

Electronic Supplementary Information

Complexation between triptycene-derived oxacalixarene and π -extended viologens: linker-length-dependent orientations of macrocycles in pseudo[3]rotaxanes in the solid state

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1. Copies of ^1H NMR and ^{13}C NMR spectra of new compounds

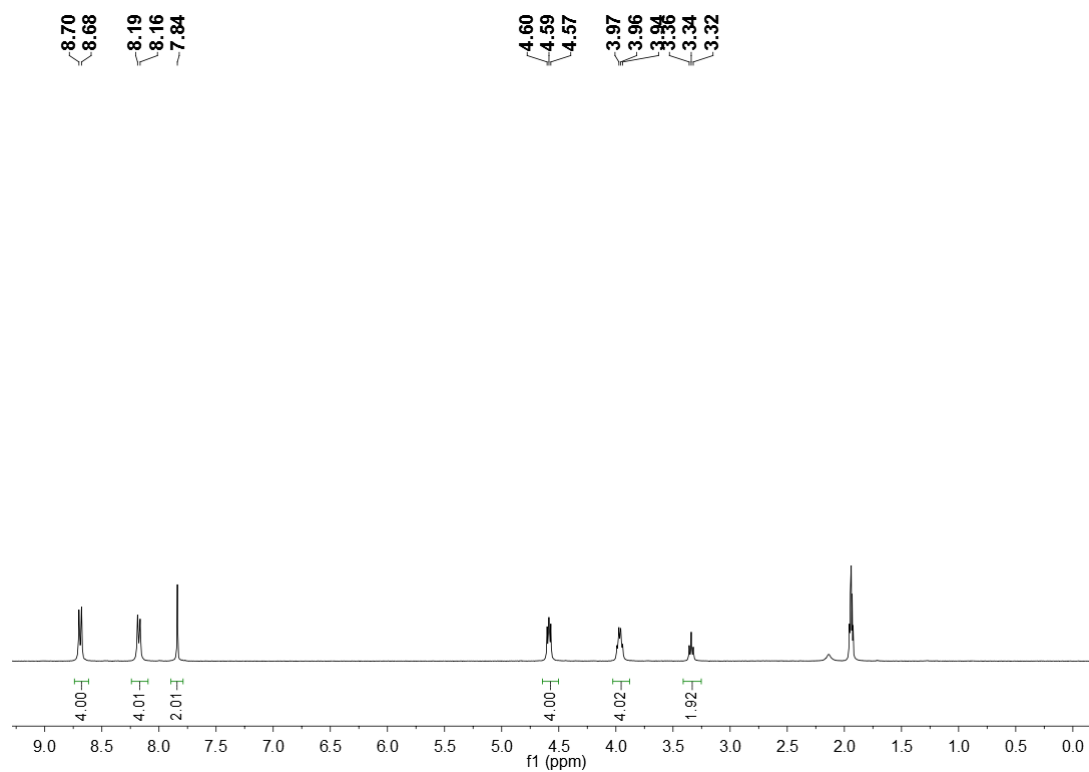


Fig. S1. ^1H NMR spectrum (300 MHz, CD_3CN) of G2.

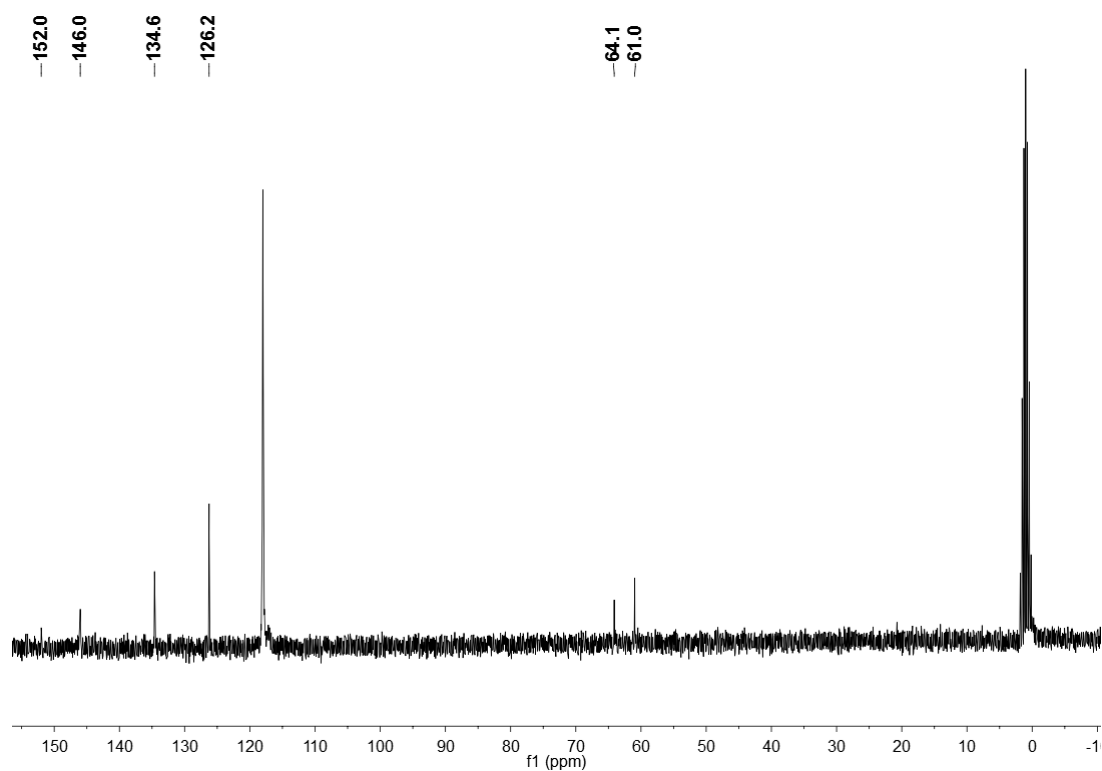


Fig. S2. ^{13}C NMR spectrum (75 MHz, CD_3CN) of G2.

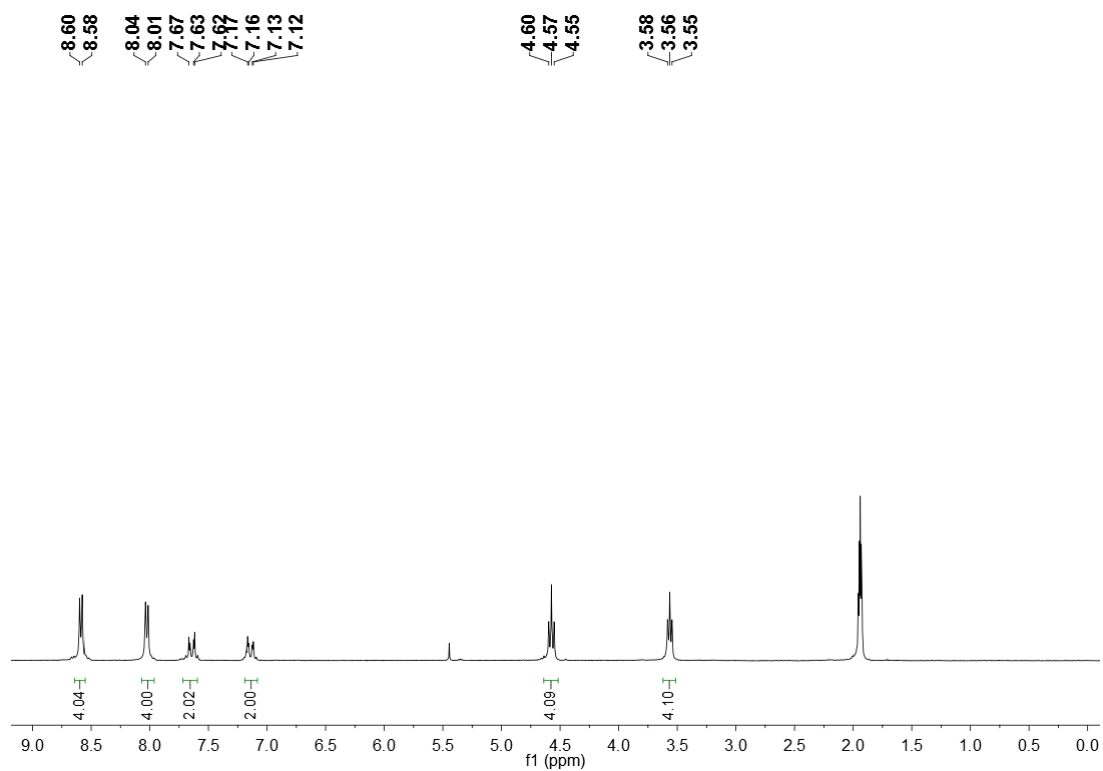


Fig. S3. ^1H NMR spectrum (300 MHz, CD_3CN) of **G4**.

