690	-3.4727850	-0.1345390
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H	-3.3657510	-2.2601900	-0.7113060
H	2.7105960	0.3905150	-0.3292290
H	0.9159270	-3.5128910	-0.0711820
H	4.9774220	-0.6579480	-0.2902200
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O	2.1458390	2.8194800	-0.2452720
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C	-3.8006210	5.8472480	-0.0892500
C	5.2302070	0.9329620	2.9254260
C	7.4941650	1.1782430	2.0685550
C	-4.3646780	4.5772570	-0.2906670
C	6.6131170	0.7355940	3.0670840
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H	2.7755420	5.8985550	-0.6791080
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H	-8.8514010	2.6524610	-0.6658670
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H	4.9152760	5.3212510	-1.5579040
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C	3.6186140	1.8828020	-4.3071520
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C	-1.4808200	1.6715300	4.4300320
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H	-9.1804180	5.9824300	2.2688820
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C	-4.3927630	2.8734130	-4.1338910
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H	-4.0388960	0.8347040	-6.0008820
C	-4.9627010	4.0286360	3.4243760
C	8.2154730	5.2307920	0.4211410
H	8.5045130	4.4732640	1.1435310
C	8.2819160	4.9372570	-0.9423160
H	8.6390180	3.9600940	-1.2560370
C	7.9385090	5.9071850	-1.9040490
C	7.5740880	7.1916130	-1.4718460
H	7.3649760	7.9771720	-2.1914280
C	7.5140110	7.4907640	-0.0982210
H	7.2596020	8.4998530	0.2106000

C	7.8117040	6.5075190	0.8588740
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C	3.5398230	0.7325850	-3.4983920
H	4.3134200	0.5189350	-2.7662080
C	-0.1642960	0.9779830	4.6393540
C	-7.2756130	7.3148450	-0.2526620
H	-6.7630880	8.0930470	0.3044650
C	0.1551520	-0.7410970	-4.5312110
C	7.9957140	5.5657330	-3.3874560
H	7.8907300	6.4548000	-4.0120530
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C	-5.0601120	5.1447630	-3.5939000
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C	2.4416890	-0.1288500	-3.5796830
H	2.4011990	-0.9893040	-2.9223190
C	7.1142020	3.2654780	-3.7597040
H	8.1369150	2.9415250	-3.6199660
C	4.7547080	2.8230200	-4.1624570
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H	5.5207630	6.1624200	-4.0282760
C	6.0753140	2.3654890	-3.9537990
H	6.3035270	1.3079530	-3.9691000
C	-1.1068760	0.0731230	-4.4231650
C	-6.0173860	3.4669470	2.6700520
H	-6.0434680	2.4123440	2.4286090
C	-5.7262120	2.6438630	-4.5352010
H	-6.0412600	1.6765730	-4.9036260
C	5.6816760	4.1539780	4.0937730
H	5.8858630	3.2264090	4.6117040
C	6.7571510	4.9166130	3.6595150
H	7.7807760	4.6186440	3.8426240

N	6.5643160	6.0724060	2.9643740
C	5.2998020	6.5348250	2.7522160
H	5.2054860	7.4880710	2.2489230
C	4.1973180	5.8076240	3.1667180
H	3.2143140	6.2254560	2.9956560
C	4.3566630	4.5572870	3.8130770
C	4.5664910	4.2249740	-4.2081680
H	3.5833200	4.6475720	-4.3695120
C	-7.0639550	4.2532390	2.2232960
H	-7.8666850	3.8363320	1.6305580
C	-7.0710900	7.2105210	-1.6376330
H	-6.4103420	7.9167930	-2.1310980
C	-6.1418770	6.1532570	3.2720580
H	-6.2401150	7.2077040	3.4950170
C	-7.3808430	5.9816140	-3.8448460
H	-8.2546700	5.6769340	-4.4233610
H	-6.9720210	6.8810640	-4.3103020
C	-5.0701900	5.4024890	3.7390520
H	-4.3103940	5.9061210	4.3223860
C	-3.3289560	1.8379480	-4.2080780
C	-8.8948350	5.5185100	-0.3604500
H	-9.6507900	4.9035870	0.1185410
C	7.7258470	6.8079940	2.3493960
H	8.6309740	6.4933650	2.8731240
H	7.5889270	7.8742530	2.5402420
C	2.0968220	1.9273960	5.3945420
H	2.0967960	1.2700460	6.2563170
C	3.1766790	2.7968160	5.1997230
H	3.9848810	2.7958070	5.9240240
C	3.1939350	3.6900150	4.1091700
C	2.0858280	3.7022650	3.2373220
H	2.0656390	4.3698510	2.3811290
C	1.0140190	2.8322470	3.4308300

H	0.1780940	2.8575560	2.7398330
C	1.0080810	1.9114310	4.4986650
C	-3.0809630	-4.8847190	-3.8944830
N	7.3262540	-4.6826740	3.4076630
C	-2.2034420	-5.0641320	-4.9827810
H	-2.3022260	-5.9223890	-5.6398050
C	-1.1931090	-4.1275350	-5.2431430
H	-0.5157900	-4.3033690	-6.0721780
C	1.3705530	-0.9824710	4.6864230
C	1.9768970	-1.6777820	5.7493130
H	1.4978120	-1.6993700	6.7225160
C	3.1914750	-2.3508370	5.5657270
H	3.6431460	-2.8443780	6.4200310
C	3.8194980	-2.3717240	4.3014850
C	3.2123250	-1.6633920	3.2453140
H	3.6444790	-1.6639610	2.2521750
C	2.0208030	-0.9676880	3.4399560
H	1.5873060	-0.4280040	2.6039170
N	7.4400600	-6.4633360	-3.3566290
N	-5.8542070	-7.7784810	-2.3652640
C	9.6633140	-5.9824390	-0.6001310
H	10.5487280	-5.7754030	-1.1930520
C	-1.0276800	-2.9813990	-4.4365110
C	2.5231830	-2.6613560	-5.5177950
H	2.4146080	-1.9140430	-6.2959670
C	8.5263100	-5.5116360	3.0298480
H	9.4221500	-4.9451420	3.2954380
H	8.5045980	-6.4111430	3.6500250
C	7.5071160	-5.1475150	-3.7019660
H	8.4639510	-4.6592860	-3.5726440
C	1.6197110	-3.9188740	-3.6597410
H	0.8153680	-4.1281540	-2.9628500
C	8.5262330	-5.8790620	1.5545760

C	5.1314610	-6.5223560	-3.9689040
H	4.2311130	-7.1079770	-4.1028510
C	5.1380700	-5.1327100	-4.2253180
C	3.7194940	-3.3878560	-5.4254730
H	4.5116720	-3.1976610	-6.1429590
C	5.0619730	-3.1394520	4.0454480
C	-8.0699930	-7.8144950	1.8404440
H	-9.0268610	-7.5831480	2.2982010
C	-8.0231840	-8.0949090	0.4628140
H	-8.9444610	-8.0720360	-0.1113050
C	-6.8098260	-8.4339500	-0.1535290
C	-5.6425970	-8.5070270	0.6315600
H	-4.7015180	-8.8139600	0.1833450
C	-5.6894720	-8.2310260	1.9998140
H	-4.7812070	-8.3343310	2.5872550
C	-6.9040630	-7.8718990	2.6178980
C	2.7964850	-4.6592590	-3.5795900
H	2.8902560	-5.4244190	-2.8151270
C	-2.9453830	-3.7117070	-3.1245130
H	-3.6195170	-3.5512740	-2.2919610
C	-0.0011900	-0.3685800	4.7986770
C	7.4357760	-6.5718490	0.9918620
H	6.5892460	-6.8535120	1.6127260
C	0.1862110	-2.1049720	-4.5833970
C	-6.7526740	-8.7524970	-1.6414210
H	-6.3538440	-9.7543240	-1.8159060
H	-7.7425090	-8.7005950	-2.1007560
C	6.2863480	-7.1624030	-3.5417080
H	6.3134910	-8.2233060	-3.3292950
C	-1.9446170	-2.7765700	-3.3895380
H	-1.8604810	-1.8911820	-2.7689780
C	-6.1100910	-6.4463190	-2.2436120
H	-6.9942170	-6.1709950	-1.6847750

C	-4.0895950	-5.8967890	-3.4777110
C	8.5724940	-6.6572910	-1.1639830
C	-4.7873830	-8.1987730	-3.0981280
H	-4.6495410	-9.2671690	-3.2043210
C	-5.2611360	-5.5006330	-2.7877990
H	-5.5138440	-4.4576850	-2.6498600
C	1.4678050	-2.8929300	-4.6141900
C	5.9121870	-2.8060810	2.9633040
H	5.7262370	-1.9378940	2.3464780
C	6.3827940	-4.4696500	-4.1497910
H	6.4653770	-3.4160790	-4.3815760
C	-5.5070780	-4.1743900	4.5483820
H	-5.8337080	-3.1602820	4.3568790
C	-6.3992770	-5.2145260	4.3257820
H	-7.4053750	-5.0457540	3.9649250
N	-6.0331780	-6.5104580	4.5305050
C	-4.8008170	-6.7979520	5.0336250
H	-4.5869210	-7.8370460	5.2476400
C	-3.8697990	-5.7926720	5.2567820
H	-2.9060550	-6.0642240	5.6677930
C	-4.1850850	-4.4446310	4.9705680
C	-3.9009140	-7.2843220	-3.6615910
H	-3.0477350	-7.6720960	-4.2031140
C	7.0124590	-3.5854270	2.6616180
H	7.6552200	-3.3654800	1.8203540
C	7.4598910	-6.9567420	-0.3507230
H	6.6289190	-7.5344840	-0.7467800
C	6.5641670	-5.0060160	4.4895480
H	6.8645210	-5.8710020	5.0670010
C	8.5950200	-7.0914220	-2.6261520
H	9.5206570	-6.7943190	-3.1226250
H	8.5007910	-8.1755180	-2.7240700
C	5.4395660	-4.2599740	4.8204200

