

Electronic Supplementary Information

Formation of charge-transfer complexes based on tropylium cation and 2,6-helic[6]arenes: a visible redox stimulus-responsive process

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1. Materials and methods

Hosts **1** and **2** were prepared according to literature procedures.^{S1} Tropylium tetrafluoroborate and other reagents were commercially available and used as received. ¹H NMR spectra and 2D Noesy spectra were recorded on the Bruker® Avance III 400 MHz NMR spectrometers at 298 K. Electrospray ionization mass spectra (ESI-MS) were recorded on the Thermo Fisher® Exactive high-resolution LC-MS spectrometer. The UV-vis spectra were recorded on PerkinElmer® UV/Vis/NIR spectrometer (Lambda 950) at room temperature.

Reference:

S1. G.-W. Zhang, P.-F. Li, Z. Meng, H.-X. Wang, Y. Han and C.-F. Chen, *Angew Chem. Int. Ed.*, 2016, **55**, 5304–5308.

2. ^1H NMR studies on complexation between the hosts and the guest

The ^1H NMR titration experiments were carried out by gradually adding guest into the solution of the hosts. According to the changes of the chemical shift of the proton in the host, the association constants K_a were calculated by using a nonlinear curve fitting method.

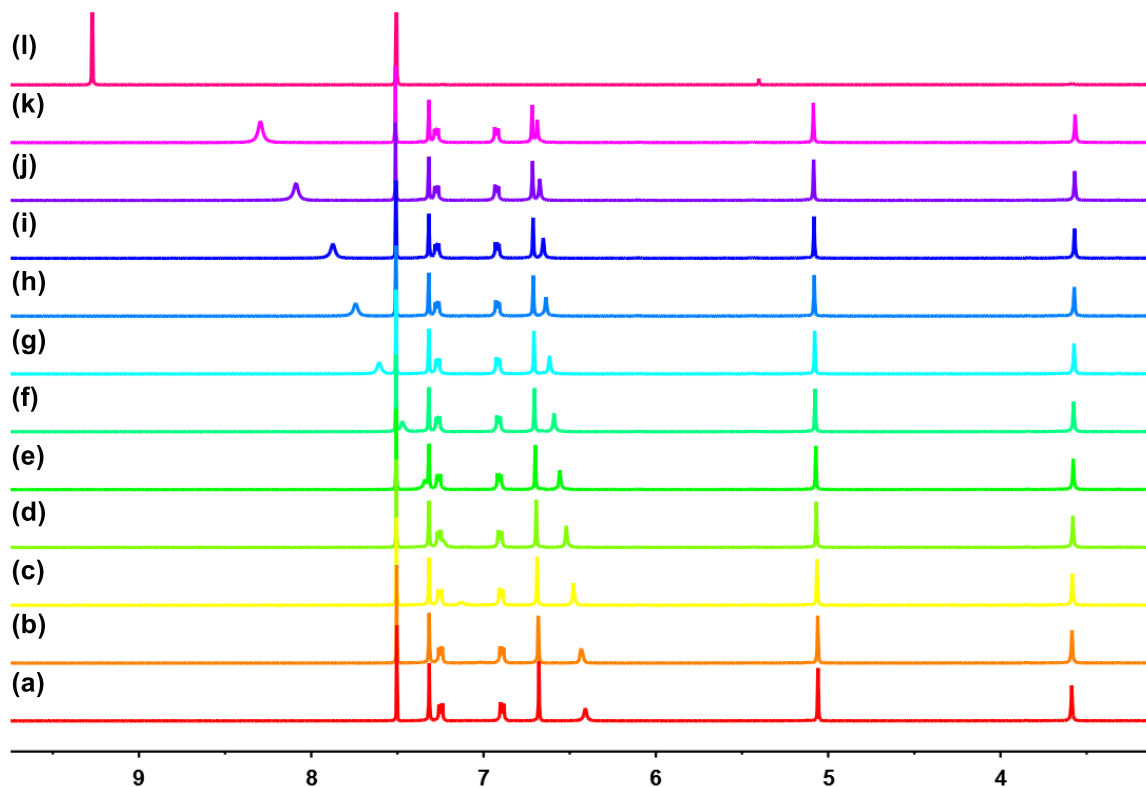


Fig. S1 ^1H NMR spectra (400 MHz, 1:1 v/v $\text{CDCl}_3/\text{CD}_3\text{CN}$) of **1** with different equivalents of **G**: a) 0.00, b) 0.20, c) 0.30, d) 0.40, e) 0.50, f) 0.60, g) 0.80, h) 1.00, i) 1.40, j) 1.80, k) 2.20, l) **G**. $[\mathbf{1}]_0 = 2.00$ mM.

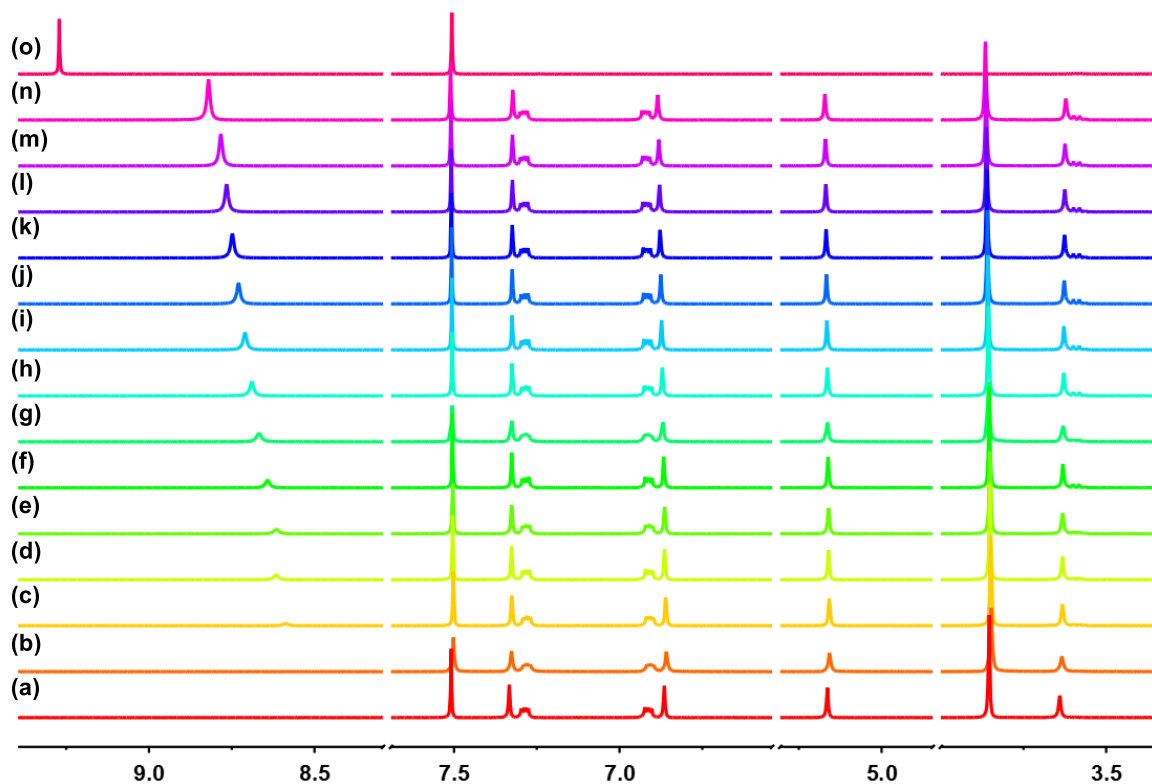


Fig. S2 ^1H NMR spectra (400 MHz, 1:1 v/v $\text{CDCl}_3/\text{CD}_3\text{CN}$) of **1** with different equivalents of **G**: a) 0.00, b) 0.20, c) 0.40, d) 0.60, e) 0.80, f) 1.00, g) 1.20, h) 1.40, i) 1.60, l) 1.80, m) 2.00, n) 2.50, o) **G**. $[\mathbf{1}]_0 = 2.00$ mM.

