Supporting information for:

Sulfate-induced large amplitude conformational change in a Solomon link

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Table of contents

1. Methods and general information

Synthesis. The Solomon link was synthesized according to a published procedure[S1] and isolated by reversed-phase flash chromatography as a trifluoroacetate salt (**SL^{8+}·$8CF_3CO_2^-$**). The full characterization of the Solomon link in D_2O can be found in reference S1.

NMR analyses. Spectra were measured using a Bruker Advance III HD-Nanobay 400 MHz spectrometer equipped with a 5-mm Prodigy CryoProbe, or a Bruker Avance III 500 MHz spectrometer equipped with a 5-mm DCH ^{13}C-^{1}H/D helium-cooled cryogenic probe. NMR solvent: CD_3OD (ARMAR Isotopes, Acros Organics). All signals were internally referenced to the solvent residue (CD_3OD: 3.310 ppm).

^{1}H NMR titrations. All the titrations were performed in CD_3OD. Tetrabutylammonium salts were purchased from Fluka (tetrabutylammonium chloride), Acros Organics (tetrabutylammonium bromide, tetrabutylammonium iodide, tetrabutylammonium perchlorate), Sigma-Aldrich (tetrabutylammonium thiocyanate, tetrabutylammonium nitrate, tetrabutylammonium triflate, tetrabutylammonium hexafluorophosphate, tetrabutylammonium perrhenate) and Alfa Aesar (tetrabutylammonium sulfate, 50% w/w aq. soln.).

Mass spectrometry. Mass spectrometry experiments were performed on an Agilent 6560 ESI-IM-QTOF mass spectrometer equipped with AJS ESI ion source. Samples were injected using direct infusion from a syringe pump with a flowrate of 5 µl/min. Nitrogen was used as dry-, sheath and nebulizer gas from nitrogen generator. A dry-gas temperature of 225 º C, drying gas flow rate of 5 l/min, nebulizer pressure of 30 psi, sheath gas temperature of 225 º C and sheath gas flow of 10 l/min were used. Capillary voltage of 2000 V and fragmentation voltage of 400 V were set as source parameters. The mass spectrometer was calibrated with an ES tuning mix from Agilent Technologies. Data was acquired with MassHunter Acquisition B.09.00 and analysed using MassHunter Qualitative analysis B.08.00 as software packages from Agilent Technologies, USA.

In IM-MS experiments both He (5.5) and N_2 (5.0) were used as drift gas. Pressures for drift tube and high-pressure funnel were set as 3.95 and 3.70 Torr (3.80 Torr for N_2), respectively. The drift tube entrance and exit voltages for He measurements (values for N_2 in parenthesis) were set as 875 V and 133 V (1574 V and 224 V). A trap filling time of 5000 µs and trap release time of 350 µs were used. For multi-field measurements, the drift tube entrance voltage was varied from 563 to 875 V with 52 V increments (1074 V to 1674 V with 100 V increments). ES tuning mix was measured as a quality control sample for the collision cross section (CCS) values.[S2,S3]

The stock solution of Solomon link was prepared as 0.5 mM in MeOH. The stock solutions of salts were 1, 2 or 5 mM in MeOH. Samples were prepared with 1 µM host concentration and 1:1 host:guest ratio in methanol. For those experiments, both analytical grade tetrabutylammonium hydrogen sulfate and tetramethylammonium sulfate were used and gave the same results.

Theoretical CCS values were calculated with IMoSSuite 1.12[S4] by using experimental parameters (gas, temperature, and pressure). Coordinates for the calculations were obtained from DFT calculated structures (see sections 10 and 11). Several theoretical approaches were tested: Project approximation (PA), trajectory method with Lennard-Jones parameters (TMLJ), diatomic trajectory method (DTM), and exact hard sphere scattering (EHSS/DHSS). The number of rotations was 3 with 300 000 gas molecules per rotation in all calculations. The best comparison to experimental data was obtained using TMLJ method with helium gas. EHSS and DTM methods with helium also resulted to similar results (error < 3%).

UV-Vis spectroscopy. UV-Vis spectra were measured using a Perkin Elmer Lambda 650 spectrophotometer (2009) with a 1 nm step rate and standard 10 mm quartz cuvettes. Emission spectra were recorded on a Cary Variant Eclipse spectrofluorimeter (2009) with an excitation wavelength of 400 nm.

High-performance liquid chromatography (HPLC). Chromatograms were obtained from Shimadzu LC-20AT liquid chromatograph equipped with an SPD-M10A VP diode array detector, SCL-10A VP system controller, and DGU-14A degasser. XBridge C18 column (3.5-micrometer diameter particle size, 4.6*150 mm) was used for all analytical experiments. 20 microliter aliquots (0.085 mM) were

injected and eluted with H_2O/MeCN solution (TFA 0.1%) in a gradient mode (5-50% of MeCN) within 30 minutes.

Theoretical methods. The geometries included in this study have been fully optimized (no imaginary frequency) at the BP86-D3/def2-TZVP[S5,S6] level of theory with the latest available correction for dispersion (D3)[S7] using the program TURBOMOLE version 7.0.[S8] In order to reproduce solvent effects, we have used the conductor-like screening model COSMO[S9] (which is a variant of the dielectric continuum solvation models)[S10] with the parameters for methanol.

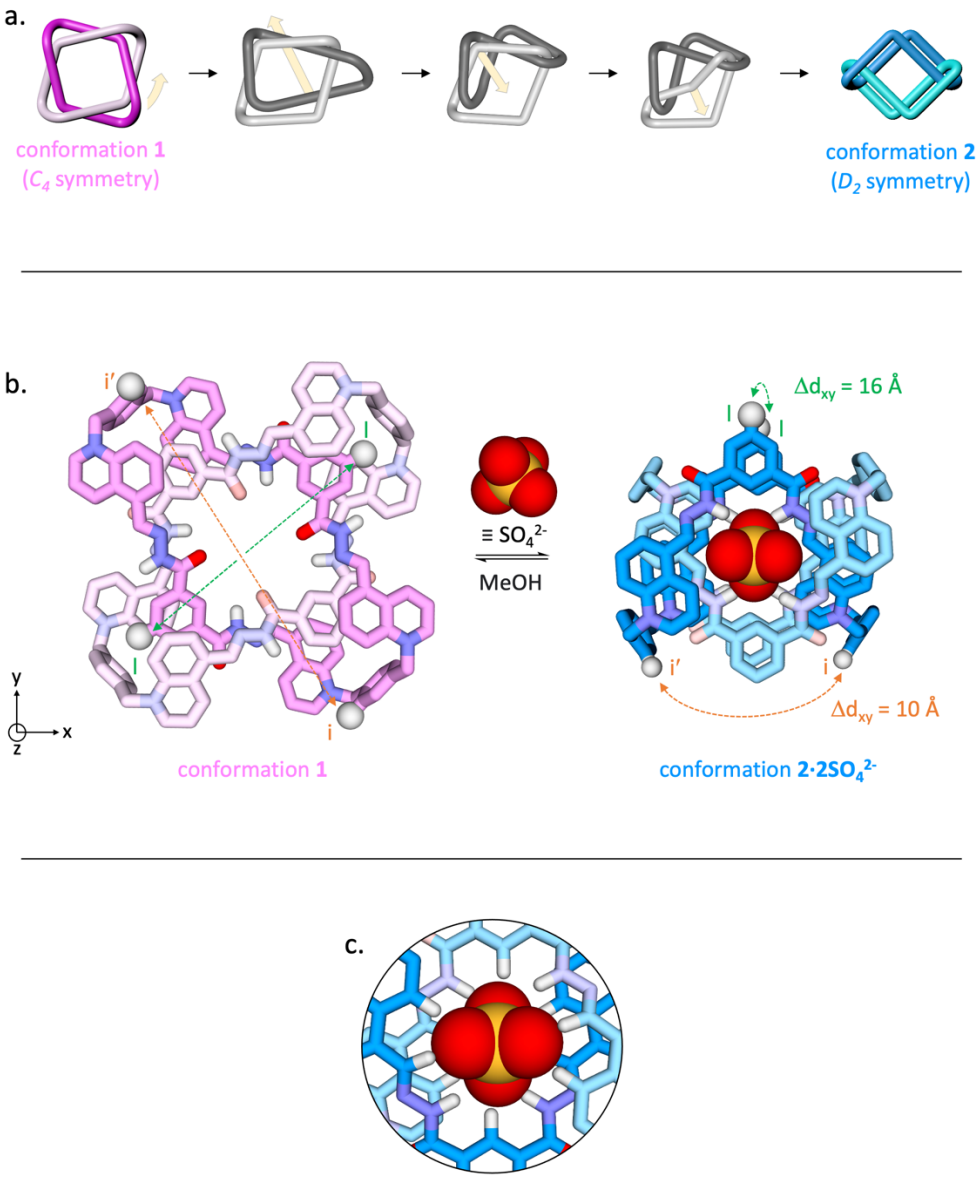


Figure S1. (a) Reidemeister moves allowing the transition between the C_4- and D_2-symmetric conformations of the Solomon link. (b) The conformational transformation significantly changes the relative distance between many atoms of the Solomon link. In this figure, we highlight the change in relative distance between protons i and i′, or between two protons l located on the same macrocycle. (c) Zoom on one of the two binding sites of conformer **2**. One sulfate anion binds in each binding site *via* the formation of four N-H···O-S and ten C-H···O-S hydrogen bonds.

2. NMR characterization of conformer 1 in CD_3OD

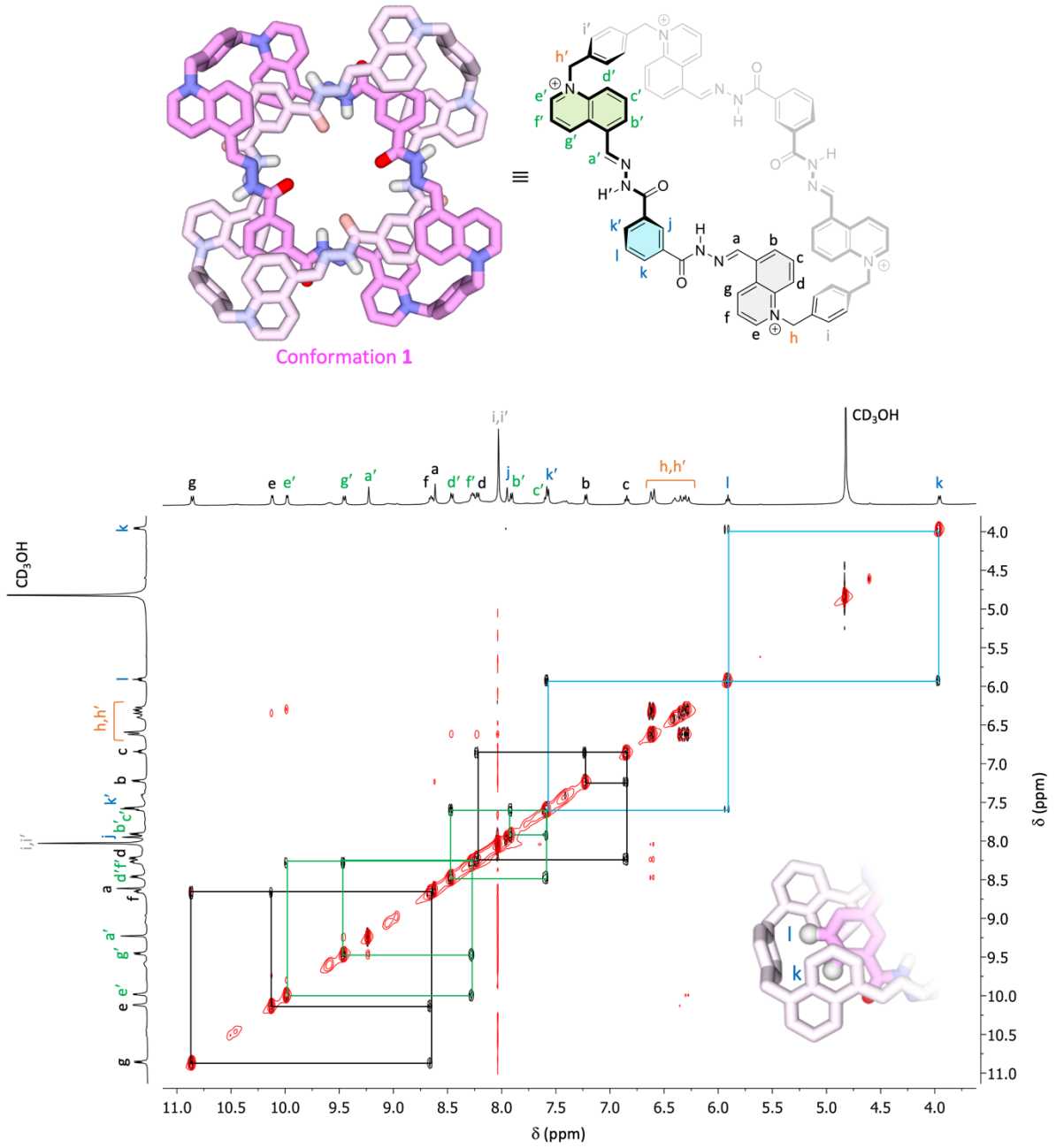


Figure S2. Overlap of the COSY (black) and NOESY (red) spectra of the Solomon link in conformation **1** (0.93 mM in CD_3OD, 298 K, 500 MHz). COSY correlations are highlighted with rectangles. For the NOESY spectrum, d_8 = 300 ms. Protons **k** and **l** are particularly upfield shifted because they face the xylylene units in a T-shape relationship.

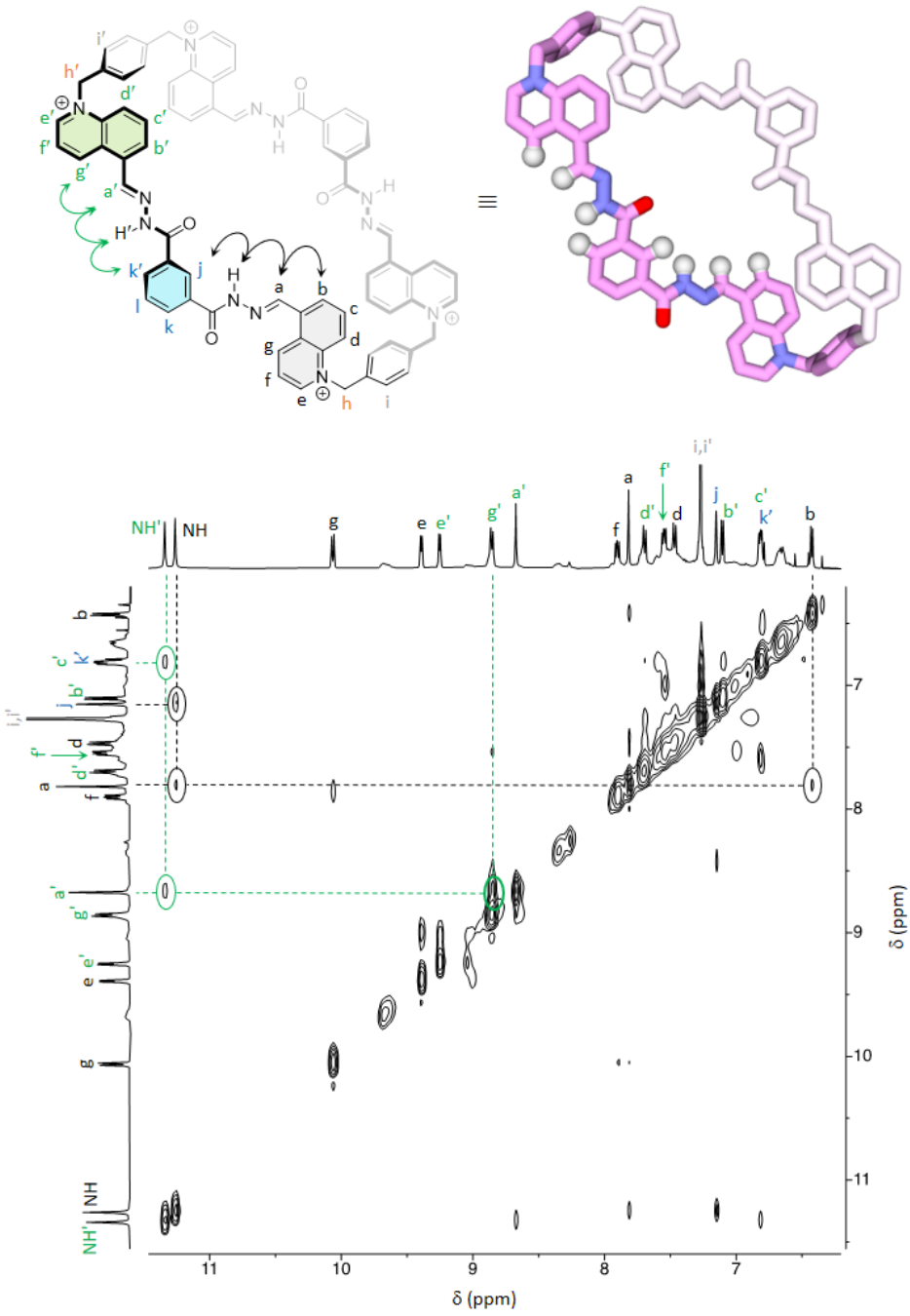


Figure S3. NOESY spectrum of the Solomon link in conformation **1** (0.93 mM in CD_3OH, 298 K, 500 MHz, d_8 = 300 ms). The highlighted NOE correlations were used to determine the conformational state of the acylhydrazone linkages.