H	4.8524540	-4.5845670	5.6692810
C	3.8729880	-4.3893580	-4.4466580
C	9.6397670	-5.5956170	0.7519870
H	10.5082790	-5.0985320	1.1728000
C	-6.9641470	-7.6218750	4.1214140
H	-7.9725530	-7.3530980	4.4423150
H	-6.6700230	-8.5138170	4.6801850
C	-2.3826550	-1.1047520	5.4776950
H	-2.5957970	-0.1304570	5.8995320
C	-3.3877810	-2.0820260	5.5087880
H	-4.3459440	-1.8338800	5.9549820
C	-3.1444900	-3.3852620	5.0280490
C	-1.8575280	-3.6810570	4.5379080
H	-1.6287600	-4.6747790	4.1649220
C	-0.8680980	-2.6999020	4.4851710
H	0.0964020	-2.9678060	4.0715560
C	-1.1079720	-1.3792590	4.9304860

PPP*→3*S

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C	13.2730360	4.4138470	-1.8765330
H	12.9693090	4.5093710	-2.9273520
H	13.4465720	3.3562950	-1.6529110
C	14.5665110	5.1823370	-1.5840260
H	14.6408080	6.0998640	-2.1845910
H	14.5883760	5.4498640	-0.5253620
C	15.9133560	3.8633370	-3.1574510
H	15.7432140	4.6944870	-3.8593600
H	15.1921160	3.0624830	-3.3657570
C	17.3411810	3.3206480	-3.3261100
H	17.7443830	3.6185160	-4.2960330
H	17.9692080	3.7483470	-2.5312070
C	16.5661250	-2.3274230	-1.1734380

H	17.4110240	-2.7683320	-1.7257960
C	16.5089810	-2.9944990	0.1995040
H	16.6491530	-4.0787790	0.0631710
H	17.3225110	-2.6091920	0.8192650
C	14.1031850	-3.4313060	0.5013150
H	14.3492070	-4.4623030	0.1982160
H	13.6872830	-2.8926680	-0.3582750
C	13.1107000	-3.5068810	1.6577430
H	12.2846650	-4.1809910	1.4012880
H	13.6215630	-3.8900290	2.5434530
C	3.1810240	-3.1667310	-0.0058600
C	2.1725500	-3.8519530	-0.0664790
C	-4.6333540	-0.5211430	-0.4403240
C	-4.7210160	0.6951710	-0.4955070
O	-10.0007300	8.4191130	-2.4861760
C	-11.1165050	8.4948990	-1.5561150
H	-10.7950940	9.0009190	-0.6375910
H	-11.4742020	7.4843170	-1.3093830
C	-12.2567570	9.2417460	-2.2390920
H	-12.3858100	8.8469120	-3.2490140
H	-13.1808760	9.0666680	-1.6636030
O	-12.0427070	10.6574880	-2.4140650
C	-12.1421970	11.4556170	-1.2115190
H	-11.4876530	11.0834920	-0.4153080
H	-13.1790400	11.4579250	-0.8391460
C	-11.7635800	12.8744000	-1.5951170
H	-12.3532020	13.1944180	-2.4626770
H	-11.9445630	13.5498830	-0.7490810
O	-10.3559900	12.9081990	-1.9571380
C	-9.8429990	14.1693640	-2.4669630
H	-10.6196210	14.6352690	-3.0858340
H	-8.9848200	13.9150000	-3.0911390
C	-9.3893320	15.0983280	-1.3493880

H	-9.3341150	16.1334230	-1.7232840
H	-10.1086800	15.0709310	-0.5148770
O	-8.0918810	14.6503820	-0.9220820
C	-7.6798930	15.2098530	0.3537530
H	-8.3810870	14.8688750	1.1267070
H	-7.6776650	16.3090140	0.3027330
C	-6.2919530	14.7093060	0.6858940
H	-6.1140000	14.7941810	1.7690080
H	-6.2039980	13.6589960	0.3939840
O	-5.3227610	15.5325890	-0.0237770
C	-3.9496660	15.1410130	0.1726030
H	-3.6811690	15.1573700	1.2401860
H	-3.3687820	15.9038650	-0.3516160
C	-3.6086020	13.7628580	-0.3925960
H	-4.2657530	13.5379940	-1.2420720
H	-2.5596590	13.7378400	-0.7185150
O	-3.8041680	12.7768550	0.6612380
C	1.4628890	4.8284650	-0.2351970
C	2.5619290	4.2994210	-0.1874370
O	12.2205860	4.9448000	-1.0193680
O	15.7463240	4.3586940	-1.7960550
O	17.4344590	1.8740690	-3.3373440
O	15.3058580	-2.7632690	0.9769040
O	12.5958540	-2.2095420	2.0628960
C	17.2056850	1.2495130	-2.0492050
H	16.3133160	1.6742800	-1.5887890
H	18.0775640	1.4003200	-1.3944600
C	16.9783290	-0.2324770	-2.3136070
H	17.8463210	-0.6654450	-2.8301460
H	16.0826230	-0.3645270	-2.9330790
H	15.6417570	-2.4897180	-1.7413320
O	16.7928880	-0.8989800	-1.0253720
C	-2.9236260	-13.0046880	-2.6763190

H	-2.1589210	-12.7878480	-3.4334600
H	-3.8764250	-12.5613400	-2.9812370
C	-3.0938270	-14.5151570	-2.4969300
H	-2.7585930	-15.0363990	-3.4049190
H	-2.4925120	-14.8528180	-1.6504740
C	-5.4105160	-14.6512040	-3.2814120
H	-4.8558940	-14.5410080	-4.2254210
H	-5.9316910	-13.7120810	-3.0611000
C	-6.4159110	-15.7906560	-3.4455850
H	-6.7858800	-15.7889430	-4.4743160
H	-5.9210860	-16.7523320	-3.2470370
C	-9.1908400	-13.2285040	-1.3146560
H	-9.4399720	-13.8354510	-2.1935870
C	-10.4582640	-12.5632600	-0.7720820
H	-11.0710230	-12.2272400	-1.6266970
H	-11.0318790	-13.2962070	-0.1973750
C	-9.9788920	-10.1814210	-0.5137390
H	-10.8085140	-9.9428400	-1.2011960
H	-9.0375330	-10.2110240	-1.0728520
C	-9.9316760	-9.1120930	0.5751610
H	-10.1408340	-8.1226610	0.1494400
H	-10.6946000	-9.3438660	1.3203440
O	-2.4948850	-12.4370720	-1.4086910
O	-4.4583990	-14.9320710	-2.2036630
O	-7.6073160	-15.6427830	-2.6372350
O	-10.2423110	-11.4534070	0.1316200
O	-8.6895400	-9.0835390	1.3210040
C	-7.4895900	-16.0751220	-1.2621920
H	-6.5495750	-15.7153280	-0.8268980
H	-7.4989200	-17.1757970	-1.2134220
C	-8.6818250	-15.5096000	-0.4974370
H	-8.7232870	-15.9543740	0.5018310
H	-9.6080440	-15.7628750	-1.0303640

H	-8.4487170	-12.4835400	-1.6051620
O	-8.5669100	-14.0809960	-0.3023980
C	-8.7921040	7.9498560	-1.9877990
C	-6.2530870	7.0402520	-1.1047560
C	-7.6222390	8.6028240	-2.4051400
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C	-6.3753500	8.1537010	-1.9678620
H	-5.4879590	8.6724370	-2.3059590
C	-8.6983160	6.8419210	-1.1300790
H	-9.5899360	6.3117680	-0.8123210
C	-7.4397290	6.3967320	-0.7036950
H	-7.3800360	5.5168810	-0.0698720
C	0.1572980	5.4289930	-0.3014140
C	-2.4376790	6.5744690	-0.4169580
C	-0.7305820	5.0949710	-1.3455140
H	-0.4144170	4.3894570	-2.1060370
C	-2.0053590	5.6605520	-1.3993730
H	-2.6756210	5.3927170	-2.2086770
C	-0.2605080	6.3623130	0.6696120
H	0.4196500	6.6370950	1.4686770
C	-1.5341540	6.9337920	0.6021740
H	-1.8330070	7.6645470	1.3469480
C	-3.7998740	7.1929600	-0.4807970
C	-4.2616180	9.1693450	1.0109720
H	-4.6253690	8.4721510	1.7597140
C	-4.2214040	10.5357590	1.2920700
H	-4.5635870	10.9354110	2.2399660
C	-3.8139060	8.6690530	-0.2275730
C	-3.2915300	9.5761520	-1.1596280
H	-2.9033670	9.2039370	-2.1034330
C	-3.2791140	10.9533090	-0.9070070
H	-2.9059660	11.6285930	-1.6674690
C	-3.7603870	11.4360820	0.3202550