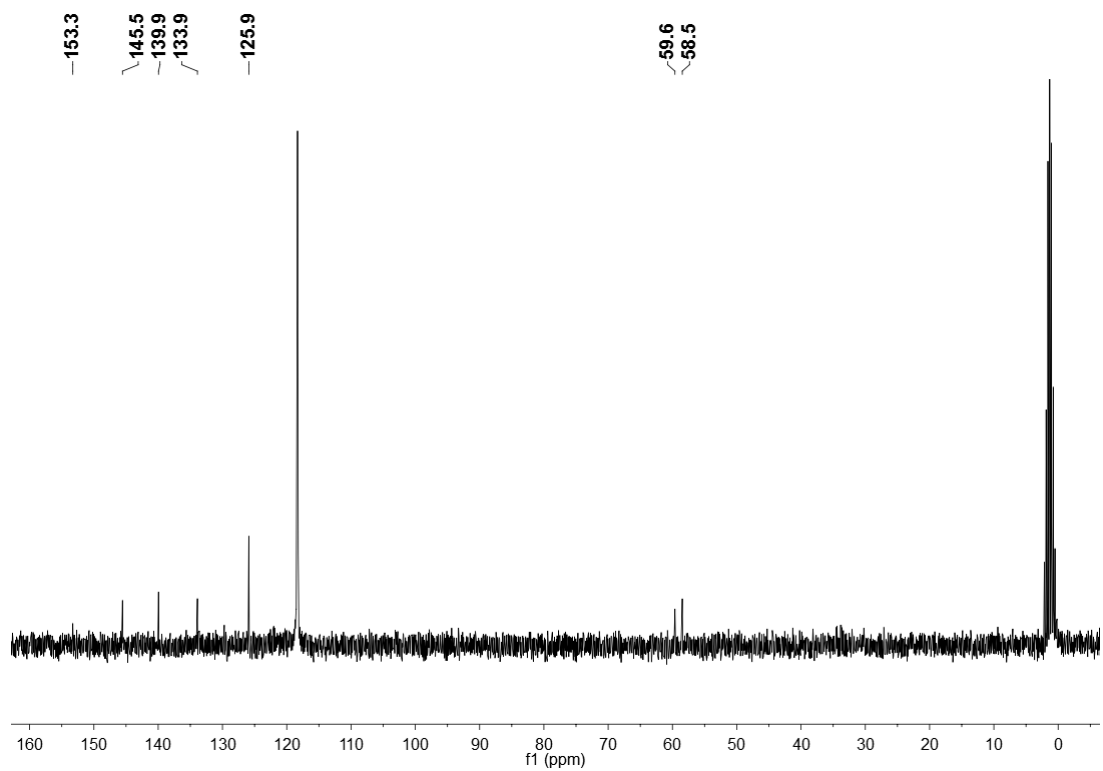


Fig. S4. ^{13}C NMR spectrum (75 MHz, CD_3CN) of **G4**.

2. ^1H NMR studies on complexation between the host **H** and the guests **G1-G4**

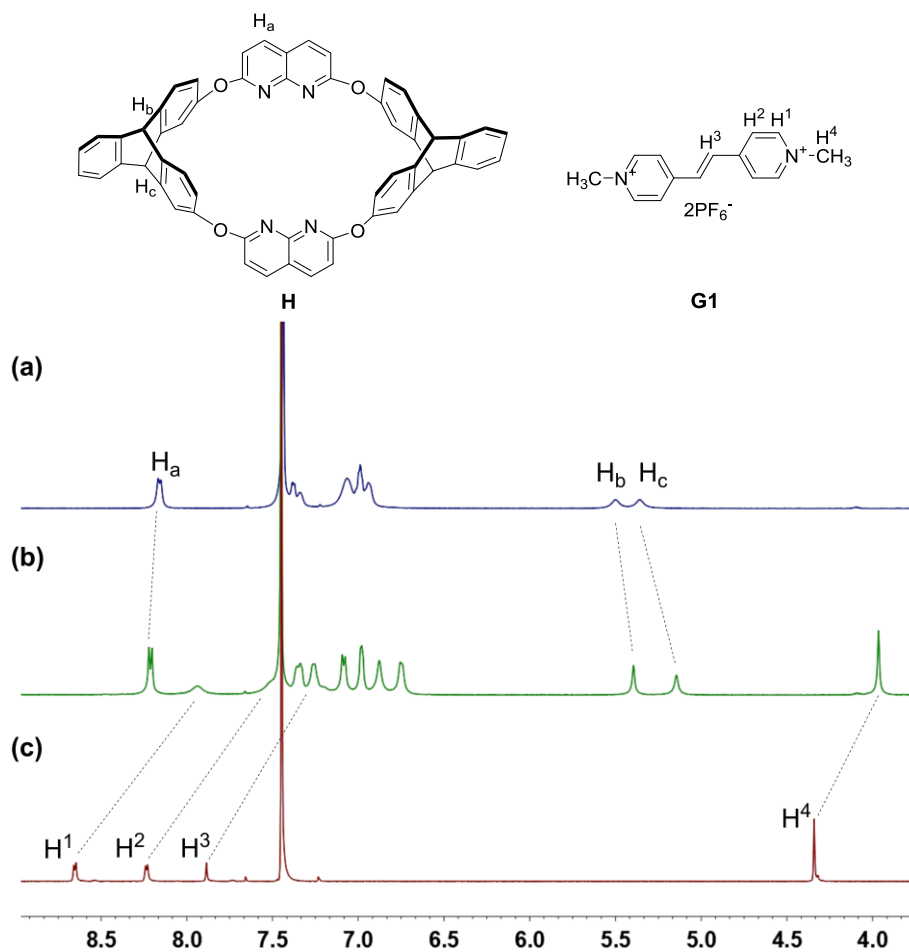


Fig. S5. Partial ^1H NMR spectra (500 MHz, $\text{CDCl}_3/\text{CD}_3\text{CN}$, 2:1 v/v, 298K) of (a) free host **H**, (b) **H** and 0.5 equiv. of **G1**, (c) free guest **G1**. $[\text{H}]_0 = 3.0$ mM.

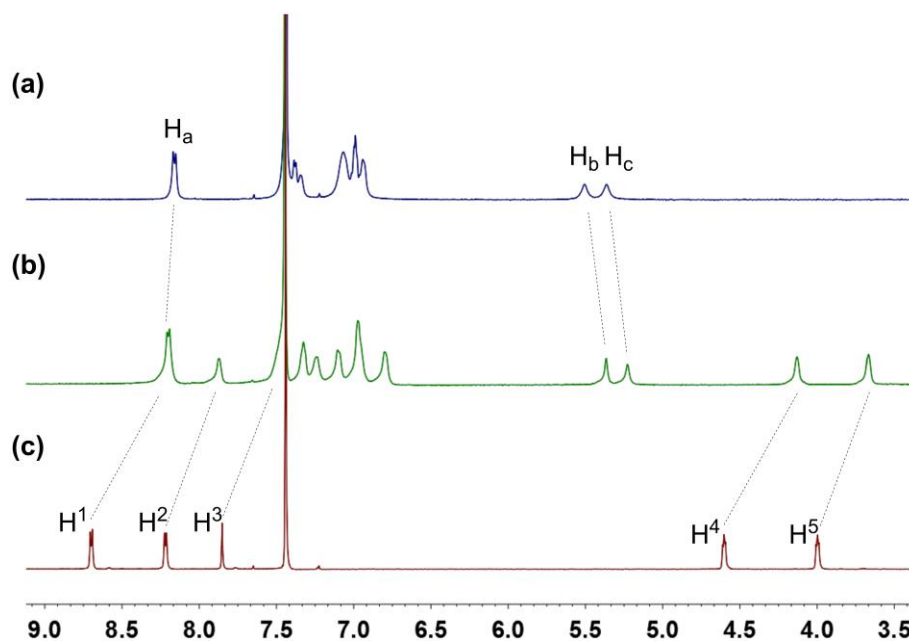
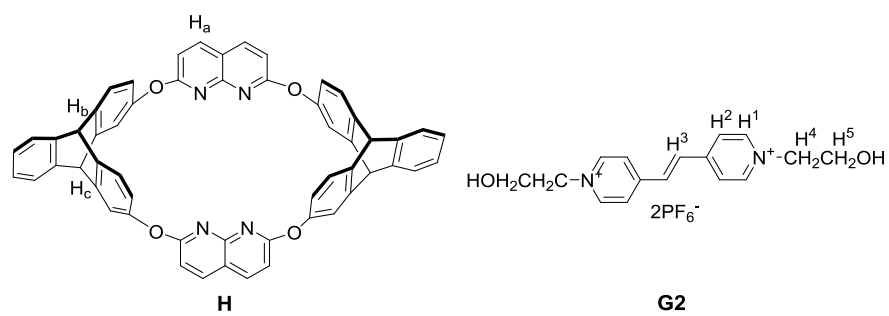


Fig. S6. Partial ^1H NMR spectra (500 MHz, $\text{CDCl}_3/\text{CD}_3\text{CN}$, 2:1 v/v, 298K) of (a) free host **H**, (b) **H** and 0.5 equiv. of **G2**, (c) free guest **G2**. $[\text{H}]_0 = 3.0$ mM.

