

SUPPORTING INFORMATION

First-principles theoretical modelling of one-handed helical ladder polymers circularly polarized luminescence

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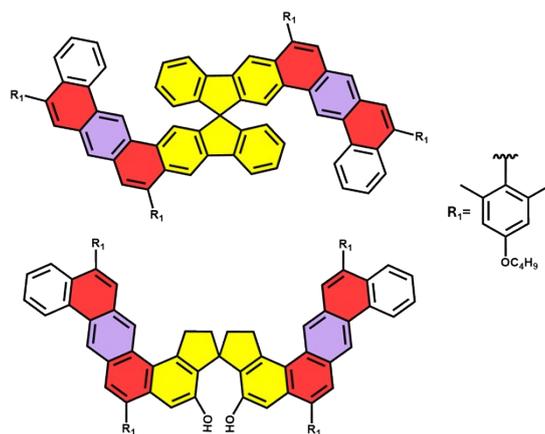


Fig. S1. Design of models 5 (top, constitutional isomer of model 4) and 6 (bottom, constitutional isomer of model 3).

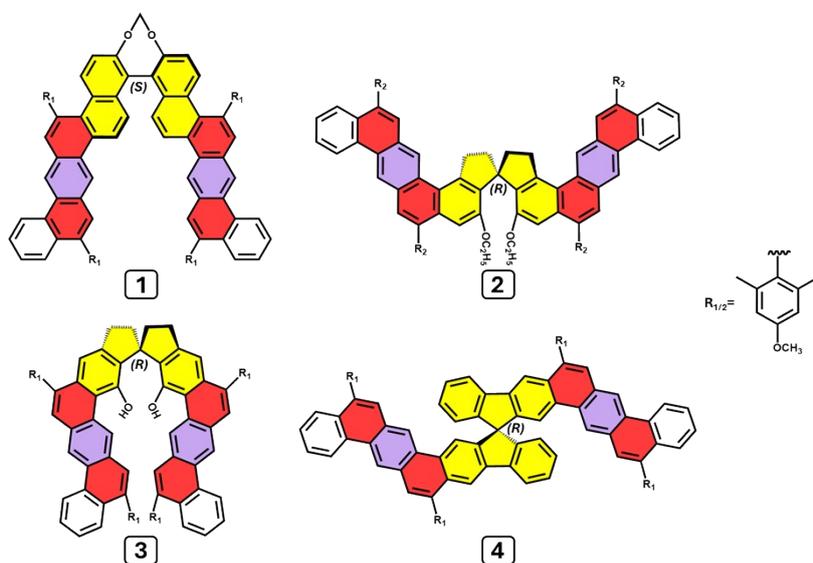


Fig. S2. Proposed truncated form of monomeric species.

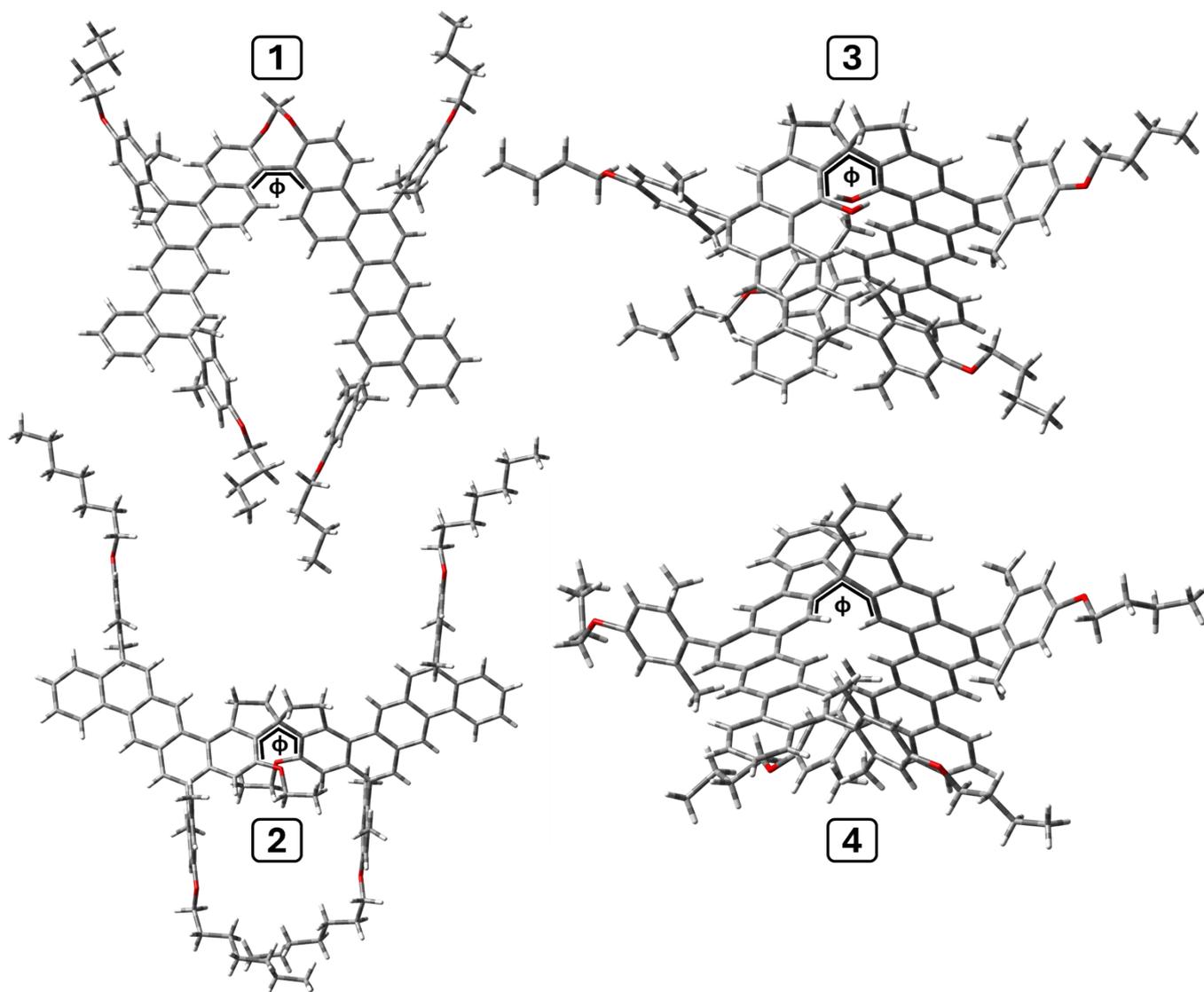


Fig. S3. Representations of dihedal angles (ϕ) involved in the chiral modules (2,2'-tethered binaphthyl for model 1, 1,1'-spirobiindane for models 2,3 and 9,9'-spirobifluorene for model 4).

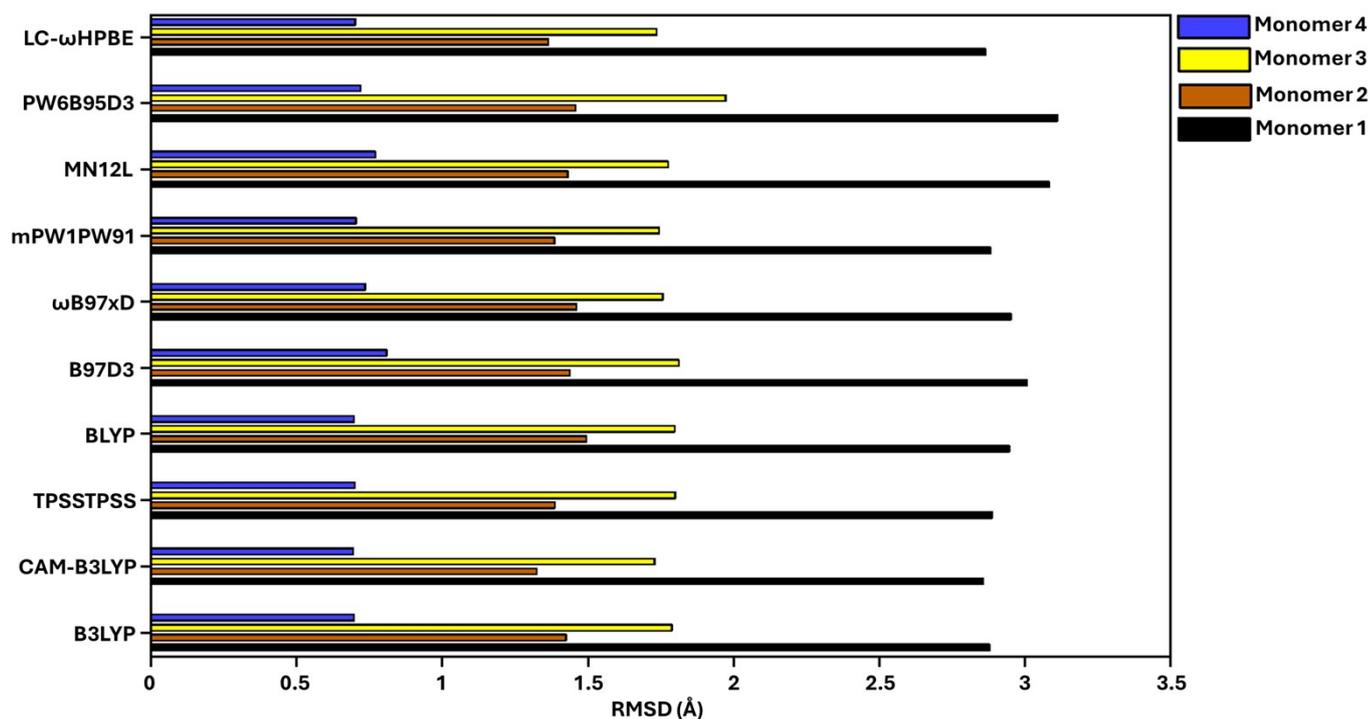


Fig. S4. Cumulative RMSD delta histograms (\AA) at the functional/6-311G(d,p) level in the gas phase for monomers 1,2,3 and 4.

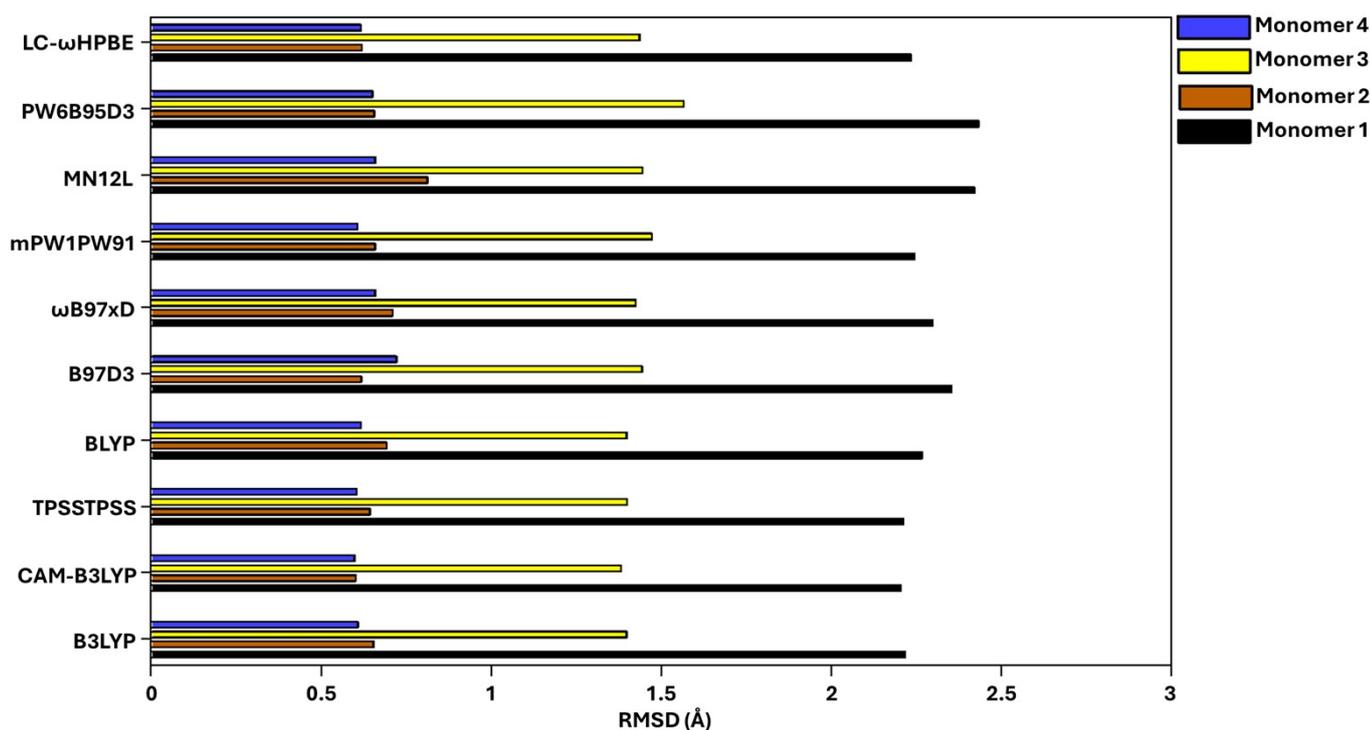


Fig. S5. Cumulative RMSD delta histograms (\AA) at the functional/6-311G(d,p) level in the gas phase of truncated forms for monomers 1,2,3 and 4.

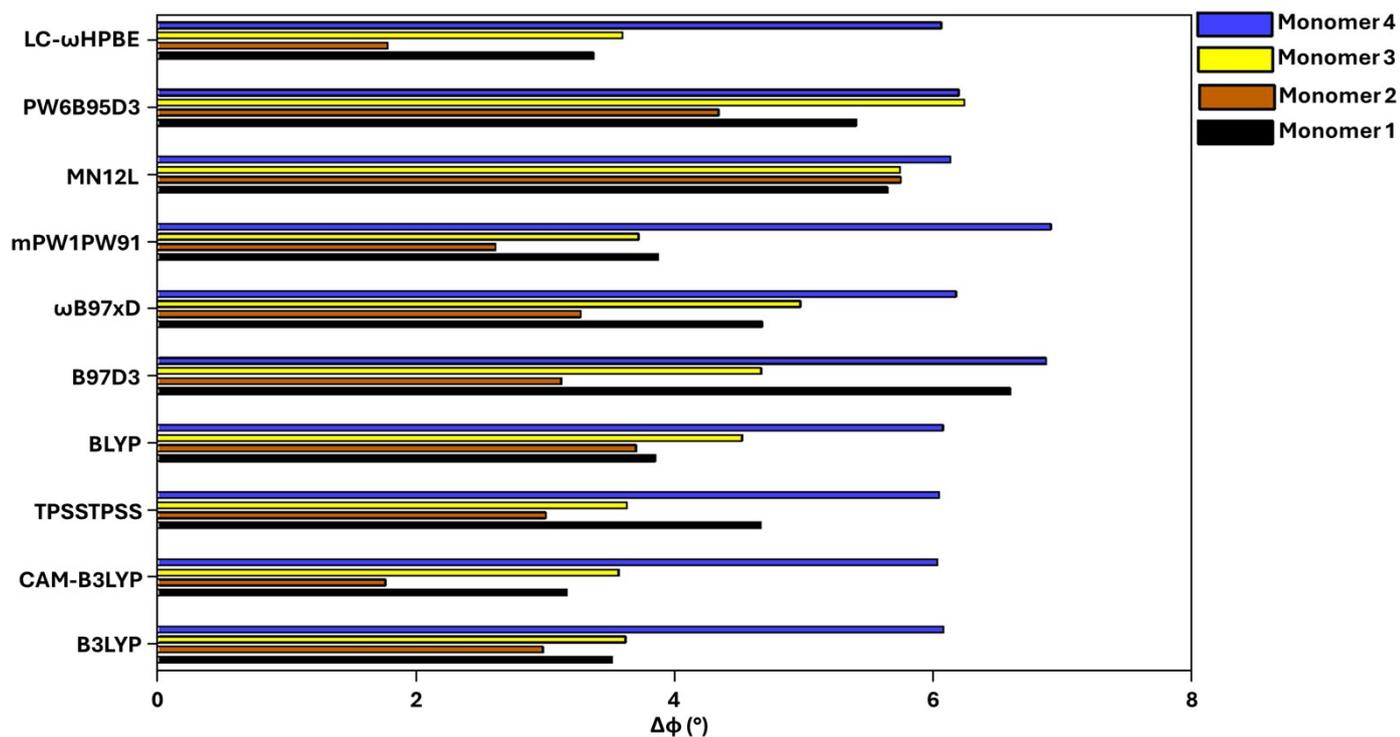


Fig. S6. Cumulative dihedral angle delta histograms ($^{\circ}$) at the functional/6-311G(d,p) level in the gas phase for monomers 1,2,3 and 4.

Table. S1. Average dihedral angles optimized at CAM-B3LYP/6-311G(d,p) level in gas phase for Pol1[1], Pol1[2], Pol1[3], Pol1[4] and Pol1[10]. Helical pitch measurements were contemplated as the spatial distance between the CH_2 groups (methylene dioxy spacers) in the periodic units.

Model	Pol1[1]	Pol1[2]	Pol1[3]	Pol1[4]	Pol1[10]
Dihedral angle $\langle\phi\rangle$	55.35	54.88	54.94	54.43	55.95
Helical pitch $\langle\Omega\rangle$				2.69	2.66

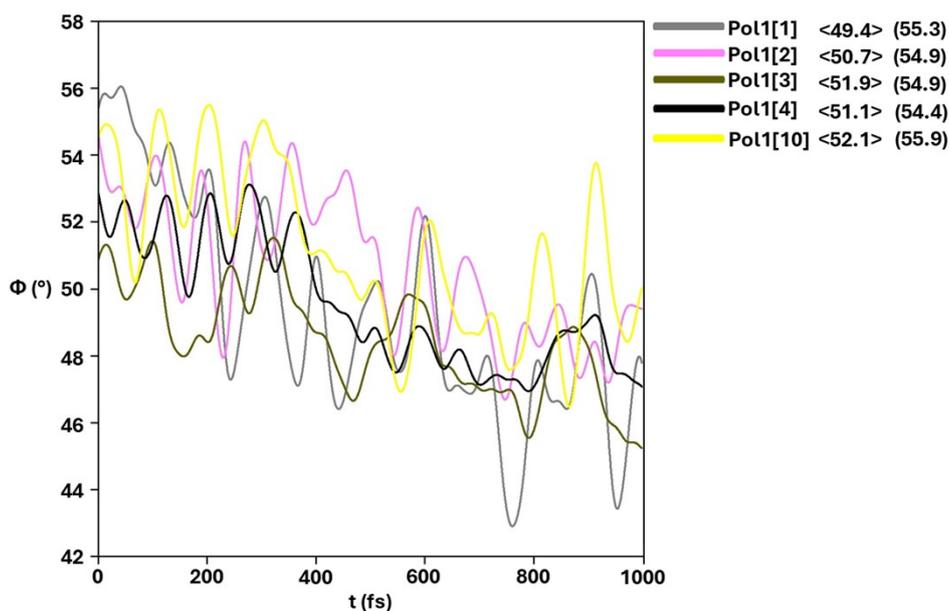


Fig. S7. Dihedral angle evolution plots of excited state trajectories (S1) computed at CAM-B3LYP/6-311G(d,p) level for Pol1[1], Pol1[2], Pol1[3], Pol1[4] and Pol1[10]. $\langle\rangle$ and $()$ refer to average values in S1 and S0, respectively.

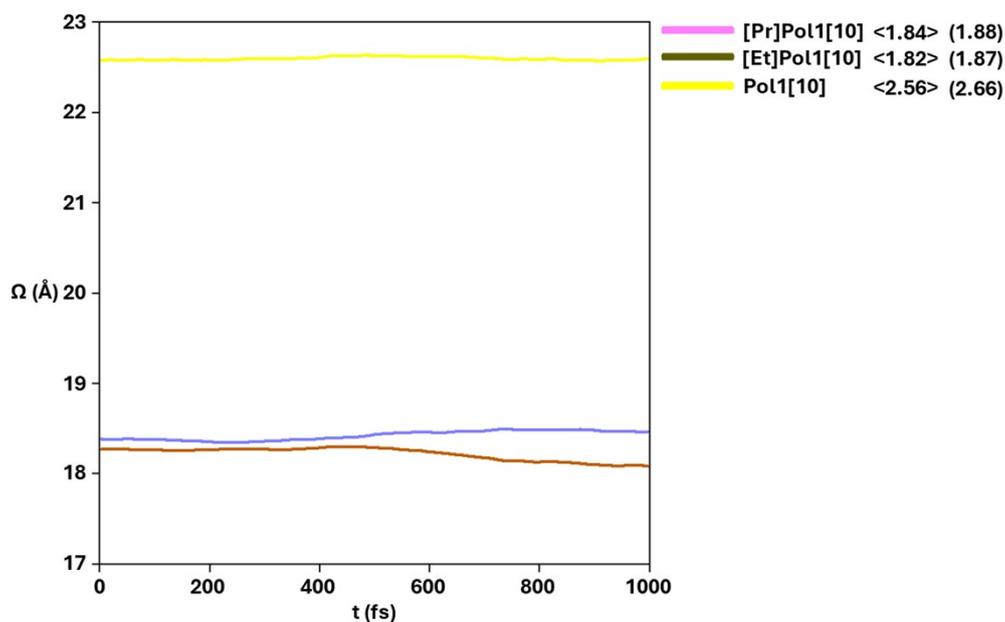


Fig. S8. Helical pitch evolution plots of excited state trajectories (S1) computed at CAM-B3LYP/6-311G(d,p) level for Pol1[10], [Et]Pol1[10] and [Pr]Pol1[10]. <> and () refer to average values in S1 and S0, respectively (reported in nm).

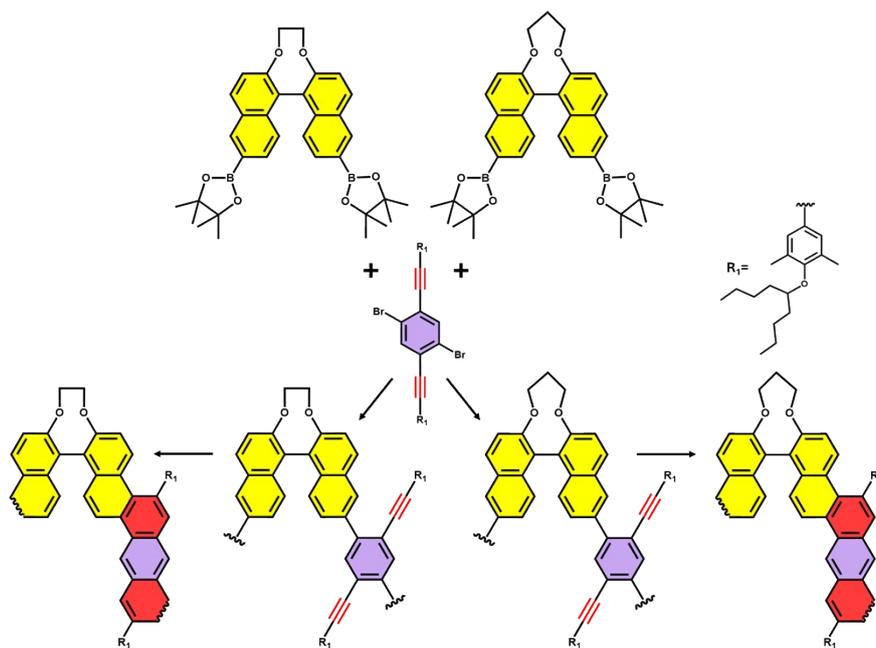


Fig. S9. Synthetic routes involving ethylenedioxy and propylenedioxy tethered binaphthyl scaffolds.

Table S2. Collection of dihedral angles and helical pitches for Pol1[1], Pol1[10], [Et]Pol1[1], [Et]Pol1[10], [Pr]Pol1[1], [Pr]Pol1[10] in S0 and S1 at CAM-B3LYP/6-311G(d,p) level. <> refers to average values during S1 dynamics. Obviously, helical pitches for monomeric species are not present.

Model	Pol1[1]	Pol1[10]	[Et]Pol1[1]	[Et]Pol1[10]	[Pr]Pol1[1]	[Pr]Pol1[10]
Dihedral angle (S0)	55.35	55.95	65.81	65.70	65.77	75.40
Dihedral angle (S1) <>	49.40	52.10	61.04	65.40	61.00	75.01
Helical pitch (S0)		2.66		1.87		1.88
Helical pitch (S1) <>		2.56		1.82		1.84

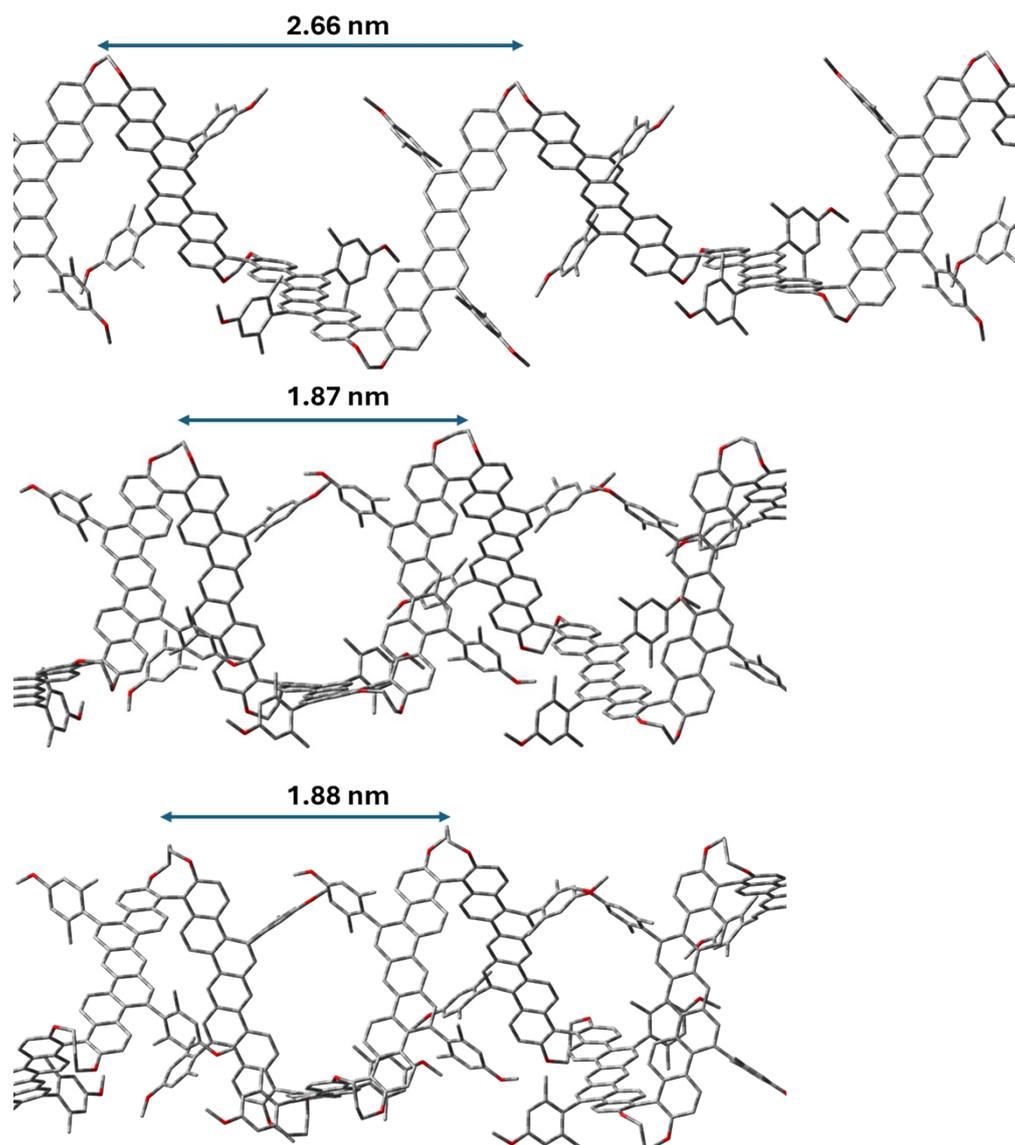


Fig. S10. Helical pitch measurement for the S0 minima (CAM-B3LYP/6-311G(d,p)) of Pol1[10], [Et]Pol1[10] and [Pr]Pol1[10].

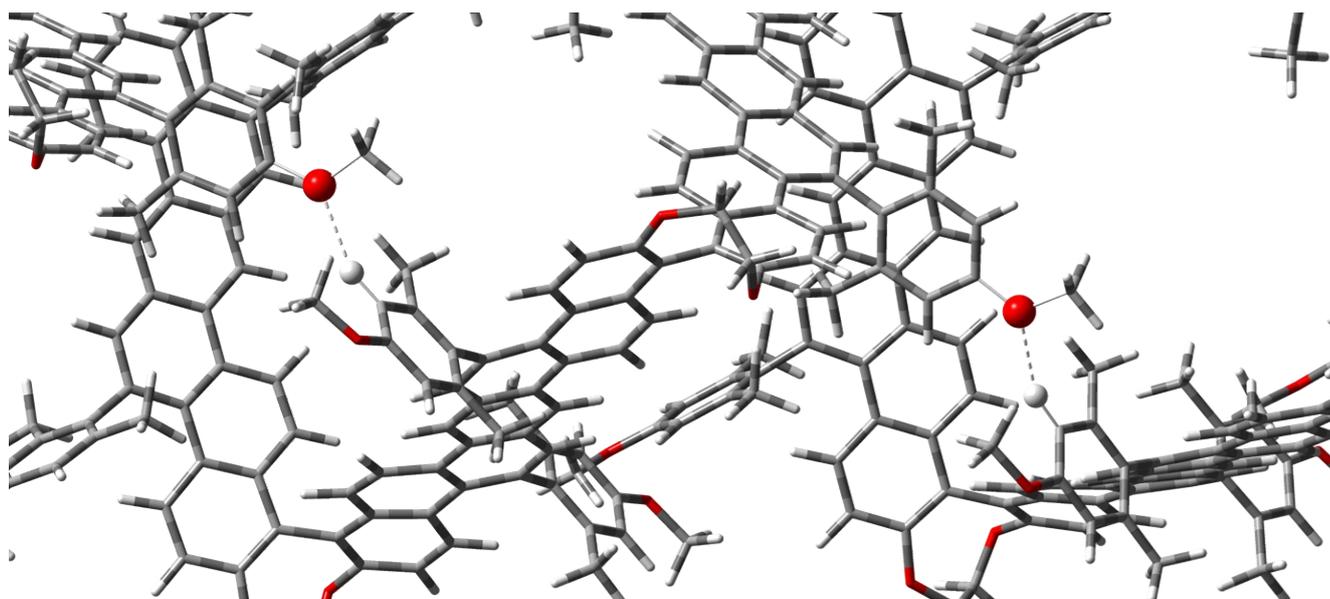


Fig. S11. Intramolecular hydrogen bonds involving the lateral alkoxy pendants. This situation is constantly maintained all along the repeating units both for [Et]Pol1[10] (as shown in the picture) and [Pr]Pol1[10].

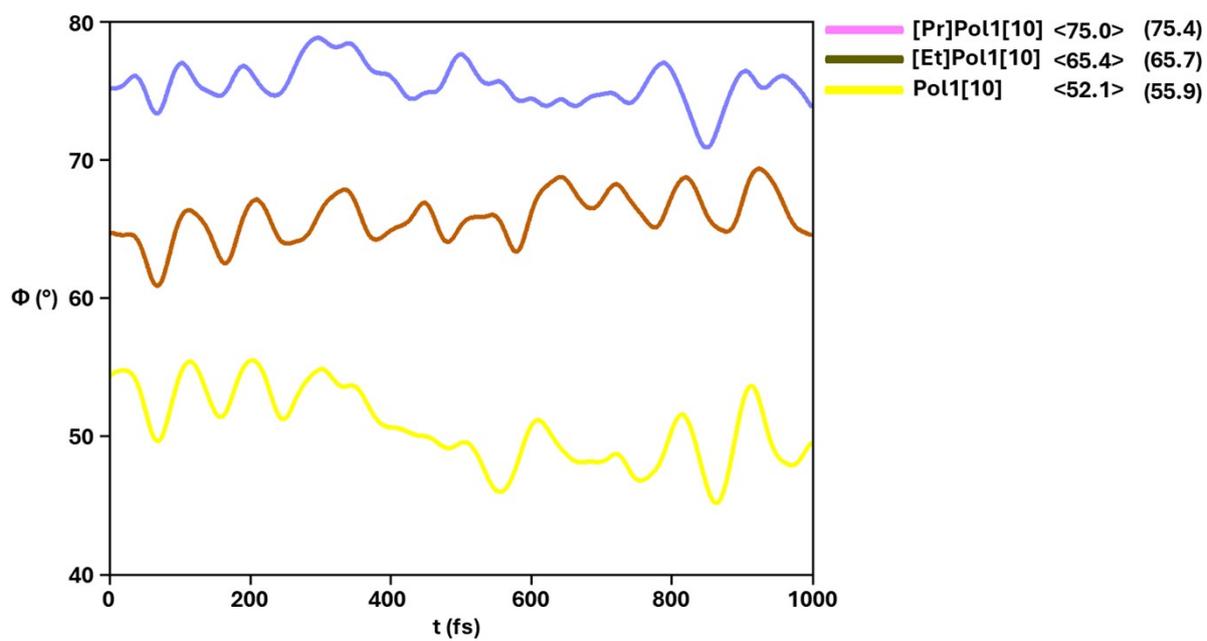


Fig. S12. Dihedral angle evolution plots of excited state trajectories (S1) computed at CAM-B3LYP/6-311G(d,p) level for Pol1[10], [Et]Pol1[10] and [Pr]Pol1[10]. < > and () refer to average values in S1 and S0, respectively.

Table S3. Computed rotational strengths (R length, expressed in cgs units) for (S)-Poll[1] by means the following functionals. (unchanged situation for (R) enantiomer)

R (length)				
B97D3	HCTH	M11L	PBEPBE	TPSSTPSS
-0.0481	-0.0059	0.1261	-0.0384	-0.0451
-1.5849	-1.5912	-1.8092	-1.4697	-1.3662
-1.4160	-0.7442	-1.9251	-0.6415	-1.8324
-1.7636	-1.9227	-2.5153	-1.4167	-1.8298
-1.0695	-1.3396	-2.1974	-1.1020	-1.0775
-3.1923	-3.3180	-4.0873	-2.7333	-3.6062
-1.4018	-1.8668	-5.5826	-2.3176	-1.4536
-1.2279	-1.7310	-2.7049	-1.2408	-1.3788
-3.2182	-3.5943	-3.1842	-2.5463	-2.8834
-1.8509	-1.8739	-0.3426	-2.1565	-1.7902
-1.8609	-1.6420	-4.2938	-1.4984	-2.0898
-1.7348	-1.8060	-2.1739	-1.6230	-1.7970
-3.2775	-2.9722	-4.1375	-2.4264	-3.0482
-0.6955	-0.9912	-0.6910	-0.6590	-0.7643
-3.3890	-4.1580	-5.5225	-3.3203	-3.7623
-1.0603	-1.2111	-2.2377	-1.0209	-1.0889
-3.4612	-3.5852	-4.8277	-3.0150	-3.4399
-4.7042	-4.6371	-6.0931	-3.9897	-4.7318
-3.3925	-3.7625	-4.4391	-3.2289	-3.6212
-2.3256	-2.6653	-2.8770	-2.5123	-2.4007
-0.7547	-0.8070	-1.0155	-0.2590	-0.5841
-1.3763	-1.3761	-1.8511	-1.2025	-1.3673
-2.0958	-2.0278	-2.6838	-1.8527	-2.0624
-1.8603	-1.9289	-2.5817	-1.4348	-1.9050
-0.2024	-0.4925	-0.4811	0.1822	-0.1534
-0.6782	-1.0208	-1.5058	-0.2134	-0.6307

Table S4. Computed rotational strengths (R length, expressed in cgs units) for (S/M) forms of Poll[1], Poll[2], Poll[3], Poll[4] and Poll[10] by means APFD and O3LYP functionals. <> refer to average values. (approximately specular R length values for (R) enantiomers)

R length									
Poll[1]		Poll[2]		Poll[3]		Poll[4]		Poll[10]	
O3LYP	APFD	O3LYP	APFD	O3LYP	APFD	O3LYP	APFD	O3LYP	APFD
-0.9715	-69.9454	-115.6053	-361.8523	-15.3955	-830.8016	-52.9215	-1758.1034	-270.1445	-4517.0103
-46.1853	-214.3646	-53.6649	-124.4385	-1.5107	-230.9479	-1.5359	-295.9896	-10.8815	-660.1753
-66.0271	-207.0947	-86.5274	-101.5480	-1.6031	-203.1128	-5.3896	-387.5100	-134.579	-790.5642
-76.5703	-175.6733	-69.3052	-167.9111	-154.0206	-279.0279	-159.2768	-499.1338	-244.8428	-597.9958
-65.7676	-159.4823	-35.3544	-34.2734	-189.1144	-277.7161	-197.8030	-248.2007	-297.0714	-471.9713
-54.1896	-98.6333	-64.3246	-73.2159	-156.6734	-218.4772	-191.6797	-232.6465	-284.2518	-860.1406
-9.7967	-71.2527	-19.4422	-335.9054	-142.5950	-208.1416	-245.0784	-328.9371	-127.3732	-834.7380
-37.1941	-83.1781	-40.9706	-257.4247	-58.7293	-218.7280	-187.5929	-404.5172	-287.1307	-407.7287
-75.2803	-164.4008	-8.1640	-109.5628	-121.4382	-201.8259	-194.2301	-239.6191	-30.1632	-585.8230
-133.6420	-249.9126	-2.9854	-171.0352	-143.2457	-202.2982	-174.7363	-214.7405	-290.6368	-878.2326
-70.4739	-214.7494	-33.0010	-142.9961	-4.48421	-303.9182	-25.9210	-540.4874	-240.1242	-681.8582
-0.0141	-14.7204	-20.5355	-188.3082	-154.8276	-191.5892	-211.0518	-363.6913	-206.9869	-481.1437
-45.2513	-156.9990	-5.7772	-170.4162	-7.7024	-402.2212	-196.8048	-293.7394	-109.9594	-520.4923
-5.8293	-50.2425	-35.8467	-32.6622	-158.5335	-268.9695	-148.1336	-210.2387	-370.4400	-589.1336
-6.3493	-61.9056	-15.1672	-190.9934	-167.0185	-250.3089	-189.8091	-254.3460	-100.0213	-1155.3771
-2.6288	-68.2125	-28.9333	-287.5694	-1.0807	-212.0311	-133.6119	-169.6583	-179.1443	-639.0760
1.0448	-91.4332	-19.6522	-181.5359	-144.0968	-199.0748	-125.2440	-153.5939	-201.6047	-361.1268
-9.6026	-72.2300	-41.5739	-271.5183	-158.1298	-203.3724	-116.3260	-134.5448	-10.2479	-571.5982
-6.8384	-85.2035	-106.0075	-129.9744	-0.5900	-190.2942	-103.9797	-252.6193	-18.4940	-642.1437
0.4383	-18.3865	-0.2684	-99.4128	-2.6293	-246.1223	-98.0722	-498.8580	-21.7579	-753.8646
-19.5925	-28.2445	-55.6833	-61.6185	-0.4216	-321.9008	-5.3471	-346.9751	-257.0245	-631.2261
-79.1940	-106.4759	-56.0355	-172.0734	-159.6536	-284.9633	-187.7703	-405.5549	-281.1825	-459.1142
-3.2346	-138.8583	-55.4363	-174.2680	-34.3835	-379.1635	-318.6160	-599.6179	-91.1872	-508.7868
-1.9304	-192.9242	-51.1824	-162.5506	-0.5682	-345.4528	-4.6960	-1096.0200	-146.6653	-977.7660
-2.2620	-125.7374	-43.0168	-156.0224	-10.5257	-251.9978	1.1815	-265.6806	-34.9423	-785.5094
-2.2153	-144.8776	-63.8672	-399.0879	-21.7090	-277.2367	-219.5188	-281.8876	-126.3113	-581.1991
<-31.5214>	<-117.8899>	<-43.3972>	<-175.3144>	<-77.3338>	<-276.9113>	<-134.3832>	<-402.9581>	<-168.1987>	<-805.5306 >

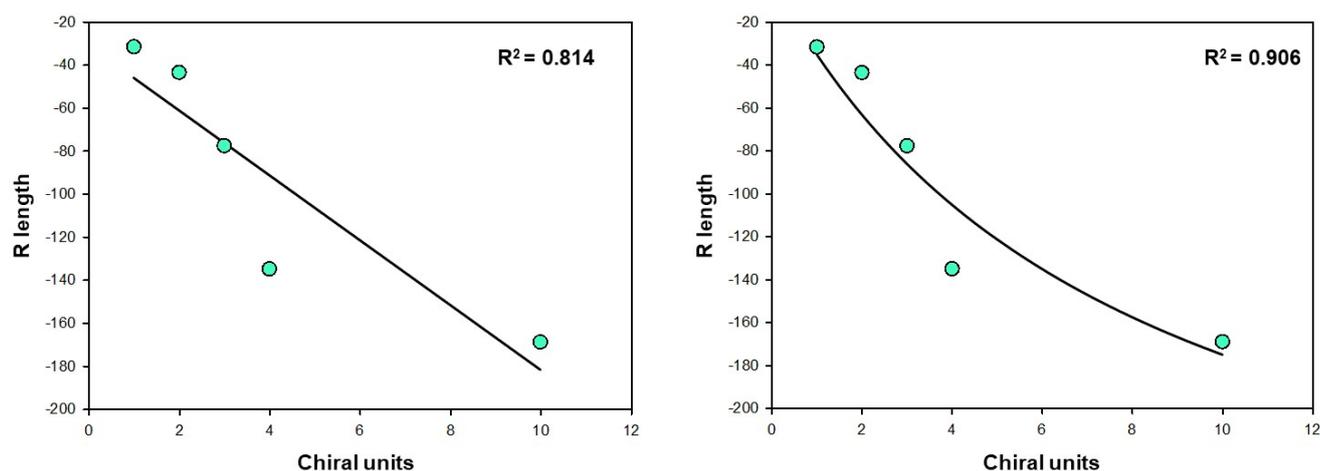


Fig. S13. (Left) Linear regression between computed (O3LYP) rotational strengths and the number of chiral units (binaphthyl scaffolds). (Right) Hyperbolic regression between computed (O3LYP) rotational strengths and the number of chiral units (binaphthyl scaffolds). Systems considered are the (*S/M*) forms of Pol1[1], Pol1[2], Pol1[3], Pol1[4] and Pol1[10]

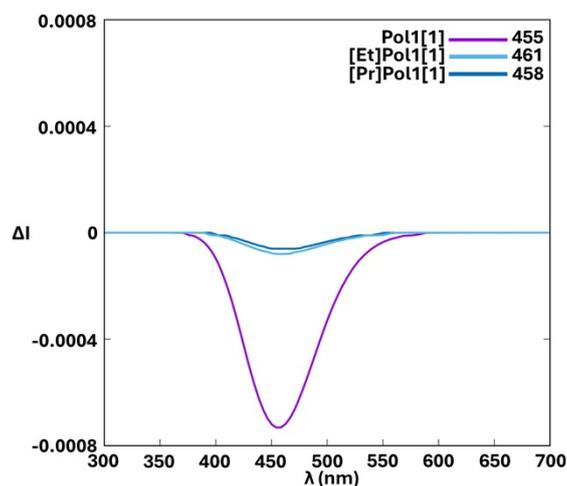


Fig. S14. Simulated (O3LYP/6-311G(d,p)) CPL spectra for (*S/M*) forms of Pol1[1], [Et]Pol1[1] and [Pr]Pol1[1].

Table S5. Computed rotational strengths (expressed in cgs units) for (*S/M*) forms of Pol1[1], [Et]Pol1[1], [Pr]Pol1[1], Pol1[10], [Et]Pol1[10] and [Pr]Pol1[10] at APFD/6-311G(d,p) level. <> refer to average values.

R length					
Pol1[1]	[Et]Pol1[1]	[Pr]Pol1[1]	Pol1[10]	[Et]Pol1[10]	[Pr]Pol1[10]
-69.9454	-14.8934	-13.6033	-4517.0103	-3340.6246	-1836.6984
-214.3646	-30.0709	-51.8807	-660.1753	-437.2798	-370.0416
-207.0947	-29.4506	-83.9970	-790.5642	-379.8986	-320.1353
-175.6733	-63.6351	-129.3183	-597.9958	-401.8004	-350.2473
-159.4823	-120.9391	-138.4588	-471.9713	-372.6240	-335.3830
-98.6333	-134.2321	-95.4411	-860.1406	-491.6072	-373.1225
-71.2527	-121.2779	-26.0672	-834.7380	-498.9465	-388.1040
-83.1781	-61.8930	-60.1061	-407.7287	-335.6832	-353.3525
-164.4008	-10.7745	-100.1603	-585.8230	-312.2827	-313.0389
-249.9126	-46.9503	-126.1060	-878.2326	-375.9853	-299.3374
-214.7494	-137.6916	-124.6628	-681.8582	-493.7224	-492.6168
-14.7204	-90.4012	-6.4895	-481.1437	-364.9502	-339.9428
-156.9990	-190.0928	-56.7789	-520.4923	-538.2057	-831.1611
-50.2425	-125.3833	-70.1272	-589.1336	-399.0494	-375.5731
-61.9056	-79.0331	-96.2097	-1155.3771	-324.2283	-298.8166
-68.2125	-83.2145	-78.8362	-639.0760	-400.6738	-281.6010
-91.4332	-102.5546	-36.3773	-361.1268	-288.9555	-310.0818
-72.2300	-86.3083	-79.8810	-571.5982	-439.6286	-447.2792
-85.2035	-164.7523	-107.4412	-642.1437	-312.5732	-331.3764

-18.3865	-85.8700	-37.8995	-753.8646	-285.1594	-281.4943
-28.2445	-39.9596	1.1563	-631.2261	-402.8081	-304.5786
-106.4759	-104.8503	-34.1805	-459.1142	-518.4202	-460.6774
-138.8583	-11.8280	-54.6477	-508.7868	-398.6807	-418.4251
-192.9242	-143.8893	-84.7556	-977.7660	-401.3683	-428.1784
-125.7374	-88.4569	-80.2009	-785.5094	-428.4817	-482.0547
-144.8776	24.7249	-54.5123	-581.1991	-465.4999	-458.4402
<-117.8899>	<-82.4491>	<-70.2685>	<-805.5306>	<-515.73606>	<-441.6060>

Table S6. Computed angles between electric (μ_E) and magnetic (μ_M) transition dipole moments (APFD/6-311G(d,p)) for (*S/M*) forms of Pol1[1], [Et]Pol1[1], [Pr]Pol1[1], Pol1[10], [Et]Pol1[10] and [Pr]Pol1[10]. < > refer to average values.