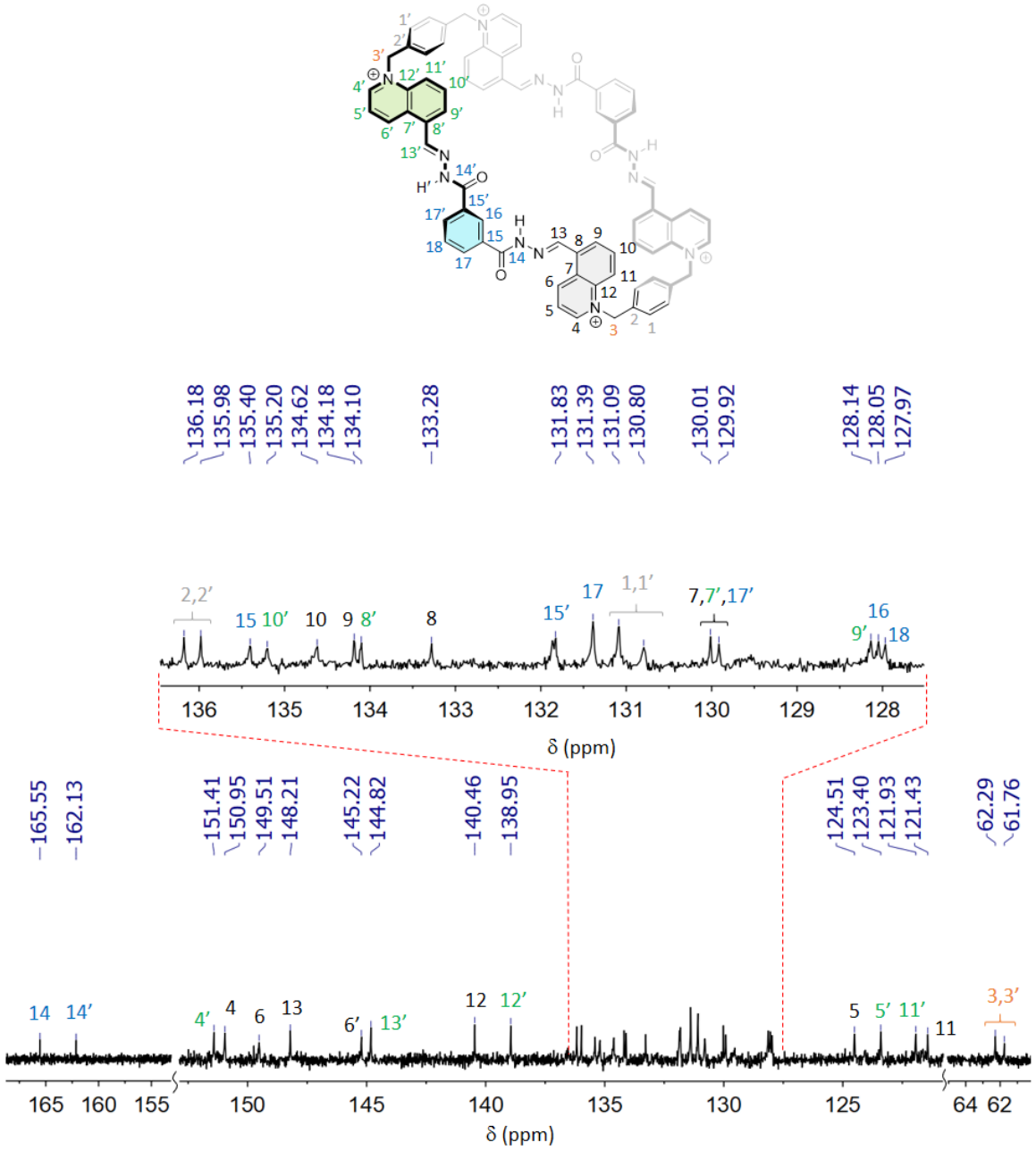


Figure S4. ^{13}C NMR spectrum of the Solomon link in conformation **1** (0.93 mM in CD_3OD, 298 K, 125 MHz).

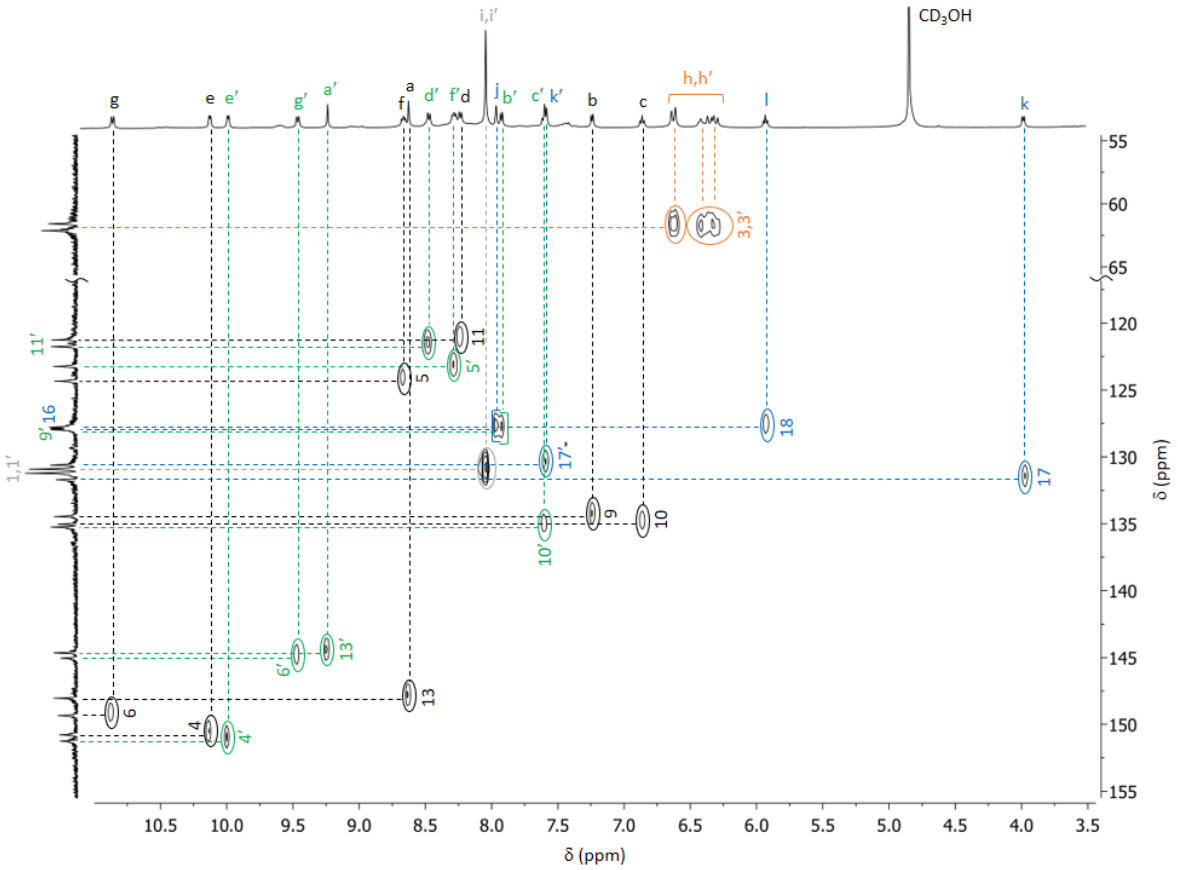


Figure S5. HSQC spectrum of the Solomon link in conformation **1** (0.93 mM in CD_3OD, 298 K, 125 MHz).

3. ^{1}H NMR anion titrations in CD_3OD

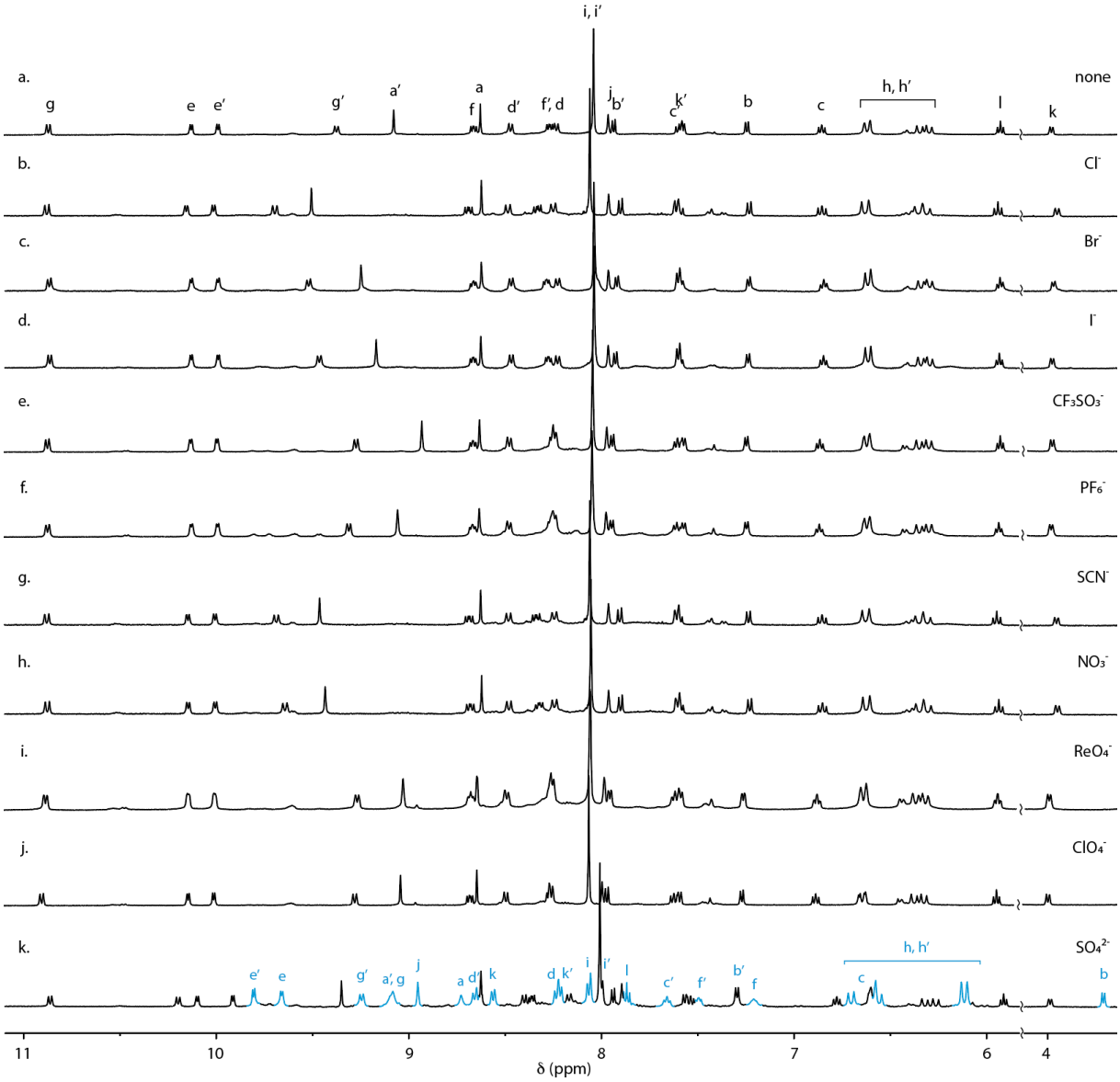


Figure S6. ^{1}H NMR spectra of the Solomon link (0.93 mM in CD_3OD, 298 K, 500 MHz) (a) before and after addition of 2 equiv. of (b) Cl^-, (c) Br^-, (d) I^-, (e) $CF_3SO_3^-$, (f) PF_6^-, (g) SCN^-, (h) NO_3^-, (i) ReO_4^-, (j) ClO_4^- and (k) SO_4^{2-}. The signals corresponding to conformers **1** and **2** are coloured in black and blue, respectively. In cases b-j, the Solomon link remains in conformation **1**. The addition of the anions only results in a shift of the protons g′ and a′, indicating an interaction between these anions and the NH′ located on the external surface of the Solomon link (in conformation **1**). In case k, the addition of SO_4^{2-} results in the appearance of conformer **2**.

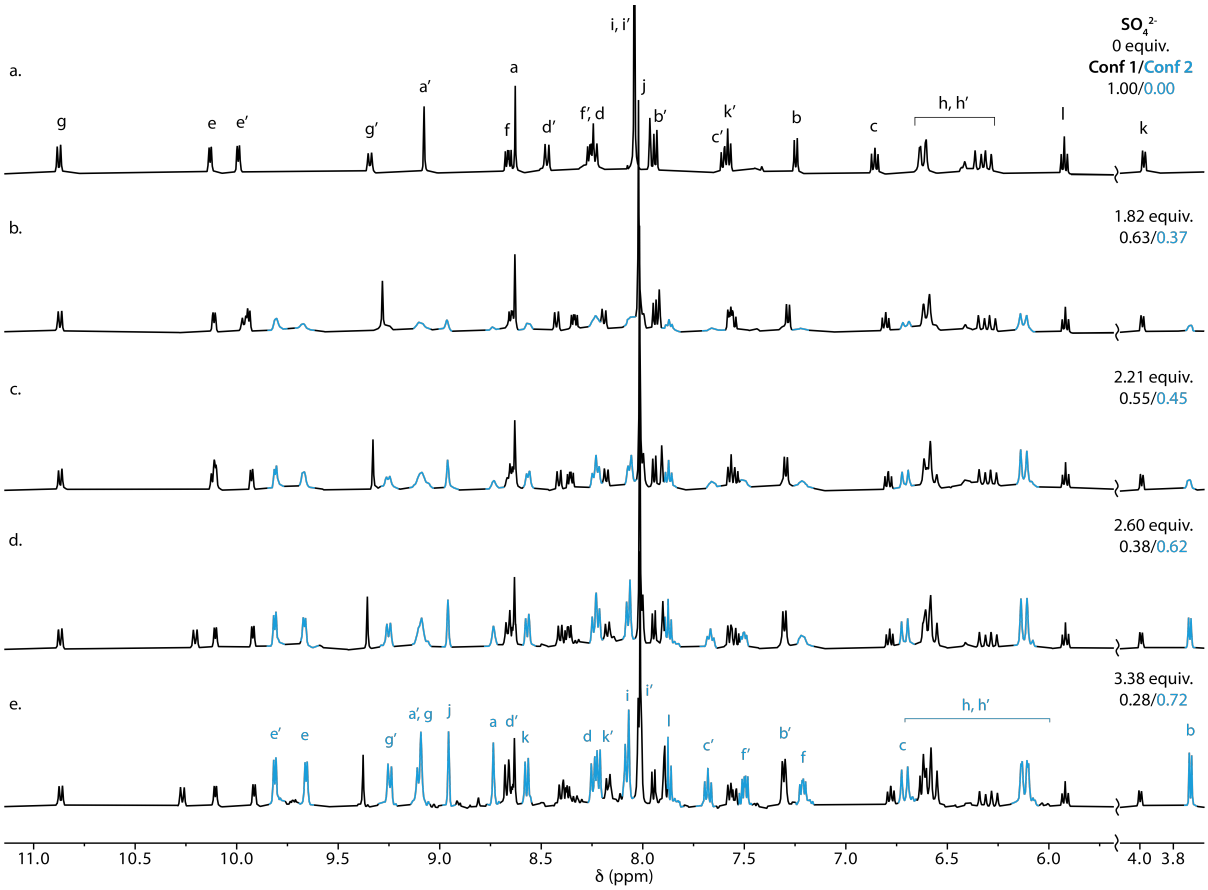


Figure S7. ^{1}H NMR spectra of the Solomon link (0.93 mM in CD_3OD, 298 K, 500 MHz) (a) before and after addition of (b) 1.82 equiv., (c) 2.21 equiv., (d) 2.60 equiv., and (e) 3.38 equiv. of SO_4^{2-}. The signals corresponding to conformers **1** and **2** are coloured in black and blue, respectively.