3. 2D NMR spectra of the complexes

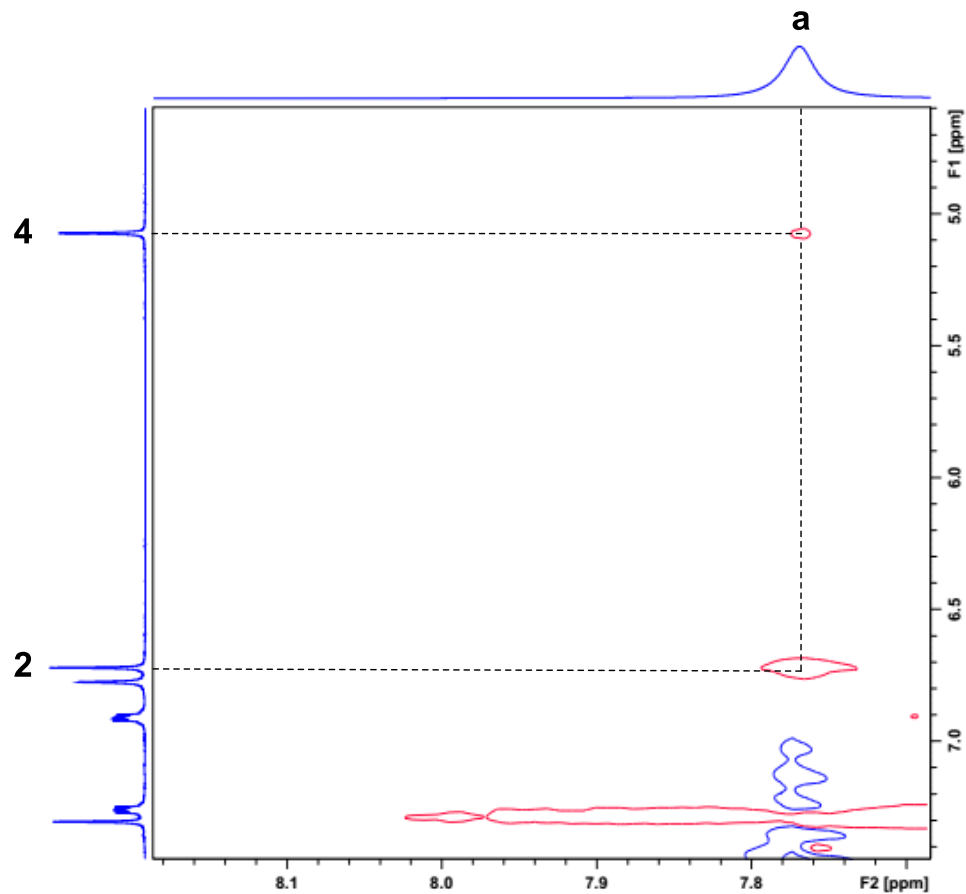


Fig. S3 2D NOESY spectrum (400MHz, CDCl₃/CD₃CN, 1/1, v/v) of **1** and **G** (15.0 mM for each).

4. Nonlinear curve fitting and molar ratio plots for the complexes

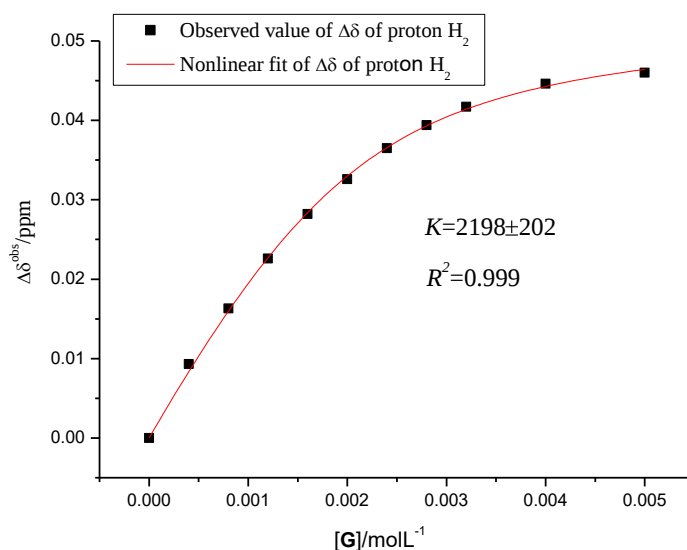


Fig. S4 Plots of $\Delta\delta_{\text{obs}}$ (ppm) for the bridgehead proton H_2 of **1** vs G concentration in $\text{CDCl}_3/\text{CD}_3\text{CN}$ (1/1, v/v) at 298 K.

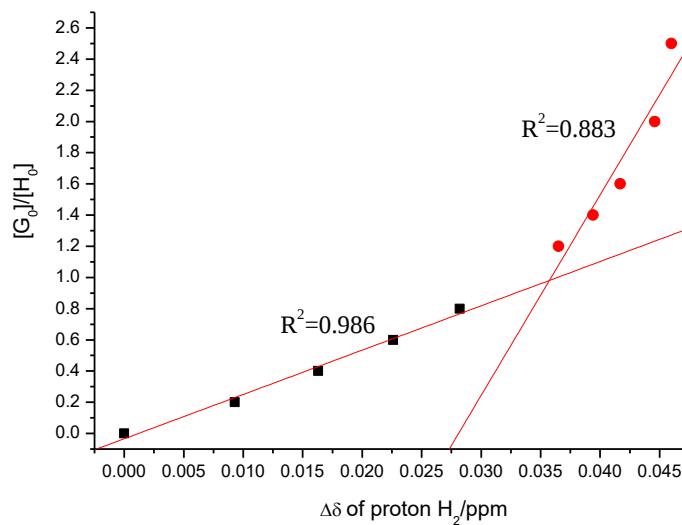


Fig. S5 Molar ratio plot for the complexation of **1** and G in $\text{CDCl}_3/\text{CD}_3\text{CN}$ (1/1, v/v) at 298 K.

