Supporting Information

Hybrid interaction network of guanidinium-biphenyldisulfonic acid for the structure determination of liquid molecules

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1. Spectra of as-synthesized host

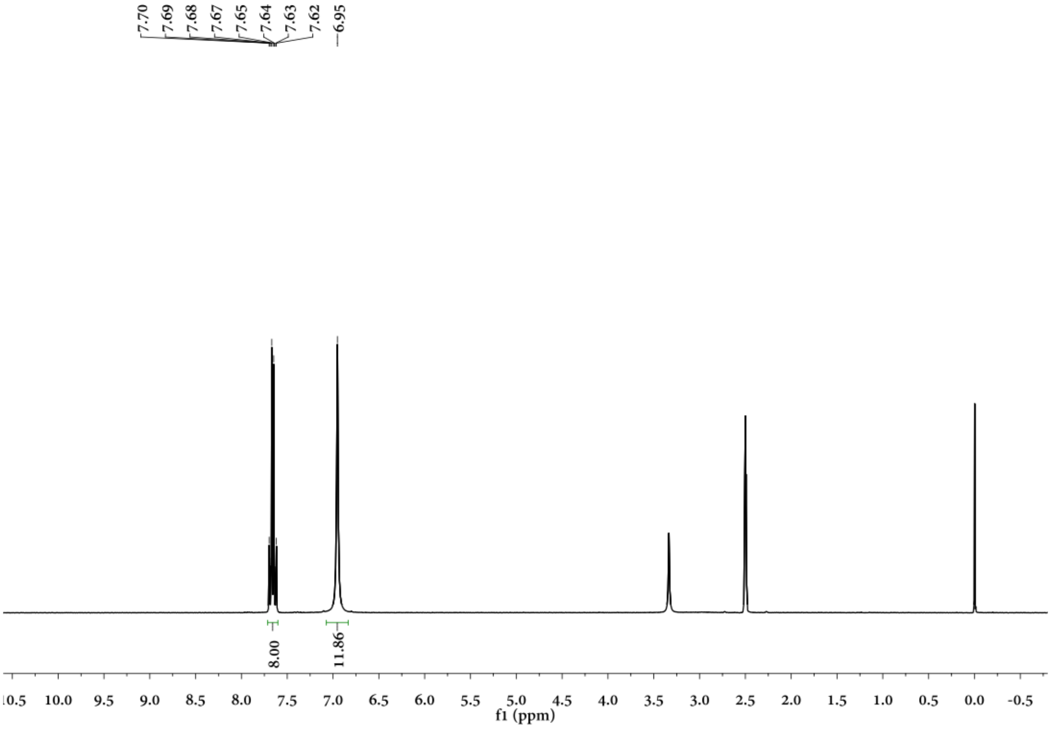

Figure Sa. ^{1}H-NMR spectra of guanidinium−biphenyldisulfonic acid (GBPS) (400 MHz, DMSO).

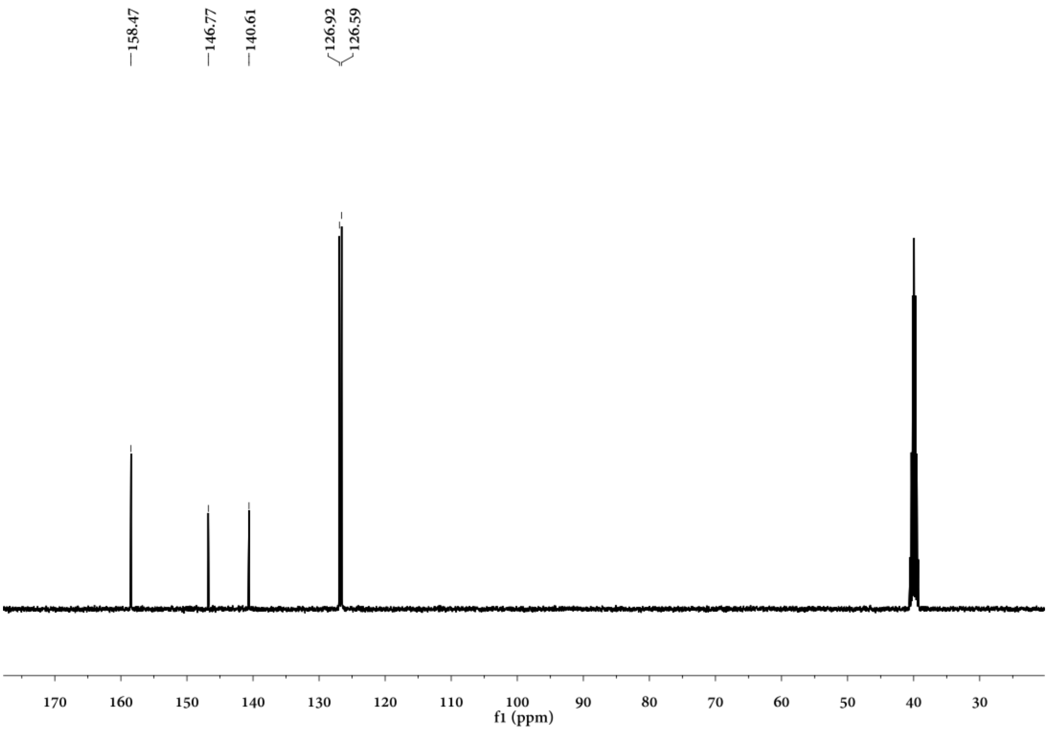

Figure Sa. ^{13}C-NMR spectra of guanidinium−biphenyldisulfonic acid (GBPS) (100 MHz, DMSO).

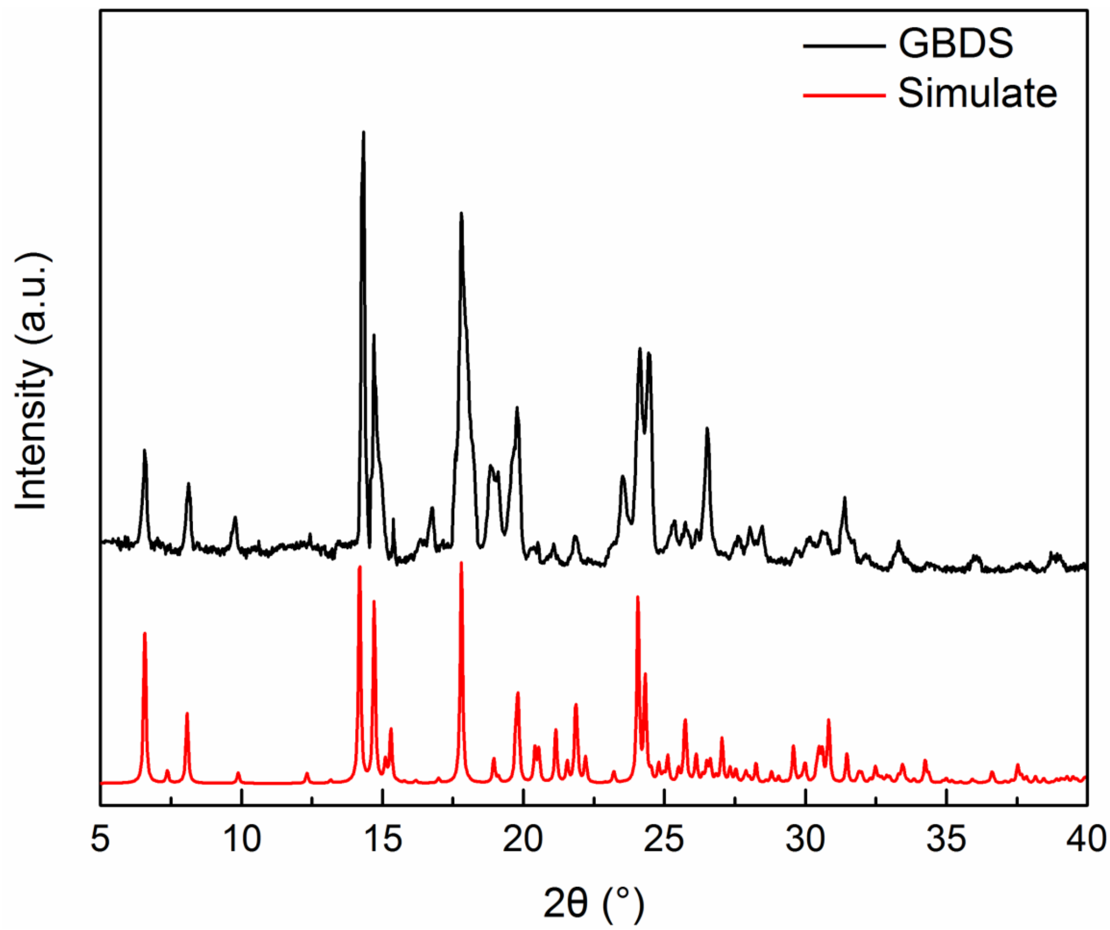

Figure Sc. PXRD spectra of guanidinium−biphenyldisulfonic acid (GBPS).

