

SUPPORTING INFORMATION

Deciphering the circularly polarized luminescence of covalent organic frameworks (COF) through ab-initio modelling

Giovanni Bella, Giuseppe Bruno, Francesco Nicolò and Antonio Santoro

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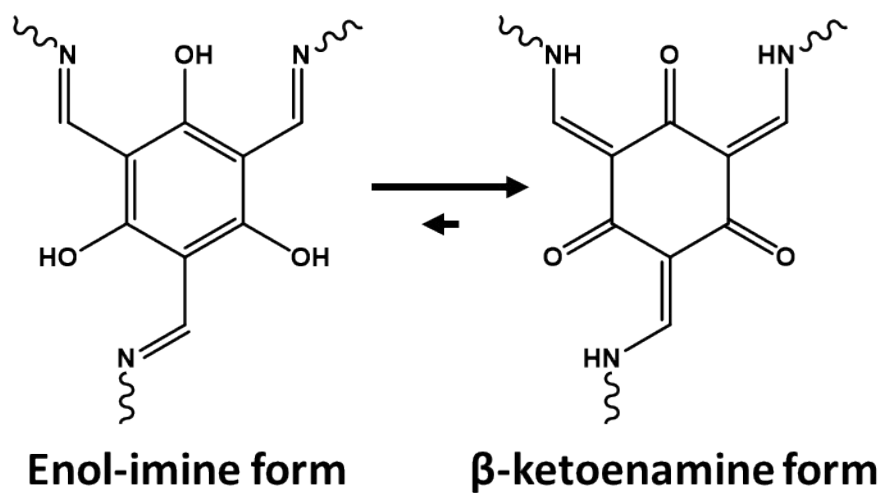


Fig. S1. Tautomerism process between the enol-imine form and the more favourite β-ketoenamine form in the 1,3,5-triformyl phloroglucinol scaffold.

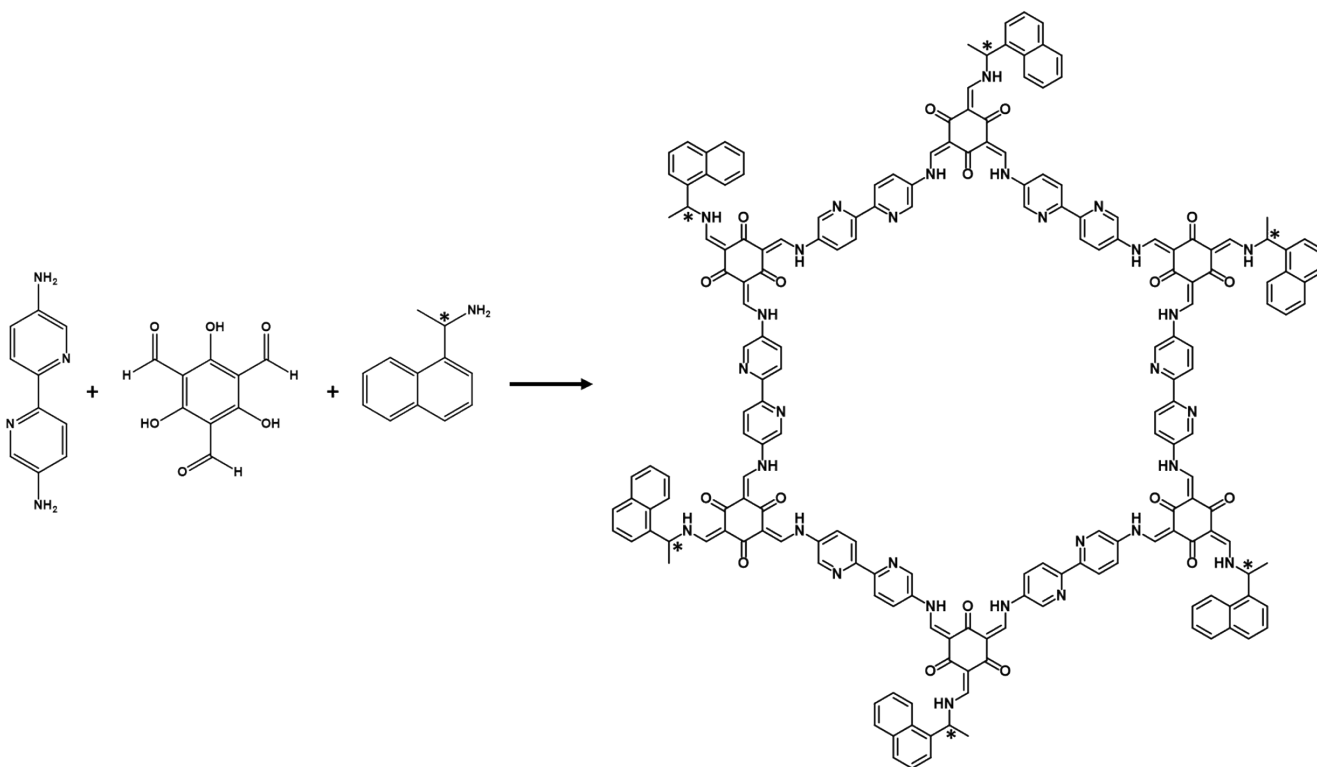


Fig. S2. Starting computational model of COF1 family (COF1[1]), digit in parenthesis refers to the number of hexagonal units in the COF.

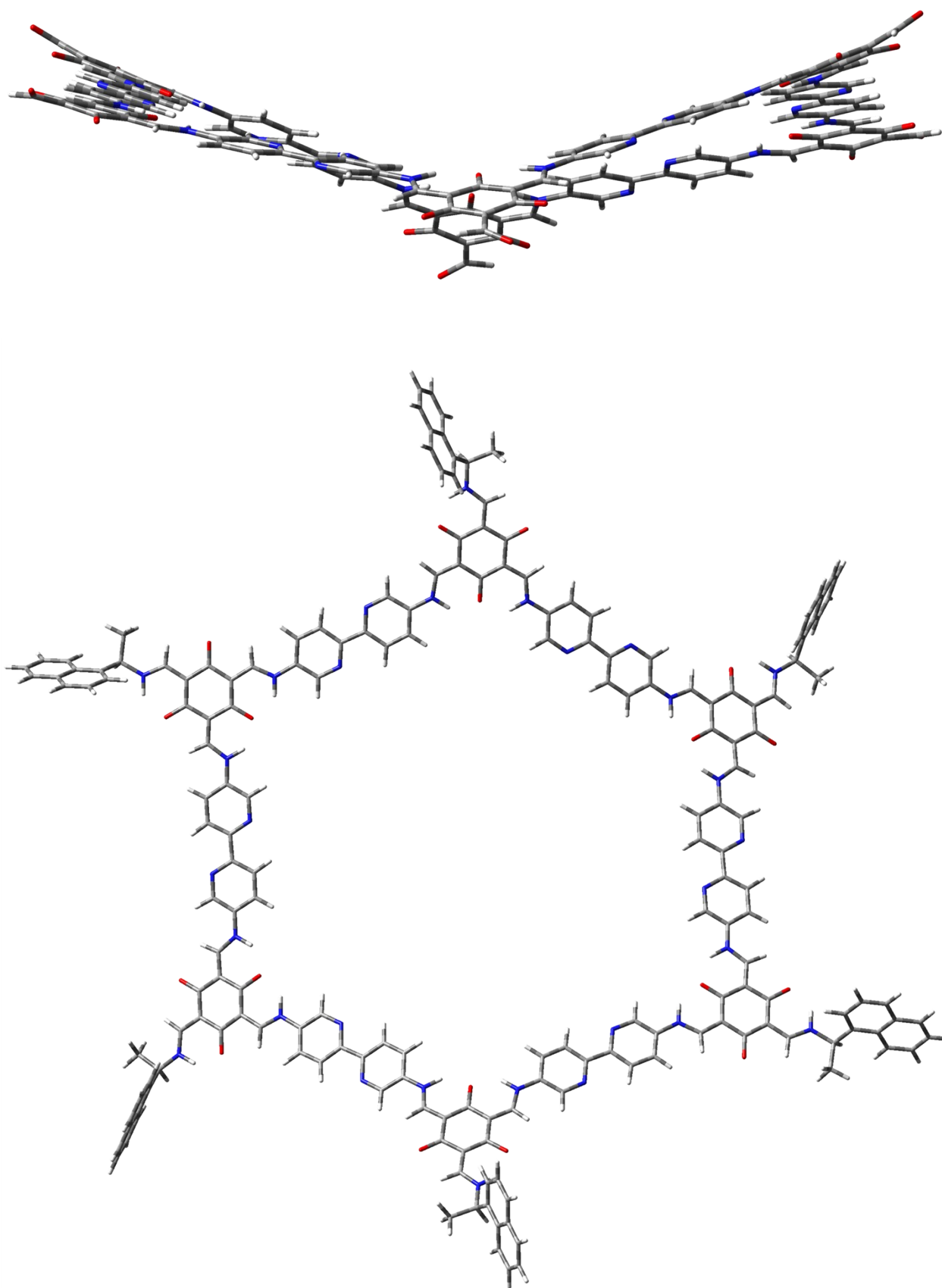


Fig. S3. Lateral (top) and frontal (down) perspectives of DFT-optimized COF1[1] at ω B97XD/6-311G(d,p) level in gas phase. For convenience only the (R) enantiomer is illustrated.

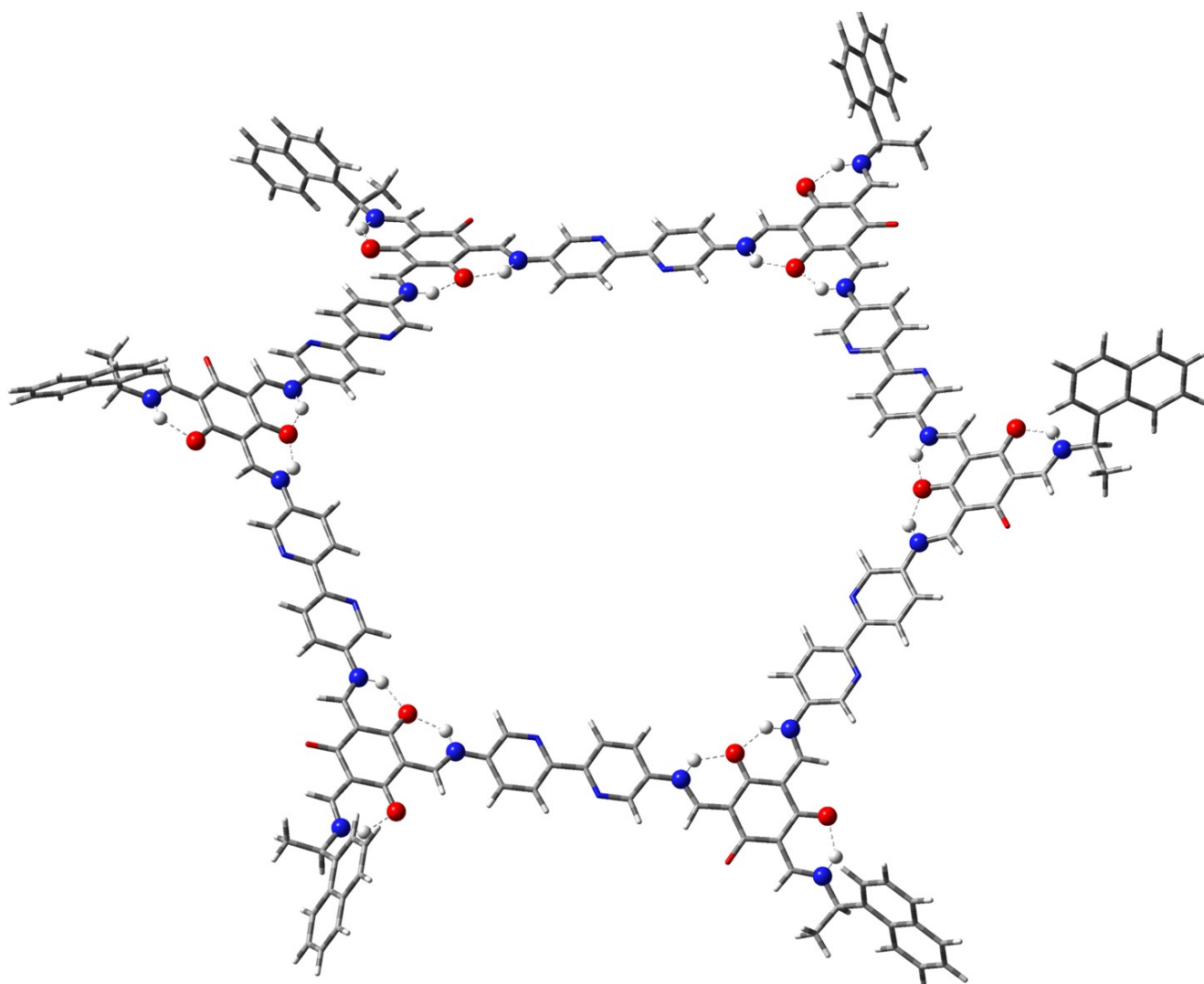


Fig. S4. Predominant hydrogen bonding schemes in COF1[1](A), ball and stick display format was used to highlight atoms involved in the H-bonds. For convenience only the (R) enantiomer is illustrated.

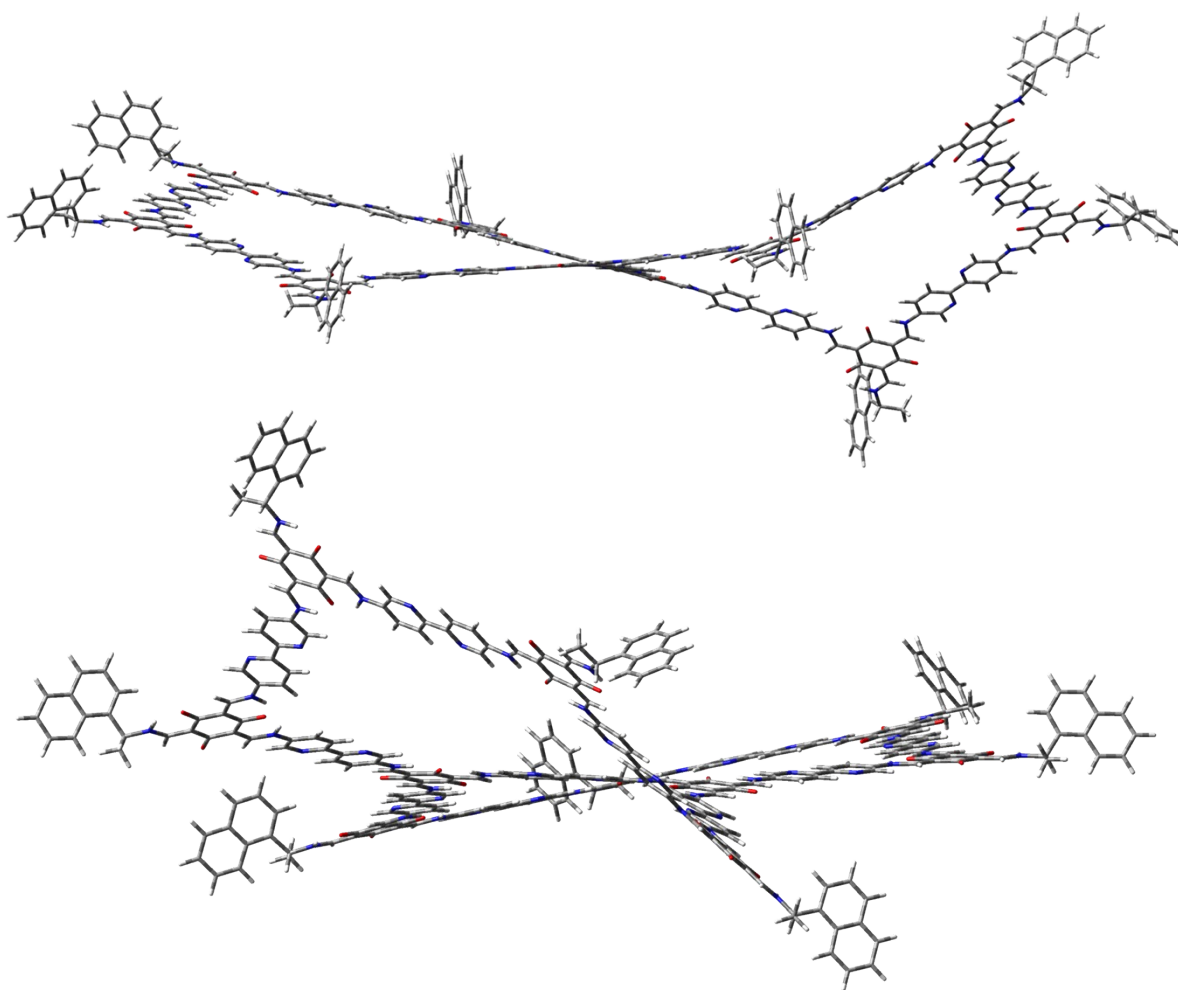


Fig. S5. Lateral perspectives along the y-axis (top) and the x-axis (down) of DFT-optimized COF1[2] at ω B97XD/6-311G(d,p) level in gas phase. For convenience only the (R) enantiomer is illustrated.

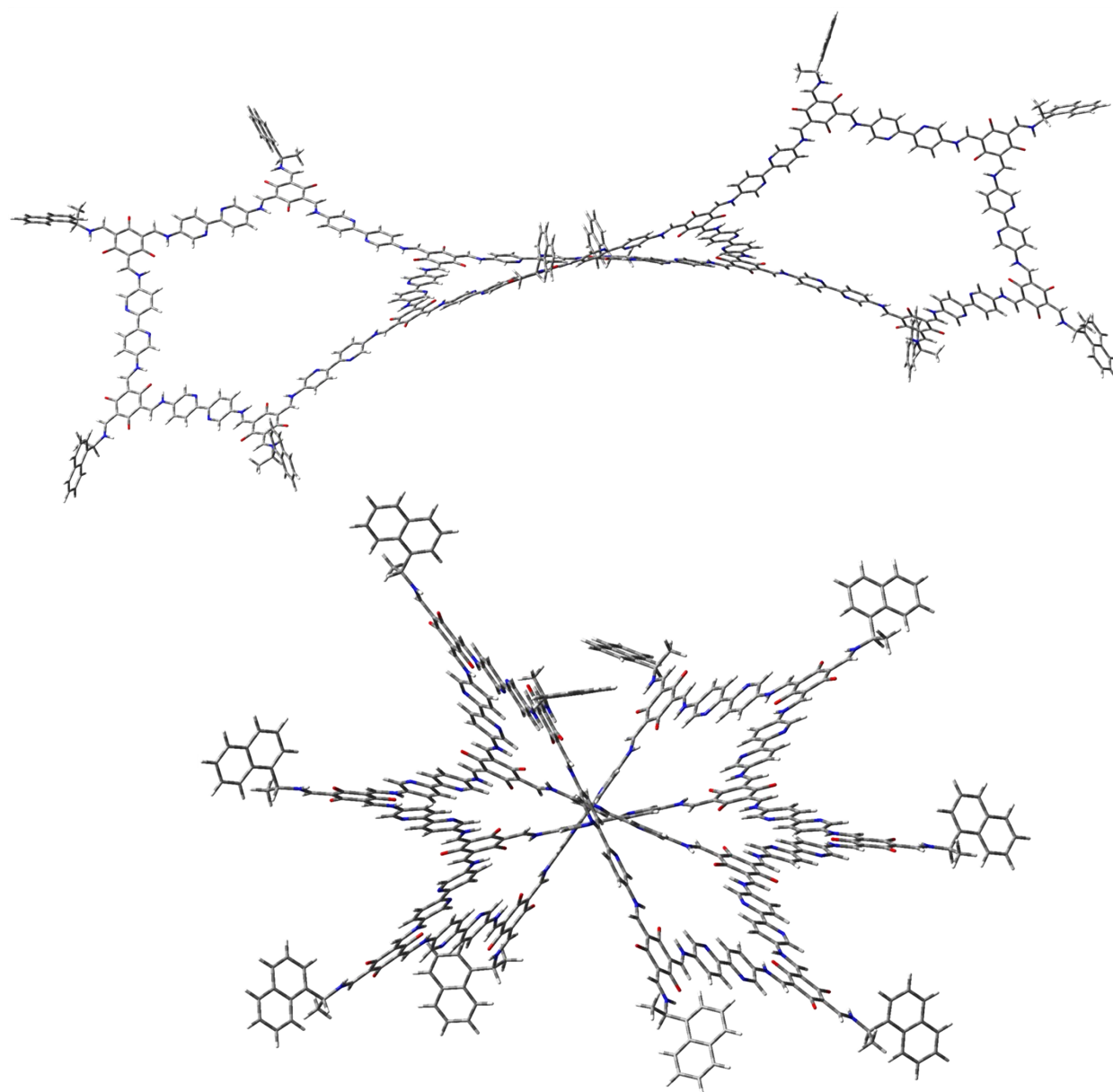


Fig. S6. Lateral perspectives along the y-axis (top) and the x-axis (down) of DFT-optimized COF1[3] at ω B97XD/6-311G(d,p) level in gas phase. For convenience only the (R) enantiomer is illustrated.

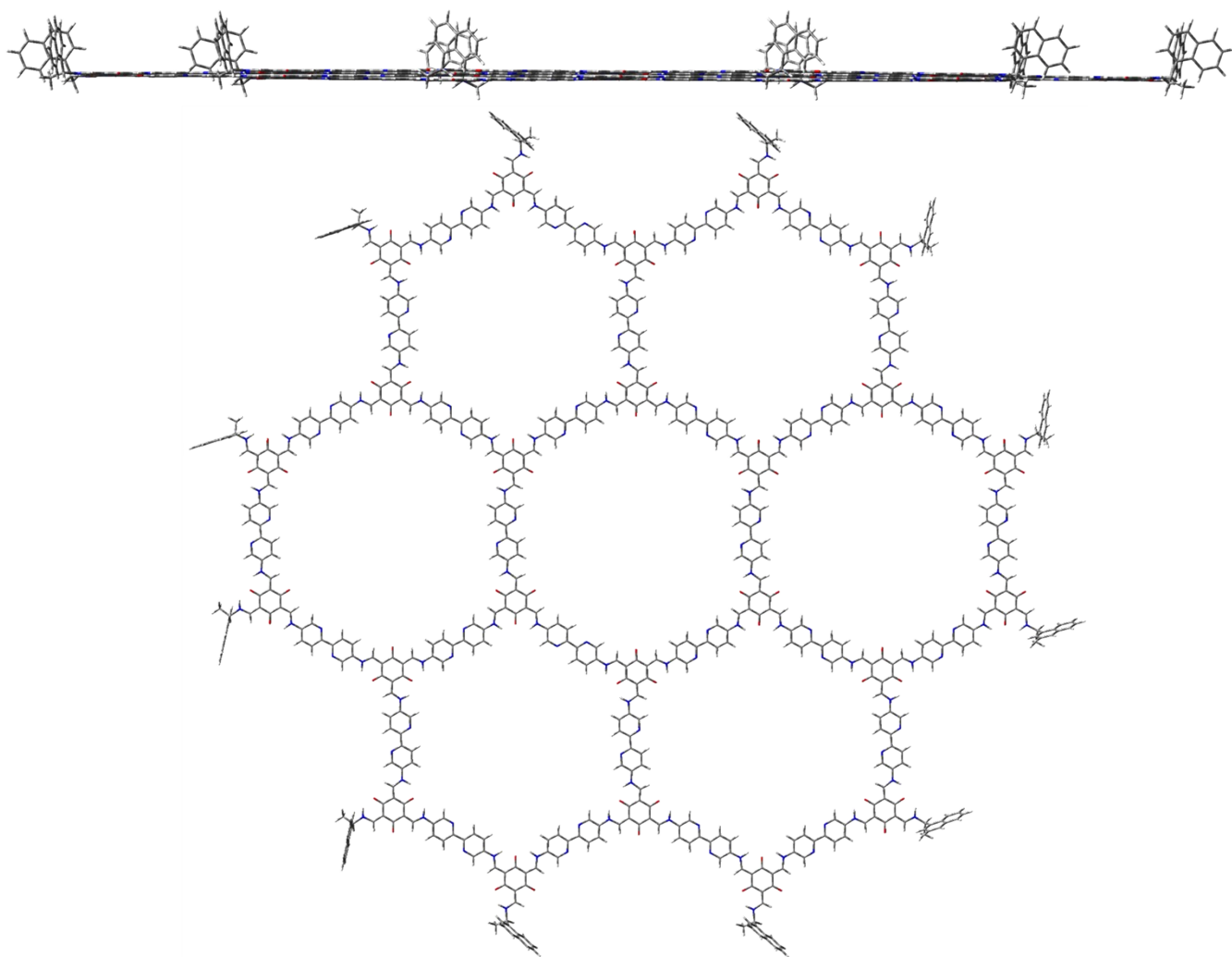


Fig. S7. Lateral (top) and frontal (down) perspectives of DFT-optimized COF1[7] at ω B97XD/6-311G(d,p) level in gas phase. For convenience only the (R) enantiomer is illustrated.

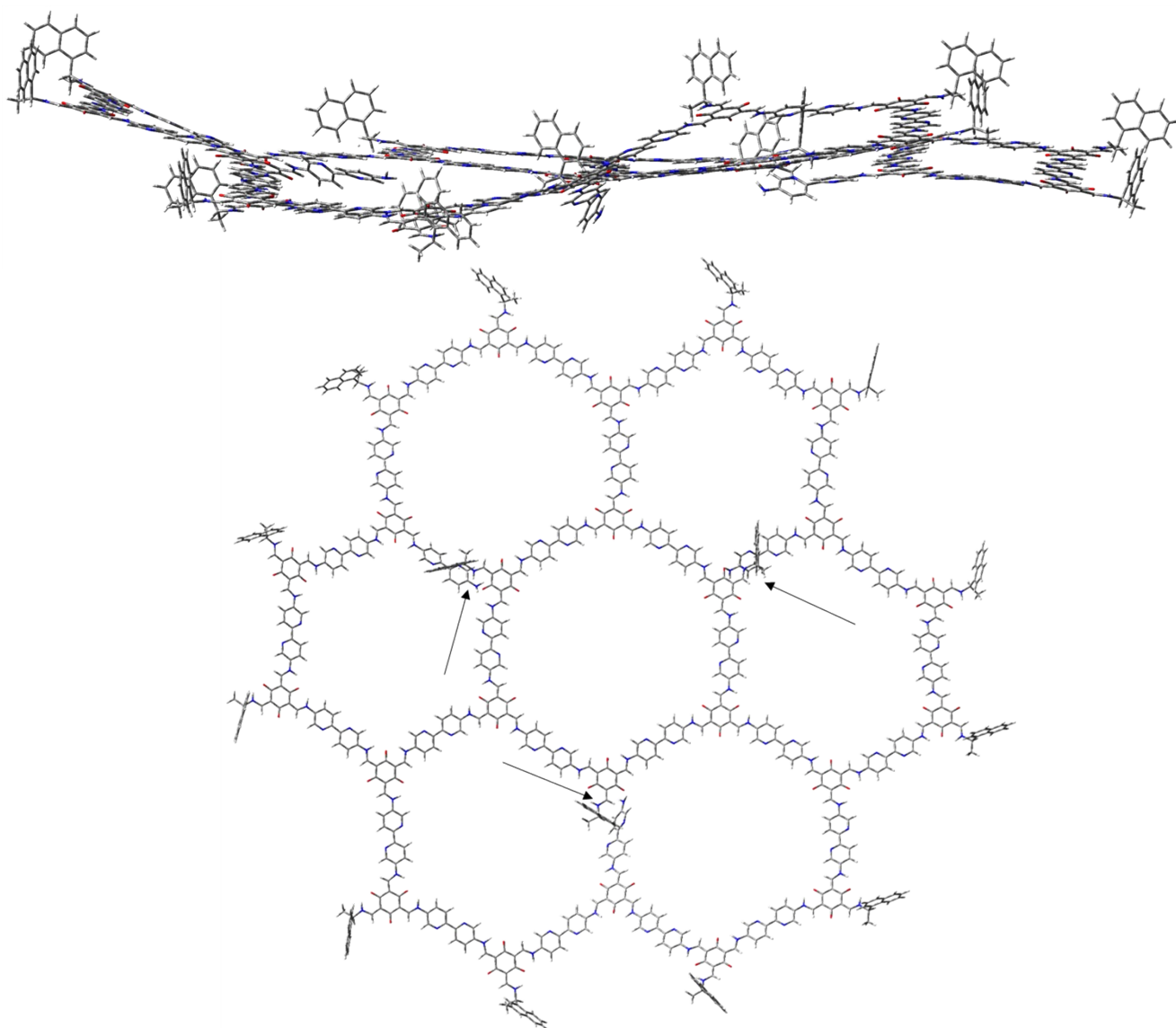


Fig. S8. Lateral (top) and frontal (down) perspectives of DFT-optimized COF1[X] at ω B97XD/6-311G(d,p) level in gas phase. Arrows indicate the chemical cracks in which NEA pendants generated internal mono-condensed bipyridines. For convenience only the (R) enantiomer is illustrated.

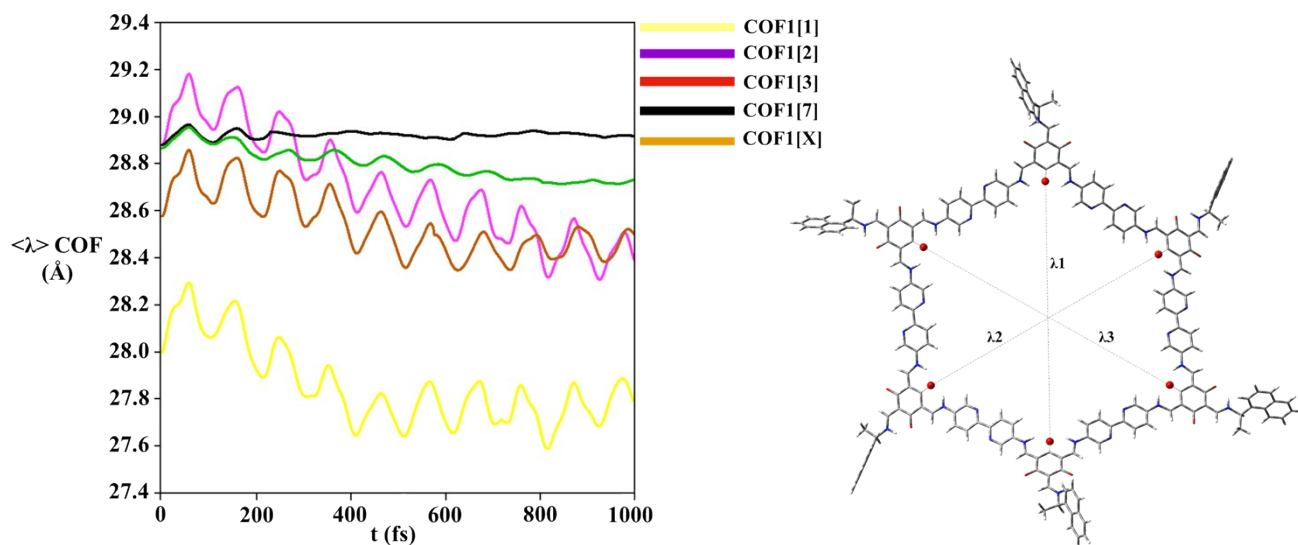


Fig. S9. (Left) Hexagonal aperture evolution plots of BOMD trajectories (S1) computed at ω B97XD/6-311G(d,p) level in gas phase for COF1[1], COF1[2], COF1[3], COF1[7] and COF1[X]. (Right) Hexagonal aperture was calculated as the average distance between the three couples of keto oxygens in each hexagonal unit. It must be noted that this geometrical parameter is different from the pore diameter calculated in table 1 in the manuscript.