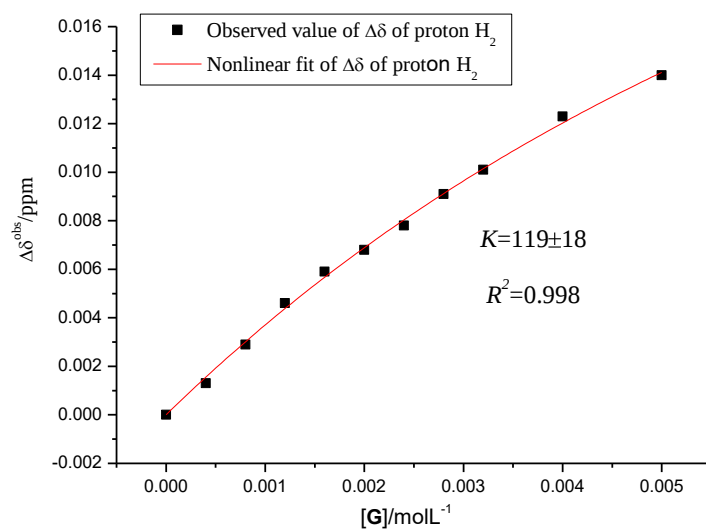


Fig. S6 Plots of $\Delta\delta_{\text{obs}}$ (ppm) for the bridgehead proton H_2 of **2** vs **G** concentration in $\text{CDCl}_3/\text{CD}_3\text{CN}$ (1/1, v/v) at 298 K.

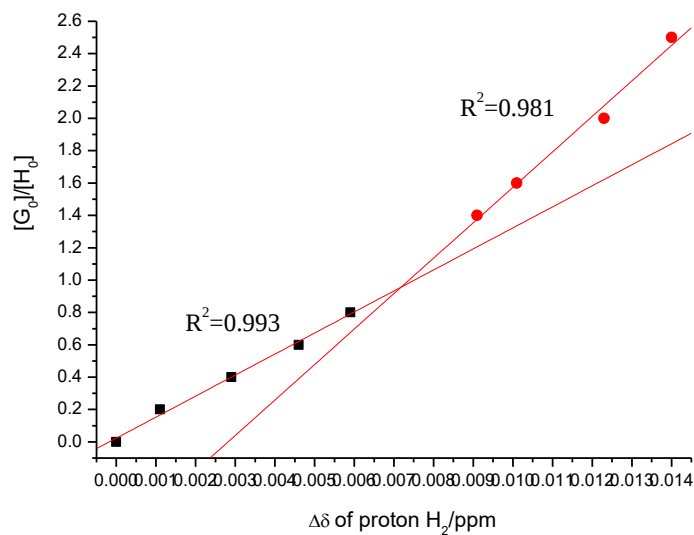


Fig. S7 Molar ratio plot for the complexation of **2** and **G** in $\text{CDCl}_3/\text{CD}_3\text{CN}$ (1/1, v/v) at 298 K..

5. ESI spectra of the complexes

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T: FTMS {1,1} + p ESI Full ms [200.00-2000.00]

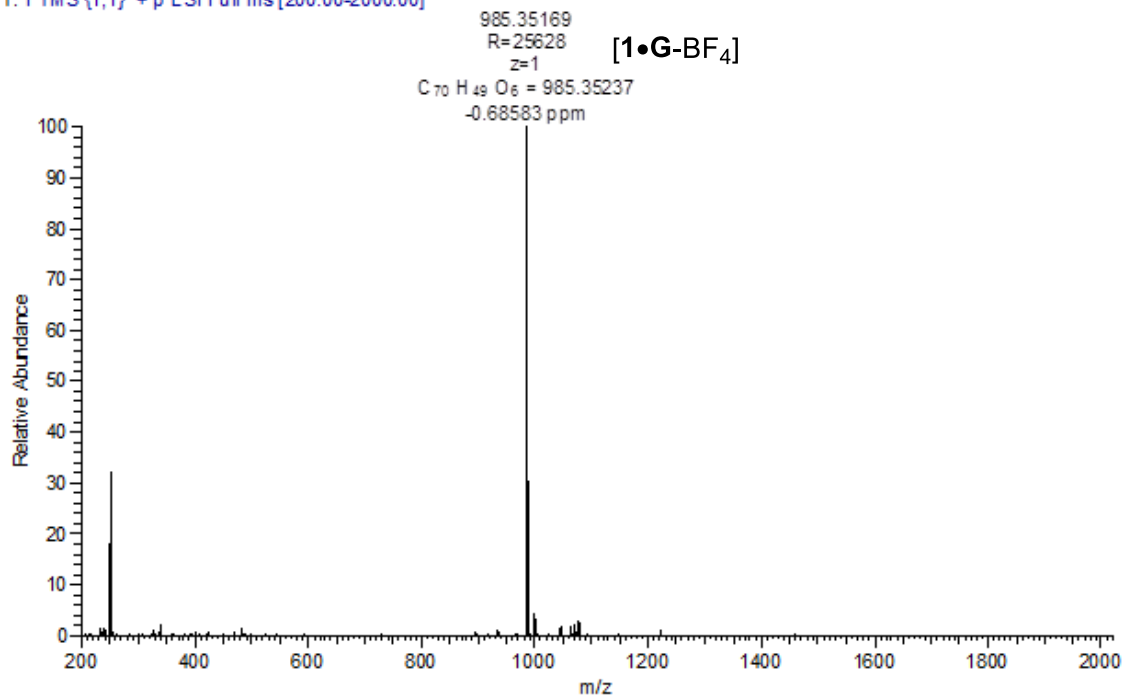


Fig. S8 ESI-MS spectrum of complex 1·G.

ZGW-1 #82-83 RT: 0.73-0.74 AV: 2 NL: 1.01E 6
T: FTMS {1,1} + p ESI Full ms [200.00-2000.00]

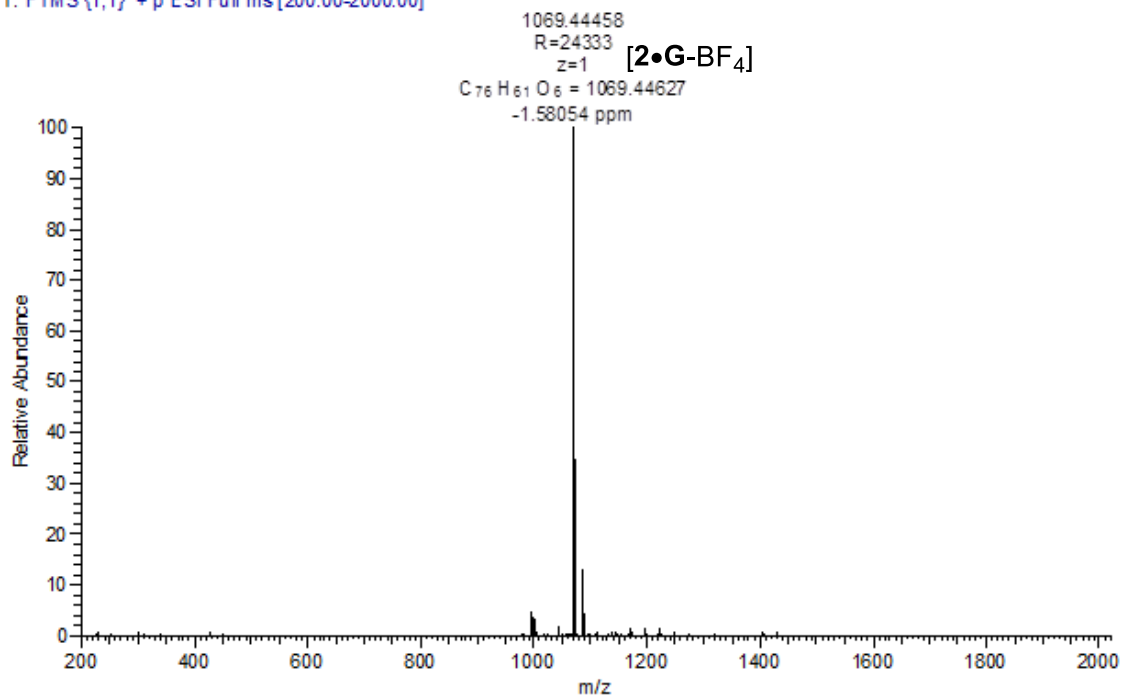
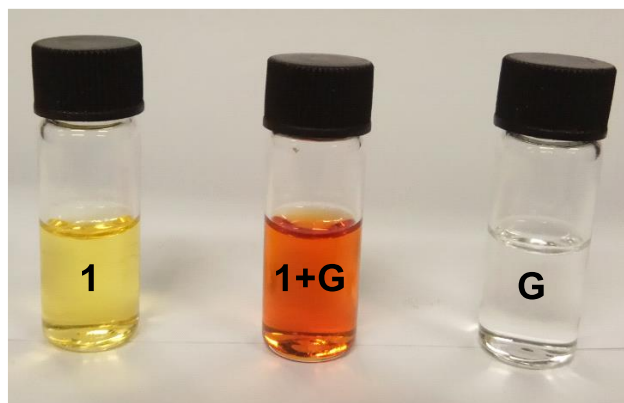