2. Figures for the NMR and interactions of inclusion complexes

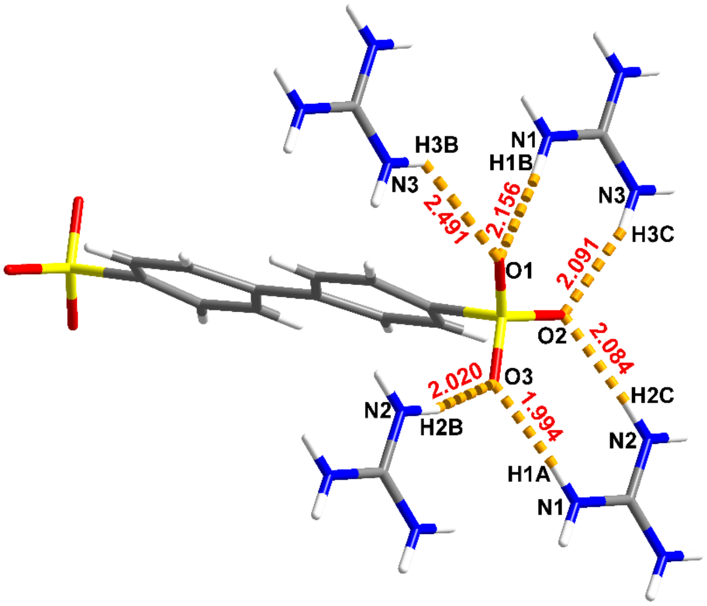

Figure S1a N–H ··O hydrogen bonds in GBPS ⊃**1**

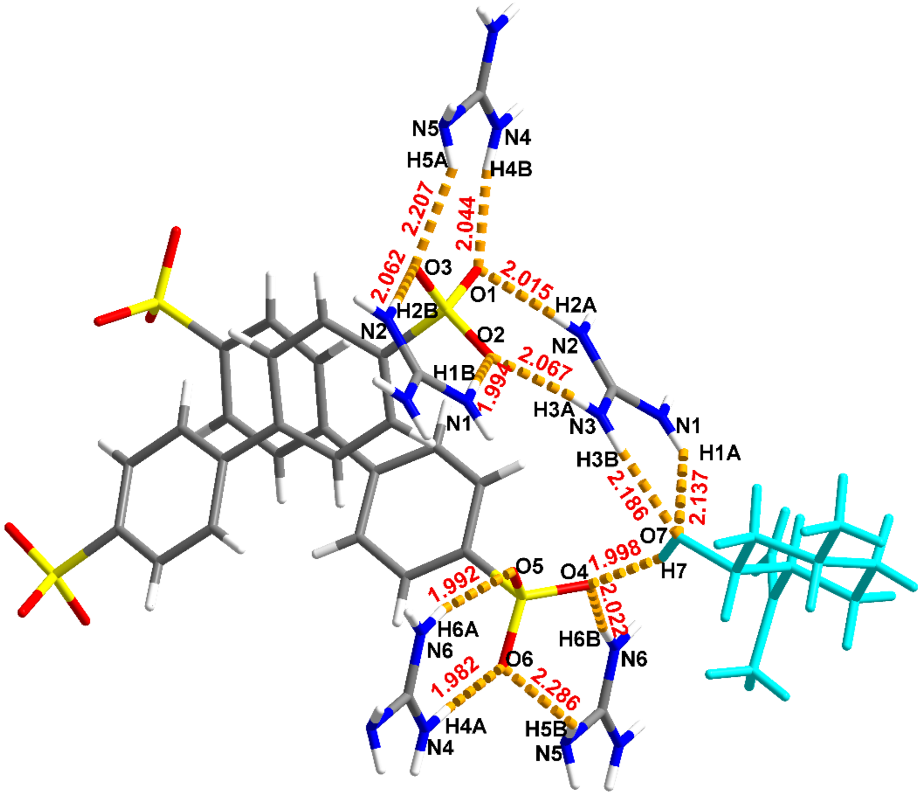

Figure S2a   N–H ··O and O–H ··O hydrogen bonds in GBPS ⊃**2**

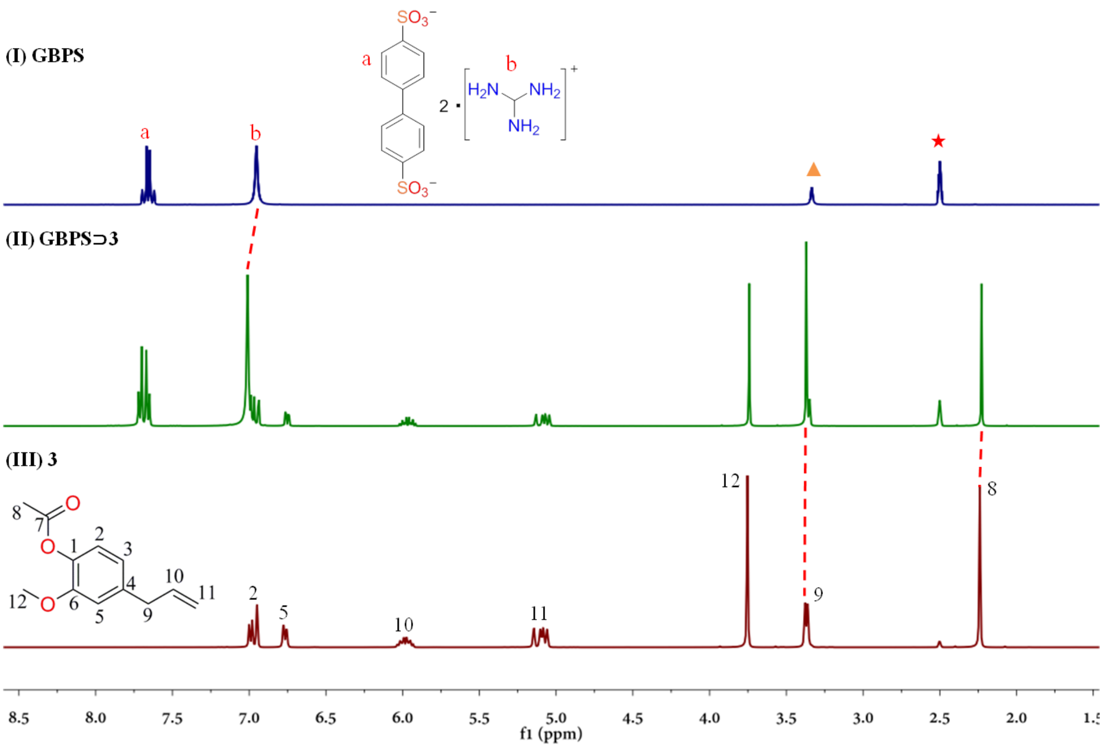

Figure S3a. [1]H-NMR of (I) GBPS, (II) GBPS ⊃**3** and (III)**3** (400 MHz, DMSO) (▲ is water peaks, ★ is DMSO-d_6)