C	-4.9236190	6.4600990	-0.7357330
C	-4.3946060	4.3068190	0.4668050
H	-4.0361840	4.8995790	1.3022250
C	-4.3483880	2.9123500	0.5335600
H	-3.9591260	2.4198320	1.4178480
C	-4.8847480	4.9618280	-0.6782760
C	-5.3575540	4.1786980	-1.7483900
H	-5.7605180	4.6694640	-2.6289110
C	-5.3046440	2.7834650	-1.6944160
H	-5.6557490	2.1902910	-2.5318380
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C	0.9592190	-4.6225500	-0.1272140
C	-1.4706980	-6.0803110	-0.2754650
C	-0.0575870	-4.4244500	0.8308700
H	0.0939190	-3.6997380	1.6233950
C	-1.2505580	-5.1443030	0.7553350
H	-2.0264900	-4.9790880	1.4951690
C	0.7567100	-5.5799670	-1.1427730
H	1.5373690	-5.7478900	-1.8770320
C	-0.4372250	-6.3044280	-1.2058960
H	-0.5788060	-7.0439630	-1.9878570
C	-7.5869730	-8.3776760	0.8456610
C	-5.2147430	-7.0314210	0.1054430
C	-6.4479890	-8.4528090	1.6606040
H	-6.4925680	-9.0578750	2.5582600
C	-5.2745630	-7.8047640	1.2813490
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C	-7.5464700	-7.6316910	-0.3442520
H	-8.4026930	-7.5763290	-1.0072370
C	-6.3695880	-6.9478700	-0.6884900
H	-6.3513120	-6.3490850	-1.5947530
C	-3.9741320	-6.2485900	-0.1978420
C	-3.5479610	-4.0095410	-1.2853700

H	-2.9406930	-4.5149960	-2.0286560
C	-3.7107260	-2.6251210	-1.3499920
H	-3.2305760	-2.0548320	-2.1377080
C	-4.1551220	-4.7660020	-0.2624730
C	-4.9663920	-4.0947410	0.6732400
H	-5.4664660	-4.6667090	1.4485090
C	-5.1253190	-2.7070000	0.6216140
H	-5.7384360	-2.1997960	1.3589280
C	-4.4926480	-1.9517660	-0.3877120
C	-2.7532490	-6.8425610	-0.3555750
C	-3.2511930	-8.8177500	-1.8043540
H	-3.8374840	-8.1550800	-2.4327550
C	-3.1611060	-10.1723390	-2.1378020
H	-3.6989090	-10.5331370	-3.0032780
C	-2.6269240	-8.3004720	-0.6594850
C	-1.8445380	-9.1713410	0.1233300
H	-1.3136340	-8.7827620	0.9873620
C	-1.7700990	-10.5329280	-0.1782750
H	-1.2122600	-11.2181210	0.4505350
C	-2.4674480	-11.0395910	-1.2844710
C	11.0880550	4.1488480	-0.8575290
C	8.8622530	2.5138630	-0.2562660
C	10.8470720	2.9878400	-1.6042040
H	11.5206710	2.6677760	-2.3887760
C	9.7481530	2.1771200	-1.2890640
H	9.5984760	1.2576900	-1.8440400
C	10.1763830	4.5382490	0.1404250
H	10.3647150	5.4513860	0.6933440
C	9.0739510	3.7320920	0.4272040
H	8.3760570	4.0368690	1.2016420
C	4.3465290	-2.3255770	0.0530410
C	6.6029730	-0.6115570	0.1898230
C	4.6168510	-1.4086180	-0.9845100

H	3.9467290	-1.3575720	-1.8356160
C	5.7284500	-0.5671510	-0.9137290
H	5.9215520	0.1389480	-1.7143260
C	5.2339970	-2.3921580	1.1474450
H	5.0397100	-3.1006880	1.9455180
C	6.3507620	-1.5539140	1.2057210
H	7.0295740	-1.6194780	2.0504630
C	7.7882660	0.2989830	0.2637410
C	9.8080720	0.1291620	1.7564650
H	9.4836380	1.0388980	2.2504760
C	10.9436020	-0.5374360	2.2153170
H	11.4993270	-0.1700400	3.0685100
C	9.0681210	-0.3667000	0.6646830
C	9.5056920	-1.5589880	0.0609310
H	8.9428130	-1.9694380	-0.7714760
C	10.6667200	-2.2200610	0.4868380
H	11.0062090	-3.0971610	-0.0521020
C	11.3908670	-1.6979320	1.5666960
C	7.6805580	1.6413030	0.0235320
C	5.3850730	2.1167980	0.9717300
H	5.6032560	1.4314420	1.7837820
C	4.1487600	2.7632830	0.9256420
H	3.4080620	2.5809520	1.6965460
C	6.3555210	2.3339940	-0.0265400
C	6.0627540	3.2496230	-1.0558660
H	6.8104670	3.4497150	-1.8169170
C	4.8232280	3.8925380	-1.1147810
H	4.6037300	4.5830100	-1.9219870
C	3.8457350	3.6528720	-0.1265390
C	-2.9958630	-13.7054870	3.1760720
C	-4.2299050	-14.5245190	3.6311640
C	-4.9749670	-13.5224060	1.7190200
C	-3.5115740	-12.9831860	1.8923960

H	-2.6819870	-12.9957010	3.9469380
H	-2.1397660	-14.3510510	2.9631970
H	-3.5010050	-11.8958850	1.9730720
H	-2.9311010	-13.2309820	0.9987290
C	-4.8534670	-14.9946670	2.2724540
C	-5.2798070	-13.5101260	4.1520540
H	-6.1214990	-13.9803770	4.6692490
H	-4.8632100	-12.7535730	4.8233500
C	-5.7700280	-12.8778590	2.8505700
H	-4.0075790	-15.3314220	4.3319190
C	-6.2118950	-15.7118130	2.4276660
H	-6.5373920	-16.1144280	1.4628880
H	-6.1109660	-16.5550550	3.1202150
H	-7.0153370	-15.0646290	2.7943900
C	-3.9358960	-15.8967710	1.4281770
H	-3.8337610	-16.8736730	1.9150610
H	-4.3649030	-16.0602370	0.4320690
H	-2.9340270	-15.4854560	1.2879790
O	-6.6692520	-12.0320470	2.7308380
C	-5.6017570	-13.4283420	0.3530460
H	-5.0052970	-13.9166860	-0.4261210
H	-6.6461710	-13.7656970	0.3223010
S	-5.7689500	-11.6709690	-0.2756060
O	-4.7775160	-10.6653990	0.4721990
O	-5.8050350	-11.7254560	-1.8880720
O	-7.4028420	-11.2507220	0.1005290
H	-7.5689430	-11.2740940	1.0777020
C	16.1719600	3.2154840	2.1134740
C	15.2473370	2.7130510	3.2467960
C	14.6275110	1.3900960	1.4815920
C	15.7211070	2.3503260	0.8981850
H	16.0424000	4.2851640	1.9272240
H	17.2258560	3.0516190	2.3521990

H	15.3620440	2.9433420	0.0554510
H	16.5426770	1.7390020	0.5214430
C	15.1518480	1.1734620	2.9652320
C	13.8196820	3.2121900	2.9058750
H	13.1051590	3.1125210	3.7273700
H	13.7877270	4.2541840	2.5732180
C	13.4281150	2.2785160	1.7677590
H	15.5776170	2.9684700	4.2550140
C	14.1594000	0.4350700	3.8853890
H	13.9990630	-0.5939130	3.5460170
H	14.5694890	0.3955910	4.9005690
H	13.1800180	0.9191340	3.9475930
C	16.4886670	0.4129430	3.0268070
H	16.8950470	0.4718210	4.0429820
H	16.3264070	-0.6446920	2.7891330
H	17.2459580	0.7959380	2.3396730
O	12.3187780	2.2397630	1.2096170
C	14.4096710	0.0884650	0.7462800
H	15.3595220	-0.3910310	0.5026110
H	13.7621680	-0.6144530	1.2748350
S	13.6147710	0.1858590	-0.9609010
O	14.1358860	1.4791160	-1.7632880
O	13.7181230	-1.2293580	-1.7137530
O	11.9289880	0.3760590	-0.6635430
H	11.8033300	1.1204880	-0.0001110
C	-7.9905930	9.9180790	4.8185200
C	-8.9381560	8.7417000	4.4923500
C	-8.4495730	9.5671020	2.4137030
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H	-8.4552390	10.6351700	5.5010570
H	-7.0675570	9.5700970	5.2899440
H	-8.1095360	11.5507190	3.3083840
H	-6.6595080	10.5721550	3.1710580

C	-8.3380490	8.1721820	3.1607290
C	-10.2843060	9.3548630	4.0242110
H	-11.1133360	8.6420670	4.0111850
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C	-9.1919820	7.0467770	2.5398900
H	-8.7518630	6.7170620	1.5952840
H	-9.2122230	6.1875800	3.2199040
H	-10.2275250	7.3348290	2.3343990
C	-6.8981820	7.6457000	3.2809800
H	-6.8676910	6.8190750	4.0002710
H	-6.5564480	7.2568660	2.3139400
H	-6.1839540	8.4039610	3.6117340
O	-10.7681000	10.1050170	1.7174870
C	-7.9587670	9.5767730	0.9875160
H	-6.9065080	9.3022900	0.8878370
H	-8.5783980	8.9744880	0.3245520
S	-8.0181140	11.2924920	0.2008260
O	-8.6613990	12.3859450	1.2049100
O	-6.5598930	11.6152890	-0.3999370
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H	-9.5370030	11.7909220	-1.5002990