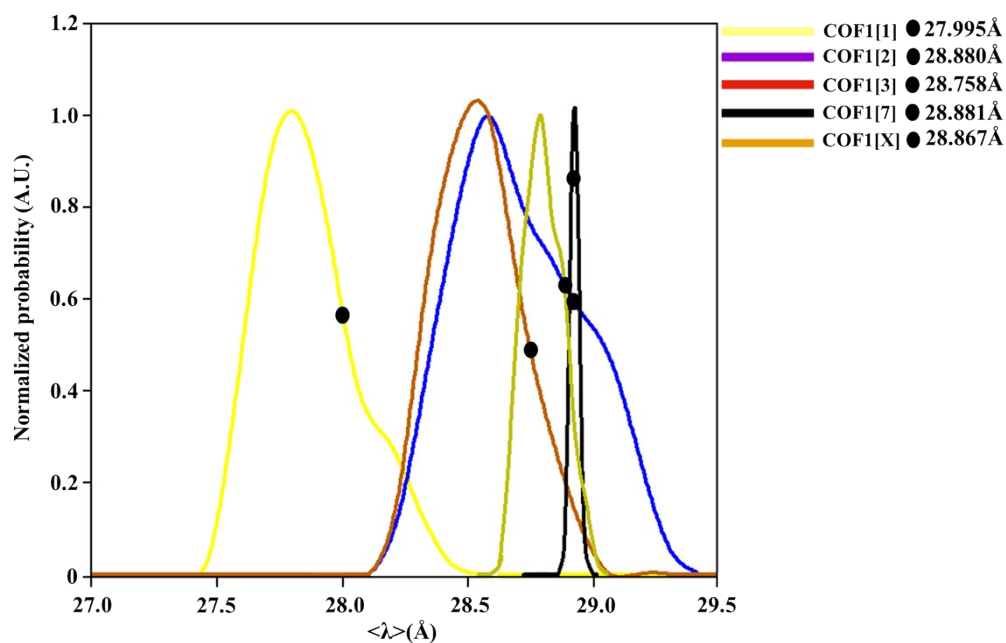


Fig. S10. Distribution functions of the hexagonal apertures ($\langle \lambda \rangle$) as obtained from the first excited state molecular dynamics for COF1[1], COF1[2], COF1[3], COF1[7] and COF1[X] in gas phase. Black circles indicate the relative values for the S0 optimization.

Table S1. Computed rotational strengths for COF1[1], COF1[2], COF1[3], COF1[7] and COF1[X] at M11L/6-311G(d,p) level. Numbers in <> are referred to the mean values. Δ are related to differences between mean values.

Time (fs)	Rlength (cgs units)				
	COF1[1]	COF1[2]	COF1[3]	COF1[7]	COF1[X]
0	-124.2523	-139.0383	-177.8022	-243.2334	-275.2970
40	-86.6169	-96.9243	-123.9468	-169.5592	-159.7767
80	-29.9404	-13.5033	-61.74802	-84.4713	-94.9119
120	-69.8392	-78.1500	-99.9383	-136.7155	-143.0136
160	-97.0586	-108.6085	-138.8886	-189.9996	-176.3836
200	-37.8673	-42.3735	-43.0672	-58.9159	-66.1980
240	-66.2229	-74.1034	-44.7634	-61.2364	-68.8052
300	-153.0945	-171.3127	-219.0747	-299.6942	-336.7364
340	-83.5357	-93.4765	-208.4978	-285.2250	-320.4788
380	-14.0427	-15.7137	-20.0947	-27.4896	-30.8873
420	-89.0393	-99.6349	-127.4132	-174.3012	-205.8449
460	-60.0049	-67.1454	-85.8656	-117.4642	-131.9827
500	-14.0492	-15.7210	-20.1040	-27.5023	-62.7016
540	21.4126	-23.9606	-30.6409	-1.9168	-12.1537
580	44.3051	-51.5774	-10.3571	-14.1686	-15.9198
620	-89.8245	-100.5136	-128.5368	-175.8383	-91.5719
660	-81.7388	-91.4657	-116.9663	-160.0099	-179.7872
700	-37.7751	-42.2703	-31.8153	-83.5233	-93.8468
740	-115.7279	-129.4995	-21.0439	-28.7881	-32.3463
780	-12.9025	-14.4378	-18.4631	-5.2576	-51.4874
820	11.5491	-16.9234	-21.6416	-29.6058	-86.2651
880	-114.0533	-127.6256	-174.3276	-238.4802	-267.9564
920	-56.1606	-62.8437	-80.3645	-109.9386	-123.5271
960	91.1864	-42.0375	-53.7576	-3.5404	-54.1180
1000	78.6540	88.0138	-12.5520	-17.1712	-19.2936
	<-48.794>	<-66.254>	<-84.193>	<-111.715>	<-119.695>
Δ	17.460	17.938	27.521	7.980	

Table S2. Computed angle between the electric dipole transition moment and the magnetic dipole transition moment for COF1[1], COF1[2], COF1[3], COF1[7] and COF1[X] at M11L/6-311G(d,p) level. Numbers in $\langle \rangle$ are referred to the mean values. Δ are related to differences between mean values.

Time (fs)	Φ_{E-M} ($^{\circ}$)				
	COF1[1]	COF1[2]	COF1[3]	COF1[7]	COF1[X]
0	95.10	96.15	95.83	109.90	101.49
40	92.80	95.43	96.10	110.22	101.77
80	90.47	92.91	93.56	107.27	99.14
120	88.95	91.28	91.92	105.35	97.44
160	88.67	90.97	90.61	103.82	96.08
200	91.61	92.14	92.79	106.36	98.34
240	91.84	94.39	95.05	109.00	100.69
300	90.80	93.27	93.92	107.68	99.51
340	97.57	98.58	92.87	106.46	98.42
380	93.22	95.88	96.55	110.75	102.24
420	94.96	95.76	96.43	110.61	102.12
460	91.61	90.14	101.58	116.60	107.44
500	93.74	94.45	95.11	109.06	99.13
540	96.57	97.50	98.18	112.65	103.93
580	90.90	93.38	94.03	107.81	99.63
620	91.94	94.50	92.16	105.63	97.69
660	99.69	100.87	90.78	104.02	96.25
700	91.95	94.52	95.18	109.15	100.82
740	92.31	92.90	93.55	107.25	100.74
780	92.44	93.04	93.69	107.42	99.28
820	89.54	91.91	92.55	106.09	98.09
880	92.59	95.20	99.27	113.92	105.06
920	94.97	96.77	97.45	111.80	103.17
960	88.20	90.47	91.11	104.40	96.60
1000	88.28	86.55	87.15	99.800	92.50
	$\langle 92.64 \rangle$	$\langle 94.12 \rangle$	$\langle 94.45 \rangle$	$\langle 108.29 \rangle$	$\langle 100.06 \rangle$
Δ	1.48	0.33	13.84	8.23	

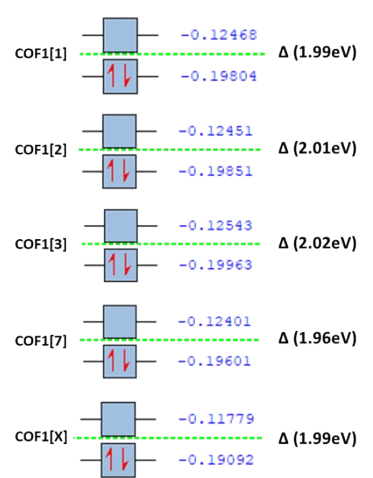


Fig. S11. Homo-Lumo absolute energies (Hartree) and their related differences (electronvolt) for COF1[1], COF1[2], COF1[3], COF1[7] and COF1[X] calculated at M11L/6-311G(d,p) level in gas phase.

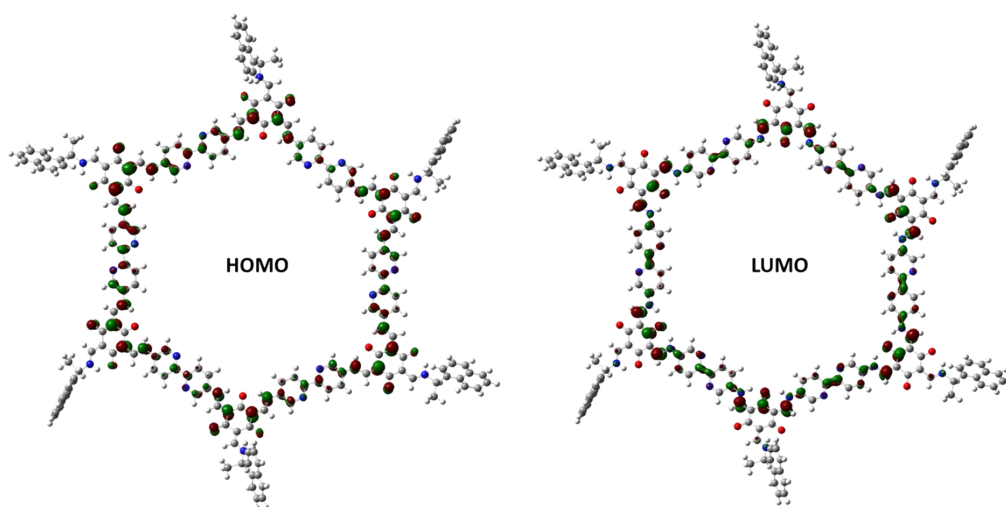


Fig. S12. Homo and Lumo orbital representations for COF1[1] calculated at M11L/6-311G(d,p) level in gas phase. For convenience only the (R) enantiomer is illustrated.

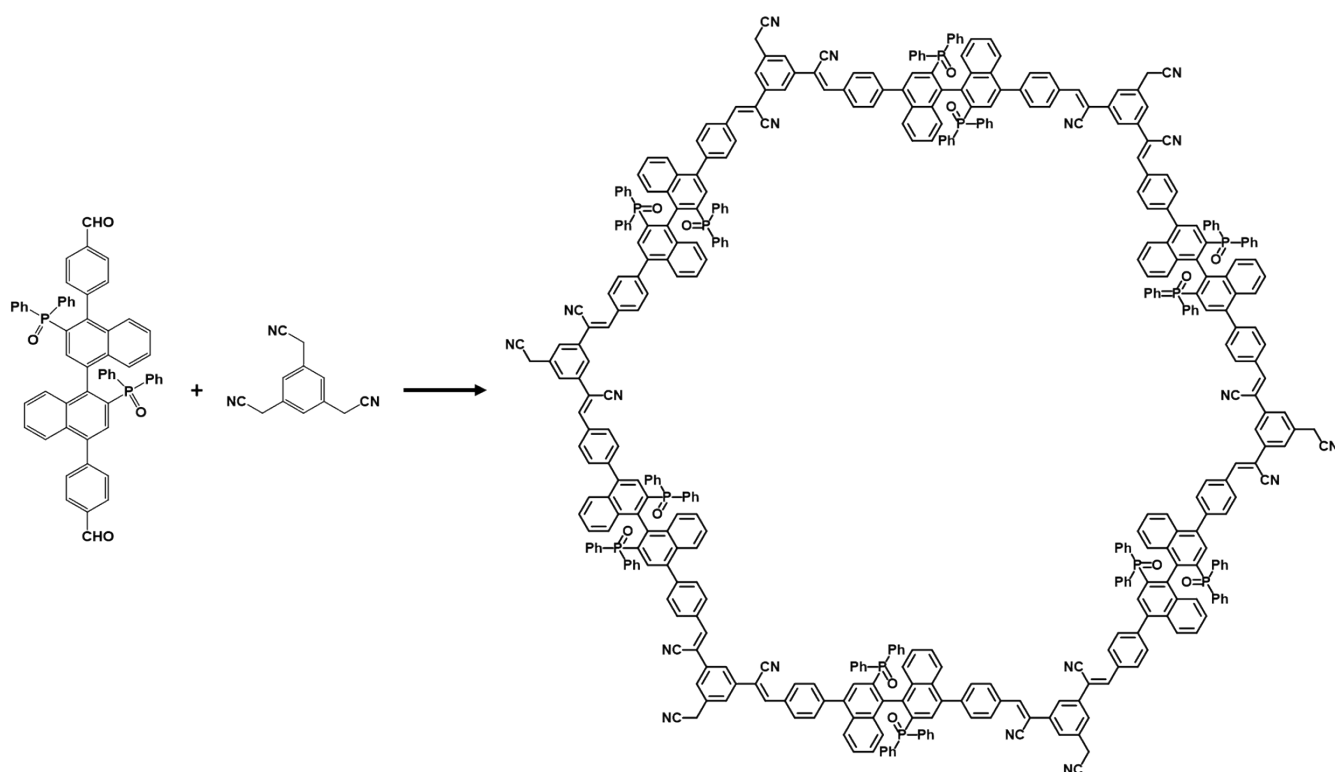


Fig. S13. Synthetic process for COF2, for a computational convenience COF2 condensation was truncated at the peripheral nitrile groups.

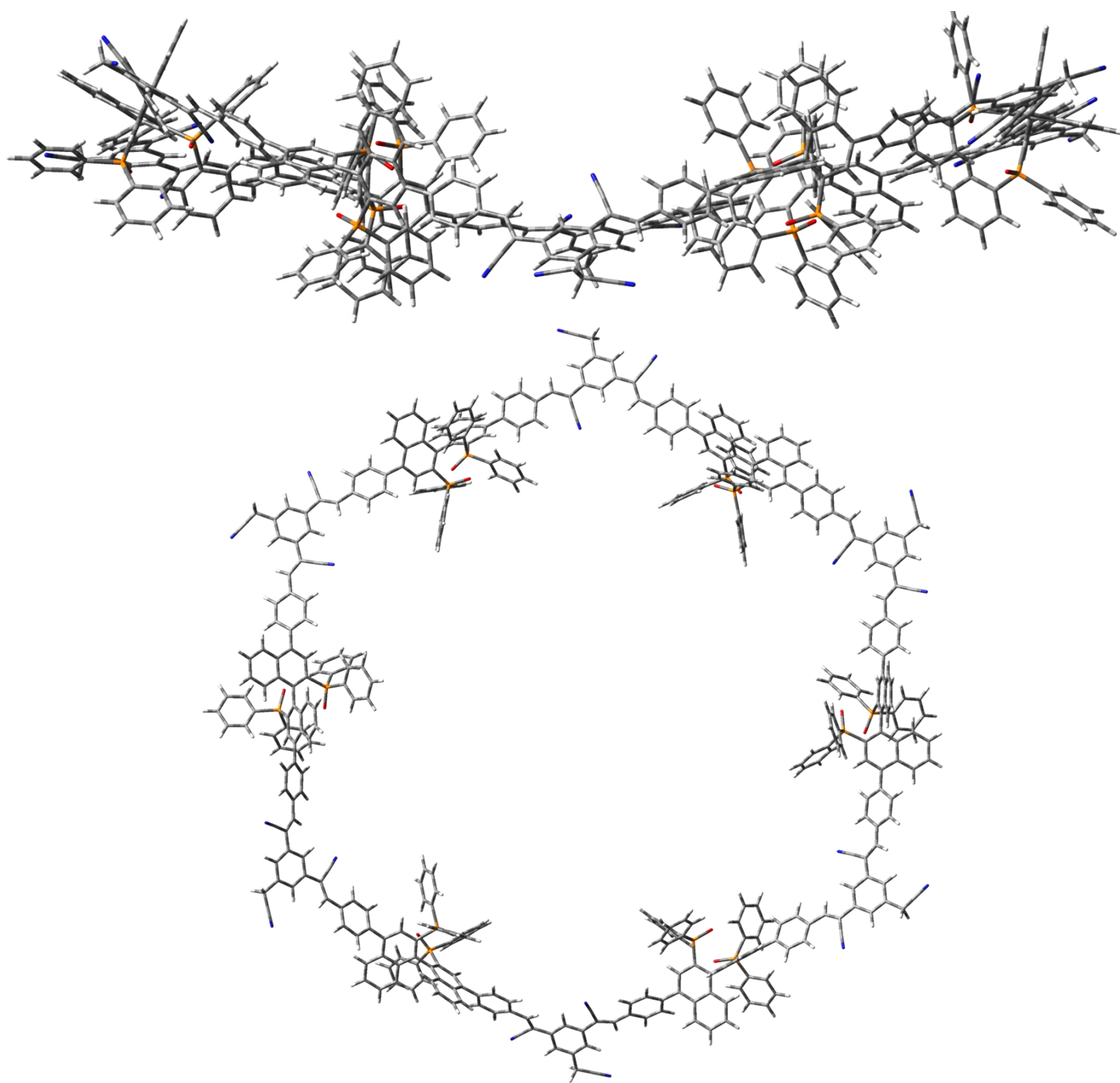


Fig. S14. Lateral (top) and frontal (down) perspectives of DFT-optimized COF2 at ω B97XD/6-311G(d,p) level in gas phase. For convenience only the (R) enantiomer is illustrated.

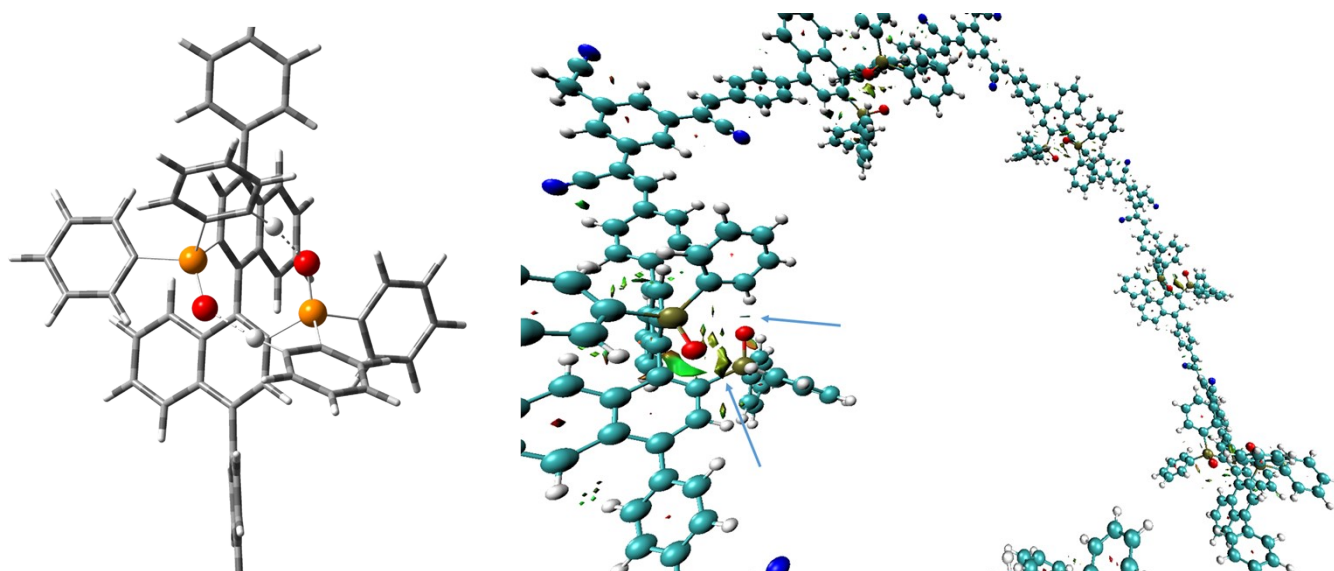


Fig. S15. (Left) Ten-members cyclic intramolecular hydrogen bonding in bisnaphthyl substituents (inside the hexagonal COF) through a ball and stick visualization. (Right) The related NCI mapped surfaces, arrows authenticate non-covalent interactions promoted by H-bonds as specified in the left part. It must be noted that this hydrogen bonding pattern is perpetuated in each bisnaphthyl unit.

Table S3. Computed rotational strengths for COF2 at M11L, M06L and MN12L/6-311G(d,p) levels.

Time (fs)	Rlength (cgs units)		
	M11L	M06L	MN12L
0	-0.6396	-0.051	-0.4523
40	-0.7946	0.0099	-1.0680
80	-1.0410	-4.6385	-1.5472
120	0.0000	-0.0017	-14.059
160	0.0000	-0.0000	0.0000
200	0.0000	0.0000	0.0000
240	0.6031	1.1827	0.9485
300	0.0003	-0.0001	0.0007
340	0.1810	-0.6926	0.3686
380	0.0004	0.0003	0.0012
420	0.0001	0.0000	0.0003
460	0.0000	0.0002	0.0097
500	-0.0000	0.0000	-0.0000
540	-0.0000	-0.0000	-0.0000
580	0.0005	0.0002	0.0007
620	0.0000	-0.0000	0.0000
660	0.0003	0.0002	0.0004
700	-0.0000	0.0000	-0.0000
740	-0.0000	-0.0000	-0.0000
780	0.0000	0.0000	0.0000
820	-0.0000	-0.0000	-0.0000
880	0.0000	0.0000	0.0000
920	0.0000	0.0000	0.0000
960	0.0006	0.0027	0.0016
1000	-0.0000	0.0000	-0.0000

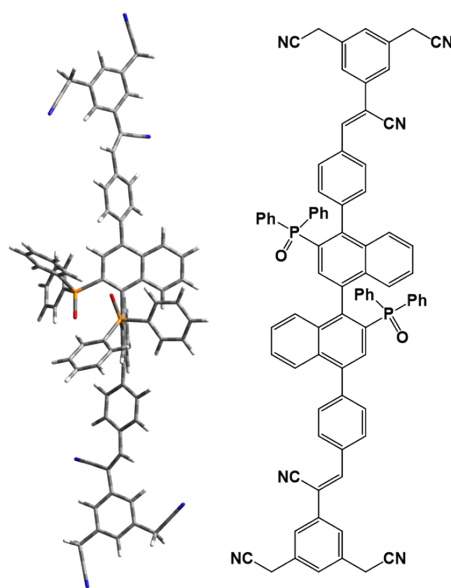


Fig. S16. (Left) DFT-optimized R-BIS2 (bis-condensed entity) at ω B97XD/6-311G(d,p) level in gas phase. (Right) R-BIS2 structure. For convenience only the (R) enantiomer is illustrated.

Table S4. Computed rotational strengths for R-BIS2 at O3LYP/6-311G(d,p) levels.

Time (fs)	λ (nm)	Rlength
		O3LYP
0	483.83	-5.5932
40	480.44	-1.7027
80	481.88	-0.6145
120	497.60	3.2478
160	461.37	4.0136
200	483.25	3.2615
240	468.75	2.7297
300	470.43	2.2585
340	460.94	2.0419
380	470.72	3.6497
420	440.58	5.8754
460	479.84	-0.2313
500	463.00	4.5546
540	448.91	2.1907
580	444.84	2.7913
620	435.48	5.7337
660	460.94	3.8769
700	472.73	1.3688
740	461.44	1.1263
780	490.06	-0.3645
820	528.59	-1.0964
880	518.67	-3.1150
920	492.91	0.1406
960	527.21	-3.7004
1000	511.38	-4.3415

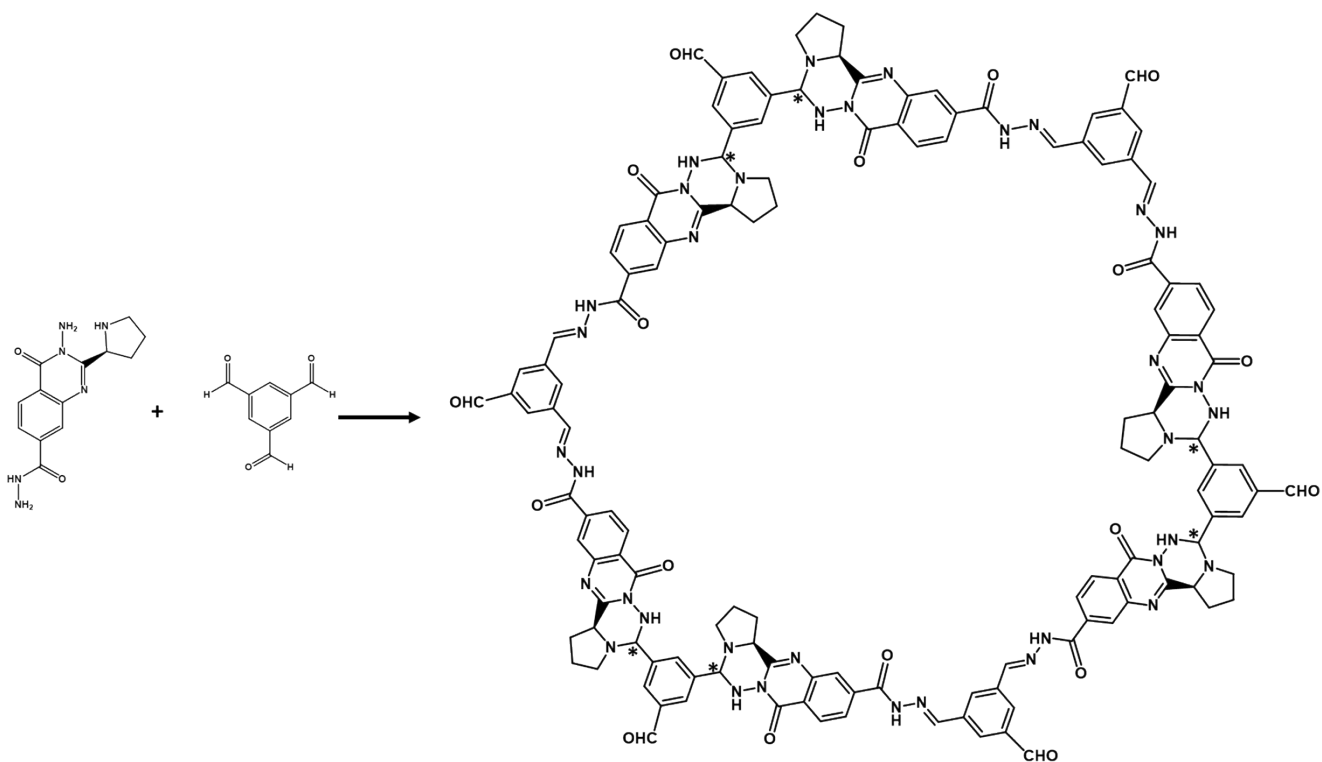


Fig. S17. Synthetic process for COF3, for a computational convenience COF3 condensation was truncated at the peripheral aldehyde groups. For a visualization convenience only L-COF3 (and the related S-monomer) is reported.

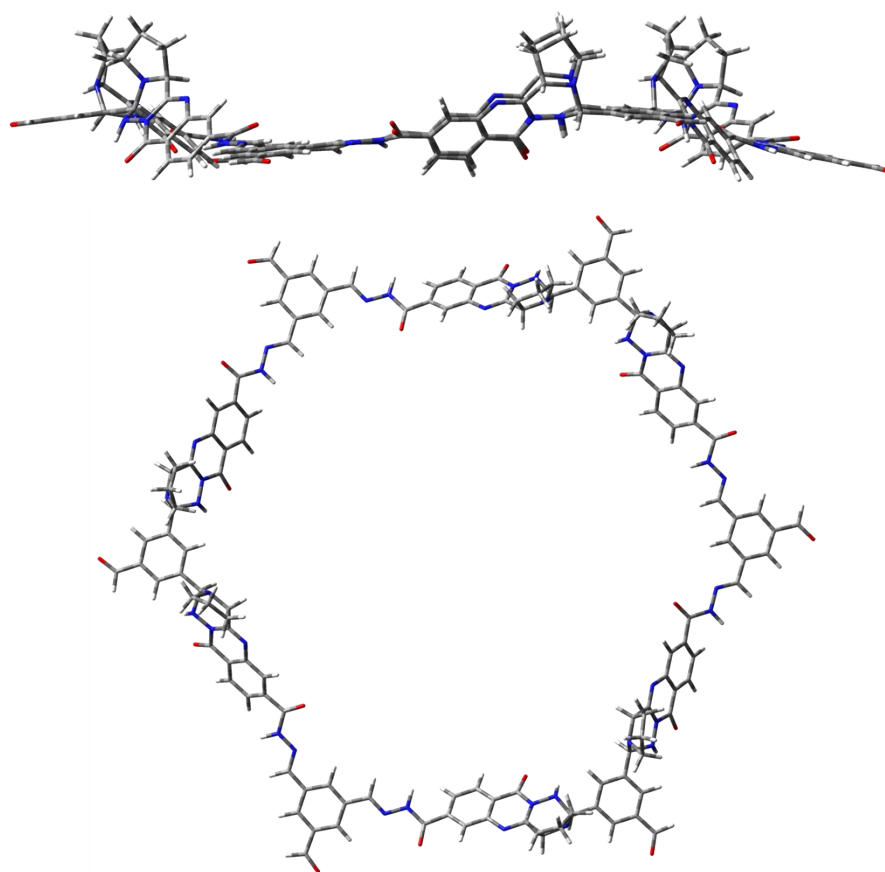


Fig. S18. Lateral (top) and frontal (down) perspectives of DFT-optimized COF3 at ω B97XD/6-311G(d,p) level in gas phase. For convenience only the (L) enantiomer is illustrated.

Table S5. Computed rotational strengths for COF3 at M11L, M06L and MN12L/6-311G(d,p) levels.