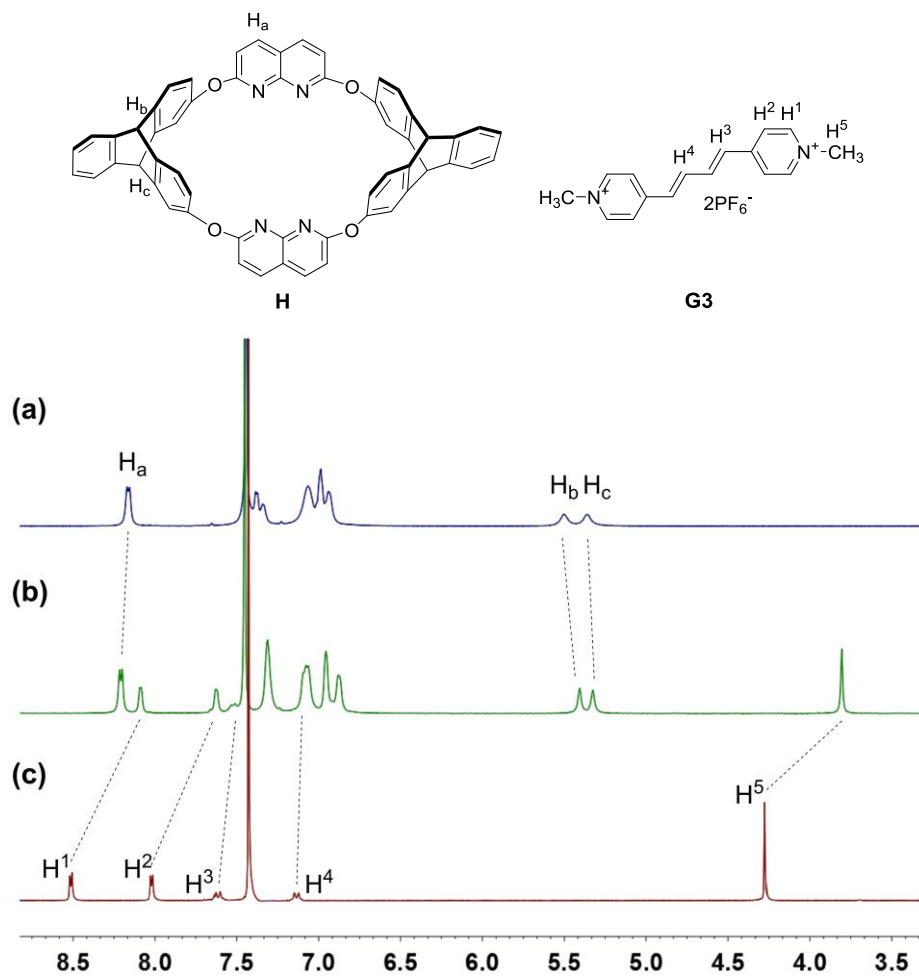


Fig. S7. Partial ^1H NMR spectra (500 MHz, $\text{CDCl}_3/\text{CD}_3\text{CN}$, 2:1 v/v, 298K) of (a) free host **H**, (b) **H** and 0.5 equiv. of **G3**, (c) free guest **G3**. $[\text{H}]_0 = 3.0$ mM.

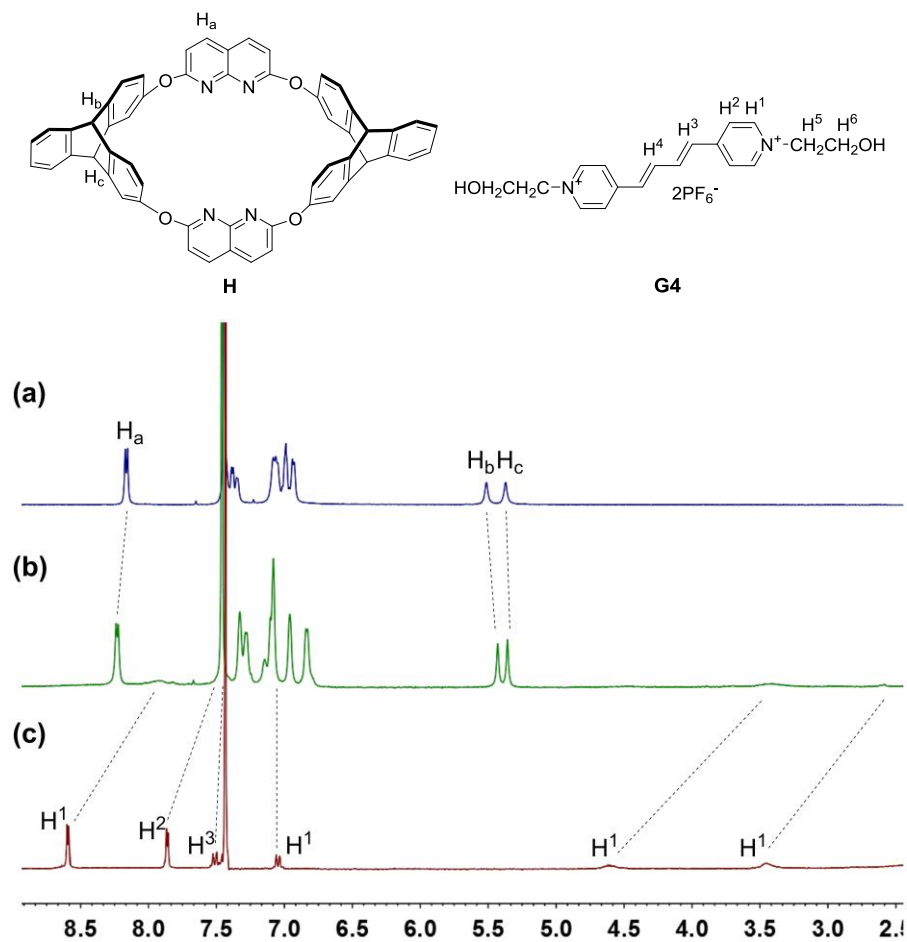
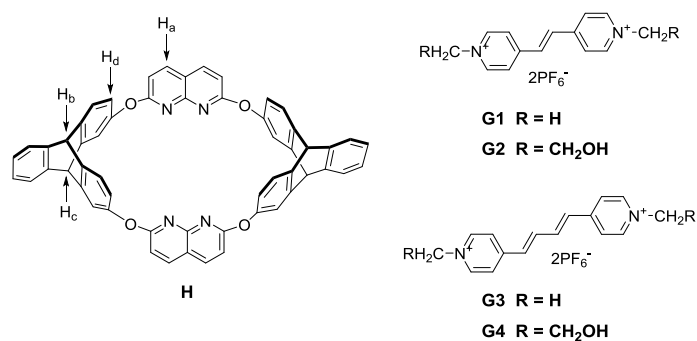


Fig. S8. Partial ¹H NMR spectra (500 MHz, CDCl₃/CD₃CN, 2:1 v/v, 298K) of (a) free host **H**, (b) **H** and 0.5 equiv. of **G4**, (c) free guest **G4**. [**H**]₀ = 3.0 mM.

3. Determination of the stoichiometries and the association constants



To determine the stoichiometries and association constants between **H** and **G1-G4**, ¹H NMR titrations were done. By a nonlinear curve-fitting method with a Matlab program, the association constants between the guests and the host were calculated and displayed in the manuscript. By a mole ratio plot, each stoichiometry was determined.

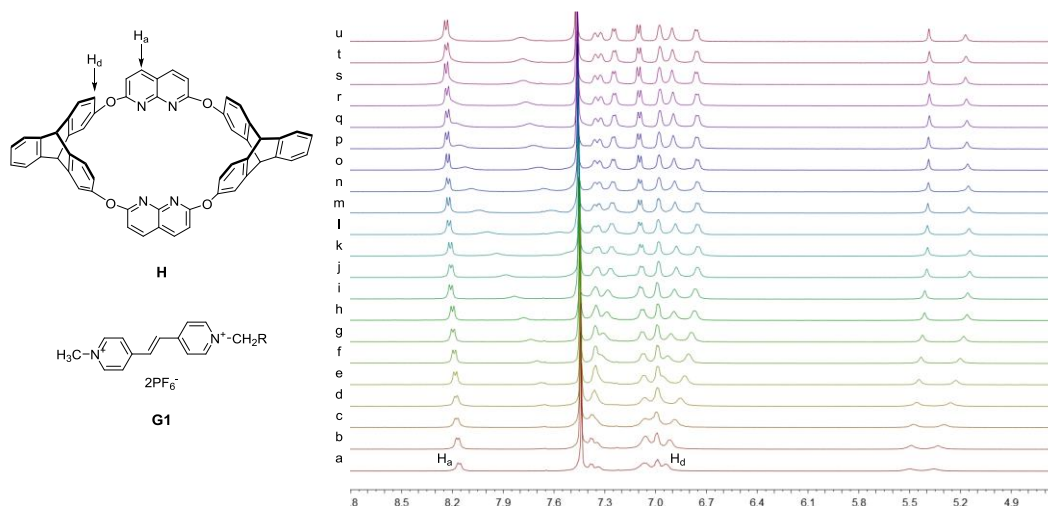


Fig. S9. ¹H NMR spectra (500 MHz, CDCl₃/CD₃CN, 2:1 v/v, 298K) of **H** at a concentration of 3.00 mM with different concentrations of **G1**: (a) 0.00 mM; (b) 0.18 mM; (c) 0.37 mM; (d) 0.55 mM; (e) 0.73 mM; (f) 0.92 mM; (g) 1.10 mM; (h) 1.28 mM; (i) 1.46 mM; (j) 1.65 mM; (k) 1.83 mM; (l) 2.01 mM; (m) 2.20 mM; (n) 2.38 mM; (o) 2.56 mM; (p) 2.74 mM; (q) 2.93 mM; (r) 3.11 mM; (s) 3.29 mM; (t) 3.47 mM; (u) 3.66 mM.

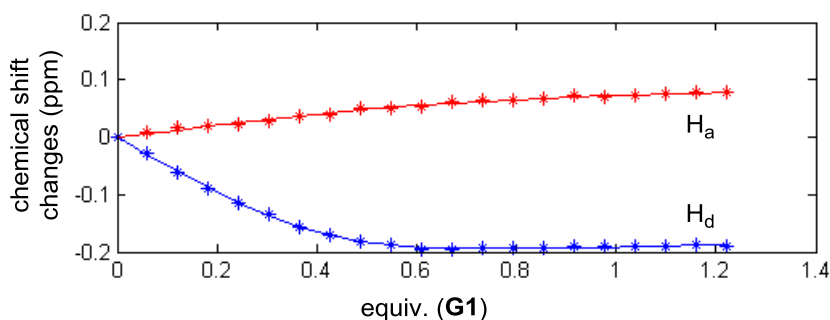


Fig. S10. Plot of chemical shift changes of **H** observed upon the titration of **G1**.