Fig. S9 ESI-MS spectrum of complex 2·G.

6. Color changes and UV-vis spectra of the complex 1·G

(a)



(b)

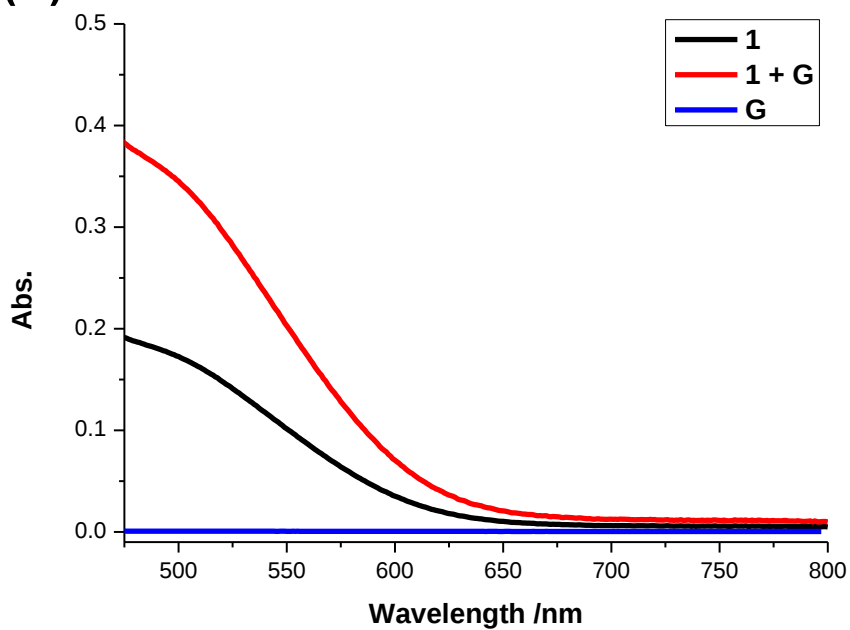


Fig. S10 Color changes (a) and UV-vis spectra (b) of **G** (4.00 mM) upon complexation with 1.0 eq. of host **1** in 1:1 (v/v) CHCl₃-CD₃CN solution at 298 K.

7. Redox stimulus-responsive process of the complex 1·G

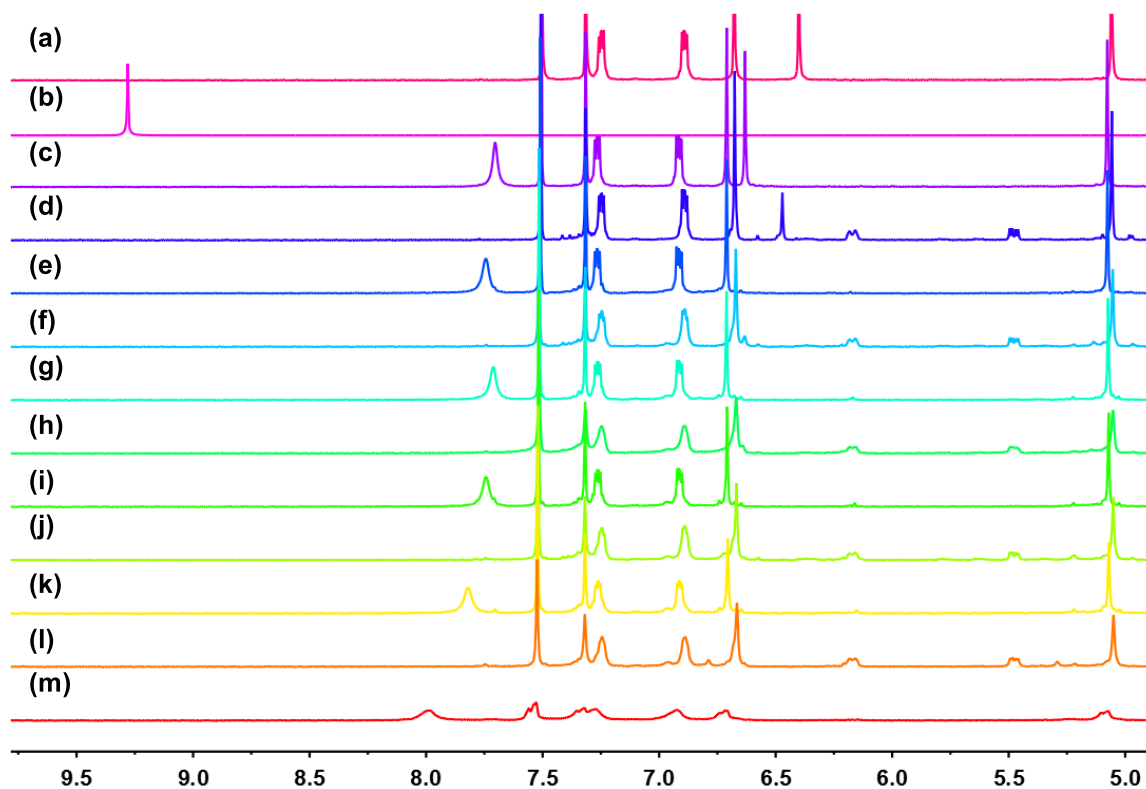
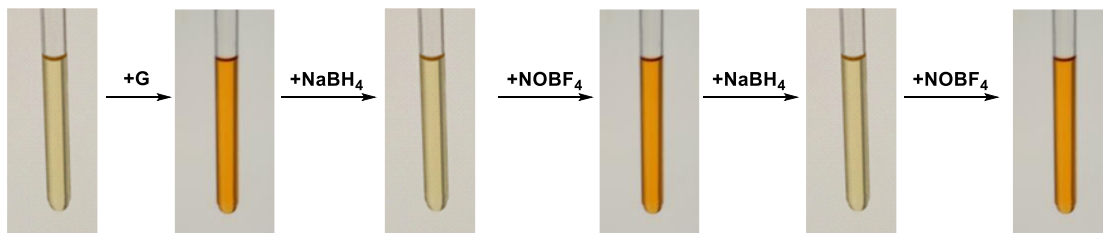