Time (fs)	Rlength (cgs units)		
	M11L	M06L	MN12L
0	-2.0000	-1.1999	-6.3000
40	0.0000	-2.9999	-1.5000
80	0.0000	0.0000	4.0000
120	-1.0000	-9.3000	-0.5076
160	0.0000	4.0000	-2.7000
200	0.0000	5.0000	0.0151
240	0.0000	4.0000	2.2000
300	-1.0000	-2.0000	-0.0281
340	0.0000	-1.3000	-3.1000
380	0.0000	9.0000	5.2000
420	0.0000	0.0000	1.0000
460	-1.0000	-5.0000	4.0000
500	0.0000	0.0000	0.0000
540	0.0000	0.0000	0.0000
580	0.0000	0.0000	0.0000
620	0.0000	2.0000	2.0000
660	0.0000	1.0000	0.0000
700	0.0000	-1.0000	-1.0000
740	-2.4974	-2.0327	-0.7724
780	-1.1000	-3.7000	0.0340
820	-2.0000	-7.0000	0.0000
880	0.0000	0.0000	0.0000
920	0.0000	0.0000	0.0000
960	0.0000	-2.0000	-4.0000
1000	0.0000	-2.0000	1.3000

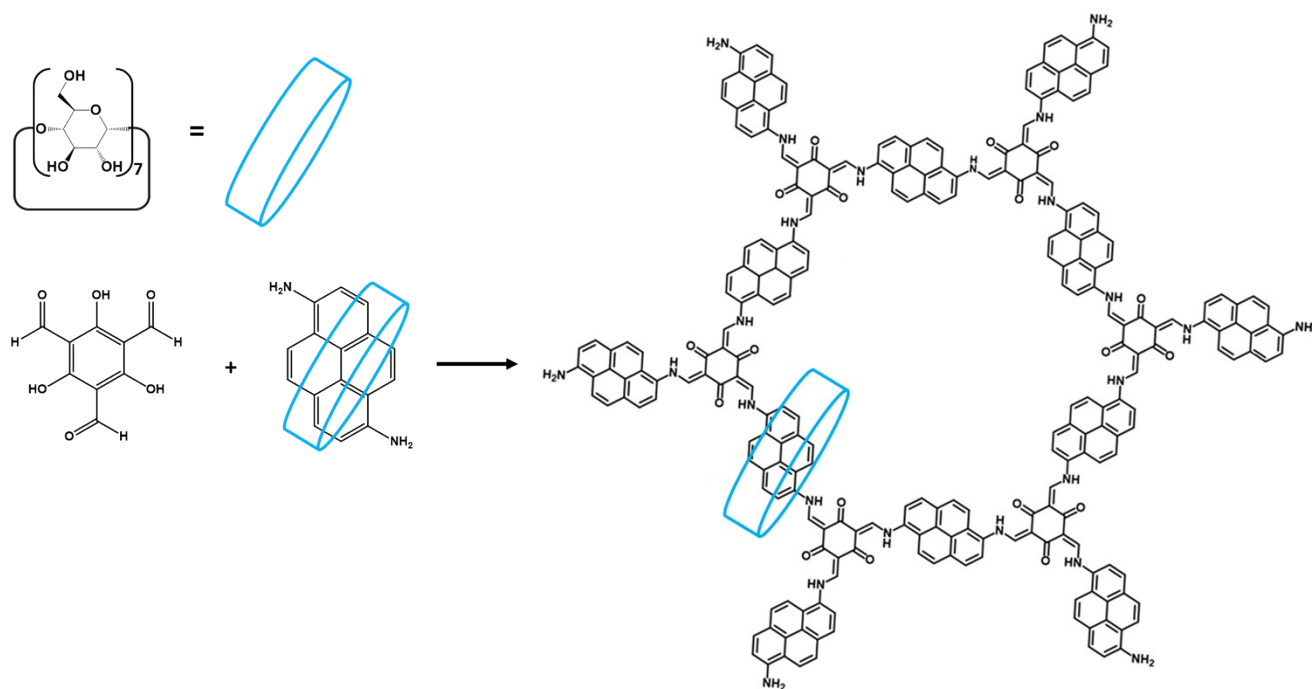


Fig. S19. Synthetic process for COF4, for a computational convenience COF4 condensation was truncated at the peripheral aldehyde groups. It must be noted that the number of mechanically interlocked cyclodextrins compatibly varies with the feeding ratio. For an easy drawing only one cyclodextrin was depicted.

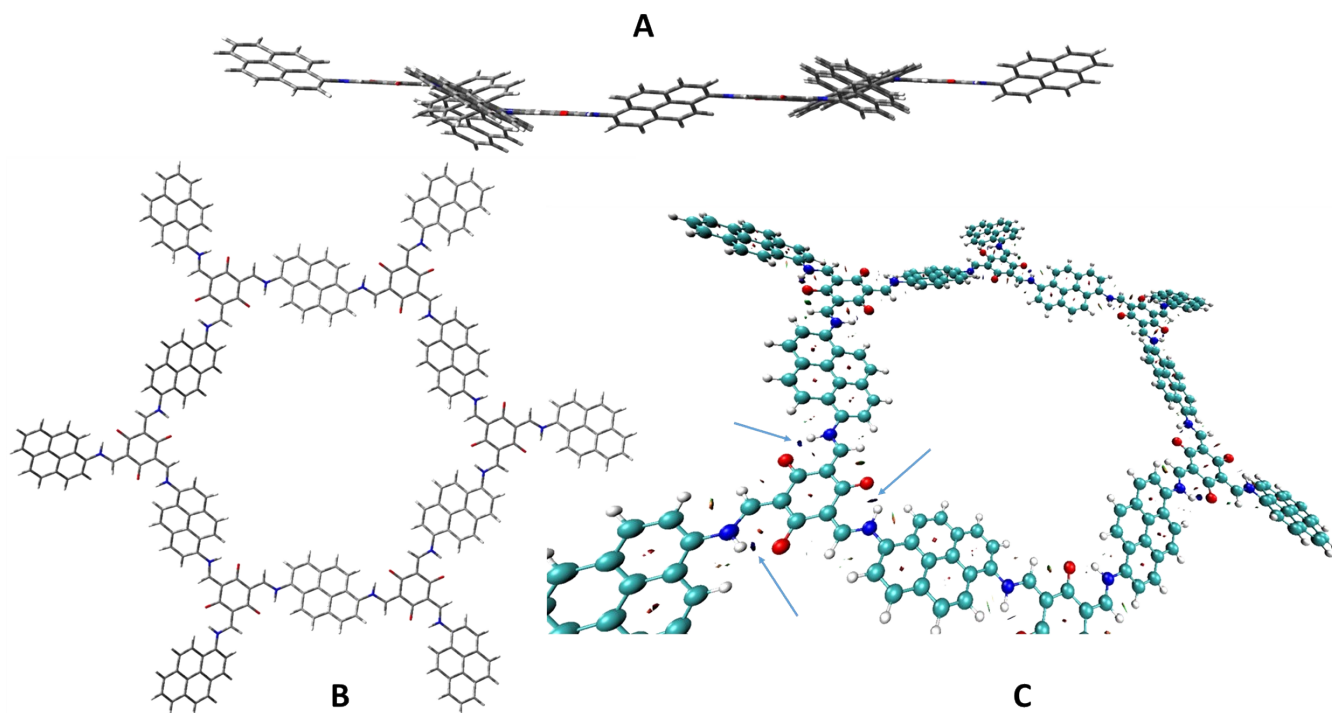


Fig. S20. Lateral (A) and frontal (B) perspectives of DFT-optimized naked COF4 at ω B97XD/6-311G(d,p) level in gas phase. (C) The related NCI mapped surfaces, arrows authenticate non-covalent interactions promoted by the most relevant H-bonds. It must be noted that this hydrogen bonding pattern is perpetuated in each pyrene-phloroglucinol couple.

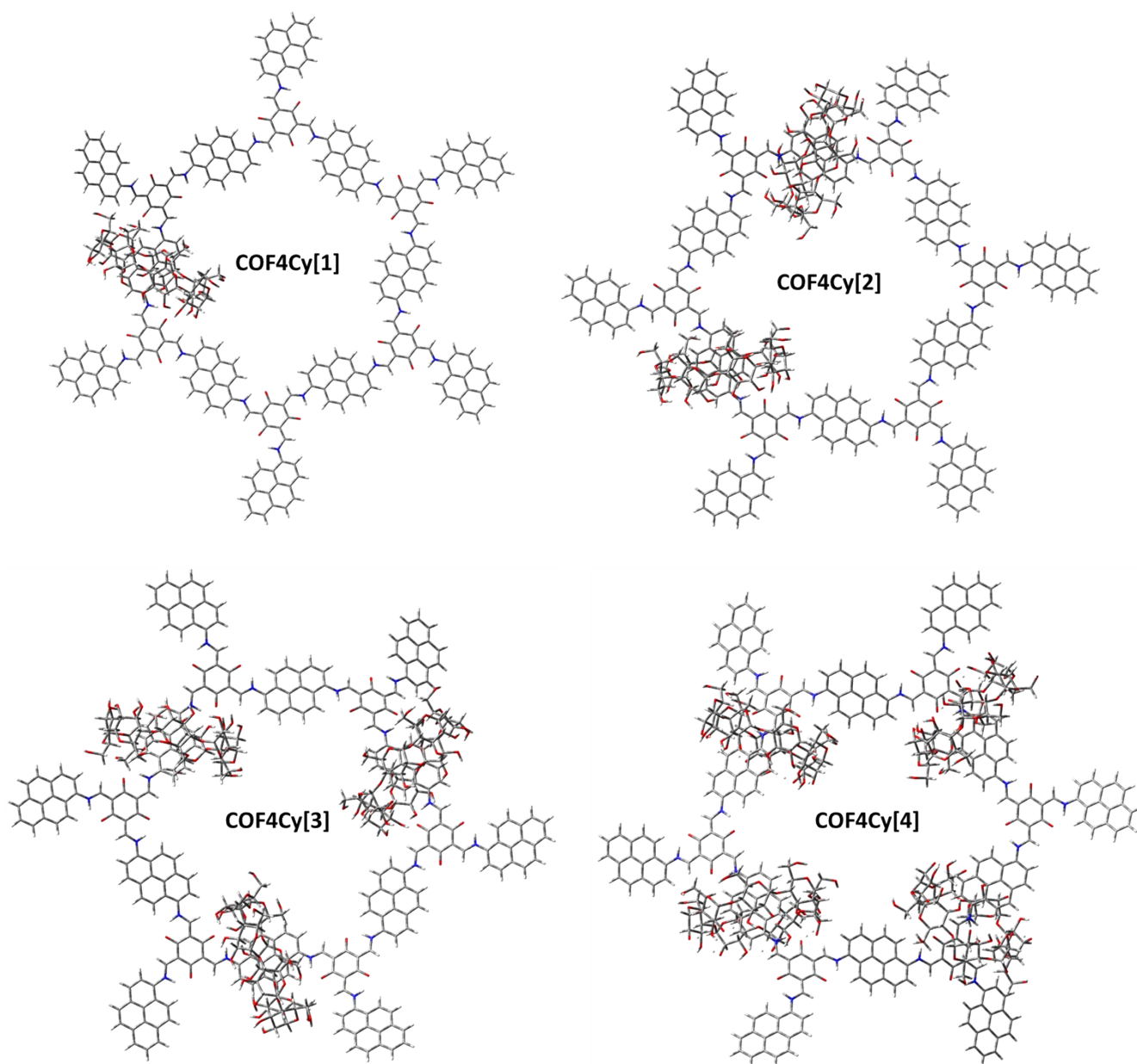


Fig. S21. Frontal perspectives of DFT-optimized COF4Cy[1], COF4Cy[2], COF4Cy[3] and COF4Cy[4] at ω B97XD/6-311G(d,p) level in gas phase.

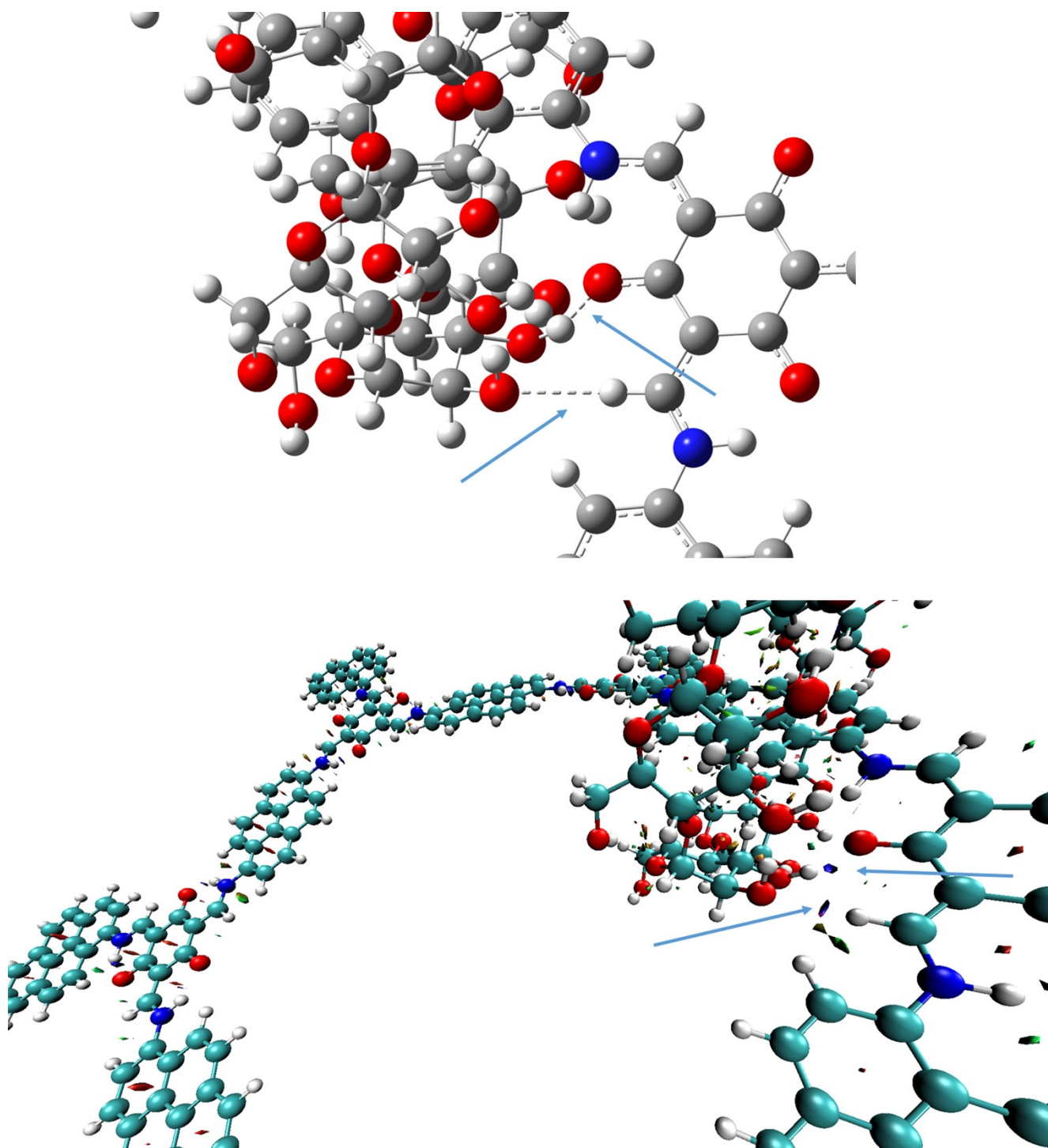


Fig. S22. (Top) Hydrogen bonds between the hydroxyl groups of the smaller rim and the β -ketoenamine fragment (the oxygen and the C-H positively polarized) through a ball and stick visualization. (Down) The related NCI mapped surfaces, arrows authenticate non-covalent interactions promoted by H-bonds as specified in the top part. It must be noted that this hydrogen bonding pattern is perpetuated in each cyclodextrin/pyrene dyad.

Table S6. Computed rotational strengths for COF4Cy[1] at M11L, M06L and MN12L/6-311G(d,p) levels.

Time (fs)	Rlength (cgs units)		
	M11L	M06L	MN12L
0	0.6411	0.2137	0.1172
40	1.2604	2.4145	2.6101
80	3.1086	3.2409	2.9395
120	2.5178	2.5590	2.2491
160	0.2478	1.1170	0.4190
200	3.7407	3.4042	3.1317
240	1.1492	1.6454	0.4415
300	1.1821	0.5473	8.5176
340	3.0744	3.2636	3.1965
380	3.2304	4.4934	3.3437
420	-1.737	-2.088	-2.064
460	-2.994	-3.121	-2.930
500	-2.045	-1.903	-2.297
540	0.7696	1.1338	0.5235
580	5.9767	1.3177	7.6955
620	1.7155	1.6912	0.4646
660	1.5763	2.0659	3.9795
700	-1.836	-3.112	-4.708
740	-6.747	-5.003	-6.672
780	6.9472	4.4850	4.2142
820	1.1326	0.9192	8.7197
880	1.9542	2.0966	1.9752
920	4.8004	5.0321	5.2571
960	2.6755	1.6834	6.8519
1000	-1.388	-2.168	-2.522

Table S7. Computed rotational strengths for COF1Cy[1], COF1Cy[2], COF1Cy[3] and COF1Cy[4] at ω B97xD/6-311G(d,p) level. Numbers in $\diamond$ are referred to the mean values.

Time (fs)	Rlength (cgs units)			
	COF4Cy[1]	COF4Cy[2]	COF4Cy[3]	COF4Cy[4]
0	-461.4246	-1195.7058	254.0401	-381.0602
40	520.5838	873.2915	-1403.2692	-2104.9038
80	87.2893	1010.1937	-1644.2095	-1466.3143
120	-71.5288	702.7537	-2121.4200	-2182.1300
160	-133.3050	-988.6350	-1784.3165	-2676.4748
200	-1.0051	-979.3772	-1351.7044	-2027.5566
240	286.5183	-1382.3382	-1838.2600	-2757.3900
300	674.7747	-1052.0981	-1593.5160	-2390.2740
340	339.4117	-1069.1622	-1309.6917	-1964.5376
380	205.8801	-1271.8092	-297.7821	1346.6732
420	-95.2188	1233.1573	1107.3981	1661.0972
460	-255.2227	1664.7329	-1162.9185	-1744.3778

500	-310.5343	-1078.7094	-1550.6393	2325.9590
540	-297.9006	-1327.9762	-1150.0036	1725.0054
580	87.6425	-647.8357	1015.5870	1523.3805
620	122.1658	680.4542	1007.9443	-1511.9165
660	230.8096	573.1545	1250.1350	1875.2025
700	303.0314	403.4662	-1409.4095	-2114.1143
740	101.8446	-547.2247	976.1746	-1464.2619
780	-1434.3975	1569.3330	799.1708	1198.7564
820	-1636.3756	1813.1123	808.2853	1212.4280
880	-1209.2415	-1515.0811	913.4628	1370.1944
920	-917.3088	-1018.3300	1038.9265	1558.3898
960	354.1080	-1193.1308	736.8126	1105.2189
1000	-739.6546	-1333.9282	879.4656	1319.1984
	<-204.340>	<-215.297>	<-267.879>	<-302.350>

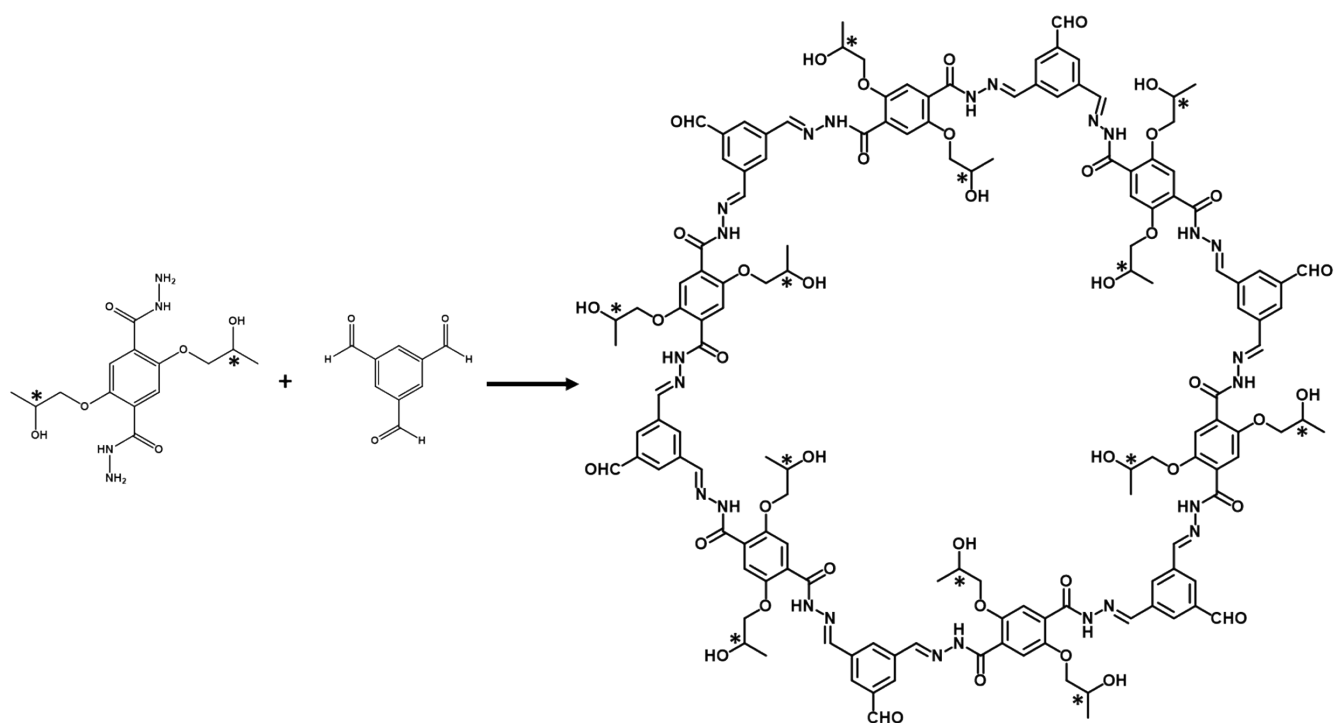


Fig. S23. Synthetic process for COF5, for a computational convenience COF5 condensation was truncated at the peripheral aldehyde groups.

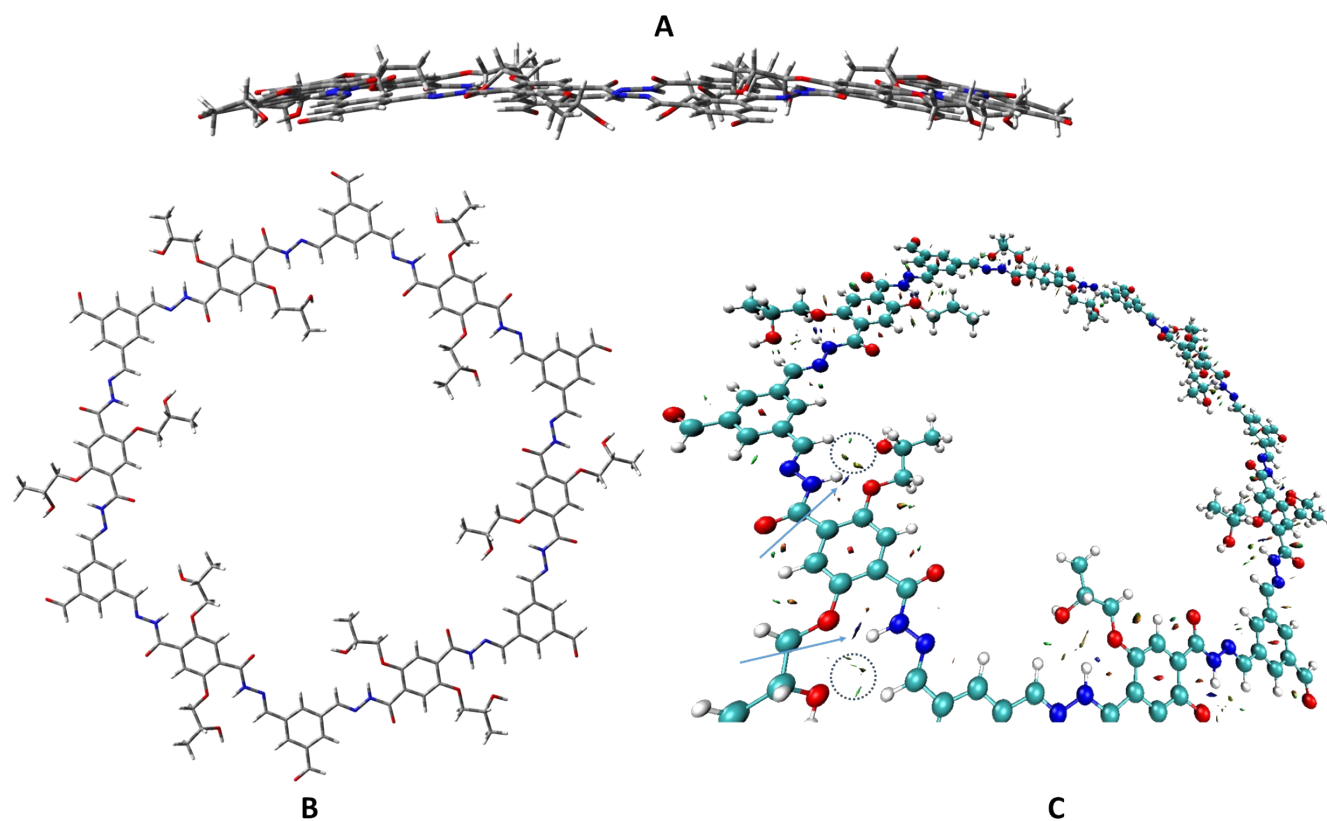


Fig. S24. Lateral (A) and frontal (B) perspectives of DFT-optimized naked COF5 at ω B97XD/6-311G(d,p) level in gas phase. (C) The related NCI mapped surfaces, arrows authenticate non-covalent interactions promoted by the cyclic six-members H-bonds, dotted circles indicate the secondary electrostatic interactions. It must be noted that this hydrogen bonding pattern is perpetuated in each terephthalate chain.

Table S8. Computed rotational strengths for COF5 at M11L, M06L and MN12L/6-311G(d,p) levels.

Time (fs)	Rlength (cgs units)		
	M11L	M06L	MN12L
0	-0.2623	-0.1116	-0.0999
40	0.1643	-0.0542	-0.0439
80	-7.0000	-3.9000	-9.8000
120	0.0122	0.0891	0.0962
160	-8.2000	-5.7000	-5.1000
200	-0.0158	-0.0137	-0.0137
240	0.0195	0.0122	-0.0556
300	-0.0526	-0.0764	-0.0828
340	-0.2140	-0.2862	-0.2757
380	-0.1365	-0.1767	-0.2035
420	0.0639	0.0885	0.0851
460	-6.8000	-9.5000	-5.7000
500	9.0000	-1.0000	-5.9999
540	0.0512	0.0617	0.0761
580	-0.0646	-0.0330	-3.5000
620	-0.0157	-0.0184	-0.0140
660	-0.2054	-0.2282	-0.0577
700	-2.9999	-2.6000	-2.3000
740	-0.0115	-0.0100	-1.9000

780	-0.0320	-0.0593	-0.0525
820	0.0523	0.1071	0.1070
880	-0.0973	-0.0736	-0.0603
920	0.7324	0.8621	0.8606
960	0.0294	0.0528	0.0698
1000	-0.5387	-0.2044	-0.0549

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

R-COF1[1]

	X	Y	Z
C	-2.9216410	16.7854010	2.9720500
C	-2.6671700	15.4526170	2.3739550
C	-3.7268750	14.4682640	2.2299390
C	-5.0745980	14.8078830	2.6613800
C	-5.3703240	16.1193560	3.2700950
C	-4.2900820	17.0798920	3.4130590
O	-1.9766520	17.6362180	3.0925190
O	-3.4740330	13.2899850	1.7158060
O	-6.5711350	16.3959180	3.6620520
C	-1.3669640	15.1931620	1.9487440
H	-0.6426670	15.9899200	2.0906880
C	-6.1382390	13.9218740	2.5105110
H	-7.1095310	14.2624180	2.8557010
N	-0.9590570	14.0284890	1.3900990
N	-6.0302590	12.6833530	1.9714410
C	0.3359620	13.7409270	0.9102790
C	1.3460250	14.7182910	0.7488070
C	0.6487230	12.4061560	0.5539810
C	2.5958590	14.3269530	0.2599530
H	1.1656830	15.7622950	0.9841810
H	-0.1000860	11.6230770	0.6591030
C	2.8285730	12.9706700	-0.0666780
H	3.3987330	15.0398610	0.1148420

C	4.1429360	12.5241320	-0.5862210
C	4.4133750	11.1614760	-0.8510830
C	6.3007300	13.1331920	-1.2601790
C	5.6707420	10.7958570	-1.3432310
H	3.6341700	10.4305950	-0.6700190
C	6.6464290	11.7942070	-1.5688960
H	7.0160530	13.9422550	-1.3772990
H	5.8979640	9.7550310	-1.5613690
N	1.8522190	12.0296750	0.0828410
N	5.0895200	13.4847540	-0.7897730
C	-10.6164120	-10.5807290	-2.8226140
C	-10.2032940	-11.9704920	-2.9484870
C	-11.1086080	-12.9845010	-3.5227530
C	-12.4296600	-12.5695440	-3.9602480
C	-12.8926100	-11.1821190	-3.8345390
C	-11.9523530	-10.1969170	-3.2475900
O	-9.7934550	-9.6891040	-2.3283620
O	-10.7208010	-14.2139080	-3.6283010
O	-14.0591050	-10.8247270	-4.2115500
C	-12.4143140	-8.8900040	-3.1136400
H	-13.4277250	-8.6967030	-3.4524190
C	-8.9488260	-12.4036510	-2.5277650
H	-8.7304760	-13.4596050	-2.6548480
C	-13.3262110	-13.4927940	-4.5278650
H	-14.2931580	-13.1026050	-4.8309180
N	-11.6869020	-7.8692130	-2.5992850
N	-8.0009560	-11.5992290	-1.9893550
C	-12.1228990	-6.5429160	-2.3935160
C	-13.4697780	-6.1343580	-2.5596820
C	-11.1876470	-5.5643610	-1.9832920
H	-14.2434800	-6.8362610	-2.8560040
C	-11.6149650	-4.2503620	-1.7654810
C	-12.9772660	-3.9246780	-1.9596110

H	-10.9315670	-3.4703910	-1.4512140
C	-13.4918110	-2.5530240	-1.7359780
C	-14.8634260	-2.2527150	-1.9070300
C	-15.3234300	-0.9529380	-1.6780910
H	-15.5325290	-3.0469200	-2.2159030
C	-13.0431030	-0.3407930	-1.1354570
C	-14.4001800	0.0408440	-1.2756240
H	-16.3758890	-0.7272270	-1.8157500
H	-12.2981550	0.3927270	-0.8319540
N	-13.8794950	-4.8692040	-2.3521560
N	-12.6004030	-1.5928290	-1.3559890
C	12.8248520	11.1294210	-3.8796460
C	12.3302230	12.5054990	-4.0074480
C	10.9969410	12.8894270	-3.5777710
C	10.1124000	11.8544440	-3.0086310
C	10.5563130	10.4744090	-2.8844690
C	11.9035690	10.1217750	-3.3006270
O	14.0019180	10.7993560	-4.2487350
O	10.5815270	14.1092390	-3.6852900
O	9.7496960	9.5616700	-2.3999670
C	12.3942330	8.8254230	-3.1648080
H	13.4145350	8.6549870	-3.4951810
C	13.2084340	13.4500730	-4.5686760
H	14.1861910	13.0829540	-4.8658020
C	8.8458500	12.2569870	-2.5919790
H	8.5982370	13.3068130	-2.7180040
N	11.6844940	7.7889450	-2.6571260
N	7.9170920	11.4253390	-2.0607910
C	3.7454920	-14.3340930	2.2561000
C	5.0883040	-14.7088650	2.6736930
C	5.3581360	-16.0334070	3.2660600
C	4.2567420	-16.9694640	3.4080500
C	2.8919070	-16.6387460	2.9806020