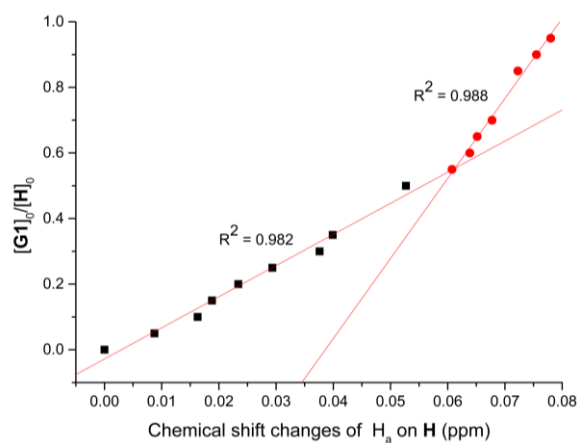


Fig. S11. Mole ratio plot for the complexation between **H** and **G1**, indicating a 2:1 stoichiometry.

m

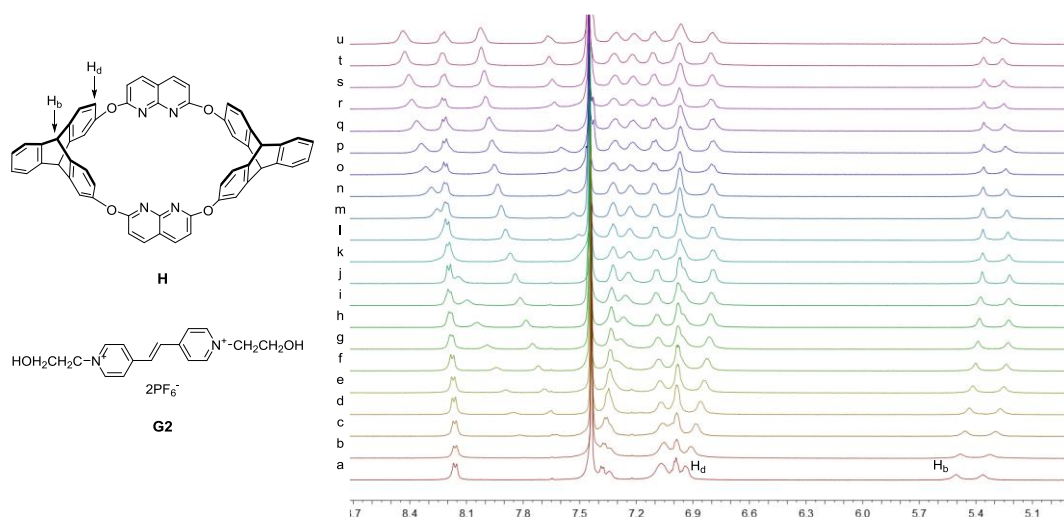


Fig. S12. ^1H NMR spectra (500 MHz, $\text{CDCl}_3/\text{CD}_3\text{CN}$, 2:1 v/v, 298K) of **H** at a concentration of 3.00 mM with different concentrations of **G2**: (a) 0.00 mM; (b) 0.22 mM; (c) 0.44 mM; (d) 0.67 mM; (e) 0.89 mM; (f) 1.11 mM; (g) 1.33 mM; (h) 1.55 mM; (i) 1.78 mM; (j) 2.00 mM; (k) 2.22 mM; (l) 2.44 mM; (m) 2.66 mM; (n) 2.89 mM; (o) 3.11 mM; (p) 3.33 mM; (q) 3.55 mM; (r) 3.77 mM; (s) 4.00 mM; (t) 4.22 mM; (u) 4.44 mM.

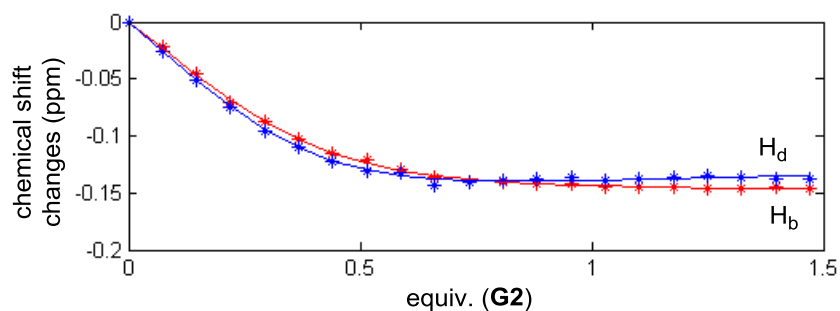


Fig. S13. Plot of chemical shift changes of **H** observed upon the titration of **G2**.

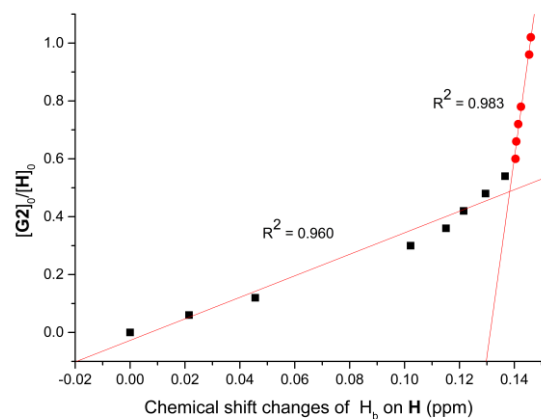


Fig. S14. Mole ratio plot for the complexation between **H** and **G2**, indicating a 2:1 stoichiometry.

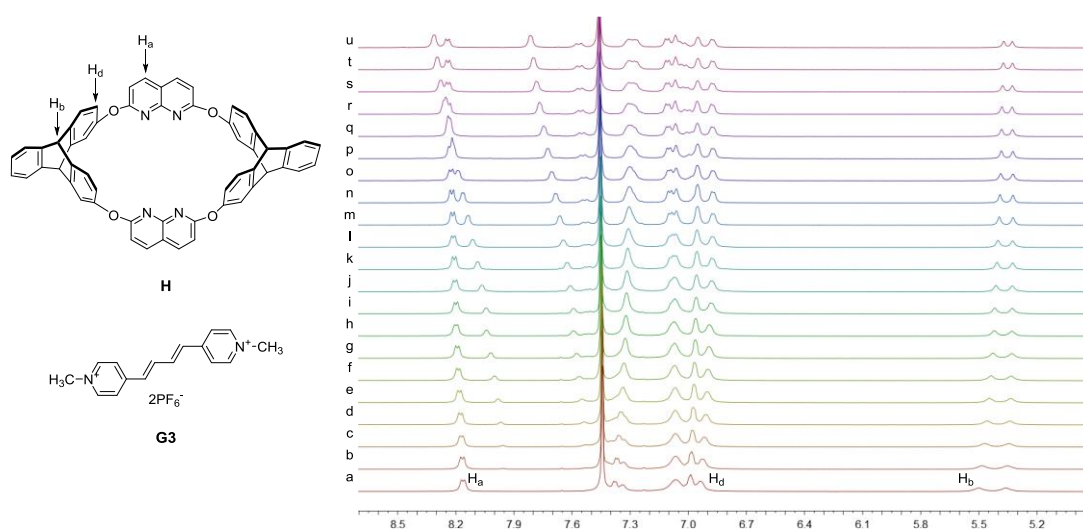


Fig. S15. ^1H NMR spectra (500 MHz, $\text{CDCl}_3/\text{CD}_3\text{CN}$, 2:1 v/v, 298K) of **H** at a concentration of 3.00 mM with different concentrations of **G3**: (a) 0.00 mM; (b) 0.12 mM; (c) 0.24 mM; (d) 0.36 mM; (e) 0.48 mM; (f) 0.60 mM; (g) 0.72 mM; (h) 0.84 mM; (i) 0.96 mM; (j) 1.08 mM; (k) 1.20 mM; (l) 1.32 mM; (m) 1.44 mM; (n) 1.56 mM; (o) 1.68 mM; (p) 1.80 mM; (q) 1.92 mM; (r) 2.04 mM; (s) 2.16 mM; (t) 2.28 mM; (u) 2.40 mM.

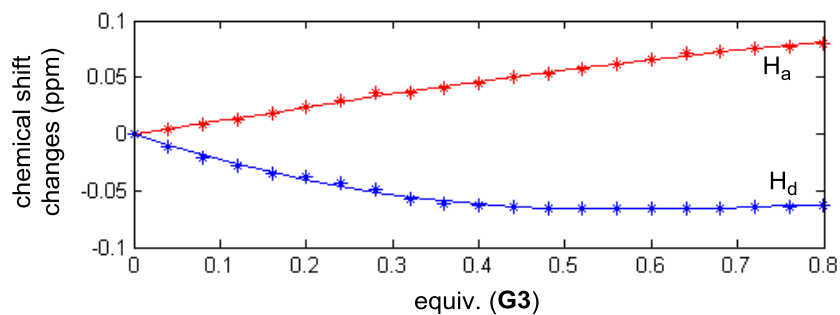


Fig. S16. Plot of chemical shift changes of **H** observed upon the titration of **G3**.