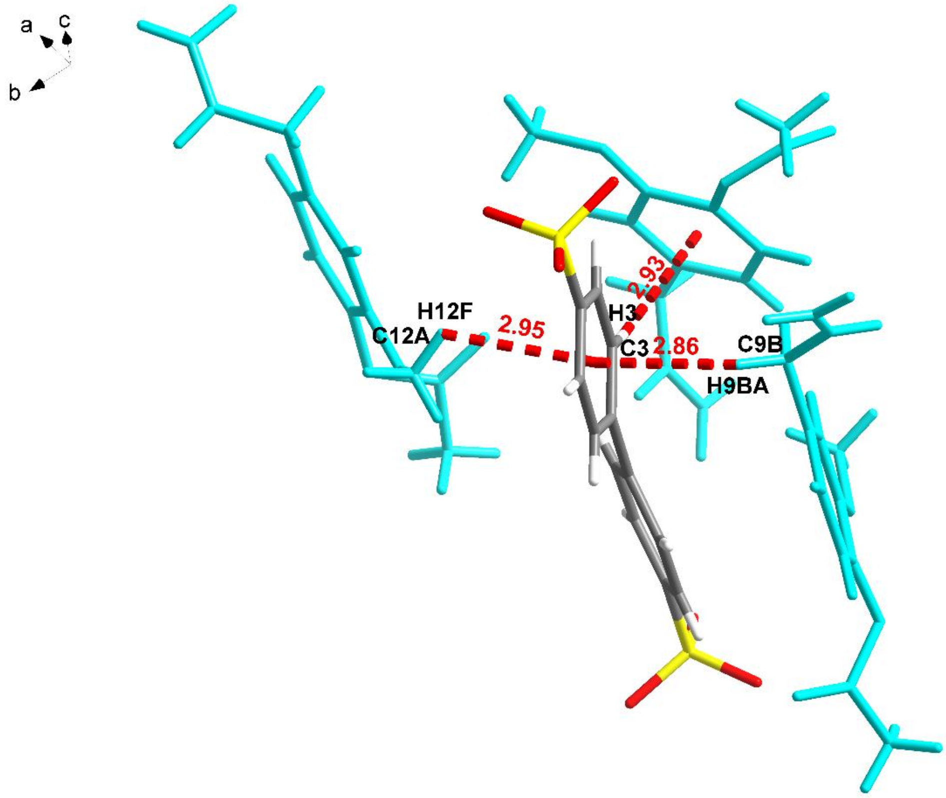

Figure S3b C–H ··π interactions in GBPS ⊃**3**

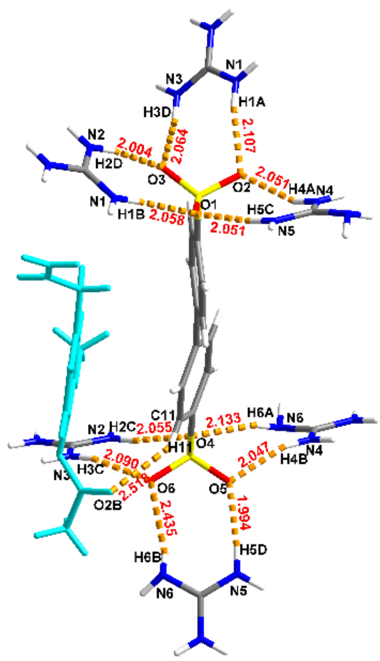

Figure S3c C–H ··O and N–H ··O hydrogen bonds in GBPS ⊃**3**

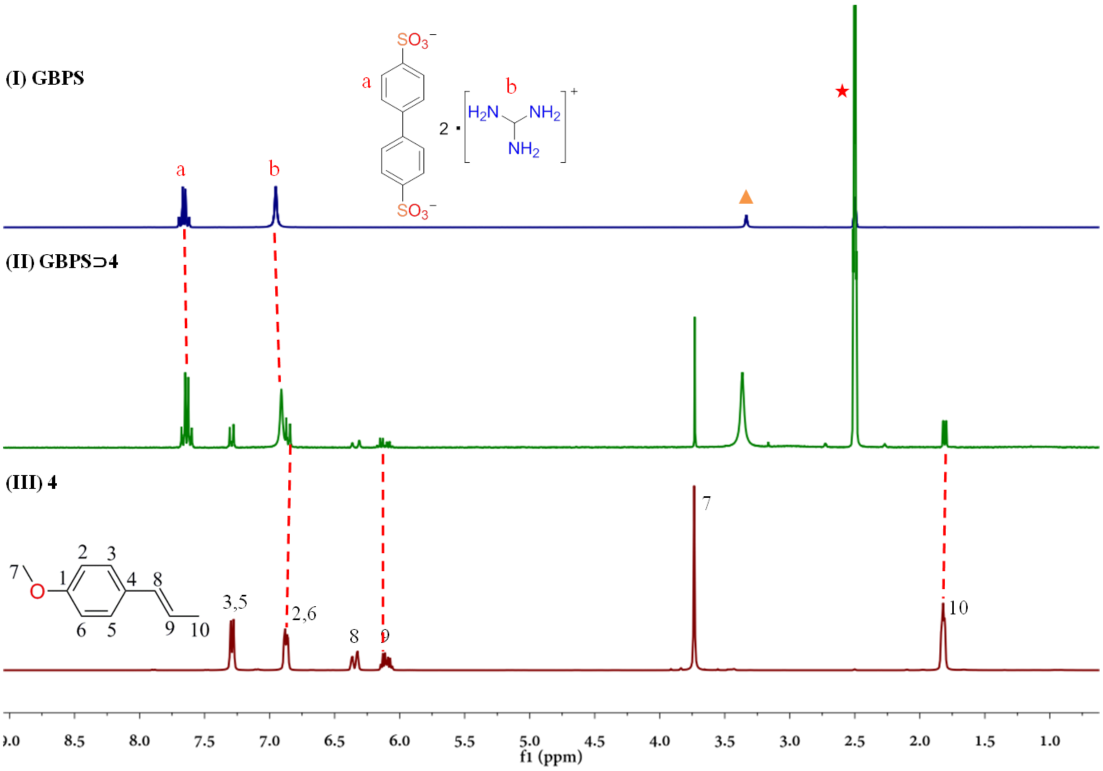

Figure S4a [1]H-NMR of (I) **GBPS**, (II) **GBPS⊃4** and (III)**4** (400 MHz, DMSO) (▲ is water peaks, ★ is DMSO-d_6).

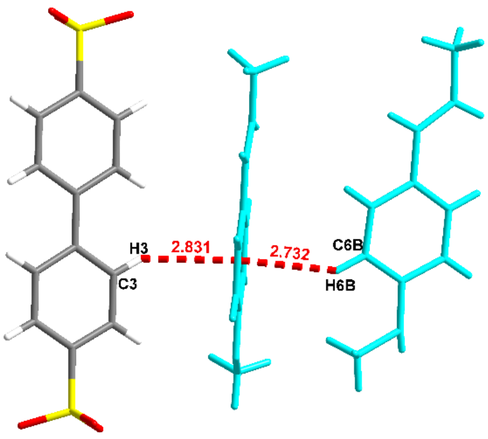

Figure S4b C–H ··π interactions in GBPS ⊃**4**

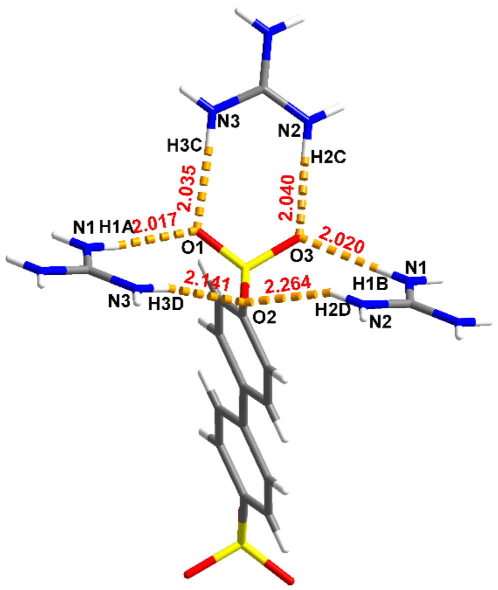

Figure S4c N–H ··O interactions in GBPS ⊃**4**

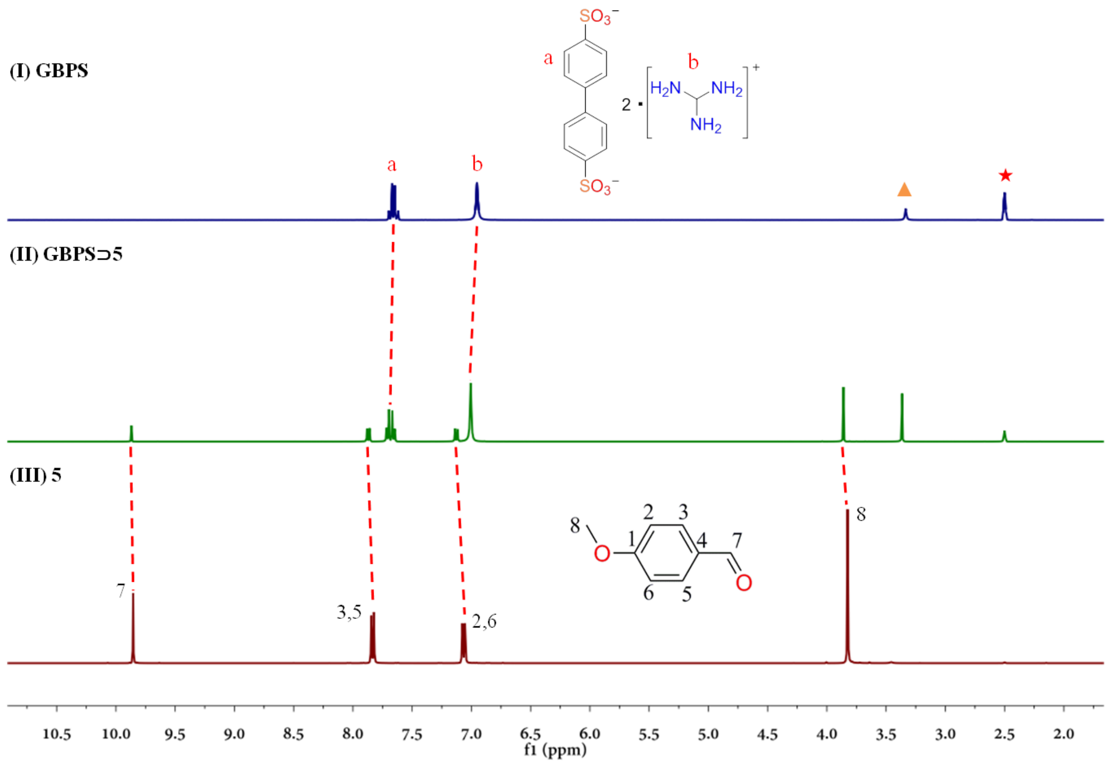

Figure S5a. [1]H-NMR of (I) GBPS, (II) GBPS ⊃**5** and (III) **5** (400 MHz, DMSO) **(**▲ is water peaks**,** ★ is DMSO-d_6**)**.