μ_E - μ_M angle (°)					
Pol1[1]	[Et]Pol1[1]	[Pr]Pol1[1]	Pol1[10]	[Et]Pol1[10]	[Pr]Pol1[10]
90.09	90.20	91.16	174.62	160.14	148.52
96.25	90.87	94.29	109.95	110.42	106.23
97.12	91.37	96.30	120.62	107.19	112.09
97.04	93.36	93.24	106.88	101.27	106.38
97.05	94.85	93.06	101.01	99.68	95.02
94.60	95.37	96.95	111.55	105.23	105.67
93.25	95.27	92.47	108.70	105.41	96.90
93.92	91.55	95.08	99.36	101.19	106.41
95.98	90.98	96.26	102.41	99.07	91.61
97.76	91.64	93.26	106.37	99.59	90.20
97.79	95.16	93.01	102.78	103.38	109.65
90.20	94.61	90.73	100.74	108.00	104.91
95.50	96.69	93.89	100.21	104.03	92.39
91.53	95.74	91.12	104.21	100.62	97.96
92.42	93.77	91.55	117.73	99.92	93.70
92.67	95.16	93.49	106.38	103.53	100.38
93.71	95.87	91.18	101.22	90.00	106.01
92.63	95.08	91.11	104.50	104.99	103.14
93.51	91.90	95.12	103.48	97.43	92.30
90.31	94.77	92.53	112.42	100.87	103.78
91.50	92.14	90.92	110.05	107.79	109.07
95.39	94.74	92.27	100.87	107.04	97.73
95.58	94.12	93.23	102.29	101.27	106.33
96.28	95.38	94.74	110.13	99.30	105.76
95.70	93.81	94.23	104.84	101.39	108.47
96.63	95.90	93.58	103.000	110.48	102.91
<94.39>	<93.85>	<93.26>	<108.70>	<104.97>	<103.59>

Eq. S1. (Rosenfeld equation)

Computationally, rotational strengths (R) can be defined as a product of wavefunction overlap integrals between the electric (μ_E) and magnetic (μ_M) transition dipole moments:

$$R = \text{Im} [\langle \psi_j | \mu_E | \psi_i \rangle \cdot \langle \psi_i | \mu_M | \psi_j \rangle]$$

where Im is an imaginary component of the scalar product between real vector μ_E and imaginary vector μ_M .

Such expression can be reformulated as follow:

$$R = |\mu| |m| \cos \theta$$

where θ is the angle between the two transition dipole moments.

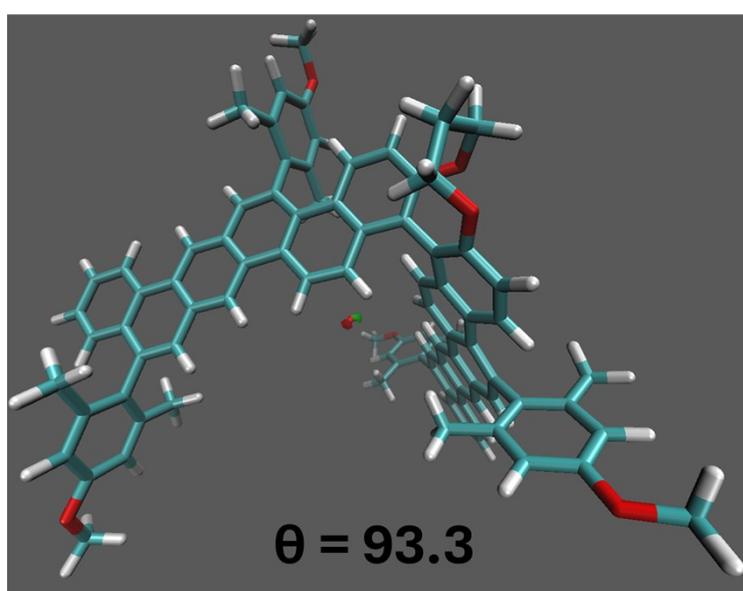
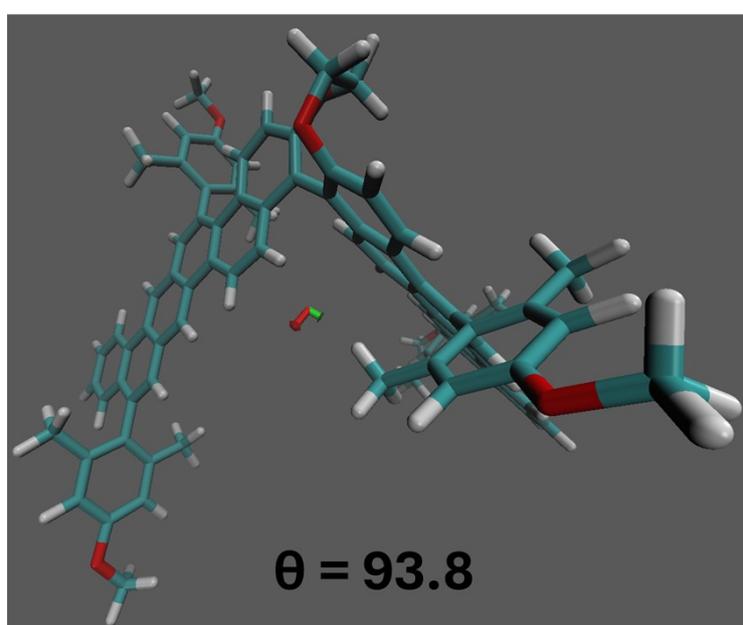
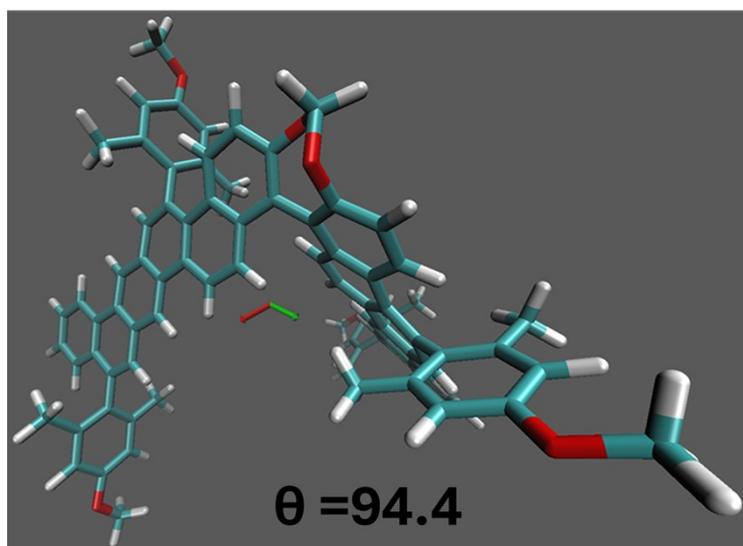


Fig. S15. Electric (green arrow) and magnetic (red arrow) transition dipole moments for (*S*) forms of Pol1[1] (top), [Et]Pol1[1] (middle) and [Pr]Pol1[1] (bottom). Both vector positions were mediated all along the S1 trajectories.

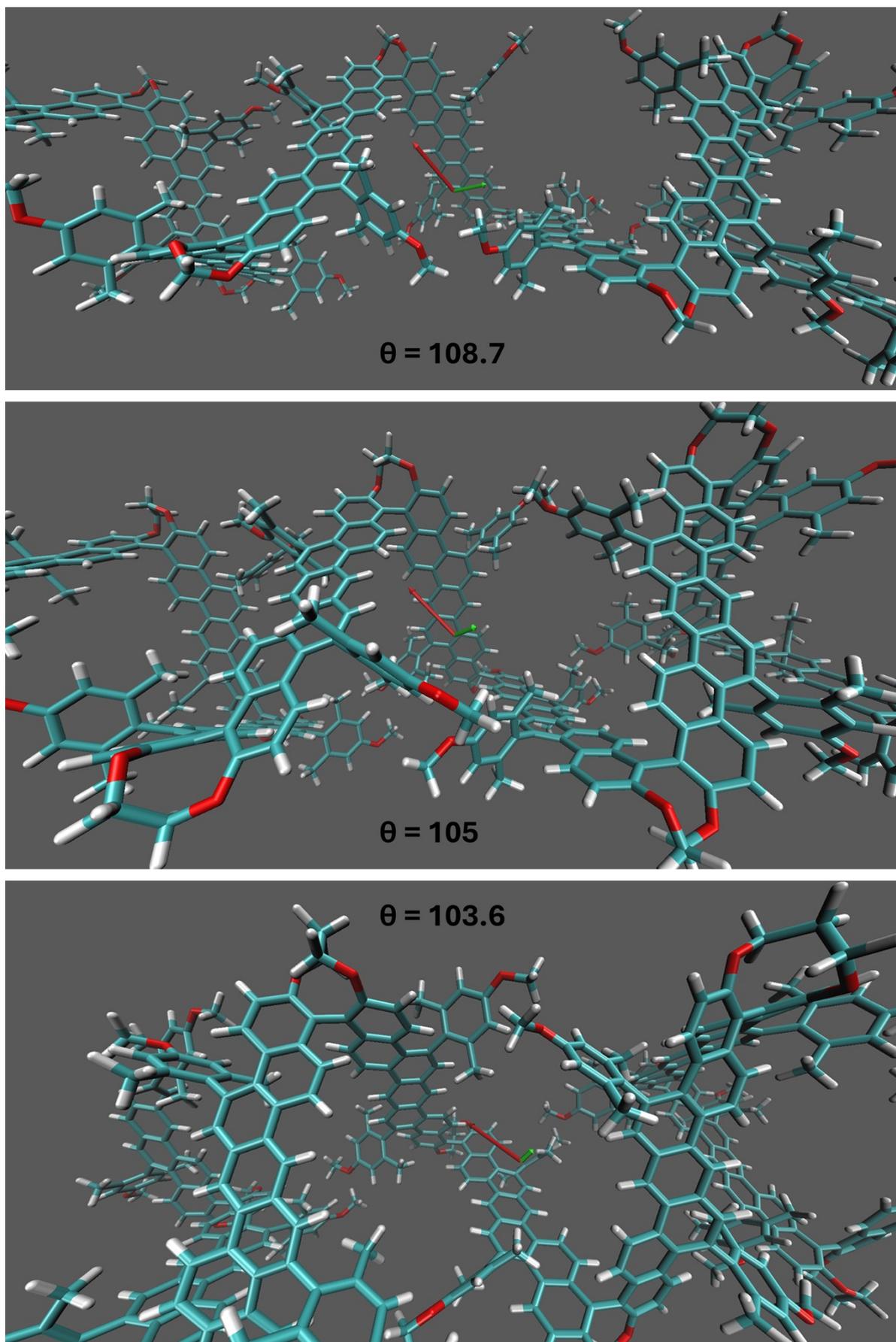


Fig. S16. Electric (green arrow) and magnetic (red arrow) transition dipole moments for (*S/M*) forms of Pol1[10] (top), [Et]Pol1[10] (middle) and [Pr]Pol1[10] (bottom). Both vector positions were mediated all along the S1 trajectories.

Table S7. Computed electric (μ_E) and magnetic (μ_M) transition dipole moments (μ_E expressed in 10^{-18} *esu*cm, μ_M expressed in 10^{-21} *erg/Gauss) for (S/M) forms of Pol1[1], [Et]Pol1[1], [Pr]Pol1[1], Pol1[10], [Et]Pol1[10] and [Pr]Pol1[10] at APFD/6-311G(d,p) level. <> refer to average values.

Pol1[1]		[Et]Pol1[1]		[Pr]Pol1[1]		Pol1[10]		[Et]Pol1[10]		[Pr]Pol1[10]	
< μ_E >	< μ_M >	< μ_E >	< μ_M >	< μ_E >	< μ_M >						
4.11	4.59	3.30	3.25	2.75	2.40	6.20	20.51	4.67	17.96	4.42	11.39

Table S8. Computed dihedral angle ϕ ($^\circ$) at CAM-B3LYP/6-311G(d,p) level for Pol2[1], Pol2[7], Pol3[1], Pol3[7], [para]Pol4[1], [para] Pol4[7], [meta]Pol4[1] and [meta]Pol4[7].

Dihedral angle < ϕ >								
Pol2[1]	Pol2[7]	Pol3[1]	Pol3[7]	[para]Pol4[1]	[para]Pol4[7]	[meta]Pol4[1]	[meta]Pol4[7]	Pol5[7]
42.174	42.507	44.259	46.916	57.890	57.836	58.207	61.979	44.565

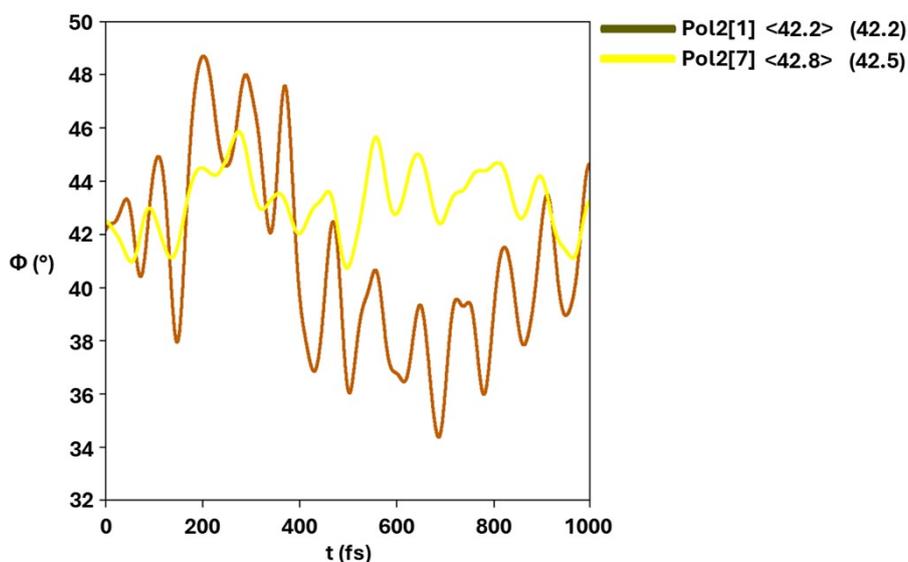


Fig. S17. Dihedral angle evolution plots of excited state trajectories (S1) computed at CAM-B3LYP/6-311G(d,p) level for Pol2[1] and Pol2[7]. <> and () refer to average values in S1 and S0, respectively.

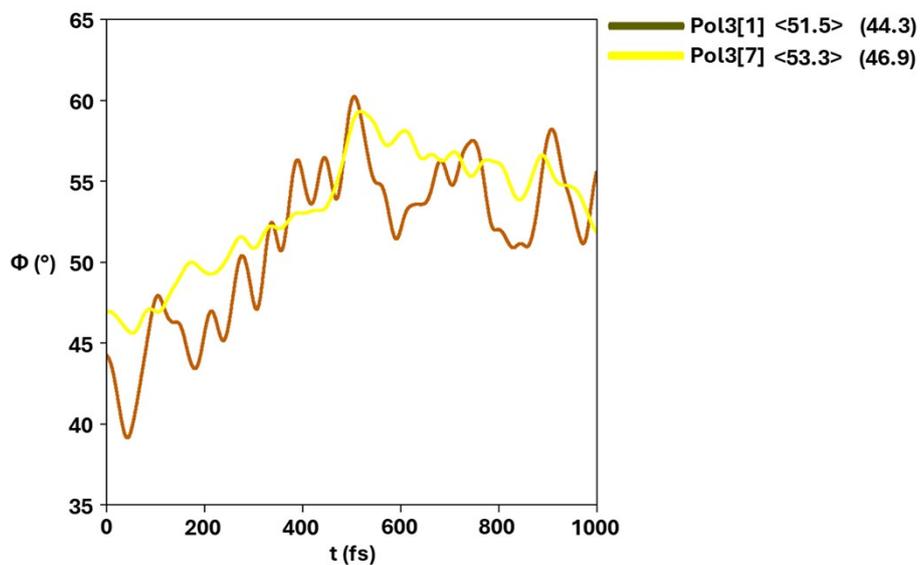


Fig. S18. Dihedral angle evolution plots of excited state trajectories (S1) computed at CAM-B3LYP/6-311G(d,p) level for Pol3[1] and Pol3[7]. <> and () refer to average values in S1 and S0, respectively.

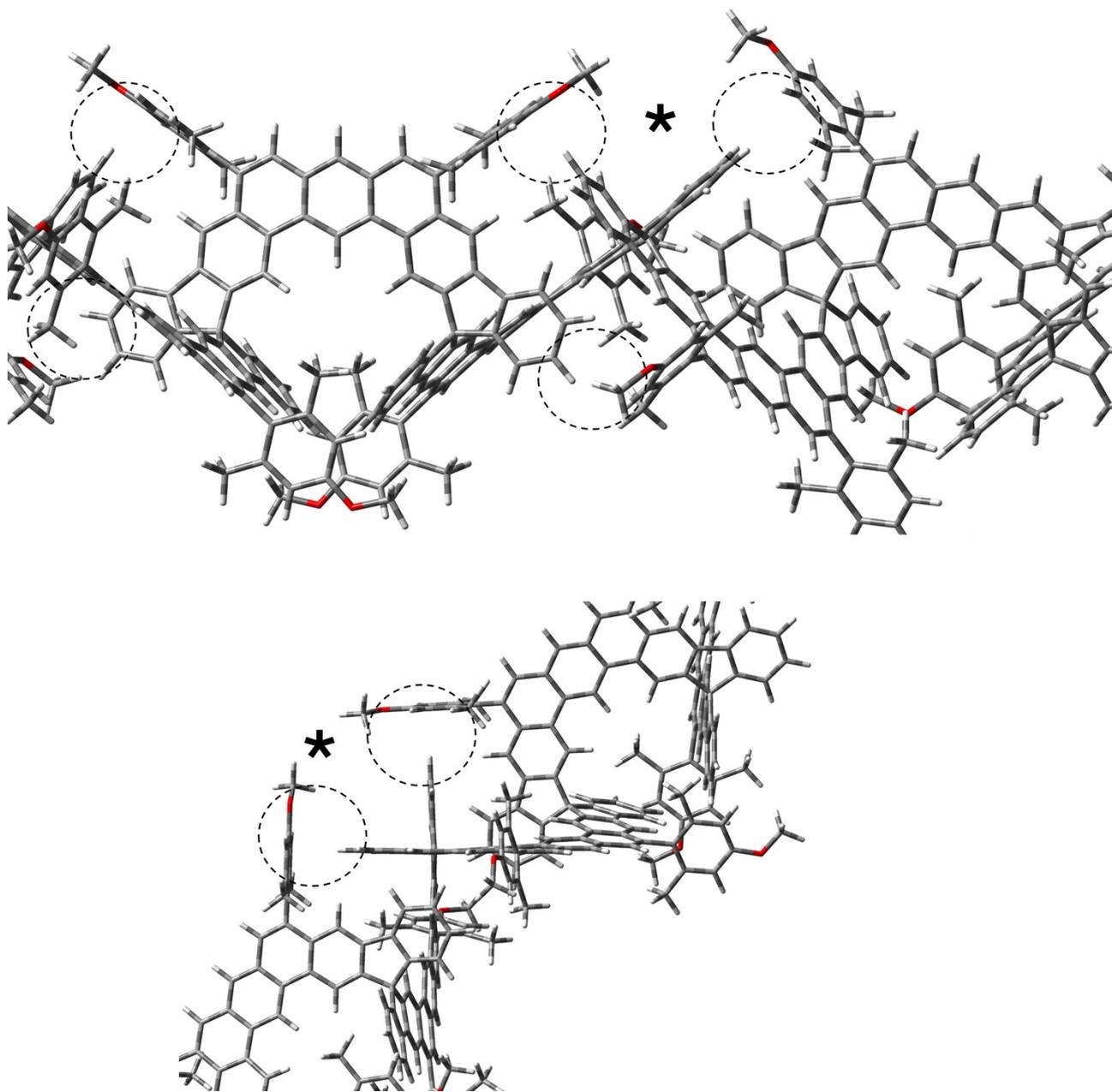


Fig. S19. Spirobifluorene/2,6-dimethyl-4-alkoxyphenyl steric hindrance in [meta]Po14[7]. * refers to a zoomed vision.

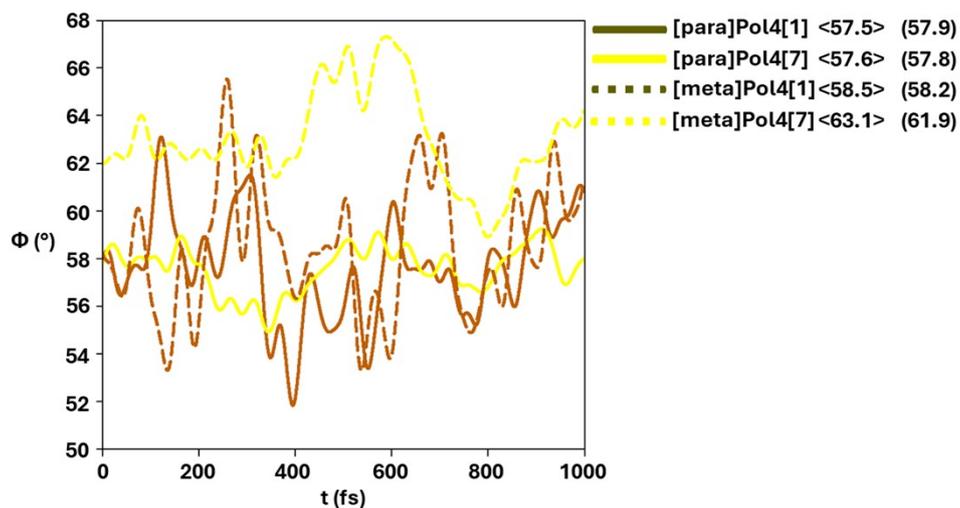


Fig. S20. Dihedral angle evolution plots of excited state trajectories (S1) computed at CAM-B3LYP/6-311G(d,p) level for [meta]Pol4[1], [meta]Pol4[7], [para]Pol4[1] and [para]Pol4[7]. <> and () refer to average values in S1 and S0, respectively.

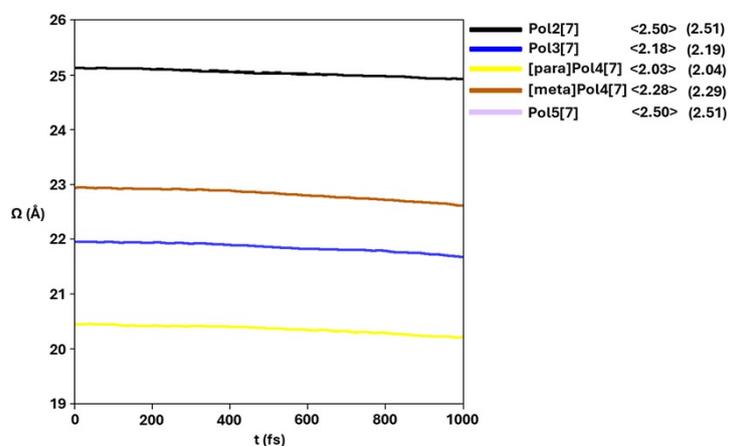


Fig. S21. Helical pitch evolution plots of excited state trajectories (S1) computed at CAM-B3LYP/6-311G(d,p) level for Pol2[7], Pol3[7], [para]Pol4[7], [meta]Pol4[7] and Pol5[7]. <> and () refer to average values in S1 and S0, respectively (reported in nm). It must be noted that Pol5[7] curve is completely covered by Pol2[7] one.

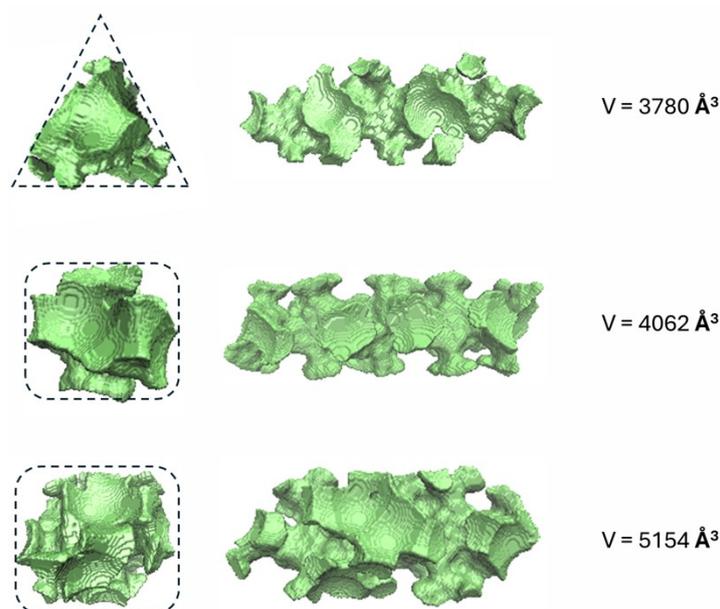


Fig S22. Calculated cavity volume (V_{occ}) for Pol1, Pol3 and [para]Pol4.

Table S9. Computed rotational strengths (R length, expressed in cgs units) for (*M*) forms of Pol2[7] and Pol3[7]. <> refer to average values.

R length			
APFD		O3LYP	
Pol2[7]	Pol3[7]	Pol2[7]	Pol3[7]
132.9630	2300.3640	2.1197	258.4935
20.6875	288.0321	0.1380	427.8997
7.0408	164.1297	1.5691	68.1286
18.3909	90.8031	14.8586	35.8707
37.4913	20.7921	24.3702	20.2745
60.7922	27.9805	23.5548	45.0654
65.2149	43.2823	41.0249	80.6516
50.9749	291.0870	24.2822	22.9659
4.4111	361.8345	13.9930	25.1596
11.6800	539.4311	18.8396	105.4907
31.1228	634.5935	12.8846	263.5463
83.3273	229.3186	12.3081	83.6646
10.3092	395.9009	20.2480	108.7786
15.4353	300.0251	6.0669	129.7563
28.5227	170.3141	5.6205	40.5722
61.0639	99.9838	21.7621	16.4982
76.3581	145.6820	58.4168	37.6992
78.9204	50.3579	29.9457	3.0172
140.2514	147.9751	8.2598	0.3659
108.7253	122.5157	39.8628	44.5759
58.6995	100.4377	13.2920	38.8922
23.6292	233.5421	12.3222	119.4294
87.0496	289.7582	4.7354	112.4519
171.3252	577.9852	19.3862	56.0196
203.3994	2300.3640	8.4707	59.9186
133.3260	288.0321	2.8560	119.8589
<66.1966>	<392.8662>	<16.9687>	<89.4248>
Pol3[7]/Pol2[7] 5.93		Pol3[7]/Pol2[7] 5.56	

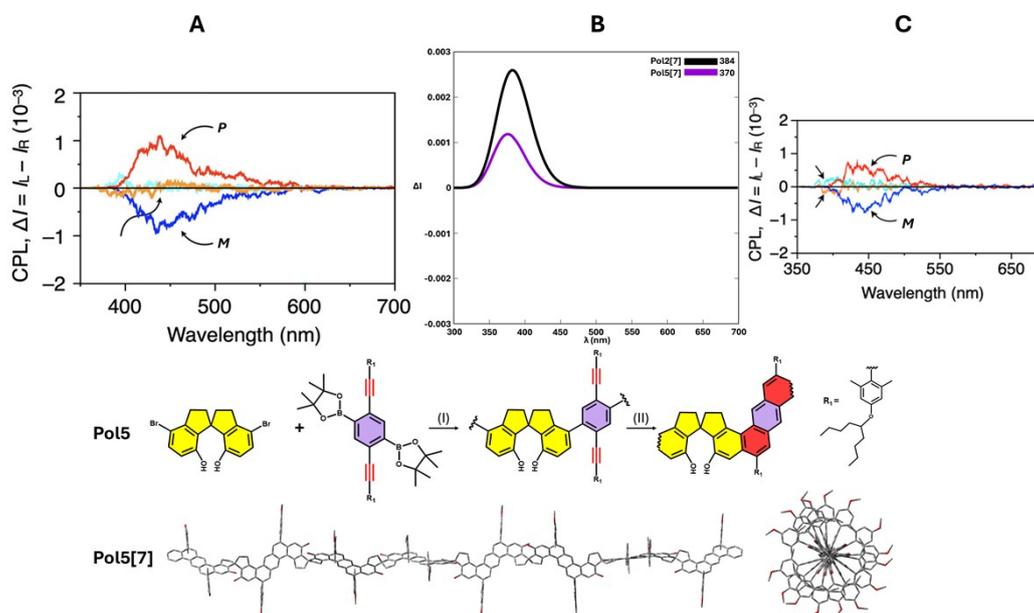


Fig S23. (A) Experimental CPL spectra of (*P*)/(*M*)-Pol2 in chloroform (quasi-silent non-specified signals refer to unzipped polymers) Adapted with permission from ref.¹ © 2024. (B) APFD TD-DFT predicted CPL spectra along the excited trajectories for (*P*)-Pol2[7] and (*P*)-Pol5[7] in chloroform. (C) Experimental CPL spectra of (*P*)/(*M*)-Pol5 in chloroform (quasi-silent non-specified signals refer to unzipped polymers) Adapted with permission from ref. 26 in the manuscript © 2023 Wiley-VCH Verlag GmbH & Co. KGaA.

Table S10. Computed rotational strengths (R length, expressed in cgs units) for (*P*) form of [meta]Pol4[7] and (*M*) form of [para]Pol4[7]. <> refer to average values.

R length			
APFD		O3LYP	
[meta]Pol4[7]	[para]Pol4[7]	[meta]Pol4[7]	[para]Pol4[7]
16.1607	-48.6115	1.3732	0.0505

72.7124	-10.6724	8.4445	0.0064
62.2489	-7.4605	29.2021	0.0051
20.3600	-12.7105	8.2476	0.0066
47.9208	-5.1374	17.6409	0.0034
38.6094	-3.3447	26.6182	0.0020
104.7958	-10.9567	94.4004	0.0008
43.7830	-16.2047	52.3651	0.0009
43.7642	-18.3420	25.4867	0.0011
80.6492	-19.7405	104.164	0.0045
92.8327	-23.6181	96.5685	0.0064
40.3191	-7.4406	17.9834	0.0034
78.3759	-0.0352	48.5891	0.0044
134.3308	-27.2219	153.778	0.0120
62.9978	-22.6861	81.5519	0.0053
53.1502	-20.9839	46.3056	0.0010
101.7518	-14.1569	101.170	0.0004
44.7763	-0.0200	50.1471	0.0015
46.7717	-3.1129	10.8519	0.0003
46.9716	-1.2032	12.9169	0.0015
27.7512	-23.2077	29.8347	0.0003
76.9486	-13.4547	83.3061	0.0011
70.5768	-12.2793	70.7827	0.0007
85.8474	-0.0006	80.0495	0.0005
70.5887	-6.3095	17.5640	0.0011
53.8940	-8.3969	3.7412	0.0048
<62.2649>	<-12.9734>	<48.9647>	<0.0048>

Table S11. Computed electric (μ_E), magnetic (μ_M) transition dipole moments (μ_E expressed in 10^{-18} *esu*cm, μ_M expressed in 10^{-21} *erg/Gauss) and their angle for (*P*) form of [meta]Pol4[7] and (*M*) form of [para]Pol4[7]. < > refer to average values.

Transition dipole moments	[meta]Pol4[7]		[para]Pol4[7]	
	APFD	O3LYP	APFD	O3LYP
< μ_E >	0.71	0.52	0.40	0.00
< μ_M >	0.72	0.64	1.38	1.6e-4
< θ >	68.30	66.56	95.17	90.00

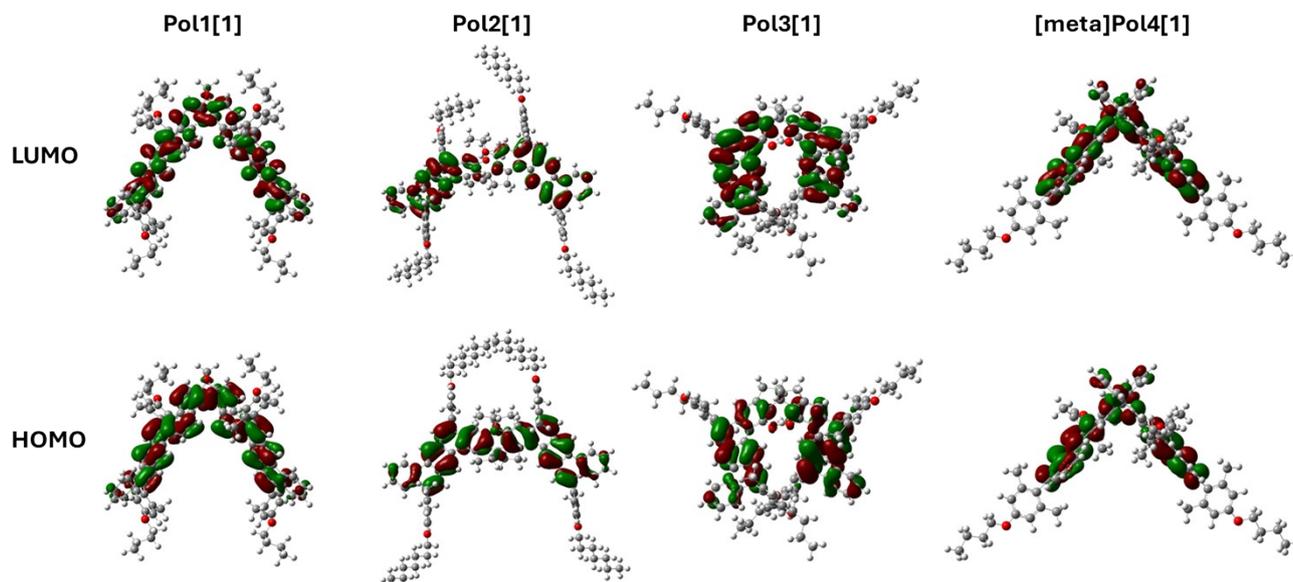


Fig S24. Computed (APFD/6-311G(d,p)) HOMO and LUMO orbitals for Pol1[1], Pol2[1], Pol3[1] and [meta]Pol4[1]. It must be noted that [para]Pol4[1] and Pol5[1] were not reported because are identical to [meta]Pol4[1] and Pol2[1], respectively.

Table S12. Calculated (O3LYP/6-311G(d,p)) and experimental g_{lum} values. Computed dissymmetry factors were approximated by $4(|\langle \mu_M \rangle| / |\langle \mu_E \rangle|) \cdot \cos \theta_{EM}$.

Calc	Exp ²	Calc	Exp ³	Calc	Exp ⁴	Calc	Exp ⁵	Calc	Exp ¹
Pol1[10]	Pol1	Pol2[7]	Pol2	Pol3[7]	Pol3	Pol4[7]	Pol4	Pol5[7]	Pol5
-2.5*10 ⁻³	-2.6*10 ⁻³	5.7*10 ⁻⁴	~5*10 ⁻⁴	2.1*10 ⁻³	~1*10 ⁻³	1.6*10 ⁻³	2.4*10 ⁻³	8.1*10 ⁻⁴	~5*10 ⁻⁴
(M)		(P)		(P)		(P)Meta		(P)	

References:

1. W. Zheng, T. Ikai and E. Yashima, *Angew. Chem. Int. Ed.*, 2021, **60**, 11294-11299.
2. T. Ikai, N. Mishima, T. Matsumoto, S. Miyoshi, K. Oki and E. Yashima, 2,2'-Tethered Binaphthyl-Embedded One-Handed Helical Ladder Polymers: Impact of the Tether Length on Helical Geometry and Chiroptical Property, *Angew. Chem. Int. Ed.*, 2024, **63**, e202318712.
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Cartesian coordinates (CAM-B3LYP/6-311G(d,p))

Monomer 1(S)

	X	Y	Z
O	-5.4410940	-5.3859770	7.0234260
C	-4.8855180	-3.2735890	3.4975650
C	-4.0761930	-3.0497140	4.6250120
C	-4.2989170	-3.7804500	5.7784150
H	-3.6881700	-3.6261750	6.6594860
C	-5.3155180	-4.7288750	5.8421180
C	-6.1216940	-4.9427440	4.7331590
H	-6.9183510	-5.6731910	4.7586570
C	-5.9150620	-4.2145460	3.5607080
C	-2.9650360	-2.0348970	4.5900070
H	-2.1936170	-2.3203900	3.8708120
H	-2.4957040	-1.9405400	5.5692090
H	-3.3350820	-1.0527910	4.2889190
C	-6.7944470	-4.4867380	2.3669530
H	-7.4656550	-3.6494240	2.1636180
H	-7.4050720	-5.3754320	2.5294710
H	-6.2014150	-4.6402790	1.4627590
C	-6.4596960	-6.3651620	7.1633460
H	-6.3248920	-7.1522670	6.4107820
H	-7.4409700	-5.9041240	7.0034480

C	-6.3603590	-6.9417530	8.5601860
H	-7.2096230	-7.6175850	8.7089460
H	-6.4758920	-6.1259770	9.2806920
C	-5.0536710	-7.6843780	8.8230490
H	-4.9566610	-8.5045270	8.1029100
H	-4.2186370	-7.0065220	8.6327530
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H	-5.0271010	-7.4311720	10.9799040
H	-4.0236720	-8.7631400	10.4058640
H	-5.7790780	-8.9356910	10.4476100
O	0.0049910	-6.9276810	1.1744320
O	-5.7341390	7.0336850	-6.4391870
C	-0.0000450	-7.7017620	0.0000040
C	-0.8748810	-5.8693360	1.1847390
C	-1.9976510	-5.9351320	2.0104920
H	-2.1537180	-6.8246800	2.6075830
C	-2.8716310	-4.8843440	2.0689890
H	-3.7195580	-4.9722220	2.7233370
C	-2.7036060	-3.7283630	1.2698810
C	-3.6419870	-2.6100910	1.2731500
C	-4.6962890	-2.4391210	2.2657250
C	-5.5638250	-1.4012880	2.1520220
H	-6.3281720	-1.2809030	2.9122890
C	-5.5127110	-0.4405830	1.1046840
C	-6.4516400	0.5896030	1.0251810
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C	-6.4115630	1.5456900	0.0229170
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H	-4.5456260	7.3416260	-4.0133880
C	-5.7959930	6.2159300	-5.3567670
C	-6.5700100	5.0690820	-5.5050020
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C	-6.7043950	4.1620700	-4.4682800
C	-4.5631260	5.8408600	-1.7974350
H	-5.2545150	5.8213910	-0.9522840
H	-4.0850790	6.8204750	-1.8229840
H	-3.7934400	5.0931790	-1.5939300
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H	-8.0291710	2.9376770	-5.6388370
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H	-5.9497900	10.9829270	-9.4045900
H	-7.6153350	10.4251930	-9.5714740
H	-6.2882890	9.4320920	-10.174340
O	5.4410000	-5.3860440	-7.0234360
C	4.8854640	-3.2736500	-3.4975720
C	4.0761630	-3.0497370	-4.6250290
C	4.2988720	-3.7804760	-5.7784330
H	3.6881450	-3.6261710	-6.6595110
C	5.3154350	-4.7289420	-5.8421270
C	6.1215880	-4.9428500	-4.7331580
H	6.9182140	-5.6733310	-4.7586490
C	5.9149700	-4.2146490	-3.5607060
C	2.9650490	-2.0348720	-4.5900360
H	2.1936070	-2.3203350	-3.8708540
H	2.4957360	-1.9404900	-5.5692440
H	3.3351330	-1.0527830	-4.2889370
C	6.7943270	-4.4868860	-2.3669400
H	7.4655680	-3.6496020	-2.1635910
H	7.4049140	-5.3756050	-2.5294540
H	6.2012750	-4.6404060	-1.4627560
C	6.4595660	-6.3652670	-7.1633490
H	6.3247230	-7.1523700	-6.4107900
H	7.4408560	-5.9042680	-7.0034370
C	6.3602240	-6.9418490	-8.5601920
H	7.2094650	-7.6177110	-8.7089450
H	6.4757960	-6.1260730	-9.2806930
C	5.0535120	-7.6844230	-8.8230730
H	4.9564620	-8.5045720	-8.1029400
H	4.2185000	-7.0065380	-8.6327840
C	4.9649110	-8.2351350	-10.241776
H	5.0269750	-7.4312060	-10.979927
H	4.0234900	-8.7631400	-10.405905
H	5.7788900	-8.9357550	-10.447632
O	-0.0050760	-6.9276850	-1.1744260

O	5.7342510	7.0335970	6.4391950
C	0.8748070	-5.8693490	-1.1847370
C	1.9975780	-5.9351600	-2.0104880
H	2.1536370	-6.8247130	-2.6075750
C	2.8715690	-4.8843820	-2.0689870
H	3.7194980	-4.9722710	-2.7233310
C	2.7035540	-3.7283960	-1.2698850
C	3.6419470	-2.6101350	-1.2731560
C	4.6962520	-2.4391810	-2.2657300
C	5.5638060	-1.4013630	-2.1520250
H	6.3281550	-1.2809900	-2.9122900
C	5.5127070	-0.4406590	-1.1046850
C	6.4516540	0.5895100	-1.0251790
H	7.2241830	0.6171610	-1.7825810
C	6.4115910	1.5455970	-0.0229140
C	7.3759540	2.6356560	0.0955340
C	8.4312200	2.8015880	-0.8165750
H	8.5457860	2.1080210	-1.6384470
C	9.3330960	3.8328050	-0.6938050
H	10.1367410	3.9347790	-1.4131930
C	9.2117610	4.7453090	0.3560760
H	9.9204930	5.5585560	0.4559520
C	8.1881970	4.6073660	1.2634180
H	8.0876700	5.3111930	2.0798160
C	7.2551070	3.5606810	1.1570600
C	6.1767300	3.4272240	2.1243020
C	5.2936930	2.4156270	1.9982160
H	4.4893590	2.3165150	2.7195860
C	5.3684060	1.4477000	0.9384220
C	4.4313600	0.4251350	0.8535470
H	3.6649510	0.3987180	1.6155660
C	4.4694340	-0.5392000	-0.1546820
C	3.5154850	-1.6284620	-0.2739830
C	2.4252800	-1.6990630	0.6384270
H	2.3273710	-0.9477630	1.4077020
C	1.4852640	-2.6645850	0.5659200
H	0.6662780	-2.6711020	1.2705900

C	1.5839860	-3.7101590	-0.3923380
C	0.6194410	-4.7594680	-0.4119830
C	6.0482080	4.4028620	3.2491190
C	5.2741880	5.5544040	3.0950350
C	5.1507950	6.4564420	4.1521190
H	4.5457480	7.3415620	4.0133940
C	5.7960930	6.2158410	5.3567740
C	6.5700890	5.0689800	5.5050090
H	7.0641560	4.9045950	6.4547450
C	6.7044600	4.1619670	4.4682860
C	4.5632260	5.8407980	1.7974390
H	5.2546160	5.8213130	0.9522890
H	4.0852000	6.8204240	1.8229870
H	3.7935240	5.0931330	1.5939350
C	7.5496400	2.9300630	4.6599980
H	6.9486980	2.0215650	4.5814010
H	8.0292100	2.9375480	5.6388450
H	8.3292170	2.8607070	3.8980480
C	4.9602890	8.2213070	6.3630010
H	3.9152260	7.9694370	6.1500140
H	5.3318710	8.8560210	5.5486840
C	5.0776400	8.9376630	7.6921650
H	4.3982550	9.7969090	7.6751960
H	4.7194580	8.2672970	8.4797520
C	6.4949920	9.4028800	8.0125610
H	7.1632180	8.5392540	7.9877480
H	6.8365660	10.0811240	7.2226370
C	6.5939330	10.0999290	9.3646850
H	7.6154970	10.4250690	9.5714900
H	6.2884320	9.4319900	10.1743530
H	5.9499620	10.9828310	9.4046030
H	-0.8988720	-8.3197980	-0.0676890
H	0.8987780	-8.3198040	0.0677000

Monomer 2(R)

	X	Y	Z
O	0.4545130	-2.6944300	1.6184970

O	-8.7061810	8.2704400	-1.7950700
O	-3.3774980	-7.7024850	5.7020620
C	-3.3994720	-1.0479690	1.4376560
C	-4.0309620	-4.2145040	3.5530180
C	-5.5108670	-2.4163270	2.7565040
H	-6.3328120	-2.9349780	3.2386940
C	-3.1728680	-2.2529820	2.1491340
C	-5.7893800	-1.1704990	2.1075300
C	-3.6694440	-4.1858480	4.9111050
C	-2.2921960	-0.5171270	0.7250680
C	-4.2685950	-2.9359010	2.8154300
C	-6.3520660	1.3260850	1.0078790
C	-1.0431930	-1.0986990	0.7880090
C	-7.4058600	0.5805760	1.5900580
C	-7.0818060	-0.6532560	2.1391350
H	-7.8396260	-1.2485810	2.6319940
C	-8.4282010	4.6817080	-1.4502780
C	-8.0827180	4.5386190	-0.0955980
C	-8.6261140	5.9478230	-1.9733820
H	-8.8914820	6.0837070	-3.0146770
C	-5.0604430	0.8032450	0.9642340
H	-4.3021130	1.4325710	0.5322460
C	-4.7344830	-0.4524650	1.4742070
C	-4.1739360	-5.4409630	2.9021220
C	-6.6254770	2.6284220	0.4679700
H	-5.7995260	3.1825160	0.0340820
C	-1.8865940	-2.8215100	2.2139100
H	-1.7598340	-3.7288140	2.7848390
C	0.0000310	-0.3344760	-0.0000470
C	-3.9605020	-6.6301650	3.6005220
H	-4.0780790	-7.5694310	3.0781160
C	-0.8206540	-2.2389320	1.5696390
C	-8.1513250	6.9404660	0.1616180
H	-8.0413200	7.8059930	0.8000290
C	-3.4610070	-5.3757470	5.5869160
H	-3.1846580	-5.3790150	6.6342420
C	-9.8477200	0.4589050	2.1433880

H	-9.7092440	-0.5294820	2.5602020
C	-8.7485210	1.1486290	1.6037650
C	-2.2265660	0.6865600	-0.1954710
H	-2.2440540	1.6158150	0.3844300
H	-3.0635640	0.7268350	-0.8931980
C	-8.9657460	2.4341570	1.0570890
C	-8.4893570	7.0804640	-1.1768330
C	-7.9483290	5.6726490	0.7074850
C	-11.3193850	2.2809680	1.6155870
H	-12.3112630	2.7167170	1.6212360
C	-3.6050240	-6.6001080	4.9413500
C	-7.8582730	3.1781050	0.4810730
C	-11.1080060	1.0085060	2.1521400
H	-11.9361280	0.4521430	2.5747240
C	-10.2635560	2.9772300	1.0779440
H	-10.4204440	3.9629150	0.6584910
C	-3.5106060	-2.8765530	5.6382780
H	-2.7922670	-2.2269090	5.1334230
H	-4.4556770	-2.3307200	5.6781700
H	-3.1670270	-3.0389940	6.6600240
C	-4.5638040	-5.5031000	1.4478020
H	-3.9271960	-4.8587980	0.8383860
H	-4.4867480	-6.5218080	1.0662090
H	-5.5910780	-5.1628120	1.2987990
C	-10.3285570	10.6278530	-2.4885140
H	-10.5218730	9.6770250	-2.9922560
H	-11.0199260	10.6733230	-1.6383370
C	-0.8936610	0.5165250	-0.9334460
H	-0.4245400	1.4659650	-1.1991360
H	-1.0632480	-0.0416330	-1.8554360
C	-10.6208880	11.7833860	-3.4402880
H	-10.4162520	12.7346730	-2.9342070
H	-9.9282930	11.7359420	-4.2888990
C	-8.8945050	10.6287400	-1.9684950
H	-8.1933600	10.5978130	-2.8082490
H	-8.6951170	11.5578920	-1.4236810
C	-8.5852540	3.4752640	-2.3382810