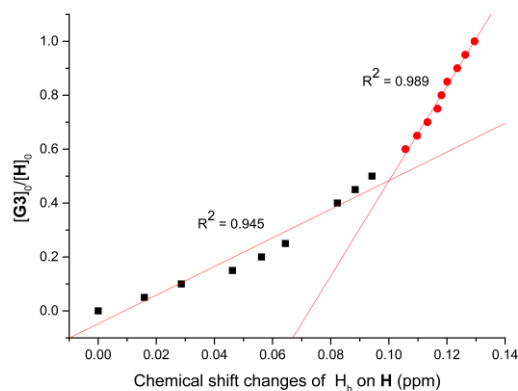


Fig. S17. Mole ratio plot for the complexation between **H** and **G3**, indicating a 2:1 stoichiometry.

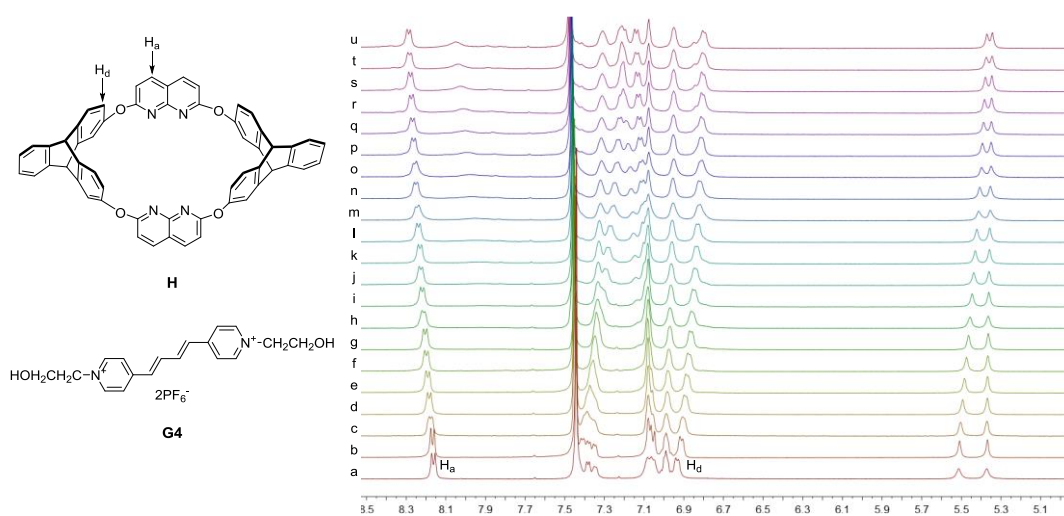


Fig. S18. ^1H NMR spectra (500 MHz, $\text{CDCl}_3/\text{CD}_3\text{CN}$, 2:1 v/v, 298K) of **H** at a concentration of 3.00 mM with different concentrations of **G4**: (a) 0.00 mM; (b) 0.15 mM; (c) 0.30 mM; (d) 0.45 mM; (e) 0.60 mM; (f) 0.75 mM; (g) 0.90 mM; (h) 1.05 mM; (i) 1.20 mM; (j) 1.35 mM; (k) 1.50 mM; (l) 1.65 mM; (m) 1.80 mM; (n) 1.95 mM; (o) 2.10 mM; (p) 2.25 mM; (q) 2.40 mM; (r) 2.55 mM; (s) 2.70 mM; (t) 2.85 mM; (u) 3.00 mM.

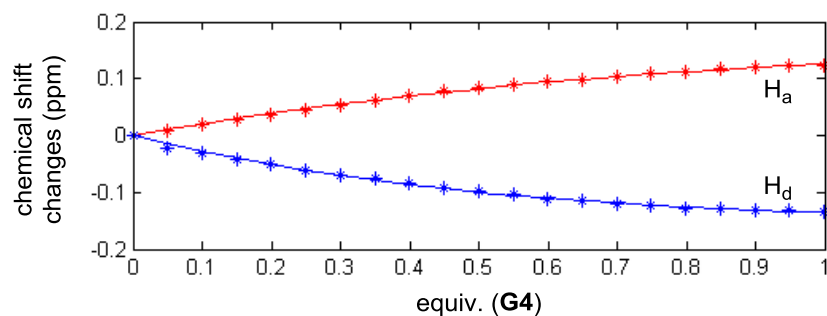


Fig. S19. Plot of chemical shift changes of **H** observed upon the titration of **G4**.

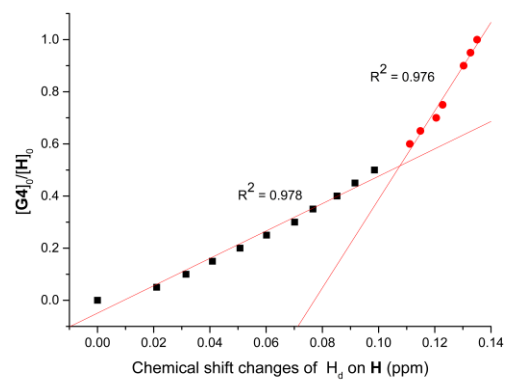


Fig. S20. Mole ratio plot for the complexation between **H** and **G4**, indicating a 2:1 stoichiometry.

4. Crystal structures

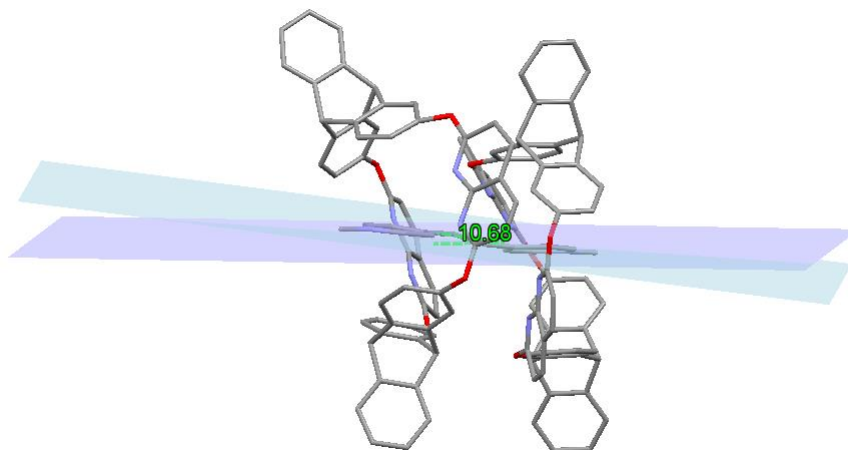


Fig. S21. The dihedral angle between the planes of the two pyridinium rings in complex $\text{H}_2\cdot\text{G1}$.

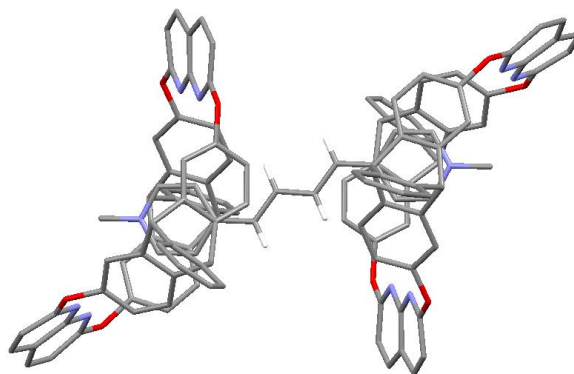


Fig. S22. The crystal structure of complex $\text{H}_2\cdot\text{G3}$ showing that the protons on the two double bonds are nearly out of the shielding regions of the host molecules.

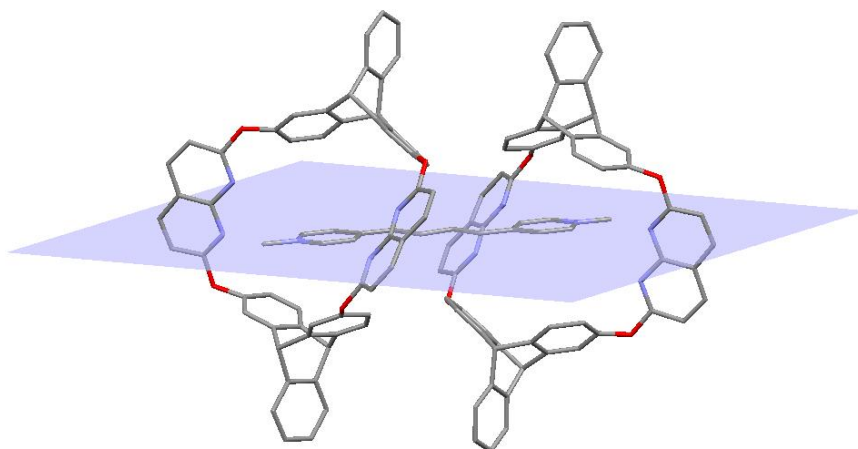


Fig. S23. The plane of the two pyridinium rings in complex $\text{H}_2\cdot\text{G3}$.

5. Cartesian Coordinates of Computed Structures¹

All DFT calculations were carried out with Gaussian 09 program using B3LYP hybrid functional. Geometries were fully optimized employing the 3-21G* basis set on all atoms.