C	2.6645610	-15.2952230	2.3958280
O	3.5161560	-13.1431560	1.7586140
O	6.5552780	-16.3417750	3.6453960
O	1.9285240	-17.4681840	3.1010460
C	1.3682820	-15.0009490	1.9797060
H	0.6225230	-15.7785330	2.1183200
C	6.1707290	-13.8455290	2.5242250
H	7.1370750	-14.2115310	2.8570620
C	4.4611940	-18.2476820	3.9582600
H	3.5876900	-18.8891570	4.0259480
N	0.9886050	-13.8195770	1.4355350
N	6.0848310	-12.5991110	1.9995070
C	-0.2958070	-13.4978680	0.9458490
C	-1.2755030	-14.4794690	0.6551370
C	-0.6300240	-12.1453220	0.7043140
H	-1.0699120	-15.5381280	0.7849710
C	-1.9015190	-11.8275220	0.2150510
H	0.0957720	-11.3616140	0.9081950
C	-2.8282140	-12.8670230	-0.0309040
H	-2.2021380	-10.8044720	0.0223280
C	-4.1904770	-12.5909480	-0.5455670
C	-5.0819380	-13.6455960	-0.8513010
C	-6.3607090	-13.3547670	-1.3352570
H	-4.7510800	-14.6652640	-0.6940660
C	-5.7860400	-11.0064050	-1.1776300
C	-6.7358650	-12.0022620	-1.5131300
H	-7.0477070	-14.1659150	-1.5542960
H	-6.0341260	-9.9531090	-1.2959510
C	7.1504840	-11.7036970	1.7693870
C	6.8627550	-10.3810970	1.3586130
C	8.5135790	-12.0654760	1.9090580
C	7.9133670	-9.4909750	1.1145670
H	5.8298590	-10.0630920	1.2370200

H	8.8070130	-13.0687180	2.2034890
C	9.2467640	-9.9312270	1.2828400
H	7.7374910	-8.4695170	0.7987190
C	10.3999740	-9.0361280	1.0280950
C	11.7291800	-9.4996420	1.1658120
C	11.1621870	-6.9193350	0.4012750
C	12.7966050	-8.6350630	0.9060410
H	11.8905310	-10.5258830	1.4736040
C	12.5209850	-7.3060560	0.5067380
H	10.9051110	-5.9048930	0.1013530
H	13.8146050	-8.9940560	1.0177040
N	-2.4998930	-14.1726740	0.1876260
N	-4.5548250	-11.2867290	-0.7110610
N	9.5242760	-11.2072890	1.6761430
N	10.1348600	-7.7520610	0.6511620
C	17.8711260	-3.6210980	-0.7534180
C	16.4456250	-3.2410620	-0.7297230
C	15.4137400	-4.2197430	-0.4213020
C	15.7996310	-5.5906760	-0.1314930
C	17.2199500	-6.0157330	-0.1435680
C	18.2289990	-4.9985280	-0.4628210
O	18.7733760	-2.7360310	-1.0282530
O	14.1521420	-3.8669100	-0.4048050
O	17.5402560	-7.2248000	0.1151720
C	16.1356000	-1.9124620	-1.0093750
H	16.9705630	-1.2527190	-1.2240720
C	14.8531150	-6.5677890	0.1668570
H	15.2334420	-7.5651870	0.3662620
N	14.8789240	-1.4072330	-1.0203240
N	13.5168940	-6.3519410	0.2127600
C	14.5107730	-0.0737380	-1.2930840
C	15.4237020	0.9296490	-1.6949660
C	13.1482410	0.2913820	-1.1615680

C	14.9482370	2.2226520	-1.9325380
H	16.4797640	0.7163550	-1.8252060
H	12.4112620	-0.4503650	-0.8585600
C	13.5720210	2.5061360	-1.7700700
H	15.6089040	3.0239520	-2.2414240
C	13.0386190	3.8690970	-2.0018450
C	11.6704570	4.1732290	-1.8135160
C	13.4972050	6.0842020	-2.6087560
C	11.2228350	5.4791130	-2.0370160
H	10.9990410	3.3831600	-1.4987820
C	12.1434870	6.4714690	-2.4473110
H	14.2600150	6.7974720	-2.9062790
H	10.1746980	5.7347610	-1.8996620
N	12.6909550	1.5363090	-1.3900200
N	13.9268180	4.8263520	-2.3952910
C	-17.0885410	6.0031560	-0.1737690
C	-18.0984640	4.9852730	-0.4872160
C	-17.7417520	3.6053420	-0.7662970
C	-16.3166950	3.2234150	-0.7366640
C	-15.2833030	4.2024880	-0.4338160
C	-15.6687090	5.5760960	-0.1553770
O	-17.4076930	7.2146430	0.0750160
O	-18.6447670	2.7194900	-1.0362160
O	-14.0227200	3.8481470	-0.4121500
C	-14.7232540	6.5551350	0.1379650
C	-19.4410340	5.4038080	-0.5108570
H	-19.6236360	6.4518550	-0.2933540
C	-16.0101850	1.8922300	-1.0055290
H	-16.8478320	1.2346880	-1.2161340
N	-13.3864780	6.3433020	0.1896320
N	-14.7562890	1.3797290	-1.0112350
C	-12.3976210	7.3058130	0.4820450
C	-11.0349770	6.9339930	0.3734230

C	-12.6866250	8.6313070	0.8838370
H	-10.7671880	5.9227950	0.0719760
C	-11.6284770	9.5072930	1.1416580
H	-13.7080260	8.9789760	0.9995610
C	-10.2945370	9.0587410	1.0001820
H	-11.8003760	10.5312530	1.4511720
C	-9.1523750	9.9684890	1.2533930
C	-7.8129830	9.5480810	1.0825740
C	-6.7748380	10.4532030	1.3267200
H	-7.6223320	8.5297350	0.7651220
C	-8.4495250	12.1126020	1.8805950
C	-7.0814130	11.7707260	1.7399390
H	-5.7376310	10.1501460	1.2037660
H	-8.7572920	13.1115710	2.1748740
N	-10.0160580	7.7780290	0.6218470
N	-9.4477090	11.2401860	1.6481180
C	-4.5202260	18.3473550	3.9778750
H	-3.6616190	19.0086280	4.0454760
C	19.5722080	-5.4153410	-0.4805710
H	19.7558380	-6.4614580	-0.2547870
C	-9.4506490	22.9112620	7.8581610
C	-9.1127750	21.8118310	8.6339830
C	-8.1976710	20.8225960	8.1535840
C	-7.6165160	20.9681290	6.8394000
C	-7.9875000	22.1188770	6.0674060
C	-8.8798430	23.0625840	6.5602510
H	-8.2978840	19.5938170	9.9465830
H	-10.1474720	23.6571440	8.2318460
H	-9.5424170	21.6852790	9.6256510
C	-7.8526110	19.6926520	8.9588990
C	-6.6972690	19.9589260	6.3692420
H	-7.5720460	22.2665780	5.0750570
H	-9.1481090	23.9240930	5.9536430

C	-6.3913540	18.8765290	7.1886910
C	-6.9666510	18.7386500	8.4850310
H	-5.7063760	18.1118090	6.8345160
H	-6.7057620	17.8775240	9.0946440
C	-6.0234090	20.1047120	4.9959110
N	-5.7066110	18.7752750	4.4259610
C	-4.7879780	21.0307610	5.0733960
H	-4.0161250	20.6101950	5.7286480
H	-4.3538490	21.2137290	4.0827460
H	-5.0883590	21.9948810	5.4949400
H	-6.7442310	20.5613840	4.3032780
N	-20.4811470	4.6049980	-0.7785470
N	-13.0635240	-14.7924140	-4.7107180
N	5.6405620	-18.7080300	4.3925820
N	20.6117750	-4.6171660	-0.7522350
N	12.9165730	14.7433170	-4.7523670
H	-10.1441260	-5.8361650	-1.8419300
C	-21.9093930	4.9881080	-0.8554180
H	-22.2104490	4.8091970	-1.8971990
C	-22.1435230	6.4841910	-0.5442190
H	-23.2127680	6.7036100	-0.6216930
H	-21.8287280	6.7319160	0.4763280
H	-21.6114950	7.1346290	-1.2493260
C	-22.7606360	4.0898170	0.0555120
C	-24.1444360	3.8313460	-0.2652100
C	-22.2167300	3.5562380	1.2200730
C	-24.7911050	4.3421950	-1.4394070
C	-24.9280730	3.0191560	0.6360400
C	-22.9948770	2.7565630	2.1063590
H	-21.1741270	3.7427600	1.4600880
C	-26.1252420	4.0639060	-1.7084830
H	-24.2379700	4.9582490	-2.1420450
C	-26.3001200	2.7509190	0.3322140

C	-24.3246510	2.4927130	1.8205800
H	-22.5338890	2.3547790	3.0048580
C	-26.8920850	3.2600440	-0.8145960
H	-26.5912340	4.4598370	-2.6074950
H	-26.8750170	2.1357670	1.0214850
H	-24.9252050	1.8815810	2.4909600
H	-27.9351780	3.0501320	-1.0369270
C	-13.9430590	-15.8055350	-5.3375320
H	-13.4242150	-16.1267580	-6.2516090
C	-15.3175040	-15.2301220	-5.7494480
H	-15.9168820	-16.0244840	-6.2046580
H	-15.8693840	-14.8575620	-4.8784600
H	-15.2168920	-14.4192730	-6.4813420
C	5.9300740	-20.0503110	4.9466870
H	6.6368280	-20.5155620	4.2453280
C	22.0406960	-4.9988990	-0.8233740
H	22.3439250	-4.8257800	-1.8654940
C	13.7764180	15.7772640	-5.3724280
H	13.2551940	16.0887040	-6.2885390
C	4.6744500	-20.9490750	5.0207710
H	4.9553000	-21.9245310	5.4295200
H	3.9158850	-20.5189090	5.6852280
H	4.2308500	-21.1106740	4.0306110
C	22.2759930	-6.4928090	-0.5027970
H	23.3456440	-6.7114000	-0.5769650
H	21.9596240	-6.7348530	0.5186250
H	21.7460400	-7.1480530	-1.2050130
C	15.1655240	15.2335950	-5.7783200
H	15.7492570	16.0420160	-6.2290630
H	15.7212610	14.8719090	-4.9051980
H	15.0868210	14.4220300	-6.5121130
C	6.6140190	-19.9347680	6.3179290
C	7.5124190	-20.9695910	6.7724100

C	6.3368090	-18.8547290	7.1506020
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C	8.1030790	-20.8516990	8.0851280
C	6.9214090	-18.7441120	8.4453910
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C	8.7264580	-23.0889710	6.4641280
H	7.4300290	-22.2472430	4.9942720
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C	7.7877190	-19.7231050	8.9043900
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C	9.3067510	-22.9649170	7.7607260
H	8.9721480	-23.9496330	5.8468480
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C	24.9228180	-4.3523410	-1.4047460
C	25.0534230	-3.0173570	0.6634500
C	23.1166010	-2.7489480	2.1279410
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H	24.3720700	-4.9731130	-2.1051040
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C	24.4466710	-2.4849940	1.8436340
H	22.6530920	-2.3426770	3.0231200
C	27.0209760	-3.2638740	-0.7814260
H	26.7256970	-4.4742160	-2.5681470
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H	25.0449360	-1.8692920	2.5118760
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C	14.2161490	18.5670120	-6.4150330
C	14.2927070	19.4305560	-4.1074460
C	14.0028130	17.9504270	-2.1856900
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C	14.4352880	19.8482760	-6.9050440
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C	14.5182200	20.7381750	-4.6422870
C	14.2225960	19.2200430	-2.6949520
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C	14.5891620	20.9489760	-6.0117110
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C	-14.1028910	-17.0256460	-4.4173520
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C	-14.5458560	-19.4490020	-4.0823560
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C	-14.6797650	-19.8590570	-6.8815130
H	-14.3023440	-17.7706870	-7.0953360
C	-14.7960380	-20.7506140	-4.6208720
C	-14.4804030	-19.2422800	-2.6690760
H	-14.1842380	-17.8201020	-1.0822370
C	-14.8628430	-20.9576370	-5.9910780
H	-14.7308520	-20.0245940	-7.9548780
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H	-15.0529250	-21.9505320	-6.3905320

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H	-12.1206270	-15.0754640	-4.3931140
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H	5.1183790	-12.3334300	1.7414090
H	6.4160200	-18.0314560	4.2878470
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H	11.9652980	15.0040620	-4.4405760
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H	-5.0610960	12.4395120	1.7030300
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R-COF1[2]

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C	16.1768900	15.4415210	-8.1107420
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C	27.1249950	-9.8989710	6.9635860
C	28.2179370	-9.0987340	7.5285000
C	28.3881870	-7.6915930	7.2106920
C	27.4273800	-7.0531030	6.2902990
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O	29.3581770	-7.0015400	7.7155110
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C	28.1814210	-2.8881860	5.1049500
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O	2.9184380	6.4613590	-2.5208320
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H	-1.1557540	11.0314710	-1.8137870
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C	14.7323120	-18.3456730	-1.6958610
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O	12.4472180	-18.3259930	-2.4316630
O	16.9874670	-18.2287280	-0.8998030
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H	23.8950170	-12.2792430	4.5815850
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H	9.0782550	-10.6522080	-1.3076030
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C	4.1986350	-10.6652740	-2.0558870
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C	-0.7476320	-6.1842790	-2.1994400
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C	1.7428670	-10.4902560	-2.2309680
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C	0.8711030	0.2544250	-2.0353700
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C	24.1286960	10.7666310	-2.4909600
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C	22.9267350	10.0211380	-2.5014360
H	24.1561400	11.7121510	-3.0193300
C	21.7216400	10.5229900	-3.2029650
C	20.5004120	9.8101480	-3.1851170
C	19.3912290	10.3358460	-3.8556540
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C	-29.1643820	-4.3551940	1.0208590
H	-28.1263180	-4.0526160	0.9221740
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C	-17.4295600	-17.2784360	-4.1257120
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H	-24.8954130	-22.3807770	-13.8703550
H	-25.7942570	-21.6222980	-11.7158030
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C	-47.0149020	-5.3278740	-11.1642450
H	-46.7321030	-4.8630440	-12.1191530
C	-48.2250740	-4.5501690	-10.5981050
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H	-48.5335600	-4.9487200	-9.6244640
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C	-48.4083580	-8.5600520	-12.8449220
C	-47.4460490	-9.1362920	-10.6746580
H	-46.5720480	-7.4925400	-9.5611720
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C	-48.0939520	-9.5236600	-11.8364490
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C	-49.3856760	-8.0208800	-15.0298270
H	-49.2765570	-5.9252560	-15.6137180
H	-49.3385790	-9.9988020	-14.1806770
H	-48.3697770	-10.5636860	-11.9971500
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H	-48.3142950	4.6443550	11.5625110
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R-COF1[7]

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C	14.6509840	-6.6125990	-0.2799390
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C	19.4807460	-5.3816470	-0.2925550
H	20.2070130	-4.5395420	-0.2931830
C	16.0929380	-1.9113010	-0.2750450
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C	13.1321500	-11.2495490	-0.2862670
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C	11.7848190	-10.8242400	-0.2821980
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C	28.2013050	-8.5232960	-0.3350880
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H	5.9287130	-13.4676620	-0.2808820
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H	48.3445030	0.0365380	-0.4414970
H	44.9166950	-0.7546500	-0.4114030
H	43.1807290	5.4749610	-0.3997560
H	37.0063320	-8.0910120	-0.3787930

H	40.2407820	15.8444580	-0.4081760
H	38.7701320	22.1415220	-0.4141820
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H	28.2900750	24.7328680	-0.3431860
H	25.7931820	27.2301310	-0.3283280
H	21.0506040	22.8299830	-0.2982780
H	13.1229310	15.5095070	-0.2670270
H	23.8045790	40.9490420	-0.3139430
H	16.5134600	39.1853410	-0.2941100
H	22.7818950	37.5871400	-0.3019420
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H	2.6422620	41.0056820	-0.2943690
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H	-22.8828200	34.6517070	-0.3463700
H	-26.2912070	33.6917860	-0.3475730
H	-34.1517430	26.2765230	-0.3281850
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N	-3.6482640	-48.5245840	-0.3101450
N	25.6324210	-41.1339030	-0.2484420
N	-23.3883950	-42.0771340	-0.3292600
N	3.6699080	48.4214150	-0.3045400
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H	-23.7293590	-41.0881850	-0.3401640
H	-44.8199120	-20.2624060	-0.4074280

H	-48.3767430	-0.1708810	-0.4460560
H	-40.3401540	28.2585610	-0.3437860
H	-24.4221790	40.9648610	-0.4077800
H	4.6965180	48.2199330	-0.3158350
C	26.0852480	-42.5535000	-0.1625520
H	27.0330740	-42.6543330	-0.7696120
C	-3.2223940	-49.9532660	-0.2344950
H	-2.2799970	-50.0687710	-0.8474130
C	-24.4041920	-43.1685330	-0.2557910
H	-24.0297950	-44.0348720	-0.8773970
C	-45.4579960	-22.3559820	-0.3418530
H	-45.1233240	-23.1565150	-1.0662710
C	-50.5084540	-0.6684380	-0.3989870
H	-51.0269770	-1.3572220	-1.1299940
C	-42.4799350	27.8060520	-0.2549880
H	-43.0448000	27.0525560	-0.8797150
C	-25.9273920	42.5519300	-0.3339680
H	-26.8693090	42.6326890	-0.9531740
C	3.2356720	49.8473460	-0.2284030
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C	26.3577620	-42.9394690	1.2844510
C	27.5879470	-43.6007560	1.6269200
C	25.4240600	-42.6736550	2.2610020
C	28.6013670	-43.9044850	0.6611150
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C	29.0315550	-44.6321670	3.3376210
C	26.8224630	-43.6744060	3.9696180
H	24.8981110	-42.8063100	4.3598890
C	29.9799610	-44.9102650	2.3868600

H	30.5308830	-44.7661240	0.2921040
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H	27.0130390	-43.9602350	5.0035280
H	30.9096660	-45.4123130	2.6505750
C	25.0128590	-43.4570840	-0.7732790
H	25.3261490	-44.5095770	-0.7317920
H	24.0551510	-43.3932510	-0.2395370
H	24.8203540	-43.2099940	-1.8253090
C	-4.3151970	-50.8325320	-0.8443480
H	-5.2688240	-50.7530830	-0.3054010
H	-4.5081160	-50.5764640	-1.8941570
H	-4.0221840	-51.8911490	-0.8098270
C	-25.7192750	-42.6670820	-0.8543640
H	-26.1308230	-41.8089170	-0.3062910
H	-25.6023440	-42.3629980	-1.9025710
H	-26.4834060	-43.4562660	-0.8215600
C	-24.6019910	-43.6169700	1.1852540
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C	-25.0225140	-43.0924520	3.5266670
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C	-24.7652690	-46.8080450	3.1902430
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H	-25.1869020	-42.3256400	4.2831800
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H	-24.9251960	-47.0948290	4.2291750
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C	-1.5034470	-51.4154390	2.8918140
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C	0.6451950	-52.3877900	2.2830170
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H	-2.2935810	-51.4043520	4.9190160
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C	-52.2769980	-1.6416390	1.1750470
C	-50.4108590	-0.3715240	2.0964850
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C	-50.9232890	-0.5631060	3.4103250
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H	-52.6094800	-2.0814470	-0.9319780
C	-53.9988740	-2.5612500	2.6795540
C	-52.0824030	-1.2696720	3.6047630
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H	-54.7084060	-3.3507910	-0.5475550
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H	-46.7953880	-21.4337910	-1.8116960
H	-47.5719100	-22.6324770	-0.7642000
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H	-50.2372360	1.5016390	-0.1817750
H	-50.3683210	0.9557440	-1.8625310
H	-51.8041350	1.0229230	-0.8277260
C	-45.5359290	-22.9343270	1.0636350
C	-45.4942550	-24.3593770	1.2513100
C	-45.6657530	-22.0998760	2.1512790
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C	-45.3275010	-26.6354640	0.3854290
H	-45.2798950	-24.8868040	-0.8509010
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H	-45.7853690	-24.3971650	4.6829630
H	-45.3976250	-28.2306190	1.8572780
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H	-42.1333560	28.8787630	4.2897860
C	-46.5328720	25.6403560	2.2157180
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H	-46.1436230	26.2845400	4.2243290
H	-44.2182590	27.6497950	4.8909730
H	-47.4450160	25.0981780	2.4607310
C	-26.2224620	42.9490820	1.1054870
C	-27.4659330	43.5961120	1.4264610
C	-25.2965350	42.7072110	2.0955890
C	-28.4720840	43.8750780	0.4457020
C	-27.7119920	43.9761600	2.7729240
C	-25.5525400	43.0851540	3.4436270
H	-24.3493440	42.2148780	1.8703930
C	-29.6444280	44.4966720	0.7924860
H	-28.2897650	43.5780620	-0.5895170
C	-28.9440960	44.6247670	3.1090890
C	-26.7291400	43.7056700	3.7769450
H	-24.7971740	42.8699540	4.1988920
C	-29.8850570	44.8792170	2.1444180
H	-30.4090580	44.7053160	0.0450150
H	-29.1164280	44.9089630	4.1467450
H	-26.9358750	43.9998050	4.8054470
H	-30.8247840	45.3708330	2.3918690
C	-42.7014950	29.1989420	-0.8465930
H	-43.7665740	29.4675880	-0.8116750
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C	-24.8607690	43.4640540	-0.9418800
H	-23.9085790	43.4197010	-0.3964480

H	-24.6526950	43.2091830	-1.9890710
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C	3.8908740	49.9717880	2.1965840
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H	4.8211910	49.4526440	1.9612050
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H	0.9026190	50.9438040	-0.4590270
C	0.3100160	51.9909690	3.2498120
C	2.5022930	51.0036140	3.8947020
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C	-0.6309890	52.2778060	2.2943040
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H	24.1359910	43.8752560	-0.8904460
C	43.5054790	-27.0925150	-0.9620610
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H	51.7566800	-1.2041920	-0.9062120
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H	25.7240860	42.1682850	-1.8312950
H	26.5830800	43.2886480	-0.7613830
C	43.7647570	-25.5975250	1.0395670
C	44.9338930	-24.8083700	1.3203440
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C	45.6427090	-24.0831340	0.3085500
C	45.4109590	-24.7427130	2.6567930
C	43.6085770	-26.1954420	3.3962380
H	42.2391420	-26.8719520	1.8662060
C	46.7569010	-23.3450920	0.6164160
H	45.2750400	-24.1268060	-0.7193890
C	46.5769900	-23.9649840	2.9523580
C	44.7225280	-25.4521330	3.6911730
H	43.0727920	-26.7387390	4.1745000
C	47.2332980	-23.2850120	1.9585590
H	47.2937450	-22.7943240	-0.1550490
H	46.9291700	-23.9262070	3.9828230
H	45.0996760	-25.3882460	4.7114120
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C	52.6859060	1.3537100	2.6671400

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H	52.6145330	1.9067130	-0.7222800
C	53.8988600	2.0586760	2.9562290
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C	44.8342460	23.8075560	3.3838210
H	44.7151190	22.2943320	1.8443220
C	43.9719430	27.9859310	0.6340500
H	43.8866150	26.3211120	-0.7122730
C	44.4221420	27.5005630	2.9653490
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H	45.0320990	23.0648080	4.1565660
C	44.1671320	28.4179330	1.9783540
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H	44.5713850	27.8167760	3.9973780
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H	24.8619040	41.5352100	2.0235100
C	24.4258530	47.2485640	0.7706250
H	24.2951760	45.5832810	-0.5703410
C	24.7928290	46.7557740	3.1150050
C	24.9993740	44.3883900	3.8563350
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R-COF1[X]

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O	-14.1430170	-3.9566710	1.7883340
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H	-13.6149490	-6.2345560	1.6339340
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H	-20.1913510	-4.6227140	2.3819850
C	-16.1097310	-1.9547490	2.1812050
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C	-9.3283340	-11.3190240	0.8953860
C	-8.3094920	-12.2583570	0.7479880
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O	14.6059440	-11.0897350	-1.3449040
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C	50.8309370	-1.6601710	0.8244540
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C	53.4161510	-4.0248240	4.4973920
H	51.7333920	-3.0792510	5.4261840
C	53.6528410	-3.7565040	2.1004040
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C	54.1184150	-4.2737060	3.2821320

H	53.8036010	-4.4499120	5.4226780
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H	55.0228040	-4.8797440	3.3126710
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S-COF2

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H	-25.5894520	-6.2324450	0.1425900
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C	23.9190920	12.5438390	-3.2053430
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H	24.2106800	13.5648130	-3.4414870
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H	21.1594330	10.6307780	-2.6018170
C	24.5388920	10.2253840	-2.8061550
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C	21.3742560	8.1912740	-2.4684530
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H	4.3930640	-23.9772590	-3.0637480
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H	9.3071050	-17.5161770	-2.9123220
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C	9.3639710	-25.9358590	1.7459180
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H	7.9693270	-26.5077910	4.8224310
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C	7.1535240	-20.2385510	6.7506940
H	9.1160020	-19.6351940	7.4450640
H	8.4559710	-18.4607030	2.2150550
C	9.2735750	-16.8118130	3.3087220
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C	12.6811850	-21.0735110	-1.8916160
C	13.7234230	-22.4775070	0.5696080
O	10.9260620	-22.6136940	-0.2670610
H	14.1211620	-19.8244530	1.0235440
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H	11.0606890	-22.2318520	-2.7067790
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H	12.8848890	-22.4127910	2.5791570
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C	13.2162150	-20.2888100	-4.5422760
H	11.5307870	-21.5409460	-5.0801660
H	16.6759060	-23.9795780	-0.2878030
C	15.8649080	-23.8900100	1.7220300
H	14.7955720	-23.6513850	3.5940460
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C	22.7791380	-5.1052730	1.3537520
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H	23.8978730	-4.6741130	3.1195980
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C	22.4220840	-3.1584740	-0.1498580
P	24.6356870	-1.8881920	3.2118720
C	23.1128770	-2.3057400	0.7882570
H	21.5805740	-6.4602690	-0.7147090
C	21.1612850	-4.8488160	-2.0601850
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H	20.8886620	-3.0298950	-3.2298340
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H	28.5571740	-4.8771800	2.5364730
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H	27.2858130	-4.4418300	6.6478330
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H	22.5282310	1.1348080	6.5330530
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C	19.9872760	0.2933060	2.1360090
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C	23.2236020	1.9797400	-0.1157190
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H	19.2358720	2.3342250	2.2801190
H	24.9698000	0.4610540	-3.1949190
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C	25.5578810	-3.2091000	-4.3901130
H	26.0033900	-3.6355450	-2.2976210
H	27.8672960	-0.1815140	-2.6502650
C	29.1745060	1.0686100	-1.4653110
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H	26.8000770	0.2247950	1.5334560
H	24.6819580	-0.1216020	-5.5866870
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H	25.7143420	-4.2318940	-4.7240700
H	29.8361320	1.2932800	-2.2984500
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C	15.4807010	16.4517970	-2.1131940
C	15.6307830	17.8127260	-1.8644240
C	14.1473780	15.9131560	-2.2229840
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C	13.8968900	14.5505200	-2.5863010
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P	14.9230990	20.5007540	-1.3793040
C	13.2225260	18.1904710	-1.7268420
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H	12.4373160	13.0205120	-2.9713150
C	11.4920540	14.9082530	-2.4296150
H	10.8461640	16.8893770	-1.9403290
C	16.3093240	20.5645960	-3.8342650
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C	16.4128720	19.7912890	1.0104060
C	14.8601170	21.6697770	1.1620000
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C	11.3537630	19.7361880	-2.5043300
H	10.4810770	14.5163640	-2.5047760
H	15.3918550	20.1338430	-4.2379510
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C	18.6677850	21.7087650	-2.7776410
H	17.6722720	21.6203990	-0.8599610
H	16.8807280	18.9900700	0.4442020
C	16.7553330	19.9675360	2.3638930
C	15.2051370	21.8442860	2.5152270
H	14.1236790	22.3060240	0.6773350
C	12.1195320	18.4415240	0.9443040
C	10.3097310	19.9197810	0.1410910
P	11.9637220	19.7466850	-4.2876550
C	10.1933280	20.5093140	-2.2213250
H	17.3078840	20.6745320	-5.7457970
C	18.5684780	21.4424170	-4.1563540
H	19.5728430	22.1529020	-2.3702670
H	17.4859220	19.3081750	2.8261620
C	16.1533450	20.9952890	3.1170820

H	14.7364080	22.6353130	3.0955620
H	13.0152460	17.8618630	0.7476130
C	11.6057050	18.4916720	2.2314090
C	9.7920510	19.9326550	1.4762480
C	9.6703630	20.6281420	-0.9381130
C	10.8504460	18.5706320	-5.2306800
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O	13.5008440	19.2898620	-4.4911210
H	9.7355140	21.0857350	-3.0201500
H	19.4000970	21.6784460	-4.8165830
H	16.4200980	21.1304950	4.1628570
H	12.1009950	17.9563170	3.0373500
C	10.4219210	19.2373870	2.4988010
H	8.8809740	20.4834730	1.6841120
C	9.4425140	18.6300540	-5.1931390
C	11.4956270	17.5784910	-5.9942540
C	10.8997630	21.6960380	-6.1019660
C	12.1626200	22.5586420	-4.1870110
H	10.0101260	19.2553910	3.5048980
H	8.9330420	19.3876770	-4.6030080
C	8.6817590	17.6988020	-5.9238260
C	10.7323970	16.6486420	-6.7248500
H	12.5824380	17.5483290	-5.9976890
H	10.4873230	20.8621160	-6.6635810
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C	11.9876230	23.8659740	-4.6750990
H	12.7268100	22.3779080	-3.2711140
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C	9.3262200	16.7080380	-6.6916130
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H	10.1837740	23.1799710	-7.5057350
C	11.2724890	24.0946020	-5.8677640
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C	-7.7223150	22.5431410	1.4064690
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H	-7.4411310	23.4604470	1.9155630
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P	-10.1415150	22.9636150	2.7965300
C	-9.4075260	20.8267960	0.9898810
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C	-9.5908890	22.5257840	4.5334410
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H	-9.0251090	28.5335990	1.8073080
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C	-14.4435660	22.7298670	-1.8224760
C	-13.9631120	23.2050050	0.5331000
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C	-12.4551980	19.2530140	-4.0761900

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H	-14.1528990	22.3026600	-2.7785160
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H	-13.2899530	23.1372400	1.3888190
H	-13.0722800	18.3956500	-4.3338160
C	-11.5140830	19.7505790	-4.9996810
H	-9.9823080	21.2393200	-5.3682600
H	-16.3370650	23.4693630	-2.5670170
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H	-15.4875840	24.3105970	1.5901790
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H	-17.0139830	24.4750740	-0.3827450
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C	-23.8384500	2.8980720	1.6819420
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P	-25.4444650	2.2622030	2.4346920
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C	-23.0406840	0.5646810	1.0542160
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H	-28.0887930	5.1610960	-0.6290700
C	-28.6764570	5.4935910	1.4322170
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H	-25.6488520	0.0015540	6.8470340
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C	-22.8127740	-0.5027010	-3.2805830
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C	-27.0047720	-0.4673810	-0.7129260
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H	-22.9845320	-1.4356700	-2.7498670
C	-21.9542770	-0.4935430	-4.3955240
C	-22.3234260	1.9024350	-4.6640820
H	-23.6583830	2.8072450	-3.1948230
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H	-26.8014560	-0.0801130	0.2864310
H	-21.4793710	-1.4166490	-4.7188910
C	-21.7105180	0.7085390	-5.0895870
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R-COF2