H	-9.3170010	2.7745900	-1.9300560
H	-8.9127120	3.7682030	-3.3359160
H	-7.6443190	2.9292880	-2.4342030
C	-8.5849690	9.4692090	-1.0445630
H	-7.5683410	9.5541760	-0.6441440
H	-9.2848180	9.4518770	-0.1996560
C	-7.5843630	5.5493360	2.1647020
H	-7.6085790	6.5223260	2.6562520
H	-8.2723570	4.8844480	2.6912220
H	-6.5832680	5.1308340	2.2890480
C	-12.0545530	11.7893070	-3.9615160
H	-12.7484500	11.8397110	-3.1138800
H	-12.2599650	10.8370380	-4.4645530
C	-3.5199470	-8.9867210	5.1145220
H	-2.8322260	-9.0862130	4.2651820
H	-4.5428810	-9.1118640	4.7417460
C	-12.3498200	12.9386800	-4.9207170
H	-12.1434660	13.8896670	-4.4175810
H	-11.6573030	12.8870700	-5.7678870
C	0.7349590	-3.8760560	2.3561350
H	0.1497630	-4.7093080	1.9515760
H	0.4441440	-3.7371260	3.4032790
C	-13.7854260	12.9348830	-5.4348370
H	-13.9690190	13.7663360	-6.1186380
H	-14.0089920	12.0085230	-5.9706180
H	-14.4989250	13.0187660	-4.6107230
C	-3.2075450	-10.0205790	6.1763310
H	-3.4221690	-11.0101520	5.7585310
H	-3.8970150	-9.8745280	7.0135610
C	-1.7667490	-9.9673760	6.6745640
H	-1.0870520	-10.1300280	5.8292400
H	-1.5584150	-8.9614200	7.0485870
C	-1.4723080	-10.9928890	7.7646340
H	-1.6923320	-11.9994790	7.3887820
H	-2.1532140	-10.8283190	8.6079980
C	-0.0320690	-10.9466920	8.2653260
H	0.6502800	-11.1147930	7.4234570

H	0.1888420	-9.9393780	8.6376120
C	0.2647370	-11.9645750	9.3626700
H	0.0426800	-12.9706220	8.9903200
H	-0.4160960	-11.7952410	10.2038990
C	2.2166480	-4.1433840	2.2334810
H	2.4817290	-5.0562070	2.7706150
H	2.4959760	-4.2586990	1.1855590
H	2.7916550	-3.3156870	2.6505530
C	1.7068980	-11.9098900	9.8550460
H	1.8913540	-12.6471190	10.6392680
H	2.4088000	-12.1085460	9.0406930
H	1.9463320	-10.9242140	10.2628240
O	-0.4535610	-2.6946730	-1.6184860
O	8.7032050	8.2735080	1.7951470
O	3.3802980	-7.7013830	-5.7019570
C	3.3998060	-1.0467480	-1.4377200
C	4.0324640	-4.2131030	-3.5530060
C	5.5117000	-2.4143460	-2.7565610
H	6.3338340	-2.9326970	-3.2387510
C	3.1736490	-2.2518660	-2.1491630
C	5.7897540	-1.1684020	-2.1076150
C	3.6709680	-4.1846180	-4.9111020
C	2.2923310	-0.5162980	-0.7251470
C	4.2696250	-2.9343920	-2.8154540
C	6.3515370	1.3283910	-1.0079770
C	1.0435450	-1.0983410	-0.7880670
C	7.4055980	0.5832700	-1.5901730
C	7.0819890	-0.6506830	-2.1392400
H	7.8400230	-1.2457350	-2.6320990
C	8.4265220	4.6846870	1.4502400
C	8.0810470	4.5415180	0.0955660
C	8.6239890	5.9508560	1.9733810
H	8.8893420	6.0868010	3.0146720
C	5.0601050	0.8050800	-0.9643220
H	4.3015530	1.4341280	-0.5323230
C	4.7345980	-0.4507510	-1.4742880
C	4.1758610	-5.4394900	-2.9020680

C	6.6244840	2.6308170	-0.4680480
H	5.7983370	3.1846050	-0.0341420
C	1.8875890	-2.8208800	-2.2139150
H	1.7611690	-3.7282460	-2.7848210
C	3.9628660	-6.6287900	-3.6004350
H	4.0807670	-7.5679980	-3.0779970
C	0.8214330	-2.2386870	-1.5696550
C	8.1487690	6.9433990	-0.1615690
H	8.0384270	7.8089080	-0.7999460
C	3.4629730	-5.3746130	-5.5868810
H	3.1866500	-5.3780130	-6.6342140
C	9.8474880	0.4625090	-2.1435670
H	9.7093620	-0.5259130	-2.5604150
C	8.7480500	1.1518160	-1.6038970
C	2.2262490	0.6873990	0.1953460
H	2.2434080	1.6166390	-0.3845890
H	3.0632210	0.7280030	0.8930850
C	8.9648170	2.4374070	-1.0571910
C	8.4867940	7.0834740	1.1768760
C	7.9462180	5.6755270	-0.7074730
C	11.3185010	2.2850910	-1.6157410
H	12.3102200	2.7212010	-1.6213960
C	3.6074100	-6.5989020	-4.9412730
C	7.8570830	3.1809410	-0.4811430
C	11.1075740	1.0125690	-2.1523300
H	11.9358890	0.4565220	-2.5749510
C	10.2624290	2.9809520	-1.0780560
H	10.4189680	3.9666830	-0.6585790
C	3.5116820	-2.8754030	-5.6383220
H	2.7931470	-2.2259720	-5.1334720
H	4.4565740	-2.3292660	-5.6782670
H	3.1681260	-3.0379980	-6.6600520
C	4.5657170	-5.5014390	-1.4477360
H	3.9287980	-4.8574200	-0.8383440
H	4.4891120	-6.5201770	-1.0661350
H	5.5928310	-5.1606800	-1.2987100
C	10.3248110	10.6314460	2.4886020

H	10.5184630	9.6806680	2.9923110
H	11.0161370	10.6771710	1.6384040
C	0.8933990	0.5169060	0.9333160
H	0.4239240	1.4661850	1.1989530
H	1.0631860	-0.0411420	1.8553360
C	10.6167880	11.7870490	3.4403990
H	10.4118210	12.7382820	2.9343510
H	9.9242360	11.7393520	4.2890300
C	8.8907410	10.6318660	1.9686320
H	8.1896350	10.6006800	2.8084080
H	8.6910240	11.5609660	1.4238500
C	8.5840520	3.4782690	2.3381940
H	9.3160870	2.7779090	1.9299460
H	8.9113830	3.7712980	3.3358440
H	7.6433380	2.9319080	2.4340820
C	8.5815650	9.4722570	1.0446770
H	7.5648950	9.5568940	0.6442930
H	9.2813920	9.4551840	0.1997460
C	7.5822500	5.5521330	-2.1646830
H	7.6061570	6.5251410	-2.6562130
H	8.2704300	4.8874630	-2.6912360
H	6.5812770	5.1333320	-2.2890110
C	12.0504680	11.7934310	3.9615830
H	12.7443210	11.8440870	3.1139260
H	12.2562100	10.8412160	4.4645870
C	3.5231550	-8.9855510	-5.1143670
H	2.8354370	-9.0852430	-4.2650480
H	4.5461180	-9.1103400	-4.7415500
C	12.3453850	12.9428760	4.9208050
H	12.1387030	13.8938080	4.4177000
H	11.6529100	12.8910160	5.7679940
C	-0.7335600	-3.8764190	-2.3561020
H	-0.1480350	-4.7094370	-1.9515390
H	-0.4428140	-3.7373920	-3.4032520
C	13.7810070	12.9395380	5.4348820
H	13.9643470	13.7710330	6.1186990
H	14.0048930	12.0132370	5.9706330

H	14.4944540	13.0236760	4.6107490
C	3.2111390	-10.0195490	-6.1761540
H	3.4260790	-11.0090370	-5.7583130
H	3.9005930	-9.8732950	-7.0133610
C	1.7703460	-9.9668440	-6.6744440
H	1.0906690	-10.1297120	-5.8291450
H	1.5616860	-8.9609660	-7.0484940
C	1.4762970	-10.9924750	-7.7645090
H	1.6966500	-11.9989850	-7.3886320
H	2.1571810	-10.8276860	-8.6078480
C	0.0360630	-10.9467780	-8.2652600
H	-0.6462630	-11.1151070	-7.4234160
H	-0.1851800	-9.9395430	-8.6375630
C	-0.2603490	-11.9647730	-9.3626070
H	-0.0379590	-12.9707400	-8.9902390
H	0.4204600	-11.7952100	-10.2038100
C	-2.2151430	-4.1443250	-2.2334240
H	-2.4798760	-5.0572400	-2.7705720
H	-2.4944090	-4.2597710	-1.1855010
H	-2.7904780	-3.3168440	-2.6504720
C	-1.7025090	-11.9105890	-9.8550410
H	-1.8866780	-12.6478880	-10.6392650
H	-2.4043740	-12.1094810	-9.0407150
H	-1.9422670	-10.9249990	-10.2628360

Monomer 3(R)

	X	Y	Z
O	-0.0719200	-2.3887340	-1.3790620
H	-0.6777090	-1.9654890	-2.0025210
O	0.4275680	0.8383360	-2.5520070
H	1.0892880	0.1410690	-2.6562480
O	-5.6510490	-4.2916950	6.7109760
O	9.9356630	-2.7484970	-3.0474180
O	-9.1920380	-0.3740690	-5.5551570
O	4.9241530	7.7389040	3.1327280
C	0.3527830	-1.6269630	-4.2346070
C	1.2242120	-0.9641700	-5.3403010

H	0.7911560	-1.1024070	-6.3321980
H	1.2743270	0.1113020	-5.1547870
C	2.6271970	-1.5753550	-5.1920970
H	2.7372160	-2.4752870	-5.8058080
H	3.4206170	-0.8876190	-5.4895860
C	2.6863380	-1.9469460	-3.7321050
C	1.4013350	-1.9652190	-3.1861370
C	1.1945660	-2.3466330	-1.8703890
C	2.2876840	-2.7017100	-1.0342620
C	2.1467830	-3.0986650	0.3697720
C	0.9392290	-3.1845750	1.0628470
H	0.0156900	-2.9503650	0.5642070
C	0.8699610	-3.5670640	2.4021180
C	-0.4026480	-3.6352110	3.0640210
H	-1.2865590	-3.3806580	2.4890010
C	-0.5318150	-3.9987700	4.3575960
C	0.6541370	-4.3380420	5.1255910
C	0.5519400	-4.7195300	6.4761330
H	-0.4292480	-4.7551730	6.9322950
C	1.6665600	-5.0422990	7.2122420
H	1.5660860	-5.3336940	8.2508830
C	2.9289930	-4.9927500	6.6157500
H	3.8121810	-5.2455910	7.1901400
C	3.0523920	-4.6221320	5.2975750
H	4.0398680	-4.5902970	4.8574660
C	1.9306130	-4.2869240	4.5200770
C	2.0448970	-3.8913530	3.1216930
C	3.2502000	-3.8095550	2.4365370
H	4.1813820	-4.0458320	2.9349050
C	3.3245390	-3.4270640	1.1003660
C	4.6044000	-3.3650780	0.4605530
H	5.4791280	-3.6217970	1.0488800
C	4.7549400	-3.0034790	-0.8278110
C	3.5848590	-2.6589770	-1.6182050
C	3.7672030	-2.2854590	-2.9630150
H	4.7680350	-2.2751270	-3.3739240
C	-0.3943940	-2.8947660	-4.7402750

H	0.1742200	-3.4175890	-5.5108870
H	-0.5224360	-3.5873200	-3.9050870
C	-1.7723220	-2.4079800	-5.2179680
H	-1.7541930	-2.1366020	-6.2784300
H	-2.5519690	-3.1616880	-5.0951420
C	-2.0081660	-1.1748800	-4.3831670
C	-3.1643020	-0.4709990	-4.1773820
H	-4.1002190	-0.7991110	-4.6098190
C	-3.1455660	0.7007690	-3.3977790
C	-4.3925920	1.4184140	-3.1917590
C	-4.3988360	2.5416360	-2.4490700
H	-5.3307220	3.0760430	-2.2967670
C	-3.2149430	3.0723290	-1.8423780
C	-3.3018860	4.2388130	-1.0881040
H	-4.2787480	4.6955460	-0.9961260
C	-2.1968150	4.8106740	-0.4710910
C	-2.2520120	6.0296120	0.3265000
C	-3.4503090	6.7332060	0.5370290
H	-4.3701720	6.3705630	0.0986420
C	-3.4869400	7.8813240	1.2924600
H	-4.4258480	8.4022400	1.4373280
C	-2.3149200	8.3740490	1.8717810
H	-2.3406040	9.2782520	2.4680570
C	-1.1285650	7.7068420	1.6825270
H	-0.2166900	8.0830070	2.1287100
C	-1.0671980	6.5302650	0.9132040
C	0.1933200	5.8337490	0.7201020
C	0.2212720	4.7066410	-0.0222510
H	1.1609800	4.1843340	-0.1667450
C	-0.9531080	4.1560730	-0.6387150
C	-0.8607360	2.9877000	-1.3944960
H	0.1089200	2.5325790	-1.4898970
C	-1.9673280	2.4069940	-2.0143450
C	-1.9380060	1.1812780	-2.8177990
C	-0.7617330	0.4212190	-3.0603230
C	-0.8087880	-0.7383380	-3.8170790
C	-1.8829340	-4.0509160	4.9944630

C	-2.4112400	-2.9170050	5.6143580
C	-3.6768230	-2.9695220	6.1992700
H	-4.0683280	-2.0803340	6.6735950
C	-4.4135120	-4.1448510	6.1697210
C	-3.8821650	-5.2741090	5.5546240
H	-4.4768730	-6.1793150	5.5476560
C	-2.6285460	-5.2418280	4.9687450
C	-1.6329450	-1.6273680	5.6605040
H	-0.6392570	-1.7776570	6.0878130
H	-2.1521310	-0.8799880	6.2611370
H	-1.4877790	-1.2163570	4.6591260
C	-2.0808750	-6.4811490	4.3108090
H	-1.9221730	-6.3241270	3.2417840
H	-2.7654910	-7.3204050	4.4346450
H	-1.1147510	-6.7623530	4.7358610
C	-6.2550350	-3.1825460	7.3551880
H	-6.3567620	-2.3487140	6.6496720
H	-5.6268850	-2.8452330	8.1889170
C	-7.6131720	-3.6252980	7.8565780
H	-7.4751070	-4.4781220	8.5277930
H	-8.1973160	-3.9868470	7.0051240
C	-8.3668120	-2.5096350	8.5740080
H	-8.4880660	-1.6572630	7.8968820
H	-7.7675380	-2.1476850	9.4163820
C	-9.7349610	-2.9548090	9.0791640
H	-10.3680140	-3.2912200	8.2541610
H	-10.2560930	-2.1419290	9.5886650
H	-9.6425000	-3.7849660	9.7840210
C	6.1207640	-2.9597590	-1.4344310
C	6.6567420	-4.0975160	-2.0404110
C	7.9380440	-4.0551940	-2.5908780
H	8.3352870	-4.9471600	-3.0551390
C	8.6833980	-2.8858890	-2.5401960
C	8.1446560	-1.7528850	-1.9382360
H	8.7467790	-0.8529440	-1.9132990
C	6.8755580	-1.7751980	-1.3864240
C	5.8691740	-5.3805400	-2.1093720

H	5.6945460	-5.7925990	-1.1130880
H	6.3973270	-6.1310420	-2.6982210
H	4.8879900	-5.2207570	-2.5614930
C	6.3211590	-0.5321390	-0.7415660
H	5.3666500	-0.2454200	-1.1885820
H	7.0132700	0.3029360	-0.8501370
H	6.1373380	-0.6865700	0.3237630
C	10.5511730	-3.8631790	-3.6714680
H	9.9458650	-4.1975780	-4.5231030
H	10.6257600	-4.6961340	-2.9615880
C	11.9267610	-3.4308180	-4.1325780
H	12.4876570	-3.0719350	-3.2645930
H	11.8149720	-2.5782770	-4.8090040
C	12.6935560	-4.5531400	-4.8253070
H	12.7886270	-5.4049810	-4.1433460
H	12.1171960	-4.9125030	-5.6846520
C	14.0792830	-4.1184230	-5.2900170
H	14.0138300	-3.2890520	-5.9987970
H	14.6096860	-4.9359260	-5.7822020
H	14.6896700	-3.7848800	-4.4470190
C	-5.6645870	0.9195480	-3.7988250
C	-6.0452250	1.3430110	-5.0836810
C	-7.2322100	0.8850580	-5.6287170
H	-7.5467220	1.1966670	-6.6172310
C	-8.0533790	0.0109730	-4.9230010
C	-7.6772040	-0.4102330	-3.6554960
H	-8.2978550	-1.0909700	-3.0896540
C	-6.4843100	0.0400840	-3.0891800
C	-5.1782570	2.2886160	-5.8728400
H	-5.0898620	3.2554560	-5.3727860
H	-5.5923270	2.4560690	-6.8672260
H	-4.1646820	1.8973180	-5.9853880
C	-6.0999590	-0.4339440	-1.7113340
H	-5.1020110	-0.8775220	-1.7079640
H	-6.8048900	-1.1805220	-1.3446420
H	-6.0803630	0.3931430	-0.9983970
C	-10.0796040	-1.2644920	-4.8955980

H	-10.4125320	-0.8235820	-3.9476260
H	-9.5629130	-2.2047540	-4.6719700
C	-11.2594880	-1.5080850	-5.8132660
H	-11.8920550	-2.2763480	-5.3552690
H	-10.8864390	-1.9255890	-6.7537900
C	-12.0846530	-0.2556510	-6.0935070
H	-12.4613160	0.1446650	-5.1456310
H	-11.4297670	0.5110110	-6.5134470
C	-13.2515900	-0.5192780	-7.0383070
H	-13.8280480	0.3894410	-7.2226410
H	-13.9344060	-1.2679320	-6.6271300
H	-12.8989630	-0.8897400	-8.0044700
C	1.4480070	6.3597550	1.3389540
C	1.8264000	5.9433170	2.6267480
C	2.9954640	6.4310090	3.1847420
H	3.3093960	6.1230380	4.1745650
C	3.8002370	7.3280080	2.4893690
C	3.4260970	7.7426250	1.2191930
H	4.0348350	8.4401100	0.6608230
C	2.2510700	7.2627270	0.6399390
C	0.9772020	4.9725640	3.4045840
H	-0.0477200	5.3358800	3.5076490
H	1.3854070	4.8138960	4.4028170
H	0.9208410	4.0050260	2.9013470
C	1.8680650	7.7296780	-0.7407980
H	1.8686930	6.9017600	-1.4530420
H	2.5624290	8.4887680	-1.1022040
H	0.8623530	8.1553540	-0.7517660
C	5.7961650	8.6503900	2.4823250
H	5.2561010	9.5744810	2.2403000
H	6.1592200	8.2121440	1.5457350
C	6.9499570	8.9382510	3.4202580
H	7.6780050	9.5557600	2.8828130
H	7.4494100	7.9930150	3.6549540
C	6.5293340	9.6360340	4.7102580
H	5.7760360	9.0244870	5.2117620
H	6.0416900	10.5852530	4.4615410

C	7.7021370	9.8930410	5.6496240
H	8.4595520	10.5239880	5.1762390
H	8.1865720	8.9565960	5.9384930
H	7.3778970	10.3937740	6.5640970

Monomer 4(*R*)

	X	Y	Z
C	0.1371300	0.1878660	3.8359230
C	1.4311260	-0.0181510	4.6162710
C	1.7183950	-0.9842080	5.5628080
H	0.9769670	-1.7249600	5.8390880
C	2.9759780	-0.9886280	6.1548710
H	3.2168480	-1.7388750	6.8984150
C	3.9291350	-0.0379270	5.8018420
H	4.9041040	-0.0561840	6.2741200
C	3.6422940	0.9325280	4.8521550
H	4.3865120	1.6721390	4.5805920
C	2.3863180	0.9376180	4.2600910
C	1.8058800	1.8251180	3.2453890
C	2.3274500	2.9084450	2.5807890
H	3.3396520	3.2435970	2.7696830
C	1.5450240	3.6023790	1.6389820
C	2.0937400	4.7490650	0.9343310
C	1.3303950	5.4068490	0.0367060
H	1.7418840	6.2629720	-0.4875850
C	-0.0190890	5.0201690	-0.2620470
C	-0.7671030	5.7306780	-1.1975470
H	-0.2891870	6.5746130	-1.6777150
C	-2.0752220	5.3878890	-1.5184200
C	-2.8839780	6.1120570	-2.4928160
C	-2.3940420	7.2310280	-3.1879150
H	-1.3865280	7.5788120	-3.0049260
C	-3.1673370	7.9045840	-4.1037020
H	-2.7616120	8.7642080	-4.6235420
C	-4.4730780	7.4807860	-4.3621170

H	-5.0849530	8.0096970	-5.0829080
C	-4.9787710	6.3895770	-3.6973140
H	-5.9899020	6.0555000	-3.8922560
C	-4.2058030	5.6853240	-2.7560530
C	-4.7538280	4.5332070	-2.0599960
C	-3.9912550	3.8776620	-1.1601020
H	-4.3998020	3.0180380	-0.6392670
C	-2.6438120	4.2696030	-0.8555710
C	-1.8966700	3.5599110	0.0810320
H	-2.3746100	2.7154140	0.5598450
C	-0.5883020	3.9033110	0.4031740
C	0.2172230	3.1790610	1.3791750
C	-0.2887920	2.0643510	2.0754840
H	-1.2986980	1.7202840	1.8965440
C	0.4900310	1.4042750	2.9863630
C	-1.0881190	0.3931990	4.7205270
C	-1.2962920	1.3585300	5.6882710
H	-0.5345130	2.0989660	5.9032120
C	-2.5011040	1.3629090	6.3814100
H	-2.6800070	2.1127660	7.1426220
C	-3.4804960	0.4129550	6.1068630
H	-4.4136390	0.4314690	6.6571420
C	-3.2730070	-0.5568160	5.1360850
H	-4.0376250	-1.2954980	4.9255670
C	-2.0697400	-0.5618780	4.4431340
C	-1.5751200	-1.4482890	3.3830510
C	-2.1505930	-2.5297880	2.7613340
H	-3.1442990	-2.8642260	3.0320050
C	-1.4491430	-3.2217260	1.7563390
C	-2.0559550	-4.3647450	1.0946890
C	-1.3717400	-5.0180300	0.1322890
H	-1.8270360	-5.8706820	-0.3605210
C	-0.0505080	-4.6324570	-0.2747070
C	0.6161970	-5.3391860	-1.2725210
H	0.0973050	-6.1779570	-1.7179780
C	1.8961210	-5.0000110	-1.6949890
C	2.6199910	-5.7196580	-2.7371550

C	2.0672950	-6.8265660	-3.4039200
H	1.0737520	-7.1677770	-3.1470440
C	2.7606050	-7.4957020	-4.3846970
H	2.3076260	-8.3456260	-4.8809310
C	4.0459450	-7.0795550	-4.7397910
H	4.5946000	-7.6046000	-5.5124360
C	4.6118150	-6.0002790	-4.1046640
H	5.6074830	-5.6719490	-4.3746070
C	3.9209300	-5.3004880	-3.0984930
C	4.5316390	-4.1604380	-2.4355840
C	3.8460150	-3.5068010	-1.4744770
H	4.3008170	-2.6552520	-0.9793530
C	2.5228240	-3.8909320	-1.0701830
C	1.8562190	-3.1836550	-0.0729840
H	2.3760180	-2.3458720	0.3728560
C	0.5752770	-3.5219810	0.3491350
C	-0.1465520	-2.7993440	1.3896300
C	0.4159660	-1.6864070	2.0441510
H	1.4075120	-1.3418120	1.7826220
C	-0.2848010	-1.0276290	3.0171930
C	3.4948120	5.1961830	1.2005820
C	3.7563560	6.1317750	2.2152570
C	5.0587170	6.5411580	2.4454900
H	5.2850960	7.2664010	3.2174480
C	6.1136930	6.0408780	1.6884380
C	5.8559590	5.1106380	0.6907400
H	6.6562200	4.6961860	0.0938050
C	4.5506280	4.6867120	0.4417670
C	2.6384530	6.6970450	3.0515560
H	1.9372690	7.2689490	2.4400220
H	3.0293650	7.3553710	3.8274370
H	2.0629670	5.9038040	3.5339010
C	4.3016590	3.6772370	-0.6492900
H	3.7400930	2.8181700	-0.2762600
H	5.2409970	3.3142130	-1.0672260
H	3.7139160	4.1098120	-1.4618970
C	8.4901920	6.0972810	1.2837650

H	9.2238690	6.8908790	1.4366730
H	8.2715300	6.0523530	0.2128190
C	9.0407450	4.7757340	1.7984380
H	9.8963250	4.5014940	1.1703610
H	8.2940220	3.9867560	1.6679640
C	9.4707480	4.8351330	3.2615210
H	10.2437360	5.6028920	3.3771500
H	8.6221150	5.1625610	3.8670600
C	9.9935690	3.4994790	3.7777210
H	9.2281540	2.7223720	3.7043200
H	10.2966970	3.5679670	4.8244140
H	10.8605630	3.1634210	3.2023270
C	-6.1499190	4.0779510	-2.3382430
C	-7.2214570	4.5931710	-1.5890520
C	-8.5085520	4.1573870	-1.8522440
H	-9.3514370	4.5387940	-1.2890970
C	-8.7563370	3.2185880	-2.8488530
C	-7.6995460	2.7120800	-3.5917710
H	-7.8684780	1.9840990	-4.3730730
C	-6.3949830	3.1386200	-3.3416000
C	-6.9862240	5.6119300	-0.5048590
H	-6.3723500	5.2000310	0.2989940
H	-7.9308310	5.9457770	-0.0753080
H	-6.4576060	6.4867260	-0.8900180
C	-5.2659740	2.5727580	-4.1639660
H	-4.6766510	3.3656990	-4.6293550
H	-5.6459870	1.9238500	-4.9535080
H	-4.5794350	1.9894900	-3.5464720
C	-10.3855690	1.9184520	-4.0228480
H	-9.8657420	0.9718020	-3.8301310
H	-10.0647280	2.2863900	-5.0052320
C	-11.8858900	1.7184190	-3.9925900
H	-12.3691550	2.6866970	-4.1529400
H	-12.1724340	1.3864120	-2.9903080
C	-12.3656490	0.7135470	-5.0354160
H	-11.8661100	-0.2476340	-4.8728410
H	-12.0629220	1.0502190	-6.0327820

C	-13.8767550	0.5113790	-5.0053970
H	-14.1977870	-0.2105740	-5.7588120
H	-14.4026040	1.4499500	-5.1978440
H	-14.2047350	0.1433430	-4.0299290
C	-3.4293200	-4.8133940	1.4775320
C	-3.6009890	-5.7596920	2.5023250
C	-4.8778690	-6.1710580	2.8431260
H	-5.0359650	-6.8987630	3.6296420
C	-5.9934150	-5.6598480	2.1868990
C	-5.8253400	-4.7221580	1.1779130
H	-6.6774200	-4.3083600	0.6568410
C	-4.5463640	-4.2950040	0.8197890
C	-2.4137210	-6.3315080	3.2317960
H	-1.7696180	-6.8982650	2.5560710
H	-2.7348030	-6.9961820	4.0338840
H	-1.7974900	-5.5420870	3.6677930
C	-4.3927390	-3.2760170	-0.2798640
H	-3.8041650	-2.4181140	0.0519660
H	-5.3650880	-2.9125880	-0.6134220
H	-3.8744330	-3.6998260	-1.1427870
C	-8.3789610	-5.6567980	1.9807800
H	-8.3433650	-5.8684080	0.9047200
H	-8.4563100	-4.5716240	2.1129520
C	-9.5570830	-6.3591320	2.6229520
H	-10.4753630	-5.9167760	2.2214340
C	-9.5659010	-7.8680900	2.3971990
H	-8.6273300	-8.2852870	2.7687180
H	-9.5888500	-8.0690150	1.3202940
C	-10.7462190	-8.5571830	3.0723890
H	-10.7279130	-8.3982230	4.1537880
H	-10.7326390	-9.6345640	2.8959710
H	-11.6986290	-8.1714590	2.6982950
C	5.9068680	-3.7146060	-2.8147250
C	7.0210260	-4.2364290	-2.1548570
C	8.3016060	-3.8094020	-2.5071660
H	9.1514800	-4.2250830	-1.9838720
C	8.4740400	-2.8689240	-3.5126780

C	7.3614380	-2.3543770	-4.1710100
H	7.5240260	-1.6240550	-4.9541290
C	6.0829050	-2.7653160	-3.8359420
C	6.8624000	-5.2594670	-1.0596900
H	6.3314790	-4.8420460	-0.2014000
H	7.8336710	-5.6167140	-0.7163510
H	6.2841270	-6.1207960	-1.4009000
C	4.8988870	-2.1904030	-4.5682250
H	4.2849380	-2.9780770	-5.0105950
H	5.2236790	-1.5224130	-5.3660570
H	4.2514840	-1.6264650	-3.8933050
C	10.8570340	-2.8777180	-3.3021000
H	10.9285970	-3.9649730	-3.4291790
H	10.8283220	-2.6641140	-2.2264720
C	12.0369570	-2.1864660	-3.9515650
H	12.0127180	-2.3925170	-5.0257110
H	11.9136100	-1.1055560	-3.8360850
C	13.3733020	-2.6279180	-3.3627150
H	13.4801770	-3.7123930	-3.4732320
H	13.3812160	-2.4283570	-2.2857260
O	7.3419430	6.5337910	2.0015700
O	-10.0567160	2.8649720	-3.0197620
O	-7.1958840	-6.1333040	2.6043820
O	9.6782540	-2.3937240	-3.9239770
C	14.5622410	-1.9319480	-4.0163350
H	14.5988950	-2.1406580	-5.0885200
H	15.5070480	-2.2623670	-3.5803790
H	14.4993800	-0.8477880	-3.8930590
H	-9.5458700	-6.1438570	3.6960520

(S)[Et]Pol1[1]

	X	Y	Z
O	1.7522610	9.5927700	-2.5666840
C	2.8936780	5.7232630	-1.6026850
C	1.6750240	6.2636910	-1.1571090
C	1.3367730	7.5590980	-1.5058920
H	0.4027550	7.9968750	-1.1755670

C	2.1873170	8.3373830	-2.2854000
C	3.3954910	7.8084520	-2.7164910
H	4.0731060	8.3937580	-3.3224150
C	3.7561390	6.5045420	-2.3738830
C	0.7299430	5.4476000	-0.3165230
H	0.3678330	4.5752050	-0.8656740
H	-0.1331820	6.0417670	-0.0162400
H	1.2224710	5.0752930	0.5840670
C	5.0645400	5.9509610	-2.8774460
H	5.7776990	5.8038250	-2.0634500
H	5.5174250	6.6255990	-3.6046580
H	4.9266190	4.9778490	-3.3538650
C	2.5679610	10.4440520	-3.3573390
H	2.7554050	9.9786320	-4.3332070
H	3.5330970	10.5978950	-2.8614250
C	1.8377030	11.7599810	-3.5268720
H	2.5080940	12.4555990	-4.0434500
H	1.6485680	12.1815480	-2.5346440
C	0.5257700	11.6356650	-4.2958660
H	0.7310910	11.2235510	-5.2901660
H	-0.1131950	10.9102950	-3.7874130
C	-0.2039890	12.9669700	-4.4336160
H	-0.4491410	13.3839360	-3.4532620
H	-1.1377320	12.8538540	-4.9880450
H	0.4085630	13.7031430	-4.9615000
O	-0.4653750	2.9051880	-6.3466430
O	8.3704940	-5.4322270	5.5575120
C	0.2794810	2.7817990	-5.2106700
C	0.9005740	3.9977030	-4.8668140
H	0.7315600	4.8405150	-5.5244510
C	1.6796550	4.1206370	-3.7595950
H	2.1185340	5.0810790	-3.5603220
C	1.9429790	3.0168800	-2.9110130
C	2.8043480	3.0936040	-1.7393820
C	3.2989900	4.3444020	-1.1736300
C	4.1474090	4.3146930	-0.1148080
H	4.4880380	5.2570130	0.3010050

C	4.5978380	3.1153100	0.5039930
C	5.4923640	3.1484510	1.5749810
H	5.8379030	4.1198720	1.9040510
C	5.9314820	1.9933830	2.2028650
C	6.8673140	1.9863170	3.3236130
C	7.3980150	3.1707040	3.8611300
H	7.1131770	4.1260690	3.4418660
C	8.2788370	3.1505180	4.9173290
H	8.6711430	4.0809340	5.3100700
C	8.6655120	1.9329400	5.4810510
H	9.3592760	1.9133010	6.3129140
C	8.1616360	0.7580580	4.9754300
H	8.4566550	-0.1897310	5.4075110
C	7.2601230	0.7553000	3.8960640
C	6.7347940	-0.4955420	3.3714910
C	5.8697190	-0.4698980	2.3369900
H	5.4778460	-1.4030670	1.9460150
C	5.4357070	0.7523050	1.7179340
C	4.5407050	0.7225390	0.6550040
H	4.2020960	-0.2501430	0.3261040
C	4.0971620	1.8838050	0.0212810
C	3.1701820	1.8960400	-1.0976190
C	2.6146950	0.6716640	-1.5550540
H	2.8890410	-0.2516750	-1.0667580
C	1.7301120	0.6139930	-2.5745930
H	1.3301250	-0.3435220	-2.8734870
C	1.3573080	1.7822830	-3.2941690
C	0.4544630	1.6746030	-4.4064620
C	7.1502230	-1.7988760	3.9735280
C	6.4136520	-2.3552970	5.0207800
C	6.8012650	-3.5768690	5.5721390
H	6.2168510	-3.9916590	6.3815820
C	7.9180730	-4.2414570	5.0859390
C	8.6521770	-3.6816700	4.0448340
H	9.5201500	-4.2196940	3.6838620
C	8.2833560	-2.4710590	3.4844270
C	5.1971120	-1.6545290	5.5686840

H	5.4286580	-0.6294240	5.8656110
H	4.8036910	-2.1801260	6.4392280
H	4.4033800	-1.5955570	4.8207720
C	9.0989020	-1.8909990	2.3587890
H	8.5092670	-1.8114090	1.4430210
H	9.9696290	-2.5128400	2.1504950
H	9.4474960	-0.8840750	2.5989970
C	7.6699470	-6.0648000	6.6177390
H	6.6373810	-6.2667850	6.3111050
H	7.6434120	-5.4036900	7.4931270
C	8.3922750	-7.3546500	6.9467020
H	8.4178580	-7.9766320	6.0464300
H	7.7964320	-7.8970580	7.6889550
C	9.8093530	-7.1444670	7.4717430
H	10.3760540	-6.5701230	6.7355660
H	9.7680850	-6.5301580	8.3781570
C	10.5256260	-8.4558410	7.7736490
H	9.9877570	-9.0380880	8.5269880
H	11.5358550	-8.2807840	8.1490030
H	10.6081760	-9.0741710	6.8759270
O	-1.1013670	-7.7201000	-6.0756390
C	-2.5086850	-4.5543200	-3.7961700
C	-1.2959070	-5.1973270	-3.4930300
C	-0.8665400	-6.2478330	-4.2841910
H	0.0648350	-6.7581220	-4.0715310
C	-1.6200970	-6.6824530	-5.3708260
C	-2.8227830	-6.0552490	-5.6639000
H	-3.4263640	-6.3760180	-6.5015650
C	-3.2744580	-4.9949060	-4.8769720
C	-0.4547100	-4.7492550	-2.3280030
H	-0.1087180	-3.7217420	-2.4634280
H	0.4204300	-5.3887010	-2.2131090
H	-1.0239020	-4.7735150	-1.3965090
C	-4.5750180	-4.3213170	-5.2329240
H	-5.3476410	-4.5226240	-4.4876230
H	-4.9408180	-4.6689020	-6.1995930
H	-4.4603230	-3.2361700	-5.2807140

C	-1.8177340	-8.2211420	-7.1945280
H	-1.9636300	-7.4211020	-7.9312450
H	-2.8043240	-8.5748090	-6.8743060
C	-1.0109040	-9.3546820	-7.7924780
H	-1.6089820	-9.8135950	-8.5873500
H	-0.8667040	-10.1202880	-7.0237170
C	0.3410520	-8.9161340	-8.3473840
H	0.1813210	-8.1589480	-9.1231740
H	0.9070940	-8.4274200	-7.5513030
C	1.1455340	-10.0765320	-8.9219500
H	1.3461190	-10.8319800	-8.1577170
H	2.1069730	-9.7389790	-9.3139450
H	0.6079440	-10.5672500	-9.7380310
O	0.8968250	0.2105190	-6.7521300
O	-9.1027740	2.8170320	6.5895360
C	0.1150740	-0.3650360	-5.7827030
C	-0.4028990	-1.6467690	-5.9865620
H	-0.1234280	-2.1841870	-6.8845750
C	-1.2391190	-2.2133220	-5.0637170
H	-1.6084450	-3.2027460	-5.2617160
C	-1.6414080	-1.5198610	-3.8966970
C	-2.5651340	-2.0726120	-2.9102760
C	-3.0155830	-3.4598710	-2.9044390
C	-3.9253810	-3.8673650	-1.9832050
H	-4.2329710	-4.9076430	-1.9863740
C	-4.4848680	-3.0132560	-0.9934140
C	-5.4392060	-3.4849720	-0.0902280
H	-5.7418940	-4.5199140	-0.1823790
C	-5.9883170	-2.6737600	0.8899150
C	-6.9893950	-3.1287030	1.8506710
C	-7.4736920	-4.4472130	1.8567340
H	-7.1020720	-5.1600080	1.1332300
C	-8.4169760	-4.8631240	2.7672750
H	-8.7712410	-5.8867700	2.7472050
C	-8.9155960	-3.9669800	3.7148770
H	-9.6587000	-4.2911740	4.4334390
C	-8.4590260	-2.6703790	3.7324970

H	-8.8406560	-1.9701450	4.4646190
C	-7.4952330	-2.2237580	2.8110090
C	-7.0206190	-0.8489790	2.8420330
C	-6.0937940	-0.4466990	1.9486660
H	-5.7394490	0.5784850	1.9724770
C	-5.5447640	-1.3241540	0.9515200
C	-4.5904040	-0.8588200	0.0550800
H	-4.2974730	0.1777720	0.1463370
C	-4.0345560	-1.6740650	-0.9320450
C	-3.0413830	-1.2249610	-1.8930540
C	-2.5337790	0.1009340	-1.7938260
H	-2.8854720	0.7451750	-1.0019910
C	-1.6009320	0.5823060	-2.6418640
H	-1.2267220	1.5890430	-2.5211380
C	-1.1283700	-0.2035210	-3.7277760
C	-0.1978030	0.3533310	-4.6539380
C	-7.5554350	0.1101190	3.8557640
C	-6.9206760	0.2527380	5.0909450
C	-7.4196000	1.1565770	6.0292750
H	-6.9130290	1.2534760	6.9794040
C	-8.5462400	1.9139060	5.7418160
C	-9.1784540	1.7658670	4.5110430
H	-10.0563280	2.3679880	4.3112760
C	-8.6985520	0.8749120	3.5669350
C	-5.6958230	-0.5573560	5.4296950
H	-5.8765220	-1.6262160	5.2973640
H	-5.3911900	-0.3895530	6.4630520
H	-4.8560710	-0.2957820	4.7821710
C	-9.4055260	0.7376560	2.2440230
H	-8.7576340	1.0341030	1.4163590
H	-10.2999660	1.3600590	2.2162240
H	-9.7032310	-0.2967400	2.0581310
C	-8.5092650	3.0250730	7.8623950
H	-7.4756500	3.3671150	7.7376160
H	-8.4921250	2.0822900	8.4235350
C	-9.3322930	4.0649520	8.5937250
H	-8.8181150	4.3066740	9.5303790

H	-9.3446530	4.9809190	7.9947020
C	-10.7613990	3.6178640	8.8865260
H	-11.2449220	3.3453230	7.9458140
H	-10.7342140	2.7073540	9.4955380
C	-11.5780030	4.6883550	9.6014500
H	-12.5952100	4.3459490	9.8017770
H	-11.6471100	5.5977230	8.9986980
H	-11.1247610	4.9606410	10.5586490
C	0.1349210	0.9424550	-7.7117590
H	0.8559440	1.5533280	-8.2544800
H	-0.3424620	0.2494810	-8.4176610
C	-0.9507480	1.8190710	-7.1170260
H	-1.6785370	1.2340510	-6.5526040
H	-1.4797450	2.2932420	-7.9452460

(S)[Pr]Pol1[1]

	X	Y	Z
O	-2.7221830	-9.4594590	2.4553170
C	-3.4597480	-5.5308830	1.3457830
C	-2.3057940	-5.8885660	2.0642160
C	-2.1022380	-7.2126030	2.4102450
H	-1.2206230	-7.5122640	2.9635450
C	-3.0251430	-8.1947240	2.0634730
C	-4.1693180	-7.8411560	1.3627690
H	-4.9008030	-8.5860640	1.0818270
C	-4.3944910	-6.5107780	1.0063650
C	-1.2851190	-4.8523820	2.4518850
H	-0.8232950	-4.4055400	1.5682510
H	-0.4960680	-5.2945020	3.0602990
H	-1.7426910	-4.0388360	3.0184110
C	-5.6359830	-6.1633130	0.2252320
H	-6.3388370	-5.5821920	0.8262200
H	-6.1470950	-7.0654430	-0.1124580
H	-5.3969060	-5.5575170	-0.6515260
C	-3.6186230	-10.5128500	2.1364220
H	-3.7476460	-10.5751210	1.0484960
H	-4.5984420	-10.3145550	2.5855590

C	-3.0333560	-11.8004400	2.6778960
H	-3.7706590	-12.5968900	2.5287990
H	-2.8994430	-11.6922700	3.7588210
C	-1.7090890	-12.1908130	2.0283200
H	-1.8598150	-12.3068230	0.9492210
H	-0.9996190	-11.3699540	2.1540670
C	-1.1271280	-13.4760870	2.6055990
H	-0.9373050	-13.3747420	3.6773980
H	-0.1818350	-13.7363470	2.1252100
H	-1.8114650	-14.3181690	2.4698950
O	0.2295520	-5.6914410	-3.9498370
O	-7.7808870	8.1350240	1.8857890
C	-0.4824510	-4.9655580	-3.0423150
C	-1.2600120	-5.7961200	-2.2133620
H	-1.1800880	-6.8635120	-2.3735710
C	-2.0750130	-5.2944720	-1.2476450
H	-2.6333560	-5.9919730	-0.6503910
C	-2.2105140	-3.8999840	-1.0436530
C	-3.0897340	-3.3201540	-0.0378430
C	-3.7234680	-4.0890430	1.0279910
C	-4.5782240	-3.4739880	1.8841560
H	-5.0233370	-4.0605730	2.6808220
C	-4.9043640	-2.0907100	1.8173400
C	-5.8118790	-1.5198650	2.7111510
H	-6.2661770	-2.1741720	3.4438610
C	-6.1303840	-0.1713530	2.6756510
C	-7.0756650	0.4620000	3.5906790
C	-7.7417270	-0.2603990	4.5945890
H	-7.5582980	-1.3204460	4.7054290
C	-8.6300000	0.3480470	5.4505010
H	-9.1283690	-0.2360210	6.2149150
C	-8.8877710	1.7153760	5.3332250
H	-9.5870160	2.1978780	6.0054970
C	-8.2499280	2.4473820	4.3599670
H	-8.4446780	3.5079320	4.2631340
C	-7.3382210	1.8457980	3.4741360
C	-6.6703530	2.6327130	2.4491990

C	-5.7991270	2.0312460	1.6134920
H	-5.3010630	2.6185030	0.8490860
C	-5.4942190	0.6287580	1.6875260
C	-4.5869450	0.0589120	0.8021810
H	-4.1383260	0.7150600	0.0692300
C	-4.2654020	-1.2984740	0.8351700
C	-3.3307170	-1.9348830	-0.0770620
C	-2.6386490	-1.1429640	-1.0316830
H	-2.8194740	-0.0789540	-1.0710280
C	-1.7358800	-1.6670100	-1.8892080
H	-1.2306430	-1.0149160	-2.5857260
C	-1.4784290	-3.0656020	-1.9286210
C	-0.5546790	-3.5923780	-2.8944140
C	-6.9472560	4.0959430	2.3228910
C	-6.1694630	5.0208830	3.0217510
C	-6.4273960	6.3858910	2.8925830
H	-5.8128160	7.0860700	3.4410590
C	-7.4560860	6.8295540	2.0738740
C	-8.2317740	5.9044880	1.3820090
H	-9.0290820	6.2761750	0.7501120
C	-7.9911100	4.5463030	1.4967280
C	-5.0468040	4.5665590	3.9186420
H	-5.3960600	3.8410820	4.6564430
H	-4.6086060	5.4103410	4.4524140
H	-4.2547900	4.0790240	3.3460640
C	-8.8486550	3.5700180	0.7350330
H	-8.2579020	3.0063010	0.0098620
H	-9.6429230	4.0886290	0.1979610
H	-9.3088120	2.8395310	1.4041490
C	-7.0307180	9.1356720	2.5572680
H	-5.9778240	9.0715730	2.2600460
H	-7.0896990	8.9803020	3.6419110
C	-7.6120290	10.4824320	2.1803540
H	-7.5561120	10.5917270	1.0927290
H	-6.9713320	11.2604590	2.6097220
C	-9.0511680	10.6787390	2.6475440
H	-9.6663410	9.8730080	2.2409350

H	-9.0906970	10.5779300	3.7379280
C	-9.6242050	12.0303470	2.2367970
H	-9.0370830	12.8538390	2.6527160
H	-10.6529320	12.1487440	2.5829270
H	-9.6254770	12.1424920	1.1493810
O	1.8733770	3.4095940	-9.0943490
C	2.9593720	1.8176870	-5.4218180
C	1.8009230	2.6001090	-5.5712690
C	1.4789700	3.1078240	-6.8172000
H	0.5913910	3.7124790	-6.9574550
C	2.2875490	2.8622030	-7.9232120
C	3.4370510	2.0993200	-7.7741650
H	4.0817920	1.8964730	-8.6180070
C	3.7806320	1.5796050	-6.5253100
C	0.9018730	2.8815080	-4.3973220
H	0.4574770	1.9608570	-4.0116100
H	0.0927770	3.5542890	-4.6813800
H	1.4562620	3.3371860	-3.5744520
C	5.0251890	0.7382520	-6.4009010
H	5.8024440	1.2537880	-5.8324900
H	5.4310790	0.4976000	-7.3839970
H	4.8216460	-0.1977200	-5.8761390
C	2.6521810	3.2075250	-10.2642200
H	2.7443510	2.1333440	-10.4686690
H	3.6586470	3.6142240	-10.1138490
C	1.9568930	3.9099240	-11.4116800
H	2.6075460	3.8481740	-12.2908570
H	1.8631000	4.9714610	-11.1621290
C	0.5838150	3.3313750	-11.7402530
H	0.6939110	2.2723290	-11.9991560
H	-0.0374380	3.3664980	-10.8425930
C	-0.1074320	4.0685330	-12.8815820
H	-0.2580900	5.1226240	-12.6342570
H	-1.0861690	3.6366640	-13.0996030
H	0.4860450	4.0263450	-13.7990780
O	-0.8742480	-3.5030990	-5.6385780
O	8.6688030	0.5360220	7.6715160