(H, H)-H₂-G1

O	11.8498	10.1812	10.4167
O	11.3162	19.1177	12.0594
O	6.0655	9.5525	6.6174
O	6.6572	18.0963	7.0104
N	9.9069	9.983	9.1475
N	7.9837	9.7814	7.8872
N	8.2061	18.4176	8.7404
N	9.7677	18.7496	10.4095
C	11.2866	11.1465	11.2703
C	12.1135	12.297	11.447
H	12.8803	12.4505	10.9066
C	11.7417	13.1644	12.4362
C	10.5898	12.9849	13.2204
C	9.7793	11.8962	12.9528
H	8.9665	11.7905	13.4344
C	10.1327	10.9491	11.9887
H	9.5846	10.1873	11.8319
C	12.589	14.3688	12.8937
H	13.3995	14.5163	12.3283
C	12.9266	14.0178	14.3483
C	14.1576	13.8962	14.9313
H	14.9404	14.0318	14.4082
C	14.278	13.5791	16.2723
H	15.1401	13.5373	16.6688
C	13.1961	13.3279	17.0168
H	13.3065	13.0707	17.9233
C	11.8946	13.4376	16.487
H	11.1314	13.2741	17.0276
C	11.7616	13.8005	15.1323
C	10.4959	13.97	14.3564
H	9.6838	13.8204	14.9208
C	10.5452	15.3777	13.7872
C	9.6807	16.4465	14.0324
H	8.9395	16.3348	14.6159
C	9.904	17.6748	13.4195
H	9.2985	18.3947	13.5504
C	11.0309	17.8323	12.6081
C	11.8846	16.8214	12.3639
H	12.6211	16.955	11.778
C	11.6926	15.5731	12.9677
C	10.7214	19.4794	10.9061
C	11.2343	20.6957	10.3453
H	11.9249	21.1882	10.7718
C	10.6928	21.1005	9.1915

H	11.0165	21.8921	8.7782
C	9.6489	20.3711	8.5764
C	9.214	19.2022	9.2271
C	9.0611	20.7097	7.3487
H	9.3761	21.4654	6.8655
C	8.0394	19.956	6.8426
H	7.6131	20.1793	6.0239
C	7.6407	18.8094	7.6093
C	5.9105	17.0746	7.6762
C	5.4111	16.1157	6.7771
H	5.6521	16.1295	5.8593
C	4.5564	15.1524	7.2751
C	4.2549	15.1065	8.6139
C	4.697	16.0816	9.4599
H	4.4275	16.0756	10.3698
C	5.5587	17.1005	8.9805
H	5.8766	17.7825	9.5605
C	3.9122	13.9859	6.4412
H	4.1338	14.0218	5.4655
C	2.428	14.1135	6.7369
C	1.3675	14.2033	5.783
H	1.5686	14.2411	4.8558
C	0.0655	14.2372	6.1965
H	-0.6361	14.3289	5.5626
C	-0.217	14.1335	7.5265
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H	0.5524	13.9819	9.4067
C	2.0954	14.0218	8.1102
C	3.3112	13.9105	8.9792
H	3.0892	13.8743	9.9544
C	4.1055	12.6876	8.5049
C	4.4626	11.6071	9.2484
H	4.2368	11.5712	10.1702
C	5.1673	10.5383	8.6517
H	5.4332	9.7826	9.1613
C	5.4598	10.632	7.284
C	5.0671	11.7227	6.5267
H	5.2503	11.7506	5.5949
C	4.4167	12.7516	7.1302
C	7.3235	9.1285	6.9918
C	7.7262	7.9764	6.2936
H	7.1545	7.5393	5.6732
C	9.0077	7.5134	6.5599
H	9.3612	6.7696	6.0832
C	9.773	8.1614	7.5467
C	9.2324	9.3	8.1858
C	11.0876	7.7467	7.9298
H	11.4933	7.0069	7.4941
C	11.7547	8.3947	8.902
H	12.618	8.1216	9.1936

C	11.064	9.5453	9.4785
N	7.5288	14.7875	11.2406
N	13.5651	11.9022	4.7759
C	6.6636	15.2701	12.3715
H	5.7733	14.8673	12.2959
H	6.5848	16.2451	12.3283
H	7.0686	15.0108	13.2266
C	8.5224	15.5472	10.7486
H	8.6382	16.4266	11.0847
C	9.3526	15.1026	9.8006
H	10.0729	15.6389	9.4904
C	9.1269	13.7825	9.2611
C	8.0527	13.0627	9.7332
H	7.8591	12.2053	9.3744
C	7.2538	13.5971	10.7421
H	6.512	13.1046	11.0685
C	9.9738	13.1923	8.1955
H	9.6729	12.3967	7.7693
C	11.1106	13.7068	7.807
H	11.4096	14.5223	8.1928
C	12.6321	11.1265	5.425
H	12.529	10.2153	5.1768
C	11.8467	11.6589	6.4312
H	11.234	11.1086	6.906
C	11.9652	13.0148	6.7415
C	12.8891	13.7466	6.0616
H	12.9714	14.6719	6.2613
C	13.6989	13.2103	5.1121
H	14.3563	13.7466	4.6831
C	14.4176	11.3638	3.6958
H	15.2375	10.9909	4.0843
H	14.6508	12.0836	3.0726
H	13.9338	10.6579	3.2183
O	12.6105	18.486	7.9907
O	8.6061	11.5281	4.8086
O	12.9239	6.3529	3.2558
O	14.9129	12.1893	9.5918
N	13.4234	16.4126	8.5338
N	14.2369	14.291	9.0428
N	11.449	8.0558	3.8029
N	9.9771	9.8005	4.2958
C	12.1961	17.958	6.7237
C	13.0927	17.9759	5.6921
H	13.9721	18.3089	5.8323
C	12.7257	17.5093	4.4565
H	13.3391	17.5293	3.7309
C	11.4546	17.0148	4.2885
C	10.5509	17.0148	5.3295
C	10.9049	17.4794	6.5901
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C	9.1638	16.4565	4.9502

H	8. 5167	16. 4804	5. 7136
C	8. 6653	17. 266	3. 726
C	7. 513	17. 9859	3. 6321
H	6. 907	18. 0537	4. 3594
C	7. 2615	18. 6319	2. 3874
H	6. 46	19. 1344	2. 2822
C	8. 0986	18. 5522	1. 3812
H	7. 8804	18. 9749	0. 5584
C	9. 2908	17. 8662	1. 4942
H	9. 8863	17. 8383	0. 7553
C	9. 6209	17. 2381	2. 6345
C	10. 8901	16. 4126	3. 0222
H	11. 5632	16. 3787	2. 2822
C	10. 3783	15. 0348	3. 3966
C	9. 4034	15. 0507	4. 4325
C	8. 8631	13. 8623	4. 903
H	8. 2395	13. 8663	5. 6192
C	9. 2442	12. 6798	4. 3171
C	10. 2108	12. 618	3. 2466
H	10. 4774	11. 7925	2. 8595
C	10. 7239	13. 8204	2. 8166
H	11. 3393	13. 8204	2. 0934
C	8. 8149	10. 3449	4. 1725
C	7. 6998	9. 7686	3. 4789
H	6. 8583	10. 2073	3. 4422
C	7. 9022	8. 5563	2. 8676
H	7. 1938	8. 1415	2. 3901
C	9. 1758	7. 9142	2. 9491
C	10. 1702	8. 5762	3. 6645
C	9. 4895	6. 6859	2. 3362
H	8. 8236	6. 2093	1. 8533
C	10. 7763	6. 1774	2. 4414
H	11. 0367	5. 3718	2. 0098
C	11. 668	6. 9252	3. 2156
C	13. 9776	7. 0887	3. 8253
C	14. 9157	7. 6151	2. 9782
H	14. 8023	7. 5593	2. 0367
C	16. 0592	8. 2432	3. 5231
H	16. 736	8. 5822	2. 9512
C	16. 1855	8. 3569	4. 8857
C	15. 2368	7. 7886	5. 7212
C	14. 1277	7. 1704	5. 1849
H	13. 4658	6. 8015	5. 7595
C	15. 556	7. 9341	7. 2108
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C	16. 9716	7. 2861	7. 3916
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H	18. 8305	5. 0707	8. 8753
C	19. 5641	6. 309	7. 3997

H	20.4501	5.9621	7.397
C	19.2188	7.3539	6.5429
H	19.8723	7.7228	5.9591
C	17.9185	7.8544	6.5394
C	17.3646	8.9192	5.6678
H	18.0606	9.312	5.0662
C	16.7192	9.9899	6.5845
C	17.024	11.3379	6.6821
H	17.6491	11.7347	6.0859
C	16.4101	12.0956	7.6581
H	16.6162	13.0188	7.7342
C	15.5019	11.5333	8.5222
C	15.1439	10.1794	8.4197
H	14.4944	9.7965	8.9967
C	15.77	9.4217	7.4474
C	15.0389	13.5552	9.7278
C	16.0252	14.0059	10.6423
H	16.6264	13.4116	11.0766
C	16.0462	15.3717	10.8635
H	16.67	15.7267	11.4866
C	15.1897	16.2371	10.2053
C	14.29	15.6669	9.2713
C	15.1307	17.6868	10.3644
H	15.7082	18.1275	10.9741
C	14.2612	18.3707	9.6568
H	14.1952	19.3139	9.7628
C	13.4303	17.7047	8.7396

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N	-2.40304	-0.59919	3.67004
C	-3.07149	-0.98849	4.95485
H	-4.10247	-1.25252	4.71624
H	-2.53131	-1.82942	5.38805
H	-3.06002	-0.13206	5.62958
C	-2.93543	0.41846	2.93819
H	-3.79105	0.92616	3.37643
C	-2.36866	0.76075	1.72438
H	-2.79986	1.58051	1.16745
C	-1.23593	0.08015	1.24168
C	-0.70693	-0.96556	2.03094
H	0.14504	-1.55159	1.69972
C	-1.30929	-1.28068	3.22753
H	-0.9507	-2.08367	3.85515
N	2.63712	0.69684	-4.05265
C	3.3743	0.79401	-5.35832
H	3.8906	1.75571	-5.3864
H	2.65133	0.70018	-6.16702
H	4.08973	-0.03147	-5.39569
C	3.34107	0.36616	-2.93622
H	4.41442	0.24662	-3.07292