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C	8.8949540	-21.3636220	1.4614660
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C	17.4064210	-14.4791980	0.1924330
C	18.5860990	-16.4634770	-0.5524550
C	18.5272520	-13.6895920	-0.0915300
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C	19.7068060	-15.6774620	-0.8418140
H	18.6111370	-17.5292940	-0.7618790
C	19.7123660	-14.2727390	-0.6167440
H	18.4726320	-12.6258360	0.1038000
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H	0.1278850	26.0602970	4.7222560
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H	26.7887040	-12.8512940	-2.6910550
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C	16.4861390	17.1736760	-1.7349310
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H	23.2357920	13.7170520	-3.2446030
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H	9.8160760	-22.4280020	-0.8128340
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C	13.0647780	-20.3059840	-1.1885870
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H	13.9588650	-19.7049010	-1.3165570
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H	10.1823970	-16.9520660	5.6148210
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C	14.9753970	-16.2484420	-0.2980840
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C	13.6516680	-19.0738910	6.9862890
H	15.0333430	-17.4107370	6.8333980
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C	12.2933220	-16.6793620	-2.7318340
H	14.9720700	-15.3284840	-0.8754610
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C	16.1243660	-20.2360020	2.6445420
H	14.0433450	-20.3544330	2.1550180
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H	14.1041610	-19.4742520	7.8907490
C	12.4318060	-13.5352180	-1.9599910
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C	13.4474970	-16.5442720	-3.5299720
C	11.1118830	-17.2133110	-3.2824230
H	18.2729390	-17.7676070	1.6578290

C	17.3313310	-19.4923520	2.5075790
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C	12.5598130	-12.1391350	-1.8271630
C	12.7995630	-12.3920800	0.5868150
H	12.7059890	-14.4298400	1.3465520
H	14.3693480	-16.1456730	-3.1140470
C	13.4150800	-16.9373120	-4.8807400
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H	12.9349660	-11.9513880	1.5715830
H	14.3058440	-16.8320820	-5.4953260
C	12.2319260	-17.4662560	-5.4344270
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C	22.9589260	-1.6438840	-2.3364530
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C	23.4941400	-0.8073890	-5.9897510
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C	21.2521820	-0.5433840	2.6283090
C	19.7813270	-0.3901260	0.6744370
C	24.5759070	0.2127230	1.6208890
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C	23.8326440	3.4942130	-2.1224670
H	23.5489950	1.1874270	-6.8663280
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C	20.3437820	-1.4269160	3.2426820
C	18.8805820	-1.2727530	1.2973040
H	19.5664860	0.0227250	-0.3121540
H	24.3749010	-0.7289370	1.1163630
C	25.7547260	0.3507110	2.3768680
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H	23.2620650	3.3378090	2.0529970
P	19.7634480	2.5212270	-2.6869720
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H	20.5593340	-1.8204910	4.2331490
C	19.1583330	-1.7930210	2.5776950
H	17.9613710	-1.5473040	0.7853570
H	26.4465490	-0.4843930	2.4556590
C	26.0377750	1.5679580	3.0282770
H	25.3614540	3.5906790	3.4152390
O	19.7084410	1.0018750	-2.1380220
C	18.5293620	3.6562920	-1.8621090
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H	20.4391990	5.3230660	-2.6696040
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H	18.4557250	-2.4731420	3.0543070
H	26.9493790	1.6725660	3.6123340
C	18.7308310	3.9675830	-0.4976610
C	17.3811220	4.1147360	-2.5376530
C	19.4999650	3.6590560	-5.3431960
C	18.9891620	1.2859400	-5.0761000
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C	26.2026810	4.9977470	-1.6548940
H	27.1909020	3.0612780	-1.4986630
H	19.6146390	3.5947920	0.0217390
C	17.7781610	4.7529810	0.1759430
C	16.4339350	4.9010790	-1.8538430
H	17.2170270	3.8639530	-3.5822610
H	19.8188270	4.6130550	-4.9310520
C	19.2064910	3.5659130	-6.7162710
C	18.6962380	1.1957320	-6.4497030
H	18.9253880	0.4181410	-4.4243030
H	27.1074760	5.5653030	-1.4516730
H	17.9294540	4.9931980	1.2255680
C	16.6321580	5.2219520	-0.4976880
H	15.5486390	5.2559230	-2.3760230
H	19.2931890	4.4466260	-7.3479890
C	18.8023570	2.3347300	-7.2703650
H	18.3902560	0.2435450	-6.8761590
H	15.8996300	5.8289310	0.0297430
H	18.5755280	2.2648380	-8.3318600
C	12.5937940	18.8676280	-0.7302900
C	12.2702400	18.9561960	0.6201400

C	11.6375300	19.3355410	-1.7022410
C	11.0472710	19.5152520	1.0807580
H	12.9804780	18.5728710	1.3470210
C	11.8481230	19.2007200	-3.1124450
C	10.3982160	19.9143850	-1.2405580
P	10.7756060	19.5237530	2.9437580
C	10.1103420	20.0024670	0.1716720
H	12.7507350	18.7168750	-3.4689000
C	10.9080930	19.6521130	-4.0280620
C	9.4551150	20.3781990	-2.2147520
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C	11.5958550	17.9554620	3.5448150
C	11.7645070	20.9662000	3.6164580
C	8.8076710	20.6270370	0.6029220
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C	9.7028150	20.2596400	-3.5737780
H	8.5236650	20.8201280	-1.8772300
C	12.5626610	17.9750050	4.5695110
C	11.1451160	16.7276580	3.0075530
C	13.0958430	21.2410250	3.2434080
C	11.0994110	21.8059700	4.5313090
C	7.6515600	19.8776120	0.8156900
C	8.7501310	22.0604150	0.7650050
H	8.9703720	20.6140310	-4.2943640
H	12.9001450	18.9171780	4.9931710
C	13.0940430	16.7641570	5.0539460
C	11.6817710	15.5240880	3.4992270
H	10.3859190	16.7206390	2.2240510
H	13.6161000	20.6090860	2.5282320
C	13.7622720	22.3522160	3.7924120
C	11.7685990	22.9162410	5.0792720
H	10.0675950	21.5810990	4.7897970
P	7.6015420	17.9987690	0.6684100

C	6.4433760	20.5180700	1.2064290
C	7.5171840	22.7055610	1.1475380
C	9.9057830	22.8758920	0.5349790
H	13.8401030	16.7799380	5.8448640
C	12.6548680	15.5383470	4.5190470
H	11.3350300	14.5781330	3.0901630
H	14.7889740	22.5630880	3.5032870
C	13.1001150	23.1895230	4.7124020
H	11.2542780	23.5641390	5.7849010
O	9.0368950	17.2583260	0.7350400
C	6.4150720	17.4435440	2.0004120
C	6.8044790	17.6304550	-0.9869830
H	5.5759540	19.9076360	1.4400250
C	6.3524040	21.8938880	1.3942030
C	7.4863760	24.1349490	1.2302010
C	9.8494420	24.2567620	0.6488030
H	10.8411520	22.3984730	0.2625780
H	13.0636840	14.6033710	4.8959620
H	13.6169520	24.0478530	5.1356960
C	6.6980800	17.8149470	3.3348220
C	5.3309570	16.5910310	1.7104410
C	5.5836650	18.1965270	-1.4068810
C	7.5028080	16.7484830	-1.8342500
H	6.5514560	24.6306410	1.4682000
C	8.6219350	24.8949260	0.9876570
H	10.7389240	24.8554390	0.4705170
H	7.5502670	18.4597930	3.5532860
C	5.8755440	17.3366180	4.3703570
C	4.5136200	16.1183530	2.7548640
H	5.1219260	16.2901210	0.6873860
H	5.0390720	18.8839130	-0.7643420
C	5.0607070	17.8753530	-2.6730130
C	6.9773860	16.4284420	-3.1001130

H	8.4471620	16.3339480	-1.4901240
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C	4.7842840	16.4917150	4.0849150
H	3.6767240	15.4613780	2.5304340
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C	5.7566030	16.9897350	-3.5202820
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H	4.1529970	16.1249430	4.8913190
H	5.3504610	16.7418560	-4.4983780
C	-10.2619820	20.7715240	1.5585070
C	-10.8282980	19.8732160	2.4576790
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C	-11.9551860	19.0700540	2.1285940
H	-10.3399440	19.7259810	3.4165560
C	-10.4108290	21.9007140	-0.6858890
C	-12.0031630	20.1064190	-0.0844610
P	-12.5449490	17.8580920	3.4461030
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C	-11.0112430	22.0329390	-1.9300220
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H	-13.4306240	19.6340490	-1.6587050
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H	-10.0640130	16.6414790	2.4971430
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C	-16.2208300	18.1319490	0.2417980
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C	-15.2463430	20.2544590	6.4331160
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C	-12.2950360	14.4012020	-0.0526610
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H	-14.6283360	15.3494600	-0.9425560
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C	-17.5151430	18.6817560	0.5128730
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H	-14.3680130	20.7348060	1.5544250
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H	-15.8923020	20.7931040	7.1227930
C	-12.8359070	14.0375150	1.2020410
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C	-12.4246760	16.1346120	-3.2197010
C	-10.2179400	16.8585690	-2.4651120
H	-18.3982590	18.1028470	0.2655560
C	-17.6586180	19.9248810	1.1128190
H	-16.6242410	21.6545120	1.9431110
H	-13.0859450	14.8081190	1.9326930
C	-13.0383060	12.6767460	1.4945790
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H	-11.5189230	13.6896400	-1.9543760
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C	-12.0249290	16.3158710	-4.5566830
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H	-9.5437840	17.0712370	-1.6390580
H	-18.6507120	20.3207800	1.3155310
H	-13.4529800	12.3935650	2.4590100
C	-12.7022420	11.6844530	0.5515590
H	-11.8900930	11.2910940	-1.4205830
H	-12.7247650	16.1078660	-5.3623930
C	-10.7221070	16.7660880	-4.8498290
H	-8.8165250	17.3902500	-4.0271480
H	-12.8616470	10.6340560	0.7849450
H	-10.4149390	16.9050840	-5.8839470
C	-22.2787480	1.6056830	-3.1552170
C	-22.7271210	1.0156020	-1.9780000
C	-21.7455060	0.7608630	-4.1936640
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H	-23.0961940	1.6600390	-1.1852850
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C	-21.7290430	-0.6684190	-3.9921250
P	-23.3497030	-1.0038440	-0.1104750
C	-22.2261030	-1.2417610	-2.7634850
H	-21.1448750	2.3666560	-5.5363310
C	-20.6642730	0.4577660	-6.3795470

C	-21.1923730	-1.4986890	-5.0295500
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H	-20.2377000	0.8814930	-7.2853750
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C	-23.7829280	0.9410680	1.9551190
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C	-25.8903280	-2.1224060	0.2488090
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C	-23.3222150	-3.4991350	-3.1346720
H	-20.2724760	-1.6040120	-6.9680750
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H	-20.7449660	0.1239610	0.5717590
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C	-27.3588680	0.0390330	-0.8031840
C	-27.2953390	-2.1849940	0.1959960
H	-25.3001230	-2.9487440	0.6372170
P	-19.6485830	-2.5544810	-1.2803850
C	-21.1803400	-4.8425440	-1.9098180
C	-23.3382760	-4.9391130	-3.0391780
C	-24.4244020	-2.8439030	-3.7745900
H	-24.0741520	2.3504140	3.5723350
C	-21.9797690	2.1777050	3.0357250
H	-19.9847340	1.7777910	2.2837590
H	-27.9234850	0.8730450	-1.2128340
C	-28.0308600	-1.1047840	-0.3278400
H	-27.8117260	-3.0706370	0.5582200

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C	-18.2776520	-2.7282310	-2.5456650
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C	-20.1490120	-3.7809200	1.2107600
C	-17.8611500	-4.0629140	0.3794500
C	-17.9142450	-3.9556590	-3.1358620
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H	-24.4178760	-6.7390750	-3.6194760
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C	-19.7965410	-4.4739310	2.3826060
C	-17.5191940	-4.7559330	1.5563680
H	-17.1062600	-3.8979340	-0.3846290
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C	-16.8788600	-3.9966610	-4.0877500
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C	-10.2645590	-14.8765990	1.9025090
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C	-8.8712500	-17.6055810	4.6692040
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H	-9.6752270	-16.8455760	-0.8513960
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H	-12.5033410	-17.1099030	6.0131660
C	-10.4113290	-17.3369330	6.5415370
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O	-9.2650870	-18.7932200	-1.4300660
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C	-8.3037930	-21.2344770	-2.5270670
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C	-7.4551420	-22.6166790	4.2236760
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L-COF3

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C	-5.6084180	12.8620630	-1.5754450
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C	-7.9041700	12.3482440	-0.7456600
C	-8.8776660	14.0278920	0.7947940
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H	2.4770840	12.9962640	-0.4307460
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H	1.5894120	18.9369810	-0.2231250
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C	-0.2664660	12.9775250	-0.3237340
H	0.3306300	15.0332570	-0.2613660
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C	-1.6121480	13.2255330	0.0861850
C	0.1254120	11.6844650	-0.7356310
C	-2.5499500	12.1345170	0.0764980
C	-2.0691730	14.5268940	0.5211550
C	-0.7875840	10.6284390	-0.7346800
H	1.1390920	11.5038500	-1.0780800
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H	-1.3830510	15.3674240	0.5566210
H	-0.4681120	9.6411970	-1.0588660

C	-4.8481070	11.2504210	0.4865210
C	-4.3306330	13.6497890	0.9084110
C	-3.0844520	9.7491750	-0.3258750
H	-3.6988280	15.7085980	1.2382560
C	-6.1904970	11.4961600	0.9091010
C	-4.3863990	9.9451670	0.0668960
C	-5.6720700	13.8461110	1.3121400
H	-2.7530350	8.7613200	-0.6371370
N	-7.1051280	10.4164090	0.9085340
C	-6.5865300	12.7910130	1.3094790
H	-5.0602620	9.0942330	0.0628160
H	-5.9951810	14.8365810	1.6224540
C	-8.3327430	10.3665790	1.4635630
H	-6.8516360	9.5167630	0.4599700
H	-7.6120390	12.9830140	1.6079930
C	-9.1450850	9.2252040	1.4193110
H	-8.7209620	11.2329910	1.9890250
C	-8.6904400	8.0026290	0.7663690
C	-10.4481290	9.2932160	2.0862510
C	-9.5772450	6.8347330	0.7666330
O	-7.5240330	7.9397780	0.2031930
C	-11.3001860	8.1058880	2.0841510
O	-10.8363690	10.3825160	2.6694540
C	-10.8950910	6.8854440	1.4000560
C	-9.0998850	5.6591060	0.1773340
C	-12.5306790	8.0949480	2.7619310
O	-11.6827450	5.8478110	1.3669170
H	-8.1026440	5.6810740	-0.2506770
N	-9.8277430	4.5209900	0.1379360
H	-13.1180150	7.1838220	2.7235500
N	-13.0127330	9.1472100	3.4461870
H	-10.7627110	4.6647980	0.5684710
C	-9.4446140	3.2377080	-0.3043010

H	-12.3895100	9.9731730	3.3861780
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C	-10.0635620	0.8764640	-0.6757730
C	-11.8322340	2.4785390	-0.0433880
C	-7.7500820	1.6300270	-1.0046830
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C	-11.0344970	-0.1843520	-0.6579260
C	-8.7018560	0.5816620	-1.0046780
C	-12.7612620	1.4682030	-0.0540670
H	-12.1644420	3.4849770	0.1906760
H	-6.7166680	1.4108790	-1.2624510
C	-12.4003690	0.1107120	-0.3512230
C	-10.6388250	-1.5373460	-0.9236630
C	-8.3432360	-0.7735630	-1.3171990
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C	-13.3485510	-0.9403510	-0.3209130
C	-11.6115430	-2.5760890	-0.8116440
C	-9.2653480	-1.7905230	-1.2804450
H	-7.3144180	-0.9947980	-1.5677080
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H	-14.3871780	-0.7180530	-0.0912730
N	-11.1693970	-3.9155090	-0.9086390
H	-8.9540060	-2.7961090	-1.5450090
H	-13.6916310	-3.0605310	-0.4334770
H	-10.1848700	-4.1508220	-0.6769290
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C	4.2451580	-16.2757610	0.9430260
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C	3.3196360	-17.4076860	1.0067820
O	5.5247000	-16.4594710	1.0482010
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H	-0.6326510	-16.6027490	0.6341670
O	1.0677590	-18.2296090	0.9376730
H	4.9492440	-18.7469210	1.2737240
N	3.1246940	-19.8040970	1.2655920
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C	-2.4018690	-12.8545410	0.1577120
C	-2.9591740	-15.2543540	0.2091070
C	-3.8010020	-12.5569260	0.0023700
C	-1.4631880	-11.7551060	0.2064810
C	-4.3154270	-14.9574700	0.0628290
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C	-4.2472830	-11.1938320	-0.1066260
C	-4.7627780	-13.6200130	-0.0441640
C	-1.8932580	-10.4540610	0.1046870
H	-0.4001460	-11.9373180	0.3283580
H	-5.0412240	-15.7660500	0.0257110
C	-5.6460740	-10.8943990	-0.2663840
C	-3.2866430	-10.1303820	-0.0545510
C	-6.1566490	-13.2952260	-0.1989260
H	-1.1742740	-9.6391980	0.1441870
C	-6.0433220	-9.5264310	-0.3767320
C	-6.5856430	-11.9939860	-0.3061860
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H	-6.8773050	-14.1091470	-0.2287560

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H	-8.0937900	-10.0076280	-0.7345300
H	-5.3790670	-7.4473870	-0.4251670
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C	-8.0205620	-8.0363870	-0.5550520
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C	-11.3383060	-6.3138070	-1.1442220
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O	-9.7737940	-10.2278590	-1.1032790
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C	22.7202820	-9.1697710	0.8220350
C	23.5856520	-11.8598390	0.9455760
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C	24.0858520	-9.4598600	0.8636140
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C	23.0966590	-14.2990330	1.0291380
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H	20.9725750	-14.7972900	0.9971780
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C	25.8754180	-14.8582680	1.1149400
C	26.3903010	-12.4133370	1.0313240
H	26.6698370	-10.2910650	0.9546340
C	24.9402320	-15.9068500	1.1342990
H	22.8433160	-16.4485620	1.1068580
H	26.9403100	-15.0776280	1.1478770
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H	25.2850080	-16.9366260	1.1823050
C	21.4555390	10.8953600	-1.0235670
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C	24.6707050	8.9128570	-1.0372520
H	22.6307880	8.3651930	-0.9178540
H	21.6602430	14.3048550	-1.2462740
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C	2.1097420	24.0440030	-0.1482920
C	6.2922520	23.1373090	-0.2018660
H	5.7573990	21.0911910	-0.2566370
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C	-16.4884650	-9.1766710	-2.7782840
C	-15.1203090	-13.2459630	-2.6971430
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C	-16.4643230	-12.9692910	-3.0384940
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H	-15.8322940	-8.3434940	-2.5455090
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H	-18.1416980	-7.8714150	-3.1320780
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H	0.7943280	-20.9285730	1.1985480
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C	0.6835820	-24.3360720	1.5781020
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H	-1.3026930	-25.1969990	1.5129410
H	1.9091170	-28.0266620	2.0993280
H	4.2718950	-27.2448900	2.2044540
H	-0.5185100	-27.5381800	1.8441480
C	-16.4417620	3.0342990	1.6108700
H	-16.9375760	3.2924990	2.5517220
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H	-17.0545840	0.5108870	1.9104600
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H	-18.2484740	2.7110070	0.4873440
O	-17.4079930	1.1500570	-1.5496160
H	-17.9173710	0.4741080	-1.0490880
C	-16.5627360	1.8888950	-0.6068970
H	-15.6908680	1.2708920	-0.3727230
O	-15.0766190	2.7668110	-2.2892590
C	-16.0957670	3.1665450	-1.3068520
H	-16.9494290	3.6466680	-1.8053360
O	-16.1788870	4.2874360	0.9378750
C	-15.4273310	4.1695390	-0.3350270
H	-14.4133840	3.8231590	-0.1154010
O	-16.7219610	6.1031880	-1.1463130
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C	-15.3221220	2.9535490	-3.7039980
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O	-16.1697870	0.5855990	-3.9303400

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C	-15.2480760	1.5864640	-4.4190270
H	-15.4999390	1.7572770	-5.4746500
O	-13.7632880	-0.2245440	-5.1111380
H	-14.5649290	-0.7523850	-4.9008530
C	-13.8126120	1.0231270	-4.3518080
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O	-11.4772370	1.4765660	-4.9051640
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C	-10.7060470	1.4742950	-6.1438040
H	-11.2057330	2.0938310	-6.8952750
O	-11.7385120	-0.7196450	-6.8163390
H	-12.4274570	-0.5571040	-6.1055850
C	-10.5143310	0.0262480	-6.6438870
H	-10.0628880	0.0802690	-7.6429150
O	-9.3681250	-2.0887200	-6.2750830
H	-10.2339750	-2.3948860	-6.6291130
C	-9.5508730	-0.7477790	-5.7216240
H	-9.9780140	-0.8272220	-4.7122540
O	-7.3037100	-0.7586740	-4.7516810
C	-8.1998010	-0.0364830	-5.6605820
H	-7.7516810	0.0178880	-6.6629790
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C	-8.4173640	1.3931870	-5.1139600
H	-8.7713820	1.3381040	-4.0763420
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C	-6.1086330	-1.3987050	-5.2878310
H	-5.9839660	-1.1649200	-6.3497160
O	-7.2525670	-3.6148110	-5.6930300
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C	-6.1783190	-2.9183980	-5.0264650
H	-5.2461500	-3.3632540	-5.3954920
O	-6.3628890	-4.5592970	-3.2023520
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C	-6.3019210	-3.1306890	-3.5101530
H	-7.2326100	-2.6564970	-3.1818760
O	-5.5495780	-2.4901570	-1.3258180
C	-5.1275960	-2.5316220	-2.7370570
H	-4.2364880	-3.1611710	-2.8496740
O	-4.9221340	-0.8801080	-4.6390820
C	-4.8381770	-1.0718110	-3.1760920
H	-5.5991650	-0.4349860	-2.7082520
O	-2.8726910	-1.2424890	-1.6130640
H	-3.3886560	-1.0428550	-0.7990020
C	-3.4085090	-0.6064130	-2.8093840
H	-2.7347880	-0.9056680	-3.6162210
H	-3.3804790	0.4888320	-2.7233810
C	-4.7765960	-3.1377200	-0.2807240
H	-3.8232370	-3.5032250	-0.6698180
O	-5.8971640	-5.3118490	-0.6235820
H	-6.1736240	-4.9791040	-1.5266700
C	-5.6289990	-4.2662570	0.3385970
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O	-7.7334890	-4.6729640	1.5807670
H	-8.2183390	-5.1814840	0.8620320
C	-6.9093060	-3.6561780	0.9544890
H	-7.4831440	-3.1539140	0.1688410
O	-7.7439610	-1.9653870	2.4982470
C	-6.5206510	-2.6264330	2.0223400

H	-6.0204890	-3.1370880	2.8576660
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C	-5.5877070	-1.5363580	1.4487460
H	-6.1645260	-0.9131270	0.7541620
O	-4.1412650	-1.4773630	3.4456090
H	-3.4296170	-1.9129170	2.9289010
C	-4.9511620	-0.6720540	2.5388780
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H	-5.7299660	-0.2173750	3.1558580
C	-8.0320740	-2.0067040	3.9213720
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O	-9.3989410	-4.0909200	3.6040960
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C	-9.3547810	-2.7641770	4.1635340
H	-9.4676770	-2.8815730	5.2503060
O	-11.7835830	-2.6721360	3.9604860
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O	-11.7377100	0.1862900	3.8752610
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O	-8.1156630	-0.6655890	4.4630820
C	-9.2757050	0.1664100	4.0504890
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C	-12.6886770	0.6799360	4.8611200
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H	-13.2226520	-1.8563840	4.3527720
C	-14.0628810	0.0125640	4.6326690
H	-14.7335560	0.3524290	5.4321460
O	-15.9649480	-0.1310730	3.0928910

H	-15.9453340	-1.0455550	3.4559250
C	-14.6375450	0.4590270	3.2749110
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O	-15.1932630	2.3317260	1.8477050
C	-14.7613600	1.9803520	3.2044780
H	-15.4903520	2.3450290	3.9415830
O	-12.8291120	2.1172360	4.7505470
C	-13.3753520	2.6156690	3.4644940
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O	-14.2372470	4.5576120	4.7298230
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C	-13.4124190	4.1352280	3.5961880
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H	-13.8681150	4.5770700	2.7083520
O	-12.5213440	4.6657290	-6.2930990
H	-13.4592830	4.9535900	-6.3056650
O	-9.1567610	1.1873300	6.2891870
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H	-8.2035520	1.9684210	4.5679560
H	-9.9848920	2.1164960	4.6629530
O	-6.7566490	2.4463110	-6.5969030
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COF4Cy[2]

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C	8.7714230	-4.1311170	-0.8484910
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H	11.7828900	-7.9356310	0.0237340
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C	11.2687950	12.5964610	0.9853410
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N	9.5170620	19.9623990	2.0022610
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C	2.9033970	15.7375500	1.0087180
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C	0.4935660	16.2413590	0.8332820
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C	-0.3205430	18.5839040	0.9175790
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C	-1.3968730	19.5009620	0.8847440
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H	-14.0774170	12.5065020	-1.8972270
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C	-12.9454420	-17.9035830	3.8643900
C	-10.5367380	-18.4264210	3.5976050
C	-13.7233000	-15.5693460	3.6243800
H	-12.2778180	-14.0853220	3.1957810
H	-8.4059930	-18.7036790	3.3298460
C	-14.0243890	-16.9580100	3.8770080
C	-13.2171000	-19.2921970	4.1161900
C	-10.8348890	-19.8155690	3.8533640
H	-14.5404700	-14.8515910	3.6381700
C	-15.3406630	-17.4062890	4.1363880
C	-14.5475620	-19.7006800	4.3712530
C	-12.1198890	-20.2328010	4.1019980
H	-10.0141990	-20.5292630	3.8449510
C	-15.5966480	-18.7659590	4.3806500
H	-16.1563180	-16.6869170	4.1458280
H	-14.7530560	-20.7516550	4.5618670
H	-12.3339560	-21.2818370	4.2936340
H	-16.6127800	-19.0971280	4.5787930
C	10.8293430	-15.2649400	-1.4467830
C	10.4526030	-16.6280950	-1.6475340
C	12.1852880	-14.8787710	-1.5240130
C	11.4814900	-17.5914790	-1.9322830
C	9.0808390	-17.0895880	-1.5805460
C	13.1760040	-15.8216990	-1.8071230
H	12.5000250	-13.8544070	-1.3558140

C	11.1432220	-18.9722320	-2.1379560
C	12.8554250	-17.1829690	-2.0161090
C	8.7630930	-18.4118340	-1.7770530
H	8.2726600	-16.3936440	-1.3767690
H	14.2118330	-15.4972380	-1.8633350
C	9.7759280	-19.3999980	-2.0604860
C	12.1716460	-19.9348780	-2.4233750
C	13.8698930	-18.1685060	-2.3053480
H	7.7257440	-18.7346160	-1.7223490
C	9.4596970	-20.7636460	-2.2644160
C	11.8143020	-21.2896350	-2.6212390
C	13.5442330	-19.4888080	-2.5006830
H	14.9048620	-17.8396220	-2.3657310
C	10.4719930	-21.6975740	-2.5417550
H	8.4221090	-21.0844350	-2.2049460
H	12.5929040	-22.0178940	-2.8372690
H	14.3164410	-20.2234030	-2.7180640
H	10.2153660	-22.7424840	-2.6965060
C	20.8108320	3.6461920	-1.4157400
C	21.8448710	2.7256520	-1.7655070
C	21.0918350	5.0265070	-1.3136080
C	23.1674290	3.2349040	-2.0089690
C	21.6248270	1.2989940	-1.8883460
C	22.3787450	5.5129590	-1.5538430
H	20.3103720	5.7288080	-1.0429800
C	24.2333760	2.3392490	-2.3619560
C	23.4360800	4.6413590	-1.9028720
C	22.6483480	0.4470280	-2.2261710
H	20.6402750	0.8745510	-1.7167970
H	22.5731260	6.5793230	-1.4691230
C	23.9853150	0.9306060	-2.4741940
C	25.5554220	2.8476170	-2.6053870
C	24.7721770	5.1277570	-2.1523320

H	22.4594920	-0.6206310	-2.3131120
C	25.0459800	0.0619510	-2.8224160
C	26.5894740	1.9459270	-2.9514450
C	25.7900680	4.2689790	-2.4892870
H	24.9563560	6.1962960	-2.0669640
C	26.3352070	0.5681250	-3.0581390
H	24.8546680	-1.0053690	-2.9067170
H	27.5900220	2.3307880	-3.1355870
H	26.7933860	4.6455900	-2.6751760
H	27.1413620	-0.1103880	-3.3249830
C	9.7804450	21.3355150	2.2179730
C	11.1389070	21.7564340	2.3506750
C	8.7333170	22.2799940	2.3024650
C	11.4109830	23.1511660	2.5699410
C	12.2596590	20.8416320	2.2747480
C	9.0064910	23.6329790	2.5154880
H	7.6997770	21.9653720	2.2030870
C	12.7649090	23.6107290	2.7082560
C	10.3347070	24.0979150	2.6529160
C	13.5526550	21.2866840	2.4078730
H	12.0967830	19.7808390	2.1102920
H	8.1847070	24.3422900	2.5772570
C	13.8545420	22.6806450	2.6286060
C	13.0375850	25.0048180	2.9274750
C	10.6341150	25.4927170	2.8735930
H	14.3783720	20.5812070	2.3475720
C	15.1820290	23.1493860	2.7670680
C	14.3793720	25.4337380	3.0607760
C	11.9297730	25.9298470	3.0055380
H	9.8054560	26.1947610	2.9335650
C	15.4387030	24.5139860	2.9811070
H	16.0057350	22.4417350	2.7063500
H	14.5855370	26.4888040	3.2267110

H	12.1447080	26.9830890	3.1716520
H	16.4635610	24.8608460	3.0858730
C	-11.3514130	20.7723190	-0.3873880
C	-11.0541680	22.1693380	-0.3905530
C	-12.6879730	20.3306510	-0.5063120
C	-12.1384190	23.1052710	-0.5163520
C	-9.7074100	22.6900230	-0.2731400
C	-13.7350900	21.2465760	-0.6299370
H	-12.9194310	19.2707040	-0.4992020
C	-11.8773050	24.5177810	-0.5219720
C	-13.4910900	22.6392950	-0.6378020
C	-9.4634460	24.0420900	-0.2792330
H	-8.8609390	22.0165660	-0.1792870
H	-14.7563380	20.8841470	-0.7191430
C	-10.5325790	25.0037190	-0.4025470
C	-12.9607210	25.4539360	-0.6472140
C	-14.5620630	23.5991690	-0.7624370
H	-8.4437050	24.4099830	-0.1901900
C	-10.2924400	26.3977610	-0.4095360
C	-12.6788470	26.8405360	-0.6499060
C	-14.3098960	24.9495810	-0.7670740
H	-15.5801180	23.2270140	-0.8529360
C	-11.3579820	27.3051960	-0.5321130
H	-9.2719310	26.7628380	-0.3188850
H	-13.4989010	27.5488750	-0.7445750
H	-15.1240890	25.6646410	-0.8613150
H	-11.1595020	28.3739310	-0.5359990
C	-19.8518260	1.5561390	-4.6348080
C	-20.7142710	2.4630000	-5.3236410
C	-20.1055990	0.1670990	-4.6638150
C	-21.8387580	1.9304280	-6.0446600
C	-20.5105270	3.8974700	-5.3335980
C	-21.1993000	-0.3396980	-5.3693800