C	-0.0162650	-2.5896320	-5.0977290
C	0.6368120	-1.6515900	-5.9068900
H	0.4303400	-1.6419540	-6.9704400
C	1.5143200	-0.7538230	-5.3656400
H	1.9902660	-0.0548050	-6.0287610
C	1.8180420	-0.7472110	-3.9820360
C	2.7732720	0.1722020	-3.3726760
C	3.3525140	1.3192110	-4.0629310
C	4.2837450	2.0814530	-3.4351650
H	4.6874840	2.9405520	-3.9602670
C	4.7454100	1.8353980	-2.1126210
C	5.7275400	2.6390100	-1.5308040
H	6.1295130	3.4452680	-2.1304600
C	6.1820350	2.4260800	-0.2390560
C	7.2082360	3.2423950	0.4033520
C	7.8170670	4.3268610	-0.2496030
H	7.5262650	4.5780700	-1.2605270
C	8.7827310	5.0879710	0.3668700
H	9.2340810	5.9185100	-0.1625150
C	9.1790980	4.7898220	1.6721210
H	9.9394960	5.3871370	2.1606350
C	8.5996520	3.7343360	2.3355300
H	8.9015030	3.4975450	3.3478480
C	7.6107340	2.9429890	1.7245170
C	7.0056370	1.8296290	2.4389910
C	6.0574500	1.0878400	1.8309810
H	5.6058220	0.2579640	2.3643430
C	5.6098690	1.3478560	0.4902350
C	4.6280680	0.5531780	-0.0891540
H	4.2350680	-0.2553640	0.5113160
C	4.1676590	0.7662130	-1.3892880
C	3.1499830	-0.0460180	-2.0344590
C	2.5141870	-1.0788770	-1.2906580
H	2.7898580	-1.2356050	-0.2585070
C	1.5489060	-1.8604110	-1.8198190
H	1.0745960	-2.6193670	-1.2138570
C	1.1699010	-1.7295240	-3.1834800

C	0.2076230	-2.6230760	-3.7416840
C	7.4308980	1.5099540	3.8356110
C	6.7687860	2.0870900	4.9207220
C	7.1643010	1.7767950	6.2220970
H	6.6379720	2.2329200	7.0489430
C	8.2150990	0.8980870	6.4439050
C	8.8752950	0.3282230	5.3595450
H	9.6926570	-0.3538040	5.5592420
C	8.4975920	0.6232030	4.0611540
C	5.6246910	3.0448590	4.7087640
H	5.9110880	3.8671670	4.0496500
H	5.2910100	3.4690570	5.6561260
H	4.7722900	2.5468740	4.2415400
C	9.2321840	-0.0099200	2.9086670
H	8.5698810	-0.6482970	2.3200090
H	10.0629100	-0.6185310	3.2659870
H	9.6303660	0.7460030	2.2281010
C	8.0409880	1.0748100	8.8253370
H	6.9803200	0.7993890	8.8324880
H	8.1098690	2.1698040	8.8093670
C	8.7472760	0.5146030	10.0422570
H	8.1994720	0.8421140	10.9326360
H	8.6765610	-0.5772030	10.0117570
C	10.2097430	0.9364160	10.1482510
H	10.7301880	0.6351820	9.2364330
H	10.2650820	2.0299990	10.1891380
C	10.9066830	0.3421250	11.3668540
H	11.9501410	0.6585920	11.4227830
H	10.8930930	-0.7504550	11.3333410
H	10.4162150	0.6498750	12.2945010
C	-0.2990870	-4.5161280	-6.4676440
H	-0.9756780	-5.3635100	-6.3659780
H	-0.3172300	-4.1917090	-7.5143140
C	1.1243740	-4.9389410	-6.1083550
H	1.3198490	-5.8411790	-6.6948270
H	1.8432760	-4.1885380	-6.4460770
C	1.3892630	-5.2182010	-4.6221940

H	1.7931140	-4.3432290	-4.1202620
H	2.1257720	-6.0188290	-4.5307730

(R)Pol1[1]

	X	Y	Z
O	4.9062540	5.4463310	-7.4071920
C	4.5462580	3.2431850	-3.9113560
C	5.5651970	4.1971110	-4.0783350
C	5.6430850	4.9112460	-5.2616860
H	6.4136210	5.6578270	-5.4103370
C	4.7347820	4.6903100	-6.2927120
C	3.7380290	3.7381490	-6.1333630
H	3.0257560	3.5433950	-6.9229630
C	3.6403370	3.0099840	-4.9479760
C	6.5515870	4.4802360	-2.9751470
H	6.0427560	4.6724630	-2.0276430
H	7.1631000	5.3494350	-3.2178760
H	7.2189980	3.6326320	-2.8061720
C	2.5419840	1.9899590	-4.8026380
H	2.9397030	1.0183580	-4.5035960
H	1.9999910	1.8647860	-5.7402940
H	1.8237520	2.2913750	-4.0361440
C	4.0118930	5.2799020	-8.4977290
H	2.9837310	5.4750620	-8.1681730
H	4.0632680	4.2485510	-8.8645550
C	4.4176660	6.2544930	-9.5835250
H	3.7996680	6.0549690	-10.4657690
H	5.4530970	6.0438390	-9.8690510
C	4.2803190	7.7178160	-9.1738810
H	3.2379650	7.9171430	-8.9012370
H	4.8729960	7.8884500	-8.2723940
C	4.7153560	8.6798940	-10.2734470
H	5.7633860	8.5223500	-10.5415290
H	4.6068790	9.7197310	-9.9587750
H	4.1188170	8.5433630	-11.1796810
O	-0.1057410	6.9091720	-1.1700760
O	6.1957670	-7.1261430	5.8584140

C	-0.0019850	7.6836400	-0.0004280
C	0.7706490	5.8512050	-1.2541990
C	1.8213960	5.9187970	-2.1698340
H	1.9287160	6.8101590	-2.7749380
C	2.6874800	4.8682230	-2.3024270
H	3.4789270	4.9584160	-3.0238560
C	2.5854520	3.7107580	-1.4944010
C	3.5206580	2.5932100	-1.5770920
C	4.4807170	2.4189450	-2.6601950
C	5.3607510	1.3863680	-2.6177640
H	6.0534110	1.2628450	-3.4434490
C	5.4087950	0.4334900	-1.5629670
C	6.3576830	-0.5905900	-1.5594220
H	7.0614210	-0.6187580	-2.3811130
C	6.4112980	-1.5403530	-0.5517500
C	7.3896210	-2.6236190	-0.5112670
C	8.3631640	-2.7884400	-1.5103210
H	8.4016220	-2.0990890	-2.3427410
C	9.2791550	-3.8132920	-1.4604310
H	10.0180160	-3.9147760	-2.2462660
C	9.2553360	-4.7200770	-0.3989210
H	9.9751760	-5.5285800	-0.3565810
C	8.3134730	-4.5827640	0.5930380
H	8.2888990	-5.2821130	1.4190470
C	7.3673970	-3.5428210	0.5618580
C	6.3760580	-3.4102130	1.6181940
C	5.4790050	-2.4045760	1.5638620
H	4.7391330	-2.3065270	2.3513470
C	5.4551030	-1.4427000	0.4962080
C	4.5076260	-0.4262670	0.4872580
H	3.8102930	-0.3991530	1.3129850
C	4.4517220	0.5318580	-0.5259870
C	3.4848460	1.6153880	-0.5671760
C	2.4749870	1.6842900	0.4336390
H	2.4443690	0.9335670	1.2091260
C	1.5285190	2.6463500	0.4382250
H	0.7706910	2.6510990	1.2083170

C	1.5442190	3.6917220	-0.5254030
C	0.5811620	4.7408490	-0.4632460
C	6.3509880	-4.3812680	2.7539860
C	7.0885830	-4.1267930	3.9116370
C	7.0541250	-5.0329560	4.9718100
H	7.6312800	-4.8172230	5.8601300
C	6.2914430	-6.1885980	4.8806050
C	5.5608120	-6.4406090	3.7234680
H	4.9742540	-7.3499410	3.6767640
C	5.5817080	-5.5537080	2.6611400
C	7.9264860	-2.8803910	4.0367620
H	8.6281000	-2.7876250	3.2049800
H	8.4988470	-2.8870770	4.9647560
H	7.3049580	-1.9823660	4.0279750
C	4.7804810	-5.8554740	1.4219210
H	4.0049080	-5.1040200	1.2592400
H	4.2990390	-6.8303430	1.4995080
H	5.4122510	-5.8562790	0.5308690
C	6.9121250	-6.9355870	7.0691750
H	6.5868780	-6.0058850	7.5496580
H	7.9856820	-6.8536540	6.8575250
C	6.6353510	-8.1255220	7.9642080
H	5.5558410	-8.1876530	8.1338680
H	7.0978800	-7.9318400	8.9382260
C	7.1481050	-9.4470150	7.3996770
H	6.7060570	-9.6037640	6.4132580
H	8.2305630	-9.3747820	7.2456600
C	6.8373160	-10.6336500	8.3047740
H	7.2904540	-10.5096180	9.2922420
H	7.2145310	-11.5668500	7.8817840
H	5.7595060	-10.7466640	8.4482780
O	-4.9103260	5.4455130	7.4058390
C	-4.5483430	3.2415680	3.9107140
C	-5.5677700	4.1950710	4.0771440
C	-5.6463200	4.9094940	5.2602770
H	-6.4172490	5.6557520	5.4085090
C	-4.7382010	4.6892630	6.2916160

C	-3.7409610	3.7375200	6.1328080
H	-3.0288140	3.5433170	6.9226570
C	-3.6426060	3.0090720	4.9476500
C	-6.5539890	4.4774070	2.9736040
H	-6.0449910	4.6695620	2.0261760
H	-7.1659610	5.3464050	3.2158930
H	-7.2209690	3.6294430	2.8047250
C	-2.5437210	1.9895390	4.8028770
H	-2.9408900	1.0176680	4.5039820
H	-2.0019190	1.8648720	5.7407110
H	-1.8254250	2.2910950	4.0364950
C	-4.0162270	5.2797500	8.4966930
H	-2.9880490	5.4752830	8.1674080
H	-4.0672610	4.2484680	8.8637580
C	-4.4227680	6.2544320	9.5821220
H	-3.8049520	6.0554040	10.4646040
H	-5.4581920	6.0433860	9.8673830
C	-4.2859510	7.7177140	9.1721560
H	-3.2436010	7.9174430	8.8997880
H	-4.8784230	7.8878570	8.2704410
C	-4.7217630	8.6798700	10.2713460
H	-5.7698040	8.5219140	10.5391480
H	-4.6136660	9.7196770	9.9564460
H	-4.1254400	8.5438400	11.1777970
O	0.1022500	6.9093430	1.1692790
O	-6.1914080	-7.1306020	-5.8571650
C	-0.7736130	5.8509380	1.2535280
C	-1.8243780	5.9180920	2.1691700
H	-1.9321320	6.8094550	2.7741970
C	-2.6899270	4.8670930	2.3018770
H	-3.4813970	4.9569540	3.0233210
C	-2.5873300	3.7095950	1.4939630
C	-3.5219820	2.5915840	1.5767680
C	-4.4820820	2.4170260	2.6597910
C	-5.3615040	1.3839210	2.6175110
H	-6.0541900	1.2602040	3.4431450
C	-5.4089010	0.4307760	1.5629300

C	-6.3571940	-0.5938550	1.5595340
H	-7.0609650	-0.6222700	2.3811880
C	-6.4102010	-1.5438460	0.5520450
C	-7.3878860	-2.6276950	0.5117240
C	-8.3613430	-2.7929290	1.5107940
H	-8.4002130	-2.1034690	2.3431050
C	-9.2767250	-3.8183320	1.4610620
H	-10.0155330	-3.9201260	2.2469070
C	-9.2523540	-4.7252780	0.3997020
H	-9.9717120	-5.5342170	0.3574860
C	-8.3105570	-4.5875720	-0.5922650
H	-8.2855560	-5.2870480	-1.4181540
C	-7.3650970	-3.5470640	-0.5612450
C	-6.3738080	-3.4140550	-1.6175790
C	-5.4773240	-2.4079050	-1.5633770
H	-4.7374800	-2.3095650	-2.3508520
C	-5.4540130	-1.4458340	-0.4958850
C	-4.5071200	-0.4288570	-0.4870750
H	-3.8097530	-0.4015080	-1.3127640
C	-4.4518210	0.5294950	0.5259920
C	-3.4855620	1.6135850	0.5670390
C	-2.4756910	1.6828620	-0.4337350
H	-2.4446170	0.9320150	-1.2090820
C	-1.5297650	2.6454520	-0.4384650
H	-0.7719200	2.6504840	-1.2085360
C	-1.5460610	3.6909670	0.5249930
C	-0.5835490	4.7405940	0.4627080
C	-6.3481650	-4.3852800	-2.7532130
C	-7.0859730	-4.1314600	-3.9108730
C	-7.0510090	-5.0377870	-4.9708890
H	-7.6283400	-4.8225700	-5.8592190
C	-6.2876070	-6.1929400	-4.8795190
C	-5.5567590	-6.4442970	-3.7223770
H	-4.9696340	-7.3532560	-3.6755470
C	-5.5781530	-5.5572260	-2.6602020
C	-7.9246620	-2.8856040	-4.0361670
H	-8.6264030	-2.7932230	-3.2044490

H	-8.4969440	-2.8927290	-4.9642070
H	-7.3037100	-1.9871800	-4.0273970
C	-4.7766840	-5.8582760	-1.4209650
H	-4.0015810	-5.1063040	-1.2584410
H	-4.2946290	-6.8328540	-1.4984070
H	-5.4084190	-5.8593290	-0.5298890
C	-6.9079030	-6.9406700	-7.0679430
H	-6.5832300	-6.0108450	-7.5485760
H	-7.9815050	-6.8593590	-6.8562870
C	-6.6304240	-8.1305780	-7.9627940
H	-7.0931020	-7.9373350	-8.9368290
H	-5.5508800	-8.1920750	-8.1324790
C	-7.1423510	-9.4522940	-7.3980360
H	-6.7001640	-9.6086230	-6.4116130
H	-8.2248460	-9.3806920	-7.2439800
C	-6.8308860	-10.6388810	-8.3029640
H	-7.2075130	-11.5722440	-7.8798100
H	-5.7530160	-10.7512620	-8.4465050
H	-7.2841500	-10.5152770	-9.2904290
H	-0.9035330	8.3013220	0.0078800
H	0.8991920	8.3018620	-0.0088050

(M)Poll[10]

	X	Y	Z
O	21.8803850	-8.7954460	-4.6087230
C	22.5806850	-8.8079520	-5.8636500
C	21.1626570	-7.6249430	-4.3251350
C	19.7640770	-7.6834910	-4.3306180
H	19.2893730	-8.6404060	-4.5277020
C	19.0289070	-6.5621520	-4.0766640
H	17.9567680	-6.6484790	-4.0641310
C	19.6372160	-5.2967100	-3.8472020
C	21.0127750	-2.9092050	-3.3129680
H	21.5420530	-1.9732410	-3.1468950
C	21.7168510	-4.0154860	-3.5786110
H	22.8026580	-3.9774570	-3.6278290

C	21.0718740	-5.2717900	-3.8016330
C	21.8371980	-6.4614690	-4.0023000
O	23.2846070	-7.5777880	-6.1050340
C	24.0039850	-7.0647750	-5.0143550
C	25.3989280	-7.1252760	-5.0546380
H	25.8774140	-7.5668730	-5.9187830
C	26.1391640	-6.6242690	-4.0107650
H	27.2099620	-6.6869190	-4.0775160
C	25.5242040	-6.0780440	-2.8536510
C	24.1585700	-5.3549780	-0.5063180
H	23.6219320	-5.1305690	0.4055300
C	23.4441330	-5.7221870	-1.5990230
H	22.3657410	-5.7830300	-1.5434430
C	24.0946820	-6.0801600	-2.8149980
C	23.3280730	-6.5089370	-3.9450820
H	21.8953660	-8.9031230	-6.7061050
H	23.2637450	-9.6542670	-5.7911880
O	13.3480780	7.5069820	-2.8763250
C	13.9881660	8.4906040	-2.0457950
C	12.4956800	6.6130420	-2.2107850
C	11.1212140	6.7178680	-2.4391450
H	10.7657150	7.4601450	-3.1421740
C	10.2505230	5.8788610	-1.7884690
H	9.2027060	5.9705360	-2.0081490
C	13.0251640	5.6338910	-1.3916590
O	22.2781710	6.4801750	1.5742590
C	19.7247690	3.9260580	-0.5242940
C	19.6871470	4.0146750	0.8850390
C	20.5551650	4.8808280	1.5387630
H	20.5452940	4.9711840	2.6183470
C	21.4652990	5.6536430	0.8189620
C	21.5132850	5.5651940	-0.5676560
H	22.2128030	6.1597460	-1.1409330
C	20.6487650	4.6982540	-1.2466020
C	18.7106050	3.1908840	1.6852330
H	17.6767480	3.4660670	1.4534080
H	18.8659350	3.3370020	2.7562520

H	18.8145580	2.1244350	1.4650660
C	20.7024100	4.6356710	-2.7535620
H	21.0641690	3.6646560	-3.1058050
H	21.3659030	5.4072350	-3.1522310
H	19.7103260	4.7798410	-3.1941150
C	23.2515180	7.3027820	0.9029600
H	22.7711410	8.0122330	0.2203950
H	23.9723000	6.6936970	0.3482030
O	14.5105430	7.9213660	-0.8333760
O	13.8493900	-7.8495870	-5.8885680
C	15.2041670	6.7105100	-0.9831730
C	16.5926270	6.7209650	-0.8259830
H	17.0839680	7.6556810	-0.5902830
C	17.3079910	5.5570170	-0.9649460
H	18.3741060	5.6013440	-0.8350440
C	16.6811940	4.3302520	-1.3106400
C	17.4237080	3.0874130	-1.5230600
C	18.8504620	2.9309170	-1.2319050
C	19.4798990	1.7640250	-1.5548300
H	20.5375310	1.6695020	-1.3294860
C	18.8206360	0.6413410	-2.1326880
C	19.5276360	-0.5257080	-2.4449710
H	20.5928060	-0.5268150	-2.2494490
C	18.8905430	-1.6600770	-2.9504360
C	19.5846540	-2.8926430	-3.2930730
C	18.8784260	-4.0672710	-3.6460660
C	17.4279050	-3.9576400	-3.8162960
C	16.8039490	-2.7716560	-3.5626050
H	15.7314900	-2.7064190	-3.7214210
C	17.4790060	-1.6014990	-3.1024070
C	16.7768530	-0.4286800	-2.8090090
H	15.7046190	-0.4507280	-2.9533790
C	17.4160660	0.7184180	-2.3389380
C	16.7320350	1.9705140	-2.0426960
C	15.3324630	2.0732230	-2.2998960
H	14.8113040	1.2302850	-2.7343630
C	14.6267660	3.1946380	-2.0268080

H	13.5660620	3.2315230	-2.2384650
C	15.2645490	4.3580140	-1.5071940
C	14.5110570	5.5506540	-1.2684770
C	16.5164730	-5.0348310	-4.3322790
C	15.7126210	-5.7657130	-3.4430550
C	14.8142830	-6.7186720	-3.9387860
H	14.2097340	-7.2806470	-3.2381650
C	14.7081240	-6.9313350	-5.3088100
C	15.4960210	-6.1975850	-6.1938330
H	15.3862090	-6.3829810	-7.2549400
C	16.3972310	-5.2489050	-5.7237420
C	15.8256220	-5.5655090	-1.9519980
H	16.8640900	-5.6550360	-1.6148030
H	15.2300830	-6.3065100	-1.4123250
H	15.4834950	-4.5699500	-1.6493730
C	17.2445070	-4.4721460	-6.7009190
H	17.1189290	-3.3941920	-6.5660390
H	16.9780420	-4.7230430	-7.7290100
H	18.3076460	-4.6900890	-6.5674990
C	12.9990510	-8.6441260	-5.0390680
H	12.3166430	-8.0159420	-4.4569960
H	13.5896020	-9.2666870	-4.3577840
H	13.2857250	9.2542190	-1.7103560
H	14.7798380	8.9044690	-2.6715710
H	23.7654180	7.8472540	1.6922560
H	12.4283880	-9.2801580	-5.7126120
O	22.6668280	-1.5155500	9.3225480
C	25.3787480	-2.8807000	6.4519820
C	25.1349930	-1.5027390	6.6412290
C	24.2238090	-1.0966320	7.6101610
H	24.0211990	-0.0459220	7.7784540
C	23.5457480	-2.0343310	8.3875170
C	23.7733840	-3.3928660	8.1986620
H	23.2560050	-4.1337640	8.7943280
C	24.6847090	-3.8242370	7.2261660
C	25.8593430	-0.4688580	5.8165680
H	26.9365920	-0.4920510	6.0086400

H	25.4972310	0.5352930	6.0463950
H	25.7209530	-0.6460000	4.7460510
C	24.9314100	-5.3038370	7.0535170
H	24.5701110	-5.6651240	6.0855790
H	24.4269660	-5.8768620	7.8353710
H	26.0001700	-5.5379370	7.0968520
C	21.9303370	-2.4223680	10.1643060
H	22.6032830	-3.0313500	10.7774630
H	21.2802160	-3.0776360	9.5745170
O	30.8232490	-2.2011780	10.0609070
O	31.3602080	-5.9054870	-6.0481880
C	31.6752110	-3.2617420	10.5222680
C	30.0893970	-2.4718020	8.8963870
C	28.7083520	-2.6530590	9.0128310
H	28.2576880	-2.5946060	9.9938040
C	27.9509280	-2.8945500	7.8934650
H	26.8908630	-3.0195650	8.0179660
C	28.5348930	-3.0138910	6.6054080
C	27.7624100	-3.3208370	5.4021910
C	26.2992310	-3.3305760	5.3561520
C	25.6662380	-3.7137230	4.2092420
H	24.5808600	-3.7047410	4.1927050
C	26.3435310	-4.0921770	3.0117830
C	25.6314490	-4.4846640	1.8752860
H	24.5531500	-4.5164480	1.9573200
C	26.2728670	-4.8172050	0.6806240
C	25.5808000	-5.2518780	-0.5250780
C	26.2843980	-5.5812790	-1.7057540
C	27.7361250	-5.3995620	-1.7085310
C	28.3679810	-5.0040680	-0.5667000
H	29.4453260	-4.8675510	-0.5911800
C	27.6927880	-4.7228850	0.6583880
C	28.4043910	-4.3331340	1.7959440
H	29.4822640	-4.2825380	1.7077270
C	27.7648790	-4.0178770	2.9953220
C	28.4620960	-3.6243870	4.2128300
C	29.8864660	-3.5536810	4.2016360

H	30.4223260	-3.8073120	3.2978110
C	30.6011290	-3.1737080	5.2881900
H	31.6798520	-3.1293430	5.2353810
C	29.9569360	-2.8781610	6.5230360
C	30.7306730	-2.5295950	7.6757220
C	28.6417270	-5.5375690	-2.8986330
C	28.7504700	-4.4852670	-3.8221630
C	29.6515100	-4.5856410	-4.8880780
H	29.7193760	-3.7666690	-5.5927770
C	30.4443100	-5.7193710	-5.0277760
C	30.3460770	-6.7618580	-4.1069430
H	30.9779400	-7.6314830	-4.2439070
C	29.4575730	-6.6823510	-3.0400080
C	27.8961390	-3.2494290	-3.6916400
H	26.8345150	-3.4859150	-3.8159510
H	28.1651220	-2.5069150	-4.4462780
H	28.0074090	-2.7902210	-2.7050910
C	29.3512050	-7.8342400	-2.0711530
H	29.6875990	-7.5519210	-1.0686320
H	29.9570130	-8.6797120	-2.4059780
H	28.3155770	-8.1756510	-1.9709550
C	31.5210740	-4.8736960	-7.0398530
H	31.8614680	-3.9384460	-6.5865450
H	30.5894390	-4.6976690	-7.5853420
O	40.3052890	-3.9215240	7.1909100
C	37.3393020	-1.2222790	6.0231200
C	37.4846590	-2.4790840	5.3945020
C	38.4863180	-3.3436210	5.8201720
H	38.6178660	-4.3149230	5.3566710
C	39.3502010	-2.9804190	6.8513970
C	39.2185900	-1.7426100	7.4693560
H	39.8785730	-1.4455750	8.2720960
C	38.2184200	-0.8545370	7.0547900
C	36.5634240	-2.8963030	4.2764070
H	35.5318140	-2.9982310	4.6287050
H	36.8720190	-3.8561800	3.8574950
H	36.5549300	-2.1567400	3.4703510

C	38.0815950	0.4772070	7.7545720
H	38.3437170	1.3110310	7.0949050
H	38.7336450	0.5249180	8.6297170
H	37.0527230	0.6492130	8.0870470
C	41.2403760	-3.6152100	8.2430180
H	40.7274730	-3.4486020	9.1962290
H	41.8431470	-2.7352250	7.9948060
O	32.4144430	-3.8722830	9.4521470
O	29.9583840	8.1765600	-1.6321810
C	32.9997510	-2.9907420	8.5318270
C	34.3910350	-2.8535860	8.5380700
H	34.9669440	-3.4240810	9.2558540
C	35.0030780	-2.0183520	7.6368460
H	36.0747940	-1.9398930	7.6662120
C	34.2571520	-1.2395850	6.7129060
C	34.8759640	-0.3059580	5.7738940
C	36.3148520	-0.2474360	5.5156320
C	36.8126730	0.7115180	4.6831540
H	37.8819950	0.7284490	4.4940700
C	36.0039090	1.6739680	4.0113440
C	36.5804580	2.6384790	3.1805160
H	37.6595830	2.6329280	3.0945880
C	35.8082990	3.5698040	2.4827370
C	34.0869460	5.3598500	1.0661620
C	33.5860280	4.3974250	1.8935830
H	32.5089320	4.2926370	1.9737550
C	34.3966660	3.4907460	2.6372630
C	33.8198700	2.5253910	3.4675070
H	32.7411060	2.5207690	3.5394860
C	34.5928270	1.6029820	4.1765240
C	34.0415120	0.5860550	5.0631310
C	32.6266910	0.4906820	5.2156440
H	31.9888560	1.1829460	4.6832640
C	32.0447490	-0.4483200	5.9995760
H	30.9670570	-0.4921620	6.0811360
C	32.8328350	-1.3540020	6.7681140
C	32.2039280	-2.3010850	7.6375890

C	33.0396940	6.1293340	0.3102570
C	32.7008610	5.7502380	-0.9978360
C	31.6723330	6.4219600	-1.6724800
H	31.4264450	6.1194460	-2.6803590
C	30.9847860	7.4573140	-1.0432090
C	31.3145180	7.8281560	0.2564020
H	30.7614030	8.6385090	0.7165350
C	32.3309090	7.1732670	0.9468580
C	33.4406680	4.6365610	-1.6997920
H	34.4940230	4.8957470	-1.8503270
H	33.0018560	4.4302330	-2.6770000
H	33.4200060	3.7128250	-1.1135120
C	32.6832290	7.6098920	2.3461080
H	32.4697450	6.8265700	3.0798160
H	32.1177450	8.5007510	2.6286430
H	33.7506000	7.8407840	2.4340240
C	29.5743090	7.8616410	-2.9854290
H	29.2100910	6.8318390	-3.0676740
H	30.4091420	8.0078720	-3.6799500
H	31.1011550	-4.0794920	10.9595310
H	32.3360050	-2.7888480	11.2498830
H	21.3203840	-1.7915000	10.8075510
H	41.8848950	-4.4878290	8.3245060
H	32.2801500	-5.2437570	-7.7248490
H	28.7692270	8.5530790	-3.2279380
C	43.8222850	-2.9825340	-5.9740960
C	45.4760190	-0.9107480	-5.1471900
H	46.1398250	-0.1147600	-4.8312690
C	46.0260820	-2.0707370	-5.6582180
H	47.1032570	-2.1694980	-5.7352610
C	45.1928020	-3.1175910	-6.0759210
O	47.8729740	8.4062650	-0.4427890
C	44.8990330	5.9166850	-1.9958250
C	45.2041180	5.9302880	-0.6167660
C	46.2020290	6.7782960	-0.1467690
H	46.4537810	6.8123390	0.9070850
C	46.9056970	7.6039130	-1.0219950

C	46.6176670	7.5865110	-2.3818500
H	47.1542340	8.2214620	-3.0739420
C	45.6191110	6.7388330	-2.8776050
C	44.4533600	5.0500670	0.3509440
H	43.3928450	5.3179290	0.3875720
H	44.8602780	5.1473980	1.3589600
H	44.5085600	3.9985220	0.0560160
C	45.3090680	6.7510970	-4.3551050
H	45.5670480	5.7991860	-4.8309860
H	45.8627600	7.5424180	-4.8661210
H	44.2419070	6.9118080	-4.5375210
C	48.6424540	9.2843350	-1.2833450
H	48.0013450	10.0140760	-1.7919330
H	49.2168310	8.7228290	-2.0294570
O	39.7886860	9.7843940	-0.5847790
O	38.3565610	-5.8324230	-7.1203650
C	38.9166980	10.4518400	-1.5112540
C	40.4171810	8.6232600	-1.0559210
C	41.7934700	8.6631200	-1.2913060
H	42.3242970	9.5904170	-1.1192420
C	42.4513860	7.5371490	-1.7209750
H	43.5123030	7.6037210	-1.8852740
C	41.7625180	6.3220520	-1.9826560
C	42.4283850	5.1123570	-2.4684740
C	43.8816400	4.9477690	-2.5259800
C	44.4106940	3.8004720	-3.0369130
H	45.4905610	3.6925170	-3.0563200
C	43.6280250	2.7137790	-3.5219680
C	44.2317910	1.5606170	-4.0401100
H	45.3142000	1.5386400	-4.0738560
C	43.4875650	0.4750380	-4.4911340
C	44.0814240	-0.7444600	-5.0314610
C	43.2395280	-1.8061130	-5.4565800
C	41.7900050	-1.6755140	-5.3573540
C	41.2581060	-0.5328970	-4.8567040
H	40.1778260	-0.4338280	-4.7825490
C	42.0660580	0.5709270	-4.4096850

C	41.4670440	1.7192460	-3.8933100
H	40.3844680	1.7328890	-3.8554270
C	42.2127350	2.8132880	-3.4394510
C	41.6265840	4.0279080	-2.8925500
C	40.2076130	4.1214530	-2.7780560
H	39.5932480	3.3028110	-3.1277510
C	39.5947050	5.1973800	-2.2305170
H	38.5154420	5.2237900	-2.1526080
C	40.3455160	6.3279990	-1.7951090
C	39.6803520	7.4710560	-1.2491500
C	40.8984230	-2.7917610	-5.8012670
C	40.4936620	-3.7755250	-4.8858630
C	39.6427920	-4.8064230	-5.3024610
H	39.3396740	-5.5571750	-4.5834060
C	39.2002510	-4.8551570	-6.6197420
C	39.6063600	-3.8834660	-7.5321930
H	39.2473040	-3.9534880	-8.5515950
C	40.4510890	-2.8513550	-7.1386000
C	40.9632760	-3.7396620	-3.4526710
H	42.0559440	-3.7217000	-3.3927740
H	40.6013860	-4.6119940	-2.9024050
H	40.6060120	-2.8439530	-2.9356940
C	40.8787720	-1.8094710	-8.1425680
H	40.5397670	-0.8105550	-7.8514240
H	40.4718720	-2.0314700	-9.1316930
H	41.9692210	-1.7615650	-8.2268260
C	37.8894100	-6.8677750	-6.2345020
H	37.3104680	-6.4502080	-5.4039420
H	38.7226190	-7.4571340	-5.8369980
O	38.0588430	9.5350340	-2.2109440
C	37.4580160	8.5347100	-1.4322090
C	36.0825060	8.6104100	-1.1992860
H	35.5294030	9.4425130	-1.6145530
C	35.4525790	7.6350610	-0.4652990
H	34.3922830	7.7262840	-0.3098650
C	36.1694340	6.5541570	0.1141390
C	35.5349680	5.5169030	0.9275800

C	36.3634280	4.6004940	1.6139680
C	37.7784590	4.6827320	1.4579860
H	38.4131530	4.0045830	2.0103450
C	38.3644970	5.5829690	0.6302950
H	39.4402550	5.6076910	0.5368450
C	37.5848670	6.5338590	-0.0875460
C	38.2224270	7.4965980	-0.9348180
H	39.4780330	10.9629360	-2.2966810
H	38.3457250	11.1492620	-0.8961380
H	49.3250930	9.8043540	-0.6134160
H	37.2494720	-7.5036710	-6.8427750
O	-30.9089650	-8.4360590	-5.0188140
C	-30.1960770	-8.4658530	-6.2660180
C	-31.6222690	-7.2576570	-4.7529740
C	-33.0181280	-7.3119440	-4.7672190
H	-33.5002630	-8.2624300	-4.9594460
C	-33.7538430	-6.1790050	-4.5197350
H	-34.8242090	-6.2660820	-4.5098220
C	-33.1356180	-4.9202210	-4.2984580
C	-31.7547340	-2.5191760	-3.8131850
H	-31.2159480	-1.5935550	-3.6695870
C	-31.0474030	-3.6490730	-4.0604470
H	-29.9682190	-3.6098190	-4.1116010
C	-31.7052610	-4.8973420	-4.2568230
C	-30.9430620	-6.0958500	-4.4402730
O	-29.4797170	-7.2444570	-6.5140430
C	-28.7695330	-6.7238500	-5.4221320
C	-27.3739750	-6.7921310	-5.4439280
H	-26.8876900	-7.2456790	-6.2989470
C	-26.6439750	-6.2849040	-4.3977050
H	-25.5729700	-6.3535550	-4.4507510
C	-27.2680730	-5.7219290	-3.2529700
C	-28.6637590	-4.9534770	-0.9353990
H	-29.2138890	-4.7125200	-0.0368820
C	-29.3646700	-5.3317890	-2.0331720
H	-30.4430090	-5.3842160	-1.9914550
C	-28.6981930	-5.7110570	-3.2337930

C	-29.4539120	-6.1499790	-4.3677370
H	-30.8727400	-8.5656070	-7.1156660
H	-29.5207720	-9.3178130	-6.1756290
O	-47.4046700	5.8303010	-4.8226520
C	-45.0081570	4.6147290	-1.6228660
C	-44.9437920	3.9737550	-2.8798960
C	-45.7602720	4.4152880	-3.9154380
H	-45.7291320	3.9430620	-4.8898900
C	-46.6435120	5.4758550	-3.7225120
C	-46.7190400	6.1051240	-2.4850110
H	-47.3993360	6.9305420	-2.3192080
C	-45.9083000	5.6746440	-1.4271630
C	-43.9960680	2.8248300	-3.1159970
H	-42.9533900	3.1488960	-3.0419540
H	-44.1460140	2.3956870	-4.1088640
H	-44.1392170	2.0330670	-2.3750360
C	-45.9941130	6.3878510	-0.0990570
H	-46.4248920	5.7484470	0.6778790
H	-46.6146320	7.2839570	-0.1778020
H	-45.0039430	6.6901640	0.2570610
C	-48.3418450	6.9161240	-4.6988370
H	-47.8346300	7.8539270	-4.4487570
H	-49.1031860	6.7016620	-3.9413490
O	-39.5838510	7.8203050	-3.4301270
O	-40.4178280	-2.6139440	9.9561590
C	-38.8888320	8.8555380	-2.7161420
C	-40.3464030	6.9395650	-2.6483200
C	-41.7399830	7.0147460	-2.7335710
H	-42.1824580	7.7557490	-3.3861990
C	-42.5202760	6.1524880	-2.0027290
H	-43.5885790	6.2351870	-2.0938490
C	-41.9525130	5.2028940	-1.1134830
C	-42.7569010	4.3041680	-0.2865240
C	-44.1906340	4.0945010	-0.4765310
C	-44.8746800	3.2940930	0.3920480
H	-45.9351980	3.1332190	0.2237710
C	-44.2702110	2.6280910	1.4973370

C	-45.0317060	1.8451150	2.3733970
H	-46.0962890	1.7808340	2.1855730
C	-44.4600890	1.1716980	3.4477490
C	-45.2245530	0.3498820	4.3847000
C	-44.5544470	-0.2953810	5.4577730
C	-43.1129100	-0.1417680	5.6213230
C	-42.4208790	0.6225420	4.7399540
H	-41.3491600	0.7394090	4.8593630
C	-43.0501800	1.3002010	3.6362800
C	-42.2934610	2.0758470	2.7579120
H	-41.2313040	2.1434130	2.9533770
C	-42.8663510	2.7558190	1.6759310
C	-42.1134000	3.5841130	0.7457460
C	-40.6949730	3.6665850	0.8759840
H	-40.2027790	3.1148320	1.6636650
C	-39.9323820	4.3994240	0.0285210
H	-38.8588190	4.4240730	0.1523780
C	-40.5276370	5.1903470	-0.9970440
C	-39.7153310	6.0157980	-1.8383520
C	-42.4061910	-0.8188080	6.7506110
C	-41.8873540	-2.1115540	6.5826020
C	-41.2152410	-2.7359510	7.6405430
H	-40.8209120	-3.7333140	7.4935960
C	-41.0645810	-2.0764420	8.8555560
C	-41.5825460	-0.7945780	9.0267250
H	-41.4515530	-0.3109510	9.9874000
C	-42.2529500	-0.1569500	7.9882450
C	-42.0466480	-2.8430830	5.2722660
H	-43.1005680	-2.9301860	4.9895170
H	-41.6280820	-3.8501860	5.3329980
H	-41.5454180	-2.3154010	4.4551360
C	-42.8094090	1.2297790	8.1971260
H	-42.3452650	1.9533800	7.5193340
H	-42.6380450	1.5659760	9.2223200
H	-43.8862380	1.2608160	8.0034160
C	-39.8604490	-3.9376460	9.8562250
H	-39.0895210	-3.9885220	9.0796830

H	-40.6356520	-4.6828520	9.6471710
O	-30.3770700	7.1264600	0.5502660
C	-32.9728910	4.4364110	-1.3137780
C	-32.9707770	4.6089860	0.0884020
C	-32.0877200	5.5185150	0.6625300
H	-32.0653060	5.6713920	1.7347140
C	-31.2059020	6.2510320	-0.1286550
C	-31.1962670	6.0790390	-1.5081910
H	-30.5188050	6.6411910	-2.1355240
C	-32.0736860	5.1662420	-2.1079210
C	-33.9185050	3.8308210	0.9675670
H	-34.9585280	4.0977840	0.7608360
H	-33.7213970	4.0310360	2.0213670
H	-33.8230490	2.7555930	0.7988660
C	-32.0613310	5.0119920	-3.6091160
H	-31.6905120	4.0265980	-3.9137640
H	-31.4233690	5.7681310	-4.0732630
H	-33.0675980	5.1121950	-4.0300070
C	-29.4278990	7.9097130	-0.1976660
H	-29.9301250	8.5686460	-0.9131240
H	-28.7161690	7.2712040	-0.7323380
O	-38.2344110	8.3633570	-1.5354460
O	-38.9930580	-7.4932890	-6.1421210
C	-37.5321190	7.1578180	-1.6799990
C	-36.1352080	7.1936520	-1.6441880
H	-35.6419570	8.1484410	-1.5129050
C	-35.4127640	6.0311990	-1.7645830
H	-34.3401240	6.0964630	-1.7308760
C	-36.0456970	4.7770550	-1.9732120
C	-35.3044670	3.5304840	-2.1596540
C	-33.8645780	3.3983870	-1.9337830
C	-33.2411650	2.2199700	-2.2249690
H	-32.1739580	2.1395250	-2.0410210
C	-33.9174390	1.0670180	-2.7220270
C	-33.2169610	-0.1061970	-3.0194440
H	-32.1451070	-0.0936140	-2.8698370
C	-33.8655930	-1.2607600	-3.4617230

C	-33.1792640	-2.5050160	-3.7846310
C	-33.8915650	-3.6835610	-4.1021280
C	-35.3467790	-3.5798970	-4.2381230
C	-35.9664040	-2.3905340	-3.9883320
H	-37.0427080	-2.3312440	-4.1157430
C	-35.2823760	-1.2105940	-3.5727100
C	-35.9808760	-0.0347980	-3.2875890
H	-37.0563850	-0.0629640	-3.4008010
C	-35.3313690	1.1279380	-2.8688770
C	-36.0134860	2.3821890	-2.5773190
C	-37.4299260	2.4498260	-2.7252730
H	-37.9702440	1.5768620	-3.0627090
C	-38.1333220	3.5763170	-2.4522820
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C	-37.4730040	4.7757800	-2.0585870
C	-38.2252080	5.9732240	-1.8348010
C	-36.2690290	-4.6664340	-4.7091820
C	-37.0402770	-5.3878910	-3.7846270
C	-37.9583700	-6.3439030	-4.2387040
H	-38.5381000	-6.8994240	-3.5115180
C	-38.1137940	-6.5693110	-5.6024950
C	-37.3588440	-5.8447170	-6.5223540
H	-37.5082710	-6.0407960	-7.5766270
C	-36.4406130	-4.8923600	-6.0929160
C	-36.8753630	-5.1716760	-2.3012380
H	-35.8270730	-5.2681530	-1.9995780
H	-37.4599520	-5.8991710	-1.7320580
H	-37.1983990	-4.1698590	-2.0009720
C	-35.6310300	-4.1252380	-7.1071760
H	-35.7604990	-3.0452150	-6.9877630
H	-35.9255420	-4.3944370	-8.1242550
H	-34.5609470	-4.3324050	-6.9991850
C	-39.8133940	-8.2753330	-5.2535370
H	-40.4709780	-7.6381100	-4.6533440
H	-39.2026430	-8.8950510	-4.5886680
H	-39.5723110	9.6235950	-2.3519710
H	-38.1730080	9.2518340	-3.4370510

H	-48.8135340	7.0049430	-5.6751500
H	-28.8976650	8.5090290	0.5400880
H	-39.4146820	-4.1390660	10.8282240
H	-40.4127740	-8.9143610	-5.8983440
C	-46.6178310	0.1730530	4.2604500
C	-45.3026000	-1.0838720	6.3583430
C	-46.6668640	-1.2388160	6.2147180
H	-47.2222750	-1.8486420	6.9189480
C	-47.3283790	-0.6034190	5.1545850
H	-48.3984360	-0.7220740	5.0350080
H	-44.7815550	-1.5709030	7.1748740
H	-47.1503990	0.6534440	3.4500850
O	-30.2742230	-0.8068230	8.7419910
C	-27.5285700	-2.3046550	5.9695530
C	-27.7473580	-0.9170210	6.1169720
C	-28.6703790	-0.4658920	7.0547720
H	-28.8549950	0.5929880	7.1898580
C	-29.3846990	-1.3681220	7.8416840
C	-29.1808270	-2.7358030	7.6942520
H	-29.7264030	-3.4494570	8.2977550
C	-28.2581830	-3.2122010	6.7537290
C	-26.9839870	0.0791090	5.2809130
H	-25.9115450	0.0389690	5.4961360
H	-27.3292940	1.0963870	5.4763090
H	-27.1042630	-0.1239350	4.2127240
C	-28.0384960	-4.7005640	6.6263850
H	-28.3861610	-5.0809800	5.6607420
H	-28.5709370	-5.2424120	7.4117160
H	-26.9759970	-4.9547910	6.6994460
C	-31.0535210	-1.6759590	9.5861880
H	-30.4109730	-2.2817580	10.2332300
H	-31.6954850	-2.3352320	8.9925820
O	-22.1413470	-1.6520260	9.6748550
O	-21.3684080	-5.7259330	-6.3375270
C	-21.3282830	-2.7230730	10.1796740
C	-22.8598970	-1.9308130	8.5017520
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H	-24.7182020	-1.9737530	9.5605000
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C	-26.5951980	-2.8034920	4.9048290
C	-27.2144380	-3.2033890	3.7567320
H	-28.2990530	-3.1750860	3.7171470
C	-26.5198480	-3.6214080	2.5833400
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C	-26.5594400	-4.4052200	0.2687650
C	-27.2398700	-4.8589540	-0.9374040
C	-26.5208490	-5.2172770	-2.1013780
C	-25.0651190	-5.0562610	-2.0810610
C	-24.4475690	-4.6495890	-0.9368330
H	-23.3677780	-4.5324140	-0.9439900
C	-25.1381770	-4.3324350	0.2706810
C	-24.4417260	-3.9287710	1.4118180
H	-23.3620460	-3.8966290	1.3426360
C	-25.0981300	-3.5755640	2.5920720
C	-24.4164210	-3.1682020	3.8137790
C	-22.9910550	-3.1300620	3.8311720
H	-22.4432130	-3.4195900	2.9455600
C	-22.2894750	-2.7397430	4.9228390
H	-21.2094180	-2.7221840	4.8913510
C	-22.9519280	-2.3975220	6.1362720
C	-22.1935970	-2.0371920	7.2962020
C	-24.1397860	-5.2366690	-3.2509090
C	-23.9853340	-4.2027070	-4.1877560
C	-23.0657600	-4.3426640	-5.2331120
H	-22.9627050	-3.5376340	-5.9480170
C	-22.3002230	-5.4981150	-5.3394160
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H	-21.8333770	-7.4102440	-4.5166210
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H	-25.8766460	-3.1594700	-4.2347110
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C	-23.5050030	-7.5358800	-2.3716790
H	-23.1851240	-7.2422740	-1.3677880
H	-22.9100940	-8.3986550	-2.6779130
H	-24.5493060	-7.8527950	-2.2899900
C	-21.1583650	-4.7115510	-7.3387040
H	-20.8066400	-3.7770910	-6.8900860
H	-22.0725280	-4.5203350	-7.9094460
O	-12.6669660	-3.6879010	7.0700370
C	-15.5216510	-0.9353990	5.7555890
C	-15.3940160	-2.2107130	5.1606540
C	-14.4296020	-3.0922470	5.6329840
H	-14.3139110	-4.0772430	5.1974550
C	-13.5850730	-2.7292320	6.6798880
C	-13.6973670	-1.4724060	7.2638260
H	-13.0500080	-1.1745670	8.0787480
C	-14.6595660	-0.5665410	6.8019070
C	-16.2981270	-2.6286290	4.0284140
H	-17.3411000	-2.6963270	4.3577380
H	-16.0056660	-3.6059000	3.6386590
H	-16.2681580	-1.9074730	3.2057570
C	-14.7772520	0.7852670	7.4653870
H	-14.4797070	1.5948780	6.7918470
H	-14.1442440	0.8389770	8.3536110
H	-15.8075250	0.9912090	7.7700270
C	-11.7685900	-3.3894960	8.1535130
H	-12.3152050	-3.1846840	9.0807440
H	-11.1261910	-2.5342240	7.9146100
O	-20.5818090	-3.3774180	9.1405150
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C	-19.9547240	-2.5340450	8.2113980
C	-18.5617240	-2.4309040	8.2445540
H	-18.0152970	-2.9960560	8.9887400
C	-17.9091400	-1.6340880	7.3363890
H	-16.8375280	-1.5812930	7.3872860