Table S1. Values used for the Hill plot $\log\theta/(1-\theta) = f(\log[SO_4^{2-}])$ and the speciation curve $\theta = f(\log K'[SO_4^{2-}])$. Values were obtained from the NMR titration of the Solomon link (0.93 mM in CD_3OD) with SO_4^{2-} at 313 K.

log $[SO_4^{2-}]$	log $K'[SO_4^{2-}]$	$\theta = [2]/[SO_4^{2-}]$	$\theta(1-\theta)$	$\log \theta(1-\theta)$
-3.95	-1.05037	0.012	0.01215	-1.91558
-3.79	-0.89037	0.0245	0.02512	-1.60006
-3.65	-0.75037	0.035	0.03627	-1.44046
-3.49	-0.59037	0.06725	0.0721	-1.14207
-3.35	-0.45037	0.095	0.10497	-0.97892
-3.256	-0.35637	0.117	0.1325	-0.87777
-3.18	-0.28037	0.154	0.18203	-0.73985
-3.1	-0.20037	0.2064	0.26008	-0.58489
-3.05	-0.15037	0.26	0.35135	-0.45426
-2.99	-0.09037	0.3262	0.48412	-0.31505
-2.95	-0.05037	0.37	0.5873	-0.23114
-2.9	0	0.43	0.75439	-0.12241
-2.87	0.02963	0.47	0.88679	-0.05218
-2.84	0.05963	0.5345	1.14823	0.06003
-2.78	0.11963	0.6622	1.96033	0.29233
-2.75	0.14963	0.73	2.7037	0.43196
-2.7	0.20963	0.79	3.7619	0.57541
-2.65	0.27963	0.83	4.88235	0.68863
-2.61	0.32963	0.84	5.25	0.72016
-2.57	0.38963	0.85	5.66667	0.75333
-2.5	0.44963	0.86	6.14286	0.78837

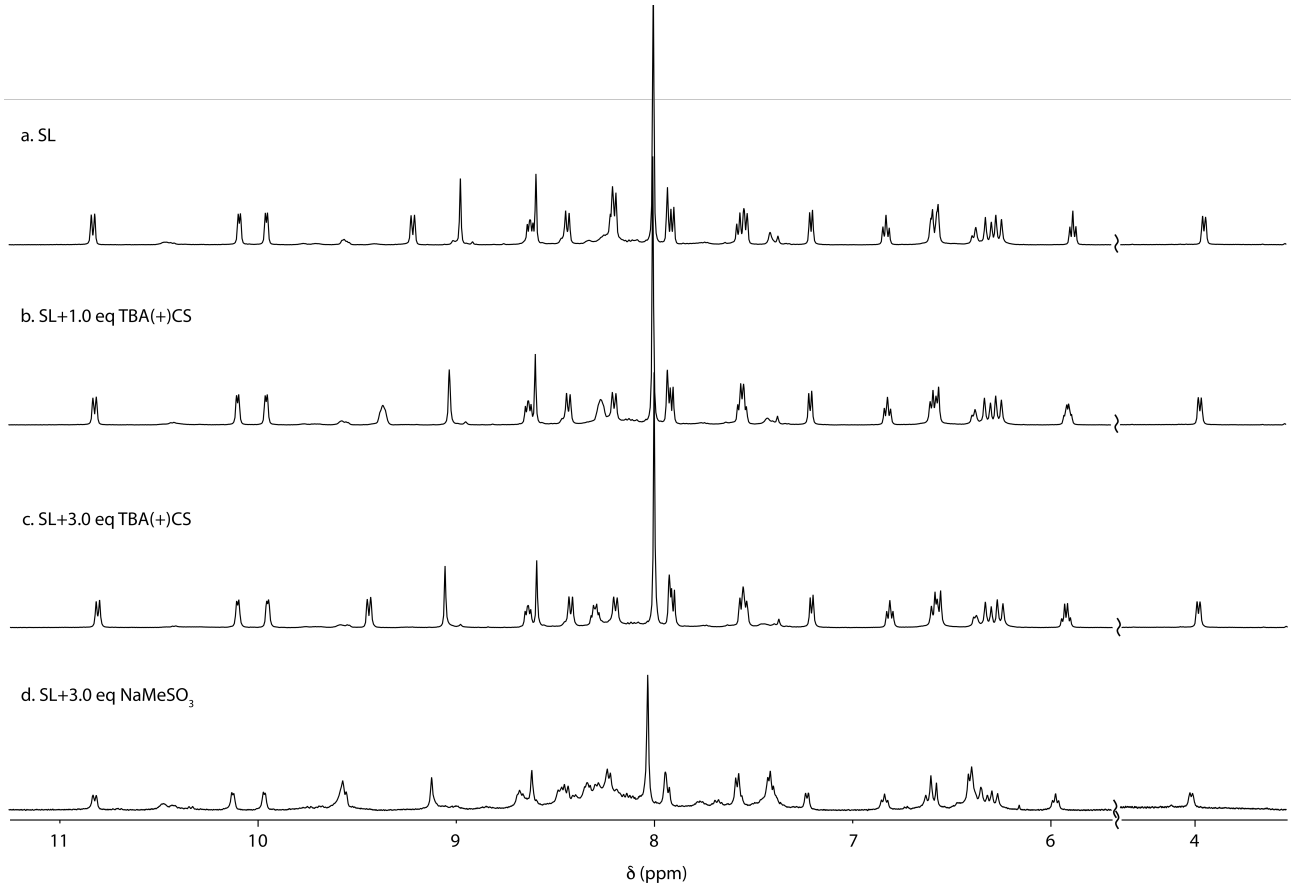


Figure S8. ^{1}H NMR spectra of the Solomon link (0.85 mM in CD_3OD, 303 K, 500 MHz) (a) before and after addition of (b) 1 equiv. of tetrabutylammonium (+)-camphor-10-sulfonate (TBA(+)CS), (c) 3 equiv. of TBA(+)CS, and (d) 3 equiv. of $NaMeSO_3$. No conformational switch was observed upon addition of the two alkane sulfonates.

4. NMR characterization of conformer 2 in CD_3OD

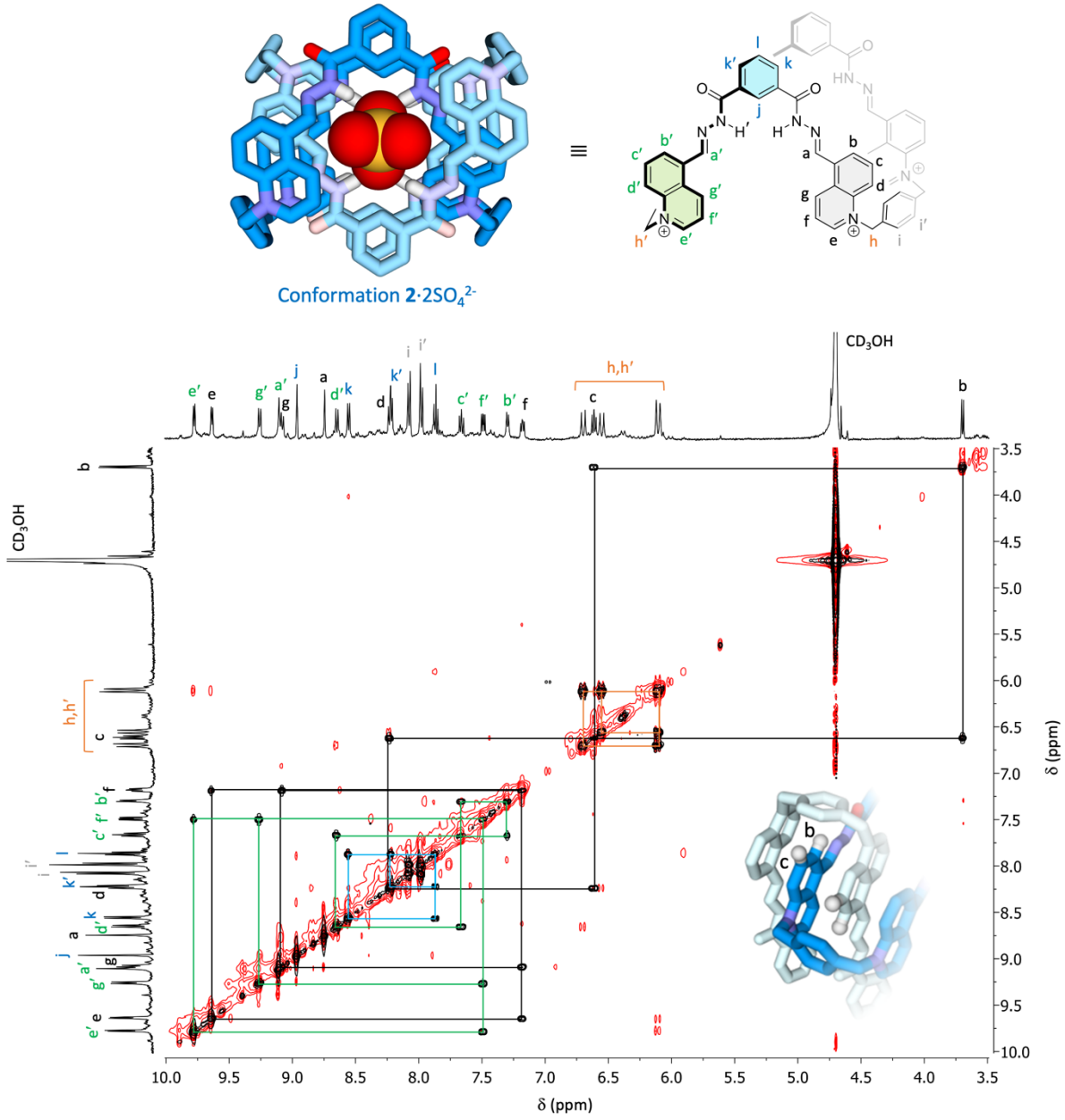


Figure S9. Overlap of the COSY (black) and NOESY (red) spectra of the Solomon link in conformation **2** (0.93 mM in CD_3OD with 2.6 equiv. of SO_4^{2-}, 313 K, 500 MHz). COSY correlations are highlighted with rectangles. For the NOESY spectrum, d_8 = 300 ms. Protons **b** and **c** are particularly upfield shifted because they face the xylylene units in a T-shape relationship.

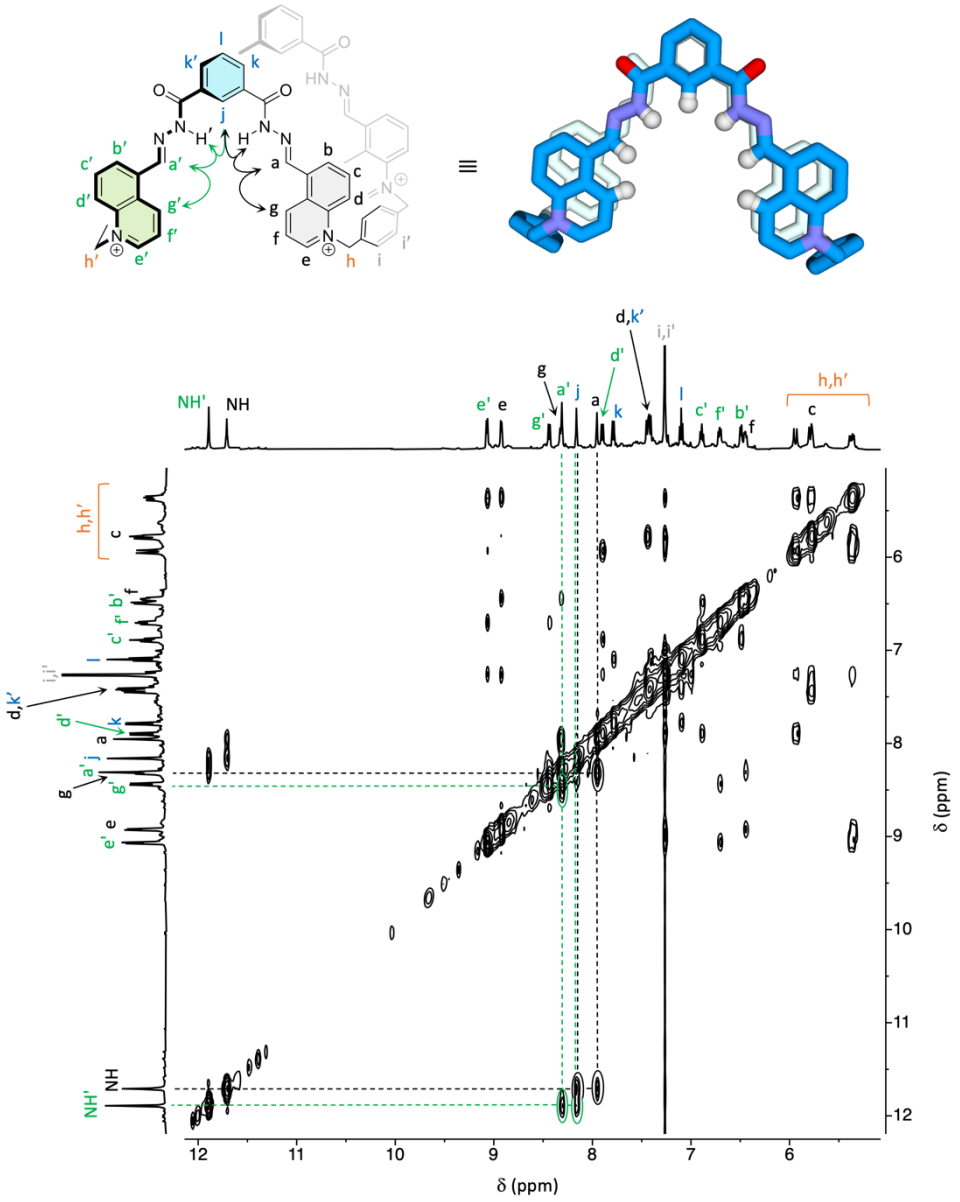


Figure S10. NOESY spectrum of the Solomon link in conformation **2** (0.93 mM in CD_3OD with 2.6 equiv. of SO_4^{2-} at 313 K, 500 MHz, d_8 = 300 ms). The highlighted NOE correlations were used to determine the conformational state of the acylhydrazone linkages.

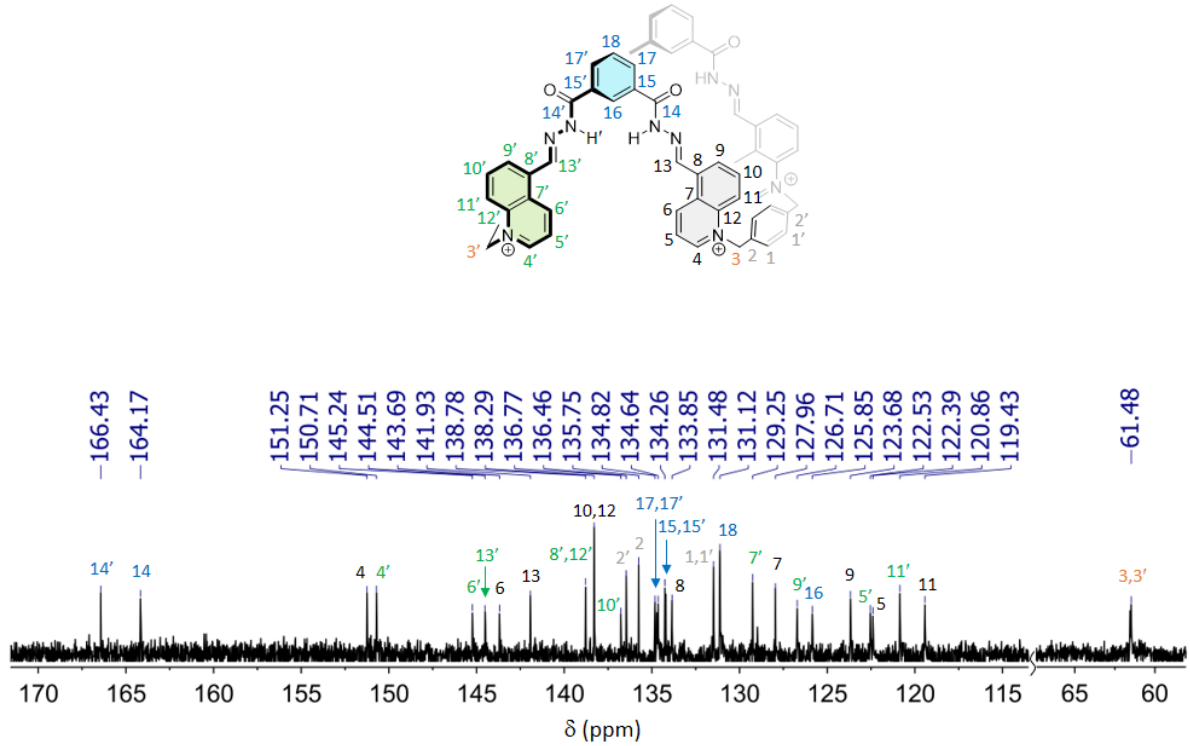


Figure S11. ^{13}C NMR spectrum of the Solomon link in conformation **2** (0.93 mM in CD_3OD with 2.6 equiv. of SO_4^{2-}, 313 K, 125 MHz).