PPP→3S

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H	0.6302790	15.6869800	-2.0071200
H	0.9910190	15.0630330	-0.3631210
C	3.2668060	16.3331650	-2.4466540

H	2.5718320	16.6590080	-3.2395290
H	3.8072870	15.4449850	-2.8001240
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H	4.7776820	17.7208200	-3.0876270
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C	8.4874620	14.3621830	1.4532240
H	9.5172650	14.1945970	1.1084830
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C	8.5943360	10.8162840	1.2793520
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C	4.4949190	1.4976080	0.1422960
C	4.7313990	0.3003240	0.1166690
C	-0.9395290	-4.6924250	-0.0542740
C	-2.0939650	-4.2990160	-0.1028880
O	-11.6035110	-5.7340000	-1.8231230
C	-12.3460230	-6.4985610	-0.8397260
H	-12.6203770	-5.8545750	0.0061300
H	-11.7147630	-7.3180330	-0.4664460
C	-13.5931330	-7.0982010	-1.4911500
H	-13.3426920	-7.4562960	-2.4915560
H	-13.9060580	-7.9545480	-0.8702870
O	-14.7133740	-6.2047720	-1.6682020
C	-15.1866130	-5.5999570	-0.4354830
H	-14.6599340	-4.6560100	-0.2724560
H	-14.9866320	-6.2727940	0.4127800
C	-16.6793870	-5.3150220	-0.4844280
H	-17.1955330	-6.1070650	-1.0444440

H	-17.0495740	-5.3028140	0.5509300
O	-16.9165360	-4.0280530	-1.1077690
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H	-18.9969780	-4.1617660	-0.8302260
H	-18.3554190	-2.6616360	-1.5516070
C	-18.2123300	-2.7382920	0.5882570
H	-19.2545480	-2.4785730	0.8355310
H	-17.8193020	-3.4040640	1.3705070
O	-17.4047840	-1.5407590	0.5205970
C	-17.3053830	-0.8264670	1.7768200
H	-17.2361250	-1.5451930	2.6056510
H	-18.1920710	-0.1918440	1.9134550
C	-16.0505110	0.0279650	1.7992980
H	-15.9075740	0.4220650	2.8187910
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O	-16.2001470	1.1284590	0.8712110
C	-15.1260670	2.0898430	0.8778660
H	-14.8850530	2.4097500	1.9034190
H	-15.5268070	2.9446140	0.3274510
C	-13.8378090	1.6332660	0.1919930
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O	-12.9747710	0.9870900	1.1774410
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O	0.6290540	12.9095970	-1.5404020
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C	-13.6193500	-1.5398690	-2.7205300
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C	-12.1785960	-2.1080230	-0.8458620
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H	-13.7416720	-1.2705640	-3.7646150
H	-15.7434430	-1.5844060	-2.2765100
H	-15.4731660	-2.1833700	0.0445270
H	-11.1685570	-2.2489050	-0.4783930
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C	-13.1255860	-2.5382330	1.4835560
C	-14.1099990	-3.5916340	2.0230280
O	-15.3174670	-3.4055360	2.1673930
O	-13.5159770	-4.7771870	2.3398730
H	-12.5368850	-4.6581880	2.2599430
O	-11.8273260	-3.0766520	1.8356220
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C	5.6860540	12.1258590	-2.7009500
C	5.7486780	13.4793000	-2.3316560
C	5.3176650	13.8809410	-1.0603760
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C	4.7345360	11.5943300	-0.5249350
C	5.1705300	11.1897320	-1.7941200
H	6.0243200	11.8077850	-3.6820430
H	6.1331840	14.2223520	-3.0239740
H	5.3603380	14.9297340	-0.7953770
H	4.3189990	10.8601440	0.1560850
H	5.1001930	10.1432470	-2.0681870
C	4.4553480	13.3820900	1.2657500
C	3.0207880	12.9936750	1.6682350
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H	3.9121940	11.9338530	2.9688910
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H	4.5352740	14.4703470	1.3301160
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H	4.1413930	16.5678230	0.4689230
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C	6.1383800	17.2014330	1.0630650
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C	11.2142050	-8.2510340	-1.7686590
H	11.2089080	-8.3134470	-2.8650100
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C	12.5677420	-8.6486360	-1.1671070
H	13.4010230	-8.2230220	-1.7447170
H	12.5950640	-8.2858750	-0.1419510
C	12.7001450	-10.8203690	-2.3095980
H	13.3643500	-10.3466470	-3.0526880
H	11.6812200	-10.8447580	-2.7184850
C	13.1966310	-12.2400440	-2.0501880
H	13.2084950	-12.7931890	-2.9940250
H	14.2191840	-12.1981550	-1.6481190
C	9.5305750	-14.4511370	0.4455930
H	9.9497930	-15.4638850	0.3426040
C	8.2357540	-14.5518040	1.2468570
H	7.6046840	-15.3522800	0.8364420
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C	6.4233600	-13.1033680	0.3048100
H	6.3368570	-13.9785580	-0.3526920
H	6.6900350	-12.2342690	-0.3029040
C	5.0968020	-12.8797980	1.0313560
H	4.2776100	-12.8277100	0.3024330
H	4.9038030	-13.7082300	1.7152300

O	10.9601840	-6.8741930	-1.3639170
O	12.7305270	-10.0912310	-1.0643550
O	12.3503020	-13.0130430	-1.1590280
O	7.4783070	-13.3143830	1.2833930
O	5.1284140	-11.7119520	1.8851910
C	7.8439590	-10.8849050	-2.8072860
C	8.9870790	-11.5990170	-2.4132300
C	9.4892940	-11.4584680	-1.1126190
C	8.8591490	-10.6095480	-0.1897760
C	7.7347870	-9.8746710	-0.5958110
C	7.2269470	-10.0186640	-1.8943010
H	7.4465510	-10.9945610	-3.8113690
H	9.4868160	-12.2667090	-3.1087310
H	10.3774530	-12.0083570	-0.8279620
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H	6.3527700	-9.4478140	-2.1866220
C	9.3607040	-10.5472900	1.2444640
C	9.6970760	-9.1188960	1.7121970
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H	10.2718140	-11.1455990	1.3274160
C	12.6165440	-12.8146310	0.2577760
H	12.3296010	-11.8019060	0.5587920
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C	11.8695210	-13.8721010	1.0547580
H	12.2608500	-13.8784240	2.0775790
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C	-10.5529030	-4.9445660	-1.3856490

C	-8.5294760	-3.1145470	-0.6412070
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C	-9.0293480	-3.1502890	-1.9613100
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C	-10.0302540	-4.9621410	-0.0817730
H	-10.4033610	-5.6550330	0.6630050
C	-9.0162820	-4.0571210	0.2746510
H	-8.6114990	-4.0828410	1.2821770
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H	-5.6544640	-0.5044080	-1.8534410
C	-5.6389190	2.2295300	0.9020190
H	-5.6344650	2.9977050	1.6676400
C	-6.6406660	1.2540720	0.8890750
H	-7.4192190	1.2775800	1.6451480
C	-7.7058240	-0.8189240	-0.0891400
C	-9.6746280	-0.5634800	1.4471660
H	-9.1089240	-1.1146260	2.1937600
C	-10.9456570	-0.0742180	1.7648050
H	-11.3807760	-0.2383290	2.7445310
C	-9.0963370	-0.3278790	0.1823400
C	-9.8200530	0.4432030	-0.7385340
H	-9.3825920	0.6646220	-1.7069050
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C	-11.6879540	0.6278540	0.8008030
C	-7.4412710	-2.1393490	-0.3020110
C	-5.1737670	-2.3542030	0.7855240
H	-5.4986240	-1.6523370	1.5460000

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H	-3.2075260	-2.5882680	1.6364140
C	-6.0611250	-2.7127980	-0.2497800
C	-5.6291500	-3.6530830	-1.2047740
H	-6.3082680	-3.9711050	-1.9893350
C	-4.3333910	-4.1767310	-1.1619530
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C	-3.4385820	-3.7895970	-0.1436510
C	4.9759030	-1.1172620	0.0945920
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C	4.4237530	-1.9511710	1.0898030
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C	4.6344240	-3.3302710	1.0534620
H	4.2013190	-3.9611490	1.8223790
C	5.7647970	-1.7004510	-0.9187000
H	6.2051590	-1.0658120	-1.6801500
C	5.9807940	-3.0811950	-0.9419860
H	6.5997860	-3.5168570	-1.7200410
C	5.0158770	-10.4275200	1.3537870
C	4.8263300	-7.7319440	0.5189690
C	5.5472370	-9.4017290	2.1503570
H	6.0169370	-9.6743650	3.0870090
C	5.4708620	-8.0732750	1.7274410
H	5.9041810	-7.2891840	2.3394830
C	4.3777250	-10.1119500	0.1447760
H	3.9525850	-10.8822870	-0.4888420
C	4.2719870	-8.7689340	-0.2488530
H	3.7408410	-8.5256220	-1.1645260
C	4.6015350	-6.2898900	0.1797690
C	2.6869960	-5.0743910	-0.9312650
H	3.3793850	-4.7359900	-1.6946740
C	1.3461310	-4.6926910	-0.9950740
H	0.9965600	-4.0596190	-1.8032800