C	-18.6160070	-0.8612500	6.3781650
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C	-16.5079530	0.0514770	5.2024350
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H	-14.8958300	0.9661830	4.1950110
C	-16.7387100	1.9445710	3.6463470
C	-16.1217100	2.8780610	2.8099360
H	-15.0415010	2.8448390	2.7496400
C	-16.8553220	3.8093810	2.0743100
C	-18.5045260	5.5997630	0.5706690
C	-19.0436260	4.6694740	1.4111970
H	-20.1256230	4.5964200	1.4755710
C	-18.2716470	3.7605840	2.1919760
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H	-19.9705330	2.8489320	3.0742290
C	-18.1553580	1.9079280	3.7790150
C	-18.7505120	0.9266390	4.6781340
C	-20.1698910	0.8707700	4.8012770
H	-20.7789210	1.5639770	4.2388700
C	-20.7915020	-0.0338710	5.5979030
H	-21.8697740	-0.0493620	5.6566220
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C	-20.7142720	-1.8463090	7.2835700
C	-19.5225590	6.3875290	-0.2035870
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H	-21.1804860	6.3400910	-3.1681750
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H	-21.6695710	9.0183260	0.1326370
C	-20.1700440	7.4874590	0.3997960
C	-19.2230510	4.8027180	-2.1554320
H	-18.1552330	4.9939830	-2.3042060
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H	-20.3054960	8.8757250	2.0404000
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H	-23.3654940	7.1410860	-3.5528530
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H	-11.1584810	-4.2818930	8.2829080
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O	-4.7595750	-4.7786670	-8.8089420
C	-5.5369280	-5.9840740	-8.9014060
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H	-2.1685380	-4.8710410	-8.6550280
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H	-10.0449670	-4.0495460	-6.6608540
C	-8.2862710	-2.9738720	-5.9838030
C	-6.7664700	-0.7755910	-5.1057430
H	-6.1664590	0.0763730	-4.8186120
C	-6.1269720	-1.8897960	-5.5394790
H	-5.0478550	-1.9052920	-5.5903990
C	-6.8572960	-3.0316000	-5.9779670

C	-6.1643010	-4.1792950	-6.4793950
H	-4.9067300	-6.8602280	-9.0552910
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C	9.6666690	-3.1418110	4.6539780
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H	10.3840770	-6.3682030	3.8045780
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H	11.8476210	-4.0572340	7.0972380
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H	7.7127320	-4.3896170	2.9306270
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H	9.0040630	-3.6940540	1.9587330
C	10.5276790	-1.7727240	6.6086010
H	11.0182020	-0.9599310	6.0637340
H	11.0740590	-1.9274320	7.5422730
H	9.5215740	-1.4205710	6.8583220
C	12.7492560	-6.4509730	6.9838910
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H	13.5395650	-5.6992210	6.8877090
O	3.9843060	-4.8735120	7.4631930
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C	3.3446460	-4.1778030	8.5452200
C	4.8233170	-4.0955320	6.6512860
C	6.2037900	-4.2929360	6.7461510
H	6.5770800	-5.0326470	7.4418910
C	7.0582550	-3.5573020	5.9635180
H	8.1137840	-3.7359900	6.0626020
C	6.5849970	-2.5576780	5.0730880
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C	9.5088540	2.1048010	1.4474780
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C	9.7906460	4.0746040	-0.0712640
C	8.3337890	4.2275000	-0.0676100
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H	6.4927940	3.5073310	0.6677640
C	8.0964500	2.2694300	1.4074200
C	7.2546970	1.3878460	2.0920330
H	6.1909400	1.5752740	2.0283910
C	7.7513860	0.3044370	2.8199140
C	6.9167970	-0.6242530	3.5708460
C	5.5080620	-0.4099340	3.6141100
H	5.0865930	0.4428580	3.1022540
C	4.6695250	-1.2382130	4.2840540
H	3.6075100	-1.0384530	4.2923430
C	5.1704140	-2.3452710	5.0274860
C	4.2769110	-3.1753210	5.7782730
C	7.5587950	5.3257530	-0.7331400
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C	6.1015870	6.0892680	-2.5152610
H	5.5946990	5.8867090	-3.4498020
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H	6.5332640	8.5394630	-0.2233710
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H	6.5245160	3.7756150	-3.6142020
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C	8.1437220	6.8681830	1.2028500
H	7.8811380	6.1314000	1.9635210
H	7.8808090	7.8588310	1.5724940
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H	5.2108590	7.9900600	-4.4531670
O	-4.8250970	-0.0752160	7.0544990
C	-2.3902660	-1.9723660	4.2397020
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C	-3.1071720	-0.0039220	5.4490850
H	-3.0398540	1.0535100	5.6724240
C	-4.0546740	-0.7623180	6.1328540
C	-4.1814240	-2.1227350	5.8715390
H	-4.9129270	-2.7271350	6.3924440
C	-3.3545080	-2.7359010	4.9181950
C	-1.2580980	0.2532230	3.7828740
H	-0.2321960	-0.0520910	4.0369800
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H	-1.3592160	0.1634440	2.6930140
C	-3.4951820	-4.2203600	4.6674740
H	-3.8891200	-4.4250600	3.6670500
H	-4.1726290	-4.6704720	5.3935600
H	-2.5335020	-4.7246990	4.7403050
C	-5.8269520	-0.7917430	7.7970600
H	-5.3807730	-1.5862420	8.4049790
H	-6.5825640	-1.2252880	7.1326610
O	2.8083020	-2.9084250	8.1350270
O	3.1876400	-6.5857340	-7.9899110
C	2.1065360	-2.9082490	6.9214210
C	0.7183490	-2.7539830	6.9600360
H	0.2331640	-2.6454070	7.9224640
C	-0.0051680	-2.7348680	5.7932100
H	-1.0713980	-2.6141740	5.8610870
C	0.6143370	-2.9124440	4.5272050
C	-0.1358690	-2.9525440	3.2736900
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H	-3.2442250	-2.4883260	1.9058720
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C	-2.2855170	-3.4130320	-0.3981540
H	-3.3420730	-3.1782050	-0.3702390
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C	-1.7053930	-4.3348110	-4.0349370
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C	0.3739820	-4.4618360	-2.7516670
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C	-0.2729740	-4.0621690	-1.5460610
C	0.4481560	-3.9051990	-0.3582780
H	1.5113730	-4.1031720	-0.3991840
C	-0.1640230	-3.5075910	0.8315470
C	0.5387100	-3.3523580	2.0983280
C	1.9381580	-3.6202130	2.1526150
H	2.4526560	-3.9418020	1.2574880
C	2.6576230	-3.4833090	3.2929700
H	3.7193900	-3.6937050	3.2914760
C	2.0294360	-3.1189050	4.5195490
C	2.7917250	-3.0425120	5.7289690
C	0.6133850	-5.0818680	-5.0642000
C	1.4657860	-4.1906520	-5.7350530
C	2.3366650	-4.6681010	-6.7232590
H	2.9785760	-3.9653070	-7.2361270
C	2.3640240	-6.0228610	-7.0307240
C	1.5275980	-6.9120600	-6.3583780
H	1.5764260	-7.9627510	-6.6186830
C	0.6535470	-6.4588510	-5.3754760
C	1.4380530	-2.7125050	-5.4290490
H	0.4206860	-2.3119750	-5.4940570
H	2.0659330	-2.1567790	-6.1295030
H	1.7943380	-2.5025010	-4.4154800
C	-0.2489780	-7.4374700	-4.6675790
H	-0.1168280	-7.3888150	-3.5826870
H	-0.0445830	-8.4597980	-4.9916110
H	-1.3032770	-7.2224750	-4.8711040
C	4.0857380	-5.7303800	-8.7244650
H	4.7981460	-5.2347650	-8.0570880
H	3.5380280	-4.9757580	-9.2981750
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C	-6.2660590	6.9753630	-0.2953160
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C	-5.8291290	7.7368610	-2.5429780
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H	-7.9174750	4.1751580	-0.0488890
C	-7.0958070	6.8349570	-4.5145290
H	-6.8169840	5.8762250	-4.9644900
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H	-8.1626540	6.9757910	-4.7154750
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C	-13.1608380	-3.8042520	-6.8563230
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H	-10.8702400	-2.8622310	-2.7277500
C	-11.9692380	-1.7935580	-7.7589890
H	-12.2254890	-0.7864850	-7.4182750
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H	-10.9194610	-1.7624200	-8.0666800
C	-14.6521360	-6.7317350	-5.1983870
H	-14.9862890	-6.3058500	-4.2465830
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H	-13.1316520	5.7604860	0.2202900
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C	-14.2668900	7.6024570	-1.3651950
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C	-13.8996738	0.1168774	0.0200344
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H	-6.5197858	-2.7527017	-4.2277076
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O	-0.4840038	5.3550774	6.2911204
H	3.7019432	1.8259463	3.7950534
H	3.7140572	3.1567874	2.6185534
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C	6.1192022	-2.2076497	2.4987074
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H	4.0075822	-3.6465726	3.7227304
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H	1.8678972	-3.1306516	4.9602634
H	1.6065512	-1.7360517	3.8874534
H	1.5624072	-3.3762907	3.2272784
C	8.7822122	-1.2819746	-0.0302396
C	9.0112462	-0.9199926	-1.3605426
C	9.9430672	-1.5754136	0.7468004
C	10.2934852	-0.7720516	-1.8994276
H	8.1875382	-0.7752906	-2.0395836
C	11.2253472	-1.4074927	0.2140004
C	9.7950592	-2.0890997	2.0783614
C	10.4409882	-0.4577967	-3.2916496
C	11.4546662	-0.9692156	-1.0930806
H	12.0485952	-1.6712147	0.8568414
H	10.6965022	-2.3193417	2.6384254
C	8.5810892	-2.3176426	2.6367934
C	11.6546012	-0.3458577	-3.8853676
H	9.5392572	-0.3303907	-3.8832056
C	12.7759232	-0.7570077	-1.6871236
C	8.4889932	-2.8965726	4.0136034
C	12.8617592	-0.4920427	-3.0846626
C	11.7454182	-0.0583567	-5.3510726
C	14.0020112	-0.7789987	-0.9661606
C	8.4887522	-2.0486017	5.1425094
C	8.4144112	-4.2877427	4.1890084
C	14.1171532	-0.3531837	-3.7151456
C	11.8347962	-1.1220596	-6.2759116
C	11.7292872	1.2664704	-5.8148956
C	15.2235972	-0.6226417	-1.6031546
C	14.2391832	-0.9356807	0.5271974
C	8.4186592	-2.6024736	6.4165894

C	8.5637912	-0.5508656	4.9809004
C	8.3452212	-4.8255726	5.4800824
C	8.4060432	-5.2155087	2.9987824
H	14.1358662	-0.1731276	-4.7805796
C	15.2862532	-0.4469366	-2.9905636
C	11.9018982	-0.8435187	-7.6369476
C	11.8577632	-2.5537267	-5.8018736
C	11.7969322	1.5257653	-7.1895496
C	11.6400602	2.4222393	-4.8484746
C	16.4013372	-0.7242597	-0.6538096
H	14.0911652	-1.9774527	0.8411664
H	13.5619902	-0.3210857	1.1260144
C	15.7048332	-0.5025156	0.7202874
H	8.4183932	-1.9749846	7.2994474
C	8.3492582	-3.9835326	6.5864124
H	7.7581902	-0.1803857	4.3386224
H	8.4877092	-0.0503687	5.9489924
H	9.5047182	-0.2460016	4.5125124
H	8.2902182	-5.9004456	5.5957834
H	8.2996592	-6.2564946	3.3136614
H	7.5824982	-4.9796106	2.3171704
H	9.3297782	-5.1283807	2.4184964
O	16.5505022	-0.3684326	-3.5408546
H	11.9688002	-1.6403177	-8.3675466
C	11.8810862	0.4727744	-8.0932806
H	12.6909142	-2.7312996	-5.1141336
H	10.9417532	-2.8084127	-5.2599076
H	11.9579522	-3.2415936	-6.6445706
H	11.7819882	2.5536554	-7.5287326
H	12.4297222	2.3691533	-4.0921896
H	11.7313592	3.3777804	-5.3708816
H	10.6879102	2.4205243	-4.3088406
C	17.5750382	0.2183413	-0.8344156
C	17.1024702	-2.1089887	-0.7684506
H	16.2094652	-1.0447787	1.5251584
H	15.7383802	0.5643974	0.9579554
O	8.2833492	-4.4244696	7.8983724

C	16.6973172	-0.1037496	-4.9577176
O	11.9526712	0.6326624	-9.4678256
C	18.7994522	-0.3996127	-0.6308206
C	17.5064832	1.5872644	-1.1191306
C	18.5685082	-1.8768286	-0.3561036
H	16.6024412	-2.8703576	-0.1627986
H	17.0670012	-2.4303066	-1.8131616
C	8.2281712	-5.8401506	8.1529414
H	16.1987362	0.8412614	-5.2050396
H	16.2171482	-0.9043796	-5.5332326
C	18.1839382	-0.0355266	-5.2315196
C	11.9185182	1.9635934	-10.0146346
C	20.0225892	0.3222714	-0.7111246
O	16.2399292	2.1249133	-1.2381596
C	18.6725192	2.3066823	-1.2719416
H	18.7204452	-2.1071086	0.7067354
H	19.2465012	-2.5197266	-0.9234786
H	9.1166372	-6.3499577	7.7655384
H	7.3314392	-6.2904576	7.7139394
H	8.1932772	-5.9395587	9.2360264
H	18.3700522	0.1784293	-6.2880356
H	18.6428092	0.7493163	-4.6252476
H	18.6625902	-0.9839406	-4.9768026
H	12.7701582	2.5595093	-9.6692186
H	10.9871202	2.4778583	-9.7549006
H	11.9765002	1.8360673	-11.0937786
C	19.9306402	1.6942553	-1.0851956
C	21.3464912	-0.2473336	-0.4529796
C	16.0874172	3.5173344	-1.6084596
H	18.6493232	3.3544373	-1.5357186
C	21.1341852	2.4863473	-1.2944566
C	22.5040322	0.5467323	-0.71117826
C	21.5816322	-1.5150397	0.0862864
H	16.5816322	3.6942364	-2.5714016
H	16.5687262	4.1530274	-0.8554516
C	14.5996912	3.7808643	-1.6911756
C	21.0367162	3.9243794	-1.6966326

C	22.3504052	1.9089714	-1.1354276
C	23.7886802	0.0279883	-0.5194336
C	22.8662562	-2.0260727	0.2982594
H	20.7611912	-2.1398507	0.3976964
H	14.4094022	4.8175903	-1.9837916
H	14.1396942	3.1156094	-2.4259686
H	14.1254672	3.5973833	-0.7242636
C	20.9418352	4.9296584	-0.7090926
C	21.0519072	4.2825483	-3.0538486
H	23.2495182	2.4928174	-1.3086636
C	24.0238292	-1.2680616	-0.0523856
H	24.6091322	0.6978403	-0.7160246
C	23.0198202	-3.3121897	0.9156494
C	20.8683702	6.2641973	-1.0939046
C	20.9200772	4.5696964	0.7554494
C	20.9779632	5.6321914	-3.4205446
C	21.1467592	3.2286504	-4.1299846
C	25.3476852	-1.8615317	0.1453084
H	22.1206812	-3.8576656	1.1863714
C	24.2360112	-3.8434986	1.1920184
H	20.7971882	7.0549073	-0.3571256
C	20.8883312	6.6156033	-2.4420296
H	20.0905742	3.8934353	0.9861874
H	21.8388282	4.0545763	1.0524844
H	20.8146202	5.4633763	1.3747694
H	20.9923402	5.8895044	-4.4719236
H	20.3598442	2.4757793	-4.0188546
H	21.0551162	3.6740823	-5.1237186
H	22.1009362	2.6945393	-4.0845326
C	25.4395452	-3.1216297	0.8044684
C	26.5707862	-1.2782297	-0.2875566
C	24.3335172	-5.1693986	1.8788604
O	20.8102182	7.9728813	-2.7097086
C	26.6975572	-3.6985187	1.0824464
C	27.7951542	-1.8709117	-0.0185866
C	26.8016682	-0.0077477	-1.0897746
C	24.3418492	-6.3621966	1.1234724

C	24.4050892	-5.2331446	3.2797614
C	20.8440612	8.4134304	-4.0795056
H	26.7206302	-4.6460067	1.6016994
C	27.8636892	-3.0688226	0.7025694
C	28.9688262	-1.0569057	-0.5272966
H	26.6506242	0.8834034	-0.4662436
H	26.1230122	0.0787734	-1.9423426
C	28.2671762	-0.1183127	-1.5514036
C	24.4169492	-7.5877466	1.7771514
C	24.2702992	-6.3208816	-0.3825756
C	24.4796092	-6.4769106	3.9188114
C	24.4045032	-3.9728687	4.1099464
H	19.9949912	8.0181554	-4.6474466
H	21.7775142	8.1184144	-4.5704746
H	20.7809132	9.4989713	-4.0373696
O	29.1300252	-3.5460516	0.9779354
C	30.1462892	-1.7757337	-1.1563026
C	29.6658152	-0.2865637	0.6317214
H	28.7677282	0.8515343	-1.6248146
H	28.3014022	-0.5926546	-2.5361686
H	24.4239432	-8.5177126	1.2219284
C	24.4836242	-7.6467557	3.1674864
H	25.0728232	-5.7048217	-0.8010876
H	24.3543252	-7.3252247	-0.8041086
H	23.3272302	-5.8846967	-0.7262076
H	24.5323692	-6.5064756	4.9996034
H	24.5090882	-4.2034557	5.1729714
H	25.2253862	-3.3078527	3.8229454
H	23.4781502	-3.4062067	3.9743504
C	29.2816652	-4.8249707	1.6422164
C	31.3680652	-1.2284917	-0.7952126
C	30.0831682	-2.8454187	-2.0571856
C	31.1315782	-0.1004306	0.1959194
H	29.1616522	0.6584153	0.8539654
H	29.6317702	-0.9080027	1.5309434
O	24.5552822	-8.9190257	3.7115134
H	28.7836812	-5.6032667	1.0516054

H	28.8034182	-4.7856907	2.6284754
C	30.7689692	-5.0793226	1.7545914
C	32.5939252	-1.7329507	-1.3112996
O	28.8188952	-3.2771277	-2.4069966
C	31.2520972	-3.4038986	-2.5287746
H	31.2804092	0.8779864	-0.2797736
H	31.8088372	-0.1465317	1.0527334
C	24.6133022	-9.0598336	5.1428534
H	30.9578682	-6.0428296	2.2368414
H	31.2260462	-5.0857406	0.7621734
H	31.2473692	-4.2929696	2.3431054
C	32.5076382	-2.8742076	-2.1602986
C	33.9153632	-1.1745436	-1.0185836
C	28.6720982	-4.4377126	-3.2621966
H	31.2332232	-4.2580297	-3.1906056
H	23.7226752	-8.6390866	5.6215524
H	25.5074552	-8.5804246	5.5555064
H	24.6556182	-10.1313267	5.3279764
C	33.7145082	-3.5231107	-2.6524806
C	35.0762842	-1.8661806	-1.4783566
C	34.1451672	0.0334743	-0.3544666
H	29.1727382	-5.2966117	-2.7993856
H	29.1504102	-4.2439136	-4.2299896
C	27.1856812	-4.6765466	-3.4136846
C	33.6230002	-4.7244297	-3.5399986
C	34.9283122	-3.0394297	-2.2910646
C	36.3587132	-1.3927957	-1.1821636
C	35.4276412	0.5177464	-0.0768326
H	33.3222032	0.6634963	-0.0606166
H	27.0000212	-5.5546697	-4.0389886
H	26.7285222	-4.8374207	-2.4343846
H	26.7047642	-3.8103477	-3.8741106
C	33.6166822	-6.0214237	-2.9821456
C	33.5550552	-4.5667317	-4.9336466
H	35.8298192	-3.5337186	-2.6407106
H	37.1822262	-1.9596076	-1.5835906
C	36.5881922	-0.2251827	-0.4491906

C	35.5761842	1.7981094	0.5535784
C	33.5470372	-7.1288047	-3.8210506
C	33.6847392	-6.2178787	-1.4882306
C	33.4860792	-5.6943987	-5.7609786
C	33.5537282	-3.1913336	-5.5547696
C	37.9092822	0.2975663	-0.0953726
H	34.6749522	2.3476484	0.8086784
C	36.7903322	2.3446003	0.8085414
H	33.5416972	-8.1346967	-3.4194176
C	33.4839102	-6.9680896	-5.2034966
H	32.8802012	-5.6765866	-0.9798866
H	33.6015952	-7.2762347	-1.2304686
H	34.6262542	-5.8399786	-1.0777686
H	33.4360832	-5.5533716	-6.8330666
H	33.4535272	-3.2517976	-6.6412496
H	32.7294212	-2.5824396	-5.1697406
H	34.4775282	-2.6502597	-5.3279186
C	37.9965072	1.5944954	0.4886944
C	39.1338302	-0.4034106	-0.2764166
C	36.8828212	3.7034584	1.4283084
O	33.4175032	-8.1388326	-5.9414746
C	39.2522772	2.1699683	0.7796314
C	40.3556382	0.1744143	0.0331134
C	39.3687782	-1.8196077	-0.7765096
C	36.9874822	4.8486173	0.6082544
C	36.8534752	3.8485913	2.8242374
C	33.3642602	-8.0524367	-7.3773336
H	39.2720432	3.1638323	1.2035714
C	40.4203912	1.4824864	0.5276494
C	41.5321122	-0.7298577	-0.2783036
H	39.2277532	-1.8805287	-1.8637896
H	38.6856172	-2.5429356	-0.3237496
C	40.8306982	-2.1147306	-0.3907356
C	37.0565842	6.1079244	1.1945664
C	37.0245492	4.7183164	-0.8939436
C	36.9235012	5.1256144	3.3950074
C	36.7473422	2.6419184	3.7244784

H	34.2549122	-7.5589467	-7.7805536
H	32.4697142	-7.5165627	-7.7123716
H	33.3261492	-9.0814716	-7.7291606
O	41.6852192	1.9945164	0.7402664
C	42.6969132	-0.7799447	0.6909874
C	42.2467502	-0.2962937	-1.5911626
H	41.3376962	-2.7715696	-1.1035116
H	40.8555332	-2.5967616	0.5905634
H	37.1352022	7.0025043	0.5890204
C	37.0229552	6.2477763	2.5804694
H	37.8575352	4.0857643	-1.2174926
H	36.1096982	4.2549414	-1.2760806
H	37.1347412	5.6967064	-1.3671936
H	36.8986652	5.2180783	4.4732624
H	37.5328632	1.9119903	3.5043844
H	36.8326502	2.9286373	4.7755704
H	35.7919542	2.1250503	3.5905474
C	41.8328272	3.3128494	1.3235094
C	43.9272082	-0.8354546	0.0539714
C	42.6152352	-0.8246277	2.0877614
C	43.7104642	-0.7551047	-1.4485286
H	41.7538442	-0.7057146	-2.4777066
H	42.2147192	0.7946804	-1.6592426
O	37.0981242	7.5475123	3.0544414
H	41.3324952	3.3372643	2.2991074
H	41.3546492	4.0571804	0.6753644
C	43.3193562	3.5623034	1.4554584
C	45.1433722	-0.9282636	0.7859924
O	41.3435872	-0.8310287	2.6264964
C	43.7742092	-0.8490467	2.8338884
H	43.8646422	-1.7345027	-1.9205106
H	44.3946802	-0.0541507	-1.9337506
C	37.0536652	7.7721253	4.4755214
H	43.5053392	4.5408073	1.9076824
H	43.7768372	2.7915233	2.0804094
H	43.7997892	3.5328744	0.4747244
C	45.0381962	-0.8876027	2.2065724

C	46.4729482	-1.0444446	0.1840004
C	41.1773452	-0.7799626	4.0648794
H	43.7408022	-0.8396286	3.9140254
H	37.8978262	7.2924774	4.9824414
H	36.1160302	7.4070424	4.9079134
H	37.1180542	8.8510883	4.6013634
C	46.2340962	-0.8708856	3.0368294
C	46.7207642	-1.2719316	-1.1724736
C	47.6226972	-0.9764896	1.0271734
H	41.6761012	0.1142664	4.4576024
H	41.6458892	-1.6606367	4.5207904
C	39.6872062	-0.7443966	4.3253824
C	47.4558312	-0.8868076	2.4494954
C	46.1224392	-0.8212426	4.5282394
C	48.0105162	-1.3541136	-1.7074136
H	45.9067502	-1.4318336	-1.8597906
C	48.9123852	-1.0373246	0.4892694
H	39.4866442	-0.6888047	5.3993184
H	39.2406282	0.1249794	3.8367384
H	39.2082672	-1.6411376	3.9253814
H	48.3492602	-0.8540806	3.0659354
C	46.1041492	0.4213423	5.1983974
C	46.0469482	-2.0117947	5.2689064
C	48.1779742	-1.6524857	-3.1008856
C	49.1600222	-1.1858297	-0.8781256
H	49.7266362	-1.0010377	1.1937324
C	46.0153492	0.4510994	6.5862684
C	46.1798422	1.7144933	4.4257244
C	45.9586322	-1.9603436	6.6655074
C	46.0579072	-3.3526166	4.5764204
C	49.3999792	-1.7917017	-3.6711686
H	47.2848122	-1.7917346	-3.7026836
C	50.4894752	-1.2325546	-1.4896856
H	46.0008882	1.3904843	7.1252744
C	45.9447342	-0.7325476	7.3176734
H	45.3837582	1.7760844	3.6765834
H	46.0882382	2.5736074	5.0943194

H	47.1274952	1.8024883	3.8854484
H	45.9030802	-2.8884636	7.2198284
H	45.9491682	-4.1670286	5.2968534
H	45.2438822	-3.4303777	3.8485634
H	46.9898002	-3.5089436	4.0243944
C	50.5954662	-1.5791466	-2.8678316
C	49.5118142	-2.1456867	-5.1207806
C	51.7047852	-0.9395786	-0.8109826
O	45.8589692	-0.5843206	8.6926944
C	51.8598182	-1.7090687	-3.4821166
C	49.6161412	-3.4987427	-5.5120986
C	49.5003142	-1.1383136	-6.0983556
C	52.9354342	-1.0562946	-1.4390286
C	51.9200332	-0.4514157	0.6124794
C	45.7994152	-1.7638257	9.5156324
H	51.8938912	-1.9936746	-4.5241196
C	53.0182742	-1.4805496	-2.7705016
C	49.7024012	-3.8170996	-6.8632976
C	49.6342852	-4.5987326	-4.4802976
C	49.5872702	-1.4798567	-7.4538056
C	49.3953252	0.3157834	-5.7080826
C	54.0990072	-0.7396797	-0.5199556
H	51.7698202	-1.2655877	1.3338104
H	51.2325562	0.3523503	0.8885734
C	53.3816982	0.0348164	0.6236384
H	46.6938782	-2.3831797	9.3903464
H	44.9097612	-2.3623516	9.2922364
H	45.7470682	-1.4010296	10.5402354
O	54.2903782	-1.6318557	-3.2865736
H	49.7810072	-4.8465426	-7.1907166
C	49.6860442	-2.8143687	-7.8305466
H	50.4573372	-4.4646476	-3.7708926
H	48.7106832	-4.6092967	-3.8933416
H	49.7480862	-5.5761217	-4.9547446
H	49.5755032	-0.6896026	-8.1935126
H	50.1747532	0.5915244	-4.9905676
H	49.4915502	0.9641034	-6.5825686

H	48.4359432	0.5335214	-5.2285456
C	55.2740362	0.0477754	-1.0658716
C	54.8037672	-2.0386236	-0.0317086
H	53.8753572	-0.1135136	1.5884304
H	53.4094212	1.1027073	0.3896784
C	54.4574662	-1.9881226	-4.6809366
O	49.7770572	-3.2459616	-9.1441346
C	56.4961292	-0.4182997	-0.6056726
C	55.2081782	1.1684044	-1.9023196
C	56.2628942	-1.6430357	0.2641484
H	54.2955172	-2.4783677	0.8313264
H	54.7849282	-2.7698506	-0.8446566
H	53.9617502	-1.2389496	-5.3100606
H	53.9863882	-2.9600276	-4.8713746
C	55.9478562	-2.0312966	-4.9388226
C	49.7476742	-2.2680627	-10.1997896
C	57.7195582	0.2094413	-0.9697496
O	53.9429572	1.5981854	-2.2511666
C	56.3756212	1.7628043	-2.3318186
H	56.3980722	-1.4015826	1.3267914
H	56.9506822	-2.4600726	0.0310724
H	56.1492492	-2.2800827	-5.9848546
H	56.3970522	-1.0611137	-4.7128276
H	56.4235022	-2.7813847	-4.3027326
H	50.5931812	-1.5756036	-10.1267346
H	48.8116792	-1.6995007	-10.1909816
H	49.8208652	-2.8365747	-11.1247826
C	57.6316792	1.2936614	-1.8902786
C	59.0402752	-0.1901757	-0.4803986
C	53.7941672	2.7027664	-3.1769736
H	56.3550012	2.6007863	-3.0139156
C	58.8375582	1.9282724	-2.4030306
C	60.2007562	0.4230074	-1.0413646
C	59.2688262	-1.1058166	0.5504004
H	54.2998622	2.4587893	-4.1190706
H	54.2660332	3.5998124	-2.7581376
C	52.3074322	2.8984214	-3.3793046

C	58.7447752	3.0611383	-3.3762626
C	60.0519232	1.4769374	-2.0036116
C	61.4830252	0.0391234	-0.6354406
C	60.5509042	-1.4732607	0.9718274
H	58.4445452	-1.5399406	1.0914664
H	52.1202782	3.7131343	-4.0848886
H	51.8565782	1.9823914	-3.7687896
H	51.8216512	3.1384473	-2.4306886
C	58.6364432	4.3889004	-2.9070436
C	58.7778662	2.8125683	-4.7574326
H	60.9529512	1.9361093	-2.3993376
C	61.7122422	-0.9344206	0.3406744
H	62.3060972	0.5645904	-1.0904676
C	60.6979322	-2.3703706	2.0820184
C	58.5676342	5.4354894	-3.8204616
C	58.5954792	4.6811463	-1.4279166
C	58.7082902	3.8805194	-5.6608356
C	58.8877012	1.4033714	-5.2864886
C	63.0335032	-1.3844996	0.7826244
H	59.7959632	-2.7491476	2.5534554
C	61.9111562	-2.7285747	2.5695214
H	58.4864522	6.4629854	-3.4876086
C	58.6053822	5.1846754	-5.1905096
H	57.7623992	4.1618993	-0.9431286
H	59.5098542	4.3438624	-0.9300826
H	58.4829332	5.7522854	-1.2453856
H	58.7364202	3.6697063	-6.7222466
H	58.1023962	0.7619864	-4.8739036
H	58.8049872	1.3864513	-6.3760686
H	59.8432742	0.9457944	-5.0119966
C	63.1186962	-2.2405956	1.9186454
C	64.2602422	-1.0425076	0.1489574
C	62.0015172	-3.6304157	3.7602264
O	58.5304912	6.3013704	-6.0073366
C	64.3738462	-2.6415176	2.4252604
C	65.4815752	-1.4628056	0.6531794
C	64.4984962	-0.2388506	-1.1192126

C	62.0103192	-5.0321377	3.5913624
C	62.0658732	-3.0854437	5.0527834
C	58.5826252	6.1224744	-7.4345326
H	64.3917042	-3.2748527	3.3007444
C	65.5434732	-2.2350917	1.8190834
C	66.6599482	-0.9473506	-0.1496946
H	64.3478212	0.8337193	-0.9386586
H	63.8236362	-0.5252457	-1.9300396
C	65.9656552	-0.5380447	-1.4811846
C	62.0788742	-5.8574196	4.7090134
C	61.9457632	-5.6426916	2.2136624
C	62.1338272	-3.9334606	6.1650234
C	62.0642662	-1.5906357	5.2602834
H	57.7412802	5.5194893	-7.7926666
H	59.5226102	5.6531154	-7.7436386
H	58.5188032	7.1238994	-7.8555186
O	66.8074742	-2.5475947	2.2798804
C	67.8366882	-1.8688366	-0.4042476
C	67.3556242	0.2439784	0.5698044
H	66.4694832	0.3062084	-1.9607236
H	66.0025952	-1.3887447	-2.1673916
H	62.0860242	-6.9357827	4.6078094
C	62.1384502	-5.3127426	5.9899404
H	62.7489362	-5.2634427	1.5735614
H	62.0336022	-6.7303866	2.2652984
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H	62.1809592	-3.4953256	7.1537464
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H	62.8901992	-1.1140186	4.7225324
H	61.1414212	-1.1368936	4.8860124
C	66.9524872	-3.4157996	3.4311194
C	69.0600152	-1.2227846	-0.3084476
C	67.7702712	-3.2211476	-0.7599926
C	68.8243832	0.2211153	0.1058984
H	66.8555962	1.1941994	0.3612994
H	67.3144712	0.0694044	1.6485384
O	62.2039642	-6.2273017	7.0286154

H	66.4570822	-4.3731606	3.2297034
H	66.4677292	-2.9563737	4.3010744
C	68.4385352	-3.5950637	3.6522394
C	70.2850762	-1.9025406	-0.5589876
O	66.5055522	-3.7572667	-0.8949776
C	68.9376682	-3.9310086	-0.9432286
H	68.9827732	0.9035243	-0.7396146
H	69.4948882	0.5415534	0.9075074
C	62.2534212	-5.7388777	8.3817894
H	68.6224602	-4.2577207	4.5028904
H	68.9024872	-4.0265996	2.7620434
H	68.9142362	-2.6315346	3.8494564
C	70.1943952	-3.2976966	-0.8364786
C	71.6091772	-1.2750676	-0.5391036
C	66.3546132	-5.1725667	-1.1687476
H	68.9164522	-4.9864437	-1.1742526
H	61.3613492	-5.1529197	8.6272004
H	63.1466772	-5.1288976	8.5539094
H	62.2914182	-6.6266336	9.0099494
C	71.3974332	-4.1009396	-1.0026916
C	72.7672312	-2.1041156	-0.6724126
C	71.8380332	0.1007394	-0.4330126
H	66.8501612	-5.7504856	-0.3794986
H	66.8356692	-5.4152077	-2.1240466
C	64.8673272	-5.4475806	-1.2083046
C	71.2994562	-5.5679996	-1.2807666
C	72.6136302	-3.5133197	-0.8929166
C	74.0490642	-1.5496356	-0.6289186
C	73.1216762	0.6560814	-0.4009686
H	71.0144992	0.7933554	-0.3955876
H	64.6783582	-6.5087927	-1.3944556
H	64.4076792	-5.1685786	-0.2571336
H	64.3916532	-4.8628927	-1.9991336
C	71.2892272	-6.4937126	-0.2147296
C	71.2297992	-6.0306296	-2.6046846
H	73.5127202	-4.1128047	-0.9991256
H	74.8858822	-2.2300777	-0.7325616

C	74.2678432	-0.1812306	-0.4815676
C	73.2939752	2.0798803	-0.2925746
C	71.2137982	-7.8551376	-0.4895696
C	71.3592282	-6.0221196	1.2162444
C	71.1547902	-7.4053787	-2.8600676
C	71.2328742	-5.0615816	-3.7616396
C	75.5939042	0.4277954	-0.4285866
H	72.4016942	2.6967443	-0.2408666
C	74.5167642	2.6683304	-0.2533966
H	71.2053412	-8.5867826	0.3090234
C	71.1486542	-8.3105327	-1.8046946
H	70.5555142	-5.3131626	1.4402734
H	71.2758882	-6.8635196	1.9079624
H	72.3015272	-5.5045716	1.4210974
H	71.1033642	-7.7437946	-3.8869836
H	71.1274752	-5.5873836	-4.7137266
H	70.4134652	-4.3404077	-3.6781916
H	72.1606022	-4.4820047	-3.7944356
C	75.7120652	1.8386993	-0.3185066
C	76.7745242	-0.3414296	-0.4809736
C	74.6350122	4.1553854	-0.1417766
O	71.0763682	-9.6850257	-1.9608166
C	76.9976342	2.4195524	-0.2712766
C	78.0226892	0.2482093	-0.4327636
C	74.6963102	4.9496643	-1.3076496
C	74.6763262	4.7675213	1.1209054
C	71.0191292	-10.2310656	-3.2915906
H	77.0771232	3.4968494	-0.1884776
C	78.1368892	1.6420424	-0.3281646
C	74.7901682	6.3322303	-1.1903496
C	74.6628492	4.3149454	-2.6756736
C	74.7708922	6.1612184	1.2170634
C	74.6223652	3.9411034	2.3827774
H	71.9105552	-9.9662716	-3.8700186
H	70.1256862	-9.8896536	-3.8252206
H	70.9758312	-11.3104977	-3.1610606
H	74.8379252	6.9653253	-2.0678046

C	74.8254412	6.9367034	0.0644604
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H	73.7295272	3.7673564	-2.8394696
H	74.7552872	5.0718124	-3.4578686
H	74.8011532	6.6161873	2.1987634
H	75.4229892	3.1948454	2.4044794
H	74.7234042	4.5726024	3.2687884
H	73.6782362	3.3933113	2.4624774
O	74.9191352	8.3186873	0.0621724
C	74.9585312	9.0143303	1.3218044
H	75.8321222	8.7199833	1.9131484
H	74.0487302	8.8358034	1.9047454
H	75.0283922	10.0702823	1.0684174
H	79.1155212	2.1069173	-0.2907016
H	78.9135352	-0.3683226	-0.4747816
H	76.7099492	-1.4193977	-0.5568836
C	-32.7999216	-1.0467026	1.1110529
C	-31.5691882	-0.7290177	0.5570455
C	-32.8870429	-1.9251541	2.1974761
C	-30.3575069	-1.2692798	1.0704321
C	-31.7311021	-2.4183597	2.7640796
C	-30.4663614	-2.0947848	2.2269575
C	-29.0288770	-1.0239960	0.5060044
H	-31.7673238	-3.0635184	3.6303054
C	-29.2732656	-2.6093708	2.8838804
C	-27.8808400	-1.5059552	1.2039950
C	-28.7814203	-0.3862718	-0.7127067
C	-29.3885676	-3.4711222	4.1018106
C	-28.0503775	-2.2925256	2.3920209
C	-26.5910577	-1.2568728	0.7235977
C	-27.4920994	-0.1551894	-1.2033039
H	-29.5961781	-0.0774092	-1.3461468
C	-29.3797719	-2.8885925	5.3879172
C	-29.4938645	-4.8652076	3.9707458
H	-27.1585354	-2.6591156	2.8915307
H	-25.7790233	-1.6730217	1.2962128
C	-26.3417680	-0.5513778	-0.4568020

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C	-29.4718150	-3.7039794	6.5110911
C	-29.2715069	-1.3935580	5.5557178
C	-29.5849287	-5.6686665	5.1140037
C	-29.5119290	-5.5123007	2.6074893
C	-25.0115510	-0.2485103	-0.9883901
H	-28.2215356	0.7263549	-3.0445628
C	-26.1072227	0.6600607	-3.0459844
H	-29.4660717	-3.2832158	7.5091313
C	-29.5719887	-5.0870844	6.3768082
H	-30.0636023	-0.8743844	5.0063459
H	-29.3452147	-1.1135838	6.6091109
H	-28.3203191	-1.0156885	5.1681930
H	-29.6636401	-6.7415331	4.9934781
H	-29.6418532	-6.5942663	2.6886586
H	-30.3252195	-5.1166424	1.9906420
H	-28.5821482	-5.3212709	2.0628674
C	-24.9096607	0.3126923	-2.2943256
C	-23.7911107	-0.4597647	-0.2886405
C	-25.9988389	1.2567443	-4.4139686
O	-29.6578947	-5.8004220	7.5613889
C	-23.6470448	0.5535528	-2.8778816
C	-22.5618334	-0.2003699	-0.8751636
C	-23.5676081	-0.9466522	1.1340187
C	-25.9291607	0.4172284	-5.5476138
C	-25.9780571	2.6506207	-4.5789770
C	-29.7479751	-7.2358830	7.5026494
H	-23.6167968	0.9618028	-3.8780301
C	-22.4854430	0.2729548	-2.1904454
C	-21.3930501	-0.5398585	0.0289425
H	-23.7462379	-2.0272968	1.2118449
H	-24.2314089	-0.4594886	1.8530279
C	-22.0919014	-0.6077389	1.4179605
C	-25.8444545	0.9827155	-6.8154619
C	-25.9456468	-1.0833476	-5.3959735
C	-25.8930063	3.2002812	-5.8643022
C	-26.0457701	3.5710542	-3.3848418

H	-28.8681550	-7.6711665	7.0170576
H	-30.6510553	-7.5581410	6.9733052
H	-29.7946221	-7.5667245	8.5382648
O	-21.2161894	0.4359135	-2.7093811
C	-20.1945217	0.3881263	0.0603872
C	-20.7274538	-1.8834915	-0.3884261
H	-21.6071992	-1.3282092	2.0831788
H	-22.0308620	0.3789504	1.8855331
H	-25.7917771	0.3620834	-7.7015634
C	-25.8282376	2.3667965	-6.9750584
H	-25.1222789	-1.4277302	-4.7618199
H	-26.8717480	-1.4258053	-4.9240174
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H	-25.8789980	4.2773046	-5.9721344
H	-25.2636214	3.3345011	-2.6564017
H	-25.9262657	4.6144013	-3.6871813
H	-27.0019372	3.4773146	-2.8606170
C	-21.0537063	0.9951025	-4.0363838
C	-18.9871623	-0.2910935	0.1191680
C	-20.2268024	1.7873866	0.0862245
C	-19.2570167	-1.7859515	0.0605816
H	-21.2489231	-2.7458388	0.0369936
H	-20.7681965	-1.9669792	-1.4780390
O	-25.7415259	2.8192042	-8.2816979
H	-21.5220397	1.9860623	-4.0734822
H	-21.5550298	0.3523132	-4.7700540
C	-19.5644112	1.0747844	-4.2913993
O	-21.4787168	2.3707431	0.0898468
C	-19.0422031	2.4924050	0.0963593
H	-19.1135613	-2.2497481	1.0454925
H	-18.5944093	-2.3043086	-0.6373984
C	-25.7341024	4.2376375	-8.5264668
H	-19.3665867	1.5065429	-5.2767956
H	-19.0845406	1.6954301	-3.5308255
H	-19.1161946	0.0793911	-4.2488961
C	-21.5939074	3.8134228	0.0223956
H	-19.0374899	3.5728360	0.0729455

H	-24.8696904	4.7194740	-8.0571508
H	-26.6535038	4.7097441	-8.1642158
H	-25.6695645	4.3456968	-9.6073406
H	-21.0858361	4.1776061	-0.8786381
H	-21.1050981	4.2625791	0.8954956
C	-23.0739212	4.1268119	-0.0094880
H	-23.2360288	5.2066071	-0.0760287
H	-23.5421369	3.6452585	-0.8714032
H	-23.5625064	3.7541035	0.8937885
H	-33.8425555	-2.2113292	2.5847738
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C	12.0730330	7.5827970	-4.2372400
C	11.6929720	6.9425310	-2.9212710
C	12.7385410	6.0375790	-0.9307780
H	11.9232670	8.6685650	-4.1838110
H	11.4718460	7.2220570	-5.0771610
C	10.4480190	6.7635880	-2.3661170
O	13.8921990	5.7035670	-0.2414220
C	11.4744990	5.8554950	-0.3061100
H	9.5515880	7.0443000	-2.9049460
C	10.3215380	6.2337780	-1.0622870
H	14.6829460	5.7411440	-0.8163380
C	11.3019390	5.3417710	1.0555230
C	8.9922420	6.0989670	-0.4851790
C	9.9803310	5.2412180	1.5824660
C	12.3418380	4.9564620	1.9082470
C	8.8576540	5.6214280	0.7757190
C	7.7706890	6.5093220	-1.2467900
C	9.7511280	4.7993630	2.8886320

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H	13.3601240	5.0080090	1.5596190
H	7.8682580	5.5309360	1.2131190
C	7.3313540	7.8507140	-1.2026970
C	7.0226840	5.5553400	-1.9550710
H	8.7331290	4.7530600	3.2380300
C	10.7916410	4.4391880	3.7493050
C	13.2343400	4.1677270	4.0411490
C	6.1523580	8.2074700	-1.8485360
C	8.1166390	8.8959080	-0.4503500
C	5.8351850	5.9342940	-2.5933900
C	7.4742980	4.1170810	-2.0291440
C	10.6178170	4.0206040	5.1419780
C	13.0989780	3.7872230	5.3350410
H	14.2238080	4.2223810	3.5978400
H	5.7943630	9.2295030	-1.8246290
C	5.4001390	7.2525630	-2.5285120
H	8.1946480	8.6458110	0.6122340
H	7.6418160	9.8761040	-0.5357680
H	9.1394030	8.9783630	-0.8319700
H	5.2659690	5.1838840	-3.1265540
H	8.5085190	4.0412020	-2.3786960
H	6.8425780	3.5429730	-2.7116450
H	7.4360610	3.6340000	-1.0477800
C	11.7712360	3.7213240	5.9299460
C	14.3089470	3.4478360	6.1473920
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C	14.7450180	2.1083200	6.2455090
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H	3.0451470	5.9698450	-3.0480610
H	3.8211910	6.3139470	-4.6240690
H	2.4685450	7.3271960	-4.0448650

H	16.2405430	0.7906110	7.0756820
C	16.5933280	2.8189000	7.6325070
H	12.9416210	0.9780380	5.8633730
H	14.4353990	0.0284780	5.7824720
H	13.9974500	1.1326280	4.4660030
H	16.7073230	4.9341690	8.0451490
H	14.6430870	6.2866560	5.7038830
H	15.1900520	6.5368080	7.3681470
H	13.5321780	6.0096880	7.0361460
O	17.7093550	2.4077280	8.3420160
C	18.5038130	3.3970160	9.0218010
H	17.9221270	3.9170090	9.7904770
H	18.9144780	4.1300460	8.3193990
H	19.3163180	2.8451450	9.4901690
C	9.3544790	3.9099470	5.7847500
C	9.2552080	3.5506160	7.1212990
O	8.2002950	4.1797510	5.0696380
C	7.9968990	3.4993940	7.9793050
C	10.4076530	3.2961810	7.8794880
H	7.3968580	3.9161170	5.5617490
C	6.7728160	2.8158480	7.3828570
C	7.4418420	4.9309850	8.2844330
C	8.5163300	2.7589920	9.2566090
C	10.0381190	3.0227490	9.3198410
C	11.6491400	3.3657590	7.2926430
C	6.7196820	1.5919220	6.7317120
C	5.5969400	3.5292450	7.6585910
H	7.9310110	5.3698920	9.1578730
H	7.6533570	5.5817350	7.4293430
C	5.9133310	4.7755230	8.4535960
H	7.9830960	3.0880340	10.1522400
H	8.3326710	1.6853770	9.1420870
H	10.2643130	3.9004330	9.9385830
H	10.5890480	2.1815510	9.7508220
H	12.5470080	3.1646760	7.8632460
C	5.4819180	1.0309190	6.3146570
O	7.8976230	0.9016130	6.4957160