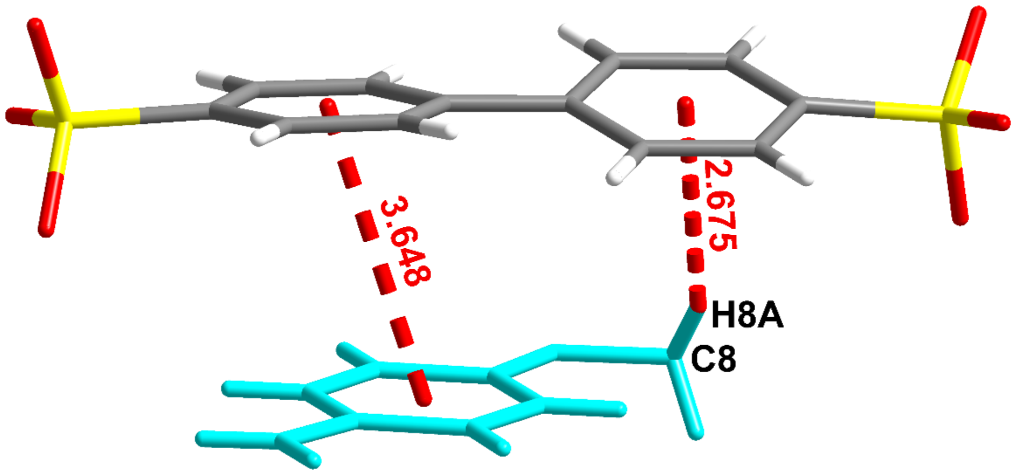

Figure S5b π ··π and C–H ··π interactions in GBPS ⊃ **5**

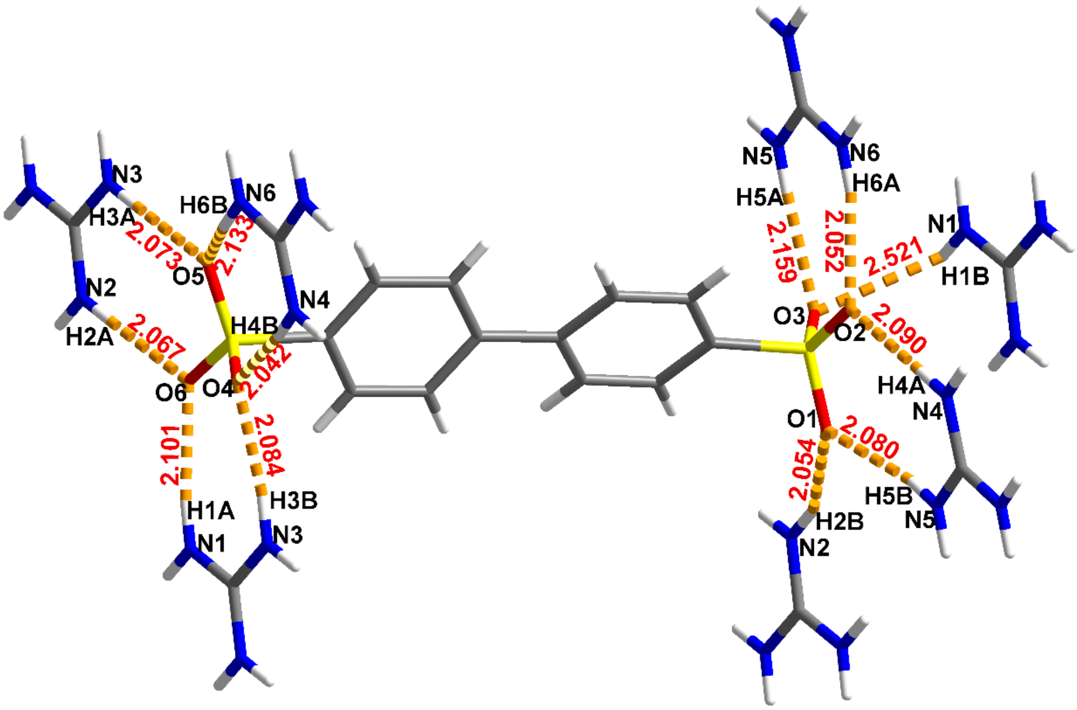

Figure S5c N–H ··O hydrogen bonds in GBPS ⊃ **5**

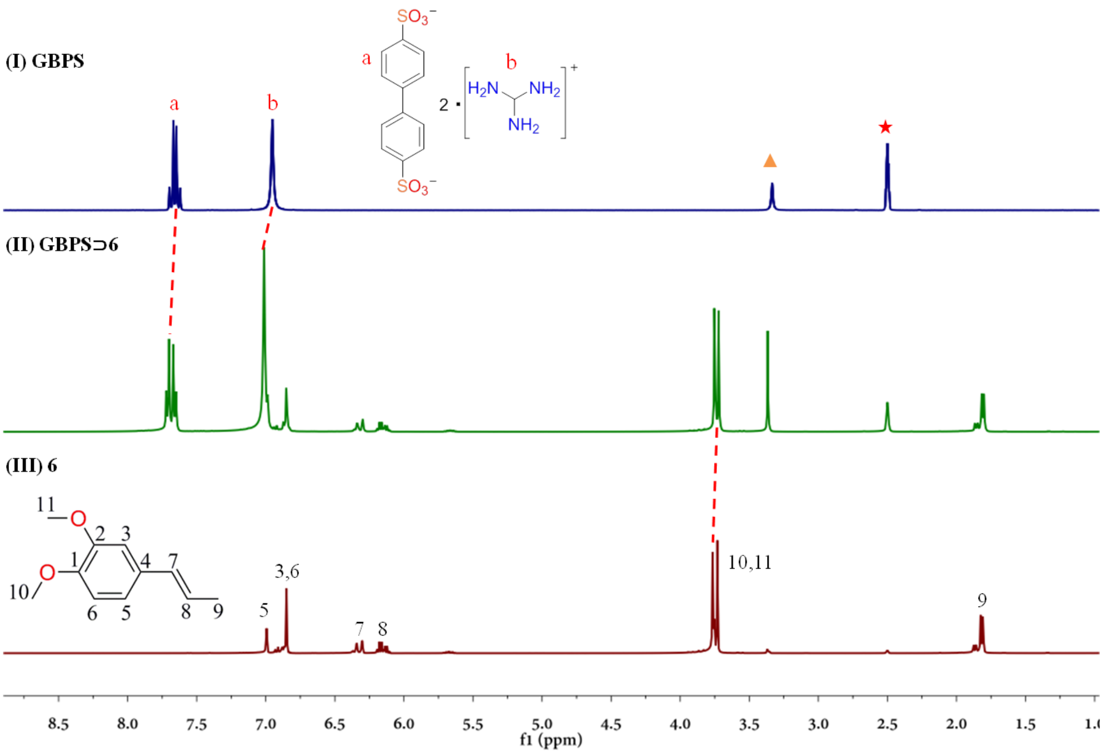

Fig. S6a [1]H-NMR of (I) **GBPS**, (II) **GBPS⊃6** and (III)**6** (400 MHz, DMSO) (▲ is water peaks, ★ is DMSO-d_6).