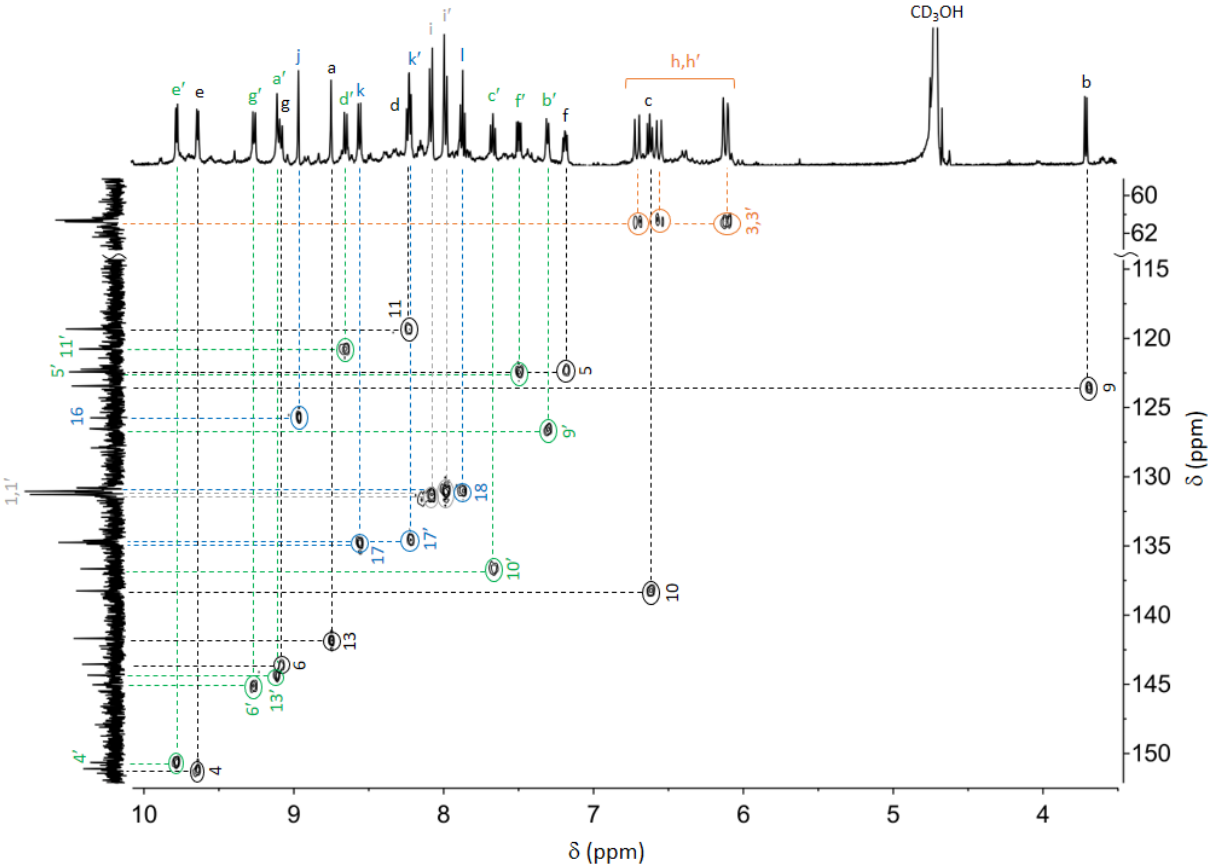


Figure S12. HSQC spectrum of the Solomon link in conformation **2** (0.93 mM in CD_3OD with 2.6 equiv. of SO_4^{2-} at 313 K, 125 MHz).

5. ESI-MS characterisation of the host-guest complexes

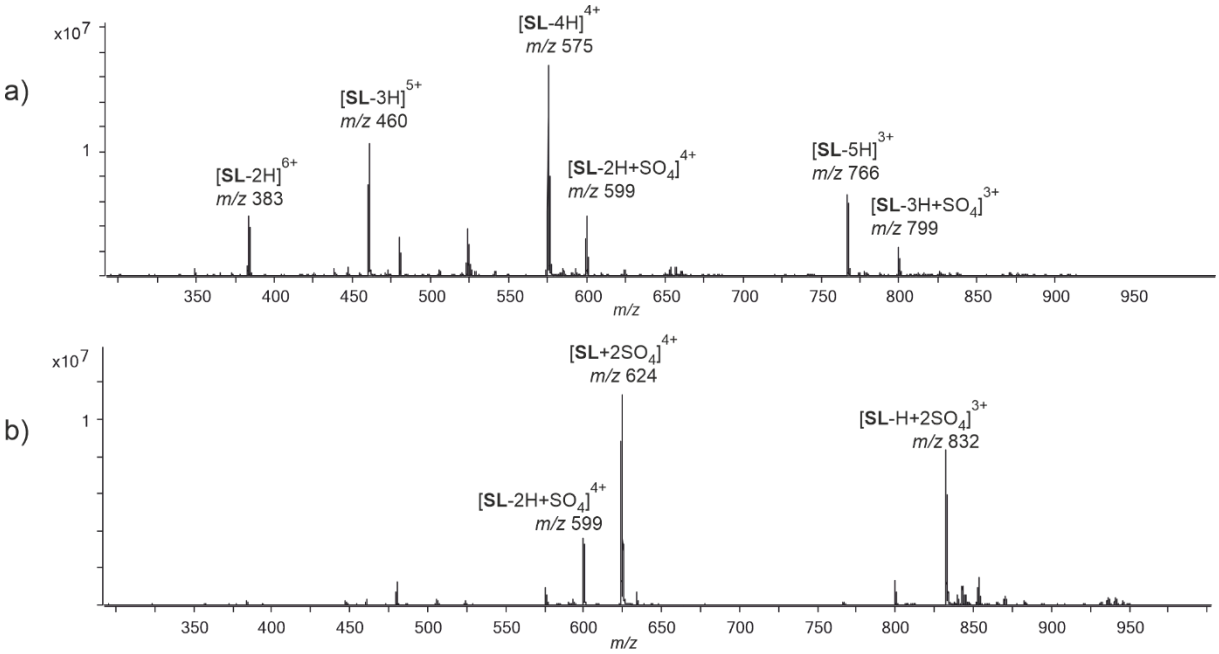


Figure S13. (+)ESI-MS spectra of (a) 1 µM Solomon link in MeOH and (b) Solomon link + $TBAHSO_4$ (both 1 µM, 1:1 ratio) in MeOH. It is interesting to note that sulfate complexes are already present before addition of $TBAHSO_4$ (profile spectrum a): the Solomon link is able to catch trace amounts of sulfate from the environment, showing its high affinity towards sulfate.

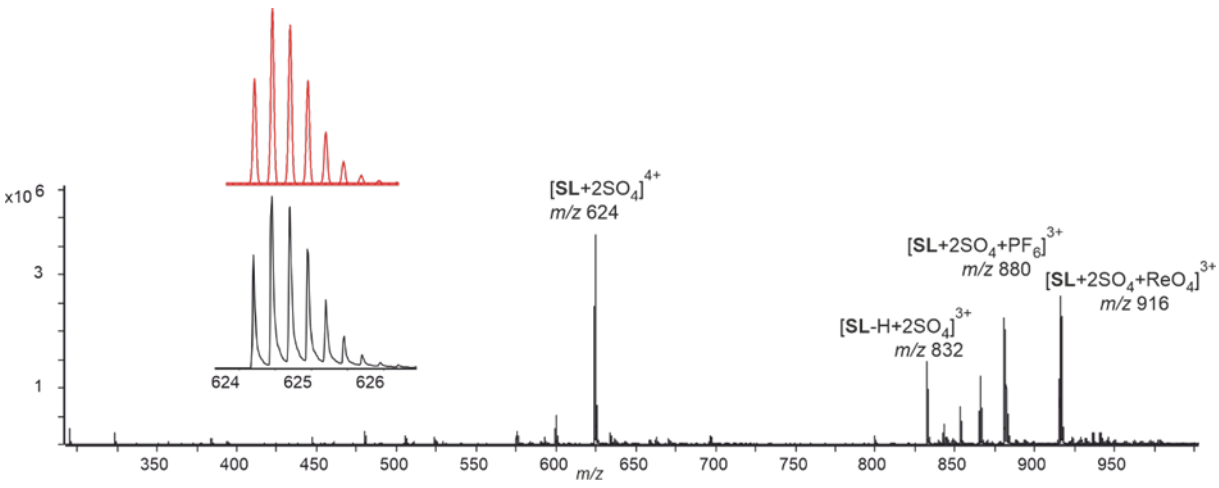


Figure S14. (+)ESI-MS spectrum of the Solomon link with mixed guests $TBAHSO_4$, $TBAClO_4$, $TBAPF_6$, $TBACF_3SO_3$ and $TBAReO_4$. All 1 µM, 1:1:1:1:1:1 molar ratio in methanol. The inset shows the theoretical (red) and experimental (black) isotopic distribution for $[\mathbf{SL}+2SO_4]^{4+}$ ion.

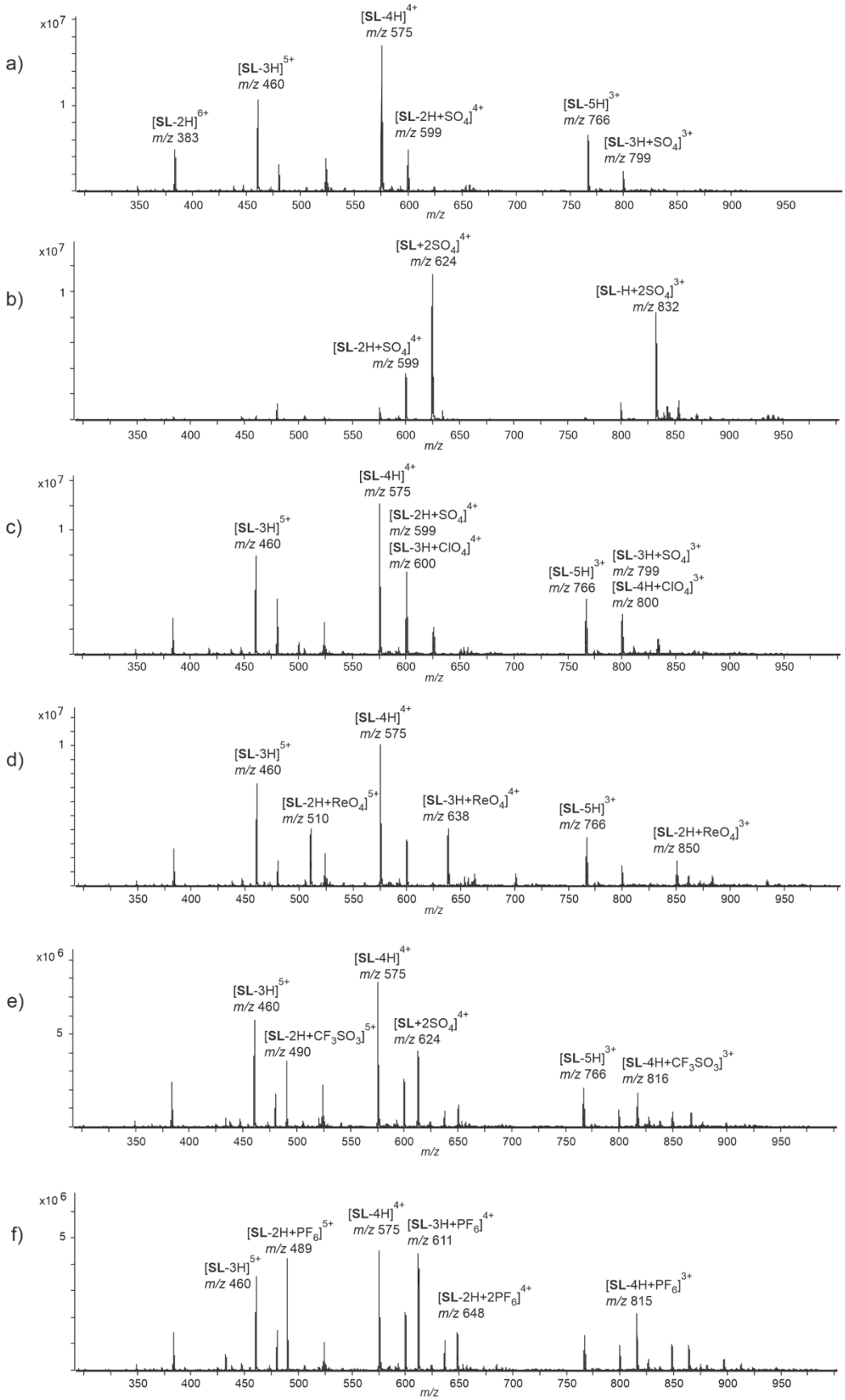


Figure S15. (+)ESI-MS spectra of (a) the Solomon link in methanol and the Solomon link with (b) $TBAHSO_4$, (c) $TBAClO_4$, (d) $TBAReO_4$, (e) $TBACF_3SO_3$ and (f) $TBAPF_6$ (1 μM each, 1:1 ratio in methanol). The experimental and theoretical mass accuracies of the peaks are shown in Table S2.

Table S2. Observed ions, their experimental and theoretical *m/z* values, mass accuracies, drift times and ^{DT}CCS values in N_2 and in He. Drift times and CCS values for ClO_4^- complexes could not be resolved from SO_4^{2-} complexes and are therefore not shown in the table.

Ion	*m/z* exp	*m/z* theor	Δ*m/z* (mDa)	DT in N_2 (ms)	$^{DT}CCS_{N2}$	DT in He (ms)	$^{DT}CCS_{He}$
[**SL**-2H]$^{6+}$	383.8174	383.8151	-2.34	15.88			
[**SL** -3H]$^{5+}$	460.3775	460.3767	-0.8	17.24	626.5	8.54	412.4
[**SL** -H+SO_4]$^{5+}$	479.9709	479.9701	-0.8	17.26	629.9	8.55	413.6
[**SL** -4H]$^{4+}$	575.2190	575.2190	0.0	19.54	568.9	10.09	395.4
[**SL** -2H+SO_4]$^{4+}$	599.7112	599.7109	-0.3	19.62	570.9	10.12	401.7
[**SL** +2SO_4]$^{4+}$	624.2026	624.2027	0.1	19.32	560.3	9.72	378.8
[**SL** -3H+PF_6]$^{4+}$	611.7135	611.712	-1.5	19.73	572.3	10.15	399.6
[**SL** -H+SO_4+PF_6]$^{4+}$	636.2048	636.2038	-1	19.49	562.1	9.83	384.2
[**SL** -2H+2PF_6]$^{4+}$	648.4562	648.4558	-0.4	19.81	571.6	10.15	395
[**SL** -3H+OTf]$^{4+}$	612.7095	612.709	-0.5	19.85	579.7	10.32	404.9
[**SL** -H+SO_4+OTf]$^{4+}$	637.2026	637.2008	-1.8	19.67	571.6	10.02	387.4
[**SL** -2H+2OTf]$^{4+}$	650.2004	650.1989	-1.5	20.33	591.1	10.48	410.1
[**SL** -3H+ClO_4]$^{4+}$	600.2097	600.2081	-1.6	19.67	573.2	10.16	399
[**SL** -H+SO_4+ClO_4]$^{4+}$	624.6996	624.6999	0.3				
[**SL** -2H+2ClO_4]$^{4+}$	625.1986	625.1972	-1.4				
[**SL** -3H+ReO_4]$^{4+}$	637.7056	637.7041	-1.5	19.63	570.0	10.14	396.8
[**SL** -H+SO_4+ReO_4]$^{4+}$	662.1959	662.1960	0.1	19.49	561.8	9.83	384.3
[**SL** -2H+2ReO_4]$^{4+}$	701.1905	701.1912	0.7	19.81	574.2	10.15	393.9
[**SL** -5H]$^{3+}$	766.6219	766.6229	1.0				
[**SL** -3H+SO_4]$^{3+}$	799.2781	799.2787	0.6				
[**SL** -H+2SO_4]$^{3+}$	831.9337	831.9345	0.8				

6. Variable temperature ^{1}H NMR in CD_3OD

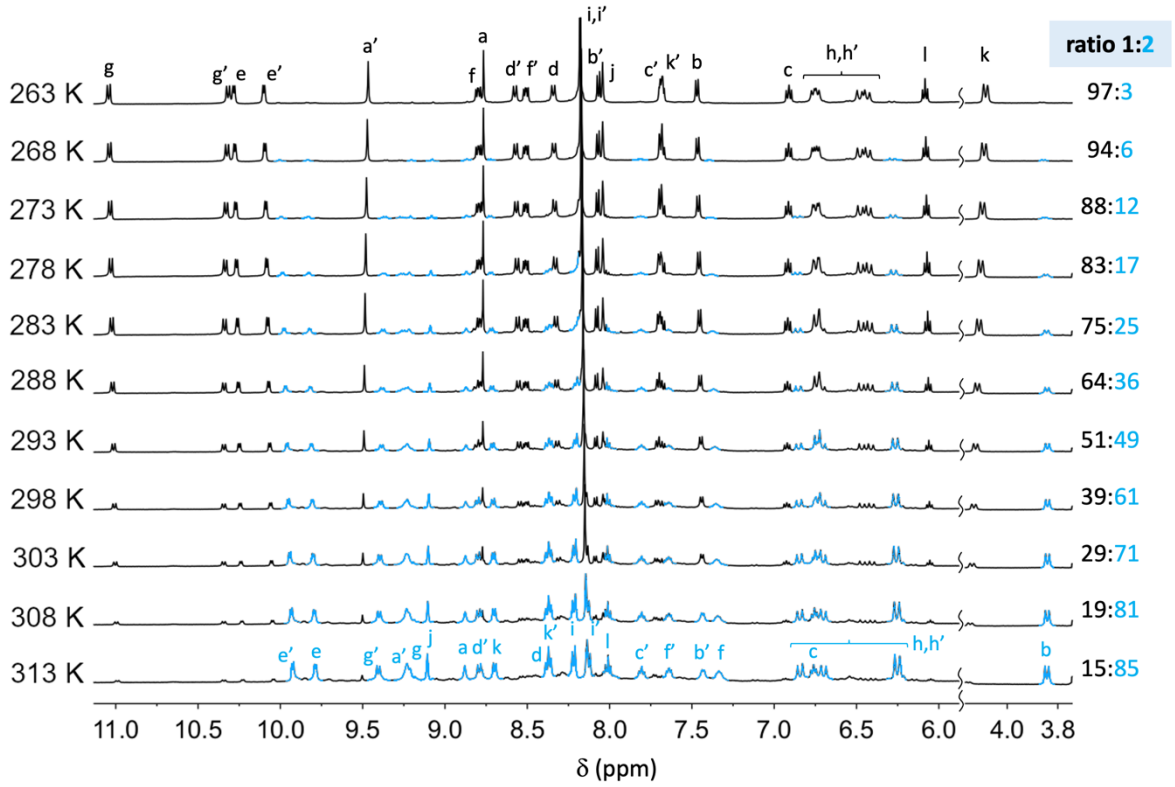


Figure S16. Variable temperature ^{1}H NMR spectra of the Solomon link (0.93 mM in CD_3OD, 500 MHz) in the presence of 2.6 equiv. of SO_4^{2-}. The signals corresponding to conformers **1** and **2** are coloured in black and blue, respectively.