C	4.3797030	3.0376490	7.2500270
H	5.6424330	4.6281140	9.5067950
H	5.3643080	5.6554590	8.1057640
C	5.3552650	-0.2707700	5.6559840
C	4.3051920	1.7977310	6.5757070
H	8.6830730	1.4602250	6.6643990
H	3.4649820	3.5831680	7.4441010
C	6.4192400	-1.1370480	5.3904400
C	4.0575020	-0.7207720	5.2707640
C	3.0023440	1.3061880	6.1480440
C	6.2350190	-2.3859420	4.7905880
H	7.4199400	-0.8469850	5.6646010
C	2.9124830	0.1062220	5.5247600
C	3.8745220	-1.9660030	4.6605460
C	1.7728760	2.1229160	6.3919390
C	7.3765910	-3.2285030	4.5829040
C	4.9379800	-2.8379410	4.4057680
H	1.9426630	-0.2613830	5.2041160
H	2.8728780	-2.2587510	4.3919780
C	1.3504550	3.0680210	5.4310790
C	1.0326900	1.9533750	7.5727870
C	7.2829100	-4.4674290	4.0430090
H	8.3462350	-2.8466840	4.8875920
C	4.8104540	-4.1679420	3.8044530
C	0.2052370	3.8200520	5.6676610
C	2.1299580	3.2731900	4.1560450
C	-0.1180840	2.7207680	7.7919980
C	1.4677170	0.9569970	8.6203510
C	5.9791040	-4.9741980	3.6388520
C	8.5119310	-5.3056310	3.8820340
C	3.5761960	-4.7337290	3.3821440
H	-0.1394090	4.5534890	4.9490710
C	-0.5274110	3.6516540	6.8418480
H	3.1671290	3.5554460	4.3644660
H	1.6805490	4.0609980	3.5473780
H	2.1657770	2.3581240	3.5568600
H	-0.6743680	2.5832690	8.7104660

H	1.4703030	-0.0644030	8.2270410
H	0.8039570	0.9866220	9.4882160
H	2.4860790	1.1624490	8.9662530
C	5.8946500	-6.2751920	3.0939340
C	8.9003620	-6.1959140	4.9088590
C	9.2998800	-5.1923740	2.7259390
O	-1.6383050	4.4603270	6.9764790
C	10.0605870	-6.9473630	4.7619590
C	8.0688510	-6.3404850	6.1596980
C	10.4659260	-5.9576710	2.5992900
C	8.9052940	-4.2554130	1.6097450
C	-2.4535510	4.3329090	8.1627010
H	10.3866910	-7.6283760	5.5379540
C	10.8422680	-6.8291980	3.6149800
H	7.9801340	-5.3898210	6.6945350
H	8.5129290	-7.0722440	6.8382300
H	7.0500460	-6.6667620	5.9253820
H	11.0642940	-5.8536840	1.7034400
H	7.8928100	-4.4672950	1.2510210
H	9.5910650	-4.3451100	0.7636230
H	8.9099570	-3.2117890	1.9393270
H	-2.8581520	3.3212250	8.2595580
H	-3.2671420	5.0428830	8.0264050
H	-1.8830380	4.5969350	9.0600850
O	11.9697880	-7.6305100	3.5700660
C	12.8313820	-7.5511410	2.4170920
H	13.2560700	-6.5488630	2.3096830
H	12.2960290	-7.8297810	1.5030990
H	13.6319610	-8.2642430	2.6036720
O	18.7101390	-4.7126660	-2.2227060
H	18.0867730	-4.5012490	-2.9464520
O	19.2592760	-1.9014970	-4.3095820
H	19.9678120	-2.5620890	-4.1721230
O	12.5982050	-4.6350690	5.4543550
O	28.8600940	-5.0952080	-3.3315130
O	9.5195980	-4.0557640	-6.7134550
O	23.8211220	6.5712040	-1.8218030

C	19.2514430	-4.7753100	-5.1667770
C	20.1500590	-4.4353030	-6.4015550
H	19.7686090	-4.9015010	-7.3137150
H	20.1401430	-3.3512970	-6.5584090
C	21.5789880	-4.8946950	-6.0310220
H	21.7668820	-5.9210360	-6.3712980
H	22.3498640	-4.2646740	-6.4844150
C	21.5833570	-4.8389840	-4.5198750
C	20.2700160	-4.7553830	-4.0339940
C	20.0198050	-4.7602750	-2.6696050
C	21.0805810	-4.8214810	-1.7250200
C	20.8819020	-4.8130610	-0.2743940
C	19.6373290	-4.7704220	0.3597290
H	18.7392920	-4.7479400	-0.2344740
C	19.5070010	-4.7532840	1.7508890
C	18.1916970	-4.7090380	2.3211510
H	17.3468790	-4.6965330	1.6395900
C	17.9757920	-4.6810020	3.6581430
C	19.1137590	-4.6927540	4.5658320
C	20.4434070	-4.7457940	4.0505120
C	20.6516270	-4.7792680	2.6011430
C	21.8971900	-4.8334610	1.9672490
H	22.7946880	-4.8607590	2.5632890
C	22.0276580	-4.8520280	0.5745990
C	23.3394080	-4.9131440	-0.0036560
H	24.1885090	-4.9447210	0.6721630
C	23.5476710	-4.9339840	-1.3429330
C	22.4082350	-4.8858660	-2.2484650
C	22.6406530	-4.8993330	-3.6431020
H	23.6600560	-4.9603550	-4.0027610
C	18.5447520	-6.1663170	-5.2927190
H	19.1316270	-6.8578860	-5.9027360
H	18.4524200	-6.6072690	-4.2944070
C	17.1386610	-5.8846490	-5.8688010
H	17.1351110	-5.9601370	-6.9636610
H	16.3881630	-6.5902130	-5.5003750
C	16.8672330	-4.4586900	-5.4465460

C	15.6864910	-3.7548260	-5.4497710
H	14.7576980	-4.2263330	-5.7455960
C	15.6701720	-2.3937700	-5.0686890
C	14.4034340	-1.6771400	-5.0730200
C	14.3707000	-0.3740380	-4.7022540
H	13.4261840	0.1611480	-4.7020690
C	15.5473920	0.3492230	-4.3165100
C	15.4283740	1.6992150	-3.9720000
H	14.4475580	2.1451860	-3.9921020
C	16.5328330	2.4806340	-3.6203940
C	16.4779500	3.9052870	-3.2849020
C	15.2739260	4.6579190	-3.2102010
C	17.6913980	5.9957630	-2.7625740
H	18.6351420	6.4986920	-2.5935760
C	17.6951820	4.6077890	-3.0274550
C	18.9663580	3.8974570	-3.0381120
C	18.9886390	2.5718740	-3.3179070
H	19.9344900	2.0391870	-3.3235000
C	17.8015690	1.8283320	-3.6290420
C	17.9180420	0.4739380	-3.9566810
H	18.8998920	0.0305170	-3.9449430
C	16.8134950	-0.3080470	-4.3083990
C	16.8711180	-1.7239970	-4.6800200
C	18.0650800	-2.4965300	-4.6785070
C	18.0581540	-3.8351600	-5.0446100
C	16.5737430	-4.6363690	4.1784530
C	15.9045650	-3.4074210	4.2949950
C	14.5711380	-3.3783480	4.7223990
H	14.0670510	-2.4234040	4.8021530
C	13.9134100	-4.5634150	5.0330530
C	14.5768060	-5.7851890	4.9283180
H	14.0242030	-6.6873690	5.1612860
C	15.9005980	-5.8345620	4.5045210
C	16.6032090	-2.1114560	3.9615170
H	17.5327650	-2.0024820	4.5292420
H	15.9657440	-1.2531240	4.1869150
H	16.8731970	-2.0613090	2.9021130

C	16.5984490	-7.1670880	4.3875660
H	16.9443240	-7.3495200	3.3651110
H	15.9298220	-7.9818270	4.6755150
H	17.4830980	-7.2108940	5.0314650
C	11.7927880	-3.4418390	5.4477810
H	11.7631400	-2.9897960	4.4508630
H	12.1604600	-2.7068160	6.1718900
C	24.9415660	-5.0038020	-1.8827110
C	25.5471650	-6.2492980	-2.1129580
C	26.8594490	-6.3079360	-2.5979510
H	27.3104670	-7.2770290	-2.7687150
C	27.5609730	-5.1347650	-2.8516810
C	26.9621370	-3.8967960	-2.6283170
H	27.5358980	-3.0024330	-2.8380180
C	25.6598060	-3.8169800	-2.1466490
C	24.7994950	-7.5328350	-1.8455940
H	24.5402840	-7.6317240	-0.7869660
H	25.3981540	-8.4014420	-2.1306760
H	23.8591610	-7.5694850	-2.4049910
C	25.0297090	-2.4665750	-1.9130840
H	24.1050520	-2.3541520	-2.4885310
H	25.7108100	-1.6635580	-2.2037200
H	24.7653460	-2.3252780	-0.8606200
C	29.5468490	-6.3357060	-3.5790530
H	29.0337010	-6.9309170	-4.3419400
H	29.6447560	-6.9273410	-2.6626280
C	13.1369520	-2.3602490	-5.4827420
C	12.7834160	-2.4353940	-6.8476540
C	11.5762790	-3.0231110	-7.2110140
H	11.2836000	-3.0944180	-8.2516570
C	10.7141680	-3.5283550	-6.2404140
C	11.0601990	-3.4709710	-4.8961890
H	10.4007790	-3.8616590	-4.1321200
C	12.2740890	-2.8895270	-4.5098020
C	13.6938390	-1.8761920	-7.9121880
H	13.8681020	-0.8060710	-7.7635430
H	13.2639370	-2.0175940	-8.9065440

H	14.6748800	-2.3617970	-7.8935480
C	12.6305950	-2.8322770	-3.0442870
H	13.6291240	-3.2406230	-2.8607790
H	11.9143070	-3.4003740	-2.4456920
H	12.6376950	-1.8026930	-2.6732010
C	8.5700620	-4.5860040	-5.7642730
H	8.2218910	-3.8093800	-5.0766870
H	9.0015820	-5.4171890	-5.1977400
C	20.2416670	4.6221700	-2.7425610
C	20.7054220	4.7262250	-1.4128100
C	21.9030940	5.3843560	-1.1546370
H	22.2828790	5.4769810	-0.1445930
C	22.6456400	5.9398480	-2.1944320
C	22.1941670	5.8448460	-3.5059130
H	22.7588870	6.2732680	-4.3239870
C	20.9909060	5.1862340	-3.7872250
C	19.9170530	4.1317890	-0.2726020
H	18.9029790	4.5427300	-0.2330430
H	20.4034030	4.3342090	0.6842640
H	19.8147630	3.0475560	-0.3798780
C	20.5148110	5.0946030	-5.2166040
H	20.4683800	4.0555270	-5.5570620
H	21.1823120	5.6412230	-5.8872720
H	19.5073470	5.5082290	-5.3280340
C	24.6478150	7.1585170	-2.8432660
H	24.9917800	6.4053260	-3.5600740
H	30.5344240	-6.0543100	-3.9391680
H	10.7941370	-3.7708230	5.7277270
H	7.7327990	-4.9439690	-6.3597480
H	25.5027040	7.5802040	-2.3183800
O	14.0601440	4.0266090	-3.4263810
H	13.3047970	4.5973920	-3.1793440
C	15.2901810	6.0184070	-2.9376220
C	14.1114390	6.9837460	-2.9446340
C	16.5054690	6.6903340	-2.7372530
C	14.7469690	8.2638950	-2.3044980
C	16.2663170	8.1730890	-2.5688680

H	16.8568360	8.6125450	-1.7595150
H	16.5433760	8.7042920	-3.4883370
H	14.5595690	8.2484280	-1.2256600
H	14.2920470	9.1747820	-2.7022250
C	18.8834060	-4.6479200	5.9566600
C	21.4891780	-4.7557710	5.0088880
H	17.8621010	-4.6028190	6.3117440
O	2.4074210	-4.0034370	3.5237290
H	1.6558190	-4.4299770	3.0650510
H	6.8006110	-6.8599810	2.9960350
O	22.8062700	-4.8094200	4.5679910
H	23.4297030	-4.8003470	5.3153470
C	3.5142650	-6.0131660	2.8484160
C	2.2694940	-6.8138900	2.4859110
C	4.6764820	-6.7885340	2.7181270
C	2.8867930	-8.0124980	1.6913640
C	1.4890290	-7.2714290	3.7627500
C	1.1718240	-6.1200020	1.6881460
C	4.3346330	-8.1693930	2.2068100
H	2.2855220	-8.9181630	1.8059540
H	2.8993170	-7.7600330	0.6256280
H	1.9105520	-8.1897570	4.1796020
H	1.5780360	-6.4929690	4.5280170
C	0.0116860	-7.4150140	3.3348930
C	-0.1024270	-6.4831680	2.1501480
C	1.3130880	-5.3339740	0.5529140
H	4.3892090	-8.8977050	3.0258120
H	5.0188320	-8.5184590	1.4277340
H	-0.2158890	-8.4435450	3.0273720
H	-0.6823970	-7.1661720	4.1431690
C	-1.2265620	-6.0397580	1.4954000
O	2.5839170	-5.0141540	0.1050170
C	0.1805560	-4.8707660	-0.1713310
H	-2.2166070	-6.3098460	1.8413210
C	-1.1039880	-5.2400210	0.3371600
H	3.2710530	-5.2607440	0.7566090
C	0.2632880	-4.0758190	-1.4000140

C	-2.3135650	-4.8089490	-0.3468730
C	-0.9506090	-3.7025500	-2.0489520
C	1.4494890	-3.6591320	-2.0146300
C	-2.2123080	-4.0778590	-1.4824210
C	-3.6699070	-5.1789660	0.1653750
C	-0.9428380	-2.9840160	-3.2466870
C	1.4573980	-2.9361160	-3.2129720
H	2.3959400	-3.9057740	-1.5619640
H	-3.1120580	-3.7632660	-2.0019000
C	-4.2980130	-6.3561650	-0.2954710
C	-4.3479760	-4.3306300	1.0552130
H	-1.8895090	-2.7405000	-3.6989640
C	0.2412560	-2.5892080	-3.8733890
C	2.7133570	-2.5445410	-3.7878240
C	-5.5902580	-6.6523240	0.1245810
C	-3.5874720	-7.2896150	-1.2437430
C	-5.6483690	-4.6474330	1.4667670
C	-3.6960420	-3.0696120	1.5670900
C	0.3086550	-1.8670330	-5.1447850
C	2.8008180	-1.8620020	-4.9558790
H	3.6194030	-2.8130590	-3.2534060
H	-6.0928780	-7.5473350	-0.2212760
C	-6.2667780	-5.7981350	0.9922010
H	-3.3749390	-6.8016740	-2.2000390
H	-4.1921390	-8.1776240	-1.4421100
H	-2.6257410	-7.6157780	-0.8351280
H	-6.1595500	-3.9793840	2.1478050
H	-2.7367800	-3.2845400	2.0486720
H	-4.3365000	-2.5647680	2.2945010
H	-3.4903440	-2.3677730	0.7529870
C	-0.8329480	-1.5020290	-5.9093960
C	1.5846190	-1.5113120	-5.6780870
C	4.1346330	-1.4708660	-5.5090690
O	-7.5586240	-6.1770120	1.3253710
O	-2.0966350	-1.8345590	-5.4518990
C	-0.7056850	-0.8343920	-7.1185530
C	1.6923040	-0.8294820	-6.9120200

C	4.7323460	-0.2527390	-5.1177210
C	4.7919340	-2.3028510	-6.4296900
C	-8.3242000	-5.3501750	2.2277150
H	-2.7990000	-1.4017520	-5.9780360
C	-1.8113440	-0.4815370	-8.1055230
C	0.5609580	-0.5074600	-7.6241470
H	2.6763560	-0.5812140	-7.2886460
C	5.9621130	0.1112580	-5.6549620
C	4.0470310	0.6615760	-4.1325690
C	6.0281480	-1.9166130	-6.9619050
C	4.1752170	-3.6096090	-6.8663350
H	-8.4505590	-4.3402460	1.8248790
H	-7.8476880	-5.2960950	3.2115630
H	-9.2946780	-5.8351220	2.3105370
C	-2.3635000	-1.7524780	-8.8346380
C	-3.0873930	0.1242100	-7.5346930
C	-1.0691500	0.5022710	-9.0695270
C	0.4308430	0.1365440	-8.9862330
H	6.4408490	1.0417320	-5.3751430
C	6.6073010	-0.7108320	-6.5777920
H	3.0462010	0.9408510	-4.4779000
H	4.6253540	1.5771550	-3.9860970
H	3.9213900	0.1803040	-3.1578980
H	6.5183230	-2.5651780	-7.6766680
H	4.0022530	-4.2751600	-6.0150150
H	4.8205660	-4.1277900	-7.5802320
H	3.2026210	-3.4508780	-7.3439120
H	-1.7628010	-1.9996190	-9.7137940
H	-2.3073270	-2.6050200	-8.1494710
C	-3.8420380	-1.4517530	-9.1695340
C	-4.2321370	-0.4177570	-8.1381510
C	-3.1966300	1.1516630	-6.6084860
H	-1.2196990	1.5270790	-8.7135200
H	-1.4718910	0.4462770	-10.084143
H	1.0795340	1.0086880	-9.1105660
H	0.7094390	-0.5799310	-9.7693880
O	7.8124680	-0.2412000	-7.0607640

H	-3.9443240	-1.0328720	-10.178696
H	-4.4675690	-2.3485860	-9.1343350
C	-5.4795770	0.0419410	-7.7882570
O	-2.0462850	1.6795980	-6.0463890
C	-4.4633070	1.6785820	-6.2358530
C	8.5101040	-1.0147590	-8.0625610
H	-6.3730850	-0.3757640	-8.2350650
C	-5.6125260	1.0843900	-6.8430560
H	-1.2616560	1.1287870	-6.2417530
C	-4.6429290	2.7833360	-5.2909540
H	8.7453410	-2.0195550	-7.7014360
H	9.4317700	-0.4694020	-8.2547000
C	-6.9458610	1.5533810	-6.4961490
C	-5.9673490	3.2307530	-5.0075000
C	-3.6052080	3.4618360	-4.6446490
C	-7.0874960	2.5790650	-5.6218310
C	-8.1621360	0.9120100	-7.0862710
C	-6.2006590	4.3040580	-4.1423150
C	-3.8381430	4.5370660	-3.7817810
H	-2.5853550	3.1611980	-4.8185220
H	-8.0810520	2.9340080	-5.3660780
C	-8.6828650	1.3690630	-8.3161480
C	-8.8150990	-0.1204660	-6.3938050
H	-7.2204040	4.6063390	-3.9698640
C	-5.1616630	4.9966460	-3.5136590
C	-2.7179260	5.1908310	-3.1686060
C	-9.8472680	0.7988780	-8.8211440
C	-7.9957620	2.4725990	-9.0812260
C	-9.9882220	-0.6775910	-6.9167280
C	-8.2763450	-0.6338050	-5.0809220
C	-5.3372440	6.1583850	-2.6391670
C	-2.8544420	6.2699060	-2.3605340
H	-1.7281690	4.7947540	-3.3734260
H	-10.2676580	1.1312960	-9.7627300
C	-10.5019370	-0.2118090	-8.1204920
H	-7.9565930	3.3972020	-8.4970220
H	-8.5185170	2.6822070	-10.017357

H	-6.9611470	2.2066050	-9.3210370
H	-10.4860520	-1.4627770	-6.3627700
H	-7.2262340	-0.9291390	-5.1690600
H	-8.8458060	-1.5004050	-4.7366360
H	-8.3245980	0.1331990	-4.3017500
C	-4.1838250	6.8018680	-2.0935990
C	-6.6012970	6.7189180	-2.3096540
C	-1.6442220	6.9040820	-1.7504880
O	-11.6758320	-0.6795060	-8.6961870
C	-4.3069410	7.9649270	-1.3006220
C	-6.7015440	7.8595450	-1.5260740
O	-7.7565450	6.1300000	-2.7962080
C	-1.2212380	6.5193610	-0.4586620
C	-0.9106960	7.8649950	-2.4643890
C	-12.4080210	-1.7285370	-8.0279990
C	-5.5489770	8.4935500	-1.0387810
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C	-7.9587570	8.6586340	-1.2057150
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C	-7.4402140	9.6318830	-0.0943730
H	-8.0049280	10.3677170	-2.6080090
H	-8.2942000	8.7972510	-3.3559180
C	-10.0315230	9.5308250	-2.2742600
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C	0.6480910	8.0479640	-0.6229110
H	-3.0246070	5.8085920	0.4998170
H	-1.5262460	5.3174230	1.3035980

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H	0.7890330	9.1753530	-2.4570230
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H	-0.7147500	9.1157310	-4.2113590
H	-2.3832560	8.6566220	-3.8370400
H	-5.6784160	10.6371960	-0.9371360
H	-5.3714160	9.8952460	0.6281090
C	-9.2609200	6.9026710	0.2267350
C	-10.3619660	8.3959600	-1.3319130
H	-7.9678800	10.5886640	-0.1260550
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H	-10.2966260	10.4904130	-1.8125580
H	-10.5777950	9.4736520	-3.2204520
O	1.7568030	8.5581060	0.0224910
C	-10.5093190	6.3782220	0.6601030
O	-8.0897010	6.4387920	0.8021170
C	-11.5888720	7.8900610	-0.9726050
C	2.5953660	9.5080310	-0.6723230
C	-10.6542830	5.3942200	1.7356970
C	-11.6802630	6.8870630	0.0185060
H	-7.2985900	6.7563280	0.3219380
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H	2.0402070	10.4220770	-0.9101320
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C	-9.5962160	4.8500760	2.4695330
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C	-12.9958500	6.3887550	0.3955140
C	-9.8013520	3.9712940	3.5376310
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C	-13.1046700	5.4769650	1.3919950
C	-12.1707320	4.0889570	3.1700340
C	-14.2232780	6.8908530	-0.2976990
C	-8.6633330	3.4847710	4.2619440
C	-11.1148090	3.5785460	3.9318930
H	-14.0851080	5.1126810	1.6826730
H	-13.1833260	3.8149490	3.4160110

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C	-11.2647850	2.7111780	5.1036210
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C	-13.9316230	5.0907490	-2.0645910
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C	-7.5423340	2.2395820	6.0681520
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H	-16.2067230	6.2584110	-3.0023240
C	-16.5398510	7.8029130	-1.5694910
H	-12.8895640	5.3492670	-2.2778610
H	-14.3950650	4.7633860	-2.9982510
H	-13.9119720	4.2409710	-1.3748420
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H	-14.4984350	8.0108960	2.3496720
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O	-13.6862610	2.7124110	5.0095430
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H	-9.2954010	1.1638180	7.4684900
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C	-5.6166140	0.7746890	6.2610080
C	-7.2823750	0.3176080	4.4378480
H	-14.4730000	2.2667440	5.3834490
C	-18.4579660	9.2828190	-1.7805940
H	-5.5276670	3.1553050	8.6641950
C	-5.1637290	1.5156060	7.3458770
H	-7.9366180	4.9439550	6.9087200
H	-7.3524150	4.6200870	8.5492370

H	-8.8673060	3.9035750	7.9764710
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H	-8.3199190	-0.0054730	4.5675370
H	-6.6618540	-0.5719390	4.3023870
H	-7.2462520	0.8985350	3.5109750
H	-18.8490480	9.0799340	-0.7778480
H	-19.2845670	9.3853200	-2.4809120
H	-17.8756680	10.2103360	-1.7617450
O	-3.9825290	1.2530350	8.0265140
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H	-2.8204050	0.3692220	6.5139850
H	-3.6207590	-0.7794180	7.6301050
H	-2.2490930	0.2160500	8.1930050
C	-12.6015740	1.5379470	6.7878830
C	-13.8538410	1.1924300	7.5862700
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C	-11.7927870	0.4029230	8.7352020
H	-13.8454370	0.1521920	9.5366330
H	-13.4565030	-0.8737530	8.1563780
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H	-14.2146450	3.3416680	7.6821100
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H	-11.5901180	1.0467640	9.6003090
H	-11.2125650	-0.5131920	8.8814030
H	-16.2449920	1.8157440	9.3543730
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C	-17.4632320	0.9277880	6.7261690
O	-13.9249170	-0.9084130	5.4543380
C	-16.3424390	-0.7671220	5.3172490
H	-18.3824120	1.4018580	7.0463930
C	-17.5239670	-0.0864530	5.7443850
H	-13.1464010	-0.3917610	5.7447160

C	-16.4606780	-1.8753230	4.3672900
C	-18.8155990	-0.4311910	5.1671920
C	-17.7469910	-2.1814800	3.8326540
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C	-18.8917570	-1.4210620	4.2451130
C	-20.0512220	0.3036510	5.5819760
C	-17.9240080	-3.2352130	2.9312490
C	-15.5891310	-3.7762190	3.0914600
H	-14.4176740	-2.5279430	4.3612920
H	-19.8518700	-1.6758680	3.8073130
C	-20.8244930	-0.1665890	6.6658340
C	-20.4563380	1.4528930	4.8846160
H	-18.9154340	-3.4192070	2.5518610
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C	-14.4732900	-4.6266500	2.7897580
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C	-21.6256580	2.1227660	5.2648300
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H	-13.5284350	-4.4118990	3.2793490
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H	-20.3925820	-2.2821890	6.7907880
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H	-20.0747420	2.9062870	3.3365000
H	-19.6033070	1.2560200	2.9054920
C	-18.2089510	-5.5552560	0.9576410
C	-15.8409960	-5.9734230	1.3010890
C	-13.4027290	-6.6042900	1.7579270
O	-23.5512150	2.2483100	6.7773190
C	-18.2547950	-6.6075480	0.0546260
C	-15.9089660	-7.0423550	0.3788660

C	-12.3972280	-6.3001270	0.8276200
C	-13.3077830	-7.7859640	2.5284560
C	-24.0322400	3.4239660	6.1002380
C	-17.0987840	-7.3485880	-0.2361710
H	-15.0133280	-7.6158920	0.1762800
C	-11.3087410	-7.1688310	0.6651920
C	-12.4757340	-5.0488090	-0.0137080
C	-12.2243690	-8.6371220	2.3480050
C	-14.3685770	-8.1358360	3.5422250
H	-24.2522460	3.2162580	5.0476980
H	-23.3104610	4.2452150	6.1645920
H	-24.9486400	3.7023440	6.6168900
H	-10.5396090	-6.9192010	-0.0547010
C	-11.2289540	-8.3364350	1.4190020
H	-13.4266910	-4.9918270	-0.5529750
H	-11.6665370	-5.0197340	-0.7474550
H	-12.4088780	-4.1448270	0.5997690
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H	-14.4894640	-7.3404860	4.2839770
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O	-10.2112330	-9.2633420	1.3148830
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H	7.9203540	-1.0805300	-8.9836770
H	24.1171700	7.9531820	-3.3785670
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H	-9.5071220	-8.9613770	-0.6436140
H	-8.5952630	-8.0969850	0.6373120
H	-8.4697320	-9.8737320	0.4839300
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(R)[meta]Pol4[1]

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H	3.2808330	-1.5539570	-7.4676940
C	2.3096550	-3.1251220	-6.3763270
H	2.8786920	-3.9078670	-6.8636040
C	1.3614220	-3.4574400	-5.4189830
H	1.1857560	-4.4942920	-5.1567870
C	0.6432770	-2.4383350	-4.8076170
C	-0.4052250	-2.4832390	-3.7815400
C	-0.9857670	-3.5380410	-3.1200340
H	-0.6805280	-4.5574260	-3.3207360
C	-1.9943270	-3.3051980	-2.1663530
C	-2.6071860	-4.4212530	-1.4651670
C	-3.5745570	-4.1849300	-0.5548660
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C	-4.0343330	-2.8617390	-0.2438670
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C	-2.4111630	-1.9777880	-1.8912330
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C	-1.8276300	0.3636780	-6.1750670

H	-1.9980090	-0.6810880	-6.4078720
C	-2.5311000	1.3597090	-6.8422950
H	-3.2555170	1.0892200	-7.6010940
C	-2.3137250	2.7018120	-6.5449560
H	-2.8708110	3.4648080	-7.0754370
C	-1.3904790	3.0714140	-5.5769300
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C	-0.6873400	2.0770930	-4.9098300
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H	3.8603120	4.8427010	-0.1150930
C	3.8718900	2.6799800	-0.2475890
C	4.8482820	2.5113130	0.7269640
H	5.2669830	3.3883180	1.2095520
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C	1.6938920	0.6453630	-2.5695640
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C	-2.7922680	-6.5638350	-2.7654230
C	-2.3810740	-7.8627600	-3.0110040
H	-2.8511920	-8.4577460	-3.7843800
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H	-0.0730160	-4.6679970	-0.2755590
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H	-1.1319580	-5.4052240	0.9114200
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H	-0.2747030	-11.4840390	-2.0464980
H	-0.1235080	-10.2319430	-0.8148010
C	1.3538380	-10.1222900	-2.4090610
H	2.0719770	-10.6714300	-1.7890210
H	1.5747630	-9.0592940	-2.2733360
C	1.5418720	-10.4997090	-3.8757670
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H	0.7840720	-9.9871590	-4.4733330
C	2.9332480	-10.1615300	-4.3987430
H	3.1334420	-9.0896220	-4.3204430
H	3.0438040	-10.4431070	-5.4478310
H	3.7084530	-10.6839230	-3.8314490
C	2.0402460	5.5771850	-1.9088890
C	2.6893450	6.2828960	-2.9364050
C	2.2815330	7.5697080	-3.2422900
H	2.7659660	8.1338010	-4.0298690
C	1.2378750	8.1737720	-2.5477780
C	0.5936970	7.4763840	-1.5357420
H	-0.2212760	7.9243580	-0.9844280
C	0.9898890	6.1781910	-1.2127360
C	3.8232360	5.6573050	-3.7055710
H	4.6714500	5.4403850	-3.0527830
H	4.1653790	6.3207000	-4.4999640
H	3.5218300	4.7096990	-4.1575350
C	0.2738530	5.4445440	-0.1080860
H	-0.0879470	4.4710220	-0.4454530

H	-0.5800100	6.0189580	0.2522360
H	0.9378550	5.2580000	0.7387690
C	-0.1292660	10.1191520	-2.2654210
H	0.0947450	10.1900490	-1.1936620
H	-1.0655830	9.5616550	-2.3823430
C	-0.2490390	11.4994240	-2.8770880
H	-1.1266970	11.9885560	-2.4404940
C	0.9870990	12.3692980	-2.6691000
H	1.8567460	11.8486650	-3.0760950
H	1.1690560	12.4820360	-1.5945010
C	0.8539630	13.7444400	-3.3134110
H	0.7036450	13.6597550	-4.3928990
H	1.7483270	14.3490320	-3.1502320
H	0.0021710	14.2943940	-2.9037790
O	-1.0607270	-9.7316690	-2.5943220
O	0.9220300	9.4372600	-2.9327710
H	-0.4493390	11.3879630	-3.9473700
C	-8.0879880	0.1605110	3.3424470
C	-7.7566450	0.3219000	4.6986210
C	-9.4292340	0.1250680	2.9567590
C	-8.7669350	0.4377870	5.6375100
C	-6.3178500	0.3691840	5.1417060
C	-10.4330820	0.2434520	3.9183250
C	-9.8137650	-0.0415260	1.5091220
H	-8.5382070	0.5622670	6.6888150
C	-10.1049560	0.3984630	5.2575990
H	-5.8069900	-0.5723860	4.9292100
H	-6.2482990	0.5603860	6.2125970
H	-5.7664880	1.1532350	4.6179320
H	-11.4657320	0.2130980	3.5995560
H	-9.3358320	0.7133720	0.8811390
H	-10.8931890	0.0430480	1.3804100
H	-9.5017050	-1.0154440	1.1257490
O	-11.0100910	0.5215800	6.2626280
C	-12.3928930	0.4884240	5.9504690
H	-12.6441810	-0.4612100	5.4622050
H	-12.6401830	1.3014140	5.2566760

C	-13.1609480	0.6412860	7.2460440
H	-12.8591170	1.5795420	7.7208530
H	-12.8632300	-0.1640770	7.9239710
C	-14.6722330	0.6206700	7.0385750
H	-14.9608390	-0.3170860	6.5516610
H	-14.9568490	1.4230250	6.3493720
C	-15.4467510	0.7740640	8.3430850
H	-16.5247780	0.7566520	8.1714360
H	-15.2029640	1.7185440	8.8360750
H	-15.2070870	-0.0333670	9.0395850
H	-6.9429780	-2.0771550	2.4724660
C	-4.9363880	2.2387440	0.0995810
C	-6.9346180	2.4852600	1.9944990
C	-6.4265930	3.6096660	1.3897490
H	-6.8075190	4.5886970	1.6544820
C	-5.4173930	3.4829530	0.4325980
H	-5.0112470	4.3637480	-0.0501500
H	-7.7171720	2.5746110	2.7371970
H	-4.1552960	2.1710720	-0.6450060
C	7.8306760	-0.1979870	3.5568040
C	7.4608720	-0.3117660	4.9078740
C	9.1823550	-0.1717750	3.2086540
C	8.4440200	-0.3903790	5.8788520
C	6.0100570	-0.3480560	5.3109700
C	10.1584460	-0.2521390	4.2022190
C	9.6078290	-0.0556970	1.7675530
H	8.1854910	-0.4777810	6.9269790
C	9.7923070	-0.3600780	5.5362480
H	5.5030350	0.5831270	5.0492540
H	5.9101960	-0.4999270	6.3857570
H	5.4760920	-1.1529320	4.8009290
H	11.1997760	-0.2296860	3.9123400
H	9.1495110	-0.8338670	1.1535070
H	10.6906570	-0.1415560	1.6727470
H	9.3049020	0.9030340	1.3409960
O	10.6683640	-0.4438230	6.5706440
C	12.0595600	-0.4161700	6.2976840

H	12.3220200	0.5163800	5.7830790
H	12.3295230	-1.2524990	5.6410820
C	12.7897790	-0.5192560	7.6197850
H	12.4771960	-1.4412280	8.1189140
H	12.4695160	0.3085270	8.2593470
C	14.3064610	-0.4994550	7.4562530
H	14.6062430	0.4216010	6.9448340
H	14.6140320	-1.3246290	6.8048940
C	15.0424680	-0.6028690	8.7877020
H	16.1250480	-0.5867690	8.6474540
H	14.7873720	-1.5302840	9.3066770
H	14.7794850	0.2277550	9.4475470
H	6.7070970	2.0033200	2.5733300
C	4.7745710	-2.4019510	0.3055560
C	5.2489110	-3.6317800	0.6965100
H	4.8580880	-4.5307670	0.2351160
C	6.7206210	-2.5734730	2.2620450
C	6.2317560	-3.7206160	1.6848410
H	6.6073740	-4.6882280	1.9952030
H	4.0141050	-2.3636690	-0.4621230
H	7.4827470	-2.6334410	3.0285550

(P)[meta]Pol4[7]

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C	1.4163500	11.4625440	2.7308580
H	1.6364710	12.5105320	2.5614380
C	0.2331390	10.9138040	2.2300370
H	-0.4564350	11.5403750	1.6755000
C	-0.0695440	9.5681290	2.4369400
H	-0.9894520	9.1459780	2.0472280
C	0.8293470	8.7811560	3.1511960
C	0.7773700	7.3608510	3.5256330
C	-0.1902160	6.4016780	3.3195960

H	-1.1025160	6.6346630	2.7832100
C	-0.0160190	5.0986610	3.8356640
C	-1.0627730	4.0978830	3.6773580
C	-0.9281750	2.8886650	4.2790310
H	-1.7195730	2.1514970	4.1833550
C	0.2543460	2.5150020	5.0064200
C	0.3612560	1.2507140	5.5915620
H	-0.4947940	0.5904880	5.5191760
C	1.5330690	0.8172380	6.2125980
C	4.0989540	-0.0339640	7.1700530
C	3.9275120	1.2185140	6.6756170
H	4.7784400	1.8896340	6.6087920
C	2.6594250	1.6900130	6.1884830
C	2.5345270	2.9748210	5.6533690
H	3.4117510	3.6106050	5.6660700
C	1.3452510	3.4286360	5.0820670
C	1.1750110	4.7740800	4.5432810
C	2.1516940	5.7774410	4.7363240
H	3.0481010	5.5622520	5.3043770
C	1.9518740	7.0433370	4.2436360
C	3.1121270	8.6282260	5.8667230
C	2.1971150	8.9088170	6.8699750
H	1.1326280	8.9093300	6.6631020
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H	1.9679880	9.4128240	8.9483670
C	4.0419090	9.1885520	8.4221280
H	4.3926570	9.4090150	9.4240950
C	4.9629220	8.9064570	7.4136450
H	6.0266590	8.9076030	7.6254010
C	4.4910800	8.6265020	6.1343340
C	5.2096070	8.3134770	4.8914390
C	6.5568270	8.2213980	4.6204990
H	7.2943220	8.3689220	5.4005180
C	6.9983790	7.9498150	3.3067710
C	8.4230320	7.8751350	3.0130640
C	8.8324840	7.6650830	1.7364580
H	9.8944360	7.6180740	1.5151360

C	7.9109100	7.5023700	0.6454850
C	8.3816180	7.3216750	-0.6574300
H	9.4550760	7.3080290	-0.8012300
C	7.5220810	7.1639100	-1.7447890
C	5.6137880	6.8134020	-3.8586310
C	5.2013500	6.9840770	-2.5768700
H	4.1389720	6.9965070	-2.3528970
C	6.1207410	7.1619110	-1.4858700
C	5.6497740	7.3460210	-0.1830430
H	4.5764630	7.3455300	-0.0372680
C	6.5090750	7.5317030	0.9007400
C	6.0454340	7.7682800	2.2650680
C	4.6687730	7.8491140	2.5779370
H	3.9240920	7.7173800	1.8032980
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C	-3.4498350	4.8902820	3.4244010
C	-4.5579920	5.1405660	2.6203790
H	-5.4775920	5.5252220	3.0442140
C	-4.5043200	4.9050080	1.2487670
C	-3.3405140	4.4178030	0.6654430
H	-3.2853190	4.2291200	-0.3985530
C	-2.2156080	4.1591720	1.4555590
C	-3.5250020	5.1556750	4.9076590
H	-3.4249970	4.2311880	5.4850650
H	-4.4786040	5.6182680	5.1720570
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C	-0.9623190	3.6282690	0.8038000
H	-0.1103350	4.2941330	0.9748320
H	-1.0972990	3.5223340	-0.2751500
H	-0.6855170	2.6501600	1.2090750
C	-5.6460080	5.0304210	-0.8989520
H	-6.6250120	5.3633180	-1.2350070
H	-5.4882950	3.9840900	-1.1794670
C	5.4548340	-0.5046200	7.5918160
C	5.9221520	-0.2591300	8.9009340
C	7.1871360	-0.7041910	9.2712980

H	7.5696770	-0.5308260	10.2696730
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C	7.5372240	-1.6382870	7.0736100
H	8.1499940	-2.1717710	6.3584880
C	6.2683810	-1.1974600	6.6801040
C	5.0635180	0.4735470	9.9020340
H	4.8588230	1.4993500	9.5800340
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H	4.0931730	-0.0173850	10.0286670
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H	4.8607960	-2.0538060	5.2779230
H	6.5386350	-2.0442400	4.7146240
H	5.5883880	-0.5507990	4.7305700
C	10.1038060	-2.5303510	7.9641850
H	10.3744900	-1.9425530	7.0808500
H	9.6509170	-3.4748850	7.6471400
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H	11.3126210	10.4069140	5.6795190
C	11.3222210	8.3256260	6.1444130
C	10.8075010	7.0667560	5.8556490
H	11.1277150	6.1918590	6.4066520
C	9.8577350	6.9137190	4.8384160
C	9.4988870	10.5308600	3.6500260
H	9.7589870	10.4599660	2.5892980
H	9.9612510	11.4345570	4.0534860
H	8.4120060	10.6517830	3.7015140
C	9.3079070	5.5402440	4.5401740
H	8.2175390	5.5183670	4.6354290
H	9.7220980	4.7953200	5.2237480
H	9.5415810	5.2295090	3.5171710
C	12.7437940	7.4696410	7.9225720
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C	4.6147060	6.6683010	-4.9622950
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C	3.1994510	7.6754510	-6.6559630
H	2.8403690	8.5659860	-7.1552540
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C	4.1523540	5.3907290	-5.3438340
C	4.6174290	9.1881850	-5.2401960
H	4.3543820	9.4305560	-4.2059980
H	4.1792310	9.9505990	-5.8887530
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C	4.6558400	4.1501960	-4.6492340
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H	4.2265600	3.2511370	-5.0968110
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C	1.2557790	7.3246220	-8.7220590
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H	0.7278300	7.9813670	-8.0236330
O	-5.6603690	5.1875570	0.5362000
O	9.2290130	-1.7911280	8.8394490
O	12.2626830	8.5718930	7.1311730
O	1.8284110	6.1910800	-8.0405410
H	10.9962090	-2.7366230	8.5515000
H	-4.8705260	5.6544660	-1.3539500
H	13.4577230	7.9028170	8.6202780
H	0.5483090	6.9077080	-9.4361600
C	2.9488590	-0.9199910	7.2918090
C	3.0929170	-2.1994220	7.8710060
C	1.6676710	-0.4890980	6.8481420
C	1.9917230	-3.0091790	8.0381810
H	4.0768450	-2.5230080	8.1890670
C	0.5504300	-1.3314640	7.0557340
C	1.8657330	-4.3595850	8.6017370
C	0.7083880	-2.5605860	7.6483520
H	-0.4400320	-1.0009010	6.7687280
C	0.5121070	-4.7302480	8.5771050
C	2.8286640	-5.2335200	9.0984640
C	-0.3543030	-3.5953070	8.0116380

C	0.1089220	-5.9715790	9.0444680
C	2.4232490	-6.4825340	9.5678210
H	3.8759510	-4.9521800	9.1192060
C	-1.3769360	-3.1131840	9.0481270
C	-1.2714610	-4.0553280	6.8788520
H	-0.9370490	-6.2570910	9.0251100
C	1.0753890	-6.8496460	9.5401660
H	3.1604680	-7.1760390	9.9566270
C	-1.1445220	-2.5118240	10.2755430
C	-2.6862350	-3.3863820	8.6194460
C	-2.6243910	-3.9987590	7.2856570
C	-0.9373980	-4.5089840	5.6266360
H	0.7767370	-7.8252260	9.9068810
H	-0.1332860	-2.3020530	10.6061390
C	-2.2374890	-2.1777230	11.0786310
C	-3.7763440	-3.0524460	9.4185200
C	-3.6172030	-4.4851280	6.4648040
C	-1.9424500	-4.9600410	4.7393300
H	0.1030960	-4.5310490	5.3278700
H	-2.0725150	-1.7050440	12.0403390
C	-3.5411640	-2.4468070	10.6533820
H	-4.7898550	-3.2492390	9.0858020
H	-4.6534820	-4.4851730	6.7811880
C	-3.2915370	-4.9975940	5.1899130
C	-1.6290960	-5.3941830	3.3817000
H	-4.3783240	-2.1837810	11.2908730
C	-4.3269040	-5.5748310	4.3434530
C	-2.6695980	-5.9423680	2.5766810
C	-0.3624520	-5.2714830	2.8099740
C	-4.0024810	-6.0307220	3.1072430
C	-5.7261950	-5.7042410	4.8547370
C	-2.3933130	-6.3776310	1.2786410
C	-0.0922230	-5.6840380	1.5023650
H	0.4498000	-4.8248780	3.3707090
H	-4.7703730	-6.4748720	2.4811690
C	-6.1099130	-6.8674080	5.5581600
C	-6.6602220	-4.6786200	4.6421230

H	-3.2157300	-6.7874120	0.7051320
C	-1.1217160	-6.2745410	0.7140860
C	1.2192760	-5.5173320	0.9391240
C	-7.4119930	-6.9827320	6.0319430
C	-5.1236310	-7.9818790	5.8055330
C	-7.9659190	-4.8144440	5.1285410
C	-6.2711600	-3.4215710	3.9028510
C	1.5246430	-5.8936490	-0.3291320
H	1.9896840	-5.0804380	1.5671410
H	-7.7323760	-7.8623990	6.5765770
C	-8.3362570	-5.9614120	5.8218570
H	-4.7625780	-8.4130630	4.8666590
H	-5.5807970	-8.7811200	6.3933700
H	-4.2430520	-7.6215030	6.3471970
H	-8.6729080	-4.0128630	4.9610940
H	-5.4662570	-2.8884900	4.4199930
H	-7.1213900	-2.7407720	3.8122390
H	-5.9076680	-3.6442190	2.8953150
C	2.9241430	-5.7408880	-0.8366500
O	-9.5992590	-6.1771110	6.3446430
C	3.8528860	-6.7754590	-0.6339500
C	3.3244960	-4.5579800	-1.4949310
C	-10.5909300	-5.1401910	6.2099780
C	5.1729460	-6.6215540	-1.0779280
C	3.4538550	-8.0669700	0.0380310
C	4.6390460	-4.4277250	-1.9332100
C	2.3428240	-3.4359270	-1.7257780
H	-10.8347050	-4.9573650	5.1579480
H	-10.2550920	-4.2061300	6.6715600
H	-11.4735970	-5.5057550	6.7299970
H	5.8746300	-7.4268410	-0.9032890
C	5.5591940	-5.4524770	-1.7238070
H	2.8314940	-7.8847190	0.9172910
H	4.3334070	-8.6296430	0.3576890
H	2.8646230	-8.6940590	-0.6420950
H	4.9697450	-3.5304990	-2.4420240
H	1.4650950	-3.7820490	-2.2812800

H	2.8048500	-2.6241120	-2.2920180
H	1.9762170	-3.0252980	-0.7797050
O	6.8451690	-5.2207430	-2.1956380
C	7.8362230	-6.2590180	-2.0411580
H	7.5298610	-7.1751430	-2.5556250
H	8.0194890	-6.4771600	-0.9840430
H	8.7395300	-5.8658120	-2.5030210
C	0.4974870	-6.5006160	-1.1643280
C	0.7905960	-6.8875840	-2.4910000
C	-0.8065450	-6.7212870	-0.6386150
C	-0.1721830	-7.5054670	-3.2589350
H	1.7820160	-6.6959570	-2.8845910
C	-1.7627750	-7.3887060	-1.4381010
C	-0.1442180	-7.9910820	-4.6459420
C	-1.4470730	-7.7812980	-2.7144520
H	-2.7465040	-7.6084860	-1.0432680
C	-1.3825470	-8.5879860	-4.9381180
C	0.8533590	-7.9247270	-5.6143240
C	-2.2974930	-8.5724400	-3.7101120
C	-1.6334790	-9.1189190	-6.1939410
C	0.5993650	-8.4581780	-6.8778430
H	1.8100850	-7.4632100	-5.3951340
C	-2.6099340	-9.9890610	-3.2079340
C	-3.7034740	-8.0281350	-3.9639700
H	-2.5892540	-9.5793160	-6.4186950
C	-0.6333500	-9.0486170	-7.1667140
H	1.3650020	-8.4120100	-7.6442200
C	-1.7223920	-10.9755640	-2.8062640
C	-3.9940020	-10.2212770	-3.1936230
C	-4.6766190	-9.0103770	-3.6672720
C	-4.0816330	-6.7921020	-4.4300300
H	-0.8157660	-9.4558400	-8.1548260
H	-0.6531300	-10.7952960	-2.8176390
C	-2.2305060	-12.2065860	-2.3856660
C	-4.5007120	-11.4485460	-2.7752540
C	-6.0143400	-8.7437060	-3.8540220
C	-5.4493400	-6.4878010	-4.6294190