H	-19.4707370	-0.5416640	-4.1427180
C	-22.7286680	2.8100640	-6.7500430
C	-22.0819870	0.5155470	-6.0686400
C	-21.3654520	4.7342530	-6.0094070
H	-19.6719490	4.3410070	-4.8054040
H	-21.3696390	-1.4132210	-5.3792820
C	-22.5019860	4.2267280	-6.7397160
C	-23.8517970	2.2775500	-7.4717180
C	-23.2163180	0.0050210	-6.8012290
H	-21.1917490	5.8080340	-6.0027190
C	-23.3878280	5.0793820	-7.4392310
C	-24.7147100	3.1637670	-8.1588970
C	-24.0665240	0.8482990	-7.4746130
H	-23.3834850	-1.0696990	-6.8083920
C	-24.4834080	4.5496460	-8.1413530
H	-23.2129090	6.1528270	-7.4293890
H	-25.5645680	2.7604270	-8.7050480
H	-24.9184000	0.4533020	-8.0236530
H	-25.1564040	5.2159820	-8.6748870
C	10.4971320	-1.0928650	4.2496940
H	9.8958840	-0.3646450	4.8043600
O	12.6009900	0.2799420	4.1600130
H	12.1794610	0.6927220	3.3394730
C	11.9969790	-0.9558610	4.5871890
H	12.0894650	-0.9784810	5.6816180
O	14.1904990	-2.0075720	4.3949850
H	14.4281550	-1.0548770	4.3248270
C	12.7861510	-2.1534830	4.0165640
H	12.7049520	-2.1696320	2.9211580
O	13.0001760	-4.5924790	4.0735890
C	12.2432270	-3.4523210	4.6075570
H	12.3338730	-3.4309320	5.7028000
O	10.0072850	-2.3856400	4.6813630

C	10.7512270	-3.5904270	4.2288150
H	10.6540020	-3.6915240	3.1394370
O	10.0879120	-4.5703350	6.3886310
H	9.6296490	-3.7280850	6.5990160
C	10.0629270	-4.7561140	4.9425330
H	9.0306070	-4.8502130	4.5770630
H	10.6061570	-5.6844930	4.7514300
C	13.7651990	-5.3961780	5.0126910
H	13.6289140	-5.0236670	6.0329250
O	15.8750470	-4.1012060	4.5116250
H	15.2306640	-3.3420940	4.3876150
C	15.2554520	-5.4012000	4.6071800
H	15.8022140	-5.9517760	5.3847400
O	16.8406380	-6.1520990	2.8988230
H	17.2299610	-5.2881290	3.1655110
C	15.4239910	-6.1377750	3.2655790
H	14.8602290	-5.6014950	2.4934280
O	15.0263780	-8.1949420	2.0502500
C	14.9220590	-7.5748690	3.3755430
H	15.5204900	-8.1380980	4.1045160
O	13.2744240	-6.7592740	5.0472070
C	13.4378150	-7.5628290	3.8109060
H	12.8312030	-7.1205500	3.0098480
C	12.9152760	-8.9533090	4.1749400
H	13.0390420	-9.6359860	3.3304360
C	15.7705940	-9.4301900	1.8616090
H	16.0673710	-9.8661100	2.8203840
O	17.9457600	-8.2279770	1.5072750
H	17.5250550	-7.4513800	1.9802780
C	16.9792960	-9.1452010	0.9449420
H	17.5170310	-10.0871940	0.7874530
O	17.5701900	-8.4570130	-1.3509630
H	18.3499430	-8.0916230	-0.8772860

C	16.4657020	-8.6027820	-0.3996930
H	16.0297990	-7.6135630	-0.2225980
O	14.7639030	-8.6579410	-2.0792840
C	15.4092840	-9.4933340	-1.0590480
H	15.8924320	-10.3678790	-1.5166330
O	14.9176130	-10.4076400	1.2183740
C	14.3197490	-9.9486090	-0.0585700
H	13.6628110	-9.1020980	0.1498510
C	13.4798920	-11.1172670	-0.5625320
H	13.0491300	-10.8771310	-1.5373060
C	14.7116460	-9.0821330	-3.4682780
H	15.1276450	-10.0882600	-3.5864640
O	16.8609130	-7.8537840	-3.9559970
H	17.0617960	-8.0186010	-2.9914570
C	15.4735060	-8.0420490	-4.3185690
H	15.4801800	-8.3996800	-5.3557220
O	15.4091250	-5.7451110	-5.1639260
H	16.3798420	-5.8644550	-5.0610200
C	14.7320820	-6.6903310	-4.2714360
H	14.7456550	-6.2911080	-3.2491930
O	12.5928510	-5.5777160	-4.7009100
C	13.2952320	-6.8716800	-4.7527890
H	13.2905480	-7.2485610	-5.7829830
O	13.3388040	-9.1726630	-3.9094400
C	12.5752030	-7.8945170	-3.8546860
H	12.5783120	-7.5476820	-2.8141530
O	10.8807640	-7.9136600	-5.7178450
H	10.6254040	-6.9707550	-5.8492330
C	11.1319430	-8.1956290	-4.3091760
H	10.9526950	-9.2654050	-4.1727780
H	10.4305930	-7.6349850	-3.6763380
C	12.2454380	-4.9772870	-5.9670850
H	12.6140620	-5.5929840	-6.7940030

O	14.2143170	-3.4219260	-5.8035650
H	14.6566890	-4.2705970	-5.5028280
C	12.7993820	-3.5442490	-6.0575880
H	12.6153470	-3.1921010	-7.0832490
O	12.6221150	-1.2699570	-5.2361360
H	13.5991870	-1.3609560	-5.3115000
C	12.0550650	-2.6071060	-5.0890770
H	12.1954350	-2.9469160	-4.0544230
O	9.8504920	-1.7108630	-4.5079580
C	10.5683380	-2.5830380	-5.4414040
H	10.4266630	-2.2273230	-6.4711540
O	10.7951560	-4.9665810	-6.1426790
C	10.0050380	-4.0186170	-5.3060270
H	10.0650710	-4.3322290	-4.2549470
O	8.4738380	-3.7396200	-7.2189880
H	9.0101890	-4.3546110	-7.7635360
C	8.5694910	-4.1388360	-5.8197750
H	8.2112170	-5.1683210	-5.6777410
H	7.9225150	-3.4516040	-5.2696270
C	9.1083710	-0.5674700	-5.0346040
H	8.9597430	-0.6656940	-6.1145560
O	11.1269330	0.9250650	-5.2510300
H	11.7012740	0.1016130	-5.2044880
C	9.8235230	0.7467510	-4.6584670
H	9.2132150	1.5773250	-5.0327680
O	10.5761290	2.0820850	-2.7485610
H	11.2962270	2.2650970	-3.3934300
C	9.9288160	0.8261590	-3.1255180
H	10.5430890	-0.0122300	-2.7780020
O	8.7786760	0.5426900	-1.0143480
C	8.5578010	0.7671310	-2.4510360
H	8.0145840	1.7072840	-2.6176020
O	7.7837700	-0.5473550	-4.4549850

C	7.7250250	-0.4309400	-2.9791680
H	8.1254540	-1.3542290	-2.5464320
C	6.2364540	-0.2928440	-2.6543460
C	8.3375770	1.5042560	-0.0069480
H	7.6913400	2.2650120	-0.4570650
O	10.3537890	2.9473040	-0.2183810
H	10.4948990	2.5430130	-1.1246420
C	9.5761800	2.1281290	0.6818860
H	9.2200270	2.8089910	1.4644030
O	11.5640720	1.5188150	2.0323020
H	12.2832950	1.7049990	1.3548460
C	10.4000120	0.9971680	1.3405540
H	10.7240010	0.2969520	0.5650470
O	10.2955170	-0.9289870	2.8207310
C	9.5344950	0.2409280	2.3559020
H	9.3044660	0.9019350	3.2036470
O	7.5304020	0.8179000	0.9738330
C	8.2194080	-0.2659260	1.7206580
H	8.4573830	-1.0832110	1.0293820
O	6.8455350	0.3393910	3.6784670
H	6.4420080	1.0697800	3.1620920
C	7.2024470	-0.7372240	2.7606380
H	6.3107980	-1.1251280	2.2479730
H	7.6373660	-1.5269960	3.3782150
O	13.6851490	-9.5308900	5.2712480
H	13.5794050	-8.9583630	6.0612510
O	5.6714700	0.8985800	-3.2754260
H	5.7618880	0.8168480	-4.2492190
H	5.7055080	-1.1964650	-2.9857350
H	6.0973040	-0.1645370	-1.5773960
O	14.2938990	-12.3191100	-0.7512900
H	14.7258200	-12.5360940	0.1032810
H	11.8501630	-8.8856330	4.4361560

H	12.6630720	-11.3054260	0.1451120
C	-10.4289930	-5.7123920	-4.2149640
H	-10.7638010	-6.0820890	-5.1895840
O	-10.6508440	-7.8577120	-2.8944050
H	-11.5424780	-7.8539420	-3.3506240
C	-9.7581240	-6.8413050	-3.3990530
H	-9.0216110	-7.3099580	-4.0715960
O	-8.3907410	-7.3920490	-1.4719420
H	-9.0378640	-8.1321980	-1.4459950
C	-9.0092400	-6.2752280	-2.1812690
H	-9.7223790	-5.7757740	-1.5124220
O	-7.2734410	-4.7063050	-1.4623630
C	-7.9388800	-5.2818380	-2.6336830
H	-7.2024680	-5.7747660	-3.2826930
O	-9.4400540	-4.7025650	-4.5312170
C	-8.6443790	-4.1429280	-3.4099720
H	-9.3103230	-3.6006130	-2.7241300
O	-6.7993080	-3.8682430	-5.0206490
H	-7.3617980	-4.2622890	-5.7216110
C	-7.6638250	-3.1744830	-4.0718560
H	-8.2256300	-2.3712770	-4.5684810
H	-6.9985930	-2.7443210	-3.3193340
C	-5.8248700	-4.8480700	-1.3107490
H	-5.3550290	-5.0838680	-2.2707650
O	-5.8595340	-7.2436030	-0.6240940
H	-6.8261020	-7.3245860	-0.8761770
C	-5.5026950	-5.9060000	-0.2274880
H	-4.4152590	-5.9205900	-0.0869100
O	-5.9621300	-6.4201480	2.1558070
H	-6.6058710	-7.1974840	2.0577590
C	-6.2001360	-5.4706970	1.0790840
H	-7.2740260	-5.4247630	0.8735230
O	-6.6414120	-3.6197740	2.5877680

C	-5.7296990	-4.0798880	1.5247440
H	-4.6985710	-4.1314650	1.9007790
O	-5.2789230	-3.5750600	-0.8950550
C	-5.8271570	-3.0459160	0.3728980
H	-6.8840480	-2.7995120	0.2176660
C	-5.0228400	-1.7755190	0.6500730
H	-5.3404290	-1.3237950	1.5936200
C	-6.1350480	-3.2510090	3.9043190
H	-5.0626320	-3.0336720	3.8578640
O	-5.8056390	-5.6193660	4.6716700
H	-5.8644950	-5.9045620	3.7025960
C	-6.4515480	-4.3578750	4.9332420
H	-6.0674090	-4.0240160	5.9053470
O	-8.2915270	-5.5404110	6.0483630
H	-7.6271650	-6.2633160	5.9924820
C	-7.9789340	-4.5382170	5.0294540
H	-8.3689770	-4.8773750	4.0633410
O	-10.1169370	-3.4425670	5.3011130
C	-8.6670830	-3.2350580	5.4269340
H	-8.4072380	-2.9839590	6.4649310
O	-6.7745240	-2.0229750	4.3181420
C	-8.2506350	-2.0745300	4.4931350
H	-8.7251320	-2.2215990	3.5171330
C	-8.6218230	-0.7039200	5.0625120
H	-9.6923320	-0.6647080	5.2799970
C	-10.9607430	-3.2016890	6.4615450
H	-10.3676390	-2.7987640	7.2890740
O	-10.7849320	-5.6344520	7.1244920
H	-9.9072750	-5.5998430	6.6435940
C	-11.6637110	-4.5194480	6.8648840
H	-12.1959590	-4.3276080	7.8059330
O	-13.4217560	-6.1117280	6.2547980
H	-12.7689420	-6.7181690	6.6722110

C	-12.7065570	-4.9177030	5.7997360
H	-12.2058350	-5.1380230	4.8473190
O	-14.7412530	-4.1686610	4.6600360
C	-13.7070650	-3.7795210	5.6307290
H	-14.1805970	-3.5487190	6.5930690
O	-11.9406000	-2.1766920	6.1698660
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O	-15.0753760	-1.3283880	5.7994680
H	-15.8079400	-1.8075490	5.3461340
C	-13.8769640	-1.2969900	4.9702950
H	-13.3148850	-0.4116270	5.2808530
H	-14.1446130	-1.1959760	3.9093160
C	-16.0834070	-4.3495000	5.1608930
H	-16.1155950	-4.2226490	6.2475170
O	-15.8099520	-6.8426750	5.1878410
H	-14.8945140	-6.5823610	5.5050030
C	-16.6141480	-5.7306000	4.7391410
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O	-17.2424570	-7.0945440	2.8059290
H	-16.8283020	-7.7740190	3.3848570
C	-16.7295350	-5.7849860	3.2072840
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O	-17.6413750	-4.7320800	1.2322970
C	-17.6794740	-4.7036560	2.6977020
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O	-16.9581100	-3.3024850	4.6370730
C	-17.1908660	-3.3113420	3.1660780
H	-16.2458340	-3.0785920	2.6592420
O	-19.4840110	-2.5083100	3.5856160
H	-19.3381980	-2.5104790	4.5556710
C	-18.2231490	-2.2111570	2.9157170
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H	-18.4580080	-2.1567730	1.8497400
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H	-19.7492020	-4.7851660	1.0694730
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H	-18.1941100	-7.2862380	1.3734200
C	-18.8020180	-6.2405280	-0.2921800
H	-19.7085090	-6.3317350	-0.9014980
O	-17.5562840	-7.4789820	-2.0209100
H	-17.8488050	-8.2386800	-1.4704570
C	-17.5585300	-6.2672950	-1.1979230
H	-16.6675350	-6.2785400	-0.5604300
O	-16.0816770	-5.0541560	-2.6379670
C	-17.4663980	-5.0688220	-2.1454860
H	-18.1754340	-5.1955060	-2.9755590
O	-18.9199190	-3.8224870	-0.5334720
C	-17.7316430	-3.7287300	-1.4185280
H	-16.8594990	-3.4858830	-0.8093790
C	-18.0178350	-2.5648250	-2.3612910
C	-15.8081160	-5.0618040	-4.0619250
H	-16.7335700	-4.9486440	-4.6368940
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C	-15.0646030	-6.3634300	-4.4225020
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O	-12.9954240	-7.6176990	-4.1424290
H	-13.6732700	-8.3310480	-4.1896740
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C	-12.8537010	-5.1706500	-4.1869050
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O	-14.9893950	-3.9259760	-4.4143920
C	-13.6224510	-3.8792400	-3.8245150

H	-13.7039680	-3.7927030	-2.7336900
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H	-13.9369380	-2.7301230	-6.1746690
C	-12.9923050	-2.6186220	-4.4185180
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H	-11.9406860	-2.5608030	-4.1296110
O	-3.6031560	-2.0737380	0.8045040
H	-3.2809900	-2.4806650	-0.0285630
O	-19.2453090	-2.7853750	-3.1279900
H	-19.9837190	-2.9198420	-2.4949720
H	-18.0793280	-1.6376810	-1.7791440
H	-17.2105470	-2.4628320	-3.0901440
O	-7.9447050	-0.4620220	6.3314570
H	-6.9759270	-0.4979990	6.1781950
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COF4Cy[3]

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C	-18.2822610	3.3249900	1.6385330
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H	-14.2148070	5.1710350	1.1549130
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C	-7.4380450	14.0634470	0.1189070
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C	10.8879750	11.5469740	-1.8495920
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C	11.9700320	13.2876790	-3.1891890
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C	12.1734730	7.0306260	-0.0923830
C	9.7412080	6.8595930	0.2463260
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C	13.6011370	5.0231090	0.3002370
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C	14.6006870	7.1602020	-0.4127650
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C	14.7640110	5.7821570	-0.0449750
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C	12.5444320	2.9124870	1.0275390
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C	16.1545620	3.7872800	0.2303220
H	16.9161760	5.7293760	-0.3016860
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C	17.3140980	-1.2643480	1.4755590
C	18.4012950	-3.4655120	1.8985930
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H	-14.6560990	-14.2998310	-2.5887240

C	-14.2877480	-19.5637530	-3.4683210
C	-15.6520720	-17.5079970	-3.2265460
C	-11.8301910	-19.4340930	-3.2345410
H	-10.9743310	-17.5425360	-2.8294000
H	-16.6857990	-15.6202040	-2.9896520
C	-13.0139710	-20.2239180	-3.4746410
C	-15.4825500	-20.3267390	-3.7044790
C	-16.8377460	-18.2959150	-3.4659910
H	-10.8643250	-19.9343100	-3.2395220
C	-12.9522570	-21.6167350	-3.7135400
C	-15.3785960	-21.7181770	-3.9393110
C	-16.7585060	-19.6480420	-3.6953650
H	-17.8015750	-17.7919630	-3.4610770
C	-14.1257180	-22.3543050	-3.9434530
H	-11.9850870	-22.1141720	-3.7181710
H	-16.2829200	-22.2955070	-4.1181820
H	-17.6579200	-20.2327000	-3.8749460
H	-14.0641980	-23.4240580	-4.1259410
C	-20.7353100	3.3085190	2.0386220
C	-21.8319870	2.4508890	2.3566290
C	-20.9159080	4.7074280	1.9746720
C	-23.1168360	3.0434700	2.6129540
C	-21.7127260	1.0093600	2.4382140
C	-22.1663500	5.2734630	2.2338320
H	-20.1050220	5.3774390	1.7090820
C	-24.2449630	2.2141550	2.9333280
C	-23.2835870	4.4684310	2.5551960
C	-22.7956040	0.2206810	2.7436660
H	-20.7567280	0.5242390	2.2655140
H	-22.2777910	6.3532520	2.1794460
C	-24.0974930	0.7885250	2.9997290
C	-25.5289240	2.8065160	3.1908850
C	-24.5831180	5.0393950	2.8189540

H	-22.6816510	-0.8596200	2.8004410
C	-25.2188390	-0.0140060	3.3154480
C	-26.6258930	1.9692340	3.5035510
C	-25.6612160	4.2442360	3.1235930
H	-24.6897470	6.1207360	2.7709740
C	-26.4703670	0.5739800	3.5641110
H	-25.1035440	-1.0944120	3.3650270
H	-27.5974940	2.4178060	3.6985410
H	-26.6360470	4.6847320	3.3207260
H	-27.3239260	-0.0542470	3.8058060
C	-7.1349320	19.8205030	0.3437130
C	-8.3953110	20.4656290	0.5285990
C	-5.9535400	20.5862440	0.2311440
C	-8.4310880	21.9016090	0.5958700
C	-9.6437950	19.7410280	0.6517590
C	-5.9974240	21.9805970	0.2964390
H	-4.9931990	20.1003190	0.0943900
C	-9.6802470	22.5857840	0.7816380
C	-7.2210990	22.6655020	0.4780510
C	-10.8356460	20.4008730	0.8295930
H	-9.6607620	18.6563990	0.6046620
H	-5.0758100	22.5505730	0.2079030
C	-10.9005130	21.8408230	0.9013670
C	-9.7166290	24.0209260	0.8488860
C	-7.2834560	24.1060180	0.5486810
H	-11.7606690	19.8357950	0.9197890
C	-12.1223200	22.5297210	1.0841810
C	-10.9590070	24.6726940	1.0325770
C	-8.4794690	24.7579720	0.7265360
H	-6.3564140	24.6674810	0.4574270
C	-12.1479650	23.9329490	1.1488100
H	-13.0456060	21.9620740	1.1746900
H	-10.9863970	25.7588710	1.0834380

H	-8.5157050	25.8438020	0.7784330
H	-13.0936830	24.4499250	1.2895460
C	13.1372480	14.9388220	-4.6145510
C	13.1925110	16.3334440	-4.9084170
C	14.1458820	14.0655560	-5.0778920
C	14.2976570	16.8296830	-5.6818980
C	12.1894110	17.2755230	-4.4576240
C	15.2249510	14.5610980	-5.8157650
H	14.0910980	12.9944130	-4.9063130
C	14.3836910	18.2264590	-6.0041750
C	15.3265730	15.9353100	-6.1333320
C	12.2753980	18.6109580	-4.7699910
H	11.3556960	16.9356530	-3.8503460
H	15.9869790	13.8703730	-6.1674740
C	13.3679190	19.1349220	-5.5546760
C	15.4881940	18.7234970	-6.7776070
C	16.4264380	16.4597280	-6.9085760
H	11.5116010	19.3017640	-4.4198100
C	13.4670150	20.5073850	-5.8830760
C	15.5508000	20.1031110	-7.0848690
C	16.5052600	17.7956880	-7.2188070
H	17.1958270	15.7681920	-7.2444780
C	14.5491820	20.9837490	-6.6419320
H	12.6957750	21.1939340	-5.5412800
H	16.3865980	20.4794550	-7.6705590
H	17.3379130	18.1797230	-7.8039860
H	14.6129080	22.0407860	-6.8872980
C	20.7928040	-3.5498950	2.5669030
C	21.9108610	-2.7442960	2.9408630
C	20.9016840	-4.9579920	2.5585300
C	23.1392570	-3.3968720	3.3052920
C	21.8661510	-1.2966350	2.9732300
C	22.0976490	-5.5839080	2.9170430

H	20.0575160	-5.5733890	2.2654770
C	24.2854830	-2.6194850	3.6859350
C	23.2326490	-4.8296040	3.2942640
C	22.9656460	-0.5581870	3.3385020
H	20.9557110	-0.7658080	2.7119610
H	22.1600850	-6.6692590	2.9021080
C	24.2117240	-1.1867940	3.7059530
C	25.5136220	-3.2710680	4.0500390
C	24.4772470	-5.4607690	3.6638840
H	22.9083310	0.5278540	3.3569820
C	25.3494810	-0.4358220	4.0833420
C	26.6294320	-2.4842190	4.4213970
C	25.5724440	-4.7149670	4.0264950
H	24.5290010	-6.5470910	3.6488950
C	26.5460080	-1.0816520	4.4370440
H	25.2901970	0.6500630	4.0979260
H	27.5589010	-2.9774640	4.6969480
H	26.5056540	-5.2002760	4.3033340
H	27.4129050	-0.4926220	4.7251640
C	6.9154910	-19.3725400	2.9452900
C	8.1528920	-19.9581330	3.3530960
C	5.7077950	-20.0935450	3.0727880
C	8.1391440	-21.2908020	3.8931340
C	9.4255110	-19.2736390	3.2485530
C	5.7057790	-21.3882030	3.5970000
H	4.7547950	-19.6686490	2.7761700
C	9.3629030	-21.9130210	4.3156070
C	6.9036720	-22.0121330	4.0156350
C	10.5931400	-19.8737760	3.6539160
H	9.4808090	-18.2680990	2.8426330
H	4.7615690	-21.9185960	3.6904760
C	10.6078770	-21.2091960	4.2008260
C	9.3490620	-23.2447110	4.8561760

C	6.9157340	-23.3480490	4.5626880
H	11.5368110	-19.3400730	3.5652180
C	11.8041990	-21.8361910	4.6212600
C	10.5672050	-23.8369610	5.2654910
C	8.0873960	-23.9411310	4.9662400
H	5.9697070	-23.8777290	4.6492430
C	11.7807330	-23.1382940	5.1483720
H	12.7462060	-21.2997340	4.5328510
H	10.5564180	-24.8447780	5.6746500
H	8.0854730	-24.9482590	5.3771590
H	12.7072500	-23.6085460	5.4677840
C	-7.4567010	7.8715380	-3.8948110
H	-6.5425740	7.5326430	-4.3937570
O	-6.9916130	10.3342680	-4.0881860
H	-6.4709370	10.2040940	-3.2320190
C	-7.8953900	9.2593380	-4.4086710
H	-7.9292330	9.2064720	-5.5053830
O	-9.7087530	10.8917210	-4.4486990
H	-8.9210340	11.4818160	-4.4317980
C	-9.3146160	9.5939110	-3.9028060
H	-9.3207820	9.6446320	-2.8054560
O	-11.6489170	8.8523480	-3.9165090
C	-10.2959410	8.5304780	-4.3896030
H	-10.2898560	8.4913070	-5.4880970
O	-8.4554140	6.8788290	-4.2323200
C	-9.8612110	7.1548250	-3.8353920
H	-9.9372990	7.1561650	-2.7396540
O	-10.4724060	5.9168780	-5.8746520
H	-9.5153480	5.7912870	-6.0532770
C	-10.6624460	5.9950910	-4.4310760
H	-10.3633040	5.0559270	-3.9446470
H	-11.7312500	6.1630070	-4.2794340
C	-12.6609390	9.1505680	-4.9162870

H	-12.2394890	9.0640140	-5.9228330
O	-12.2863750	11.6356160	-4.6540130
H	-11.3390770	11.3453050	-4.4954660
C	-13.2468070	10.5581670	-4.6684860
H	-13.9435900	10.7687640	-5.4912900
O	-14.5930020	11.9001600	-3.1250760
H	-13.9359260	12.5613080	-3.4419760
C	-14.0274010	10.5678330	-3.3413770
H	-13.3366400	10.3355220	-2.5224510
O	-15.8065440	9.5389290	-2.0607490
C	-15.1591520	9.5447960	-3.3767510
H	-15.8888260	9.8032090	-4.1561650
O	-13.7308650	8.1738770	-4.8780700
C	-14.5679760	8.1426670	-3.6538740
H	-13.9482800	7.8384540	-2.8001840
C	-15.6417280	7.0917320	-3.9394570
H	-16.3401010	7.0282650	-3.1011300
C	-17.2389910	9.7568800	-1.9342140
H	-17.7302360	9.7504840	-2.9119370
O	-16.9902710	12.2530820	-1.8533750
H	-16.0940780	12.1208140	-2.2810860
C	-17.4735980	11.0754240	-1.1665170
H	-18.5546140	11.2172000	-1.0544610
O	-17.1358330	12.1399300	1.0360750
H	-17.0928430	12.9433560	0.4717290
C	-16.8111200	10.9691070	0.2175260
H	-15.7258030	10.9401430	0.0722260
O	-16.2387170	9.5795100	2.0779790
C	-17.2332260	9.7278510	1.0084580
H	-18.2388960	9.8763260	1.4258520
O	-17.8215360	8.6669150	-1.1798240
C	-17.1975350	8.4432560	0.1461600
H	-16.1555690	8.1542820	-0.0042940

C	-17.9539660	7.2728100	0.7654480
H	-17.5897380	7.0841610	1.7779650
C	-16.6433770	9.5206350	3.4723650
H	-17.7346360	9.5242080	3.5642830
O	-16.3576120	12.0176200	3.6908080
H	-16.5684450	12.0287720	2.7145400
C	-16.0009210	10.7156470	4.2099810
H	-16.3573080	10.6980230	5.2474410
O	-13.8797000	11.6422510	5.0081300
H	-14.3646970	12.4722830	4.8007530
C	-14.4667480	10.5570290	4.2161520
H	-14.0799480	10.6120520	3.1905730
O	-12.6213950	9.0761530	4.8522650
C	-14.0870000	9.2251740	4.8571010
H	-14.4544220	9.1889810	5.8901210
O	-16.2051650	8.2784040	4.0657650
C	-14.7301710	8.0695030	4.0687620
H	-14.3873750	8.0897430	3.0270810
O	-14.1368070	6.7218800	6.1119020
H	-13.1735340	6.8757220	6.2529230
C	-14.4575710	6.6837280	4.6896150
H	-15.3690130	6.0874290	4.5957800
H	-13.6518230	6.1902730	4.1292960
C	-11.9593040	9.1460730	6.1332850
H	-12.6862840	9.3493390	6.9263550
O	-11.2761130	11.5237780	5.6810160
H	-12.2297900	11.5695770	5.3732620
C	-10.8517430	10.2147260	6.1146730
H	-10.4789150	10.3088290	7.1453520
O	-8.6662700	10.8243190	5.2596570
H	-9.1272960	11.6926530	5.2151770
C	-9.6795930	9.7739680	5.2193520
H	-10.0248430	9.6456030	4.1849950

O	-7.9940240	8.0282130	4.8841870
C	-9.0940250	8.4653660	5.7481480
H	-8.7330010	8.5974790	6.7772550
O	-11.3953170	7.8450100	6.4842820
C	-10.2006340	7.3830090	5.7215500
H	-10.4924390	7.1905460	4.6800660
O	-9.3898910	6.3199650	7.7938210
H	-10.1732060	6.6402050	8.2900640
C	-9.7708770	6.0846880	6.4060590
H	-10.5819280	5.3456980	6.3393340
H	-8.8788170	5.6876410	5.9161020
C	-6.6661690	7.8456370	5.4669510
H	-6.7261400	7.7888440	6.5583230
O	-6.0717160	10.2938790	5.4312210
H	-7.0494420	10.5014850	5.3247890
C	-5.7189600	8.9662240	4.9894690
H	-4.7274400	8.7684020	5.4138460
O	-4.7279760	9.9610750	2.9820940
H	-4.8500170	10.7611660	3.5414930
C	-5.6471690	8.9253960	3.4529580
H	-6.6481530	9.1274040	3.0554070
O	-5.4094600	7.5321280	1.4878200
C	-5.1575020	7.5722230	2.9363840
H	-4.0860140	7.4523050	3.1467620
O	-6.1251900	6.5760910	5.0354000
C	-5.9598930	6.4071750	3.5731300
H	-6.9550820	6.3754290	3.1159900
C	-5.2558270	5.0588690	3.4093160
C	-4.3260160	7.3881560	0.5191440
H	-3.3861410	7.1434430	1.0248130
O	-3.7874590	9.8164370	0.4748620
H	-4.2373000	9.8870340	1.3677100
C	-4.2147910	8.6864930	-0.3172150