C	3.1622010	-5.8857600	0.1188080
C	2.2409840	-6.3371430	1.0841020
H	2.5827980	-6.9851540	1.8851900
C	0.8986590	-5.9509420	1.0324150
H	0.2032870	-6.2898400	1.7928000
C	0.4343940	-5.1163230	-0.0052500
C	5.6191080	-5.3992300	-0.0088790
C	7.2569710	-6.6401440	-1.4382080
H	6.4141860	-6.9868170	-2.0286840
C	8.5588480	-6.9920510	-1.8142590
H	8.7221840	-7.6220290	-2.6815740
C	7.0165270	-5.8285430	-0.3178500
C	8.1249080	-5.3515440	0.4124760
H	7.9616750	-4.7110730	1.2736140
C	9.4271310	-5.7135060	0.0612030
H	10.2804560	-5.4022890	0.6500070
C	9.6440730	-6.5428870	-1.0507670
C	0.9711280	11.6073270	-1.1805820
C	1.6021750	8.9846140	-0.3627790
C	1.8923950	10.8493940	-1.9149350
H	2.3716070	11.2706100	-2.7919060
C	2.2072920	9.5506860	-1.4966740
H	2.9211200	8.9603600	-2.0635840
C	0.3422140	11.0540210	-0.0540170
H	-0.3422580	11.6717970	0.5128900
C	0.6476610	9.7489380	0.3390960
H	0.1594160	9.3247020	1.2108500
C	4.1831770	2.9018900	0.1618900
C	3.5109620	5.6579800	0.2187280
C	3.4141930	3.4758040	-0.8725650
H	3.0735740	2.8501450	-1.6903130
C	3.0865230	4.8320900	-0.8417130
H	2.4895780	5.2595200	-1.6403530

C	4.6324100	3.7296250	1.2118300
H	5.2327420	3.2999930	2.0065180
C	4.3087650	5.0893820	1.2307160
H	4.6679490	5.7156160	2.0415180
C	3.1563550	7.1112990	0.2419880
C	4.2065750	8.7733140	1.8110320
H	3.2831940	8.7726760	2.3807790
C	5.3025230	9.5051080	2.2720460
H	5.2635840	10.0670900	3.1967490
C	4.2847710	8.0217150	0.6188430
C	5.4950060	8.0371340	-0.0931440
H	5.5886260	7.4376370	-0.9939960
C	6.5907660	8.8004890	0.3382580
H	7.4999540	8.7992350	-0.2525000
C	6.4929830	9.5345890	1.5298700
C	1.8928640	7.5606020	-0.0132750
C	0.5214030	5.7022410	1.0087000
H	1.2500110	5.6373310	1.8096230
C	-0.5806170	4.8463780	1.0051740
H	-0.7079070	4.1167660	1.7973480
C	0.7077170	6.6490790	-0.0183990
C	-0.2682640	6.7419260	-1.0293110
H	-0.1572010	7.4891650	-1.8087380
C	-1.3690650	5.8807200	-1.0455790
H	-2.1053710	5.9505310	-1.8389630
C	-1.5348370	4.9146040	-0.0319110

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	X	Y	Z
C	-5.5795790	12.4783330	0.5203260
H	-4.5980460	12.9531870	0.6187300
H	-5.8221150	11.9830170	1.4696130
C	-6.6423750	13.5083090	0.1591880

H	-7.4646080	12.9959020	-0.3609400
H	-7.0282800	13.9817370	1.0643930
C	-5.4880450	14.2515700	-1.8853340
H	-6.1023540	13.5274220	-2.4393090
H	-4.5066650	13.8032650	-1.6833990
C	-5.3351100	15.5289700	-2.7040980
H	-5.1204060	15.2769500	-3.7454000
H	-6.2766720	16.0955340	-2.6539410
C	-1.2710220	16.8619140	-2.0185850
H	-1.4348580	17.7282810	-2.6709000
C	0.2258040	16.5940680	-1.8817970
H	0.7316400	16.9147970	-2.8049660
H	0.6241370	17.1510390	-1.0331880
C	0.2612040	14.2684160	-2.6785400
H	0.0756690	14.7983760	-3.6254580
H	-0.6420830	13.7180980	-2.3947570
C	1.4677530	13.3580000	-2.8869030
H	1.3176060	12.7243240	-3.7715470
H	2.3591250	13.9713960	-3.0308270
C	3.2520610	3.0639020	-0.2818450
C	4.0133300	2.1164420	-0.1686000
C	1.3179740	-4.8868940	-0.1057640
C	0.1131720	-5.0772760	-0.1537300
O	-7.5827900	-11.0251600	0.5683020
C	-8.5962800	-11.3004520	1.5749070
H	-9.3688420	-10.5252520	1.5658380
H	-8.1130610	-11.3165170	2.5622900
C	-9.2101450	-12.6612460	1.2659160
H	-8.4446410	-13.3263560	0.8623050
H	-9.6159340	-13.0971070	2.1918460
O	-10.2478210	-12.6041840	0.2540720
C	-11.5157230	-12.0778730	0.7161970
H	-11.3802630	-11.1748850	1.3249590

H	-12.0504110	-12.8315880	1.3118640
C	-12.2960520	-11.7404390	-0.5481830
H	-11.7358810	-11.0345530	-1.1695260
H	-12.5040750	-12.6525650	-1.1159070
O	-13.5668610	-11.1197040	-0.1517690
C	-14.6733100	-11.3413780	-1.0794000
H	-15.1121880	-12.3220960	-0.8645980
H	-14.2973430	-11.3133180	-2.1078000
C	-15.6834280	-10.2237130	-0.9031920
H	-16.6218750	-10.4893710	-1.4128650
H	-15.9000150	-10.0679030	0.1660230
O	-15.0819960	-9.0587100	-1.4885900
C	-15.7259890	-7.7980500	-1.1763080
H	-15.8641910	-7.7052330	-0.0909210
H	-16.6958830	-7.7308990	-1.6885360
C	-14.8019150	-6.6941030	-1.6362000
H	-15.1393690	-5.7259370	-1.2436370
H	-13.8015610	-6.9028140	-1.2428270
O	-14.7869270	-6.6757020	-3.0835360
C	-13.7916590	-5.8061560	-3.6611080
H	-13.9692030	-4.7571630	-3.3800930
H	-13.9321610	-5.9136370	-4.7388180
C	-12.3510890	-6.1666100	-3.2899510
H	-12.2751610	-7.2232370	-3.0080800
H	-11.6808770	-5.9611340	-4.1346470
O	-11.9488050	-5.3181760	-2.1668330
C	-4.5692580	0.7169300	-0.7761540
C	-4.1311590	1.8562240	-0.7751870
O	-5.5819120	11.4846230	-0.5469000
O	-6.1527770	14.6105490	-0.6401740
O	-4.2290210	16.3775110	-2.3022410
O	0.5672830	15.2108630	-1.6177250
O	1.7787430	12.5314280	-1.7351220

C	-4.2802460	16.8415730	-0.9292870
H	-4.1923000	16.0026340	-0.2329020
H	-5.2414630	17.3399830	-0.7337180
C	-3.1473580	17.8314060	-0.7231980
H	-3.2431130	18.3020660	0.2579220
H	-3.1573630	18.6018330	-1.5026260
H	-1.8204110	16.0084790	-2.4256930
O	-1.8283760	17.2005850	-0.7087780
C	13.7236790	-1.8477160	1.4003480
H	13.9559980	-1.2618560	0.5056620
H	13.3556630	-2.8239880	1.0910340
C	14.9455530	-2.1115570	2.2795450
H	15.5195560	-1.1960380	2.4786850
H	14.6166810	-2.5459810	3.2242660
C	16.5183810	-2.6651810	0.4822260
H	17.0763000	-1.7483740	0.7288120
H	15.8191300	-2.4695320	-0.3401380
C	17.4934980	-3.7498920	0.0514240
H	18.2205080	-3.3119850	-0.6494850
H	18.0292190	-4.1437630	0.9241470
C	14.7073470	-7.5589330	-3.3225040
H	15.3097450	-7.7348200	-4.2279000
C	14.0905510	-8.8927290	-2.8921610
H	13.9515810	-9.5145960	-3.7907130
H	14.7798120	-9.4033360	-2.2163030
C	11.7290960	-8.2771560	-2.9666130
H	11.8308720	-8.5999080	-4.0168580
H	11.7743000	-7.1870500	-2.9200880
C	10.3889570	-8.8200080	-2.4760420
H	9.6111540	-8.5011040	-3.1849230
H	10.4310680	-9.9112490	-2.4525700
O	12.6852410	-1.1777760	2.1804900
O	15.8011550	-3.1197720	1.6629840