Fig. S11 Partial ^1H NMR spectra (400MHz, $\text{CDCl}_3/\text{CD}_3\text{CN}$, 1/1, v/v): (a) 4.00 mM free host **1**; (b) 4.00 mM free guest **G** (c) after addition of 1.0 equiv of **2** to (b); (d) after addition of 1.0 equiv of NaBH_4 to (c); (e) after addition of 2.0 equiv of NOBF_4 to (d); (f) after addition of 1.0 equiv of NaBH_4 to (e); (g) after addition of 2.0 equiv of NOBF_4 to (f); (h) after addition of 1.0 equiv of NaBH_4 to (g); (i) after addition of 2.0 equiv of NOBF_4 to (h); (j) after addition of 1.0 equiv of NaBH_4 to (h); (k) after addition of 2.0 equiv of NOBF_4 to (j); (l) after addition of 1.0 equiv of NaBH_4 to (k); (m) after addition of 2.0 equiv of NOBF_4 to (l).

(a)



(b)

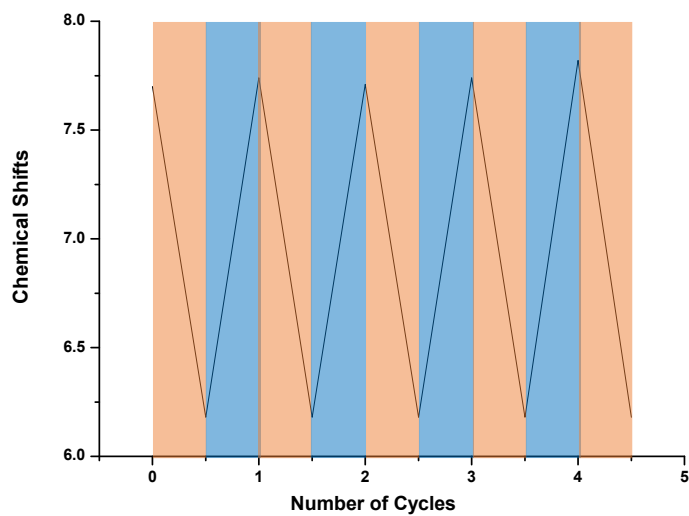


Fig. S12 (a) Color changes of 4.00 mM **1** (298 K, 1:1 v/v CDCl₃/CD₃CN) in the process of redox stimulus-responsive. (b) Redox switching of complex **1·G** monitored by ¹H NMR spectroscopy. The chemical shifts of H₂ were recorded.

8. DFT calculations for complexation between the hosts and guest

Molecular modelings of free host, free guest and the complexes were constructed by referring to the single crystal or calculated structures that involved the related interaction modes. To make sure of the accuracy, density functional theory (DFT) calculations based on the B3LYP/6-31G were carried using the Gaussian 09 program package. The actual counterions were not included in the calculations.

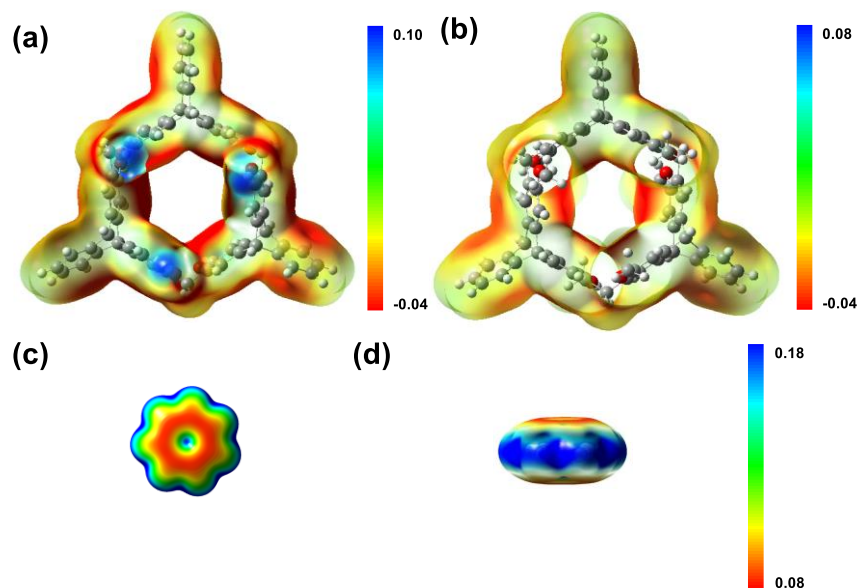


Fig. S13 ESPs mapped onto electron density isosurfaces ($\rho = 0.01$) for top view of calculated structure of (a) the host **1** and (b) of the host **2**. (c) Top view and (d) side view of calculated structure of **G**.

The atomic coordinates of host **1**:

O	1.88335897	4.21995255	-2.63687732
H	1.51887128	4.06909796	-3.55210570
O	-4.60847363	0.53165611	2.61939103
H	-4.28949313	0.76085093	3.53542764
O	-4.61888712	-0.45556000	-2.59840303
H	-4.30518092	-0.68385300	-3.51651466
O	1.82255481	-4.25128724	2.63899975
H	1.45931582	-4.10054354	3.55473403
O	2.70856800	-3.77367304	-2.58097085
H	2.76096127	-3.39649001	-3.50210870
O	2.76279997	3.73726403	2.58180939
H	2.81043538	3.36009277	3.50324149

C	1.29979960	4.56557514	-0.37531148
C	0.88227391	4.33644068	-1.70051853
C	-0.47587824	4.23435164	-2.06291803
H	-0.76400152	4.06077966	-3.09723431
C	-1.42166832	4.36580891	-1.05997308
C	-1.02456374	4.58344608	0.28911970
C	0.31794428	4.67666826	0.62548852
H	0.62974707	4.83149228	1.66182799
C	-2.93557311	4.30991123	-1.24730064
H	-3.24385515	4.14025541	-2.29650712
C	-2.19859890	4.71364595	1.25198618
H	-1.88919696	4.88167570	2.30122846
C	-3.05927849	5.83994408	0.68471138
C	-3.45408422	5.62368585	-0.66731987
C	-4.23581387	6.55663460	-1.32870607
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C	-4.63256695	7.71978694	-0.64127031
H	-5.24778833	8.45892055	-1.15481961
C	-4.24692632	7.93092495	0.68019589
H	-4.56011411	8.83545287	1.20205082
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H	-3.15671610	7.16104773	2.39027277
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C	-4.19609113	2.12811845	-0.63360522
H	-4.49158949	1.94837515	-1.67050542
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C	-3.40265246	2.56252843	2.05604673
H	-3.10326626	2.71296133	3.09105555
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H	-6.13593287	0.29046636	-0.83669186
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H	-4.52028076	-1.89808416	1.68289001
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C	-3.43848998	-2.50506797	-2.04693212
H	-3.14068803	-2.65375772	-3.08269916
C	-4.21239892	-1.38815832	-1.67228441