C	2.68748	0.21392	-1.72923
H	3.25069	-0.08431	-0.85404
C	1.29745	0.4353	-1.62682
C	0.60999	0.8261	-2.79702
H	-0.45106	1.05672	-2.81117
C	1.29729	0.92651	-3.98889
H	0.79325	1.1702	-4.91367
C	0.65298	0.19675	-0.33489
H	1.30657	-0.18966	0.44461
C	-0.64376	0.4299	-0.05131
H	-1.30244	0.89861	-0.77578
O	-5.77886	2.42399	-1.68165
O	-2.17839	5.24215	3.63616
O	-0.1524	-2.94352	6.71409
O	-4.19696	-5.51511	1.54278
N	-4.5623	3.39233	0.06943
N	-3.35209	4.32866	1.82219
N	-1.40929	-3.85857	4.93485
N	-2.77828	-4.69621	3.23659
C	-5.48382	3.49686	-0.86929
C	-6.25772	4.66377	-1.10622
H	-6.98969	4.65448	-1.89992
C	-6.03398	5.7552	-0.30662
H	-6.60086	6.6684	-0.44544
C	-5.04466	5.69438	0.71283
C	-4.7452	6.76212	1.60118
H	-5.28206	7.69922	1.51078
C	-3.77997	6.59757	2.56113
H	-3.50769	7.37163	3.26277
C	-3.10921	5.34818	2.62478
C	-4.31667	4.47851	0.86122
C	-1.14618	4.2723	3.64226
C	-0.93473	3.60243	4.85199
H	-1.59322	3.806	5.68664
C	0.14685	2.73905	4.9613
C	1.00769	2.53388	3.86853
C	0.77419	3.19027	2.66517
H	1.44801	3.05156	1.82709
C	-0.31231	4.06769	2.54642
H	-0.48726	4.60473	1.62427
C	0.57985	1.9828	6.2216
H	-0.08961	2.14015	7.06873
C	2.01889	2.45135	6.49544
C	2.49613	3.01835	7.66986
H	1.83692	3.17584	8.51611
C	3.8473	3.38803	7.75046
H	4.22743	3.83273	8.66228
C	4.7007	3.18844	6.66512
H	5.74208	3.47887	6.73599
C	4.21618	2.61623	5.47943
H	4.87339	2.46087	4.63057

C	2.87784	2.25265	5.4037
C	2.1843	1.61204	4.19345
H	2.8705	1.45409	3.36202
C	1.57809	0.31291	4.72807
C	1.85893	-0.97127	4.28076
H	2.53219	-1.1283	3.44664
C	1.2762	-2.07199	4.92274
H	1.52242	-3.07787	4.61618
C	0.40038	-1.86413	5.97879
C	0.10391	-0.57441	6.43628
H	-0.5606	-0.45474	7.28223
C	0.70891	0.51017	5.81657
C	-1.03326	-3.8706	6.20069
C	-1.49149	-4.80705	7.16858
H	-1.11174	-4.73803	8.17685
C	-2.40478	-5.74678	6.77367
H	-2.78691	-6.47927	7.47522
C	-2.87366	-5.75146	5.43222
C	-3.84403	-6.66347	4.9368
H	-4.25409	-7.41715	5.59908
C	-4.2552	-6.57828	3.63311
H	-4.99089	-7.23919	3.20006
C	-3.68883	-5.55842	2.82245
C	-2.35101	-4.77425	4.53627
C	-3.69313	-4.68751	0.51019
C	-4.65926	-4.04476	-0.27568
H	-5.70591	-4.18732	-0.03943
C	-4.24387	-3.26197	-1.34237
C	-2.87292	-3.10551	-1.61677
C	-1.92779	-3.7614	-0.84091
H	-0.87184	-3.64989	-1.05648
C	-2.33689	-4.56333	0.23274
H	-1.60712	-5.06558	0.84938
C	-5.14195	-2.48763	-2.31451
H	-6.20661	-2.61624	-2.11295
C	-4.73356	-2.95385	-3.71887
C	-5.57325	-3.49283	-4.68517
H	-6.63122	-3.623	-4.48705
C	-5.03756	-3.86718	-5.92616
H	-5.68624	-4.28576	-6.6862
C	-3.67719	-3.70049	-6.18593
H	-3.2714	-3.98895	-7.14828
C	-2.83137	-3.15572	-5.20871
H	-1.77417	-3.02217	-5.41132
C	-3.36488	-2.78425	-3.9809
C	-2.59246	-2.17998	-2.80249
H	-1.52732	-2.06058	-3.00696
C	-4.6804	-1.02941	-2.21542
C	-5.47775	0.06757	-1.92045
H	-6.54261	-0.02486	-1.74983
C	-4.89061	1.33646	-1.87517

C	-3.52772	1.51009	-2.09684
H	-3.09056	2.49659	-2.04609
C	-2.73333	0.39678	-2.39728
H	-1.67393	0.529	-2.58525
C	-3.30662	-0.86686	-2.46561
O	-1.74386	2.11307	-6.56955
O	0.47794	-3.73417	-3.41979
O	5.80929	0.49408	2.43718
O	2.61714	6.24375	-0.02341
N	-1.0266	0.13573	-5.54061
N	-0.30964	-1.81155	-4.48852
N	4.77689	2.43266	1.602
N	3.70097	4.34093	0.81021
C	-1.76136	0.73029	-6.45494
C	-2.63782	0.05537	-7.34931
H	-3.19117	0.63058	-8.07747
C	-2.71429	-1.31283	-7.26478
H	-3.35014	-1.87571	-7.93851
C	-1.92789	-2.00334	-6.3005
C	-1.91445	-3.41423	-6.14038
H	-2.52821	-4.03134	-6.78666
C	-1.10039	-3.98697	-5.19078
H	-1.02522	-5.05542	-5.0505
C	-0.31245	-3.12519	-4.38822
C	-1.08779	-1.22281	-5.44903
C	1.82885	-3.31884	-3.21477
C	2.34752	-3.49713	-1.92796
H	1.71054	-3.88015	-1.14131
C	3.68977	-3.21871	-1.70375
C	4.5146	-2.77206	-2.75185
C	3.9774	-2.57039	-4.01802
H	4.60584	-2.24127	-4.83801
C	2.62194	-2.84191	-4.25445
H	2.20833	-2.70646	-5.24373
C	4.44429	-3.40861	-0.38526
H	3.80327	-3.73855	0.43384
C	5.56672	-4.40608	-0.71227
C	5.80209	-5.61756	-0.07568
H	5.16806	-5.94471	0.74072
C	6.87521	-6.41493	-0.49946
H	7.06891	-7.3603	-0.00724
C	7.69378	-5.99547	-1.54787
H	8.52162	-6.61588	-1.86921
C	7.45316	-4.77166	-2.18917
H	8.09261	-4.44785	-3.00264
C	6.39038	-3.98376	-1.76736
C	5.98238	-2.61872	-2.34207
H	6.62524	-2.2922	-3.16146
C	5.99159	-1.66072	-1.14881
C	6.76039	-0.50981	-1.01457
H	7.43755	-0.20471	-1.80467

C	6.68662	0.24151	0.16618
H	7.29969	1.12316	0.29735
C	5.84084	-0.1759	1.18805
C	5.06494	-1.33305	1.06736
H	4.44265	-1.64002	1.89799
C	5.15264	-2.07876	-0.10028
C	5.41492	1.80747	2.57226
C	5.73419	2.38684	3.83096
H	6.26646	1.79095	4.55713
C	5.35847	3.68412	4.05723
H	5.58852	4.17263	4.99686
C	4.66274	4.40142	3.04568
C	4.22224	5.74486	3.18006
H	4.42822	6.28361	4.09775
C	3.55619	6.35378	2.14566
H	3.21396	7.37698	2.18592
C	3.32169	5.59562	0.97097
C	4.38666	3.72623	1.82125
C	2.75604	5.92727	-1.39899
C	1.60772	6.09614	-2.18212
H	0.68602	6.40091	-1.70331
C	1.69686	5.90844	-3.55514
C	2.9195	5.54266	-4.14512
C	4.05107	5.37302	-3.35686
H	5.00446	5.12413	-3.80997
C	3.97316	5.5653	-1.97066
H	4.85359	5.45123	-1.35515
C	0.56914	6.10024	-4.57782
H	-0.38017	6.38626	-4.12229
C	1.09819	7.14063	-5.57565
C	0.48826	8.34187	-5.91251
H	-0.45334	8.62917	-5.45818
C	1.10568	9.18283	-6.8495
H	0.63832	10.12258	-7.1179
C	2.31707	8.81555	-7.43526
H	2.78869	9.47021	-8.15815
C	2.93059	7.60176	-7.09301
H	3.87241	7.31919	-7.54979
C	2.31739	6.77065	-6.1646
C	2.84029	5.41482	-5.66796
H	3.78947	5.13008	-6.12539
C	0.48946	4.78902	-5.36626
C	-0.64784	4.01431	-5.55847
H	-1.60673	4.30992	-5.15465
C	-0.54068	2.84657	-6.31774
C	0.66857	2.45107	-6.87813
H	0.72683	1.54795	-7.47018
C	1.80488	3.24709	-6.69144
H	2.74355	2.95747	-7.14962
C	1.7153	4.41314	-5.94123