H	-3.4286920	8.5393610	-1.0676600
O	-5.5136140	10.1147950	-1.8731690
H	-5.6391220	10.9222280	-1.2877650
C	-5.5595910	8.9261860	-1.0419770
H	-6.3497680	9.0387280	-0.2941370
O	-7.2586510	7.9176300	-2.4565690
C	-5.8961870	7.7265170	-1.9361370
H	-5.1784880	7.6779430	-2.7673870
O	-4.6189590	6.2732390	-0.3501190
C	-5.8667500	6.3977320	-1.1466190
H	-6.7286640	6.3742210	-0.4690950
O	-4.7304690	5.1603380	-2.9536910
H	-3.9115460	5.1282630	-2.4140920
C	-5.8802590	5.1681360	-2.0555440
H	-5.8997460	4.2592060	-1.4376960
H	-6.7637170	5.1878180	-2.6984960
O	-16.4437040	7.4649930	-5.0995280
H	-15.8561130	7.5048850	-5.8844950
O	-3.9536630	5.0630620	4.0640570
H	-4.0860660	5.2160040	5.0243500
H	-5.8954250	4.2619190	3.8142710
H	-5.0589000	4.8639830	2.3515190
O	-19.3838120	7.5623160	0.8843610
H	-19.7305870	7.7759210	-0.0089880
H	-15.1636970	6.1140440	-4.0906670
H	-17.7862200	6.3741300	0.1592090
C	17.1889850	10.2203220	-2.0420860
H	17.5535230	10.6416880	-2.9840340
O	19.2620210	8.8604150	-1.6243940
H	18.8257640	8.1827830	-2.2188030
C	18.3373810	9.8345070	-1.0870690
H	18.9284030	10.7356780	-0.8859770
O	18.7923320	9.0367290	1.2000820

H	19.5571690	8.6389750	0.7266720
C	17.7306050	9.3046620	0.2230630
H	17.2190690	8.3611800	0.0103520
O	15.9525420	9.5126290	1.8494680
C	16.7373330	10.2751740	0.8658680
H	17.2824900	11.0949170	1.3545970
O	16.3923920	11.2530880	-1.4195730
C	15.7279640	10.8528100	-0.1554860
H	14.9800720	10.0875820	-0.3780620
O	16.0097040	13.1868550	0.5814240
H	16.4358910	13.4092660	-0.2739420
C	15.0409820	12.1196920	0.3541790
H	14.2688020	12.4274410	-0.3632090
H	14.5765950	11.9261930	1.3246690
C	16.1283710	9.7652580	3.2636940
H	16.8389790	10.5832440	3.4256170
O	17.7979290	7.8755540	3.4587330
H	18.1534320	8.2988510	2.6258470
C	16.5813520	8.4671540	3.9688720
H	16.7597000	8.7187780	5.0240030
O	15.8980820	6.2239360	4.6453400
H	16.8335940	6.0360170	4.4110170
C	15.4622770	7.4071030	3.9068550
H	15.2670420	7.1325710	2.8624860
O	13.1345670	6.9429420	4.4879130
C	14.1971780	7.9544610	4.5626400
H	14.4054080	8.1933160	5.6144770
O	14.8831760	10.2206830	3.8478470
C	13.7609070	9.2444060	3.8318700
H	13.4989750	9.0102680	2.7914590
C	12.6020930	9.9592260	4.5255870
H	11.7336770	9.2987460	4.5815710
C	12.4514800	6.6223970	5.7365400

H	12.7041290	7.3644980	6.5005830
O	14.2396320	4.9520240	6.3285940
H	14.8057270	5.3860980	5.6229110
C	12.8230620	5.1952950	6.1936860
H	12.4057710	5.0547970	7.1992380
O	12.5409430	2.8155340	5.7774510
H	13.4667440	2.8496240	6.1099400
C	12.1941770	4.1387900	5.2618320
H	12.5933150	4.2464030	4.2438630
O	10.0845580	3.3108640	4.3367510
C	10.6746720	4.2982450	5.2467930
H	10.2684970	4.1625210	6.2591750
O	11.0205480	6.7347030	5.5754900
C	10.3313540	5.7185920	4.7405710
H	10.6545000	5.8240660	3.6967570
C	8.8450470	6.0543140	4.8807640
H	8.2405960	5.2998600	4.3712790
C	9.1663300	2.3099510	4.8702880
H	8.9102140	2.5315020	5.9109510
O	10.9878690	0.6660390	5.4616850
H	11.5848120	1.4705670	5.5293380
C	9.7816870	0.9033500	4.7054560
H	9.0484660	0.1728890	5.0675770
O	10.6241990	-0.6494160	2.9874470
H	11.2553060	-0.8414720	3.7173220
C	10.0593610	0.6818080	3.2110630
H	10.7895250	1.4332760	2.8932480
O	9.2705730	0.9439180	0.9645440
C	8.7997580	0.8040400	2.3537660
H	8.1817730	-0.0961380	2.4577590
O	7.9127130	2.3473750	4.1479460
C	7.9864500	2.0798390	2.6966510
H	8.4965240	2.9272350	2.2224680

O	6.3057230	1.1528860	1.0695490
H	6.7600120	1.4927330	0.2650110
C	6.5085450	1.9869610	2.2465250
H	5.9395040	1.4994920	3.0421890
H	6.0977510	2.9949300	2.0949270
C	8.8393270	0.0337750	-0.0801740
H	8.0650600	-0.6441970	0.2870650
O	10.6566480	-1.5651230	0.4076440
H	10.7225900	-1.1345810	1.3087190
C	10.0753830	-0.7214510	-0.6138330
H	9.7516650	-1.4049260	-1.4080600
O	12.2435270	-0.3676280	-1.7594630
H	12.8329940	-0.6647800	-1.0026550
C	11.0749890	0.2960520	-1.2105630
H	11.3859090	0.9982020	-0.4297800
O	11.3102920	2.1190240	-2.8155300
C	10.3910090	1.0748420	-2.3414340
H	10.1494750	0.3866330	-3.1642120
O	8.2139930	0.8101860	-1.1365910
C	9.0998440	1.7685470	-1.8531270
H	9.3752390	2.5815290	-1.1695890
O	7.8211380	1.2252400	-3.8905370
H	7.2888930	0.5842510	-3.3718750
C	8.2470290	2.3031010	-3.0056780
H	7.3786480	2.8439300	-2.6016750
H	8.8403180	2.9809470	-3.6240080
C	11.6861650	2.1090280	-4.2181540
H	11.1562100	1.3086570	-4.7451950
O	13.7553880	0.7991310	-3.6552340
H	13.1595120	0.4272190	-2.9316070
C	13.2154470	1.9425220	-4.3460980
H	13.4371420	1.8007870	-5.4133510
O	15.3825060	3.0307460	-4.0874790

H	15.6134980	2.1104360	-3.8278280
C	13.9483870	3.2175470	-3.8776210
H	13.7570630	3.3903750	-2.8099310
O	14.1801330	5.6196950	-4.2575640
C	13.4760390	4.4119110	-4.7026760
H	13.6823010	4.2347360	-5.7672400
O	11.2568300	3.3273740	-4.8746210
C	11.9534560	4.5857170	-4.5033610
H	11.7437570	4.8226580	-3.4511000
C	11.3521600	5.6504310	-5.4222610
C	14.8966420	6.4021670	-5.2557060
H	14.6702420	6.0417720	-6.2639280
O	16.9844220	5.0304860	-4.9468180
H	16.3844850	4.3283060	-4.5541700
C	16.4113120	6.3556450	-4.9552940
H	16.9269260	6.8976930	-5.7580640
O	18.1378260	7.0712010	-3.3654440
H	18.5113780	6.2163080	-3.6780490
C	16.6947530	7.0563220	-3.6131390
H	16.1988390	6.4952280	-2.8114070
O	16.3724680	9.0417750	-2.2733490
C	16.1840750	8.4968130	-3.6215250
H	16.7360870	9.0999260	-4.3556190
O	14.4447020	7.7775820	-5.2307700
C	14.6741240	8.5007260	-3.9559130
H	14.1285780	7.9869390	-3.1566170
O	14.7689760	10.6080950	-5.2488760
H	14.6424950	10.1005920	-6.0793420
C	14.0961250	9.8968330	-4.1599830
H	13.0187460	9.8200350	-4.3543160
H	14.2470920	10.4989580	-3.2629490
O	12.9393980	10.2916500	5.9071420
H	13.7020970	10.9089840	5.9035220

O	11.5789870	5.3195910	-6.8251280
H	11.1428590	4.4615900	-7.0171390
H	10.2781900	5.7502310	-5.2114800
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O	8.4309850	6.0186330	6.2779670
H	8.9661720	6.6739280	6.7757440
H	12.3391030	10.8625720	3.9581520
H	8.6516170	7.0420730	4.4390110
C	-3.4726090	-13.2113100	4.1073160
H	-3.6224310	-13.7465090	5.0506330
O	-5.4733530	-14.1019770	2.8429230
H	-5.1017300	-14.9649240	3.1900720
C	-4.8238970	-12.9422290	3.4065940
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O	-5.9726330	-11.7188970	1.6543960
H	-6.4207750	-12.5918080	1.5855260
C	-4.6607650	-11.9313470	2.2593330
H	-3.9787740	-12.3418740	1.5031780
O	-3.8976830	-9.6773270	1.6841780
C	-4.1058710	-10.6104400	2.7940120
H	-4.7908250	-10.1726720	3.5328000
O	-2.8799540	-11.9490310	4.4975090
C	-2.7361380	-10.9025820	3.4544520
H	-2.0339550	-11.2496110	2.6835120
O	-3.0551200	-9.2477690	5.2524250
H	-3.1620450	-9.9806430	5.8962260
C	-2.1582650	-9.6941740	4.1917620
H	-1.1705860	-9.9540210	4.5972260
H	-2.0612440	-8.8492670	3.5057430
C	-4.5778900	-8.3816230	1.6871130
H	-4.9133370	-8.1206420	2.6957360
O	-6.8266170	-9.2536210	1.0603770
H	-6.5284620	-10.1972360	1.2164220

C	-5.7435820	-8.3900610	0.6682430
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O	-6.1887170	-8.8116990	-1.7367620
H	-6.6562440	-9.7109250	-1.6896490
C	-5.1579310	-8.7617250	-0.7105970
H	-4.7033620	-9.7522510	-0.6129750
O	-3.3674640	-8.3528380	-2.2979520
C	-4.0705020	-7.7686140	-1.1410420
H	-4.5240640	-6.8060950	-1.4150820
O	-3.6279200	-7.3624040	1.2995510
C	-3.0090450	-7.5612410	-0.0292450
H	-2.3747380	-8.4543470	0.0143330
C	-2.1525670	-6.3154490	-0.2566070
H	-1.6699150	-6.3611520	-1.2365260
C	-3.2873300	-7.6375920	-3.5658970
H	-3.4778970	-6.5692710	-3.4181790
O	-5.6508370	-8.1526730	-4.2402680
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C	-4.2579000	-8.2553840	-4.5957240
H	-4.1485860	-7.6922870	-5.5311520
O	-4.7422970	-10.2997630	-5.8650980
H	-5.6545450	-9.9609010	-5.7235750
C	-3.8664310	-9.7252040	-4.8439640
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O	-2.0771680	-11.2642460	-5.3704750
C	-2.4281380	-9.8370840	-5.3421470
H	-2.3538140	-9.4070720	-6.3508930
O	-1.9363420	-7.7365610	-4.0691470
C	-1.4507560	-9.1045080	-4.3935650
H	-1.3576890	-9.6838340	-3.4688120
C	-0.0745620	-8.8874100	-5.0257050
H	0.3434000	-9.8426530	-5.3537240
C	-1.6112600	-11.8433010	-6.6212420

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O	-3.9715450	-12.5310560	-7.2075660
H	-4.2349450	-11.7544230	-6.6328120
C	-2.5965270	-12.9478490	-7.0712600
H	-2.2792210	-13.2775030	-8.0694130
O	-3.3829500	-15.2240380	-6.6257050
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C	-2.5137820	-14.1594690	-6.1198900
H	-2.8454740	-13.8705650	-5.1134760
O	-0.9958520	-15.8602580	-5.2247820
C	-1.0779130	-14.6712390	-6.0862950
H	-0.7476510	-14.9328010	-7.0992230
O	-0.2803450	-12.3895410	-6.4612070
C	-0.1613440	-13.5569520	-5.5485240
H	-0.4940140	-13.2424730	-4.5493100
O	1.6890970	-15.0012080	-6.4587740
H	1.5459500	-15.8979130	-6.0752350
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H	1.9196190	-13.0805160	-5.7758000
H	1.5878030	-14.2650010	-4.4829140
C	-0.6987210	-17.1207610	-5.8633560
H	-0.6362530	-17.0038200	-6.9497670
O	-3.1132690	-17.7985260	-5.8034020
H	-3.2301300	-16.8277750	-6.0280080
C	-1.7574030	-18.1649640	-5.4684570
H	-1.5300380	-19.0933620	-6.0099180
O	-2.6719080	-19.4248430	-3.5788380
H	-3.4904290	-19.2457380	-4.0949430
C	-1.6717760	-18.4266180	-3.9562550
H	-1.8821530	-17.4904690	-3.4272780
O	-0.2386830	-19.0420790	-2.1103480
C	-0.2872440	-18.9434320	-3.5727250
H	-0.0996270	-19.9251230	-4.0277550

O	0.6273830	-17.5847970	-5.4609700
C	0.7958800	-17.9327450	-4.0227660
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O	2.3576790	-19.7169680	-4.6982830
H	2.2439170	-19.4983650	-5.6477580
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H	2.9411200	-17.7380430	-4.2188380
H	2.4144860	-18.7888120	-2.8746180
C	0.1121540	-20.2875040	-1.4443850
H	0.4937670	-21.0252090	-2.1569700
O	-2.2441920	-21.1513630	-1.5059760
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H	-0.8342510	-21.7226280	-0.1499780
O	-2.6188480	-20.2493060	1.2073710
H	-3.2508930	-20.7545830	0.6498200
C	-1.5426650	-19.7342590	0.3578440
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O	-0.8662130	-18.0427910	1.9102560
C	-0.4046630	-19.2875100	1.2787300
H	-0.2128470	-20.0619180	2.0346530
O	1.1838670	-20.0334910	-0.5067110
C	0.8919660	-18.9760490	0.4938980
H	0.7627610	-18.0255110	-0.0260730
C	2.1373760	-18.8959420	1.3706910
C	-0.8823600	-17.9149370	3.3547520
H	-0.3951230	-18.7749500	3.8268970
O	-3.2230180	-18.8415520	3.4787950
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C	-2.3400850	-17.7508970	3.8292660
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O	-4.2896240	-16.2912370	3.8075270
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C	-2.9171110	-16.4209680	3.3030290
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O	-2.5811700	-13.9756930	3.2484690
C	-2.0746310	-15.2420470	3.7969430
H	-2.0870140	-15.1997470	4.8955630
O	-0.1123750	-16.7618170	3.7578870
C	-0.6176710	-15.4318900	3.3159470
H	-0.5805240	-15.3785280	2.2205610
O	0.4186410	-14.5831680	5.3847980
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C	0.3542120	-14.4274190	3.9368220
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H	-0.0035360	-13.4107950	3.7602890
O	-2.9707030	-5.1076540	-0.2668820
H	-3.4169860	-5.0293490	0.6037490
O	2.4346340	-20.1851790	1.9968480
H	2.5306320	-20.8560900	1.2862340
H	2.9808550	-18.5486360	0.7624700
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O	-0.1719710	-8.0593080	-6.2223850
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COF4Cy[4]

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C	-0.8023380	-15.4010770	1.4943830
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N	-6.2123670	-12.5012240	1.4287750
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H	-8.5592820	-13.5463610	1.0788640
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C	-11.2062170	-8.9312340	0.5435880
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H	-8.5598250	-6.7549930	0.5317070
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H	-10.9830540	-6.7643650	0.2896590
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C	-14.1063050	-2.7069850	0.1061120
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C	-13.8504050	-0.2539920	0.1327920
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H	-18.6729400	-6.6292020	-1.3256740
C	-14.3922880	0.9419290	-0.4101920
C	-12.6288630	-0.2153530	0.8227120

C	-13.6844840	2.1702560	-0.2175850
C	-15.6124310	0.9603900	-1.1739070
C	-11.9362420	0.9722250	0.9894190
H	-12.2270630	-1.1246120	1.2503530
C	-14.2060650	3.3892600	-0.7554690
C	-12.4416060	2.1836770	0.4860610
C	-16.0983050	2.1218120	-1.6945620
H	-16.1460790	0.0362990	-1.3607670
H	-10.9959640	0.9739340	1.5293670
C	-13.4927440	4.6167340	-0.5757430
C	-15.4220870	3.3724570	-1.5035720
C	-11.7597810	3.4308130	0.6610030
H	-17.0133910	2.1174930	-2.2764820
C	-14.0017280	5.8031210	-1.1657100
C	-12.2696470	4.5958890	0.1720340
C	-15.8870760	4.5727870	-2.0643310
H	-10.8150300	3.4596510	1.1874190
N	-13.2187680	6.9734480	-1.0747020
C	-15.1951840	5.7638710	-1.8890740
H	-11.7390380	5.5210970	0.3562780
H	-16.7511090	4.5699310	-2.7152880
C	-13.5748450	8.2562860	-1.1831670
H	-12.1771090	6.8938390	-0.9626570
H	-15.5448670	6.6426650	-2.4069690
C	-12.6411380	9.2965640	-1.0914860
H	-14.6158300	8.5153880	-1.3264800
C	-11.2281900	9.0164750	-0.9281640
C	-13.1333890	10.6585950	-1.1658270
C	-10.3054060	10.1099260	-0.8140630
O	-10.8214220	7.7773870	-0.8899040
C	-12.1702540	11.7226100	-1.1774710
O	-14.4080370	10.9084700	-1.2302700
C	-10.7462940	11.4830860	-1.0030970

C	-8.9637320	9.8311740	-0.4980240
C	-12.5526700	13.0539820	-1.3379170
O	-9.9253370	12.4687380	-0.9849590
H	-8.6613630	8.8133630	-0.2625610
N	-8.0621530	10.8128160	-0.4343190
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C	-6.6896260	10.7436450	-0.1236260
H	-14.4807510	12.6642080	-1.4947550
C	-5.8795830	11.8677960	-0.4391550
C	-6.1294790	9.6117770	0.4861490
C	-4.4853810	11.8182820	-0.1208060
C	-6.3967560	13.0539440	-1.0727920
C	-4.7775570	9.5748870	0.7898620
H	-6.7607570	8.7642180	0.7437410
C	-3.6404940	12.9326700	-0.4217740
C	-3.9305930	10.6588030	0.5013800
C	-5.5914650	14.1194730	-1.3398010
H	-7.4421520	13.1094460	-1.3506310
H	-4.3599570	8.6986070	1.2730850
C	-4.1929320	14.1053390	-1.0205020
C	-2.2456390	12.8749990	-0.1121800
C	-2.5364570	10.6412290	0.8345910
H	-6.0004350	15.0055900	-1.8127090
C	-3.3480530	15.1955490	-1.2894900
C	-1.4287670	13.9863040	-0.4303250
C	-1.7314340	11.7029080	0.5408050
H	-2.1181720	9.7792280	1.3458960
C	-1.9907370	15.1322180	-1.0053110
H	-3.7617820	16.0856720	-1.7493900
N	-0.0390590	13.9116810	-0.1722050
H	-0.6881670	11.6818470	0.8334130

H	-1.3477760	15.9632430	-1.2678290
H	0.5099080	13.0345950	-0.3308380
N	13.7963650	0.4286130	-0.0476090
C	13.4071340	1.7035870	0.1039050
C	14.2576160	2.6920610	0.5734750
H	12.3928910	1.9972720	-0.1434600
C	13.6970450	4.0281610	0.7043770
C	15.6348160	2.3896410	0.9303270
C	14.5604280	5.0698540	1.2233380
O	12.4779230	4.2563870	0.3746320
C	16.4511220	3.4603950	1.4631500
O	16.1011640	1.1977210	0.7846570
C	14.0895700	6.3654440	1.3804800
C	15.9397900	4.8138250	1.6104680
C	17.7596260	3.1613980	1.8446250
N	12.8306090	6.7071590	1.0736870
H	14.7823780	7.1058280	1.7636140
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C	10.2363770	7.0531790	-0.0855880
C	12.1709740	10.2519740	1.9683730
H	13.7993590	8.9092050	2.2730550
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C	10.8781920	10.4463980	1.4510170
C	8.9805460	7.2293230	-0.5821760
H	10.7305140	6.1023870	-0.2431410

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C	8.2396930	10.8041210	0.4112880
C	8.2768200	8.4678770	-0.4295520
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H	8.4874030	6.4240010	-1.1153700
C	6.9183500	10.9338540	-0.0944000
C	8.9217730	11.8645150	1.1043840
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H	10.6817690	12.4983420	2.1112990
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C	6.3203980	9.8615290	-0.7708840
H	8.4504260	12.8313950	1.2436460
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H	6.6649880	12.9946240	0.4822670
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H	14.7987260	0.3196670	0.2439090
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C	2.7922760	13.5392760	0.1065270
C	4.9881150	14.6421910	0.7701720
C	2.1208260	14.7924160	0.3866730
O	2.1375210	12.4972080	-0.2709360
C	4.2608930	15.8531770	1.0854340
O	6.2661050	14.5776150	0.9459820
C	0.7486370	14.9191350	0.2198300
C	2.8288410	15.9652230	0.8771490
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O	2.1935450	17.0510570	1.1291440
H	6.0561910	16.8088170	1.7165100
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H	12.2689560	-16.2585590	-4.5054530
C	17.5607110	-16.7816190	-4.5843230
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C	17.7877310	-14.4986260	-3.6934520
H	16.0169930	-13.4280660	-3.2769710
H	13.2730530	-18.3699940	-5.2385770
C	18.4043690	-15.7092010	-4.1619720
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H	18.4312230	-13.6934970	-3.3558100
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H	15.2755960	-19.7506230	-5.7284830
C	20.3581960	-17.0692630	-4.6574270
H	20.4381220	-15.0595370	-3.8857680
H	19.9877120	-19.0507390	-5.4159980
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H	21.4357700	-17.1803470	-4.6864830
C	-4.9764790	-19.5182340	4.0962090
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H	-6.8227480	-18.5927170	4.7665570
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C	-6.0152050	-21.8451650	5.3406760
C	-2.2361450	-21.9765990	3.3821160
H	-2.5437030	-19.9511490	2.8692570
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C	-2.7242140	-23.1615990	4.0320450
C	-4.5135760	-24.2706820	5.3277660
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H	-1.2818390	-22.0294260	2.8694130
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H	-7.4817650	-22.9848050	6.4631910
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H	-1.0421360	-24.4112850	3.5386890
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C	-20.5022250	-5.7047050	-1.9526180
C	-21.0465210	-6.8925210	-2.5067730
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H	-20.8807550	-3.6538800	-1.4147740
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H	-19.2332280	-8.1169760	-2.3764280
H	-23.2028240	-3.6438310	-2.1997300
C	-22.2064780	-9.2628960	-3.6150630
C	-24.3517520	-8.0732380	-3.9215090
C	-24.5655460	-5.7304670	-3.2758940
H	-20.2390990	-10.1265110	-3.3021360

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C	-24.8984080	-9.2522620	-4.4558250
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H	-25.1512240	-4.8220250	-3.1855550
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H	-25.9326870	-9.2529840	-4.7818910
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C	-18.4863120	15.5442360	-1.7422840
C	-18.0298280	17.9238430	-2.2389580
C	-15.7340010	18.7192740	-2.4597630
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C	4.9987890	19.2634300	2.4185770
C	4.2814030	20.4806080	2.2802860
C	6.2540980	19.2524340	3.0449390
C	4.8558640	21.6812140	2.8020400
C	3.0019570	20.5605990	1.6216210
C	6.8130340	20.4257470	3.5318130
H	6.7966850	18.3250920	3.1843580
C	4.1514480	22.9193560	2.6898210
C	6.1384440	21.6529760	3.4312110
C	2.3344870	21.7429560	1.5195710
H	2.5634020	19.6712310	1.1853710
H	7.7852510	20.3956510	4.0105000
C	2.8742640	22.9635000	2.0522730
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H	1.3729390	21.7832790	1.0194330
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C	4.0095780	25.3246440	3.0952980
C	6.0161450	24.0539220	3.8442930
H	7.6654650	22.8372820	4.4193210
C	2.7614540	25.3553910	2.4745200
H	1.2274620	24.2229210	1.4719680
H	4.4426020	26.2357900	3.4931910
H	6.4427040	24.9703160	4.2371710
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C	19.9087070	3.9292990	2.7977160
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C	20.8905420	7.5390300	3.0905990
H	19.1421120	6.5632630	2.4319670
H	22.2054840	1.5618700	3.6137820
C	22.2324960	7.4414280	3.5945030
C	24.1216500	6.0103850	4.2959180
C	23.9178900	3.5806580	4.2302720
H	20.4802190	8.5273870	2.9138800
C	23.0163760	8.5738130	3.8736200
C	24.8672290	7.1714410	4.5618580
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H	24.3320370	2.5901580	4.3848880
C	24.3179620	8.4357130	4.3526580
H	22.5959590	9.5601380	3.7109680
H	25.8813010	7.0726990	4.9334340
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O	-7.7452460	5.8771880	-3.8583670
H	-8.0712420	6.2098920	-2.9282770
C	-8.6157290	4.8044810	-4.2933360
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O	-9.9028250	6.5789160	-5.2418180
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C	-10.0305400	5.3755220	-4.4040970
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O	-12.3423530	4.8708810	-5.0370490
C	-10.9587110	4.3710700	-5.0381860
H	-10.6429440	4.1167830	-6.0550640
O	-9.5549660	2.5953460	-4.0684710
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H	-11.4104550	3.2393450	-3.2368920
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H	-9.9236020	1.6301650	-5.9064100
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H	-12.6246510	2.2737910	-5.3020740
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H	-11.9761800	5.5888480	-6.9827310
O	-12.1232920	7.8756260	-5.1710290
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C	-13.1206870	7.0478880	-5.7956470
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O	-14.4934860	8.2952530	-4.2469060
H	-13.5566590	8.6861850	-4.2774570
C	-14.2413440	6.9369030	-4.7571730
H	-13.8859480	6.3046890	-3.9437040
O	-16.6110030	6.2771340	-4.5116970
C	-15.4551590	6.3363290	-5.4261380
H	-15.7245700	6.9215900	-6.3054350
O	-13.9308720	5.0116530	-6.8070100
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H	-14.8160910	4.3017470	-5.0077060
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O	-16.6156960	9.0828020	-5.6402610
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C	-17.7179660	8.4386320	-4.9421400
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H	-17.0914990	10.5879760	-4.1459610
C	-17.6045650	8.8032620	-3.4683710

H	-16.6516990	8.4225680	-3.0958410
O	-18.2948280	8.3375660	-1.2268230
C	-18.7211500	8.2366450	-2.6262650
H	-19.6674890	8.7543690	-2.8104900
O	-18.9480650	6.4418570	-4.3415230
C	-18.9155100	6.7393970	-2.8878190
H	-18.1173770	6.1905870	-2.3908570
C	-20.2950530	6.3060690	-2.3978310
H	-20.3961580	6.5677490	-1.3417970
C	-19.0054130	9.2017800	-0.2959270
H	-19.9350730	9.5774170	-0.7305300
O	-17.7962730	11.2731490	-0.9810660
H	-17.6590030	10.8191450	-1.8871700
C	-18.0472690	10.3467690	0.0869750
H	-18.5154020	10.9189880	0.8929200
O	-15.7858640	10.6923180	1.0175600
H	-15.3179230	10.9473220	0.1511170
C	-16.7759790	9.6891350	0.6467180
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O	-15.9979370	8.2681140	2.4682460
C	-17.1901540	8.9003900	1.8767350
H	-17.6588440	9.5577740	2.6124070
O	-19.3666180	8.4310260	0.8691000
C	-18.1901370	7.8028310	1.5207400
H	-17.7322740	7.0979870	0.8220210
O	-18.4545800	7.8325160	4.0228670
H	-17.5712720	7.5465140	4.4020540
C	-18.6962850	7.0828320	2.7981490
H	-19.7783510	6.9816450	2.6852070
H	-18.2513180	6.0808330	2.8375520
C	-15.6280070	8.7456670	3.7697150
H	-16.3172230	9.5091650	4.1325730
O	-13.9258960	10.3211410	2.7979890

H	-14.6782570	10.3973030	2.0822060
C	-14.1891480	9.2377040	3.7057550
H	-13.8963420	9.5539890	4.7142620
O	-11.9440870	8.6378750	3.1387040
H	-12.1625730	9.5569910	2.7672600
C	-13.2856350	8.0672270	3.2960880
H	-13.6298740	7.6527210	2.3448020
O	-12.4662940	5.9068820	4.1833300
C	-13.3607860	7.0463670	4.4052290
H	-13.1242910	7.5214570	5.3594780
O	-15.7271680	7.6512240	4.7496520
C	-14.8010780	6.5123560	4.4750450
H	-15.0724450	6.0296850	3.5326590
O	-14.3748600	6.1534570	6.8648190
H	-14.8897810	6.9917910	7.0294510
C	-14.9525680	5.5627500	5.6570330
H	-16.0099480	5.3019530	5.7885290
H	-14.3701560	4.6639620	5.4550920
C	-11.5198210	5.7173610	5.2863910
H	-12.0311040	5.8545330	6.2426800
O	-10.4817160	8.0450860	5.2102840
H	-11.0616110	8.3585230	4.4166670
C	-10.2928160	6.6112150	5.0976440
H	-9.5683170	6.3295460	5.8668580
O	-8.4829030	7.1711090	3.6355330
H	-8.7516060	7.9953860	4.1504060
C	-9.6948300	6.3309820	3.7195970
H	-10.4150230	6.6313590	2.9548460
O	-9.0442170	4.5986000	2.1187300
C	-9.3218660	4.8796850	3.5425320
H	-8.4672080	4.6107630	4.1713130
O	-11.0614570	4.3512500	5.2379210
C	-10.4984580	3.9610880	3.9220310

H	-11.2756830	4.0093800	3.1623300
C	-9.9884950	2.5443490	4.1743930
C	-7.6819310	4.8272440	1.6403610
H	-7.0144960	5.0332590	2.4808540
O	-8.0741090	7.2663180	1.1070230
H	-8.1909850	7.2724630	2.1330580
C	-7.6835990	5.9697930	0.6031450
H	-6.6668120	6.0172070	0.1929340
O	-8.6547590	6.6187040	-1.5522570
H	-9.4909450	7.1953710	-1.3834830
C	-8.6421640	5.5858850	-0.5260530
H	-9.6382750	5.4715980	-0.1005010
O	-9.2055080	3.8383110	-2.1179430
C	-8.1915940	4.2774620	-1.1476090
H	-7.2286580	4.4193680	-1.6431560
O	-7.1837050	3.6278180	1.0030910
C	-8.0572070	3.1694160	-0.1030200
H	-9.0474530	2.9094370	0.2710700
O	-6.2199490	2.2994660	-1.5068180
H	-5.5808570	2.7457060	-0.8846630
C	-7.3834510	1.9366400	-0.6968260
H	-7.1225210	1.2469930	0.1151280
H	-8.0809440	1.4549240	-1.3832960
O	-16.7205470	5.2275370	-7.6745340
H	-15.9393120	5.4536240	-8.2524090
O	-9.0412180	2.5818460	5.2831190
H	-9.5446360	3.0559960	6.0044290
H	-10.8397690	1.8805630	4.3736340
H	-9.4382390	2.1956700	3.2982880
O	-21.3076390	7.0572470	-3.1325130
H	-21.0707970	6.8986370	-4.0900960
H	-15.8481600	3.3559730	-7.1349420
H	-20.4063970	5.2215120	-2.5263050