C	-2.26281353	-4.67638686	-1.25476932
H	-1.95466992	-4.84225567	-2.30471443
C	-2.99640005	-4.27808481	1.24640396
H	-3.30320334	-4.11099665	2.29648493
C	-3.53186404	-5.58129880	0.65802479
C	-3.13873664	-5.79465021	-0.69494571
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H	-5.36553133	-8.39408083	1.12622994
C	-4.32751006	-6.50710573	1.31280509
H	-4.63356070	-6.35482391	2.34681843
C	-1.08797827	-4.56717721	-0.29027017
C	0.25347636	-4.67636590	-0.62600397
H	0.56414633	-4.83015256	-1.66285605
C	1.23596514	-4.58263783	0.37596340
C	0.82061891	-4.35253455	1.70176668
C	-0.53647819	-4.23631827	2.06387220
H	-0.82345397	-4.06527334	3.09890880
C	-1.48317916	-4.35181097	1.05972034
C	2.69100844	-4.73379541	0.03433887
H	3.23480668	-5.19143531	0.89176745
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C	3.90940894	-1.73381435	-2.03890549
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C	4.50159309	-0.96854872	-1.04814434
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C	3.90490321	-2.60769283	0.66120912
H	3.88749608	-2.94122950	1.70188947
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H	5.19872349	-0.78089800	2.30784579
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C	6.60397416	-0.26298107	0.67838552
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H	7.80611691	-0.81640580	2.38501288

C	9.00845615	-0.27482834	0.66258787
H	9.95127194	-0.44729706	1.18211884
C	9.01120977	0.14893340	-0.66402297
H	9.95615931	0.30785648	-1.18398555
C	7.80189979	0.37680569	-1.34838368
H	7.81599030	0.70792628	-2.38577510
C	4.51515518	0.90672633	1.04861534
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H	3.92727140	2.88760492	-1.70122535
C	4.51644020	1.34276568	-0.30611952
C	2.75677820	4.69654279	-0.03359253
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H	3.30661328	5.14573798	-0.89164358

The atomic coordinates of host 2:

O	-2.59195928	-3.94898629	-2.60583797
O	-2.92075088	3.72315952	2.60810607
O	-2.12724581	4.21884741	-2.59870302
O	4.68452897	0.66207133	2.60501344
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C	-4.45882471	-1.14373936	-1.03832787
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C	-5.17770539	-0.61044061	1.24135381
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C	-4.53910951	0.76826036	1.03817744
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C	-5.20678668	0.17803229	-1.24289978
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H	-3.99495611	1.23940241	3.05777551
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C	2.06249887	4.78825046	1.24195592
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C	2.93813143	3.54592241	1.03904998
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C	3.24647181	7.11513038	1.33351484
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H	4.28781093	8.99760251	1.17370591
C	4.37037377	7.89179463	-0.67066607
H	4.95060792	8.64658940	-1.18902094
C	3.99806970	6.71751194	-1.34223492
H	4.28941801	6.56499338	-2.37596460

C	3.37180834	2.67384399	2.03041499
H	3.07213309	2.83817904	3.05722780
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C	4.58663641	1.39527866	0.35110149
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C	5.49393905	0.22704221	0.00280619
H	6.13681104	0.01079498	0.85900018
H	6.11452812	0.49534033	-0.85503645
C	4.68397424	-1.01089037	-0.34637485
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C	3.57721405	-2.38266406	-2.02739798
H	3.29259670	-2.56888260	-3.05468509
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C	4.29463592	-1.92422447	0.63982416
H	4.55566870	-1.70606408	1.66860018
C	3.11412730	-4.17819903	1.24139170
H	3.39434294	-4.00192013	2.28183333
C	3.71862554	-5.46696842	0.66876802
C	3.35986610	-5.69386793	-0.67229974
C	2.44811454	-4.59816522	-1.24171751
H	2.16707240	-4.77424836	-2.28201620
C	4.54180243	-6.36465862	1.33544593
H	4.81959484	-6.19012660	2.36940860
C	5.01341855	-7.50078000	0.66043716
H	5.65719817	-8.20448774	1.17565455
C	4.65688697	-7.72667222	-0.66810622
H	5.02308365	-8.60607236	-1.18547108
C	3.82647259	-6.81782030	-1.34129941
H	3.55055700	-6.99433107	-2.37540623
C	1.60173063	-4.31774849	1.03828810
C	1.24313190	-4.53958046	-0.29657109
C	-0.09336887	-4.71002917	-0.63675306
H	-0.40353619	-4.85238807	-1.66488684
C	-1.08495513	-4.67290358	0.34998324
C	-0.71781674	-4.43162980	1.68394471
C	0.62943648	-4.25950372	2.02965107
H	0.91954543	-4.08261625	3.05677190
C	-2.55033609	-4.87304731	0.00014996
H	-3.05935461	-5.31935247	0.85746418

H	-2.62917133	-5.54673977	-0.85570051
C	-2.65557418	-3.58011486	-4.01481641
H	-3.69156080	-3.51298019	-4.36884222
H	-2.13905703	-4.38290539	-4.54210511
H	-2.14811144	-2.62660010	-4.20522798
C	-2.95926706	3.35577242	4.01806273
H	-3.98744693	3.20291124	4.36839080
H	-2.51615406	4.20188346	4.54457166
H	-2.37369662	2.44969983	4.21657262
C	-1.78619647	4.10781114	-4.01183360
H	-2.74360452	4.07447891	-4.53312364
H	-1.22052065	3.19177046	-4.22156959
H	-1.20866951	4.97405943	-4.35677490
C	4.38374854	0.87300608	4.01527900
H	3.30679292	0.80994300	4.21400428
H	4.75923049	1.84156030	4.36788068
H	4.90079427	0.06753478	4.53791144
C	4.43913906	-0.50425308	-4.01206163
H	3.36038552	-0.52568394	-4.21009152
H	4.88867788	-1.43980340	-4.36647861
H	4.89145604	0.33905300	-4.53531534
C	-1.43697722	-4.22261222	4.01298766
H	-2.39289701	-4.26014496	4.53673808
H	-0.95153422	-3.25711379	4.20171084
H	-0.78626218	-5.02897887	4.37310361

The atomic coordinates of **G**:

C	-5.09508400	-1.49429700	-0.30434900
C	-5.98884300	-0.49507100	-0.27992800
C	-5.84938800	0.82250400	-0.06816500
C	-4.77016600	1.57553400	0.18891000
C	-3.48666300	1.21683100	0.31463300
C	-2.92756000	-0.21154300	0.19090300
C	-3.77023700	-1.46217000	-0.11566100
H	-5.51038100	-2.50048900	-0.51152100
H	-7.03254500	-0.81825800	-0.47158900
H	-6.79829800	1.39504700	-0.11587300
H	-4.96427800	2.65887600	0.31743200
H	-2.75367300	2.01530600	0.52960000
H	-1.84276200	-0.34957700	0.33550800
H	-3.22315900	-2.41989500	-0.18265100

The atomic coordinates of **1·G**:

O	3.38272242	3.02376320	2.77170895
H	3.51062874	2.69008359	3.68029159
O	2.21026954	-3.73279650	-2.95206803
H	2.67529139	-3.66592488	-3.80871682
O	1.16265303	-4.15416609	2.31602272
H	0.87761498	-4.11993952	3.24909260
O	-5.38353093	0.25682327	-2.53307166
H	-5.43096092	-0.13119923	-3.42761898
O	-4.80095500	1.56130241	2.80219950
H	-4.62249833	1.91503455	3.69444954
O	2.71162260	3.56142457	-2.45419181
H	2.39232145	3.63424654	-3.37398286
C	4.10742851	2.68303406	0.51678289
C	3.96900397	2.17765448	1.82181131
C	4.34784904	0.86490289	2.15090468
H	4.20673149	0.49266822	3.16295028
C	4.87955655	0.04311619	1.16148568
C	5.06927007	0.53805288	-0.14569405
C	4.68645512	1.84255727	-0.45892779
H	4.80079183	2.22746344	-1.46694823
C	5.26007337	-1.43719920	1.30483184
H	5.09356727	-1.82424818	2.31184343
C	5.65650145	-0.51898666	-1.10158193
H	5.82463546	-0.13163662	-2.10857482
C	6.93975417	-1.04103562	-0.44160124
C	6.72425641	-1.54318908	0.85725906
C	7.78454024	-2.06178276	1.59712050
H	7.62086746	-2.44988700	2.59810106
C	9.07103893	-2.07933819	1.03321647
H	9.90229219	-2.48214155	1.60234038
C	9.28479801	-1.58063220	-0.25572881
H	10.28164089	-1.59643147	-0.68375864
C	8.21517029	-1.05802184	-1.00150783
H	8.38363884	-0.67120234	-2.00223272
C	4.41890830	-2.16444690	0.24158401
C	3.47586550	-3.16405612	0.46255446
H	3.28192753	-3.53134983	1.46363618
C	2.72845329	-3.71012029	-0.60384453
C	2.99474818	-3.22878841	-1.89598603

C	3.95816356	-2.23162639	-2.13807960
H	4.13757129	-1.88161544	-3.15269997
C	4.65634814	-1.68610969	-1.06364048
C	1.71550707	-4.82888782	-0.37258072
H	1.61248200	-5.39445891	-1.30175959
H	2.13214808	-5.50613108	0.38140562
C	0.31997366	-4.41633940	0.09036552
C	-0.78278074	-4.42325224	-0.79057651
H	-0.60880535	-4.68318662	-1.83128496
C	-2.07426397	-4.14619881	-0.33540375
C	-2.28695430	-3.83623763	1.02274119
C	-1.21706888	-3.81657064	1.91101916
H	-1.37654584	-3.59724553	2.96441526
C	0.07088970	-4.11835958	1.44175797
C	-3.76250128	-3.58995476	1.36569446
H	-3.92010505	-3.34041723	2.41676893
C	-3.38763620	-4.18838461	-1.14196173
H	-3.23375263	-4.44166593	-2.19315651
C	-4.29601439	-5.19492779	-0.41638070
C	-4.50134447	-4.86886637	0.93939596
C	-5.30199863	-5.67484835	1.74473929
H	-5.46278109	-5.42493862	2.78927021
C	-5.90350091	-6.81695827	1.18957103
H	-6.52959539	-7.45004672	1.80952389
C	-5.69978058	-7.14038050	-0.15546799
H	-6.16729799	-8.02441819	-0.57623369
C	-4.89217611	-6.32645917	-0.96765000
H	-4.73533739	-6.58018701	-2.01191086
C	-4.23731942	-2.48408862	0.41377622
C	-4.78030073	-1.24919702	0.76501798
H	-4.90681311	-0.97548298	1.80829927
C	-5.15707854	-0.31505634	-0.22233426
C	-5.00829825	-0.68637829	-1.57136107
C	-4.46073685	-1.93041965	-1.93956510
H	-4.35438537	-2.18888462	-2.99108329
C	-4.05605059	-2.81875775	-0.94470997
C	-5.66037223	1.07236876	0.15739159
H	-6.25459832	1.47108919	-0.66822789
H	-6.31041605	0.98863078	1.03186187
C	-4.53713950	2.05594888	0.47729569
C	-4.14211732	2.29151192	1.80682291

C	-3.12267342	3.20845667	2.12563288
H	-2.85500190	3.38561730	3.16501890
C	-2.48396365	3.90264043	1.09989941
C	-2.85717786	3.67635548	-0.24090702
C	-3.87021282	2.76619808	-0.54254198
H	-4.17668090	2.60065451	-1.57148371
C	-2.09124006	4.56974179	-1.22758532
H	-2.38144086	4.40015055	-2.26641479
C	-1.39920491	4.98059453	1.25031941
H	-1.11100974	5.15431274	2.28907945
C	-1.98241102	6.23616745	0.57669275
C	-2.35539372	6.01423893	-0.76458057
C	-2.90225796	7.04540324	-1.52376136
H	-3.19263453	6.87668497	-2.55654435
C	-3.07712826	8.31052401	-0.93718457
H	-3.50323180	9.11949246	-1.52127803
C	-2.70561346	8.53096824	0.39250884
H	-2.84304558	9.51086338	0.83753409
C	-2.15447385	7.48943719	1.15843096
H	-1.86619147	7.66332939	2.19092664
C	-0.59526128	4.33272894	-0.97531185
C	0.36674978	3.99627905	-1.92322305
H	0.08762191	3.83301218	-2.96187935
C	1.71262889	3.89643849	-1.53197066
C	2.12118466	4.13055478	-0.20620605
C	1.12524916	4.45587228	0.73864626
H	1.42956960	4.64641070	1.76313878
C	-0.21650003	4.55418866	0.36501050
C	3.60057924	4.07758884	0.17088660
H	4.18682289	4.46521042	-0.66701507
H	3.76304993	4.73616084	1.02831735
C	-1.65652912	0.26943022	0.54488514
C	-0.95224572	1.47270852	0.42715879
C	0.41635542	1.67129358	0.21504897
C	-1.16154315	-1.03183176	0.43922988
C	1.43549146	0.72257734	0.08450799
C	0.15815833	-1.44525313	0.21833473
C	1.31301516	-0.67025214	0.07322034
H	-2.72470304	0.36530624	0.71052995
H	-1.54288896	2.37528692	0.51521688
H	0.73157420	2.70725423	0.17998352

H	-1.89019201	-1.83073159	0.53154074
H	2.44491354	1.11439568	-0.00386631
H	0.30173342	-2.51517177	0.15863181
H	2.23266339	-1.23093942	-0.05790767

The atomic coordinates of **2·G**:

O	1.07191291	-4.68359778	-2.89036359
O	-4.74581255	0.29025724	2.32473136
O	-4.53935545	1.19442655	-2.99407128
O	2.68089592	3.95213831	2.10277403
O	3.43320744	3.03765281	-3.14959163
O	2.03575635	-4.24017553	2.36002137
C	0.03305991	-4.57981231	-1.95487535
C	0.38243710	-4.85518883	-0.61776884
C	-0.62287676	-4.77692387	0.36149338
H	-0.35421970	-4.97913019	1.39323971
C	-1.92992144	-4.43680773	0.01818886
C	-2.25543755	-4.16561749	-1.32146322
C	-1.28050452	-4.23626440	-2.31416429
H	-1.54326029	-4.02829424	-3.34468554
C	-3.13896485	-4.32922235	0.96033524
H	-2.88664043	-4.54444054	2.00083248
C	-3.71270033	-2.91862554	0.76054434
C	-4.02694361	-2.63944825	-0.58099867
C	-3.73713320	-3.81854710	-1.52079849
H	-3.98922636	-3.60320305	-2.56146435
C	-4.52234640	-5.01044268	-0.95205912
C	-4.19827808	-5.28736886	0.39336590
C	-4.82155301	-6.33662635	1.06425025
H	-4.57233547	-6.55157461	2.09961540
C	-5.77620278	-7.11717497	0.38935969
H	-6.26490754	-7.93680247	0.90705246
C	-6.09768552	-6.84235756	-0.94296775
H	-6.83644040	-7.44819608	-1.45853617
C	-5.46832872	-5.78353818	-1.62041488
H	-5.71988413	-5.57026488	-2.65557536
C	-3.94157630	-1.96533588	1.74993046
H	-3.69557367	-2.18508169	2.78230297
C	-4.48225620	-0.72041286	1.38534652
C	-4.79357148	-0.41620929	0.04577714

C	-4.55592417	-1.40007347	-0.93059680
H	-4.79183285	-1.16747071	-1.96369518
C	-5.38220608	0.93555264	-0.33592929
H	-5.94233850	1.32798777	0.51671808
H	-6.08250538	0.78962997	-1.16326155
C	-4.34248471	1.96805429	-0.75058166
C	-3.93055876	2.08006277	-2.09342694
C	-2.97715369	3.03149579	-2.49149258
H	-2.66757183	3.11474819	-3.52659193
C	-2.42626809	3.87855887	-1.53235616
C	-2.82222355	3.78506393	-0.18722742
C	-3.77122712	2.83830749	0.19424053
H	-4.08816607	2.75588330	1.22945307
C	-1.38641536	4.98094863	-1.77670140
H	-1.07657018	5.05154009	-2.82166509
C	-2.02882140	6.27679318	-1.25759117
C	-2.42766895	6.18678251	0.09325604
C	-2.12350175	4.81432431	0.71364199
H	-2.43341404	4.74331068	1.75844618
C	-0.61535467	4.59823826	0.51898304
C	-0.21805384	4.68122589	-0.82619927
C	-3.02682842	7.27484867	0.72282967
H	-3.33457336	7.20650374	1.76248847
C	-3.23090097	8.46367399	0.00089301
H	-3.69774475	9.31516469	0.48632650
C	-2.83537658	8.55300975	-1.33684015
H	-2.99462630	9.47409778	-1.88899502
C	-2.23093248	7.45456388	-1.97261533
H	-1.92304728	7.52563699	-3.01209146
C	0.32272318	4.35492542	1.51975915
H	0.00580822	4.28643822	2.55337774
C	1.67116370	4.18634465	1.16241150
C	2.08949017	4.25630456	-0.18177755
C	1.12105048	4.50727042	-1.16876026
H	1.44080663	4.55629179	-2.20474198
C	3.55514078	4.07087882	-0.55094118
H	4.17312232	4.42626409	0.27798319
H	3.77573037	4.68772986	-1.42628423
C	3.93981939	2.62964559	-0.85907746
C	3.87339067	2.13071677	-2.17530381
C	4.23876346	0.80872168	-2.47890666

H	4.19016018	0.43368209	-3.49436670
C	4.66995216	-0.02608175	-1.45032538
C	4.73955878	0.44876249	-0.12940780
C	4.37677310	1.76337339	0.15856325
H	4.41848770	2.14245209	1.17469213
C	5.25519860	-0.60982828	0.85838399
H	5.31292947	-0.23987967	1.88446155
C	6.61756354	-1.06404531	0.31176125
C	6.54361631	-1.53881462	-1.01522689
C	5.11869984	-1.48789691	-1.58739145
H	5.06109562	-1.85781354	-2.61339402
C	7.83740462	-1.04160063	0.98310586
H	7.89566651	-0.67511806	2.00415939
C	8.99467224	-1.49586572	0.32704568
H	9.94863330	-1.48023180	0.84500852
C	8.92149449	-1.96617454	-0.98730846
H	9.81862228	-2.31605576	-1.48865388
C	7.69015058	-1.98879394	-1.66503866
H	7.63459379	-2.35507817	-2.68634371
C	4.32356680	-1.82180720	0.70782437
C	4.24541533	-2.29247672	-0.61371155
C	3.43995476	-3.38783863	-0.91724130
H	3.36304370	-3.75439952	-1.93562095
C	2.69643330	-4.03575291	0.08387310
C	2.79011542	-3.55059284	1.40387167
C	3.60426765	-2.44998905	1.72358482
H	3.68066868	-2.09083040	2.74314955
C	1.81126684	-5.23021644	-0.24671256
H	1.78275608	-5.89821771	0.61830234
H	2.26039977	-5.77621876	-1.08088509
C	0.77138768	-4.48148645	-4.29294485
H	0.02351861	-5.20030060	-4.64892409
H	1.71409639	-4.64484201	-4.81499369
H	0.41671138	-3.46126052	-4.48311593
C	-4.79996103	-0.06963374	3.73221737
H	-5.46340864	-0.92723659	3.89311564
H	-5.20315585	0.80893354	4.23687284
H	-3.80238790	-0.29194444	4.12604259
C	-4.21829267	1.30053339	-4.40299070
H	-4.83047413	0.54449581	-4.89446362
H	-3.15736243	1.09333267	-4.58794321

H	-4.47092285	2.29232094	-4.79678764
C	2.35103054	4.02063726	3.51533433
H	1.65800781	3.22444617	3.80372404
H	1.92470601	4.99766666	3.77316484
H	3.29927369	3.88508483	4.03550879
C	3.40300511	2.61502997	-4.53487494
H	2.70225922	1.78470534	-4.68464640
H	4.39940814	2.31907508	-4.88473464
H	3.06287329	3.48687032	-5.09357517
C	2.11922899	-3.83086956	3.74978573
H	1.47227454	-4.52210723	4.28964575
H	1.76011528	-2.80448089	3.88702391
H	3.14532972	-3.91632909	4.12784127
C	1.02984756	-0.68035717	-1.66765784
C	1.63426784	-0.69366734	-0.38437981
C	1.05800920	-0.27986040	0.84833709
C	-0.24217623	-0.28495289	-2.03926358
C	-0.19986412	0.22347343	1.10736666
C	-1.29717234	0.22858333	-1.18743150
C	-1.27965147	0.45064918	0.16112994
H	1.66537386	-1.03425840	-2.47765593
H	2.66341030	-1.03928060	-0.34030938
H	1.71422367	-0.37197817	1.71389623
H	-0.49150449	-0.36009695	-3.09287821
H	-0.42336077	0.47913854	2.14006103
H	-2.22369147	0.46194895	-1.70807357
H	-2.19144962	0.85333735	0.59895328