O	16.7555740	-4.8138170	-0.6016630
O	12.8275750	-8.8255750	-2.1844600
O	9.9911740	-8.4526410	-1.1294200
C	17.3895280	-5.4944960	-1.7083430
H	17.9128430	-6.3930490	-1.3566820
H	18.1175130	-4.8264370	-2.1936970
C	16.3354070	-5.8765630	-2.7365920
H	16.8378350	-6.1201660	-3.6861250
H	15.6540580	-5.0296940	-2.8989460
H	13.9371840	-6.8101890	-3.5432240
O	15.5933690	-7.0431220	-2.2844770
C	-6.1055910	-7.1430800	-0.0989210
C	-5.5808870	-8.2717210	-0.7619010
H	-4.7836030	-8.1421110	-1.4877980
C	-6.0885190	-9.5485260	-0.5176180
H	-5.7112080	-10.4169370	-1.0450790
C	-7.1195240	-9.7269680	0.4226290
C	-7.6122070	-8.6219270	1.1376290
H	-8.4044380	-8.7286780	1.8657030
C	-7.1079200	-7.3462560	0.8620700
H	-7.5093640	-6.4895790	1.3956180
C	-5.6097430	-5.7687350	-0.4057590
C	-3.4302750	-4.9271950	-1.3751450
H	-3.9824140	-4.5318320	-2.2209140
C	-2.0449420	-4.7661440	-1.3180220
H	-1.5225680	-4.2459180	-2.1133660
C	-1.3106880	-5.2696910	-0.2236750
C	-1.9998590	-5.9595070	0.7955570
H	-1.4425200	-6.3614470	1.6348280
C	-3.3855680	-6.1273830	0.7249980
H	-3.9039560	-6.6714790	1.5083570
C	-4.1263610	-5.5931570	-0.3470570
C	-5.9759190	-3.3202920	-0.7366440

C	-6.2445910	-2.4763420	-1.8316550
H	-6.8096100	-2.8630190	-2.6741180
C	-5.7858610	-1.1563240	-1.8515180
H	-5.9855960	-0.5210750	-2.7077280
C	-5.0580050	-0.6359280	-0.7606730
C	-4.8124060	-1.4695660	0.3502650
H	-4.2594830	-1.0770370	1.1966120
C	-5.2668540	-2.7898590	0.3582790
H	-5.0646710	-3.4240470	1.2149980
C	-6.4539250	-4.7389240	-0.7192870
C	-8.3062310	-6.0143460	-1.8871940
H	-7.5760310	-6.7423810	-2.2204330
C	-9.6418730	-6.1827670	-2.2637620
H	-9.9278100	-7.0492020	-2.8451520
C	-10.5976150	-5.2412200	-1.8529270
C	-10.2089690	-4.1495490	-1.0610870
H	-10.9591970	-3.4168040	-0.7849150
C	-8.8731850	-4.0064030	-0.6752200
H	-8.5825220	-3.1495480	-0.0748290
C	-7.8924880	-4.9377830	-1.0788830
C	8.8458300	-2.1996810	0.7400480
C	9.6336490	-1.2556590	0.0551160
H	9.2486270	-0.7971870	-0.8504190
C	10.9062880	-0.9051820	0.5205170
H	11.5230300	-0.2002500	-0.0262420
C	11.3906160	-1.4783330	1.7049600
C	10.6064350	-2.3887330	2.4235560
H	11.0007790	-2.8143440	3.3367810
C	9.3477450	-2.7557990	1.9315380
H	8.7416250	-3.4705810	2.4790510
C	7.4419530	-2.5005780	0.3201550
C	5.7111330	-1.1421640	-0.9197580
H	5.7001880	-1.9067750	-1.6890840

C	4.8858350	-0.0235470	-1.0440130
H	4.2338190	0.0810890	-1.9042880
C	4.8844370	0.9777320	-0.0501430
C	5.7480150	0.8370760	1.0560310
H	5.7623040	1.6069710	1.8199950
C	6.5791090	-0.2810650	1.1681690
H	7.2464860	-0.3720000	2.0195340
C	6.5572650	-1.2997790	0.1959190
C	5.5106470	-4.0671400	0.0558620
C	4.9766640	-4.8838610	-0.9595880
H	5.6406440	-5.3004810	-1.7105830
C	3.6064970	-5.1533170	-1.0185300
H	3.2044240	-5.7690890	-1.8158780
C	2.7320810	-4.6303550	-0.0430300
C	3.2690610	-3.8432630	0.9973450
H	2.6067330	-3.4464320	1.7589330
C	4.6368000	-3.5684410	1.0424300
H	5.0365210	-2.9561630	1.8438040
C	6.9761990	-3.7661420	0.1104640
C	8.7332890	-4.9410560	-1.2472660
H	8.8711300	-4.0258250	-1.8128470
C	9.4409020	-6.0895480	-1.6287400
H	10.1299730	-6.0261280	-2.4595880
C	9.2975600	-7.2662760	-0.8829380
C	8.4514730	-7.2847650	0.2409100
H	8.3594000	-8.2062410	0.8048850
C	7.7305990	-6.1409200	0.5907440
H	7.0454610	-6.1761320	1.4327510
C	7.8603420	-4.9461440	-0.1478590
C	0.4615600	6.2778500	-0.6820450
C	1.5053180	6.1118740	-1.6129660
H	1.5909330	6.8049930	-2.4441750
C	2.4208120	5.0634100	-1.4873830

H	3.2100870	4.9357650	-2.2203780
C	2.3280560	4.1589890	-0.4086140
C	1.3044410	4.3429990	0.5443990
H	1.2306450	3.6590040	1.3827040
C	0.3882400	5.3876520	0.4066980
H	-0.3992690	5.5140480	1.1420650
C	-0.5305790	7.3871450	-0.8339830
C	-0.5146620	9.6097970	-2.0467000
H	-1.3958830	9.2992930	-2.5961610
C	0.0192930	10.8797000	-2.2898880
H	-0.4702240	11.5256150	-3.0083220
C	1.1605030	11.2942350	-1.5853680
C	1.7600440	10.4290170	-0.6562590
H	2.6675360	10.7489530	-0.1573060
C	1.2058420	9.1706370	-0.4145850
H	1.6812620	8.5084380	0.3023120
C	0.0485570	8.7405200	-1.0953200
C	-2.8603360	8.2856050	-0.6305200
C	-3.9789560	8.3412130	-1.4867240
H	-4.1435040	7.5428050	-2.2042570
C	-4.8669400	9.4159240	-1.4355500
H	-5.7213460	9.4756400	-2.1000060
C	-4.6616130	10.4491130	-0.5047410
C	-3.5795460	10.3932390	0.3890670
H	-3.4017630	11.1811690	1.1123790
C	-2.6921710	9.3131610	0.3128480
H	-1.8439330	9.2779430	0.9893270
C	-1.8768010	7.1670180	-0.7409010
C	-2.0636110	4.8411450	-1.7175840
H	-1.3131980	5.1112630	-2.4527620
C	-2.6134650	3.5581220	-1.7303850
H	-2.2913250	2.8335070	-2.4701350
C	-3.5857310	3.1874010	-0.7778850

C	-4.0071720	4.1438730	0.1693590
H	-4.7624520	3.8717930	0.8987930
C	-3.4594770	5.4296330	0.1690420
H	-3.7993000	6.1615110	0.8951030
C	-2.4628160	5.7918570	-0.7576710
C	2.1574480	15.9882170	3.3414340
C	2.1738130	14.6120900	4.0468530
C	0.6619560	14.3031590	2.3557270
C	1.1808390	15.7394660	2.1872920
H	1.8016480	16.7995990	3.9835920
H	3.1284990	16.2907000	2.9395440
C	1.9861710	13.6051390	2.8612260
C	0.8314690	14.4887390	4.8096990
H	0.8239270	13.6209410	5.4742310
H	0.6380150	15.3713790	5.4260520
C	-0.2126980	14.3367850	3.6588150
H	3.0612800	14.4329110	4.6566580
C	1.7883820	12.1494940	3.3185150
H	1.6575340	11.4864460	2.4571220
H	2.6809230	11.8136760	3.8595180
H	0.9263720	12.0100580	3.9740860
C	3.1152280	13.6286660	1.8100230
H	4.0268920	13.1922830	2.2331830
H	2.8330100	13.0410180	0.9293830
H	3.3583780	14.6331070	1.4509450
C	0.0813740	13.6899330	1.0969080
H	0.5097530	14.1220430	0.1856360
H	0.1311100	12.5980620	1.0895630
S	-1.7541050	14.0075820	0.8785220
O	-2.1950720	13.7617970	-0.6601850
O	-2.5926930	13.1872080	1.9849570
O	-1.9268820	15.6648330	1.2635740
H	-1.7456410	16.2849400	0.4386570