H	-3.3211700	-6.0561400	-4.6587290
H	-1.5497190	-12.9881470	-2.0676070
C	-3.6080240	-12.4404710	-2.3707380
H	-5.5694370	-11.6330800	-2.7627560
H	-6.7673540	-9.4926050	-3.6392020
C	-6.4241440	-7.4851880	-4.3450750
C	-5.8817840	-5.1895570	-5.1400400
H	-3.9857440	-13.4019440	-2.0413890
C	-7.8363410	-7.2149660	-4.5777670
C	-7.2677350	-4.9768330	-5.3971360
C	-5.0079110	-4.1321220	-5.3948070
C	-8.2116300	-6.0168900	-5.0924270
C	-8.8643310	-8.2548280	-4.2618080
C	-7.7025060	-3.7635090	-5.9367780
C	-5.4451380	-2.9130380	-5.9201930
H	-3.9502590	-4.2326490	-5.1832400
H	-9.2626810	-5.8197450	-5.2805350
C	-9.2667840	-9.1783360	-5.2511160
C	-9.4377180	-8.3109180	-2.9813680
H	-8.7639000	-3.6535380	-6.1231510
C	-6.8231460	-2.7208060	-6.2290530
C	-4.5144180	-1.8426060	-6.1514170
C	-10.2328810	-10.1311850	-4.9457160
C	-8.6591730	-9.1442720	-6.6314760
C	-10.4085740	-9.2781280	-2.6946090
C	-9.0196590	-7.3401870	-1.9040170
C	-4.8879940	-0.6517510	-6.6847240
H	-3.4756830	-2.0052320	-5.8803860
H	-10.5599650	-10.8518080	-5.6851480
C	-10.8028230	-10.1813520	-3.6753210
H	-8.8779750	-8.2011950	-7.1419020
H	-9.0448460	-9.9607530	-7.2461680
H	-7.5689830	-9.2350570	-6.5888080
H	-10.8398680	-9.3065920	-1.7022560
H	-7.9417550	-7.3900430	-1.7193320
H	-9.5339640	-7.5527260	-0.9637740
H	-9.2436990	-6.3072170	-2.1877430

C	-3.8756730	0.4301200	-6.8874220
O	-11.7534930	-11.1702430	-3.4826950
C	-3.1019370	0.4655020	-8.0581580
C	-3.6830300	1.4114990	-5.8902820
C	-12.3803950	-11.2889690	-2.1921090
C	-2.1383940	1.4671880	-8.2265020
C	-3.2936650	-0.5652890	-9.1443120
C	-2.7217770	2.3979330	-6.0776960
C	-4.5039060	1.3956990	-4.6246300
H	-12.9298080	-10.3785370	-1.9300430
H	-11.6454540	-11.5067910	-1.4099620
H	-13.0751840	-12.1216050	-2.2821870
H	-1.5492870	1.4793190	-9.1343270
C	-1.9483330	2.4262210	-7.2373600
H	-3.0198000	-1.5672940	-8.7992950
H	-2.6809430	-0.3302550	-10.018005
H	-4.3387570	-0.6167310	-9.4656930
H	-2.5486880	3.1599850	-5.3277180
H	-5.5749720	1.4613310	-4.8422690
H	-4.2358770	2.2346010	-3.9778820
H	-4.3516370	0.4695360	-4.0617260
O	-1.0206450	3.4469110	-7.3138610
C	-0.1459600	3.5146160	-8.4598720
H	-0.7169820	3.6709110	-9.3822660
H	0.4463970	2.5979340	-8.5566510
H	0.5118960	4.3630390	-8.2778210
C	-6.2772580	-0.4406840	-7.0680850
C	-6.6673400	0.7631020	-7.6955210
C	-7.2416030	-1.4623070	-6.8401360
C	-7.9727500	0.9412780	-8.0980220
H	-5.9190020	1.5267650	-7.8717610
C	-8.5773020	-1.2441400	-7.2501850
C	-8.6231610	2.0472880	-8.8146580
C	-8.9317380	-0.0705690	-7.8687480
H	-9.3249700	-2.0136290	-7.1053380
C	-9.9674660	1.7068550	-9.0410830
C	-8.1176460	3.2642810	-9.2629690

C	-10.2902770	0.3325830	-8.4514060
C	-10.8131990	2.5752790	-9.7143710
C	-8.9693130	4.1369830	-9.9399030
H	-7.0807960	3.5319440	-9.0906990
C	-10.8163130	-0.6827100	-9.4693830
C	-11.4389470	0.3648490	-7.4394460
H	-11.8508780	2.3125940	-9.8881110
C	-10.3054130	3.7960510	-10.164861
H	-8.5913440	5.0890730	-10.295311
C	-10.2148230	-1.1193290	-10.639927
C	-12.0648160	-1.1900510	-9.0727930
C	-12.4585660	-0.5379400	-7.8162210
C	-11.5786070	1.1516940	-6.3227670
H	-10.9541690	4.4854480	-10.693299
H	-9.2505140	-0.7282540	-10.945083
C	-10.8728590	-2.0730520	-11.419853
C	-12.7197920	-2.1415930	-9.8494840
C	-13.5968410	-0.6571360	-7.0499020
C	-12.7476390	1.0708410	-5.5308980
H	-10.7917210	1.8489120	-6.0645560
H	-10.4160660	-2.4236130	-12.338452
C	-12.1140600	-2.5800050	-11.026702
H	-13.6844640	-2.5356100	-9.5486240
H	-14.3851220	-1.3476910	-7.3253450
C	-13.7622500	0.1421760	-5.8972630
C	-12.9485600	1.9324510	-4.3688880
H	-12.6110120	-3.3204970	-11.643365
C	-14.9742530	0.0330600	-5.0967040
C	-14.1598300	1.8173190	-3.6265190
C	-12.0203140	2.8853550	-3.9480400
C	-15.1401530	0.8425200	-4.0201200
C	-16.0307010	-0.9611740	-5.4618800
C	-14.3910180	2.6512400	-2.5292880
C	-12.2510450	3.7187740	-2.8502080
H	-11.0825910	3.0072880	-4.4763090
H	-16.0461520	0.7655300	-3.4266270
C	-17.0909540	-0.5873210	-6.3161440

C	-15.9750450	-2.2677540	-4.9509030
H	-15.3247290	2.5235600	-1.9951690
C	-13.4696980	3.6151700	-2.1185350
C	-11.2719120	4.6947810	-2.4569730
C	-18.0724670	-1.5189750	-6.6373990
C	-17.1682850	0.8075660	-6.8854890
C	-16.9733360	-3.1902480	-5.2866510
C	-14.8488360	-2.6945890	-4.0413920
C	-11.4465290	5.5180440	-1.3919480
H	-10.3644210	4.7698540	-3.0484010
H	-18.8964380	-1.2594430	-7.2906630
C	-18.0163920	-2.8134720	-6.1252010
H	-17.2788730	1.5567850	-6.0954170
H	-18.0176390	0.9031510	-7.5656980
H	-16.2584180	1.0631120	-7.4381700
H	-16.9145460	-4.1930080	-4.8833810
H	-13.8745430	-2.5512400	-4.5195430
H	-14.9415010	-3.7493350	-3.7716420
H	-14.8365020	-2.1075510	-3.1178330
C	-10.4082190	6.5398670	-1.0515310
O	-19.0453160	-3.6566480	-6.5111880
C	-10.5205610	7.8430350	-1.5641600
C	-9.3084800	6.2011480	-0.2329610
C	-19.0495910	-5.0132180	-6.0291470
C	-9.5413110	8.7968350	-1.2630280
C	-11.6852520	8.2336400	-2.4412790
C	-8.3411530	7.1627160	0.0499820
C	-9.1694790	4.8164780	0.3521980
H	-19.1133090	-5.0481910	-4.9363710
H	-18.1573540	-5.5563950	-6.3581140
H	-19.9364130	-5.4722910	-6.4614730
H	-9.6438560	9.7954280	-1.6680280
C	-8.4578820	8.4535080	-0.4620250
H	-11.7305950	7.6164760	-3.3438470
H	-11.6095260	9.2795120	-2.7485620
H	-12.6392310	8.1022180	-1.9203040
H	-7.4777010	6.9169840	0.6566780

H	-9.9691050	4.6121530	1.0733890
H	-8.2095130	4.7083480	0.8612570
H	-9.2402470	4.0442750	-0.4193940
O	-7.4410210	9.3304120	-0.1194790
C	-7.4966330	10.6828900	-0.6077430
H	-8.3918460	11.2013560	-0.2478690
H	-7.4756850	10.7142060	-1.7024610
H	-6.6085080	11.1714610	-0.2117830
C	-12.6709090	5.4271000	-0.6087640
C	-12.8592670	6.2604540	0.5159030
C	-13.6911470	4.5091710	-0.9856160
C	-14.0402420	6.2102340	1.2227230
H	-12.0642880	6.9384820	0.8030660
C	-14.9039370	4.5004760	-0.2579720
C	-14.4895900	6.9451490	2.4133440
C	-15.0770550	5.3414640	0.8133180
H	-15.7099870	3.8387110	-0.5486300
C	-15.8037690	6.5503600	2.7149790
C	-13.8337900	7.8815560	3.2073700
C	-16.3178230	5.5384330	1.6872080
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C	-14.5044020	8.4171950	4.3067740
H	-12.8184950	8.1882200	2.9805400
C	-17.5163300	6.0748160	0.8936910
C	-16.9040110	4.2620830	2.2895760
H	-17.4847930	6.7797720	4.0391650
C	-15.8106180	8.0217440	4.6056420
H	-14.0068600	9.1458410	4.9369280
C	-17.5928520	7.2223870	0.1193930
C	-18.6290820	5.2311410	1.0365050
C	-18.2550890	4.1062050	1.9035050
C	-16.2997110	3.3366330	3.1052600
H	-16.3169710	8.4461240	5.4652330
H	-16.7331460	7.8741940	0.0099450
C	-18.7982800	7.5244150	-0.5179880
C	-19.8309590	5.5324510	0.4020110
C	-18.9837760	3.0254930	2.3464210

C	-17.0214840	2.2133730	3.5729880
H	-15.2641670	3.4763640	3.3886120
H	-18.8742170	8.4177050	-1.1276240
C	-19.9074700	6.6863300	-0.3772230
H	-20.6938690	4.8842560	0.5097630
H	-20.0208960	2.8969230	2.0604460
C	-18.3837830	2.0634700	3.1876150
C	-16.4055680	1.2078230	4.4351340
H	-20.8358200	6.9359710	-0.8785780
C	-19.1564990	0.9226510	3.6588200
C	-17.1939080	0.1053770	4.8761050
C	-15.0734610	1.2579460	4.8499910
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C	-20.5885880	0.7636610	3.2567670
C	-16.6297170	-0.8751510	5.6955380
C	-14.5072450	0.2725250	5.6641970
H	-14.4331600	2.0736240	4.5368280
H	-19.1419250	-0.8461390	4.8185660
C	-21.6128190	1.3275410	4.0485310
C	-20.9195750	0.0470200	2.0957510
H	-17.2687850	-1.6943040	6.0019480
C	-15.2983840	-0.8271900	6.1056550
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C	-22.9406530	1.1605140	3.6704260
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C	-19.8436740	-0.5581720	1.2272180
C	-14.6807700	-1.8478030	6.9482320
C	-12.5245920	-0.6019510	6.8141600
H	-12.5416050	1.1912320	5.6913820
H	-23.7462600	1.5817310	4.2591160
C	-23.2660430	0.4448760	2.5199690
H	-20.7693810	1.4850430	6.0344710
H	-22.1889970	2.5062610	5.7573850
H	-20.6162730	2.9492940	5.0745910
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H	-19.1279250	0.1998910	0.8933680

H	-20.2750390	-1.0296670	0.3409860
H	-19.2704170	-1.3163120	1.7698580
C	-15.4051910	-2.9566770	7.4330000
C	-13.3080490	-1.7353190	7.2914190
C	-11.0681770	-0.5193390	7.1440990
O	-24.6181790	0.3421650	2.2399850
H	-16.4540820	-3.0621680	7.1878500
C	-14.8088930	-3.9205340	8.2220720
C	-12.7188400	-2.7339380	8.0970450
C	-10.6424040	-0.0170580	8.3842430
C	-10.1128420	-0.9790820	6.2103810
C	-25.0323250	-0.3832200	1.0672010
H	-15.3913420	-4.7609660	8.5821330
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H	-24.7172620	-1.4309880	1.1145030
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H	-26.1190570	-0.3286350	1.0608380
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H	-8.9674880	0.3939130	9.6575570
C	-8.3452150	-0.4765950	7.7834870
H	-12.2675480	1.2857770	8.9650840
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O	-6.9820440	-0.5239330	8.0147230
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H	-6.9001360	-0.6012120	10.1142240
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H	12.9039490	6.8111550	-7.6545070
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C	13.0001090	8.3333320	-4.3887260
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H	12.0918610	6.3369470	-9.9544710
H	10.3577600	9.7417880	-6.0224520
C	12.0164610	10.8151980	-5.1493170
C	13.7219110	9.4777430	-4.0612700
C	14.3403000	6.3011050	-3.5062160
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H	11.4457420	4.1956500	-5.0270680
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C	13.2205800	10.7205990	-4.4467650
H	14.6577530	9.4076430	-3.5175360
H	15.1536600	6.8829300	-3.0892230
C	14.3936220	4.8932660	-3.4179740
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H	13.7701300	11.6220420	-4.1999300
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C	16.6308720	5.0676690	-2.1856170
C	14.7067790	0.6662170	-3.2906270
C	12.5571050	0.4067540	-4.3565370
H	11.5190600	2.2045960	-4.8189420
H	16.4589250	2.4051810	-2.3034260
C	17.7573020	5.4237550	-2.9589170
C	16.5450380	5.4828400	-0.8470670
H	15.6092050	0.2621300	-2.8488740
C	13.7347920	-0.1849240	-3.8151200
C	11.5149930	-0.4430230	-4.8681320
C	18.7728390	6.1789580	-2.3819490
C	17.8688830	4.9983520	-4.4019800
C	17.5782950	6.2426780	-0.2855560
C	15.3483900	5.1216050	-0.0013070
C	11.6203310	-1.7968240	-4.8944800
H	10.6130380	0.0299510	-5.2445100
H	19.6475830	6.4668040	-2.9520240
C	18.6861200	6.5861140	-1.0523300
H	17.9082510	3.9087040	-4.4963790
H	18.7701600	5.4116600	-4.8603220
H	17.0050350	5.3350200	-4.9841870
H	17.4951880	6.5543290	0.7476900
H	14.4188070	5.4862620	-0.4501070
H	15.4318390	5.5514950	0.9997310
H	15.2445380	4.0370270	0.1017570
C	10.5009520	-2.6353970	-5.4273350
O	19.7533010	7.3340170	-0.5830590
C	10.4511440	-2.9581150	-6.7926410
C	9.4902070	-3.1058270	-4.5587380
C	19.7293010	7.8008160	0.7785770
C	9.4010590	-3.7429210	-7.2846620
C	11.5185090	-2.4717360	-7.7430540

C	8.4550030	-3.8862630	-5.0659160
C	9.5116780	-2.7734050	-3.0865490
H	19.6982280	6.9655780	1.4863180
H	18.8744950	8.4611820	0.9590590
H	20.6548930	8.3574090	0.9111480
H	9.3784950	-3.9814100	-8.3403150
C	8.4114220	-4.2024700	-6.4227030
H	11.5343270	-1.3789670	-7.8022010
H	11.3528260	-2.8623690	-8.7500660
H	12.5159880	-2.7846660	-7.4178410
H	7.6700230	-4.2566030	-4.4158300
H	10.4396280	-3.1134810	-2.6138510
H	8.6679230	-3.2417820	-2.5740510
H	9.4547430	-1.6926840	-2.9218300
O	7.3412780	-4.9867680	-6.8231310
C	7.2157410	-5.3320240	-8.2142980
H	8.0713090	-5.9228640	-8.5591370
H	7.1169970	-4.4387260	-8.8403130
H	6.3085330	-5.9289120	-8.2849010
C	12.8373910	-2.4318770	-4.4044040
C	12.9998210	-3.8330690	-4.4923700
C	13.8788350	-1.6363320	-3.8505070
C	14.1585770	-4.4249120	-4.0377060
H	12.2043980	-4.4242680	-4.9305080
C	15.0436870	-2.2740870	-3.3672140
C	14.6045250	-5.8261560	-4.0419910
C	15.1761290	-3.6363760	-3.4568950
H	15.8459820	-1.6921520	-2.9322300
C	15.8806940	-5.8946880	-3.4552350
C	13.9870420	-6.9768220	-4.5235160
C	16.3355010	-4.5152620	-2.9782630
C	16.5457840	-7.1065160	-3.3483530
C	14.6575500	-8.1952660	-4.4153870
H	13.0038790	-6.9296490	-4.9791250
C	17.7087760	-4.0646330	-3.4727000
C	16.5240300	-4.4335410	-1.4613370
H	17.5302820	-7.1586390	-2.8966110

C	15.9263920	-8.2604680	-3.8346550
H	14.1908430	-9.1003280	-4.7878340
C	18.1628750	-3.9590330	-4.7785170
C	18.5432330	-3.7201210	-2.3937410
C	17.8070500	-3.9397850	-1.1395070
C	15.6260220	-4.7547680	-0.4769990
H	16.4351580	-9.2149790	-3.7608870
H	17.5195400	-4.2241980	-5.6102210
C	19.4644790	-3.5051170	-5.0050670
C	19.8391730	-3.2662670	-2.6206710
C	18.1608400	-3.7440660	0.1787990
C	15.9678140	-4.5838900	0.8822480
H	14.6497470	-5.1303770	-0.7544820
H	19.8340410	-3.4186560	-6.0205840
C	20.2941360	-3.1612640	-3.9350630
H	20.4874280	-3.0006600	-1.7926880
H	19.1355520	-3.3515150	0.4436460
C	17.2450930	-4.0520560	1.2109750
C	15.0364650	-4.9346600	1.9473340
H	21.3016430	-2.8104820	-4.1284500
C	17.5927090	-3.8205820	2.6070470
C	15.4005560	-4.6783630	3.3002860
C	13.7999900	-5.5311060	1.7078140
C	16.6932950	-4.1143850	3.5819690
C	18.9301860	-3.2528550	2.9630330
C	14.5100190	-4.9898110	4.3333410
C	12.9204210	-5.8591880	2.7399090
H	13.4938360	-5.7728830	0.6978180
H	16.9529170	-3.9311320	4.6202850
C	20.0209790	-4.1148850	3.2099710
C	19.1045230	-1.8630240	3.0579060
H	14.8271720	-4.7743870	5.3468170
C	13.2637570	-5.5707240	4.0915950
C	11.6761990	-6.5125460	2.4457110
C	21.2563900	-3.5750740	3.5510200
C	19.8608220	-5.6112840	3.1058930
C	20.3567470	-1.3401690	3.4027970

C	17.9572850	-0.9193860	2.7903720
C	12.3036350	-5.9070820	5.1412190
C	10.7868970	-6.8632040	3.4081450
H	11.4603340	-6.7444330	1.4071970
H	22.1098720	-4.2126030	3.7462160
C	21.4249980	-2.1953900	3.6490540
H	19.1317610	-5.9867900	3.8306790
H	20.8116670	-6.1175000	3.2868130
H	19.5015090	-5.9056070	2.1144320
H	20.4733800	-0.2662640	3.4713700
H	17.5326270	-1.0806000	1.7943760
H	18.2834800	0.1214210	2.8547980
H	17.1435460	-1.0648390	3.5076700
C	12.5480390	-5.6174780	6.4995760
C	11.0796390	-6.5435180	4.7976820
C	9.5382800	-7.5880690	3.0169000
O	22.6963750	-1.7698270	3.9947620
H	13.4722910	-5.1321690	6.7865750
C	11.6319930	-5.9386810	7.4831290
C	10.1566740	-6.8575300	5.8179590
C	9.5039850	-8.9918050	3.0578190
C	8.4200990	-6.8726760	2.5365140
C	22.9482760	-0.3573550	4.1153560
H	11.8496360	-5.7099310	8.5204750
C	10.4230080	-6.5631230	7.1404850
H	9.2254210	-7.3387130	5.5429730
C	8.3686710	-9.6736390	2.6048840
C	10.6847600	-9.7811780	3.5676970
C	7.3020260	-7.5695400	2.0869110
C	8.4217920	-5.3639380	2.5012560
H	22.3247890	0.0936610	4.8945860
H	22.7755410	0.1611640	3.1663290
H	23.9971490	-0.2721930	4.3921360
H	9.7029370	-6.8151060	7.9106850
H	8.3617430	-10.7554640	2.6362760
C	7.2814340	-8.9625620	2.1114160
H	11.5835660	-9.5793620	2.9767610

H	10.4851870	-10.8545560	3.5264780
H	10.9226150	-9.5208360	4.6040270
H	6.4332780	-7.0431210	1.7103830
H	8.6543890	-4.9443940	3.4854120
H	7.4477020	-4.9817930	2.1882050
H	9.1752350	-4.9776000	1.8078530
O	6.1319830	-9.5583010	1.6139150
C	6.0132170	-10.9941130	1.6558930
H	6.0677620	-11.3657150	2.6840390
H	6.7887540	-11.4754200	1.0512810
H	5.0333440	-11.2155650	1.2379130

(M)[para]Pol4[7]

	X	Y	Z
C	22.6072240	-2.5556660	-0.9633240
C	23.7847330	-3.5191100	-0.7955340
C	24.5440820	-4.1325130	-1.7801950
H	24.3235750	-3.9706990	-2.8295710
C	25.5989380	-4.9639020	-1.3965100
H	26.2009090	-5.4524020	-2.1544010
C	25.8858380	-5.1713780	-0.0449230
H	26.7083520	-5.8196970	0.2356470
C	25.1228680	-4.5541760	0.9461110
H	25.3458690	-4.7208560	1.9943980
C	24.0700680	-3.7276120	0.5638540
C	23.1009730	-2.9699420	1.3673360
C	22.9746450	-2.8185240	2.7299790
H	23.6724380	-3.2907080	3.4113030
C	21.9348690	-2.0249010	3.2611660
C	21.8516530	-1.8010400	4.6978450
C	20.8811890	-0.9914660	5.1900560
H	20.8323030	-0.7977060	6.2572250
C	19.8841880	-0.3860750	4.3511800
C	18.9020810	0.4403990	4.8933720
H	18.9257230	0.6598370	5.9567090
C	17.8919800	0.9960550	4.1102570
C	16.9317620	1.8975900	4.6822480

C	15.9380200	2.4627280	3.9520760
C	17.8233600	0.6721730	2.7239290
C	18.8416040	-0.1177530	2.1775350
H	18.8187210	-0.3355180	1.1193040
C	19.8899270	-0.6346820	2.9475940
C	20.9881840	-1.4195200	2.3854990
C	21.1612550	-1.5698560	0.9893500
H	20.4860980	-1.0779130	0.3002660
C	22.2037440	-2.3153760	0.4939490
C	21.4882690	-3.0753560	-1.8621380
C	20.7360640	-4.2307740	-1.7180840
H	20.8995710	-4.8952610	-0.8767100
C	19.7653010	-4.5251750	-2.6777170
H	19.1651210	-5.4213020	-2.5810700
C	19.5559560	-3.6742760	-3.7659080
H	18.8010580	-3.9284290	-4.5022220
C	20.3113680	-2.5102840	-3.9099770
H	20.1517270	-1.8521810	-4.7569400
C	21.2751970	-2.2121590	-2.9510800
C	22.2132020	-1.0850030	-2.8473440
C	22.4124850	0.0150060	-3.6523560
H	21.8026790	0.1783560	-4.5328200
C	23.4281070	0.9472930	-3.3426690
C	23.6537400	2.1005110	-4.2040600
C	24.6539000	2.9696300	-3.9109870
H	24.8259660	3.8267800	-4.5549270
C	25.5044770	2.8095170	-2.7639940
C	26.5208070	3.7246550	-2.4905110
H	26.6677460	4.5650420	-3.1625510
C	27.3531540	3.5932710	-1.3794010
C	28.3941800	4.5497500	-1.1176360
C	29.2211350	4.4525890	-0.0462620
C	29.0601140	3.3420190	0.8826730
C	28.0459400	2.3708920	0.6668120
C	27.1642640	2.4935270	-0.4935380
C	26.1441700	1.5812440	-0.7751250
H	25.9979250	0.7464000	-0.1064920

C	25.3052580	1.7046200	-1.8868750
C	24.2412890	0.7502570	-2.1905450
C	23.9977040	-0.3764570	-1.3722590
H	24.5959180	-0.5512760	-0.4873540
C	23.0080490	-1.2701950	-1.6954540
C	22.8448350	-2.4342680	5.6199220
C	22.5938700	-3.7169590	6.1545510
C	23.5167150	-4.2891980	7.0233350
H	23.3489960	-5.2708140	7.4491160
C	24.6826630	-3.6086610	7.3682610
C	24.9389370	-2.3474180	6.8423210
H	25.8415790	-1.8078920	7.0988540
C	24.0230590	-1.7534610	5.9652920
C	21.3379070	-4.4702540	5.7933370
H	20.4418000	-3.9252080	6.1059230
H	21.3225730	-5.4526350	6.2706240
H	21.2577270	-4.6160580	4.7111540
C	24.3199700	-0.3850090	5.4017830
H	24.2913100	-0.3895540	4.3075540
H	25.3082780	-0.0388050	5.7138090
H	23.5832720	0.3534860	5.7329730
C	26.7493100	-3.6287790	8.6507320
H	27.2335460	-4.3290800	9.3283240
H	26.5474700	-2.6891930	9.1758580
C	22.7749580	2.3338840	-5.3914520
C	23.0420810	1.6843580	-6.6166890
C	22.2060680	1.9054220	-7.7060210
H	22.3877110	1.4200910	-8.6570310
C	21.1120290	2.7617880	-7.5987060
C	20.8486660	3.4136180	-6.3984040
H	20.0100510	4.0916650	-6.3042090
C	21.6779540	3.2044940	-5.2888870
C	24.2230870	0.7565050	-6.7557060
H	25.1613170	1.2702060	-6.5246440
H	24.2910090	0.3625720	-7.7721800
H	24.1483360	-0.0912510	-6.0668020
C	21.3709650	3.9165360	-3.9934370

H	21.1403790	3.2054350	-3.1931080
H	20.5142970	4.5853470	-4.1088030
H	22.2203980	4.5137690	-3.6514460
C	19.1811430	3.7497390	-8.6987450
H	19.4516960	4.7885370	-8.4820760
H	18.4608410	3.3976600	-7.9526200
O	25.5288010	-4.2727300	8.2405110
O	20.3452360	2.9027200	-8.7421290
C	14.9855060	3.4180900	4.5976720
C	15.1702160	4.8111980	4.4521130
C	13.9155340	2.9343830	5.3676970
C	14.2803290	5.6886080	5.0625760
C	16.3235720	5.3567370	3.6476760
C	13.0349850	3.8359670	5.9797600
C	13.6899630	1.4514680	5.5410340
H	14.3986730	6.7608230	4.9661430
C	13.2155190	5.2059280	5.8208000
H	17.2815150	4.9906520	4.0296160
H	16.3379270	6.4484220	3.6793620
H	16.2621810	5.0480490	2.5990070
H	12.2213260	3.4474170	6.5787640
H	13.5367790	0.9576950	4.5758790
H	12.8113570	1.2595520	6.1620330
H	14.5477910	0.9649190	6.0131780
O	12.3909470	6.1667120	6.3794500
C	11.2403630	5.7411890	7.1344230
H	11.5339890	5.1685490	8.0204850
H	10.5625280	5.1396950	6.5193090
H	17.0303820	2.1417200	5.7356030
C	30.2880420	5.4767330	0.1783510
C	30.0131260	6.6272830	0.9493680
C	31.5625360	5.3025820	-0.3839250
C	31.0092780	7.5792580	1.1374480
C	28.6540420	6.8331110	1.5707470
C	32.5512870	6.2732500	-0.1825110
C	31.8849220	4.0774510	-1.2044790
H	30.8258510	8.4713440	1.7235510

C	32.2716490	7.4058500	0.5738160
H	27.8718890	6.9010430	0.8082200
H	28.6322580	7.7508110	2.1627690
H	28.3850180	5.9984180	2.2261850
H	33.5281880	6.1230340	-0.6237610
H	31.7018120	3.1588710	-0.6377940
H	32.9320890	4.0798660	-1.5164890
H	31.2633510	4.0228920	-2.1036320
O	33.1847540	8.4161140	0.8256580
C	34.5102970	8.3083030	0.2744140
H	34.4855920	8.2742830	-0.8199380
H	35.0292540	7.4215900	0.6537070
H	28.5103980	5.3759960	-1.8124240
C	27.9281590	1.3126700	1.5917970
C	28.7683700	1.2094180	2.6832540
H	28.6530390	0.3835170	3.3761060
C	29.9069180	3.2165410	2.0047540
C	29.7679030	2.1697720	2.8936480
H	30.4284110	2.0909570	3.7496270
H	27.1655530	0.5573260	1.4533300
H	30.6762690	3.9634490	2.1589770
H	35.0339920	9.2048270	0.6000650
H	10.7403560	6.6573470	7.4418790
H	27.4044430	-3.4331500	7.7951380
H	18.7398970	3.6872030	-9.6913520
C	15.7937570	2.1098400	2.5461010
C	14.7459510	2.6655390	1.7796850
C	16.7037740	1.1951460	1.9416440
C	14.5872620	2.3051370	0.4601440
H	14.0720270	3.3726680	2.2483530
C	16.4849070	0.8070860	0.5987150
C	13.6356730	2.7618690	-0.5623430
C	15.4437510	1.3432130	-0.1196900
H	17.1330280	0.0773860	0.1295120
C	13.8887380	2.0625360	-1.7541650
C	12.6383780	3.7313700	-0.5106740
C	15.0300430	1.0649470	-1.5703340

C	13.1443740	2.3172580	-2.8955670
C	11.8921920	3.9910230	-1.6602610
H	12.4475320	4.2795360	0.4049170
C	16.1806640	1.2216250	-2.5631760
C	14.6153050	-0.3911680	-1.8153730
H	13.3391550	1.7753180	-3.8145760
C	12.1425170	3.2885250	-2.8417770
H	11.1140680	4.7465670	-1.6457970
C	16.9244810	2.3566550	-2.8469650
C	16.4469030	0.0078350	-3.2181040
C	15.4865040	-0.9994850	-2.7462390
C	13.5658020	-1.0938890	-1.2736470
H	11.5506940	3.5028950	-3.7230770
H	16.7182210	3.2934090	-2.3408770
C	17.9409000	2.2731400	-3.8011240
C	17.4626450	-0.0752510	-4.1661760
C	15.3311190	-2.3282140	-3.0721550
C	13.3529660	-2.4483280	-1.6240390
H	12.9080240	-0.6050000	-0.5656550
H	18.5297580	3.1510630	-4.0385190
C	18.2089190	1.0674280	-4.4543610
H	17.6694550	-1.0101080	-4.6744250
H	16.0158500	-2.8176870	-3.7544850
C	14.2750340	-3.0780150	-2.5100810
C	12.2336560	-3.2199280	-1.0832560
H	19.0013420	1.0279150	-5.1939330
C	14.1382830	-4.4938570	-2.8240130
C	12.1868920	-4.6191020	-1.3514800
C	11.2005330	-2.6567410	-0.3233610
C	13.1509910	-5.2126360	-2.2341710
C	15.0866590	-5.1638330	-3.7667470
C	11.1936340	-5.3959410	-0.7595160
C	10.1647130	-3.4232120	0.2255980
H	11.2033940	-1.5893700	-0.1524410
H	13.0589710	-6.2737940	-2.4446990
C	14.9054200	-5.0377160	-5.1624920
C	16.1425210	-5.9450990	-3.2702010

H	11.1910850	-6.4684330	-0.9302400
C	10.2044350	-4.8368050	0.0461650
C	15.7845020	-5.6782360	-6.0292300
C	13.7658710	-4.2238300	-5.7228620
C	17.0110370	-6.5890340	-4.1612890
C	16.3665360	-6.0978390	-1.7846820
C	9.2382330	-5.6707350	0.7036550
H	15.6679530	-5.5974450	-7.1029390
C	16.8342880	-6.4491970	-5.5337880
H	12.8025940	-4.5752070	-5.3405440
H	13.7437670	-4.2851660	-6.8131590
H	13.8514050	-3.1686080	-5.4437430
H	17.8125630	-7.1976850	-3.7626140
H	16.5102700	-5.1253650	-1.3028940
H	17.2500210	-6.7089030	-1.5834950
H	15.5122550	-6.5716150	-1.2932760
C	8.2593720	-5.1660200	1.4949350
H	9.3217110	-6.7449900	0.5699850
O	17.6478980	-7.0394900	-6.4847520
C	7.3040170	-6.0881480	2.1831040
C	18.7834180	-7.8103350	-6.0465410
C	7.4928270	-6.4177570	3.5440050
C	6.2291080	-6.6480840	1.4740200
H	19.2767740	-8.1431710	-6.9573790
H	18.4722360	-8.6804790	-5.4590540
H	19.4738280	-7.1989110	-5.4557170
C	6.6020140	-7.2828900	4.1703600
C	8.6520500	-5.8474930	4.3224250
C	5.3478090	-7.5230650	2.1226230
C	5.9983500	-6.3149090	0.0193920
H	6.7236270	-7.5511850	5.2125590
C	5.5322940	-7.8319700	3.4661640
H	9.6065770	-6.0854100	3.8430140
H	8.6715420	-6.2462720	5.3390780
H	8.5935030	-4.7560850	4.3866550
H	4.5303240	-7.9546710	1.5593830
H	5.8526580	-5.2391880	-0.1232510

H	5.1136340	-6.8294910	-0.3638830
H	6.8503650	-6.6043360	-0.6017100
O	4.7072740	-8.6765080	4.1880970
C	3.5514350	-9.2405840	3.5394260
H	3.8386520	-9.8855930	2.7023420
H	2.8756960	-8.4566900	3.1809530
H	3.0518610	-9.8343280	4.3021670
C	8.1330890	-3.7222620	1.6410840
C	7.0893690	-3.1797450	2.4217130
C	9.0516370	-2.8524480	0.9845100
C	6.9388520	-1.8150200	2.5234750
H	6.4097950	-3.8538870	2.9292060
C	8.8416280	-1.4554840	1.0687420
C	5.9889490	-1.0004070	3.2936370
C	7.8006210	-0.9515130	1.8113570
H	9.4943490	-0.7740910	0.5370720
C	6.2466970	0.3551230	3.0315220
C	4.9889790	-1.3688280	4.1890130
C	7.3896920	0.5099520	2.0303410
C	5.5046600	1.3491730	3.6503980
C	4.2450540	-0.3688550	4.8153890
H	4.7942740	-2.4140710	4.4006380
C	8.5375380	1.3950320	2.5118880
C	6.9733900	1.2286730	0.7408480
H	5.7030860	2.3955270	3.4454770
C	4.5001940	0.9783540	4.5467510
H	3.4648310	-0.6314870	5.5216840
C	9.2859130	1.2773890	3.6728820
C	8.7923400	2.4291630	1.5963080
C	7.8361120	2.3178270	0.4862040
C	5.9272670	0.9496590	-0.1058600
H	3.9098950	1.7398670	5.0412830
H	9.0898230	0.4770430	4.3780200
C	10.2937220	2.2117710	3.9203080
C	9.7956030	3.3613320	1.8450660
C	7.6810360	3.0697810	-0.6566220
C	5.7129400	1.7350520	-1.2633940

H	5.2739420	0.1141110	0.1133220
H	10.8889670	2.1377340	4.8220900
C	10.5458300	3.2460920	3.0153740
H	9.9880330	4.1662410	1.1448300
H	8.3611290	3.8816570	-0.8850750
C	6.6320740	2.7839570	-1.5572160
C	4.5954040	1.4829140	-2.1733960
H	11.3286050	3.9644770	3.2338900
C	6.5012710	3.5483470	-2.7902350
C	4.5516280	2.2017230	-3.4036010
C	3.5598690	0.5814610	-1.8961040
C	5.5178670	3.2301570	-3.6681590
C	7.4575330	4.6538840	-3.1064720
C	3.5594410	1.9032520	-4.3346810
C	2.5241880	0.3215510	-2.8025490
H	3.5600770	0.0662560	-0.9457510
H	5.4311730	3.7788560	-4.6010430
C	7.2745730	5.9340250	-2.5372140
C	8.5277320	4.4305240	-3.9877550
H	3.5593070	2.4207290	-5.2894690
C	2.5675210	0.9599850	-4.0763420
C	8.1663610	6.9557870	-2.8455040
C	6.1206090	6.2061910	-1.6048780
C	9.4101820	5.4758790	-4.2900880
C	8.7520380	3.0738090	-4.6115750
C	1.6014280	0.6196820	-5.0824320
H	8.0491890	7.9457840	-2.4222720
C	9.2314590	6.7296840	-3.7150830
H	5.1632450	5.9717300	-2.0802990
H	6.1040610	7.2556320	-1.3025680
H	6.1832500	5.5929560	-0.7000120
H	10.2240450	5.2904850	-4.9793290
H	8.8993960	2.3045320	-3.8465700
H	9.6336760	3.0814740	-5.2573710
H	7.8962810	2.7601850	-5.2155410
C	0.6187640	-0.2903810	-4.8698240
H	1.6878870	1.1017390	-6.0514550

O	10.0579810	7.8147620	-3.9484540
C	-0.3368960	-0.6301920	-5.9688540
C	11.2092550	7.6417140	-4.7967810
C	-0.1528500	-1.8062570	-6.7299880
C	-1.4076690	0.2291410	-6.2635270
H	11.7110620	8.6071090	-4.8049490
H	10.9162700	7.3720450	-5.8169150
H	11.8852310	6.8781240	-4.3973030
C	-1.0441730	-2.1069950	-7.7544050
C	1.0015450	-2.7351140	-6.4479970
C	-2.2895400	-0.0894000	-7.3045580
C	-1.6331700	1.4926750	-5.4680500
H	-0.9262200	-3.0023160	-8.3522620
C	-2.1097770	-1.2559020	-8.0404430
H	1.9585720	-2.2080650	-6.5100240
H	1.0194670	-3.5612530	-7.1622610
H	0.9381450	-3.1586160	-5.4403210
H	-3.1037790	0.5886070	-7.5261690
H	-1.7768350	1.2724310	-4.4052530
H	-2.5172780	2.0268330	-5.8250390
H	-0.7794790	2.1722470	-5.5381570
O	-2.9358640	-1.6539220	-9.0768970
C	-4.0879160	-0.8499360	-9.3952410
H	-3.7959750	0.1521300	-9.7267180
H	-4.7638280	-0.7680250	-8.5373070
H	-4.5893330	-1.3709690	-10.2082500
C	0.4882730	-0.9061460	-3.5562280
C	-0.5601010	-1.8174040	-3.3041310
C	1.4070930	-0.5790520	-2.5169560
C	-0.7148750	-2.3644710	-2.0502460
H	-1.2399790	-2.0696880	-4.1090940
C	1.1928920	-1.1200350	-1.2269330
C	-1.6701340	-3.3563720	-1.5377740
C	0.1473160	-1.9824570	-0.9985470
H	1.8458920	-0.8469070	-0.4071670
C	-1.4153390	-3.5587910	-0.1715010
C	-2.6721800	-4.0750140	-2.1833590

C	-0.2690810	-2.6704250	0.3075980
C	-2.1623820	-4.4686440	0.5605200
C	-3.4210710	-4.9939940	-1.4482660
H	-2.8646180	-3.9278760	-3.2400260
C	0.8741470	-3.4225910	0.9857390
C	-0.6825900	-1.6887180	1.4112280
H	-1.9662300	-4.6224780	1.6160190
C	-3.1688350	-5.1875110	-0.0876890
H	-4.2028760	-5.5703780	-1.9311020
C	1.6179250	-4.4834660	0.4926720
C	1.1298770	-2.9006600	2.2643290
C	0.1783680	-1.8116110	2.5243460
C	-1.7248620	-0.7928390	1.4261510
H	-3.7629520	-5.9038090	0.4662170
H	1.4211340	-4.8842150	-0.4957100
C	2.6219460	-5.0302230	1.2944800
C	2.1294870	-3.4478030	3.0635490
C	0.0258300	-0.9802830	3.6111150
C	-1.9367490	0.0415510	2.5493600
H	-2.3769650	-0.7211990	0.5643730
H	3.2134690	-5.8600940	0.9280340
C	2.8750240	-4.5183140	2.5696840
H	2.3226730	-3.0532290	4.0546280
H	0.7047510	-1.0354970	4.4536450
C	-1.0189870	-0.0312370	3.6373690
C	-3.0504190	0.9884230	2.6107950
H	3.6548390	-4.9654410	3.1767590
C	-1.1468590	0.8809290	4.7657630
C	-3.0911780	1.9126090	3.6953450
C	-4.0852470	1.0282310	1.6677170
C	-2.1261470	1.8189500	4.7542500
C	-0.1922000	0.8097810	5.9147510
C	-4.0797080	2.8937030	3.7204690
C	-5.1174860	1.9734890	1.7211120
H	-4.0873410	0.3010810	0.8678140
H	-2.2106450	2.5188040	5.5800380
C	-0.3819920	-0.1482480	6.9357690

C	0.8835000	1.7087910	5.9950210
H	-4.0776180	3.6240460	4.5242080
C	-5.0710190	2.9647980	2.7444350
C	0.5084840	-0.1991440	8.0028980
C	-1.5417090	-1.1112300	6.8843640
C	1.7644860	1.6446240	7.0825320
C	1.1152610	2.7430710	4.9195330
C	-6.0338360	4.0297670	2.7557160
H	0.3861500	-0.9241210	8.7981280
C	1.5788800	0.6899440	8.0768730
H	-2.4959440	-0.5793400	6.8204660
H	-1.5619470	-1.7435440	7.7747370
H	-1.4830230	-1.7626410	6.0063170
H	2.5826080	2.3515040	7.1353300
H	1.2586850	2.2731630	3.9411010
H	2.0015570	3.3435980	5.1391790
H	0.2645650	3.4231150	4.8227600
C	-7.0162960	4.1327720	1.8266280
H	-5.9453850	4.7845040	3.5312190
O	2.4034330	0.5479710	9.1791700
C	-7.9694720	5.2843780	1.8703970
C	3.5594310	1.3993430	9.2965580
C	-7.7825460	6.3926540	1.0142250
C	-9.0407400	5.2791130	2.7782500
H	4.0581940	1.0864280	10.2115420
H	3.2724060	2.4530700	9.3772850
H	4.2358430	1.2695790	8.4449440
C	-8.6715320	7.4607780	1.0706040
C	-6.6274040	6.4330410	0.0452100
C	-9.9201620	6.3688100	2.8234560
C	-9.2693990	4.1093700	3.7053680
H	-8.5513480	8.3219250	0.4248980
C	-9.7375650	7.4501700	1.9679280
H	-5.6708620	6.3161220	0.5637730
H	-6.6081840	7.3806240	-0.4976640
H	-6.6909510	5.6226090	-0.6882280
H	-10.7347120	6.3542620	3.5362650

H	-9.4163020	3.1808170	3.1441960
H	-10.1526920	4.2711460	4.3282750
H	-8.4158540	3.9467680	4.3690880
O	-10.5610180	8.5618940	1.9366700
C	-11.7135190	8.5975490	2.8000980
H	-11.4221930	8.5766110	3.8555250
H	-12.3911380	7.7626310	2.5919080
H	-12.2127640	9.5385680	2.5785090
C	-7.1494980	3.0972520	0.8109190
C	-8.1971520	3.1641570	-0.1330010
C	-6.2341200	2.0053580	0.7762880
C	-8.3548150	2.1622460	-1.0640350
H	-8.8741650	4.0095570	-0.1051930
C	-6.4513280	0.9675370	-0.1609740
C	-9.3100650	2.0097260	-2.1700540
C	-7.4963300	1.0405450	-1.0508200
H	-5.8010720	0.1015040	-0.1741800
C	-9.0591830	0.7862790	-2.8125930
C	-10.3091440	2.8598870	-2.6352600
C	-7.9152910	0.0368330	-2.1323800
C	-9.8075140	0.3984490	-3.9132290
C	-11.0592010	2.4722520	-3.7456060
H	-10.4984240	3.8092630	-2.1473180
C	-6.7725740	-0.3568420	-3.0661770
C	-8.3326370	-1.3286400	-1.5719780
H	-9.6145070	-0.5476230	-4.4071020
C	-10.8111490	1.2510880	-4.3776580
H	-11.8386790	3.1211170	-4.1302390
C	-6.0259590	0.4580100	-3.9030460
C	-6.5205030	-1.7368020	-2.9972120
C	-7.4741200	-2.3404470	-2.0563310
C	-9.3763660	-1.6369190	-0.7324810
H	-11.4062370	0.9668120	-5.2367470
H	-6.2199320	1.5238570	-3.9536880
C	-5.0227260	-0.1198670	-4.6837380
C	-5.5218860	-2.3121360	-3.7776800
C	-7.6303470	-3.6409010	-1.6322010

C	-9.5925050	-2.9727130	-0.3181560
H	-10.0265790	-0.8458400	-0.3797360
H	-4.4288910	0.4994030	-5.3446160
C	-4.7734070	-1.4933420	-4.6233000
H	-5.3317180	-3.3785170	-3.7339480
H	-6.9530250	-4.4192010	-1.9628600
C	-8.6770140	-3.9775500	-0.7466560
C	-10.7088950	-3.3418400	0.5525420
H	-3.9941890	-1.9199860	-5.2456870
C	-8.8095000	-5.3443440	-0.2607990
C	-10.7549630	-4.6718650	1.0633570
C	-11.7420170	-2.4625920	0.9009740
C	-9.7915020	-5.6421730	0.6257520
C	-7.8570200	-6.4074480	-0.7070940
C	-11.7476450	-5.0192150	1.9766800
C	-12.7785320	-2.8245630	1.7708180
H	-11.7399950	-1.4666080	0.4808140
H	-9.8797020	-6.6532590	1.0114770
C	-8.0454820	-7.0516550	-1.9503910
C	-6.7850930	-6.7856720	0.1173440
H	-11.7500290	-6.0202340	2.3978050
C	-12.7382680	-4.1199050	2.3643970
C	-7.1572570	-8.0443550	-2.3503190
C	-9.2015600	-6.6797130	-2.8448810
C	-5.9064420	-7.7932550	-0.3018290
C	-6.5548600	-6.1158080	1.4509280
C	-13.7061580	-4.4826650	3.3606340
H	-7.2786660	-8.5531950	-3.2986320
C	-6.0905520	-8.4132740	-1.5331890
H	-10.1575920	-6.7930890	-2.3245850
H	-9.2212880	-7.3096070	-3.7369770
H	-9.1388000	-5.6354000	-3.1676990
H	-5.0912970	-8.0807990	0.3498350
H	-6.4074730	-5.0373060	1.3333470
H	-5.6713590	-6.5255780	1.9468150
H	-7.4078720	-6.2476760	2.1221080
C	-14.6910620	-3.6403340	3.7602200