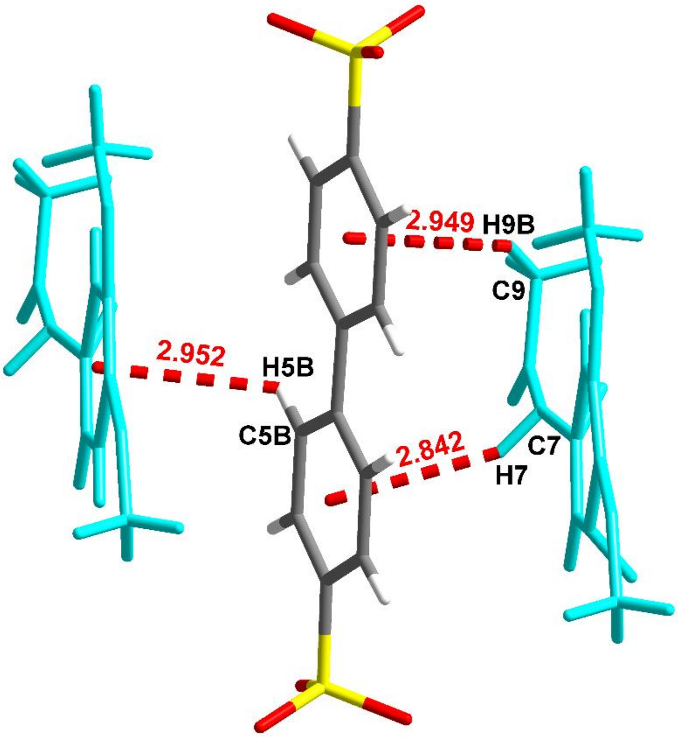

Figure S6b C–H ··π interactions in GBPS ⊃ **6**

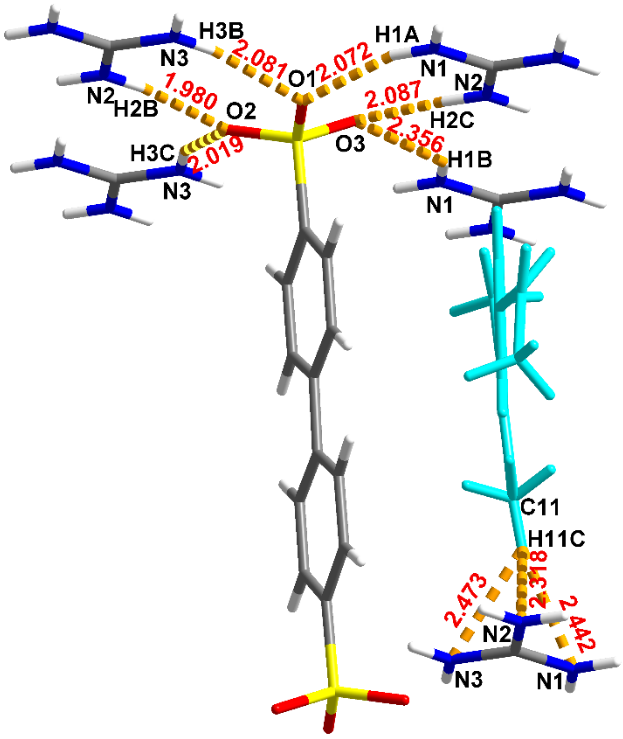

Figure S6c N–H ··O and C–H ··N hydrogen bonds in GBPS ⊃ **6**

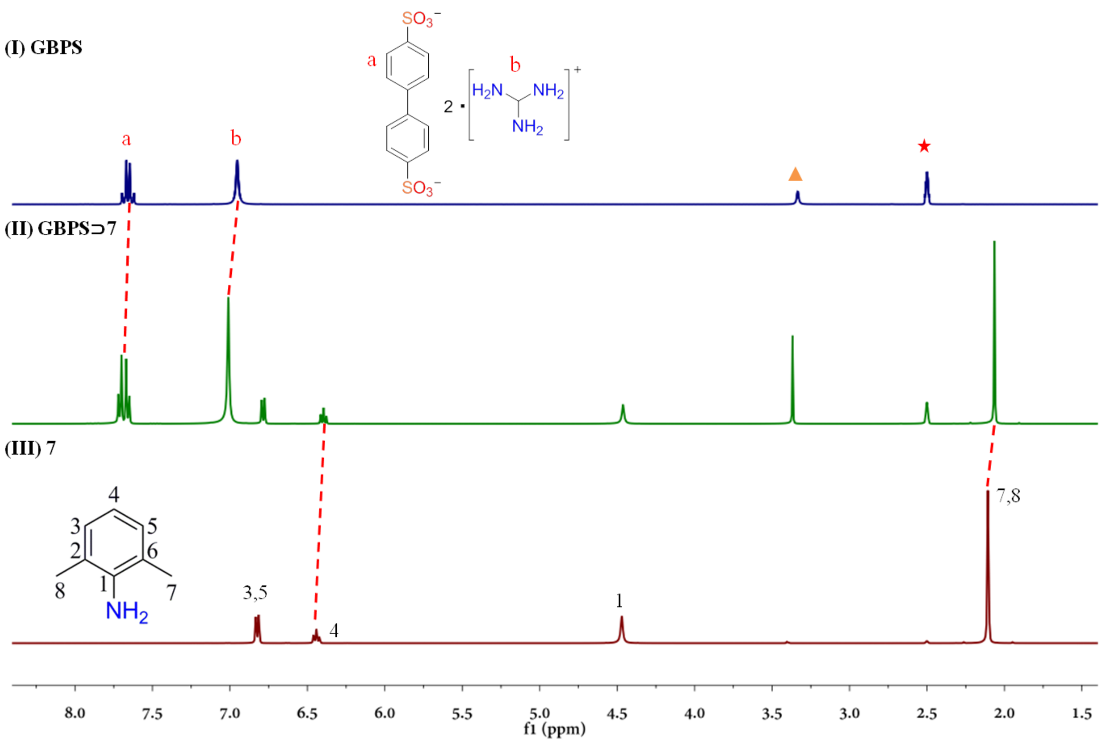

Fig. S7a [1]H-NMR of (I) **GBPS**, (II) **GBPS⊃7** and (III)**7** (400 MHz, DMSO) **(**▲ is water peaks**,** ★ is DMSO-d_6**)**.

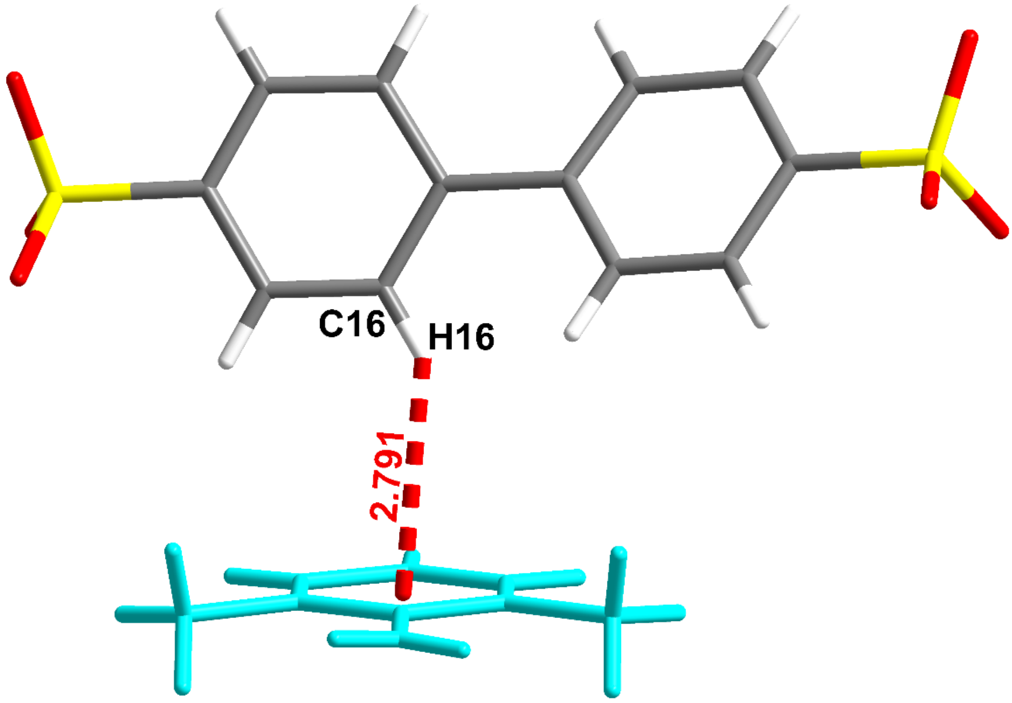

Figure S7b C–H ··π interactions in GBPS ⊃ **7**

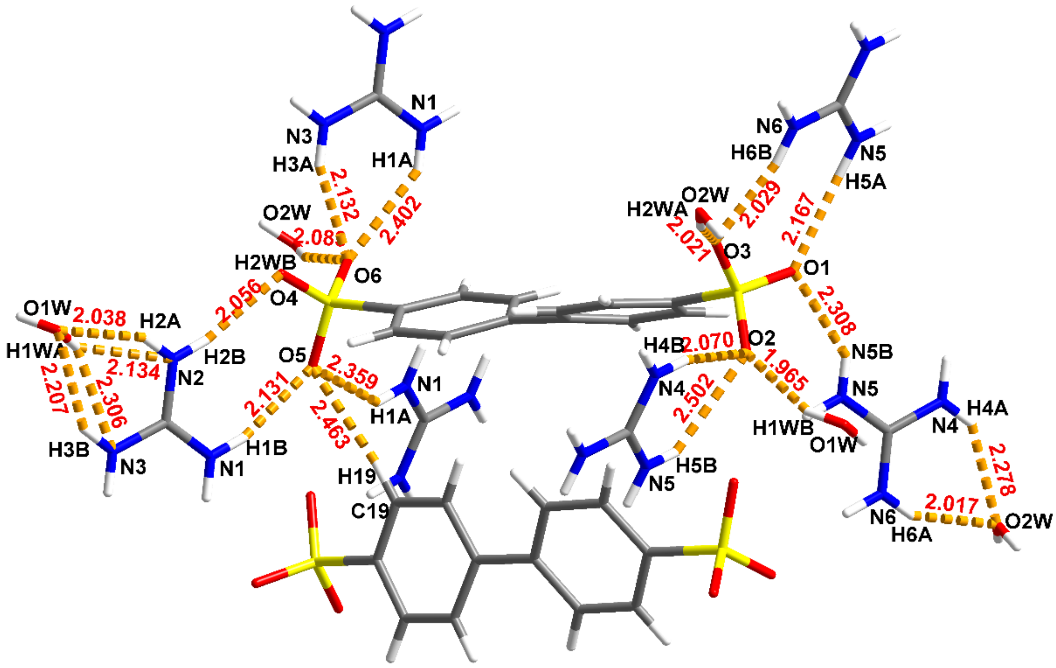

Figure S7c N–H ··O hydrogen bonds in GBPS ⊃ **7**

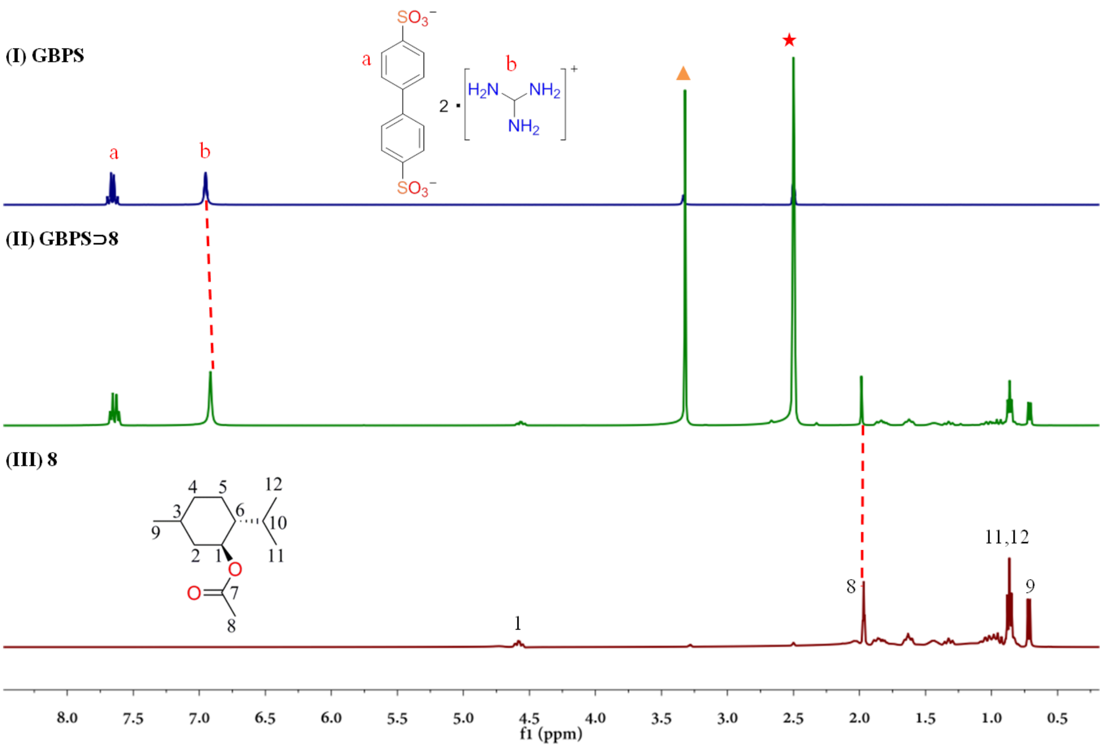

Fig. S8a ^{1}H-NMR of (I) **GBPS**, (II) **GBPS⊃8** and (III)**8** (400 MHz, DMSO) **(**▲ is water peaks**,** ★ is DMSO-d_6**)**.