C	10.0421170	15.9194880	-2.1871270
H	10.4024180	16.3260140	-3.1346500
O	11.9238040	14.2779480	-1.8675900
H	11.3245320	13.6618370	-2.4192380
C	11.1600890	15.3708040	-1.3060360
H	11.8643760	16.1773090	-1.0815620
O	11.6174270	14.4141050	0.8547870
H	12.2245890	13.9151980	0.2335470
C	10.5308490	14.8858570	-0.0052640
H	9.8386590	14.0740740	-0.2366100
O	9.1224300	15.4000470	1.8633070
C	9.8017420	16.0001400	0.6976530
H	10.4959620	16.7851980	1.0140290
O	9.3675030	17.0125580	-1.5157310
C	8.7485060	16.6461920	-0.2091160
H	7.8999200	15.9710700	-0.3292220
O	9.5624290	18.8405670	0.4326500
H	9.9422890	18.7927760	-0.4903980
C	8.3600550	18.0165070	0.3442210
H	7.5924410	18.4673280	-0.2973470
H	7.9762340	17.9150840	1.3572980
C	9.4033580	15.9891130	3.1487590
H	10.0132400	16.8899580	3.0414190
O	11.3211720	14.3566300	3.4909710
H	11.3923930	14.4215640	2.4715450
C	10.1003040	14.9334620	4.0214890
H	10.3484710	15.4052460	4.9788380
O	9.8071450	12.8414000	5.1929190
H	10.7364760	12.7708930	4.8322270
C	9.1343320	13.7887610	4.3056680
H	8.8477390	13.3065370	3.3698320
O	6.9918820	13.1869130	5.1873670
C	7.9071070	14.3132370	4.9932840

H	8.1469490	14.7888930	5.9489060
O	8.1695830	16.4389730	3.7850100
C	7.1970450	15.3478970	4.1218160
H	6.8163790	14.9025440	3.2006050
C	6.1278080	16.0421310	4.9703290
H	5.4763730	15.2819340	5.4062390
C	6.6585900	12.8386530	6.5482950
H	7.1577240	13.4951080	7.2644300
O	8.4295470	11.0340400	6.6092950
H	8.9069630	11.6825320	5.9803020
C	7.0323740	11.3664220	6.7429780
H	6.7179090	11.0669420	7.7485580
O	6.5828040	9.1387910	5.9170660
H	7.5679520	9.1483340	6.0980030
C	6.2392640	10.5441780	5.7287820
H	6.4926120	10.8835440	4.7195400
O	4.0268280	9.9841640	4.9796770
C	4.7687310	10.7384140	5.9886130
H	4.4986890	10.4088840	6.9965580
O	5.2339040	13.0303020	6.7610250
C	4.3748630	12.2112040	5.8625100
H	4.4783070	12.5428850	4.8276080
C	2.9657560	12.4169860	6.4189960
H	2.2733490	11.7464220	5.9050140
C	3.1051080	8.9785920	5.4586780
H	3.0445230	8.9759580	6.5490610
O	4.8645690	7.1589660	5.2924520
H	5.5146480	7.9345370	5.4456680
C	3.5619600	7.6349320	4.8862230
H	2.8319480	6.8734140	5.1775040
O	4.0051540	6.4862520	2.8104160
H	4.7217360	6.1887020	3.4469880
C	3.5630630	7.7622440	3.3659650

H	4.2457190	8.5704020	3.0869100
O	2.3271010	8.3491590	1.4228770
C	2.1789280	8.0867300	2.8617970
H	1.4936480	7.2544550	3.0408570
O	1.7677160	9.2824020	4.9879820
C	1.6713070	9.3773250	3.5110600
H	2.3047530	10.1949520	3.1590940
O	-0.3923880	8.8097300	2.1510470
H	-0.0006490	9.0577920	1.2603640
C	0.1669450	9.6289970	3.2265790
H	-0.3609410	9.3226230	4.1309020
H	-0.0123200	10.6980070	3.0629060
C	1.5732950	7.5338560	0.5110940
H	0.8480500	6.9058790	1.0283100
O	3.3655330	5.7560800	0.3287440
H	3.6637020	6.0855150	1.2556730
C	2.5616870	6.7449290	-0.3461040
H	1.9950280	6.2178840	-1.1206680
O	4.4408060	6.9891700	-1.8507980
H	4.5630610	6.1356390	-1.3327650
C	3.4921670	7.7488740	-1.0256650
H	4.0222570	8.3186730	-0.2607960
O	3.5110950	9.5803570	-2.6226060
C	2.6514770	8.6365900	-1.9020320
H	2.1052450	8.0169150	-2.6167170
O	0.7818070	8.4366550	-0.3321520
C	1.6156030	9.4206010	-1.0951900
H	2.0774900	10.1451150	-0.4241140
O	0.1658640	9.1816980	-3.0630150
H	-0.3342100	8.4803100	-2.5600600
C	0.6489250	10.1213150	-2.0463480
H	-0.1754570	10.5627570	-1.4752450
H	1.1933570	10.8972350	-2.5853310

C	3.2231310	9.6594870	-4.0572710
H	2.2928460	9.1329210	-4.2750570
O	4.7808580	7.7235490	-4.4900400
H	4.6761660	7.5262380	-3.4998980
C	4.4429130	9.0967640	-4.7922210
H	4.2443840	9.1389120	-5.8677360
O	6.7973800	9.4996930	-5.2464710
H	6.7476000	8.5040640	-5.1613050
C	5.6424270	9.9898670	-4.4933800
H	5.8530550	9.9804700	-3.4215400
O	6.4829860	12.2257930	-4.5166960
C	5.3515330	11.4005410	-4.9345010
H	5.1949930	11.4587780	-6.0163540
O	2.9674110	11.0292580	-4.4295320
C	4.1070580	11.9637440	-4.2479890
H	4.3020960	12.1338830	-3.1872380
C	3.6509180	13.2294040	-4.9788080
C	7.2793560	12.8471900	-5.5452680
H	6.9579730	12.5472110	-6.5451470
O	9.0397300	11.0559570	-5.3500710
H	8.2062340	10.4876180	-5.2079420
C	8.7336670	12.4622610	-5.2543490
H	9.3773980	12.9958900	-5.9622280
O	10.4746090	12.6733910	-3.5613390
H	10.6319740	11.7464940	-3.8984360
C	9.0671030	12.9469350	-3.8441240
H	8.4118770	12.4391490	-3.1305410
O	9.1119480	14.8392280	-2.3887240
C	8.8608060	14.4375020	-3.7719570
H	9.5408950	14.9539430	-4.4553290
O	7.1051040	14.2888790	-5.4787030
C	7.4354370	14.8441550	-4.1389830
H	6.7331680	14.4783530	-3.3881380

O	8.3051510	16.7379920	-5.3832090
H	8.0543820	16.1541540	-6.1542080
C	7.3581080	16.3571550	-4.3365510
H	6.3277010	16.6426550	-4.5846270
H	7.6780520	16.8609670	-3.4220170
O	6.7879140	16.7131100	6.0885700
H	7.4921970	17.2708890	5.6534220
O	3.2973030	12.8638370	-6.3468970
H	2.6527970	12.1093890	-6.2291110
H	2.8135720	13.6883250	-4.4377100
H	4.4881100	13.9273020	-5.0458120
O	2.9677050	12.0281650	7.8271260
H	3.7194050	12.5593520	8.2159790
H	5.5360820	16.7325610	4.3592080
H	2.6592800	13.4610460	6.2748850
C	12.7574350	-6.2519060	3.6740380
H	13.2752770	-6.6782290	4.5367260
O	13.2918230	-8.1489490	2.0425780
H	14.2457920	-7.7800510	2.1510020
C	12.2993480	-7.3312660	2.6891570
H	11.6287790	-7.9966260	3.2474980
O	11.1908570	-7.7059830	0.5913200
H	12.0038290	-8.3039630	0.6938640
C	11.4711330	-6.6613760	1.5776690
H	12.0512450	-5.8587900	1.1158500
O	9.2635960	-5.5667590	1.2856660
C	10.2188750	-6.1346040	2.2391580
H	9.7373630	-6.9331320	2.8067180
O	11.5864730	-5.5904070	4.2218280
C	10.6408780	-5.0292280	3.2188990
H	11.1056990	-4.2021660	2.6749050
O	8.7602830	-5.7245790	4.6142740
H	9.4596570	-6.1800180	5.1621150

C	9.4393440	-4.5653010	4.0333460
H	9.7679370	-3.8514960	4.7984360
H	8.7196720	-4.0956870	3.3621420
C	7.9219670	-6.1577860	1.3526650
H	7.6889640	-6.4433680	2.3814770
O	8.6403090	-8.4544510	0.7169760
H	9.6300060	-8.2113720	0.6202630
C	7.8252530	-7.3181780	0.3501450
H	6.7874090	-7.6604640	0.3331450
O	8.0897790	-7.8037750	-2.0588420
H	8.9927460	-8.3113730	-2.0399750
C	8.2188690	-6.7696050	-1.0239720
H	9.2589970	-6.4560720	-0.9400700
O	8.0853520	-4.9294320	-2.5634370
C	7.3891180	-5.5611050	-1.4232600
H	6.3658570	-5.8421490	-1.6906760
O	6.9781900	-5.1283810	0.9753650
C	7.3261720	-4.4985600	-0.3163430
H	8.2864340	-3.9935780	-0.2270390
C	6.1738070	-3.5330660	-0.5747760
H	6.3055230	-3.0570770	-1.5494840
C	7.4075510	-4.7402350	-3.8325330
H	6.3256800	-4.8462140	-3.7178440
O	7.7795980	-7.1230810	-4.5993080
H	7.8912540	-7.3298320	-3.5935160
C	7.9833450	-5.7206590	-4.8579950
H	7.5138490	-5.5011060	-5.8224940
O	10.0170620	-6.4219160	-5.9446680
H	9.4860990	-7.2553590	-5.7643920
C	9.4851710	-5.4605930	-4.9841910
H	9.9571330	-5.5823180	-4.0072600
O	11.1660580	-3.8049480	-5.4880740
C	9.7197080	-4.0600900	-5.4831730

H	9.2945890	-3.9220130	-6.4828220
O	7.6404070	-3.3843660	-4.2868110
C	9.0669250	-3.0318830	-4.5502050
H	9.6350740	-2.9726420	-3.6218430
C	8.9781460	-1.6835840	-5.2655870
H	9.9737430	-1.4050680	-5.6198360
C	11.7768390	-3.5529450	-6.7774200
H	11.0238680	-3.5317380	-7.5690460
O	12.4091470	-6.0140610	-7.0399810
H	11.5306260	-6.1619300	-6.5350370
C	12.8346020	-4.6371900	-7.0285610
H	13.2852800	-4.4244420	-8.0049380
O	14.9295300	-5.5359280	-6.2517500
H	14.3706800	-6.3193320	-6.5401770
C	13.9387500	-4.4979530	-5.9748300
H	13.5091530	-4.6195680	-4.9749200
O	15.6936880	-2.9955380	-5.2179020
C	14.5549410	-3.1340440	-6.1390210
H	14.8943220	-2.9790560	-7.1652780
O	12.3920410	-2.2393390	-6.7999640
C	13.5093610	-2.0666120	-5.8316100
H	13.1239270	-2.1874390	-4.8149550
O	15.2845280	-0.6518520	-6.9018700
H	16.0967250	-0.7287330	-6.3207300
C	14.1009710	-0.6522130	-6.0504890
H	13.3322810	-0.0657360	-6.5590800
H	14.3006110	-0.2010910	-5.0709000
C	16.9893050	-2.8971880	-5.8271030
H	16.9324430	-2.9108000	-6.9164800
O	17.4600500	-5.3682780	-5.5251810
H	16.4498930	-5.4339210	-5.7253050
C	17.8702000	-4.0094240	-5.2608780
H	18.8832730	-3.8799350	-5.6569050

O	18.5744470	-4.9954090	-3.1647810
H	18.3511710	-5.7147190	-3.8432150
C	17.8879520	-3.8323260	-3.7398680
H	16.8528540	-3.8194620	-3.3996740
O	18.5551740	-2.3110070	-1.9526680
C	18.5670570	-2.5269720	-3.4045310
H	19.5875270	-2.4786110	-3.7907580
O	17.5906260	-1.5971160	-5.4867450
C	17.7426850	-1.3805020	-4.0166850
H	16.7593010	-1.3477740	-3.5430550
O	19.8663080	-0.2155200	-4.3552540
H	19.7822540	-0.4529130	-5.3208200
C	18.4938440	-0.0623670	-3.8751770
H	17.9514740	0.7310640	-4.4041470
H	18.5660570	0.1856050	-2.8152600
C	19.8241210	-2.1027630	-1.2665900
H	20.5291100	-1.5768150	-1.9156090
O	20.7418430	-4.4188790	-1.7383720
H	19.9295360	-4.6616160	-2.3125600
C	20.3604900	-3.4419330	-0.7412430
H	21.2574630	-3.2278610	-0.1535810
O	19.8385230	-5.3089190	0.7216950
H	20.3632240	-5.7100240	-0.0319960
C	19.3035220	-4.0643700	0.1670340
H	18.4150840	-4.2730580	-0.4317610
O	17.6830290	-3.7196940	1.8836140
C	18.9051650	-3.1493070	1.3008580
H	19.7076970	-3.0548970	2.0410090
O	19.5471740	-1.2384490	-0.1415460
C	18.5037570	-1.7706420	0.7739460
H	17.5533220	-1.8708890	0.2606610
C	18.3881160	-0.7355860	1.8886330
C	17.7183880	-4.2237690	3.2330030

H	18.6856150	-4.0346910	3.7064110
O	18.2575130	-6.5842460	2.4511130
H	18.8052270	-6.0845440	1.7468290
C	17.3712030	-5.7132670	3.1879910
H	17.3375780	-6.0782420	4.2201950
O	15.7045250	-7.2962700	2.5241960
H	16.5961560	-7.6805670	2.2617770
C	15.9671720	-5.8610630	2.5904640
H	15.9435070	-5.4094860	1.5937430
O	13.6123290	-5.3061130	2.9806070
C	14.9792110	-5.1801740	3.5062810
H	15.0325440	-5.5872310	4.5213850
O	16.7376910	-3.5234150	4.0391800
C	15.3178480	-3.6859290	3.6019560
H	15.1568670	-3.1935090	2.6408170
O	14.9244580	-3.6992250	5.9924340
H	15.9204610	-3.6209530	5.9848110
C	14.5240010	-3.0544990	4.7453990
H	14.6916070	-1.9699760	4.7621300
H	13.4645720	-3.2725770	4.5997010
O	4.9295250	-4.2964290	-0.6253300
H	4.9421970	-4.8179900	0.2272640
O	19.7372550	-0.3557160	2.3351390
H	20.2473330	-0.2793480	1.4774280
H	17.8118100	0.1169740	1.5250210
H	17.8662150	-1.1898830	2.7358350
O	8.1294340	-1.8413090	-6.4427500
H	7.3005700	-2.2629050	-6.0768560
H	6.1584400	-2.7678800	0.2121760
H	8.5957700	-0.9205140	-4.5750120
C	-2.3276310	-10.0288190	-2.6904190
H	-1.7937470	-9.1286530	-3.0041670
O	-4.5386060	-9.3136670	-3.6953430

H	-4.5165500	-8.6874290	-2.8909110
C	-3.5298800	-10.3370080	-3.5895220
H	-3.1472150	-10.5344260	-4.5975720
O	-5.3003040	-11.9481290	-3.9666350
H	-5.7098480	-11.0661590	-4.1988450
C	-4.1865460	-11.6218680	-3.0787980
H	-4.5338410	-11.4702660	-2.0535000
O	-3.7565130	-13.9747990	-2.6875420
C	-3.1605400	-12.7220690	-3.1526950
H	-2.8284900	-12.8259010	-4.1883350
O	-1.3668710	-11.1096140	-2.7405830
C	-1.9376660	-12.4139870	-2.2943230
H	-2.1934300	-12.3860230	-1.2342690
O	-0.6343630	-13.5816200	-4.0137550
H	-0.3685220	-12.6705320	-4.3229890
C	-0.8441680	-13.4416470	-2.5685880
H	0.0749150	-13.1456690	-2.0495220
H	-1.1791420	-14.4200100	-2.2197160
C	-3.5277040	-15.1058320	-3.5673200
H	-2.7231320	-14.8919710	-4.2740360
O	-5.4864500	-14.4208920	-5.0288740
H	-5.4195010	-13.4986650	-4.5837350
C	-4.8708340	-15.4460330	-4.2072950
H	-4.7486940	-16.3249120	-4.8461520
O	-7.1439050	-16.0234650	-3.7543680
H	-7.0874220	-15.3704240	-4.5283810
C	-5.8556810	-15.7806740	-3.0848140
H	-5.9305130	-14.9186980	-2.4149980
O	-6.2331510	-17.2539510	-1.1527180
C	-5.3736940	-16.9840650	-2.3094100
H	-5.2767540	-17.8715690	-2.9434160
O	-3.0655860	-16.2328700	-2.7863490
C	-3.9943480	-16.6680340	-1.7098000

H	-4.0881610	-15.8915090	-0.9487170
C	-3.3429250	-17.9423970	-1.1796910
H	-4.0229750	-18.4206640	-0.4744670
C	-7.4599380	-17.9794370	-1.4204910
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O	-8.8674940	-15.8887940	-1.8534870
H	-8.2527230	-15.8665460	-2.6834310
C	-8.6519760	-17.0856670	-1.0802810
H	-9.5424210	-17.7281910	-1.1187450
O	-9.5309030	-15.6041980	0.5713350
H	-9.6170700	-15.2267780	-0.3702250
C	-8.4549910	-16.5962510	0.3577340
H	-7.4920150	-16.0990050	0.4649590
O	-8.1877250	-17.3206050	2.6687950
C	-8.5282130	-17.7722050	1.3040740
H	-9.5069830	-18.2564760	1.2921880
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C	-7.4585870	-18.8092480	0.8967670
H	-6.4644840	-18.4219520	1.1240450
C	-7.7332280	-20.1551480	1.5602980
H	-7.6831960	-20.0588140	2.6438530
C	-9.2115010	-17.5126580	3.6892750
H	-9.5631320	-18.5484520	3.6936890
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C	-10.3899720	-16.5281190	3.5430160
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O	-11.0178440	-14.1842180	3.6412320
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C	-9.8753480	-15.1021420	3.7130070
H	-9.1489560	-14.8816170	2.9291210
O	-8.7263450	-13.5906190	5.1691130
C	-9.2352070	-14.9647320	5.0620070

H	-9.9335530	-15.1751220	5.8741290
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O	-8.3590990	-15.3046620	7.5936310
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H	-7.2084380	-16.8633670	6.8968790
H	-6.5063100	-15.2679030	6.5488740
C	-9.3979490	-12.7283500	6.0952840
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O	-10.6547040	-11.5760860	4.2548240
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O	-7.0037940	-10.4069060	8.7508320
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O	-7.7934440	-7.4645710	5.2967080

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C	-6.3557130	-7.6101720	5.3250190
H	-5.9500810	-6.6905860	5.7574820
O	-6.2080100	-6.5791830	3.1144150
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C	-5.8413710	-7.7697070	3.9002340
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H	-4.0601320	-9.9564520	4.3963300
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O	-4.9857240	-6.1493280	0.7340270
H	-5.3705690	-6.3046070	1.6666020
C	-3.6757310	-6.7587190	0.5645470
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O	-4.3195920	-7.4491770	-1.6853980
H	-5.0820670	-6.8430850	-1.4656860
C	-3.8315350	-7.9373170	-0.3918280
H	-4.5410300	-8.6465000	0.0286620
O	-2.8479150	-9.8910010	-1.3446350
C	-2.5287320	-8.6666160	-0.6076140
H	-1.7854450	-8.0599220	-1.1332970
O	-1.7726810	-7.9262240	1.6033870
C	-1.9501410	-9.1128560	0.7328270
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O	-2.0905760	-7.4684340	5.6145710
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C	-4.0196380	-11.3228930	-0.6260230
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H	13.7835650	-6.6253630	-0.0706830

C	16.7141610	-9.0699280	0.7036860
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C	14.0503620	0.1727670	-0.6305150
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C	7.4155290	14.8715510	-0.1422390
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H	2.1040980	9.4557900	-0.2033450
H	0.9058110	12.0089540	-0.1688360
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H	-1.1296660	15.1420330	-0.0265150
C	-0.4705070	18.9003200	0.7527170
H	1.6426350	18.4018870	0.5876770
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C	-3.4144530	16.5561700	0.3240160
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H	-17.1333850	5.0011750	0.4985980
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C	-15.3706350	9.5726590	0.5243830
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C	-9.3002680	11.8461720	-0.3416280
C	-9.6897240	13.1940840	-0.1233740
C	-7.9329280	11.5850180	-0.5494910
C	-8.7273460	14.2088060	-0.0518320
O	-11.0610810	13.4542450	-0.0068480

C	-6.9748540	12.6055900	-0.5134780
H	-7.6678190	10.5495680	-0.7354840
C	-7.3568320	13.9422440	-0.2270050
H	-8.9901100	15.2426520	0.1456520
C	-11.5545350	14.7315360	0.4954090
O	-5.6193950	12.3711450	-0.7776090
C	-13.0862900	14.6292800	0.4865780
H	-11.2315090	15.5496970	-0.1625960
H	-11.1616470	14.9069050	1.5087410
C	-5.0612090	11.0245710	-0.7693440
C	-13.7484070	15.9055390	1.0248520
C	-3.5607200	11.1906520	-1.0496870
H	-5.2453740	10.5527360	0.2081960
H	-5.5244710	10.4148720	-1.5572650
H	-14.8374770	15.7932430	1.0082410
H	-13.4371680	16.1134410	2.0588880
H	-13.4847310	16.7769920	0.4125970
C	-2.8206230	9.8458050	-1.0468610
H	-1.7558090	10.0094460	-1.2430390
H	-2.9205450	9.3352530	-0.0778300
H	-3.2133890	9.1764680	-1.8225570
C	8.4133410	13.2927610	-0.3618830
C	7.4483010	12.2842470	-0.6181900
C	7.9546760	14.6125040	-0.1967280
C	6.0838520	12.5966130	-0.6363790
O	7.9252810	10.9914100	-0.8711030
C	6.5919370	14.9332200	-0.2520260
H	8.7193140	15.3608030	-0.0191040
C	5.6231640	13.9121050	-0.4393580
H	5.3207980	11.8430720	-0.8004700
C	7.0451310	9.8307820	-0.8201830
O	6.1293530	16.2524730	-0.1524280
C	7.9407730	8.6127180	-1.0879110

H	6.2709900	9.9046280	-1.5964110
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C	6.2136470	18.6174690	0.2602080
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H	7.8918060	17.3949610	-0.3226810
H	7.8287740	6.4546310	-1.2300160
H	6.6776000	7.1469160	-0.0619540
H	6.3649130	7.2796960	-1.8054860
C	7.0567880	19.8092190	0.7400960
H	6.4804540	20.7416730	0.6767180
H	7.3741040	19.6694890	1.7809650
H	7.9512990	19.9351200	0.1174840
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O	3.3698420	13.0950750	-0.6754440
N	2.2956620	15.5859100	-0.0320770
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C	0.5205980	17.1689550	0.3804220
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C	0.1705320	18.4944770	0.6915650
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H	-0.2230200	15.1958070	-0.0767840
C	-1.1905370	18.8716750	0.7811260
H	0.9308160	19.2524750	0.8664990
C	-2.2037270	17.9237680	0.5634730
C	-2.9019610	15.5607190	0.0314880
H	-3.2546050	18.1957560	0.6291350
H	-2.5687540	14.5380680	-0.1789360
N	-4.1654090	15.8850800	0.0984150

N	-5.0796280	14.8691640	-0.1085870
H	-4.7762100	13.9079450	-0.3060820
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O	-6.9202760	16.2788340	0.1486200
C	18.4296910	-8.9102530	1.0241950
O	19.4163450	-8.1524770	1.1256340
H	18.5499330	-10.0047350	1.1640800
C	1.5671460	-20.2945020	1.0245260
O	0.7531140	-21.2196540	1.2369030
H	2.6572480	-20.4868170	1.0634170
C	-16.8413910	-11.5427630	0.8562660
O	-18.0520080	-11.3078950	1.0635300
H	-16.4593040	-12.5820480	0.8825890
C	-18.4379600	8.7981010	1.0108100
O	-18.8322850	9.9631060	1.2366270
H	-19.1510090	7.9508060	1.0317490
C	-1.5596000	20.2696230	1.1067930
O	-0.7367010	21.1867060	1.3226510
H	-2.6476570	20.4704480	1.1515330
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O	18.0419320	11.2889750	1.0085890
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O	-12.0601150	3.5569040	-0.1533080
H	-11.6059990	3.4927610	0.7142420
H	-11.8884690	2.9239040	-2.0697300
O	-18.4366790	-4.9907700	1.0561240
H	-18.5524700	-4.8801700	2.0244710
H	-19.2241200	-4.3846310	-0.7084340
O	-9.1039700	-8.6126590	-0.1874580
H	-8.8368860	-8.2514240	0.6849850
H	-8.4375710	-8.7770660	-2.0931590
O	-4.8972510	-18.3992270	1.1049790
H	-5.0700920	-18.4435790	2.0701190

H	-5.7806720	-18.7800350	-0.6771310
O	2.9481060	-12.1483850	-0.1289730
H	2.7612510	-11.7199820	0.7338800
H	3.4404110	-11.6879540	-2.0392130
O	13.5245900	-13.4768720	1.2526420
H	13.4110520	-13.6150010	2.2179410
H	13.3989650	-14.4483990	-0.5185610
O	12.0703000	-3.5939890	-0.0594200
H	11.6429200	-3.5154260	0.8204990
H	11.8644770	-2.9698640	-1.9747150
O	18.4397770	4.9811540	1.0067710
H	18.5722860	4.8697660	1.9728900
H	19.1951400	4.3753380	-0.7718810
O	9.0819860	8.5973920	-0.1610340
H	8.8148880	8.2510410	0.7174350
H	8.4126430	8.7407470	-2.0672200
H	5.8858250	18.7787150	-0.7776440
O	5.0210100	18.4217640	1.1025070
H	4.6516020	19.2874370	1.3768840
O	-2.9617140	12.1444370	-0.1044280
H	-2.7819240	11.7149830	0.7594070
H	-3.4441940	11.6875470	-2.0180000
O	-13.5326580	13.4338130	1.2181260
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H	-13.4136710	14.4330550	-0.5392860

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C	-11.8307870	-0.6792580	-0.6818740
C	-12.7375190	-1.7256230	-0.4102770
C	-14.1199800	-1.4821050	-0.2908790

C	-14.6085700	-0.1761470	-0.4457210
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H	-12.3638020	-2.7394150	-0.2845520
H	-15.6745480	0.0201930	-0.3528750
C	-10.3655400	-0.9600800	-0.7866130
C	-9.4104830	0.0236080	-0.6918220
H	-9.7949870	1.0261670	-0.5110420
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C	-7.1520060	-1.1714640	-0.9864880
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H	-7.6100770	-2.1481880	-1.0806860
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C	-5.0881210	0.1638850	-0.9271790
H	-5.1734060	-1.9849910	-1.1897160
H	-5.3938150	2.2864410	-0.6184150
C	-10.0166680	-2.3445280	-0.9734660
N	-9.7831960	-3.4955730	-1.1236710
C	-14.3127070	2.2829900	-0.9270240
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H	-14.9840340	2.5217230	-0.0909420
C	-13.3144610	3.3588400	-1.0344880
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C	-1.3571740	-0.2582850	-1.8851210
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H	-3.5693840	1.2609000	0.9373320
C	-2.5756900	-1.4215510	-4.1790990

H	-4.4494490	-0.8828880	-3.2932230
C	-0.5676840	-0.8345260	-2.9331000
C	-0.7340400	0.3739400	-0.7464480
C	-1.1573660	-1.4079180	-4.0495050
H	-3.0333830	-1.8487900	-5.0678890
H	0.5137390	-0.8155160	-2.8489720
H	-0.5387150	-1.8395500	-4.8320110
C	0.7716360	0.4151960	-0.6827820
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C	1.5206510	-0.5588810	-0.0254270
C	0.7345420	2.5399770	-2.0053880
C	2.9038170	1.5663970	-1.3278850
C	2.9404930	-0.4920830	-0.0243280
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C	3.5434880	2.6970020	-1.9308910
C	3.6446950	0.5226080	-0.6651640
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C	2.8068270	3.6929540	-2.5563290
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H	4.6230000	2.7851810	-1.8776030
H	3.3125990	4.5450940	-3.0036220
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C	-2.6496870	2.3833970	3.9312830
C	-3.1848890	-0.3267930	4.4758150
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C	-3.4963990	2.0346540	5.0008490
H	-2.4382790	3.4308760	3.7335190
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H	1.1437030	6.3171620	1.6641630
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C	3.2371500	-3.7234270	3.7884640
H	2.2769910	-4.3709810	1.9621290
C	3.4570430	-2.6508450	4.6732120
H	3.0486120	-0.5618600	5.0916920
H	3.6699240	-4.6995450	3.9940130
H	4.0629750	-2.7974490	5.5646760
C	0.8808520	-3.4937100	-0.1985140
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C	-0.2691360	-5.4170200	-1.1581140
H	-1.1801380	-3.9725250	0.1993350
C	0.9047210	-5.7754790	-1.8478620

H	2.9732490	-5.2602210	-2.2506720
H	-1.1679510	-6.0197830	-1.2627960
H	0.9149460	-6.6570880	-2.4847820
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C	7.2123340	0.1984820	0.6335480
H	5.2459410	0.2380490	1.5178900
C	7.9985710	0.2810140	-0.5485130
H	7.8554970	0.5097410	-2.7157940
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C	9.4490250	0.1698890	-0.3811640
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C	11.9187320	0.0612220	-0.8732220
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N	10.1464840	0.6799990	-3.8394890
C	14.3077700	0.3652020	-1.3608360
H	12.7044330	0.9403080	-2.6887860
C	13.6166930	-0.6562850	0.7441120
H	11.5054540	-0.9126330	1.0290200
C	14.6369300	-0.2044390	-0.1217850
C	15.3693070	0.8651090	-2.3459570
H	15.6799910	-0.3053990	0.1703460
H	15.2571760	0.3433280	-3.3066930
H	15.2097280	1.9325660	-2.5532370
C	16.7577750	0.6915630	-1.8911220
N	17.8705460	0.5519310	-1.5246730

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H	14.5704030	-2.2429180	1.8702830
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H	-14.9162870	-3.4380350	-0.7690510
H	-14.7289880	-3.1455310	0.9557380
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N	-17.6097090	-2.0686850	0.1900820
C	12.9227890	-1.5956100	2.9848710
N	12.0264760	-1.8292420	3.7157530