H	-0.7973790	13.4182700	3.7432770
H	-0.9312030	15.1590490	3.6221030
O	0.9244500	16.5288480	1.2730330
C	12.8041120	-6.8755000	3.4668530
C	13.2751640	-8.1379270	2.7054960
C	13.4056360	-6.5039870	1.1163190
C	12.8619730	-5.8296680	2.3629390
H	11.7913100	-6.9528070	3.8726960
H	13.4690230	-6.5900880	4.2877240
C	14.3806490	-7.5706970	1.7515990
C	12.1350580	-8.5151260	1.7203160
H	12.2920900	-9.4950000	1.2655340
H	11.1626350	-8.5410830	2.2208620
C	12.2068360	-7.3859500	0.6456290
H	13.6081810	-8.9503660	3.3536940
C	14.9140900	-8.6069170	0.7477900
H	15.6221570	-8.1450940	0.0511210
H	15.4415850	-9.3972230	1.2956570
H	14.1268650	-9.0702510	0.1496780
C	15.5897860	-6.9197690	2.4559750
H	16.1227120	-7.6685720	3.0526550
H	16.2840600	-6.5210730	1.7075240
H	15.3250180	-6.0846750	3.1127350
C	14.1033550	-5.6112790	0.1254430
H	14.7245870	-4.8486000	0.6008610
H	14.6895530	-6.1901080	-0.5942280
S	13.0284120	-4.5906340	-1.0414040
O	13.7885470	-3.2195690	-1.4064090
O	12.5494630	-5.4646250	-2.3009590
O	11.5537800	-4.2460610	-0.1768940
H	11.7200510	-4.0865150	0.7931070
H	12.4119950	-7.7898430	-0.3468220
H	11.2849670	-6.8051910	0.5830580

O	12.4741590	-4.6494910	2.4393470
C	-14.2423010	-4.8983950	3.6031950
C	-12.8590340	-4.9030210	4.2976150
C	-12.4757270	-6.0878900	2.3782070
C	-13.9502770	-5.6718130	2.3148040
H	-15.0252660	-5.3902830	4.1878890
H	-14.6016640	-3.8961800	3.3520980
C	-11.8626410	-4.8196280	3.0919320
C	-12.6320070	-6.3381780	4.8288850
H	-11.7543980	-6.3914140	5.4781750
H	-13.4889250	-6.6917400	5.4093060
C	-12.4247100	-7.1656490	3.5226410
H	-12.7327520	-4.1162900	5.0434660
C	-10.3827870	-4.9816090	3.4814740
H	-9.7427130	-4.9318510	2.5920150
H	-10.0854510	-4.1588350	4.1419550
H	-10.1647460	-5.9208770	3.9940040
C	-11.9926250	-3.5239800	2.2644020
H	-11.7804260	-2.6557980	2.8982120
H	-11.2626160	-3.5249330	1.4488670
H	-12.9818410	-3.3816820	1.8177910
C	-11.8736980	-6.4129800	1.0252850
H	-12.4436100	-6.0004010	0.1889490
H	-10.8260650	-6.1103070	0.9417230
S	-11.7396420	-8.2334020	0.6082860
O	-11.4176540	-8.4225660	-0.9582930
O	-10.7059940	-8.9267510	1.6379990
O	-13.3056730	-8.8362800	0.9526490
H	-13.4614740	-9.7460840	0.4647800
H	-11.4642650	-7.6835970	3.5083530
H	-13.1934940	-7.9265230	3.3688930
O	-14.7355470	-5.8718640	1.3825410

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C	-8.9962580	10.5200790	1.3069780
H	-8.8065280	10.6172120	0.2322680
H	-8.2049100	11.0429910	1.8535670
C	-10.3754660	11.0774890	1.6642320
H	-11.1511620	10.3733170	1.3293710
H	-10.4686250	11.2221980	2.7408580
C	-10.9518350	12.3569100	-0.3302020
H	-11.8806950	11.7759980	-0.4614290
H	-10.1627550	11.8886010	-0.9293810
C	-11.2032790	13.7759940	-0.8264610
H	-11.6303290	13.7218530	-1.8324900
H	-11.9258760	14.2699050	-0.1604840
C	-6.7327880	15.8974490	-1.6970060
H	-7.1742630	16.7228030	-2.2732070
C	-5.2190070	16.1061120	-1.6521200
H	-4.8615680	16.3189550	-2.6717460
H	-5.0021140	16.9638720	-1.0117060
C	-4.0327840	13.9431280	-1.9748620
H	-3.9273650	14.3283700	-3.0007900
H	-4.7707840	13.1311510	-1.9764680
C	-2.6591570	13.4547580	-1.5126390
H	-2.1886210	12.8497990	-2.2962400
H	-2.0316240	14.3236640	-1.3041370
C	2.0948980	4.1642190	0.1050970
C	3.1338350	3.5236140	0.0982890
C	2.9089990	-4.0057260	-0.1991800
C	1.8332390	-4.5822570	-0.2012400
O	-3.4193680	-12.6767190	0.7778060
C	-3.9302260	-13.2405690	2.0201520
H	-4.7635020	-12.6419940	2.4023500
H	-3.1221190	-13.2323710	2.7643090

C	-4.3851910	-14.6837910	1.7940720
H	-3.6762210	-15.1972080	1.1419390
H	-4.3884940	-15.1782670	2.7798810
O	-5.6758820	-14.8594910	1.1660820
C	-6.7884900	-14.2257770	1.8517190
H	-6.9709240	-13.2466910	1.4005300
H	-6.5548000	-14.0883900	2.9192220
C	-8.0607110	-15.0560920	1.7582440
H	-7.8360590	-16.1129860	1.9619440
H	-8.7568360	-14.6807120	2.5252460
O	-8.6478170	-14.9167070	0.4421510
C	-10.0082950	-15.3905000	0.3113860
H	-10.1713770	-16.2821580	0.9365300
H	-10.1259440	-15.6682890	-0.7386030
C	-11.0643500	-14.3371390	0.6533090
H	-12.0529730	-14.8231740	0.6764060
H	-10.8727220	-13.8922050	1.6440400
O	-11.0273670	-13.3144750	-0.3674450
C	-12.0745610	-12.3116860	-0.2892140
H	-12.3257090	-12.1109990	0.7651410
H	-12.9703480	-12.6846590	-0.8033540
C	-11.6182470	-11.0018510	-0.9173160
H	-12.4015200	-10.2462780	-0.7366870
H	-10.6928400	-10.6420800	-0.4589170
O	-11.4572970	-11.1947630	-2.3451910
C	-11.1326580	-10.0030200	-3.0919200
H	-11.7917950	-9.1675420	-2.8101560
H	-11.3326430	-10.2751910	-4.1315910
C	-9.6795510	-9.5384930	-2.9840250
H	-9.0147310	-10.3985220	-2.8343850
H	-9.4044370	-9.0157970	-3.9112140
O	-9.5573870	-8.6146330	-1.8633200
C	-4.6019880	-0.5690710	-0.0844380

C	-4.5627940	0.6483970	-0.0076370
O	-9.0079680	9.0909350	1.6449180
O	-10.5906390	12.3899530	1.0699940
O	-10.0155390	14.5981590	-0.9636700
O	-4.4584650	15.0099060	-1.0853390
O	-2.6903200	12.6968520	-0.2680060
C	-6.7755480	-12.2807990	-2.2123880
C	-7.9517130	-12.6655640	-1.5552330
C	-8.3627580	-11.9837970	-0.4066740
C	-7.6184150	-10.9116060	0.0922720
C	-6.4349580	-10.5332380	-0.5551700
C	-6.0201420	-11.2153730	-1.7064870
H	-6.4450950	-12.8102330	-3.0999750
H	-8.5506440	-13.4957890	-1.9048670
H	-9.2731870	-12.3108720	0.0716450
H	-5.8634290	-9.6774450	-0.2086280
H	-5.1179500	-10.8977580	-2.2148830
C	-8.0931670	-10.1859940	1.3467990
C	-7.6470600	-10.9691980	2.5875910
O	-8.4374820	-11.5496410	3.3340400
O	-6.3054930	-10.9961970	2.8149660
H	-5.7680500	-10.5733410	2.1066350
C	-7.3466980	10.5301520	-2.3033670
C	-7.8688330	11.8191230	-2.1058000
C	-7.4334290	12.5973270	-1.0260840
C	-6.4458340	12.1202210	-0.1483810
C	-5.9440100	10.8280590	-0.3393280
C	-6.3956750	10.0346830	-1.4034070
H	-7.6900620	9.9173280	-3.1304010
H	-8.6223670	12.2190750	-2.7777100
H	-7.9049580	13.5534900	-0.8476980
H	-5.2122170	10.4176790	0.3455410
H	-6.0058700	9.0297220	-1.5138630

C	-5.8709950	13.0624020	0.9002060
C	-5.2434320	12.3638380	2.1109090
O	-5.8440550	11.6289220	2.8900600
O	-3.9213950	12.6661960	2.3160120
H	-3.4954910	13.0938040	1.5385800
C	-9.5897060	15.2668790	0.2563700
H	-9.1422440	14.5498740	0.9531770
H	-10.4653470	15.7228360	0.7437590
C	-8.6233320	16.3854220	-0.1146000
H	-8.5534630	17.0890230	0.7200020
H	-8.9931070	16.9108960	-1.0031690
H	-6.9952110	14.9512120	-2.1842670
O	-7.2517550	15.9273700	-0.3427540
C	13.8793200	2.3865720	1.3387260
H	13.9656090	2.2228540	0.2581770
H	13.8605530	1.4196570	1.8484820
C	15.0470260	3.2197370	1.8642430
H	14.9948200	4.2431830	1.4651480
H	15.0236630	3.2609930	2.9536300
C	16.7663600	2.8684160	0.1671970
H	16.9089190	3.9545150	0.0362760
H	16.0331600	2.5225960	-0.5709920
C	18.1039760	2.1767310	-0.0707900
H	18.5329940	2.5596400	-1.0019200
H	18.7848780	2.4167860	0.7587190
C	17.5043360	-2.3295770	-1.4990360
H	18.5232120	-2.5646410	-1.8405530
C	16.5629920	-3.4568250	-1.9139900
H	16.6320160	-3.6067030	-3.0011700
H	16.8655370	-4.3775920	-1.4062400
C	14.2018700	-2.9791750	-2.5458790
H	14.6758590	-2.8741340	-3.5333670
H	13.6785660	-2.0459120	-2.3208090