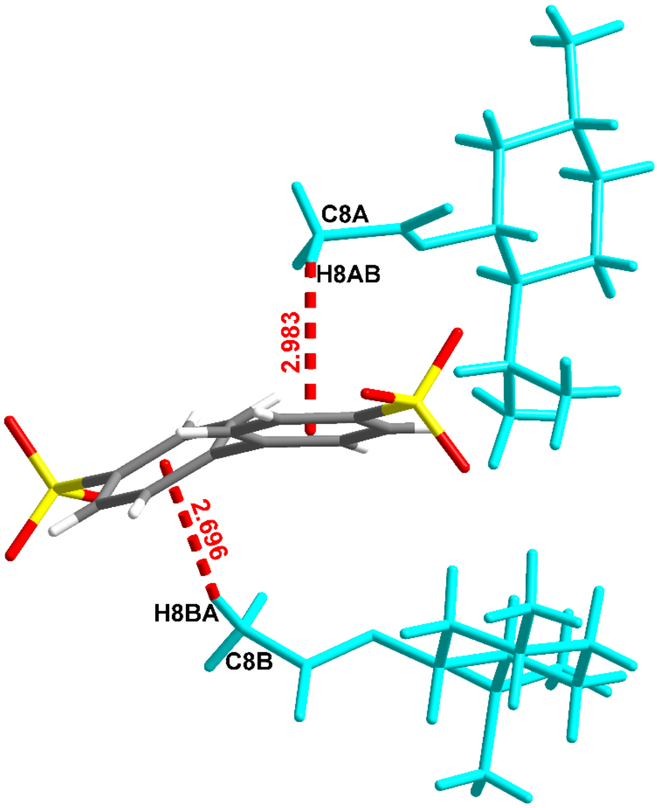

Figure S8b C–H ··π interactions in GBPS ⊃ **8**

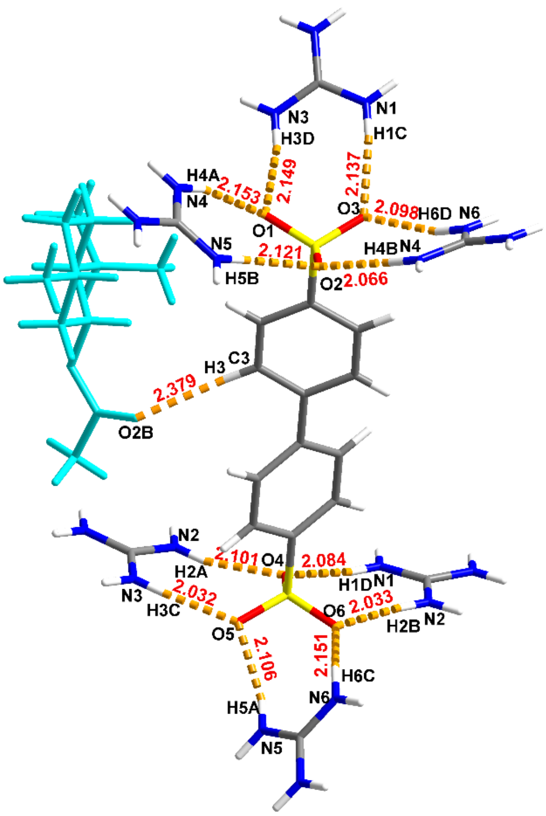

Figure S8c N–H ··O and C–H ··O hydrogen bonds in GBPS ⊃ **8**

3. Supplementary Tables

Table S1. C-H···π intermolecular interactions in host-guest complexes

Host-Guest	X-H···Cg	H···Cg(Å)	X-H···Cg(°)	X···Cg(Å)
GBPS⊃1	C_{15}-H_{15}A···Cg1 [a]	2.68	145	3.51(4)

Symmetry codes: [a] X,Y,Z; Cg3 is the centroid of C1, C2, C3, C4, C5 and C6;

Host-Guest	X-H···Cg	H···Cg(Å)	X-H···Cg(°)	X···Cg(Å)
GBPS⊃2	C_3A-H_3A···Cg1 [a]	2.95	118	3.50(16)
	C_{13}-H_{13}···Cg2 [b]	2.84	151	3.71(4)
	C_{15}-H_{15}B···Cg2 [c]	2.95	141	3.76(4)

Symmetry codes: [a] 1-X,3-Y,1-Z; [b] -X,2-Y,1-Z; [c] -1+X,-1+Y,Z;Cg1 is the centroid of C7, C8, C9, C10, C11 and C13; Cg2 is the centroid of C1, C2, C3, C4, C5 and C6.

Host-Guest	X-H···Cg	H···Cg(Å)	X-H···Cg(°)	X···Cg(Å)
GBPS⊃3	C_3-H_3···Cg4 [b]	2.93	147	3.74(4)
	C_9B-H_9BA···Cg1 [a]	2.86	136	3.62(5)
	C_{12}A-H_{12}F···Cg1 [c]	2.95	116	3.48(5)

Symmetry codes: [a] X,Y,Z; [b] -1/2+X,3/2-Y,1-Z; [c] 1-X,1-Y,1-Z; Cg1 is the centroid of C1, C2, C3, C4, C5 and C6. Cg4 is the centroid of C1B, C2B, C3B, C4B, C5B and C6B.

Host-Guest	X-H···Cg	H···Cg(Å)	X-H···Cg(°)	X···Cg(Å)
GBPS⊃4	C_3-H_3···Cg2 [a]	2.83	136	3.56(5)
	C_6B-H_6B···Cg2	2.73	137	3.47(9)

Symmetry codes: [a] -1+X,Y,Z; Cg2 is the centroid of C1A, C2A, C3A, C4A, C5A and C6A.

Host-Guest	X-H···Cg	H···Cg(Å)	X-H···Cg(°)	X···Cg(Å)
GBPS⊃5	C_{19}-H_{19}···Cg2 [a]	2.68	149	3.53(19)

symmetry codes: [a] 1-X,1-Y,1-Z; Cg2 is the centroid of C7, C8, C9, C10, C11 and C12.

Host-Guest	X-H···Cg	H···Cg(Å)	X-H···Cg(°)	X···Cg(Å)
GBPS⊃6	C_5B-H_5B···Cg1 [a]	2.95	118	3.50(16)
	C_7-H_7···Cg2 [b]	2.84	151	3.71(4)
	C_9-H_9B···Cg2 [c]	2.95	141	3.76(4)

Symmetry codes: [a] 1-X,3-Y,1-Z; [b] -X,2-Y,1-Z; [c] -1+X,-1+Y,Z;Cg1 is the centroid of C1, C2, C3, C4, C5 and C6; Cg2 is the centroid of C1A, C2A, C3A, C4A, C5A and C6A.

Host-Guest	X-H···Cg	H···Cg(Å)	X-H···Cg(°)	X···Cg(Å)
GBPS⊃7	C_5-H_5···Cg3 [a]	2.79	142	3.59(4)

symmetry codes: [a] -1/2+X,-Y,Z; Cg2 is the centroid of C15, C16, C17, C18, C19 and C20.

Host-Guest	X-H ··Cg	H ··Cg(Å)	X-H ··Cg(°)	X ··Cg(Å)
GBPS⊃8	C_8A-H_8AB ··Cg2 [a]	2.98	122	3.59(5)
	C_8B-H_8BA ··Cg1 [b]	2.70	154	3.58(4)

symmetry codes: [a] 1-X,-1/2+Y,3/2-Z; [b] X,-1+Y, Z; Cg1 is the centroid of C1, C2, C3, C4, C5 and C6; Cg2 is the centroid of C7, C8, C9, C10, C11 and C12.

Table S2. Geometric parameters of the N–H···O, O–H···O, C–H···N and C–H···O hydrogen bonding interactions in the co-crystals

Host-Guest complexes	**Interactions**	**D−H (Å)**	**D ··A (Å)**	**H ··A (Å)**	**D-H ··A (deg)**	**Symmetry code**
GBPS⊃**1**	N_1-H_1A ··O_3	0.86	1.99	2.85(5)	172	x, y, z
	N_1-H_1B ··O_1	0.86	2.16	2.99(5)	166	x,1+y,z
	N_2-H_2B ··O_3	0.86	2.02	2.84(5)	160	-1+x,y,z
	N_2-H_2C ··O_2	0.86	2.08	2.93(5)	168	x, y, z
	N_3-H_3B ··O_1	0.86	2.49	3.09(5)	127	-1+x,1+y,z
	N_3-H_3C ··O_2	0.86	2.09	2.93(5)	163	x,1+y,z
GBPS⊃**2**	N_1-H_1A ··O_1	0.88	2.07	2.93(4)	164	x, y, z
	N_1-H_1B ··O_3	0.88	2.36	2.99(4)	130	1+x,y,z
	N_2-H_2B ··O_2	0.88	1.98	2.85(4)	172	x,1+y,z
	N_2-H_2C ··O_3	0.88	2.09	2.96(4)	169	x, y, z
	N_3-H_3B ··O_1	0.88	2.08	2.94(4)	166	x,1+y,z
	N_3-H_3C ··O_2	0.88	2.02	2.86(4)	159	1+x,1+y,z
	C_{17}-H_{17}C ··N_1	0.98	2.44	3.40(3)	164	-1+x,-1+y,z
	C_{17}-H_{17}C ··N_2	0.98	2.32	3.09(2)	135	-1+x,-1+y,z
	C_{17}-H_{17}C ··N_3	0.98	2.47	3.26(2)	137	-1+x,-1+y,z
GBPS⊃**3**	N_1-H_1A ··O_2	0.86	2.11	2.93(4)	160	x, y, z
	N_1-H_1B ··O_1	0.86	2.06	2.92(4)	175	-1/2+x,y,1/2-z
	N_2-H_2C ··O_4	0.86	2.06	2.91(4)	171	-1/2+x,3/2-y,1-z
	N_2-H_2D ··O_3	0.86	2.00	2.86(4)	170	-1/2+x,y,1/2-z
	N_3-H_3C ··O_6	0.86	2.09	2.92(4)	163	-1/2+x,3/2-y,1-z
	N_3-H_3D ··O_3	0.86	2.06	2.88(4)	159	x, y, z
	N_4-H_4A ··O_2	0.86	2.05	2.85(4)	155	1-x,1-y,1-z
	N_4-H_4B ··O_5	0.86	2.05	2.86(4)	157	x, y, z
	N_5-H_5C ··O_1	0.86	2.05	2.91(4)	172	1-x,1-y,1-z
	N_5-H_5D ··O_5	0.86	1.99	2.84(4)	169	-1/2+x,y,3/2-z
	N_6-H_6A ··O_4	0.86	2.13	2.93(4)	155	x, y, z
	N_6-H_6B ··O_6	0.86	2.44	2.93(4)	117	-1/2+x,y,3/2-z
	C_{11}-H_{11} ··O_2A	0.93	2.52	3.34(5)	148	x, y, z
GBPS⊃**4**	N_1-H_1A ··O_1	0.86	2.02	2.86(4)	165	x, y, z
	N_1-H_1B ··O_3	0.86	2.02	2.86(4)	166	1+x,y,z
	N_2-H_2C ··O_3	0.86	2.04	2.87(4)	162	1/2-x,1/2+y,1/2-z