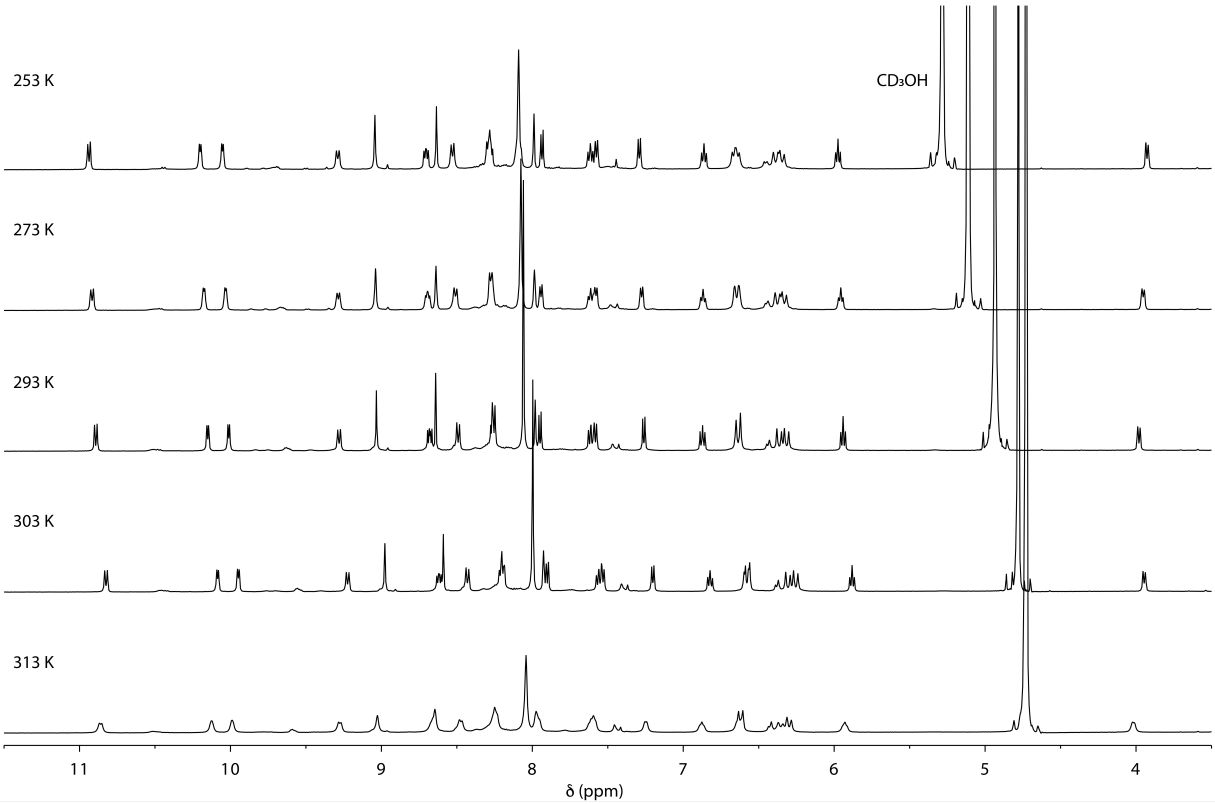


Figure S17. Variable temperature ^{1}H NMR spectra of the Solomon link (0.93 mM in CD_3OD, 500 MHz), confirming that no conformational switch occurs in the absence of sulfate.

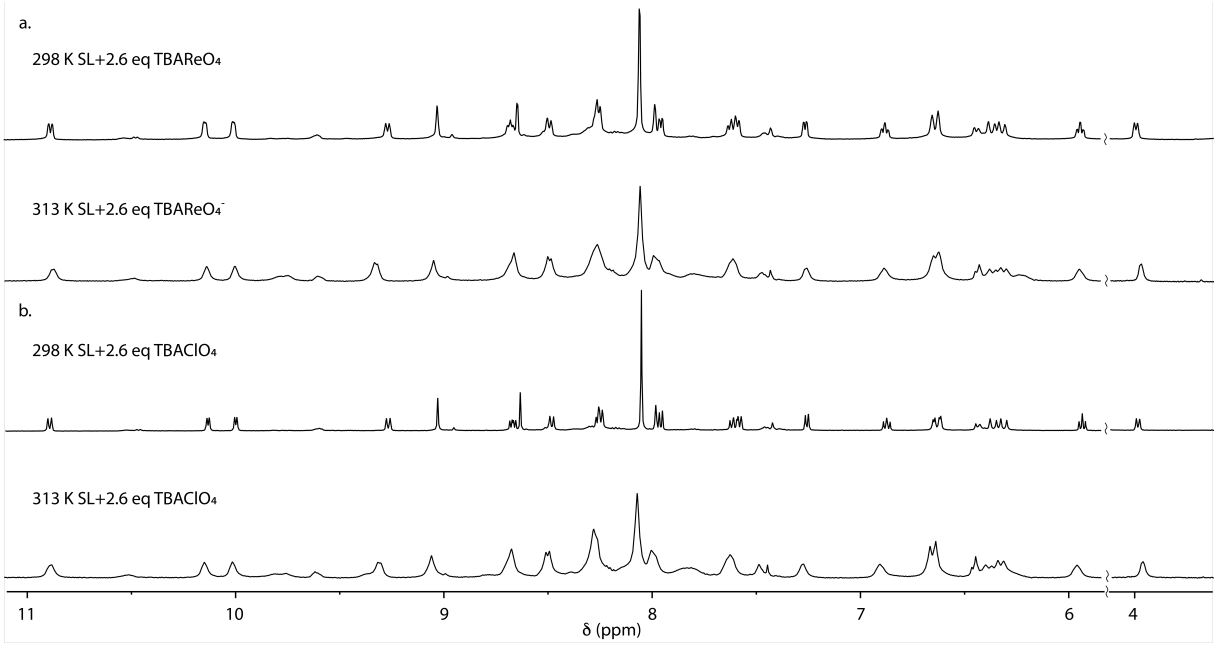


Figure S18. Variable temperature ^{1}H NMR spectra of the Solomon link (0.93 mM in CD_3OD, 500 MHz) with (a) 2.6 equiv. $TBAReO_4$ measured at 298 K and 313 K; and (b) 2.6 equiv. $TBAClO_4$ measured at 298 K and 313 K. These data show that these anions do not trigger any conformational switch, even at higher temperature.

7. UV-Vis characterisation of conformers 1 and 2 in CH_3OH

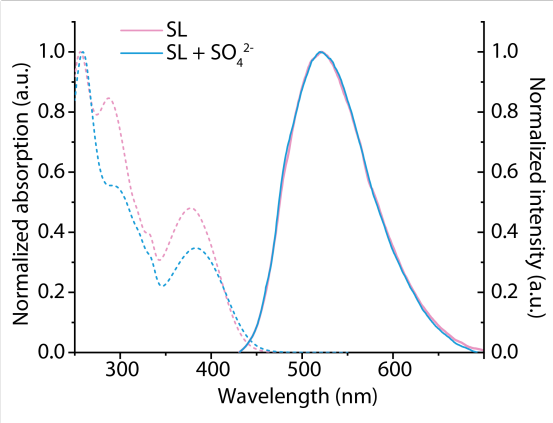


Figure S19. Normalized absorption (dashed line) and emission (solid line) spectra of the Solomon link alone (85 μM in pink) and with 3.0 equiv. of SO_4^{2-} (in blue). Solvent: MeOH. Differences in the absorption spectra reflect differences in packing of the aromatic units in conformers **1** and **2**.

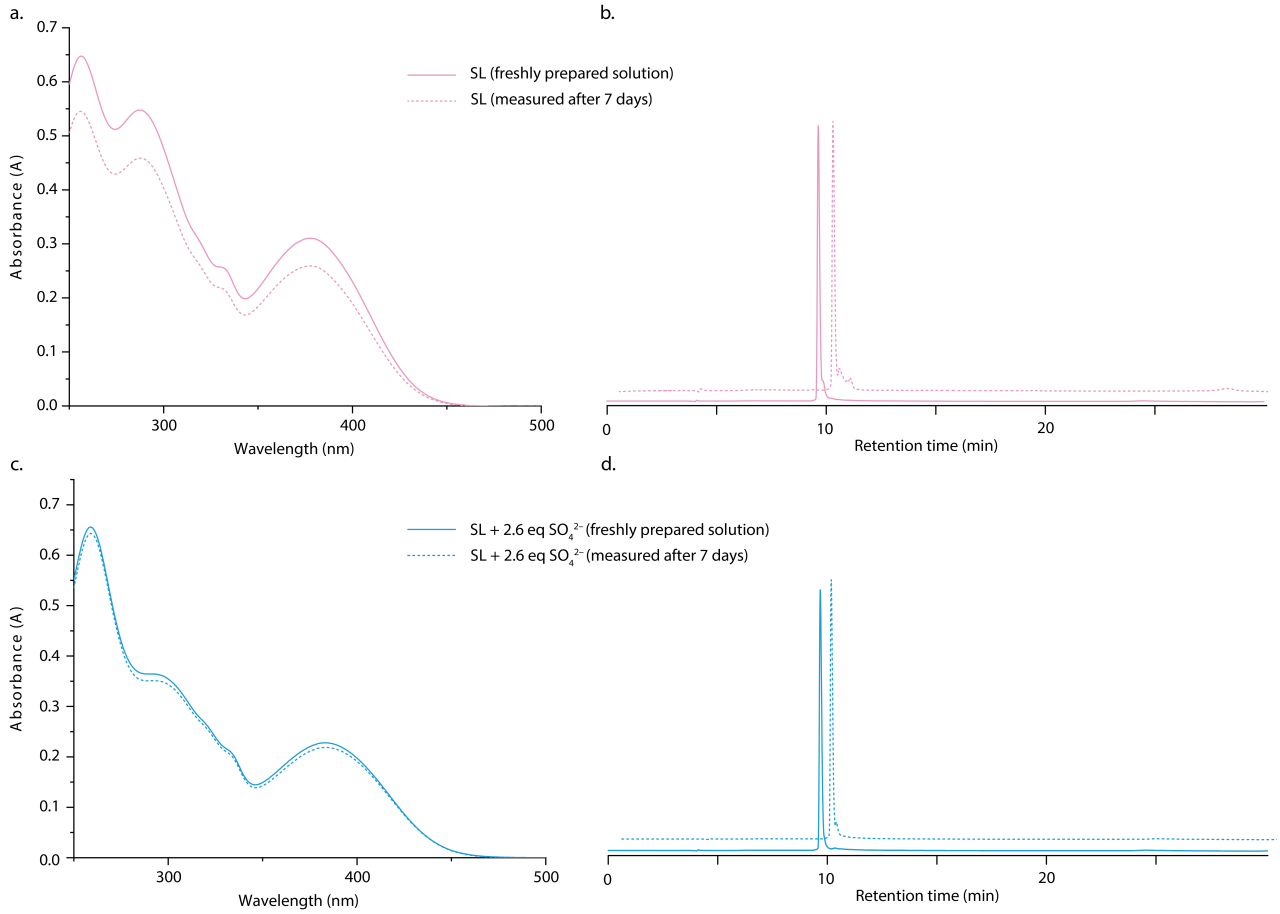


Figure S20. (a) UV-Vis spectra and HPLC chromatograms (monitored at 360 nm) of freshly prepared (solid line) and 7 days old (dashed line) solutions of the Solomon link. (b) UV-Vis spectra and HPLC chromatograms (monitored at 360 nm) of freshly prepared (solid line) and 7 days old (dashed line) solutions of the Solomon link with 3.0 equiv. of SO_4^{2-}. These data show that the unbound conformer **1** degrades slightly faster than the sulfate-bound conformer **2** in methanol, suggesting that sulfate stabilizes the Solomon link to some extent and reduces the kinetics of acylhydrazone exchange.

8. ^{1}H NMR anion titrations in solvents other than CD_3OD

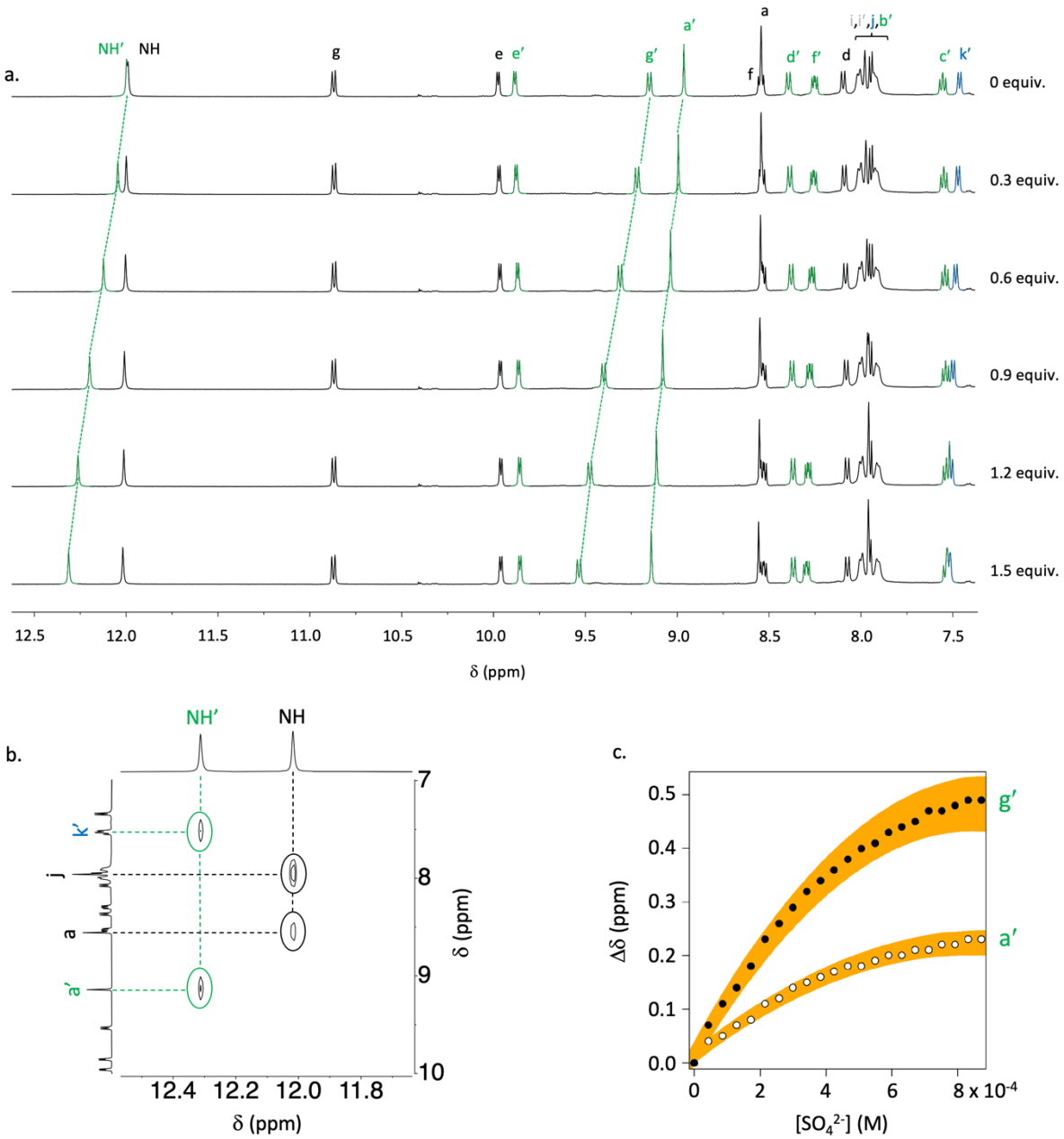


Figure S21. Titration in water. (a) Partial ^{1}H NMR spectra of the Solomon link (0.93 mM in H_2O/D_2O 95/5, 298 K, 500 MHz) during the titration with SO_4^{2-} (0–1.5 equiv.). The downfield shift of the protons NH′, a′, g′, and k′ shows that SO_4^{2-} interacts with the external surface of the Solomon link. (b) Protons NH and NH' were assigned by NOESY (d_8 = 300 ms) after addition of 1.5 equiv. SO_4^{2-}. (c) Variation of the chemical shifts of protons a′ (hollow circles) and g′ (full circles) as a function of the concentration of SO_4^{2-}. The orange band represents the standard deviation over three titrations. Precipitation of the sample in the course of the titration prevented us to quantitatively assess binding.