C	13.2223680	-4.1545720	-2.6020560
H	12.5823470	-4.0712620	-3.4914820
H	13.7725690	-5.0958220	-2.6502950
O	12.6420980	3.1334270	1.5950120
O	16.3163140	2.5968100	1.5149180
O	18.0300880	0.7405240	-0.2540360
O	15.1971770	-3.1732770	-1.5151970
O	12.4075580	-4.2847220	-1.4073060
C	13.4737270	1.0473380	-2.3678590
C	14.7585050	0.7047050	-1.9167550
C	14.9175810	-0.1303020	-0.8037290
C	13.8031470	-0.6689750	-0.1477300
C	12.5229250	-0.3055320	-0.5856950
C	12.3569610	0.5507570	-1.6830080
H	13.3462420	1.6996380	-3.2255760
H	15.6410570	1.0843180	-2.4228160
H	15.9120970	-0.3531520	-0.4527210
H	11.6378880	-0.6748950	-0.0820730
H	11.3547020	0.8235190	-1.9932450
C	13.9856220	-1.7105340	0.9649060
C	13.1632760	-1.3259070	2.2062310
O	13.5337780	-0.5569610	3.0847850
O	11.9089900	-1.8911460	2.2830050
H	11.6651780	-2.4564370	1.5203590
C	18.0191390	-0.0513710	0.9691580
H	17.0260360	-0.0509440	1.4301340
H	18.7329340	0.3770800	1.6889880
C	18.4761180	-1.4662760	0.6350190
H	18.6705880	-2.0012510	1.5680560
H	19.3946230	-1.4312120	0.0352120
H	17.1973500	-1.3688090	-1.9274810
O	17.4763080	-2.2767800	-0.0527140
C	-3.3936630	-8.5275770	0.0517930

C	-2.9778410	-9.4683330	-0.9134350
H	-2.6791830	-9.1212870	-1.8978650
C	-2.9677800	-10.8352190	-0.6352620
H	-2.7011660	-11.5639900	-1.3913500
C	-3.3482250	-11.3039330	0.6354640
C	-3.6392650	-10.3739610	1.6507910
H	-3.7738480	-10.6918260	2.6794830
C	-3.6861190	-9.0006340	1.3403860
H	-3.9381270	-8.2883450	2.1213440
C	-3.3860720	-7.0497650	-0.2130740
C	-1.6672840	-5.4852500	-1.1969150
H	-2.3889110	-5.2168470	-1.9608700
C	-0.4046840	-4.8922450	-1.2022630
H	-0.1466770	-4.1649430	-1.9641560
C	0.5455720	-5.2232210	-0.2130280
C	0.2036550	-6.1845010	0.7597180
H	0.9319520	-6.4570620	1.5158020
C	-1.0602530	-6.7822160	0.7526150
H	-1.3005240	-7.5284850	1.5029970
C	-2.0264410	-6.4229050	-0.2067260
C	-4.5549160	-4.8350830	-0.3327590
C	-5.2415050	-4.0686950	-1.2937760
H	-5.7566780	-4.5704600	-2.1069360
C	-5.2595490	-2.6728800	-1.2188540
H	-5.7774450	-2.0920230	-1.9743090
C	-4.6084250	-2.0053240	-0.1609890
C	-3.9544500	-2.7727910	0.8261390
H	-3.4634160	-2.2689250	1.6513220
C	-3.9305620	-4.1651010	0.7383310
H	-3.4186310	-4.7427110	1.5006340
C	-4.5265060	-6.3289140	-0.4206700
C	-5.9669150	-7.6364770	-2.0111180
H	-5.0959430	-7.7505570	-2.6497790

C	-7.1933590	-8.1780030	-2.4230640
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C	-8.3159600	-8.0638080	-1.5884700
C	-8.2136340	-7.3496730	-0.3801670
H	-9.0961130	-7.2692460	0.2441840
C	-6.9901520	-6.7968830	0.0053700
H	-6.9247890	-6.2374080	0.9339780
C	-5.8341670	-6.9601630	-0.7876810
C	9.1749560	1.0131040	0.4484280
C	9.5483710	2.2047660	-0.2047260
H	8.9378690	2.5797320	-1.0211250
C	10.6987820	2.9051960	0.1789430
H	11.0105250	3.8039690	-0.3411730
C	11.4754480	2.4356750	1.2480810
C	11.0772420	1.2965430	1.9602450
H	11.6540190	0.9591390	2.8141970
C	9.9430780	0.5862230	1.5493130
H	9.6537640	-0.3037950	2.0977400
C	7.9132310	0.2911640	0.0908440
C	5.7486620	1.0539290	-0.9661320
H	5.9290060	0.3591060	-1.7796200
C	4.5952140	1.8399290	-0.9701230
H	3.8810380	1.7581760	-1.7821220
C	4.3399710	2.7395600	0.0862540
C	5.2836050	2.8480890	1.1289920
H	5.1017810	3.5453340	1.9395310
C	6.4422180	2.0663720	1.1201690
H	7.1650650	2.1660050	1.9237640
C	6.6804450	1.1399460	0.0869300
C	6.5839300	-1.8220640	-0.1767580
C	6.3087870	-2.7550540	-1.1951560
H	7.0353680	-2.9128280	-1.9862600
C	5.1089540	-3.4721480	-1.2085030

H	4.9011190	-4.1750490	-2.0080320
C	4.1571930	-3.2908510	-0.1841380
C	4.4470500	-2.3865480	0.8594480
H	3.7279040	-2.2507800	1.6596450
C	5.6423870	-1.6666100	0.8606140
H	5.8503460	-0.9721860	1.6673780
C	7.8646430	-1.0480840	-0.1692800
C	9.7424960	-1.6908480	-1.7181490
H	9.4039250	-0.9110600	-2.3933670
C	10.8415200	-2.4846440	-2.0852200
H	11.3408230	-2.2875770	-3.0262900
C	11.3035680	-3.4707430	-1.2024900
C	10.6191730	-3.6949050	0.0096590
H	10.9478190	-4.5123500	0.6433940
C	9.5129110	-2.9089610	0.3477620
H	8.9867770	-3.0984760	1.2781360
C	9.0788810	-1.8648110	-0.4939080
C	-1.6250040	6.2725830	0.1583460
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H	-0.8340520	7.3474790	-1.5403510
C	0.5749290	5.8855230	-0.8294830
H	1.3174760	6.1163020	-1.5857690
C	0.8523610	4.8888330	0.1283910
C	-0.1148490	4.6109390	1.1173060
H	0.0946220	3.8567990	1.8679010
C	-1.3316220	5.2939040	1.1296100
H	-2.0654980	5.0682150	1.8955530
C	-2.9254860	7.0125560	0.1808120
C	-3.1554560	9.1138030	-1.2016990
H	-3.5462330	8.5078360	-2.0129820
C	-3.0694300	10.5069960	-1.3643580
H	-3.4312650	10.9548940	-2.2829870
C	-2.6303600	11.2909610	-0.2928270

C	-2.1736330	10.6843040	0.8879420
H	-1.8103920	11.3019060	1.6990330
C	-2.2523050	9.2991190	1.0273710
H	-1.9191790	8.8363690	1.9506820
C	-2.7954450	8.4966260	0.0052480
C	-5.3962260	7.1138240	0.6946950
C	-6.6072200	6.7731080	0.0565930
H	-6.6098670	5.9994400	-0.7055450
C	-7.8028990	7.4265800	0.3797350
H	-8.7292890	7.1885420	-0.1308870
C	-7.8070550	8.4217040	1.3673850
C	-6.6313760	8.7227740	2.0672380
H	-6.6346060	9.4823440	2.8399380
C	-5.4391070	8.0760040	1.7241940
H	-4.5350820	8.3218630	2.2700100
C	-4.1277660	6.3902390	0.3634200
C	-3.7184610	4.2066640	-0.8394080
H	-3.2051130	4.7614200	-1.6176870
C	-3.8278350	2.8181980	-0.9351220
H	-3.4026620	2.2937410	-1.7837970
C	-4.4810080	2.0821750	0.0755120
C	-5.0425760	2.7767820	1.1673280
H	-5.5566810	2.2205570	1.9435690
C	-4.9395090	4.1681450	1.2496130
H	-5.3844590	4.6932320	2.0889460
C	-4.2553200	4.9013370	0.2614210
H	-5.0913830	13.6489510	0.3999350
O	-6.8429090	13.9789630	1.4362650
H	-6.8754310	14.7796750	0.8542720
O	-9.5178780	-10.0262040	1.4000410
H	-9.8793340	-10.5918300	2.1133100
H	-7.6363980	-9.1904970	1.3835260
O	15.3241990	-1.8430510	1.4187800

H	15.9412920	-2.1999080	0.7309690
H	13.6196090	-2.6726450	0.5697190