H	-13.6191230	-5.4636640	3.8176900
O	-5.2680340	-9.4086740	-2.0309330
C	-15.6438530	-4.0631260	4.8328100
C	-4.1155130	-9.8060740	-1.2636860
C	-15.4643480	-3.6093980	6.1589880
C	-16.7023600	-4.9358810	4.5334770
H	-3.6174310	-10.5665880	-1.8615270
H	-4.4066850	-10.2315790	-0.2975580
H	-3.4369080	-8.9618840	-1.1010200
C	-16.3476460	-4.0220360	7.1508540
C	-14.3222780	-2.6898530	6.5126930
C	-17.5752010	-5.3460290	5.5498110
C	-16.9245280	-5.4367150	3.1263160
H	-16.2325000	-3.6887030	8.1748610
C	-17.4000150	-4.8846040	6.8501770
H	-13.3599050	-3.1253360	6.2268250
H	-14.3018540	-2.4907080	7.5864340
H	-14.4032770	-1.7307330	5.9909040
H	-18.3788580	-6.0287530	5.3051430
H	-17.0600710	-4.6061730	2.4261290
H	-17.8120670	-6.0722270	3.0732690
H	-16.0727720	-6.0197020	2.7651610
O	-18.2177830	-5.2286720	7.9120750
C	-19.3562150	-6.0768230	7.6665950
H	-19.0481840	-7.0629340	7.3035110
H	-20.0428220	-5.6204270	6.9455880
H	-19.8525440	-6.1816240	8.6291340
C	-14.8210760	-2.3392540	3.1182630
C	-15.8746440	-1.4732460	3.4834930
C	-13.8950980	-1.9419820	2.1100310
C	-16.0239190	-0.2595690	2.8506190
H	-16.5622140	-1.7838080	4.2611750
C	-14.1015990	-0.7088410	1.4471960
C	-16.9804570	0.8348320	3.0674310
C	-15.1487640	0.1066300	1.8039120
H	-13.4407560	-0.4048420	0.6448120
C	-16.7076920	1.8573400	2.1437680

C	-17.9980080	0.9833510	4.0055220
C	-15.5569410	1.4643560	1.2188090
C	-17.4463590	3.0305470	2.1483940
C	-18.7391140	2.1650530	4.0126140
H	-18.2102870	0.1965630	4.7203400
C	-14.4116190	2.4725410	1.1615380
C	-15.9688280	1.3909780	-0.2569600
H	-17.2349350	3.8195600	1.4349990
C	-18.4643490	3.1802490	3.0927270
H	-19.5327690	2.3055100	4.7384420
C	-13.6668500	2.9888390	2.2105920
C	-14.1552250	2.8672360	-0.1621230
C	-15.1080600	2.1837760	-1.0479120
C	-17.0120070	0.7034550	-0.8284810
H	-19.0491760	4.0920690	3.1136110
H	-13.8641950	2.6818650	3.2318820
C	-12.6612510	3.9157940	1.9286470
C	-13.1541690	3.7929840	-0.4415840
C	-15.2644860	2.2199380	-2.4155790
C	-17.2284320	0.7611610	-2.2255200
H	-17.6634870	0.1091040	-0.1999910
H	-12.0689830	4.3315200	2.7344290
C	-12.4076280	4.3160740	0.6142710
H	-12.9606580	4.1068120	-1.4610480
H	-14.5874150	2.7923970	-3.0382480
C	-16.3139620	1.5014550	-3.0291480
C	-18.3496490	0.0711330	-2.8623940
H	-11.6265440	5.0436120	0.4215490
C	-16.4551670	1.5085610	-4.4790110
C	-18.4147640	0.0535980	-4.2861020
C	-19.3725840	-0.5601060	-2.1450980
C	-17.4500700	0.7885220	-5.0550240
C	-15.4980750	2.2785040	-5.3322220
C	-19.4258460	-0.6700610	-4.9156730
C	-20.4220740	-1.2423860	-2.7714070
H	-19.3525110	-0.5174030	-1.0654710
H	-17.5461930	0.7737800	-6.1364250

C	-15.6774820	3.6666460	-5.5243690
C	-14.4290200	1.6209490	-5.9619020
H	-19.4465980	-0.7123930	-6.0006560
C	-20.4123880	-1.3385890	-4.1935920
C	-14.7834830	4.3694790	-6.3251170
C	-16.8294420	4.3927910	-4.8757970
C	-13.5442900	2.3468980	-6.7700380
C	-14.2087860	0.1389000	-5.7747960
C	-21.4095190	-2.1252920	-4.8651990
H	-14.8977530	5.4340530	-6.4881390
C	-13.7197030	3.7157350	-6.9437440
H	-17.7883840	3.9486650	-5.1598990
H	-16.8402000	5.4450360	-5.1684620
H	-16.7694900	4.3445120	-3.7836150
H	-12.7314500	1.8235230	-7.2570480
H	-14.0574560	-0.1097960	-4.7192970
H	-13.3307870	-0.1992070	-6.3308700
H	-15.0682930	-0.4436260	-6.1174470
C	-22.3843450	-2.7892800	-4.1956310
H	-21.3566260	-2.1953960	-5.9473640
O	-12.8908370	4.5120970	-7.7143940
C	-23.3762280	-3.6248710	-4.9409880
C	-11.7411200	3.9143170	-8.3434390
C	-23.1298610	-5.0006300	-5.1429510
C	-24.5485020	-3.0446410	-5.4508010
H	-11.2372750	4.7285790	-8.8601590
H	-12.0360480	3.1473720	-9.0673530
H	-11.0662360	3.4750720	-7.6010000
C	-24.0513560	-5.7645420	-5.8508530
C	-21.8801670	-5.6476640	-4.5998380
C	-25.4632210	-3.8316160	-6.1612250
C	-24.8405980	-1.5784760	-5.2422950
H	-23.8870040	-6.8213230	-6.0217210
C	-25.2115580	-5.1844710	-6.3598080
H	-20.9792760	-5.1982780	-5.0290750
H	-21.8669340	-6.7167530	-4.8233930
H	-21.8076440	-5.5258210	-3.5141540

H	-26.3615860	-3.3677520	-6.5477500
H	-24.8185220	-1.3149280	-4.1801100
H	-25.8251180	-1.3158590	-5.6369260
H	-24.0975770	-0.9470240	-5.7392770
O	-26.0569490	-6.0385930	-7.0478710
C	-27.2719990	-5.5098180	-7.6107110
H	-27.0624380	-4.7287480	-8.3491770
H	-27.9299380	-5.1073560	-6.8331450
H	-27.7569580	-6.3529380	-8.0985590
C	-22.4727580	-2.6589930	-2.7477530
C	-23.5178790	-3.2965700	-2.0447160
C	-21.5252330	-1.8643850	-2.0404410
C	-23.6476650	-3.1154220	-0.6860550
H	-24.2167400	-3.9155710	-2.5947070
C	-21.7017790	-1.6740000	-0.6496010
C	-24.6215640	-3.6544180	0.2729110
C	-22.7486390	-2.2744700	0.0073900
H	-21.0253420	-1.0340290	-0.0968200
C	-24.3364800	-3.1287340	1.5437600
C	-25.6783350	-4.5431790	0.0967310
C	-23.1534830	-2.1594260	1.4794770
C	-25.1000530	-3.4854610	2.6447330
C	-26.4455060	-4.9021470	1.2047770
H	-25.9013300	-4.9540370	-0.8819750
C	-22.0369740	-2.4594400	2.4764460
C	-23.5465650	-0.7356180	1.8883100
H	-24.8797440	-3.0787660	3.6255810
C	-26.1588690	-4.3792870	2.4683580
H	-27.2710980	-5.5947600	1.0853120
C	-21.2907110	-3.6200570	2.6089230
C	-21.8196410	-1.3656840	3.3323940
C	-22.7521590	-0.2901980	2.9653750
C	-24.5327830	0.0636000	1.3641040
H	-26.7640880	-4.6697850	3.3196770
H	-21.4574490	-4.4628440	1.9470340
C	-20.3215770	-3.6854900	3.6122240
C	-20.8575440	-1.4347830	4.3357810

C	-22.9474670	0.9689380	3.4919490
C	-24.7703680	1.3494390	1.8972890
H	-25.1334260	-0.3084270	0.5440410
H	-19.7259560	-4.5822180	3.7295820
C	-20.1080790	-2.6037870	4.4703110
H	-20.6947180	-0.5969140	5.0046820
H	-22.3376760	1.3300210	4.3114110
C	-23.9582430	1.8060810	2.9723250
C	-25.8336520	2.2102500	1.3752140
H	-19.3545870	-2.6814390	5.2467250
C	-24.1811690	3.1312190	3.5428570
C	-26.0332030	3.4975360	1.9755760
C	-26.6665730	1.8384420	0.3269020
C	-25.1771520	3.9114370	3.0570480
C	-23.3005700	3.6295020	4.6441590
C	-27.0391900	4.3341940	1.5086360
C	-27.6861590	2.6787170	-0.1523610
H	-26.5483760	0.8753470	-0.1543650
H	-25.3452150	4.8948090	3.4857300
C	-23.5700250	3.2829910	5.9864610
C	-22.1990160	4.4467020	4.3430790
H	-27.1768030	5.3056480	1.9743360
C	-27.8815970	3.9590310	0.4510110
C	-22.7319690	3.7460540	6.9952470
C	-24.7559960	2.4191960	6.3362120
C	-21.3676470	4.9027980	5.3742480
C	-21.8894270	4.8375820	2.9180330
C	-28.9188070	4.8052230	-0.0407390
H	-22.9153620	3.4953100	8.0327700
C	-21.6335040	4.5483860	6.6928310
H	-25.6919540	2.8728950	5.9960420
H	-24.8225740	2.2681620	7.4159230
H	-24.6888540	1.4361310	5.8588020
H	-20.5254270	5.5358960	5.1257690
H	-21.6620010	3.9592870	2.3046130
H	-21.0299580	5.5114030	2.8757830
H	-22.7365070	5.3426610	2.4463530

C	-29.7317610	4.4193260	-1.0773470
H	-29.0599310	5.7768820	0.4230850
O	-20.8650720	4.9464700	7.7727850
C	-30.8179130	5.3088200	-1.5904220
C	-19.6967700	5.7544660	7.5347900
C	-30.5559760	6.2062820	-2.6480530
C	-32.1039220	5.2462830	-1.0319550
H	-19.2552250	5.9216270	8.5150820
H	-19.9622570	6.7160320	7.0829510
H	-18.9786970	5.2353430	6.8910700
C	-31.5771580	7.0223170	-3.1224820
C	-29.1820030	6.2917430	-3.2654270
C	-33.1183560	6.0763900	-1.5240940
C	-32.4113860	4.2942200	0.0985460
H	-31.4041000	7.7203970	-3.9322750
C	-32.8520520	6.9595280	-2.5642060
H	-28.4316970	6.5973000	-2.5292480
H	-29.1681490	7.0138910	-4.0848720
H	-28.8581400	5.3230170	-3.6593240
H	-34.1043390	6.0149800	-1.0816750
H	-32.1768690	3.2600850	-0.1729250
H	-33.4678550	4.3414050	0.3735370
H	-31.8187790	4.5260540	0.9892540
O	-33.7907640	7.8167860	-3.1145540
C	-35.1305810	7.8097430	-2.5884220
H	-35.1447240	8.0873480	-1.5290750
H	-35.6031910	6.8296440	-2.7131390
H	-35.6741570	8.5533280	-3.1678460
C	-28.5415440	2.2975610	-1.2279440
C	-29.5261460	3.1349390	-1.6735540
H	-28.3957360	1.3254740	-1.6882250
H	-30.1719090	2.8361160	-2.4922970

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C	47.7961410	0.4772560	-0.4666190

C	49.1487950	2.4679600	-0.6127560
C	46.6127520	1.2442630	-0.4592360
C	48.0071520	3.2438220	-0.6038550
C	46.7249340	2.6584560	-0.5266000
C	45.2904990	0.6301520	-0.3831540
H	48.0819600	4.3233700	-0.6564820
C	45.5272770	3.4865860	-0.5136120
C	44.1426630	1.4676850	-0.3591590
C	45.0760820	-0.7472060	-0.3520840
C	45.6384350	4.9765300	-0.5880700
C	44.3082790	2.8943040	-0.4313950
C	42.8625550	0.9083880	-0.2721580
C	43.7984910	-1.3060730	-0.2758550
H	45.9133320	-1.4329910	-0.4038580
C	45.6380420	5.6241890	-1.8428160
C	45.7345400	5.7370610	0.5880250
H	43.4141740	3.5106590	-0.4187210
C	42.6403990	-0.4700930	-0.2006750
H	42.0363760	1.5988530	-0.2863750
C	43.6478920	-2.7335570	-0.3110820
C	45.7260310	7.0110660	-1.8978960
C	45.5454220	4.8285780	-3.1210610
C	45.8221810	7.1324030	0.5106680
C	45.7475380	5.0689910	1.9413970
C	41.3206480	-1.1001490	-0.0926490
H	44.5479090	-3.3378260	-0.3728790
C	42.4350180	-3.3360770	-0.2992760
H	45.7272490	7.5334730	-2.8466450
C	45.8157900	7.7628910	-0.7283860
H	46.3572320	4.0976870	-3.1945380
H	44.6082300	4.2659290	-3.1746890
H	45.5987270	5.4851000	-3.9924920
H	45.8951930	7.7027970	1.4277270
H	46.5585410	4.3375060	2.0162990
H	45.8789200	5.8037820	2.7394400
H	44.8155910	4.5267830	2.1290900
C	41.2300590	-2.5236880	-0.1920590

C	40.1042310	-0.4002090	0.1147330
C	42.3415450	-4.8271360	-0.3776960
O	45.8980570	9.1348630	-0.9019040
C	39.9802050	-3.1658660	-0.1617450
C	38.8808360	-1.0606610	0.1435600
C	39.8654930	1.0839460	0.3477940
C	42.3677430	-5.6013180	0.8025260
C	42.2428780	-5.4624390	-1.6254400
C	45.9928280	9.9774290	0.2612660
H	39.9179720	-4.2423060	-0.2440970
C	38.8145660	-2.4466630	-0.0171610
C	37.7077630	-0.1080930	0.2865590
H	39.9921960	1.6554040	-0.5811480
H	40.5547700	1.5082280	1.0823020
C	38.4096100	1.1585360	0.8487180
C	42.3042220	-6.9877440	0.7136780
C	42.4577810	-4.9410280	2.1557390
C	42.1792220	-6.8594450	-1.6930340
C	42.1982570	-4.6566270	-2.9006570
H	46.8959920	9.7579630	0.8406200
H	45.1135110	9.8691600	0.9051260
H	46.0425720	10.9952350	-0.1205130
O	37.6197370	-3.1443070	-0.0337780
C	36.5291220	-0.5371430	1.1439560
C	37.0112570	0.1324910	-1.0867180
H	37.8981300	2.0770050	0.5463890
H	38.3983020	1.1066540	1.9410350
H	42.3217330	-7.6058480	1.6028770
C	42.2121810	-7.6151690	-0.5266990
H	41.6357690	-4.2336650	2.3057460
H	42.4179240	-5.6852140	2.9545200
H	43.3876520	-4.3740070	2.2638500
H	42.1023170	-7.3322040	-2.6637000
H	42.0813240	-5.3069800	-3.7709480
H	41.3638760	-3.9479360	-2.8920370
H	43.1116740	-4.0690160	-3.0353140
C	35.2977530	-0.2089680	0.5798840

C	36.5880000	-1.1422040	2.4043910
C	35.5359550	0.4434930	-0.7719690
H	37.5036670	0.9245550	-1.6569340
H	37.0734710	-0.7856240	-1.6809120
O	42.1558670	-8.9994210	-0.4965340
C	34.0734250	-0.4907820	1.2419980
O	37.8408660	-1.3753010	2.9380320
C	35.4191620	-1.4897300	3.0461080
H	35.3660580	1.5261550	-0.7126160
H	34.8719470	0.0570130	-1.5490840
C	42.0441360	-9.7161060	-1.7395870
C	34.1630410	-1.1927720	2.4821570
C	32.7473950	-0.1302790	0.7344690
H	35.4535910	-2.0022730	4.0010370
H	42.9083030	-9.5307360	-2.3865030
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C	32.9599520	-1.6311310	3.1751360
C	31.5932810	-0.6162260	1.4170450
C	32.5077850	0.7085820	-0.3571400
C	33.0594960	-2.3797200	4.4664960
C	31.7473740	-1.3669320	2.6307230
C	30.3080080	-0.3350960	0.9422930
C	31.2219940	1.0069240	-0.8190840
H	33.3225770	1.1951560	-0.8669330
C	33.1602870	-3.7885870	4.4649900
C	33.0417170	-1.6838080	5.6859990
H	30.8483030	-1.7112220	3.1329740
H	29.4881250	-0.7201080	1.5254650
C	30.0702230	0.4399480	-0.1958990
C	31.0610380	1.9267490	-1.9098240
C	33.2360370	-4.4705700	5.6746950
C	33.1877570	-4.5594490	3.1686800
C	33.1193180	-2.3897770	6.8927380
C	32.9405810	-0.1780390	5.7153140
C	28.7457620	0.7433780	-0.7425420
H	31.9562620	2.3518210	-2.3536050

C	29.8430330	2.2940230	-2.3760280
H	33.3125440	-5.5505220	5.7030540
C	33.2138660	-3.7769970	6.8831350
H	34.0205550	-4.2416590	2.5328480
H	33.2941530	-5.6303540	3.3550360
H	32.2714490	-4.4032210	2.5911730
H	33.1032260	-1.8372020	7.8233570
H	33.0097510	0.1990840	6.7385090
H	33.7379190	0.2872780	5.1269780
H	31.9930860	0.1675410	5.2902670
C	28.6437270	1.7025990	-1.7975850
C	27.5363850	0.1423430	-0.3100040
C	29.7387540	3.2875400	-3.4896290
O	33.2948950	-4.5573400	8.0237560
C	27.3881340	2.0697220	-2.3116620
C	26.3075380	0.5198050	-0.8392160
C	27.3127040	-0.9581740	0.7156610
C	29.6455860	4.6660480	-3.1995240
C	29.7484720	2.8556580	-4.8251050
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H	27.3159060	2.8013730	-3.1046910
C	26.2291440	1.5027010	-1.8291640
C	25.1440030	-0.1908720	-0.1718880
H	27.4377260	-0.5767920	1.7377670
H	28.0109590	-1.7906490	0.5962130
C	25.8597420	-1.4111060	0.4705550
C	29.5733880	5.5820910	-4.2432980
C	29.6174470	5.1530850	-1.7722300
C	29.6746310	3.7942830	-5.8613590
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H	32.3333850	-3.3608100	9.4604290
H	34.1159320	-3.2323570	9.4351850
H	33.3357330	-4.7182750	10.0399620
O	25.0286110	1.9376520	-2.3612040
C	23.9631810	-0.6069730	-1.0324260
C	24.4475500	0.7342680	0.8713510
H	25.3553630	-1.7475790	1.3810100

H	25.8526620	-2.2361380	-0.2472140
H	29.5003500	6.6451290	-4.0494320
C	29.5897280	5.1504870	-5.5677920
H	28.7855560	4.7064330	-1.2180220
H	30.5347160	4.8841710	-1.2391320
H	29.5070440	6.2391780	-1.7341880
H	29.6826120	3.4434030	-6.8853000
H	29.0186620	0.8261130	-4.6902230
H	29.7726430	1.2289690	-6.2413350
H	30.7685800	0.9463310	-4.8053720
C	22.7335130	-0.3731170	-0.4196970
C	24.0192940	-1.2241800	-2.2870180
C	22.9747330	0.2870740	0.9278450
H	24.9448130	0.6936830	1.8440390
H	24.5026190	1.7699020	0.5187890
O	29.5142210	6.1489260	-6.5252460
C	21.5079840	-0.7257810	-1.0446270
O	25.2712520	-1.4922780	-2.8066030
C	22.8488890	-1.5210710	-2.9507600
H	22.8120650	-0.4299530	1.7426700
H	22.3074080	1.1335090	1.1077560
C	29.5109630	5.7781040	-7.9159400
C	21.5941980	-1.2673200	-2.3630030
H	22.8807540	-1.9555860	-3.9437120
H	28.6506430	5.1450720	-8.1579430
H	30.4339670	5.2573370	-8.1924790
H	29.4414930	6.7143880	-8.4661670
C	20.1838230	-0.5544730	-0.4420520
C	19.9483720	-0.2147470	0.8927930
C	19.0273490	-0.7950610	-1.2412460
C	18.6640730	-0.0384610	1.4173380
H	20.7654770	-0.1125620	1.5873670
C	17.7435160	-0.5980410	-0.7223550
C	19.1777090	-1.2866720	-2.5813990
C	18.5072530	0.2511260	2.8149050
C	17.5096970	-0.1806060	0.5905640
H	16.9216100	-0.8215820	-1.3819550

H	18.2768960	-1.4729370	-3.1584140
C	20.3889930	-1.5474060	-3.1303290
C	17.2909020	0.3893550	3.3956160
H	19.4043410	0.3390450	3.4203560
C	16.1869360	0.0610280	1.1708910
C	20.4851190	-2.1012110	-4.5166620
C	16.0890270	0.2984290	2.5771570
C	17.1915120	0.6523230	4.8650030
C	14.9755320	0.0921080	0.4344670
C	20.5751130	-1.2301540	-5.6249100
C	20.4750470	-3.4903930	-4.7213790
C	14.8351470	0.4756290	3.1870030
C	17.1014010	-0.4266440	5.7710190
C	17.2037620	1.9696880	5.3492550
C	13.7484000	0.2750690	1.0616060
C	14.7479060	-0.0333240	-1.0640640
C	20.6482530	-1.7609050	-6.9083540
C	20.5937390	0.2657730	-5.4318050
C	20.5497710	-4.0039710	-6.0218750
C	20.3851460	-4.4431760	-3.5541040
H	14.7659480	0.6474350	4.2524250
C	13.6740060	0.4463560	2.4463160
C	17.0349200	-0.1705780	7.1362680
C	17.0706810	-1.8502360	5.2735000
C	17.1357950	2.2058800	6.7276440
C	17.2840650	3.1409110	4.4007670
C	12.5824430	0.1908820	0.0932000
H	14.8704040	-1.0726990	-1.3964870
H	15.4455700	0.5742310	-1.6462790
C	13.2951050	0.4413950	-1.2644970
H	20.7162540	-1.1164090	-7.7760950
C	20.6338890	-3.1399600	-7.1080730
H	21.4264850	0.5753970	-4.7918740
H	20.6937920	0.7805480	-6.3898810
H	19.6766580	0.6181210	-4.9497830
H	20.5395880	-5.0773500	-6.1611100
H	20.4576740	-5.4806760	-3.8891120

H	21.1855630	-4.2634690	-2.8292220
H	19.4399990	-4.3267510	-3.0147050
O	12.4754270	0.5968550	3.1202970
H	16.9644880	-0.9791350	7.8533750
C	17.0541150	1.1379490	7.6139200
H	16.2351010	-2.0107080	4.5844930
H	17.9850320	-2.1035500	4.7279210
H	16.9647900	-2.5505720	6.1050790
H	17.1460310	3.2281210	7.0834170
H	16.4681520	3.1157800	3.6713800
H	17.2264520	4.0879630	4.9429310
H	18.2185080	3.1324250	3.8310340
C	11.4022510	1.1245120	0.3016840
C	11.8856960	-1.2008520	0.1751250
H	12.7881240	-0.0644510	-2.0912990
H	13.2888050	1.5159150	-1.4676750
O	20.7115480	-3.5556620	-8.4262950
O	16.9847180	1.2752490	8.9908840
C	10.1722820	0.4990300	0.1063250
C	11.4588960	2.4916650	0.5944770
C	10.4129120	-0.9677390	-0.2108270
H	12.3824570	-1.9402130	-0.4585920
H	11.9408450	-1.5646210	1.2068800
C	20.6885380	-4.9664250	-8.7136960
C	16.9867910	2.5982730	9.5572990
C	8.9470850	1.2084920	0.2170980
O	12.7110350	3.0658130	0.7030300
C	10.2887860	3.1961310	0.7765000
H	10.2505020	-1.1626960	-1.2785930
H	9.7452010	-1.6333790	0.3416460
H	19.7587490	-5.4288160	-8.3659920
H	21.5421210	-5.4803360	-8.2590390
H	20.7516260	-5.0428840	-9.7972600
H	16.1257890	3.1810550	9.2129760
H	17.9094990	3.1356590	9.3134470
H	16.9225620	2.4535830	10.6339470
C	9.0338330	2.5780300	0.6116270

C	7.6228000	0.6308720	-0.0247270
H	10.3210740	4.2442680	1.0524150
C	7.8289670	3.3533520	0.8703450
C	6.4665380	1.4077590	0.2810760
C	7.3872740	-0.6259020	-0.5884170
C	7.9261690	4.7819450	1.3033250
C	6.6174010	2.7624030	0.7310600
C	5.1825000	0.8804720	0.1093890
C	6.1028120	-1.1447200	-0.7799260
H	8.2045830	-1.2348410	-0.9373750
C	7.9404930	5.8130260	0.3382090
C	7.9931020	5.1044300	2.6684430
H	5.7167760	3.3306810	0.9432960
C	4.9483070	-0.4069790	-0.3807970
H	4.3607750	1.5371040	0.3421130
C	5.9460740	-2.4193240	-1.4222050
C	8.0173570	7.1383200	0.7527440
C	7.8731800	5.4919130	-1.1342570
C	8.0686300	6.4453780	3.0644570
C	7.9872090	4.0223300	3.7206240
C	3.6251250	-1.0095390	-0.5566730
H	6.8433110	-2.9499950	-1.7261930
C	4.7296820	-2.9582800	-1.6786250
H	8.0287490	7.9487470	0.0343410
C	8.0790370	7.4549810	2.1084090
H	8.6840760	4.8201560	-1.4341520
H	6.9357470	4.9885930	-1.3906110
H	7.9453520	6.4016900	-1.7344450
H	8.1181430	6.6757880	4.1208850
H	8.8083360	3.3141780	3.5695690
H	8.0893920	4.4486400	4.7213710
H	7.0602290	3.4414450	3.6924850
C	3.5275220	-2.2585210	-1.2451530
C	2.4129400	-0.4498740	-0.0789260
C	4.6297570	-4.2736640	-2.3841780
O	8.1527200	8.8049600	2.4058750
C	2.2734480	-2.8438610	-1.4905650

C	1.1856820	-1.0523970	-0.3305480
C	2.1843260	0.8022740	0.7535620
C	4.6480020	-5.4765900	-1.6455090
C	4.5320000	-4.3167850	-3.7837640
C	8.2067580	9.2115830	3.7862110
H	2.2045160	-3.7858000	-2.0172600
C	1.1117500	-2.2428500	-1.0582830
C	0.0190040	-0.2399950	0.2014690
H	2.3110680	1.7086590	0.1467620
H	2.8787310	0.8791660	1.5942540
C	0.7292280	0.6668790	1.2441330
C	4.5776640	-6.6928770	-2.3161070
C	4.7361080	-5.4559590	-0.1397700
C	4.4613900	-5.5517290	-4.4395140
C	4.4956120	-3.0446360	-4.5948540
H	9.0982940	8.8158200	4.2841250
H	7.3131530	8.8902200	4.3315250
H	8.2517620	10.2985660	3.7669090
O	-0.0869920	-2.8603370	-1.3666540
C	-1.1639110	-0.9824800	0.7994140
C	-0.6730670	0.5613550	-0.9421510
H	0.2234880	1.6299130	1.3595410
H	0.7181780	0.1582990	2.2122020
H	4.5886040	-7.6307490	-1.7745590
C	4.4864530	-6.7322290	-3.7056850
H	3.9192140	-4.8717890	0.2960780
H	4.6855930	-6.4689110	0.2661100
H	5.6701400	-4.9985090	0.2011750
H	4.3852410	-5.5660540	-5.5191350
H	4.3847570	-3.2623190	-5.6598870
H	3.6607560	-2.4050140	-4.2907790
H	5.4096670	-2.4578280	-4.4608790
C	-2.3922360	-0.4401110	0.4262370
C	-1.1108280	-2.0617400	1.6885270
C	-2.1474930	0.7192610	-0.5255640
H	-0.1753000	1.5172170	-1.1254220
H	-0.6144780	-0.0209380	-1.8681010

O	4.4227330	-7.9970570	-4.2673280
C	-3.6194430	-0.9672240	0.9087950
O	0.1398730	-2.5051340	2.0735440
C	-2.2828100	-2.6397880	2.1254720
H	-2.3121040	1.6773720	-0.0162150
H	-2.8115390	0.6993650	-1.3931950
C	4.3080410	-8.1164950	-5.6971190
C	-3.5361210	-2.1259520	1.7390640
C	-4.9424960	-0.4197740	0.5994270
H	-2.2533050	-3.5064690	2.7764340
H	5.1745070	-7.6796790	-6.2050950
H	3.3932950	-7.6397520	-6.0650210
H	4.2685350	-9.1854320	-5.8971610
C	-4.7429030	-2.8082140	2.1840180
C	-6.1004850	-1.1415520	1.0143080
C	-5.1756030	0.8010970	-0.0391620
C	-4.6498740	-4.0307370	3.0411170
C	-5.9528620	-2.3331500	1.8008300
C	-7.3832540	-0.6809000	0.7002250
C	-6.4588460	1.2718660	-0.3346550
H	-4.3575170	1.4530010	-0.2966460
C	-4.5560720	-5.3089620	2.4474140
C	-4.6667110	-3.9119000	4.4401790
H	-6.8547470	-2.8517190	2.1119390
H	-8.2063670	-1.2710090	1.0673880
C	-7.6146380	0.5010400	-0.0084490
C	-6.6130090	2.5651610	-0.9390440
C	-4.4861220	-6.4366830	3.2582810
C	-4.5298440	-5.4635970	0.9471300
C	-4.5950100	-5.0601660	5.2382730
C	-4.7606910	-2.5575030	5.0999150
C	-8.9361450	1.0114420	-0.3800580
H	-5.7148650	3.1332380	-1.1619520
C	-7.8281870	3.0993830	-1.2105850
H	-4.4150580	-7.4288980	2.8300160
C	-4.5072460	-6.3153210	4.6463670
H	-3.6944920	-4.9120130	0.5035100

H	-4.4286450	-6.5141290	0.6660290
H	-5.4444370	-5.0747180	0.4890330
H	-4.6103330	-4.9499910	6.3149650
H	-4.6913550	-2.6458830	6.1867890
H	-3.9602450	-1.8918430	4.7613780
H	-5.7058940	-2.0605360	4.8601910
C	-9.0313730	2.3249720	-0.9361390
C	-10.1488620	0.2894650	-0.2420960
C	-7.9251940	4.4687290	-1.8051910
O	-4.4321380	-7.5031920	5.3530820
C	-10.2838610	2.8789280	-1.2522020
C	-11.3744940	0.8589450	-0.5678480
C	-10.3796860	-1.1385350	0.2276760
C	-8.0147650	5.5990100	-0.9640230
C	-7.9118420	4.6364990	-3.1986770
C	-4.4592940	-7.4601170	6.7921070
H	-10.3509130	3.8758870	-1.6657170
C	-11.4462720	2.1665330	-1.0549910
C	-12.5427170	-0.0612360	-0.2633160
H	-10.2579080	-1.2208240	1.3158890
H	-9.6831840	-1.8473280	-0.2276650
C	-11.8327640	-1.4412330	-0.1885220
C	-8.0796090	6.8686060	-1.5276930
C	-8.0469070	5.4428680	0.5358990
C	-7.9782670	5.9234580	-3.7460420
C	-7.8322580	3.4437270	-4.1199810
H	-5.3906250	-7.0168540	7.1600210
H	-3.6073860	-6.8990050	7.1906410
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O	-12.6434140	2.7891570	-1.3591350
C	-13.7201680	-0.0741950	-1.2232630
C	-13.2423350	0.3448430	1.0688700
H	-12.3418810	-2.1257780	0.4961090
H	-11.8389280	-1.8901270	-1.1857030
H	-8.1497530	7.7527560	-0.9061430
C	-8.0594680	7.0320360	-2.9110780
H	-8.8826720	4.8091930	0.8499730

H	-7.1327950	4.9706240	0.9091080
H	-8.1535420	6.4134630	1.0255940
H	-7.9675470	6.0342020	-4.8227250
H	-8.6509640	2.7422070	-3.9303110
H	-7.8858680	3.7536380	-5.1665020
H	-6.8999050	2.8884390	-3.9777410
C	-14.9523000	-0.1140620	-0.5732890
C	-13.6591440	-0.1099140	-2.6207810
C	-14.7162990	-0.0793210	0.9277140
H	-12.7498270	-0.1011320	1.9369550
H	-13.1835510	1.4327240	1.1825000
O	-8.1273100	8.3402410	-3.3617920
C	-16.1754370	-0.1689530	-1.2928460
O	-12.4052040	-0.1404320	-3.2004390
C	-14.8268840	-0.0978140	-3.3520490
H	-14.8843700	-1.0708520	1.3671820
H	-15.3827870	0.6167620	1.4428870
C	-8.1264290	8.5868310	-4.7798360
C	-16.0839100	-0.1093230	-2.7165570
C	-17.5021180	-0.2618130	-0.6786590
H	-14.7910690	-0.0770140	-4.4355830
H	-8.9882280	8.1181850	-5.2667590
H	-7.2043420	8.2252080	-5.2473700
H	-8.1900280	9.6678960	-4.8868010
C	-17.2859170	-0.0389520	-3.5350690
C	-17.7432590	-0.5108330	0.6750610
C	-18.6552130	-0.1432520	-1.5095250
C	-18.4993660	-0.0289240	-2.9318120
C	-17.1841470	0.0388010	-5.0255210
C	-19.0297810	-0.5674500	1.2203430
H	-16.9291750	-0.7100440	1.3519120
C	-19.9412170	-0.1788160	-0.9607190
H	-19.3977790	0.0459070	-3.5370850
C	-17.0877200	1.2938480	-5.6663170
C	-17.1952180	-1.1366600	-5.7936520
C	-19.1925220	-0.8882590	2.6104040
C	-20.1806350	-0.3487420	0.4054550

H	-20.7602390	-0.1041400	-1.6565370
C	-17.0092600	1.3496300	-7.0537470
C	-17.0680330	2.5710800	-4.8639820
C	-17.1150320	-1.0581410	-7.1893740
C	-17.2919860	-2.4906260	-5.1334880
C	-20.4113020	-1.0036050	3.1910210
H	-18.2979940	-1.0627260	3.2006930
C	-21.5059020	-0.3702120	1.0284640
H	-16.9362700	2.2982400	-7.5712270
C	-17.0245510	0.1812840	-7.8131290
H	-16.2384010	2.5810460	-4.1495280
H	-16.9619930	3.4396020	-5.5176890
H	-17.9872800	2.6923050	-4.2827470
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H	-17.2185180	-3.2924620	-5.8721010
H	-16.4952540	-2.6335560	-4.3964580
H	-18.2398790	-2.6082030	-4.5991680
C	-21.6097380	-0.7425790	2.4047200
C	-20.5167910	-1.3784430	4.6354880
C	-22.7143490	-0.0328760	0.3676630
O	-16.9410480	0.3561370	-9.1838490
C	-22.8662330	-0.8354810	3.0277370
C	-20.6105770	-2.7371080	5.0075080
C	-20.5062060	-0.3839140	5.6258960
C	-23.9441890	-0.1280530	1.0088320
C	-22.9358610	0.4798410	-1.0469660
C	-16.9639690	-0.8041560	-10.036285
H	-22.9398280	-1.1248750	4.0670980
C	-24.0243460	-0.5514930	2.3379410
C	-20.6822280	-3.0747750	6.3546290
C	-20.6394080	-3.8225920	3.9606070
C	-20.5793630	-0.7451330	6.9766390
C	-20.4218800	1.0763420	5.2538760
C	-25.1061270	0.2005450	0.0888880
H	-22.8106070	-0.3253570	-1.7830060
H	-22.2367830	1.2749250	-1.3188960
C	-24.3885030	0.9954830	-1.0366870

H	-17.8960050	-1.3668580	-9.9184820
H	-16.1132560	-1.4639220	-9.8352490
H	-16.8953270	-0.4195300	-11.051804
O	-25.2258540	-0.6958850	3.0081520
H	-20.7554870	-4.1088680	6.6680690
C	-20.6645430	-2.0855410	7.3353940
H	-21.4718880	-3.6788230	3.2642070
H	-19.7226470	-3.8267560	3.3627750
H	-20.7491860	-4.8060770	4.4231130
H	-20.5702470	0.0349250	7.7270140
H	-21.2344570	1.3596910	4.5772860
H	-20.4821440	1.7103140	6.1419160
H	-19.4848420	1.3051250	4.7366850
C	-26.2887510	0.9616740	0.6634320
C	-25.8008690	-1.0979480	-0.4213100
H	-24.8914560	0.8818560	-2.0013850
H	-24.3954580	2.0565160	-0.7719850
O	-20.7390060	-2.5359710	8.6434980
C	-27.5168460	0.4751660	0.2192830
C	-26.2355750	2.0812530	1.5011940
C	-27.2723560	-0.7244960	-0.6812750
H	-25.3001570	-1.5050460	-1.3036690
H	-25.7494610	-1.8594660	0.3644040
C	-20.7375860	-1.5707330	9.7110240
C	-28.7436480	1.0730500	0.6119540
O	-24.9849160	2.5578020	1.8442720
C	-27.4075980	2.6446540	1.9568200
H	-27.4296410	-0.4547990	-1.7334410
H	-27.9412900	-1.5600810	-0.4611050
H	-21.5970780	-0.8956790	9.6397110
H	-19.8137020	-0.9824840	9.7162670
H	-20.8051810	-2.1520190	10.6284960
C	-28.6608090	2.1516610	1.5438670
C	-30.0659550	0.6498030	0.1449270
H	-27.3781450	3.4813940	2.6458500
C	-29.8680360	2.7467840	2.0990320
C	-31.2247760	1.2269050	0.7433330

C	-30.2969500	-0.2546670	-0.8949010
C	-29.7751940	3.8626890	3.0909470
C	-31.0780070	2.2681750	1.7203460
C	-32.5071780	0.8203320	0.3606550
C	-31.5796860	-0.6450050	-1.2921970
H	-29.4771040	-0.6610010	-1.4635110
C	-29.7630050	5.2032670	2.6465290
C	-29.7102380	3.5837360	4.4657150
H	-31.9803610	2.6950020	2.1477630
C	-32.7370380	-0.1424720	-0.6256500
H	-33.3309070	1.3190110	0.8437620
C	-31.7314860	-1.5321420	-2.4110060
C	-29.6904810	6.2331490	3.5782960
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C	-29.6390350	4.6356120	5.3872100
C	-29.7134380	2.1603570	4.9677610
C	-34.0584240	-0.6149750	-1.0447440
H	-30.8320140	-1.8866540	-2.9052700
C	-32.9457400	-1.9128170	-2.8762420
H	-29.6806870	7.2700210	3.2655290
C	-29.6309330	5.9529010	4.9420700
H	-29.0146240	5.0452910	0.6229760
H	-30.7634150	5.1773240	0.7289890
H	-29.7566130	6.6060120	1.0110930
H	-29.5909720	4.4024120	6.4430930
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H	-30.6374770	1.6414840	4.6949490
C	-34.1509250	-1.4589100	-2.1948300
C	-35.2736060	-0.3075050	-0.3818360
C	-33.0404760	-2.8101720	-4.0694510
O	-29.5618250	7.0542490	5.7777670
C	-35.4029820	-1.8857050	-2.6699600
C	-36.4988400	-0.7475900	-0.8695420
C	-35.5077690	0.4782620	0.8990920
C	-33.0242510	-4.2121150	-3.9041370
C	-33.1312230	-2.2614270	-5.3582390

C	-29.5090860	6.8455500	7.2016300
H	-35.4679090	-2.5186490	-3.5443610
C	-36.5675530	-1.5211440	-2.0309770
C	-37.6689110	-0.2334380	-0.0503910
H	-35.3803020	1.5558090	0.7305550
H	-34.8169320	0.1943390	1.6971700
C	-36.9645730	0.1492050	1.2806720
C	-33.0896500	-5.0342380	-5.0238560
C	-32.9430370	-4.8258760	-2.5285730
C	-33.1968660	-3.1067460	-6.4723120
C	-33.1653120	-0.7662370	-5.5602860
H	-28.6164120	6.2800440	7.4891950
H	-30.4017850	6.3229780	7.5610370
H	-29.4673030	7.8408190	7.6393570
O	-37.7640470	-1.9506690	-2.5769900
C	-38.8538170	-1.1570610	0.1748570
C	-38.3562060	0.9755210	-0.7529570
H	-37.4722880	0.9740740	1.7889990
H	-36.9786920	-0.7199530	1.9442240
H	-33.0799600	-6.1128350	-4.9262580
C	-33.1738230	-4.4863310	-6.3019890
H	-33.7614430	-4.4767330	-1.8907240
H	-32.9959900	-5.9154930	-2.5858100
H	-32.0101920	-4.5563200	-2.0235170
H	-33.2675330	-2.6663280	-7.4585260
H	-33.2694730	-0.5164430	-6.6189150
H	-34.0032290	-0.3128230	-5.0209140
H	-32.2532110	-0.2905620	-5.1866770
C	-40.0816240	-0.5072970	0.0606190
C	-38.8017250	-2.5099310	0.5281090
C	-39.8333100	0.9441070	-0.3176220
H	-37.8595200	1.9192210	-0.5128320
H	-38.2912400	0.8385130	-1.8377490
O	-33.2329450	-5.3982480	-7.3430050
C	-41.3098960	-1.1875460	0.2771460
O	-37.5523330	-3.0738480	0.6946560
C	-39.9744260	-3.2176260	0.6783000

H	-40.0046570	1.6019110	0.5440400
H	-40.4899730	1.2882770	-1.1204010
C	-33.3385440	-4.9063810	-8.6916710
C	-41.2267070	-2.5881650	0.5428310
C	-42.6341100	-0.5591170	0.2317100
H	-39.9461790	-4.2777710	0.9037590
H	-32.4697120	-4.2975330	-8.9637060
H	-34.2518940	-4.3184590	-8.8313430
H	-33.3748090	-5.7926100	-9.3221040
C	-42.4324360	-3.3969620	0.6588800
C	-43.7925480	-1.3926550	0.3174640
C	-42.8609780	0.8173900	0.1442470
C	-42.3368010	-4.8677670	0.9144360
C	-43.6431240	-2.8060090	0.5192090
C	-45.0732750	-0.8400850	0.2466070
C	-44.1447510	1.3715380	0.0849650
H	-42.0389760	1.5128830	0.1454660
C	-42.2437690	-5.7714890	-0.1671450
C	-42.3510770	-5.3551300	2.2312620
H	-44.5444740	-3.4076680	0.5847800
H	-45.9114940	-1.5230500	0.3142590
C	-45.2904500	0.5307840	0.1166200
C	-44.3163590	2.7965930	-0.0024750
C	-42.1714820	-7.1367910	0.0869270
C	-42.2213500	-5.2733200	-1.5908060
C	-42.2769710	-6.7336820	2.4647400
C	-42.4450680	-4.4104420	3.4048670
C	-46.6158000	1.1376240	0.0356600
H	-43.4247650	3.4162590	-0.0170240
C	-45.5391120	3.3830140	-0.0669860
H	-42.1009980	-7.8524820	-0.7228350
C	-42.1896930	-7.6176510	1.3948600
H	-41.3875470	-4.5840720	-1.7599430
H	-42.1200220	-6.1044290	-2.2920460
H	-43.1377000	-4.7287240	-1.8384570
H	-42.2902250	-7.0921560	3.4859690
H	-42.3696780	-4.9525560	4.3505000

H	-41.6481770	-3.6602670	3.3791910
H	-43.3931220	-3.8635200	3.4033520
C	-46.7335840	2.5499720	-0.0520420
C	-47.7953190	0.3649820	0.0389580
C	-45.6575140	4.8715210	-0.1555110
O	-42.1124010	-8.9927240	1.5286470
C	-48.0184040	3.1295690	-0.1264460
C	-49.0426090	0.9534710	-0.0352570
C	-45.7525100	5.6444950	1.0223610
C	-45.6654570	5.5054400	-1.4080860
C	-42.1370990	-9.5670790	2.8490790
H	-48.0978070	4.2079790	-0.1918830
C	-49.1567290	2.3488960	-0.1174450
C	-45.8460240	7.0286240	0.9268310
C	-45.7557510	4.9858920	2.3795340
C	-45.7604280	6.9003630	-1.4819490
C	-45.5752040	4.7018490	-2.6826180
H	-43.0681890	-9.3241740	3.3717690
H	-41.2848300	-9.2281130	3.4474790
H	-42.0724600	-10.6427160	2.6986190
H	-45.9195180	7.6460790	1.8135690
C	-45.8482170	7.6553200	-0.3176970
H	-46.5721800	4.2618840	2.4690600
H	-44.8257460	4.4379870	2.5605940
H	-45.8723600	5.7287890	3.1717330
H	-45.7649480	7.3727040	-2.4558270
H	-46.3738710	3.9554040	-2.7406230
H	-45.6526180	5.3490860	-3.5594850
H	-44.6282260	4.1568330	-2.7465120
O	-45.9448210	9.0361410	-0.2933310
C	-45.9538710	9.7550580	-1.5408490
H	-46.8110420	9.4692200	-2.1596260
H	-45.0286310	9.5898250	-2.1029290
H	-46.0336680	10.8058090	-1.2697000
H	-50.1349070	2.8124290	-0.1752940
H	-49.9329550	0.3349720	-0.0312210
H	-47.7311900	-0.7141290	0.0964150

H	47.7364300	-0.6020760	-0.4085150
H	49.9336500	0.4564460	-0.5457810
H	50.1247020	2.9362180	-0.6728690
H	36.8668560	-2.5880380	0.2408800
H	37.8001260	-1.8667050	3.7775530
H	24.2805100	1.3749260	-2.0865290
H	25.2271450	-1.8550910	-3.7090120
H	12.6666800	4.0023690	0.9653510
H	11.7256720	0.7270930	2.5097820
H	0.0947290	-3.3023610	2.6306270
H	-0.8374490	-2.4662600	-0.8835760
H	-13.3940200	2.1660600	-1.3481120
H	-12.4458300	-0.0929430	-4.1720470
H	-25.9734060	-0.3227330	2.5044650
H	-25.0314740	3.2989040	2.4739730
H	-38.5177150	-1.7949540	-1.9776390
H	-37.5967480	-4.0314690	0.8649440