	N_2-H_2D ··O_2	0.86	2.26	3.06(4)	154	1+x,y,z
	N_3-H_3C ··O_1	0.86	2.04	2.89(4)	172	1/2-x,1/2+y,1/2-z
	N_3-H_3D ··O_2	0.86	2.14	2.99(4)	169	x, y, z
GBPS⊃**5**	N_1-H_1A ··O_6	0.86	2.10	2.96(18)	172	1-x,1-y,1-z
	N_1-H_1B ··O_3	0.86	2.52	3.03(17)	118	1-x,1-y,2-z
	N_2-H_2A ··O_6	0.86	2.07	2.92(18)	169	2-x,1-y,1-z
	N_2-H_2B ··O_1	0.86	2.05	2.87(19)	158	x, y, z
	N_3-H_3A ··O_5	0.86	2.07	2.93(18)	176	2-x,1-y,1-z
	N_3-H_3B ··O_4	0.86	2.08	2.93(18)	170	1-x,1-y,1-z
	N_4-H_4A ··O_2	0.86	2.09	2.95(18)	173	1-x,2-y,1-z
	N_4-H_4B ··O_4	0.86	2.04	2.90(19)	174	x, y, z
	N_5-H_5A ··O_3	0.86	2.16	3.05(19)	177	2-x,2-y,1-z
	N_5-H_5B ··O_1	0.86	2.08	2.92(18)	165	1-x,2-y,1-z
	N_6-H_6A ··O_2	0.86	2.05	2.90(17)	167	2-x,2-y,1-z
	N_6-H_6B ··O_5	0.86	2.13	2.97(19)	163	x, y, z
GBPS⊃**6**	N_1-H_1A ··O_7	0.86	2.14	2.87(18)	143	x, y, z
	N_1-H_1B ··O_2	0.86	1.99	2.85(17)	172	x, y, z
	N_2-H_2A ··O_1	0.86	2.02	2.87(17)	174	x,y,1+z
	N_2-H_2B ··O_3	0.86	2.06	2.92(16)	177	x, y, z
	N_3-H_3A ··O_2	0.86	2.07	2.92(17)	171	x,y,1+z
	N_3-H_3B ··O_7	0.86	2.19	2.92(19)	144	x, y, z
	N_4-H_4A ··O_6	0.86	1.98	2.84(17)	176	x, y, z
	N_4-H_4B ··O_1	0.86	2.04	2.89(16)	169	x,1+y,1+z
	N_5-H_5A ··O_3	0.86	2.21	2.94(16)	142	x,1+y,1+z
	N_5-H_5B ··O_6	0.86	2.29	2.89(16)	127	x,y,1+z
	N_6-H_6A ··O_5	0.86	1.99	2.83(15)	165	x, y, z
	N_6-H_6B ··O_4	0.86	2.02	2.87(15)	171	x,y,1+z
	O_7-H_7 ··O_4	0.82	1.99	2.76(16)	154	x, y, z
GBPS⊃**7**	N_1-H_1A ··O_6	0.86	2.40	3.13(4)	143	-1/2+x,-1/2+y,-1/2+z
	N_1-H_1A ··O_5	0.86	2.36	3.06(4)	138	x,-3/2-y,-1/2+z
	N_1-H_1B ··O_5	0.86	2.13	2.97(4)	165	1/2+x,-1/2+y,-1/2+z
	N_2-H_2A ··O_1W	0.86	2.04	2.83(4)	152	x, y, z
	N_2-H_2B ··O_4	0.86	2.06	2.89(4)	162	1/2+x,-1/2+y,-1/2+z
	N_3-H_3A ··O_6	0.86	2.13	2.93(4)	155	-1/2+x,-1/2+y,-1/2+z
	N_3-H_3B ··O_1W	0.86	2.21	2.95(4)	144	x, y, z
	N_4-H_4A ··O_2W	0.86	2.28	3.01(5)	143	x, y, z
	N_4-H_4B ··O_2	0.86	2.07	2.89(5)	159	1/2+x,-1/2+y,1/2+z
	N_5-H_5A ··O_1	0.86	2.17	3.01(5)	167	-1/2+x,-1/2+y,1/2+z
	N_5-H_5B ··O_2	0.86	2.50	3.23(5)	140	1/2+x,-1/2+y,1/2+z
	N_5-H_5B ··O_1	0.86	2.31	3.02(4)	140	x,-3/2-y,1/2+z
	N_6-H_6A ··O_2W	0.86	2.02	2.82(5)	154	x, y, z
	N_6-H_6B ··O_3	0.86	2.03	2.87(4)	166	-1/2+x,-1/2+y,1/2+z
	O_1W-H_1WA ··N_2	0.85	2.13	2.83(4)	138	

	O_1W-$H_1WA \cdot\cdot N_3$	0.85	2.31	2.95(4)	133	x, y, z
	O_1W-$H_1WB \cdot\cdot O_2$	0.85	1.97	2.76(4)	155	x, y, z
	O_2W-$H_2WA \cdot\cdot O_3$	0.79	2.02	2.80(4)	166	x,-1/2-y,1/2+z
	O_2W-$H_2WB \cdot\cdot O_6$	0.74	2.08	2.79(4)	161	x, y, z
	C_2-$H_2 \cdot\cdot O_5$	0.95	2.46	3.41(4)	174	1/2+x,-1-y,z
GBPS⊃**8**	N_1-$H_1C \cdot\cdot O_3$	0.86	2.14	2.99(4)	171	x,-1+y,z
	N_1-$H_1D \cdot\cdot O_4$	0.86	2.08	2.93(4)	169	3/2-x,1-y,-1/2+z
	N_2-$H_2A \cdot\cdot O_4$	0.86	2.10	2.94(3)	166	2-x,-1/2+y,3/2-z
	N_2-$H_2B \cdot\cdot O_6$	0.86	2.03	2.89(4)	172	3/2-x,1-y,-1/2+z
	N_3-$H_3C \cdot\cdot O_5$	0.86	2.03	2.89(3)	176	2-x,-1/2+y,3/2-z
	N_3-$H_3D \cdot\cdot O_1$	0.86	2.15	2.96(4)	157	x,-1+y,z
	N_4-$H_4A \cdot\cdot O_1$	0.86	2.15	2.99(4)	164	x, y, z
	N_4-$H_4B \cdot\cdot O_2$	0.86	2.07	2.93(3)	178	1/2+x,3/2-y,1-z
	N_5-$H_5A \cdot\cdot O_5$	0.86	2.11	2.92(4)	158	3/2-x,1-y,-1/2+z
	N_5-$H_5B \cdot\cdot O_2$	0.86	2.12	2.96(4)	163	x, y, z
	N_6-$H_6C \cdot\cdot O_6$	0.86	2.15	2.94(4)	152	3/2-x,1-y,-1/2+z
	N_6-$H_6D \cdot\cdot O_3$	0.86	2.10	2.94(3)	165	1/2+x,3/2-y,1-z
	C_3-$H_3 \cdot\cdot O_2B$	0.93	2.38	3.26(5)	159	2-x,1/2+y,3/2-z

4. Guest volume calculations

The volume of guests were performed at 6-311++G(d, p) level using the Gaussian 09 program.[1] The length and width of the guests and host are measured by diamond.

Cartesian coordinates (Å) for the optimized geometries of **1**

C	-1.90210000	-0.35830000	0.00080000
C	-0.55340000	-0.28440000	0.00050000
C	0.16800000	0.85310000	0.00040000
C	-0.53460000	1.99740000	0.00060000
C	-1.87350000	1.96310000	0.00080000
C	-2.57490000	0.81610000	0.00100000
O	-3.93080000	0.91440000	0.00100000
O	-2.42680000	-1.63310000	0.00080000
C	1.51610000	0.78950000	0.00020000
C	2.38690000	1.81360000	0.00000000
C	3.88400000	1.63310000	-0.00030000
C	-3.80940000	-1.88380000	0.00040000
H	-0.01790000	-1.25160000	0.00040000
H	-0.05550000	2.98840000	0.00050000
H	-2.42480000	2.92000000	0.00080000
H	-4.32560000	0.03370000	-0.00140000
H	1.98390000	-0.21140000	0.00010000

H	2.05360000	2.86310000	0.00010000
H	4.19160000	0.56380000	-0.00030000
H	4.32530000	2.11310000	-0.90340000
H	4.32560000	2.11310000	0.90270000
H	-3.94970000	-2.98840000	0.00070000
H	-4.27510000	-1.48980000	0.93100000
H	-4.27430000	-1.49060000	-0.93100000