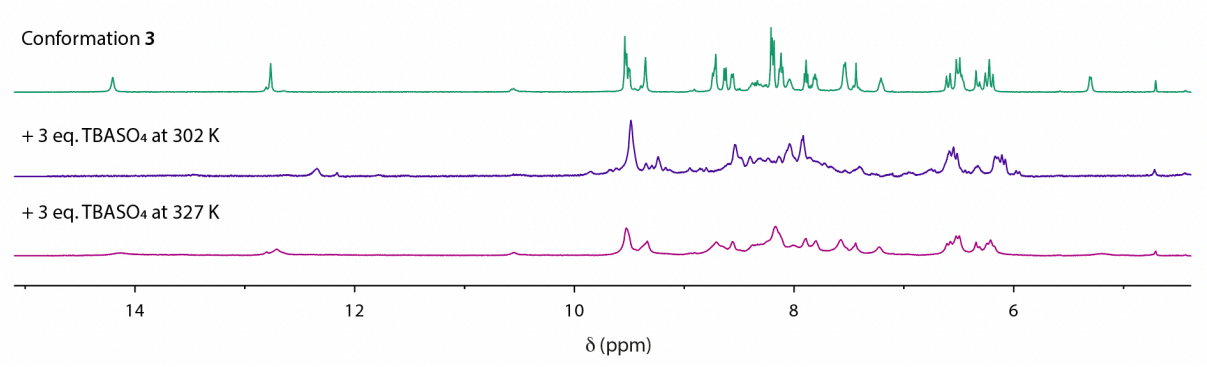


Figure S22. ^{1}H NMR spectra of the Solomon link (0.93 mM in 500 µL of CD_3CN, 500 MHz) before (green) and after the addition of 3 equiv. of SO_4^{2-} at 302 K (purple) and at 327 K (red).

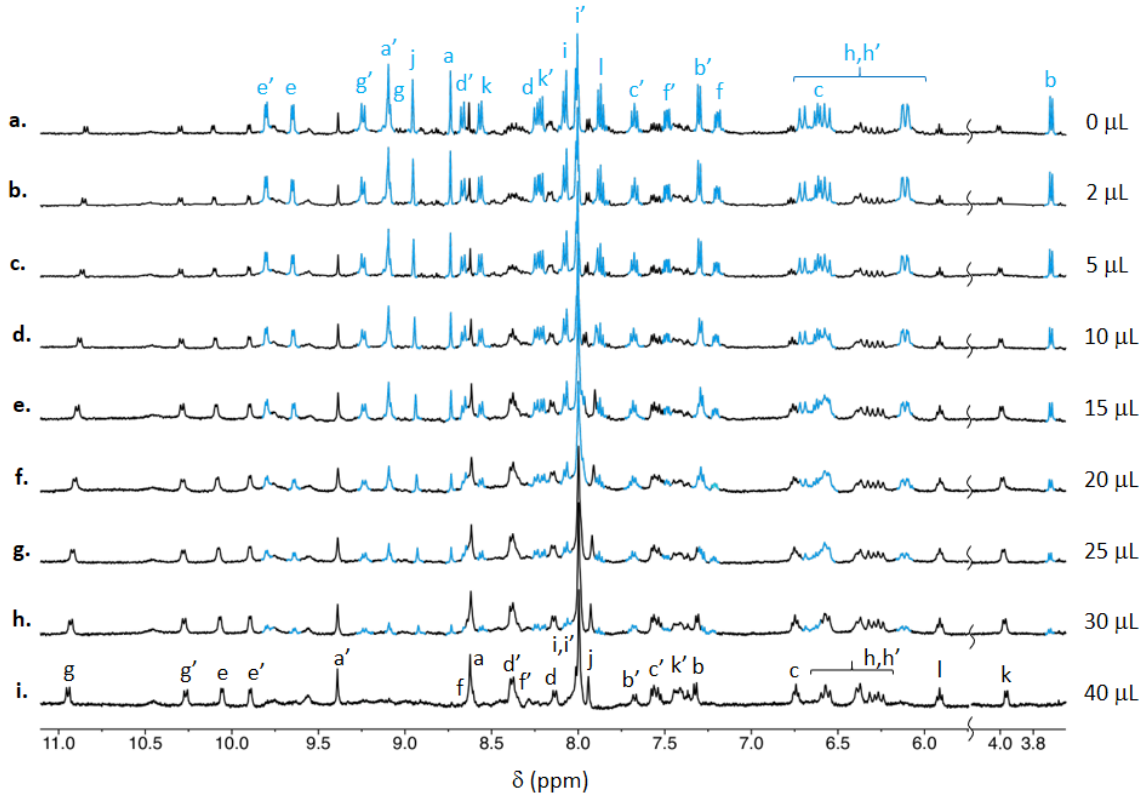
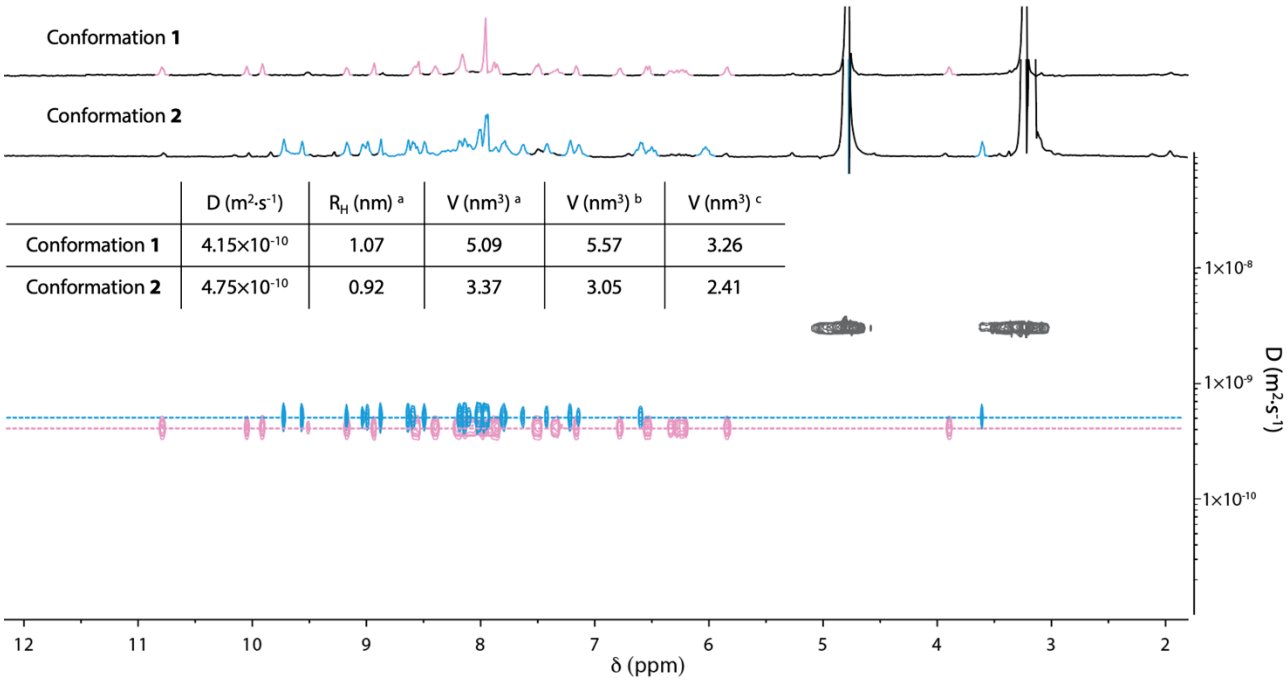


Figure S23. ^{1}H NMR spectra of the Solomon link (0.93 mM in 500 µL of CD_3OD, 298 K, 500 MHz) in the presence of 3 equiv. of SO_4^{2-} (a) before and after addition of (b) 2 µL, (c) 5 µL, (d) 10 µL, (e) 15 µL, (f) 20 µL, (g) 25 µL, (h) 30 µL, and (i) 40 µL of D_2O. The signals corresponding to conformers **1** and **2** are coloured in black and blue, respectively. Water highly solvates sulfate and stabilises conformer **1** (see ref. S11). As a result, addition of water disrupts the host-guest complex **2**·**2**SO_4^{2-}, and the Solomon link switches back to conformer **1**.

9. Evidence for the Solomon link contraction upon sulfate binding



	D ($m^2 \cdot s^{-1}$)	R_H (nm) [a]	V (nm^3) [a]	V (nm^3) [b]	V (nm^3) [c]
Conformation **1**	4.15×10^{-10}	1.07	5.09	5.57	3.26
Conformation **2**	4.75×10^{-10}	0.92	3.37	3.05	2.41

Figure S24. Overlaid DOSY of the Solomon link (CD_3OD, 313 K, 500 MHz) in conformations **1** (pink colour) and **2** (blue colour). The diffusion coefficients were measured to be $4.15 \cdot 10^{-10}$ $m^2 \cdot s^{-1}$ (**1**) and $4.75 \cdot 10^{-10}$ $m^2 \cdot s^{-1}$ (**2**). [a] Hydrodynamic radii and volumes were calculated using the Stokes-Einstein equation assuming both conformers to be spherical; volumes were also calculated using dimensions from the DFT minimized models for comparison, approximating them as spheres [b] and cylinders [c].

10. Comparison between the different conformers of the Solomon link

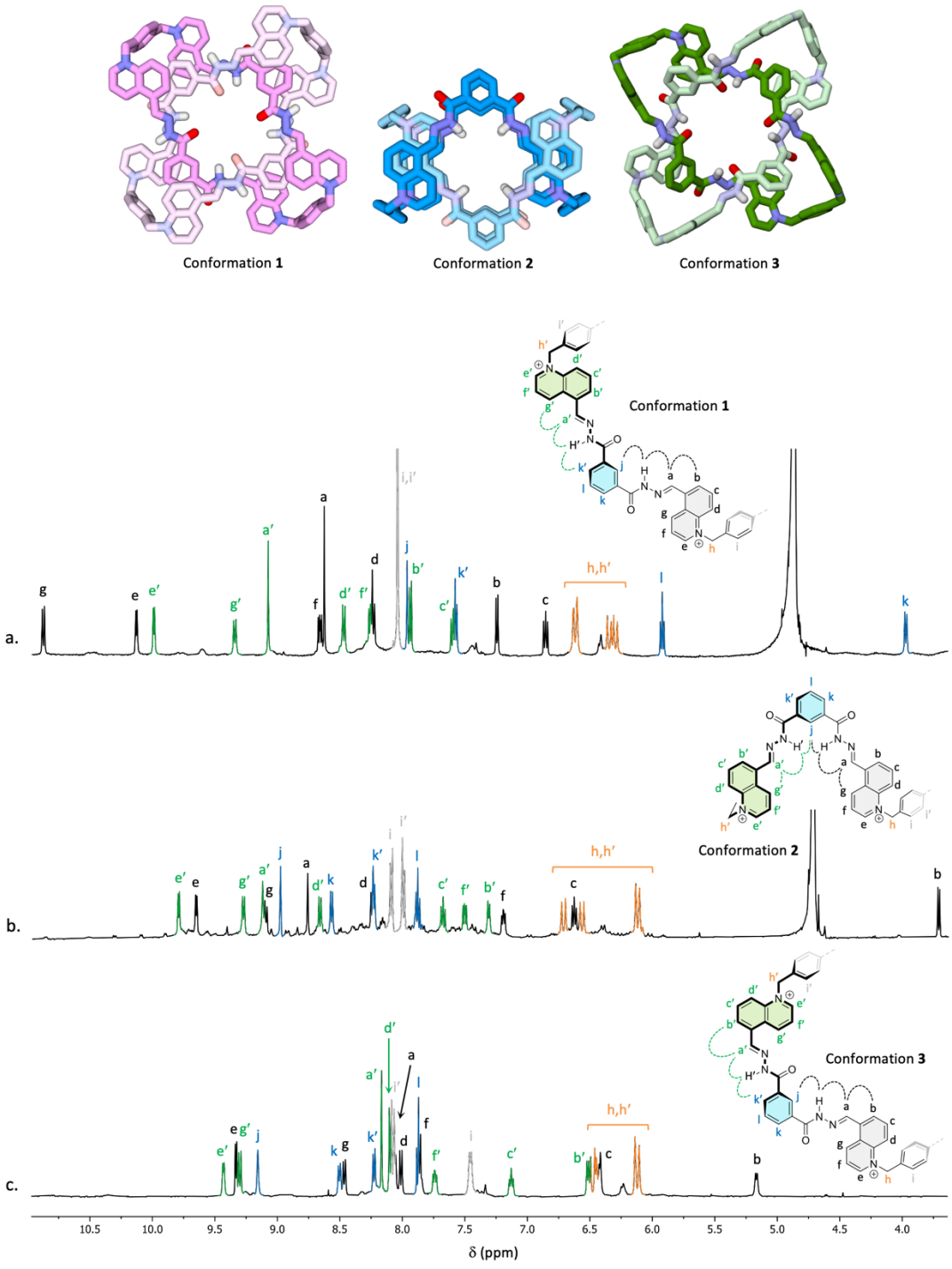


Figure S25. Comparison between the NMR spectra of the three conformers of the Solomon link currently known. Two of these conformers (**1** and **2**) are described in this article. Conformer **3** has been described elsewhere.[S11] (a) ^{1}H NMR spectrum of the Solomon link in conformation **1** (CD_3OD, 298 K, 500 MHz). The Solomon link also adopts this conformation in D_2O.[S1] (b) ^{1}H NMR spectrum of the Solomon link in conformation **2** (CD_3OD with 2.6 equiv. of SO_4^{2-}, 313 K, 500 MHz). (c) ^{1}H NMR spectrum of the Solomon link in conformation **3** (CD_3CN, 298 K, 500 MHz). Key NOE correlations are highlighted with dotted lines.

11. DFT calculations

Table S3 presents a summary of the energies associated with the sulfate-free Solomon link (conformer **1**) and the complexes formed with one or two sulfate anions (conformer **2**). Despite several attempts, satisfactory models of the intermediate complex formed with one sulfate anion proved particularly difficult to obtain. Figure S26 shows one example of the structures calculated for the complex with one sulfate anion (for the geometry with two sulfate anions, refer to Fig. 1 in the main text). Notably, the formation energy of the Solomon link bound to one sulfate anion is calculated to be -45.8 kcal·mol^{-1} (excluding entropic effects). The formation energy with two sulfate anions is significantly higher at -138.0 kcal·mol^{-1}, more than twice the energy of the interaction with only one anion.

This substantial difference arises because the introduction of the first sulfate anion incurs an energy cost to transition from conformer **1** to conformer **2**. Once this transition occurs, the entry of the second sulfate anion becomes more favourable. Consequently, it is plausible that the complex with only one sulfate anion represents a transient intermediate that has not been experimentally detected.

Table S3. Total energies of the different complexes formed between the Solomon link and sulfate. The formation energies of the complexes are also indicated.

Host-guest complex	**E (Hartries)**
1 (C_4 symmetry)	-7472.8905009067
Solomon link + SO_4^{2-} (D_2 symmetry)	-8172.6045304824
2 + 2 SO_4^{2-} (D_2 symmetry)	-8872.3925662255
Host-guest complex	**ΔE_f (kcal·mol^{-1})**
Solomon link + SO_4^{2-} (D_2 symmetry)	–45.8
2 + 2 SO_4^{2-} (D_2 symmetry)	–138.0

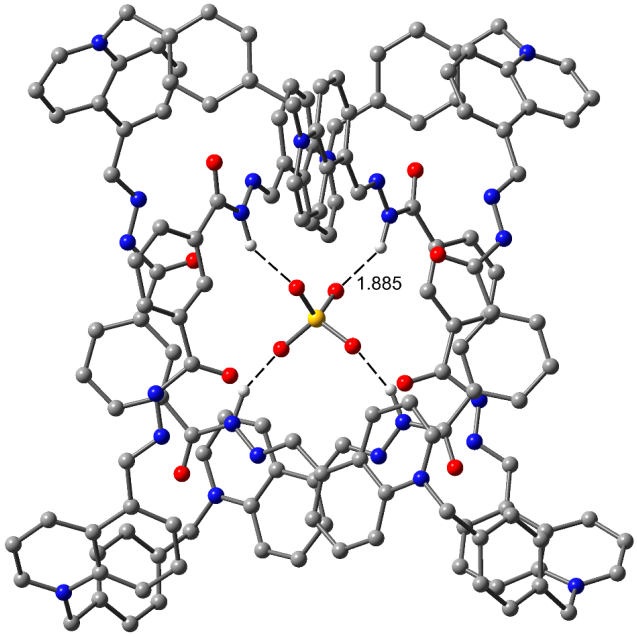


Figure S26. RI-BP86-D3/def2-TZVP optimized Solomon link bond to one sulfate. The four symmetrically equivalent NH···O H-bonds are indicated as dashed lines. Distances are given in Å.