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N	4.116	23.0276	14.007
C	4.9606	21.8535	14.2378
H	5.7545	21.9178	13.6998
H	4.4761	21.0603	14.0002
H	5.2046	21.8119	15.1667
C	4.6478	24.1315	13.4508
H	5.5461	24.1456	13.2072
C	3.8589	25.2373	13.2462
H	4.2301	25.9909	12.8473
C	2.5108	25.2599	13.6229
C	2.0082	24.0897	14.2045
H	1.1186	24.0534	14.4738
C	2.8155	23.0062	14.3767
H	2.4644	22.2326	14.758
N	-2.45032	29.9384	13.02567
C	-3.29492	31.1126	12.79487
H	-4.08882	31.0483	13.33287
H	-2.81042	31.9058	13.03247
H	-3.53892	31.1541	11.86597
C	-2.98212	28.8345	13.58187
H	-3.88042	28.8204	13.82547
C	-2.19322	27.7287	13.78647
H	-2.56442	26.9752	14.18537
C	-0.84512	27.7062	13.40977
C	-0.34252	28.8763	12.82817
H	0.54708	28.9127	12.55887
C	-1.14982	29.9599	12.65597
H	-0.79872	30.7335	12.27467
C	-0.03212	26.5261	13.64467
H	-0.45872	25.7758	13.99057
C	1.28558	26.4314	13.40247
H	1.72838	27.1868	13.08927
O	7.9532	22.34	10.6813
O	7.919	24.7318	17.1911
O	-0.7917	25.4702	18.3857
O	-0.0984	20.168	13.951
N	7.8919	23.0626	12.866
N	7.8814	23.8803	15.0189
N	-0.5263	23.7313	16.8896
N	-0.3028	21.949	15.4257
C	8.5703	22.5693	11.8727
C	9.9396	22.2611	11.87
H	10.3653	21.9585	11.0989
C	10.6135	22.4198	13.0218
H	11.5168	22.2	13.0692
C	9.944	22.9199	14.1561
C	10.5487	23.0941	15.4178
H	11.4259	22.8187	15.5591
C	9.8437	23.6683	16.4249

H	10.2149	23.782	17.2695
C	8.5319	24.0805	16.1415
C	8.5899	23.2708	14.0192
C	6.8604	25.6129	16.9946
C	5.939	25.6653	18.0585
H	5.9801	25.0493	18.7526
C	4.979	26.647	18.0474
C	4.8983	27.5585	16.9878
C	5.8046	27.4671	15.9402
H	5.7467	28.0641	15.2262
C	6.792	26.5	15.9469
H	7.4042	26.4522	15.2479
C	3.9135	26.8758	19.1196
H	3.97	26.2406	19.865
C	4.0968	28.3368	19.5513
C	4.3383	28.7856	20.8317
H	4.4009	28.1808	21.5348
C	4.488	30.1481	21.0642
H	4.6719	30.4521	21.9245
C	4.3645	31.0469	20.0357
H	4.451	31.9581	20.2033
C	4.1088	30.5959	18.7318
H	4.0123	31.2037	18.0354
C	4.0004	29.2396	18.4947
C	3.7651	28.5634	17.144
H	3.7099	29.1984	16.4008
C	2.5056	27.7393	17.3201
C	1.3543	27.8128	16.5624
H	1.3098	28.3952	15.8379
C	0.2706	27.0202	16.8825
H	-0.5139	27.0818	16.3873
C	0.3556	26.1434	17.9334
C	1.5067	26.0188	18.7088
H	1.5495	25.4129	19.413
C	2.5847	26.8327	18.3954
C	-1.1932	24.296	17.8557
C	-2.3471	23.7693	18.479
H	-2.8075	24.2596	19.1207
C	-2.7624	22.5452	18.1223
H	-3.4953	22.1566	18.5415
C	-2.0737	21.8554	17.0998
C	-2.4003	20.5612	16.6552
H	-3.0817	20.0888	17.0747
C	-1.7204	19.9957	15.6092
H	-1.9176	19.1418	15.302
C	-0.706	20.7797	15.0257
C	-0.9779	22.5034	16.4728
C	0.4924	20.9004	12.9301
C	1.6074	20.3168	12.345
H	1.9552	19.5217	12.6849
C	2.194	20.9279	11.2535

C	1.6815	22.1248	10.7596
C	0.5494	22.6898	11.3393
H	0.1927	23.4754	10.9934
C	-0.0456	22.0733	12.4364
H	-0.799	22.4469	12.8337
C	3.3891	20.4123	10.4608
H	3.746	19.5678	10.8094
C	2.8751	20.2975	9.015
C	2.887	19.1491	8.2329
H	3.2164	18.3467	8.5658
C	2.3877	19.2395	6.9257
H	2.3704	18.4824	6.3871
C	1.9255	20.4253	6.4304
H	1.6168	20.466	5.5535
C	1.9107	21.5666	7.2188
H	1.5933	22.3682	6.8743
C	2.374	21.5029	8.5203
C	2.4293	22.6298	9.5392
H	2.068	23.4727	9.1936
C	4.4117	21.5208	10.4321
C	5.7479	21.4152	10.7412
H	6.0992	20.6207	11.0692
C	6.5513	22.5191	10.5512
C	6.0785	23.7164	10.1192
H	6.6491	24.4441	10.0326
C	4.7357	23.8382	9.8099
H	4.3946	24.6531	9.5157
C	3.8986	22.7384	9.942
O	-6.28752	30.6261	16.35137
O	-6.25332	28.2343	9.84157
O	2.45738	27.4959	8.64697
O	1.76408	32.798	13.08167
N	-6.22622	29.9034	14.16667
N	-6.21572	29.0858	12.01377
N	2.19198	29.2348	10.14307
N	1.96848	31.0171	11.60697
C	-6.90462	30.3968	15.15997
C	-8.27392	30.705	15.16267
H	-8.69962	31.0076	15.93377
C	-8.94782	30.5463	14.01087
H	-9.85112	30.7661	13.96347
C	-8.27832	30.0462	12.87657
C	-8.88302	29.872	11.61487
H	-9.76022	30.1474	11.47357
C	-8.17802	29.2978	10.60777
H	-8.54922	29.1841	9.76317
C	-6.86622	28.8856	10.89117
C	-6.92422	29.6953	13.01347
C	-5.19472	27.3532	10.03807
C	-4.27332	27.3008	8.97417
H	-4.31442	27.9168	8.28007

C	-3.31332	26.319	8.98527
C	-3.23262	25.4075	10.04487
C	-4.13892	25.499	11.09247
H	-4.08102	24.902	11.80647
C	-5.12632	26.4661	11.08577
H	-5.73852	26.5139	11.78477
C	-2.24782	26.0903	7.91307
H	-2.30432	26.7255	7.16767
C	-2.43112	24.6293	7.48137
C	-2.67262	24.1804	6.20097
H	-2.73522	24.7853	5.49787
C	-2.82232	22.8179	5.96847
H	-3.00622	22.514	5.10817
C	-2.69882	21.9192	6.99697
H	-2.78532	21.008	6.82937
C	-2.44312	22.3702	8.30087
H	-2.34662	21.7623	8.99727
C	-2.33472	23.7265	8.53797
C	-2.09942	24.4027	9.88867
H	-2.04422	23.7677	10.63187
C	-0.83992	25.2268	9.71257
C	0.31138	25.1533	10.47027
H	0.35588	24.5709	11.19477
C	1.39508	25.9459	10.15017
H	2.17958	25.8843	10.64537
C	1.31008	26.8227	9.09927
C	0.15898	26.9472	8.32387
H	0.11618	27.5532	7.61967
C	-0.91902	26.1334	8.63727
C	2.85888	28.6701	9.17697
C	4.01278	29.1968	8.55367
H	4.47318	28.7065	7.91197
C	4.42808	30.4209	8.91037
H	5.16098	30.8095	8.49117
C	3.73938	31.1107	9.93287
C	4.06598	32.4048	10.37747
H	4.74738	32.8773	9.95797
C	3.38608	32.9703	11.42347
H	3.58328	33.8243	11.73067
C	2.37168	32.1864	12.00697
C	2.64358	30.4627	10.55987
C	1.17328	32.0656	14.10257
C	0.05828	32.6493	14.68767
H	-0.28952	33.4444	14.34777
C	-0.52832	32.0382	15.77917
C	-0.01582	30.8413	16.27307
C	1.11628	30.2763	15.69337
H	1.47298	29.4907	16.03927
C	1.71128	30.8928	14.59627
H	2.46468	30.5191	14.19897
C	-1.72342	32.5538	16.57187

H	-2.08032	33.3983	16.22327
C	-1.20942	32.6686	18.01767
C	-1.22132	33.817	18.79977
H	-1.55072	34.6194	18.46687
C	-0.72202	33.7266	20.10697
H	-0.70472	34.4837	20.64557
C	-0.25982	32.5408	20.60227
H	0.04888	32.5001	21.47917
C	-0.24502	31.3994	19.81387
H	0.07238	30.5978	20.15837
C	-0.70832	31.4632	18.51237
C	-0.76362	30.3363	17.49347
H	-0.40232	29.4934	17.83907
C	-2.74602	31.4453	16.60057
C	-4.08222	31.5509	16.29147
H	-4.43352	32.3454	15.96347
C	-4.88562	30.447	16.48147
C	-4.41282	29.2497	16.91347
H	-4.98342	28.5219	17.00007
C	-3.07002	29.1279	17.22277
H	-2.72892	28.313	17.51697
C	-2.23292	30.2277	17.09067

6. References

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