Cartesian coordinates (Å) for the optimized geometries of **2**

C	-2.02270000	-0.53480000	-1.11620000
C	-1.48970000	-1.66540000	-0.21880000
C	0.04430000	-1.73710000	-0.27130000
C	0.67220000	-0.39270000	0.13330000
C	0.14330000	0.72740000	-0.76550000
C	-1.38230000	0.80610000	-0.71750000
O	0.67970000	1.96130000	-0.34860000
C	-3.55630000	-0.45460000	-1.04940000
C	2.19110000	-0.44140000	0.15790000
C	2.87700000	-0.08560000	1.25700000
C	2.91780000	-0.88000000	-1.09180000
H	-1.73460000	-0.76050000	-2.17410000
H	-1.81820000	-1.49380000	0.83330000
H	-1.92160000	-2.64260000	-0.54150000
H	0.40810000	-2.54580000	0.40660000
H	0.34880000	-2.00830000	-1.30920000
H	0.31490000	-0.17080000	1.17000000
H	0.46920000	0.57390000	-1.81950000
H	-1.70960000	1.08070000	0.31290000
H	-1.73640000	1.61410000	-1.40080000
H	0.43320000	2.64260000	-0.97820000
H	-4.02330000	-1.41570000	-1.36430000
H	-3.90390000	-0.22970000	-0.01570000
H	-3.94680000	0.34340000	-1.72140000
H	3.97640000	-0.11070000	1.28230000
H	2.36860000	0.24680000	2.17410000
H	2.68430000	-1.94060000	-1.33280000
H	2.63570000	-0.24550000	-1.96050000
H	4.02330000	-0.81030000	-0.98570000

Cartesian coordinates (Å) for the optimized geometries of **3**

C	-0.20600000	1.34810000	-0.46270000
C	-0.15460000	0.02870000	-0.15540000
C	1.03850000	-0.48450000	0.21010000

C	2.17090000	0.23660000	0.26580000
C	2.10620000	1.53270000	-0.07070000
C	0.93170000	2.06700000	-0.42800000
C	3.47820000	-0.40570000	0.67390000
C	4.01900000	-1.22580000	-0.46880000
C	4.16780000	-2.55730000	-0.42790000
O	-1.31500000	-0.70660000	-0.22380000
C	-1.31560000	-2.04940000	0.19870000
O	-1.36800000	1.97630000	-0.83800000
C	-2.46180000	1.76810000	-0.04860000
C	-3.67430000	1.42120000	-0.89140000
O	-2.46210000	1.86690000	1.15900000
H	1.13030000	-1.54890000	0.47570000
H	3.01140000	2.16130000	-0.05420000
H	0.89850000	3.13660000	-0.69780000
H	4.23800000	0.35940000	0.95480000
H	3.31640000	-1.03100000	1.58180000
H	4.29370000	-0.68280000	-1.38960000
H	4.56210000	-3.11120000	-1.29390000
H	3.89920000	-3.13660000	0.46800000
H	-2.35510000	-2.43440000	0.09740000
H	-0.65640000	-2.66230000	-0.45550000
H	-1.02320000	-2.11750000	1.27020000
H	-3.49090000	0.50020000	-1.48950000
H	-4.56210000	1.23870000	-0.24490000
H	-3.91530000	2.26100000	-1.58180000

Cartesian coordinates (Å) for the optimized geometries of **4**

C	0.92610000	-0.01030000	-0.00030000
C	0.23420000	1.14540000	-0.00040000
C	-1.10730000	1.16090000	-0.00060000
C	-1.84710000	0.03640000	-0.00070000
C	-1.14800000	-1.11520000	-0.00050000
C	0.19530000	-1.14050000	-0.00040000
C	2.27500000	0.02840000	-0.00010000
C	3.12790000	-1.01050000	0.00000000
C	4.62790000	-0.85550000	0.00020000
O	-3.21740000	0.14220000	-0.00090000
C	-3.98790000	-1.03730000	-0.00030000
H	0.75500000	2.11900000	-0.00030000
H	-1.62680000	2.13500000	-0.00070000
H	-1.66640000	-2.08750000	-0.00060000
H	0.66870000	-2.13500000	-0.00020000
H	2.75880000	1.02180000	-0.00010000

H	2.77650000	-2.05410000	0.00000000
H	4.95370000	0.20840000	0.00020000
H	5.06100000	-1.34290000	0.90340000
H	5.06120000	-1.34290000	-0.90280000
H	-5.06120000	-0.74230000	-0.00030000
H	-3.79080000	-1.62890000	-0.92200000
H	-3.79060000	-1.62810000	0.92200000

Cartesian coordinates (Å) for the optimized geometries of **5**

C	1.91980000	0.02630000	-0.00030000
C	1.20360000	1.16400000	-0.00040000
C	-0.13760000	1.12160000	-0.00070000
C	-0.83110000	-0.03330000	-0.00090000
C	-0.09290000	-1.16140000	-0.00070000
C	1.25010000	-1.13950000	-0.00040000
C	3.27990000	0.06470000	-0.00010000
O	4.01550000	-0.89790000	0.00010000
O	-2.20460000	0.02180000	-0.00110000
C	-2.93230000	-1.18450000	-0.00030000
H	1.69510000	2.15200000	-0.00030000
H	-0.69660000	2.07360000	-0.00070000
H	-0.57510000	-2.15200000	-0.00080000
H	1.78150000	-2.10630000	-0.00030000
H	3.72690000	1.08730000	0.00010000
H	-4.01550000	-0.92810000	-0.00030000
H	-2.71410000	-1.76870000	-0.92200000
H	-2.71390000	-1.76760000	0.92200000

Cartesian coordinates (Å) for the optimized geometries of **6**

C	-1.05790000	-1.86570000	0.00040000
C	0.27970000	-1.79050000	0.00060000
C	0.90070000	-0.59990000	0.00500000
C	0.09350000	0.47470000	0.00920000
C	-1.25670000	0.43320000	0.00960000
C	-1.86220000	-0.78280000	0.00410000
O	-3.23290000	-0.88490000	0.00450000
C	2.24940000	-0.55670000	0.00520000
C	3.04010000	0.53040000	0.00950000
C	4.54650000	0.46310000	0.00960000
O	-1.87820000	1.66600000	0.01370000
C	-3.27870000	1.79610000	0.00170000
C	-3.84940000	-2.15140000	0.00730000
H	-1.47670000	-2.88450000	-0.00330000

H	0.85440000	-2.73340000	-0.00280000
H	0.53320000	1.48510000	0.01280000
H	2.79140000	-1.51950000	0.00150000
H	2.62920000	1.55200000	0.01330000
H	4.93380000	-0.58000000	0.00760000
H	4.95080000	0.97670000	-0.89240000
H	4.95040000	0.97310000	0.91380000
H	-3.51290000	2.88450000	0.00120000
H	-3.70420000	1.36550000	-0.93120000
H	-3.72020000	1.36360000	0.92620000
H	-4.95080000	-1.98970000	0.01040000
H	-3.58880000	-2.71340000	-0.91710000
H	-3.58330000	-2.71180000	0.93120000

Cartesian coordinates (Å) for the optimized geometries of **7**

C	-1.01780000	1.05360000	0.00020000
C	-1.04110000	-0.29120000	0.00020000
C	0.12920000	-0.96450000	0.00030000
C	1.30900000	-0.30900000	0.00030000
C	1.29570000	1.03660000	0.00030000
C	0.14400000	1.72020000	0.00030000
C	-2.37690000	-1.00640000	0.00010000
C	2.66430000	-0.98710000	0.00030000
N	0.08960000	-2.23310000	0.00030000
H	-1.95820000	1.62900000	0.00010000
H	2.24680000	1.59530000	0.00030000
H	0.15220000	2.82310000	0.00030000
H	-3.24230000	-0.30690000	0.00020000
H	-2.48070000	-1.64390000	-0.90730000
H	-2.48080000	-1.64420000	0.90730000
H	2.64160000	-2.09590000	0.00070000
H	3.24200000	-0.68150000	-0.90200000
H	3.24230000	-0.68110000	0.90240000
H	0.95390000	-2.82310000	0.00030000
H	-0.82460000	-2.74570000	0.00020000

Cartesian coordinates (Å) for the optimized geometries of **8**

C	-0.85260000	-0.62000000	-0.57720000
C	0.57590000	-0.65240000	-0.01490000
C	1.33250000	0.65930000	-0.31140000
C	0.50620000	1.84410000	0.23480000
C	-0.90550000	1.89290000	-0.36330000
C	-1.66160000	0.58660000	-0.07280000

C	1.75390000	0.80980000	-1.79900000
O	0.49350000	-0.86800000	1.36670000
C	2.38890000	2.18070000	-2.10590000
C	2.75160000	-0.28250000	-2.23660000
C	1.42110000	-1.56400000	2.08790000
C	2.57980000	-2.17390000	1.31470000
O	1.32870000	-1.70140000	3.29030000
C	-3.06560000	0.61190000	-0.69820000
H	-0.82020000	-0.59820000	-1.69100000
H	-1.38340000	-1.56350000	-0.30430000
H	1.06800000	-1.52720000	-0.48870000
H	2.28950000	0.65380000	0.26860000
H	1.02840000	2.81400000	0.07730000
H	0.41440000	1.75820000	1.34380000
H	-0.84640000	2.06300000	-1.46280000
H	-1.46590000	2.75670000	0.06740000
H	-1.78320000	0.49100000	1.03570000
H	0.85080000	0.71760000	-2.45010000
H	2.77660000	2.22650000	-3.14890000
H	1.65590000	3.01360000	-2.02550000
H	3.24140000	2.39080000	-1.42090000
H	3.08010000	-0.13330000	-3.29030000
H	2.31530000	-1.30400000	-2.20200000
H	3.66350000	-0.27380000	-1.59770000
H	2.23430000	-3.01360000	0.67090000
H	3.13310000	-1.42110000	0.71310000
H	3.32290000	-2.60770000	2.02180000
H	-3.66350000	1.46770000	-0.30960000
H	-3.01240000	0.70950000	-1.80620000
H	-3.62640000	-0.32190000	-0.46500000

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