12. Cartesian coordinates

Conformation 1 (C_4-symmetry)

C	6.8663452	4.1975156	-2.3501902
C	5.7569916	3.2950359	-2.5031432
C	4.5404272	3.7900280	-2.9567526
C	4.3823551	5.1509560	-3.2639092
C	5.4159009	6.0524254	-3.0918206
C	6.6641290	5.5923238	-2.6284339
C	3.8837194	6.1342779	3.5235627
C	2.6544232	5.5201086	3.2405272
C	1.5925581	6.2202085	2.6716909
C	1.7655763	7.6287979	2.4015783
C	3.0649631	8.2082131	2.6112240
C	4.1078356	7.4537717	3.1868444
H	5.2579175	7.1004514	-3.3278829
H	5.0709071	7.9032253	3.4044695
C	0.4085576	5.4249105	2.3568222
C	5.8809711	1.8690526	-2.1742979
C	-5.8809711	-1.8690526	-2.1742979
C	-0.4085576	-5.4249105	2.3568222
C	-5.7569916	-3.2950359	-2.5031432
C	-4.5404272	-3.7900280	-2.9567526
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C	-4.3823551	-5.1509560	-3.2639092
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C	-2.6544232	-5.5201086	3.2405272
C	-5.4159009	-6.0524254	-3.0918206
C	-1.5925581	-6.2202085	2.6716909
C	-3.8837194	-6.1342779	3.5235627
H	-5.2579175	-7.1004514	-3.3278829
C	-1.7655763	-7.6287979	2.4015783
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C	-3.0649631	-8.2082131	2.6112240
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H	-8.3080745	-2.7463905	-1.6190714
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H	4.6760576	5.5626715	4.0061954
H	3.4295566	5.5040883	-3.6569130
H	3.7097562	3.0987781	-3.0919125
H	-2.5262973	-4.4622226	3.4729389
H	-4.6760576	-5.5626715	4.0061954
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C	-0.9531623	-9.8209918	1.7444232
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C	8.9348473	6.0371107	-2.0472071
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H	-5.1897617	-9.9092099	3.0968723
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C	4.1489100	-0.7546248	-0.5485558
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O	3.1793119	-0.2095096	-0.0281171
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C	5.4249105	-0.4085576	2.3568222
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C	6.2202085	-1.5925581	2.6716909
C	5.5201086	-2.6544232	3.2405272
C	7.6287979	-1.7655763	2.4015783
C	6.1342779	-3.8837194	3.5235627
C	8.2082131	-3.0649631	2.6112240
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C	7.4537717	-4.1078356	3.1868444
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C	5.1509560	-4.3823551	-3.2639092
H	7.9032253	-5.0709071	3.4044695
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C	-9.8209918	0.9531623	1.7444232
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C	10.3188316	-2.2497664	1.8595909
C	6.0371107	-8.9348473	-2.0472071
C	-10.3188316	2.2497664	1.8595909
C	-6.0371107	8.9348473	-2.0472071
H	4.3880598	-10.1756467	-1.4730707
H	6.7923437	-9.7131344	-1.9430287
H	10.5033260	-0.1535305	1.4619930
H	11.3565222	-2.4926082	1.6338764
H	-11.3565222	2.4926082	1.6338764
H	-10.5033260	0.1535305	1.4619930
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H	9.9092099	-5.1897617	3.0968723
H	11.1850330	-4.5524600	2.0679896
C	7.9542209	-7.5041580	-2.4975539
H	8.1931070	-7.0008595	-3.4415823
H	8.4129236	-8.5001086	-2.5502649
C	-7.9542209	7.5041580	-2.4975539
H	-8.1931070	7.0008595	-3.4415823
H	-8.4129236	8.5001086	-2.5502649
C	-10.0973628	4.6623320	2.1551176
H	-9.9092099	5.1897617	3.0968723
H	-11.1850330	4.5524600	2.0679896
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N	1.2467135	-4.8763244	-1.6487523
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H	-0.5709198	-5.8417591	-1.7638622

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C	-0.7546248	-4.1489100	-0.5485558
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O	-0.2095096	-3.1793119	-0.0281171
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C	4.3995957	3.7906521	0.4616673
H	2.6990369	2.4590914	0.1400329
C	4.8511253	5.1182476	0.3669762
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C	-2.6641817	-5.8299128	-0.3506421
C	-4.3995957	-3.7906521	0.4616673
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C	-3.9870359	-6.1314013	-0.0317013
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N	-5.8782849	-0.6346795	1.7400066
N	5.8782849	0.6346795	1.7400066
C	8.4709960	-6.7396550	-1.2909487
C	9.3057174	-5.6264210	-1.4562741
C	8.1805738	-7.1808716	0.0066291
C	9.8266185	-4.9621832	-0.3436494
H	9.5837628	-5.2923149	-2.4576711
C	8.7016734	-6.5172853	1.1178591
H	7.5626553	-8.0663429	0.1662518
C	9.5229487	-5.3937554	0.9555434
H	10.4954043	-4.1135067	-0.5007257
H	8.4921737	-6.9077457	2.1146702
C	-8.4709960	6.7396550	-1.2909487
C	-9.3057174	5.6264210	-1.4562741
C	-8.1805738	7.1808716	0.0066291
C	-9.8266185	4.9621832	-0.3436494
H	-9.5837628	5.2923149	-2.4576711
C	-8.7016734	6.5172853	1.1178591
H	-7.5626553	8.0663429	0.1662518
C	-9.5229487	5.3937554	0.9555434
H	-10.4954043	4.1135067	-0.5007257
H	-8.4921737	6.9077457	2.1146702
H	4.3614374	-0.4808517	2.6380025
H	-4.3614374	0.4808517	2.6380025
N	9.5375539	-3.2714589	2.2482396
N	-9.5375539	3.2714589	2.2482396
N	6.4768531	-7.7213675	-2.4206040
N	-6.4768531	7.7213675	-2.4206040

Solomon link::1 SO_4^{2-} (D_2 symmetry)

C	6.8138492	9.0080042	-3.3495359
H	7.6490751	9.2602297	-4.0157048
H	6.4472077	9.9500344	-2.9207195
C	2.3394134	6.1113443	-5.7304692
C	3.5270937	6.8692240	-5.1785052
C	3.5362332	8.2683381	-5.1532493
C	4.6444061	6.1734523	-4.7050292
C	4.6131659	8.9615772	-4.5956463
H	2.6909956	8.8314526	-5.5545044
C	5.7290199	6.8636877	-4.1785777
H	4.6619689	5.0830625	-4.7111735
C	5.7073000	8.2617002	-4.0785804
H	4.5838466	10.0517159	-4.5482547

H	6.5797424	6.2939581	-3.8021992
C	0.8041140	3.0585918	-3.1562999
C	1.6492808	2.7620166	-4.2133033
H	1.9426304	1.7372842	-4.4310555
C	2.1173355	3.7893017	-5.0248416
N	1.8131423	5.0774267	-4.7880748
C	1.0278800	5.4414655	-3.6967758
C	0.7784175	6.7945240	-3.4064215
H	1.2269592	7.5881950	-3.9948504
C	-0.0364677	7.1169683	-2.3322936
H	-0.2218823	8.1679980	-2.1080436
C	-0.6364662	6.1257398	-1.5474292
H	-1.2891946	6.3933041	-0.7175351
C	-0.4190046	4.7710579	-1.8019642
C	-1.0766408	3.7562152	-0.9951250
N	-1.9178784	4.1340210	-0.0796374
N	-2.5048182	3.1433186	0.6081377
C	-3.4977905	3.4411164	1.5198101
C	-4.3500086	2.2756073	1.9242518
C	-5.5934143	2.5832410	2.5035449
C	-6.4864819	1.5706556	2.8462643
H	-7.4417010	1.8138001	3.3122876
C	-6.1514376	0.2352742	2.6057936
H	-6.8432441	-0.5507187	2.9139471
C	-4.9080162	-0.0826773	2.0369037
H	-5.8358794	3.6335877	2.6693373
C	-4.0026943	0.9359359	1.7079346
H	-3.0267074	0.6410738	1.3089684
O	-3.7183676	4.5833687	1.9276789
H	-2.1720054	2.1701087	0.4495198
H	2.7374452	3.5985883	-5.8988688
C	0.4592123	4.4009562	-2.8811040
C	5.5934143	-2.5832410	2.5035449
H	5.8358794	-3.6335877	2.6693373
C	4.3500086	-2.2756073	1.9242518
C	4.0026943	-0.9359359	1.7079346
H	3.0267074	-0.6410738	1.3089684
C	4.9080162	0.0826773	2.0369037
C	6.1514376	-0.2352742	2.6057936
H	6.8432441	0.5507187	2.9139471
C	4.4556709	1.4864120	1.7787571
O	3.2872041	1.8347166	1.8522855
N	5.4866074	2.3548410	1.4055269
H	6.4210440	1.9657517	1.2378070
N	5.2247055	3.6295553	1.0814361
C	6.1926812	4.3462754	0.6087620
C	5.9206423	5.6943161	0.1270605
C	6.9132542	6.4264884	-0.6156706
C	8.2749578	6.0551982	-0.7038367
C	9.1545847	6.7561636	-1.5100863
H	10.2114693	6.5027907	-1.5644406
C	8.6550001	7.7650699	-2.3328954
N	7.3728199	8.1551942	-2.2595184
H	9.2692301	8.2542728	-3.0877774
H	8.6551852	5.2173638	-0.1209982
C	6.4964252	7.6020468	-1.3258381
C	5.2114375	8.1379878	-1.1373344
H	4.9087312	9.0549746	-1.6346804
C	4.3214772	7.4722235	-0.3131634
H	3.3277599	7.8911425	-0.1580247
C	4.6489604	6.2435533	0.2724173
H	3.8915705	5.6796978	0.8143774
C	6.4864819	-1.5706556	2.8462643
H	7.4417010	-1.8138001	3.3122876
H	2.6127772	5.5740565	-6.6480626
H	1.5131738	6.7836812	-5.9911724
H	0.4481862	2.2418266	-2.5233110
C	3.4977905	-3.4411164	1.5198101
O	3.7183676	-4.5833687	1.9276789
N	2.5048182	-3.1433186	0.6081377
H	2.1720054	-2.1701087	0.4495198
N	1.9178784	-4.1340210	-0.0796374
C	1.0766408	-3.7562152	-0.9951250
C	0.4190046	-4.7710579	-1.8019642
C	-0.4592123	-4.4009562	-2.8811040
C	-1.0278800	-5.4414655	-3.6967758
C	-0.7784175	-6.7945240	-3.4064215

C	0.0364677	-7.1169683	-2.3322936
H	0.2218823	-8.1679980	-2.1080436
H	-1.2269592	-7.5881950	-3.9948504
N	-1.8131423	-5.0774267	-4.7880748
C	-2.1173355	-3.7893017	-5.0248416
H	-2.7374452	-3.5985883	-5.8988688
C	-1.6492808	-2.7620166	-4.2133033
H	-1.9426304	-1.7372842	-4.4310555
C	-2.3394134	-6.1113443	-5.7304692
H	-1.5131738	-6.7836812	-5.9911724
H	-2.6127772	-5.5740565	-6.6480626
C	-3.5270937	-6.8692240	-5.1785052
C	-4.6444061	-6.1734523	-4.7050292
H	-4.6619689	-5.0830625	-4.7111735
C	-5.7290199	-6.8636877	-4.1785777
H	-6.5797424	-6.2939581	-3.8021992
C	-5.7073000	-8.2617002	-4.0785804
C	-4.6131659	-8.9615772	-4.5956463
H	-4.5838466	-10.0517159	-4.5482547
C	-6.8138492	-9.0080042	-3.3495359
N	-7.3728199	-8.1551942	-2.2595184
C	-6.4964252	-7.6020468	-1.3258381
C	-5.2114375	-8.1379878	-1.1373344
C	-4.3214772	-7.4722235	-0.3131634
C	-4.6489604	-6.2435533	0.2724173
H	-3.8915705	-5.6796978	0.8143774
C	-5.9206423	-5.6943161	0.1270605
C	-6.1926812	-4.3462754	0.6087620
N	-5.2247055	-3.6295553	1.0814361
N	-5.4866074	-2.3548410	1.4055269
H	-6.4210440	-1.9657517	1.2378070
C	-4.4556709	-1.4864120	1.7787571
O	-3.2872041	-1.8347166	1.8522855
H	-3.3277599	-7.8911425	-0.1580247
H	-4.9087312	-9.0549746	-1.6346804
C	-6.9132542	-6.4264884	-0.6156706
C	-8.2749578	-6.0551982	-0.7038367
C	-9.1545847	-6.7561636	-1.5100863
H	-10.2114693	-6.5027907	-1.5644406
H	-8.6551852	-5.2173638	-0.1209982
C	-8.6550001	-7.7650699	-2.3328954
H	-9.2692301	-8.2542728	-3.0877774
H	-6.4472077	-9.9500344	-2.9207195
H	-7.6490751	-9.2602297	-4.0157048
C	-3.5362332	-8.2683381	-5.1532493
H	-2.6909956	-8.8314526	-5.5545044
C	-0.8041140	-3.0585918	-3.1562999
H	-0.4481862	-2.2418266	-2.5233110
C	0.6364662	-6.1257398	-1.5474292
H	1.2891946	-6.3933041	-0.7175351
H	-0.8549388	2.6956921	-1.1544332
H	7.2013768	3.9224564	0.4875765
H	0.8549388	-2.6956921	-1.1544332
H	-7.2013768	-3.9224564	0.4875765
C	-0.4190046	-4.7710579	1.8019642
C	-0.6364662	-6.1257398	1.5474292
H	-1.2891946	-6.3933041	0.7175351
C	-0.0364677	-7.1169683	2.3322936
H	-0.2218823	-8.1679980	2.1080436
C	0.7784175	-6.7945240	3.4064215
H	1.2269592	-7.5881950	3.9948504
C	1.0278800	-5.4414655	3.6967758
N	1.8131423	-5.0774267	4.7880748
C	2.3394134	-6.1113443	5.7304692
H	1.5131738	-6.7836812	5.9911724
H	2.6127772	-5.5740565	6.6480626
C	3.5270937	-6.8692240	5.1785052
C	4.6444061	-6.1734523	4.7050292
H	4.6619689	-5.0830625	4.7111735
C	5.7290199	-6.8636877	4.1785777
H	6.5797424	-6.2939581	3.8021992
C	5.7073000	-8.2617002	4.0785804
C	6.8138492	-9.0080042	3.3495359
N	7.3728199	-8.1551942	2.2595184
C	8.6550001	-7.7650699	2.3328954
H	9.2692301	-8.2542728	3.0877774
C	9.1545847	-6.7561636	1.5100863

H	10.2114693	-6.5027907	1.5644406
C	8.2749578	-6.0551982	0.7038367
H	8.6551852	-5.2173638	0.1209982
C	6.9132542	-6.4264884	0.6156706
C	5.9206423	-5.6943161	-0.1270605
C	6.1926812	-4.3462754	-0.6087620
H	7.2013768	-3.9224564	-0.4875765
N	5.2247055	-3.6295553	-1.0814361
N	5.4866074	-2.3548410	-1.4055269
C	4.4556709	-1.4864120	-1.7787571
O	3.2872041	-1.8347166	-1.8522855
C	4.9080162	-0.0826773	-2.0369037
C	4.0026943	0.9359359	-1.7079346
H	3.0267074	0.6410738	-1.3089684
C	4.3500086	2.2756073	-1.9242518
C	5.5934143	2.5832410	-2.5035449
C	6.4864819	1.5706556	-2.8462643
H	7.4417010	1.8138001	-3.3122876
H	5.8358794	3.6335877	-2.6693373
C	3.4977905	3.4411164	-1.5198101
O	3.7183676	4.5833687	-1.9276789
N	2.5048182	3.1433186	-0.6081377
H	2.1720054	2.1701087	-0.4495198
N	1.9178784	4.1340210	0.0796374
C	1.0766408	3.7562152	0.9951250
H	0.8549388	2.6956921	1.1544332
C	0.4190046	4.7710579	1.8019642
C	-0.4592123	4.4009562	2.8811040
C	-1.0278800	5.4414655	3.6967758
C	-0.7784175	6.7945240	3.4064215
C	0.0364677	7.1169683	2.3322936
H	0.2218823	8.1679980	2.1080436
H	-1.2269592	7.5881950	3.9948504
N	-1.8131423	5.0774267	4.7880748
C	-2.1173355	3.7893017	5.0248416
H	-2.7374452	3.5985883	5.8988688
C	-1.6492808	2.7620166	4.2133033
H	-1.9426304	1.7372842	4.4310555
C	-2.3394134	6.1113443	5.7304692
H	-1.5131738	6.7836812	5.9911724
H	-2.6127772	5.5740565	6.6480626
C	-3.5270937	6.8692240	5.1785052
C	-4.6444061	6.1734523	4.7050292
H	-4.6619689	5.0830625	4.7111735
C	-5.7290199	6.8636877	4.1785777
H	-6.5797424	6.2939581	3.8021992
C	-5.7073000	8.2617002	4.0785804
C	-4.6131659	8.9615772	4.5956463
H	-4.5838466	10.0517159	4.5482547
C	-6.8138492	9.0080042	3.3495359
N	-7.3728199	8.1551942	2.2595184
C	-6.4964252	7.6020468	1.3258381
C	-5.2114375	8.1379878	1.1373344
C	-4.3214772	7.4722235	0.3131634
C	-4.6489604	6.2435533	-0.2724173
H	-3.8915705	5.6796978	-0.8143774
C	-5.9206423	5.6943161	-0.1270605
C	-6.1926812	4.3462754	-0.6087620
H	-7.2013768	3.9224564	-0.4875765
N	-5.2247055	3.6295553	-1.0814361
N	-5.4866074	2.3548410	-1.4055269
H	-6.4210440	1.9657517	-1.2378070
C	-4.4556709	1.4864120	-1.7787571
O	-3.2872041	1.8347166	-1.8522855
C	-4.9080162	0.0826773	-2.0369037
C	-6.1514376	-0.2352742	-2.6057936
C	-6.4864819	-1.5706556	-2.8462643
H	-7.4417010	-1.8138001	-3.3122876
C	-5.5934143	-2.5832410	-2.5035449
H	-5.8358794	-3.6335877	-2.6693373
C	-4.3500086	-2.2756073	-1.9242518
C	-3.4977905	-3.4411164	-1.5198101
N	-2.5048182	-3.1433186	-0.6081377
N	-1.9178784	-4.1340210	0.0796374
H	-2.1720054	-2.1701087	-0.4495198
O	-3.7183676	-4.5833687	-1.9276789
H	-6.8432441	0.5507187	-2.9139471

C	-4.0026943	-0.9359359	-1.7079346
H	-3.0267074	-0.6410738	-1.3089684
H	-3.3277599	7.8911425	0.1580247
H	-4.9087312	9.0549746	1.6346804
C	-6.9132542	6.4264884	0.6156706
C	-8.2749578	6.0551982	0.7038367
C	-9.1545847	6.7561636	1.5100863
H	-10.2114693	6.5027907	1.5644406
H	-8.6551852	5.2173638	0.1209982
C	-8.6550001	7.7650699	2.3328954
H	-9.2692301	8.2542728	3.0877774
H	-6.4472077	9.9500344	2.9207195
H	-7.6490751	9.2602297	4.0157048
C	-3.5362332	8.2683381	5.1532493
H	-2.6909956	8.8314526	5.5545044
C	-0.8041140	3.0585918	3.1562999
H	-0.4481862	2.2418266	2.5233110
C	0.6364662	6.1257398	1.5474292
H	1.2891946	6.3933041	0.7175351
C	6.1514376	0.2352742	-2.6057936
H	6.8432441	-0.5507187	-2.9139471
H	6.4210440	-1.9657517	-1.2378070
C	4.6489604	-6.2435533	-0.2724173
H	3.8915705	-5.6796978	-0.8143774
C	4.3214772	-7.4722235	0.3131634
H	3.3277599	-7.8911425	0.1580247
C	5.2114375	-8.1379878	1.1373344
H	4.9087312	-9.0549746	1.6346804
C	6.4964252	-7.6020468	1.3258381
H	6.4472077	-9.9500344	2.9207195
H	7.6490751	-9.2602297	4.0157048
C	4.6131659	-8.9615772	4.5956463
H	4.5838466	-10.0517159	4.5482547
C	3.5362332	-8.2683381	5.1532493
H	2.6909956	-8.8314526	5.5545044
C	2.1173355	-3.7893017	5.0248416
C	1.6492808	-2.7620166	4.2133033
C	0.8041140	-3.0585918	3.1562999
H	0.4481862	-2.2418266	2.5233110
H	1.9426304	-1.7372842	4.4310555
H	2.7374452	-3.5985883	5.8988688
C	0.4592123	-4.4009562	2.8811040
C	-1.0766408	-3.7562152	0.9951250
H	-0.8549388	-2.6956921	1.1544332
S	0.0000000	0.0000000	0.0000000
O	0.8674417	-0.8752543	0.8654489
O	0.8674417	0.8752543	-0.8654489
O	-0.8674417	-0.8752543	-0.8654489
O	-0.8674417	0.8752543	0.8654489

Conformation 2::2 SO_4^{2-} (D_2 symmetry)

C	5.0296695	6.8888115	-4.3585100
H	5.5475511	6.6746139	-5.3003644
H	5.4665669	7.8013571	-3.9469566
C	-0.7138647	6.2490220	-4.5510591
C	0.7439272	6.6348365	-4.6223040
C	1.3375580	7.4126833	-3.6176370
C	1.5484584	6.1123509	-5.6382287
C	2.7189265	7.5772036	-3.5778508
H	0.7254573	7.8726911	-2.8418847
C	2.9312858	6.2734638	-5.5977123
H	1.1027651	5.5370488	-6.4502414
C	3.5320288	6.9636551	-4.5417961
H	3.1647111	8.1646490	-2.7751095
H	3.5435337	5.8171751	-6.3759170
C	-1.1198222	2.8614061	-1.9807837
C	-0.7438997	2.7392381	-3.3032254
H	-0.5662530	1.7658393	-3.7523657
C	-0.6268250	3.8800077	-4.0869315
N	-0.8819629	5.1031889	-3.5982157
C	-1.2378609	5.2947027	-2.2685112
C	-1.4860159	6.5793596	-1.7444460
H	-1.4392646	7.4636417	-2.3723618
C	-1.7982634	6.7259313	-0.4026173
H	-1.9820984	7.7254794	-0.0078334
C	-1.8860384	5.6224399	0.4498105
H	-2.1255648	5.7542870	1.5049440

C	-1.6775282	4.3321606	-0.0323444
C	-1.7772802	3.1884498	0.8570626
N	-2.1813100	3.3496271	2.0810517
N	-2.3015428	2.2063389	2.7942425
C	-2.5535085	2.2719331	4.1501295
C	-2.8770578	0.9666527	4.8208280
C	-2.9085979	0.9686294	6.2258577
C	-3.2064809	-0.1970974	6.9309838
H	-3.2319584	-0.1836287	8.0206763
C	-3.4702255	-1.3811159	6.2435131
H	-3.6895018	-2.3056962	6.7775207
C	-3.4624808	-1.3969946	4.8389658
H	-2.6956528	1.9011021	6.7484643
C	-3.1715630	-0.2225246	4.1305205
H	-3.1190076	-0.2495599	3.0402480
O	-2.5152831	3.3350885	4.7781839
H	-2.2406859	1.2961017	2.2593638
H	-0.3279072	3.8334202	-5.1301060
C	-1.3453703	4.1407851	-1.4194586
C	2.9085979	-0.9686294	6.2258577
H	2.6956528	-1.9011021	6.7484643
C	2.8770578	-0.9666527	4.8208280
C	3.1715630	0.2225246	4.1305205
H	3.1190076	0.2495599	3.0402480
C	3.4624808	1.3969946	4.8389658
C	3.4702255	1.3811159	6.2435131
H	3.6895018	2.3056962	6.7775207
C	3.6918118	2.7223902	4.1758717
O	3.4251484	3.7823462	4.7366747
N	4.2097745	2.6765379	2.8880432
H	4.3880686	1.7842015	2.4109969
N	4.3806732	3.8232029	2.1933696
C	4.9710254	3.7071605	1.0486326
C	5.1158312	4.8816252	0.1970268
C	5.2253379	4.7230125	-1.2270481
C	5.2324201	3.4536768	-1.8521128
C	5.3720453	3.3564401	-3.2225278
H	5.4046704	2.3929850	-3.7266429
C	5.3702079	4.5161909	-3.9887721
N	5.3164785	5.7370866	-3.4328712
H	5.3594865	4.4832015	-5.0756848
H	5.0880008	2.5441870	-1.2654559
C	5.3013611	5.9001807	-2.0487386
C	5.3458690	7.1754316	-1.4527333
H	5.4651532	8.0745376	-2.0506349
C	5.2762475	7.2892060	-0.0734835
H	5.3439185	8.2780708	0.3809525
C	5.1377781	6.1603146	0.7448184
H	5.0685871	6.2676346	1.8266930
C	3.2064809	0.1970974	6.9309838
H	3.2319584	0.1836287	8.0206763
H	-1.0921713	5.8986640	-5.5177246
H	-1.3650116	7.0677062	-4.2357257
H	-1.2619401	1.9459925	-1.4034272
C	2.5535085	-2.2719331	4.1501295
O	2.5152831	-3.3350885	4.7781839
N	2.3015428	-2.2063389	2.7942425
H	2.2406859	-1.2961017	2.2593638
N	2.1813100	-3.3496271	2.0810517
C	1.7772802	-3.1884498	0.8570626
C	1.6775282	-4.3321606	-0.0323444
C	1.3453703	-4.1407851	-1.4194586
C	1.2378609	-5.2947027	-2.2685112
C	1.4860159	-6.5793596	-1.7444460
C	1.7982634	-6.7259313	-0.4026173
H	1.9820984	-7.7254794	-0.0078334
H	1.4392646	-7.4636417	-2.3723618
N	0.8819629	-5.1031889	-3.5982157
C	0.6268250	-3.8800077	-4.0869315
H	0.3279072	-3.8334202	-5.1301060
C	0.7438997	-2.7392381	-3.3032254
H	0.5662530	-1.7658393	-3.7523657
C	0.7138647	-6.2490220	-4.5510591
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C	-1.5484584	-6.1123509	-5.6382287

H	-1.1027651	-5.5370488	-6.4502414
C	-2.9312858	-6.2734638	-5.5977123
H	-3.5435337	-5.8171751	-6.3759170
C	-3.5320288	-6.9636551	-4.5417961
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H	-3.1647111	-8.1646490	-2.7751095
C	-5.0296695	-6.8888115	-4.3585100
N	-5.3164785	-5.7370866	-3.4328712
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C	-5.3458690	-7.1754316	-1.4527333
C	-5.2762475	-7.2892060	-0.0734835
C	-5.1377781	-6.1603146	0.7448184
H	-5.0685871	-6.2676346	1.8266930
C	-5.1158312	-4.8816252	0.1970268
C	-4.9710254	-3.7071605	1.0486326
N	-4.3806732	-3.8232029	2.1933696
N	-4.2097745	-2.6765379	2.8880432
H	-4.3880686	-1.7842015	2.4109969
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O	-3.4251484	-3.7823462	4.7366747
H	-5.3439185	-8.2780708	0.3809525
H	-5.4651532	-8.0745376	-2.0506349
C	-5.2253379	-4.7230125	-1.2270481
C	-5.2324201	-3.4536768	-1.8521128
C	-5.3720453	-3.3564401	-3.2225278
H	-5.4046704	-2.3929850	-3.7266429
H	-5.0880008	-2.5441870	-1.2654559
C	-5.3702079	-4.5161909	-3.9887721
H	-5.3594865	-4.4832015	-5.0756848
H	-5.4665669	-7.8013571	-3.9469566
H	-5.5475511	-6.6746139	-5.3003644
C	-1.3375580	-7.4126833	-3.6176370
H	-0.7254573	-7.8726911	-2.8418847
C	1.1198222	-2.8614061	-1.9807837
H	1.2619401	-1.9459925	-1.4034272
C	1.8860384	-5.6224399	0.4498105
H	2.1255648	-5.7542870	1.5049440
H	-1.5038247	2.1984370	0.4868995
H	5.3137390	2.7339035	0.6863384
H	1.5038247	-2.1984370	0.4868995
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H	-1.9820984	-7.7254794	0.0078334
C	-1.4860159	-6.5793596	1.7444460
H	-1.4392646	-7.4636417	2.3723618
C	-1.2378609	-5.2947027	2.2685112
N	-0.8819629	-5.1031889	3.5982157
C	-0.7138647	-6.2490220	4.5510591
H	-1.3650116	-7.0677062	4.2357257
H	-1.0921713	-5.8986640	5.5177246
C	0.7439272	-6.6348365	4.6223040
C	1.5484584	-6.1123509	5.6382287
H	1.1027651	-5.5370488	6.4502414
C	2.9312858	-6.2734638	5.5977123
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C	5.0296695	-6.8888115	4.3585100
N	5.3164785	-5.7370866	3.4328712
C	5.3702079	-4.5161909	3.9887721
H	5.3594865	-4.4832015	5.0756848
C	5.3720453	-3.3564401	3.2225278
H	5.4046704	-2.3929850	3.7266429
C	5.2324201	-3.4536768	1.8521128
H	5.0880008	-2.5441870	1.2654559
C	5.2253379	-4.7230125	1.2270481
C	5.1158312	-4.8816252	-0.1970268
C	4.9710254	-3.7071605	-1.0486326
H	5.3137390	-2.7339035	-0.6863384
N	4.3806732	-3.8232029	-2.1933696
N	4.2097745	-2.6765379	-2.8880432
C	3.6918118	-2.7223902	-4.1758717
O	3.4251484	-3.7823462	-4.7366747
C	3.4624808	-1.3969946	-4.8389658
C	3.1715630	-0.2225246	-4.1305205

H	3.1190076	-0.2495599	-3.0402480
C	2.8770578	0.9666527	-4.8208280
C	2.9085979	0.9686294	-6.2258577
C	3.2064809	-0.1970974	-6.9309838
H	3.2319584	-0.1836287	-8.0206763
H	2.6956528	1.9011021	-6.7484643
C	2.5535085	2.2719331	-4.1501295
O	2.5152831	3.3350885	-4.7781839
N	2.3015428	2.2063389	-2.7942425
H	2.2406859	1.2961017	-2.2593638
N	2.1813100	3.3496271	-2.0810517
C	1.7772802	3.1884498	-0.8570626
H	1.5038247	2.1984370	-0.4868995
C	1.6775282	4.3321606	0.0323444
C	1.3453703	4.1407851	1.4194586
C	1.2378609	5.2947027	2.2685112
C	1.4860159	6.5793596	1.7444460
C	1.7982634	6.7259313	0.4026173
H	1.9820984	7.7254794	0.0078334
H	1.4392646	7.4636417	2.3723618
N	0.8819629	5.1031889	3.5982157
C	0.6268250	3.8800077	4.0869315
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C	0.7438997	2.7392381	3.3032254
H	0.5662530	1.7658393	3.7523657
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H	1.3650116	7.0677062	4.2357257
H	1.0921713	5.8986640	5.5177246
C	-0.7439272	6.6348365	4.6223040
C	-1.5484584	6.1123509	5.6382287
H	-1.1027651	5.5370488	6.4502414
C	-2.9312858	6.2734638	5.5977123
H	-3.5435337	5.8171751	6.3759170
C	-3.5320288	6.9636551	4.5417961
C	-2.7189265	7.5772036	3.5778508
H	-3.1647111	8.1646490	2.7751095
C	-5.0296695	6.8888115	4.3585100
N	-5.3164785	5.7370866	3.4328712
C	-5.3013611	5.9001807	2.0487386
C	-5.3458690	7.1754316	1.4527333
C	-5.2762475	7.2892060	0.0734835
C	-5.1377781	6.1603146	-0.7448184
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C	-4.9710254	3.7071605	-1.0486326
H	-5.3137390	2.7339035	-0.6863384
N	-4.3806732	3.8232029	-2.1933696
N	-4.2097745	2.6765379	-2.8880432
H	-4.3880686	1.7842015	-2.4109969
C	-3.6918118	2.7223902	-4.1758717
O	-3.4251484	3.7823462	-4.7366747
C	-3.4624808	1.3969946	-4.8389658
C	-3.4702255	1.3811159	-6.2435131
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H	-3.2319584	0.1836287	-8.0206763
C	-2.9085979	-0.9686294	-6.2258577
H	-2.6956528	-1.9011021	-6.7484643
C	-2.8770578	-0.9666527	-4.8208280
C	-2.5535085	-2.2719331	-4.1501295
N	-2.3015428	-2.2063389	-2.7942425
N	-2.1813100	-3.3496271	-2.0810517
H	-2.2406859	-1.2961017	-2.2593638
O	-2.5152831	-3.3350885	-4.7781839
H	-3.6895018	2.3056962	-6.7775207
C	-3.1715630	0.2225246	-4.1305205
H	-3.1190076	0.2495599	-3.0402480
H	-5.3439185	8.2780708	-0.3809525
H	-5.4651532	8.0745376	2.0506349
C	-5.2253379	4.7230125	1.2270481
C	-5.2324201	3.4536768	1.8521128
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H	-5.0880008	2.5441870	1.2654559
C	-5.3702079	4.5161909	3.9887721
H	-5.3594865	4.4832015	5.0756848
H	-5.4665669	7.8013571	3.9469566
H	-5.5475511	6.6746139	5.3003644

C	-1.3375580	7.4126833	3.6176370
H	-0.7254573	7.8726911	2.8418847
C	1.1198222	2.8614061	1.9807837
H	1.2619401	1.9459925	1.4034272
C	1.8860384	5.6224399	-0.4498105
H	2.1255648	5.7542870	-1.5049440
C	3.4702255	-1.3811159	-6.2435131
H	3.6895018	-2.3056962	-6.7775207
H	4.3880686	-1.7842015	-2.4109969
C	5.1377781	-6.1603146	-0.7448184
H	5.0685871	-6.2676346	-1.8266930
C	5.2762475	-7.2892060	0.0734835
H	5.3439185	-8.2780708	-0.3809525
C	5.3458690	-7.1754316	1.4527333
H	5.4651532	-8.0745376	2.0506349
C	5.3013611	-5.9001807	2.0487386
H	5.4665669	-7.8013571	3.9469566
H	5.5475511	-6.6746139	5.3003644
C	2.7189265	-7.5772036	3.5778508
H	3.1647111	-8.1646490	2.7751095
C	1.3375580	-7.4126833	3.6176370
H	0.7254573	-7.8726911	2.8418847
C	-0.6268250	-3.8800077	4.0869315
C	-0.7438997	-2.7392381	3.3032254
C	-1.1198222	-2.8614061	1.9807837
H	-1.2619401	-1.9459925	1.4034272
H	-0.5662530	-1.7658393	3.7523657
H	-0.3279072	-3.8334202	5.1301060
C	-1.3453703	-4.1407851	1.4194586
C	-1.7772802	-3.1884498	-0.8570626
H	-1.5038247	-2.1984370	-0.4868995
S	3.0439995	-0.0000000	0.0000000
S	-3.0439995	0.0000000	0.0000000
O	-3.8784934	1.2335179	-0.0202132
O	3.8784934	1.2335179	0.0202132
O	3.8784934	-1.2335179	-0.0202132
O	-3.8784934	-1.2335179	0.0202132
O	-2.1403770	-0.0041055	-1.2180729
O	2.1403770	-0.0041055	1.2180729
O	2.1403770	0.0041055	-1.2180729
O	-2.1403770	0.0041055	1.2180729

SO_4^{2-} (C_1 symmetry)

S	0.0000000	0.0000486	-0.0001021
O	-0.0000001	-0.0001679	1.5178755
O	0.0000001	-1.4312497	-0.5057776
O	1.2396160	0.7156845	-0.5059978
O	-1.2396160	0.7156844	-0.5059980

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