Electronic Supplementary Information

Stepwise Enhancement of Fluorescence Induced by Anion Coordination and Guest Molecule Interaction

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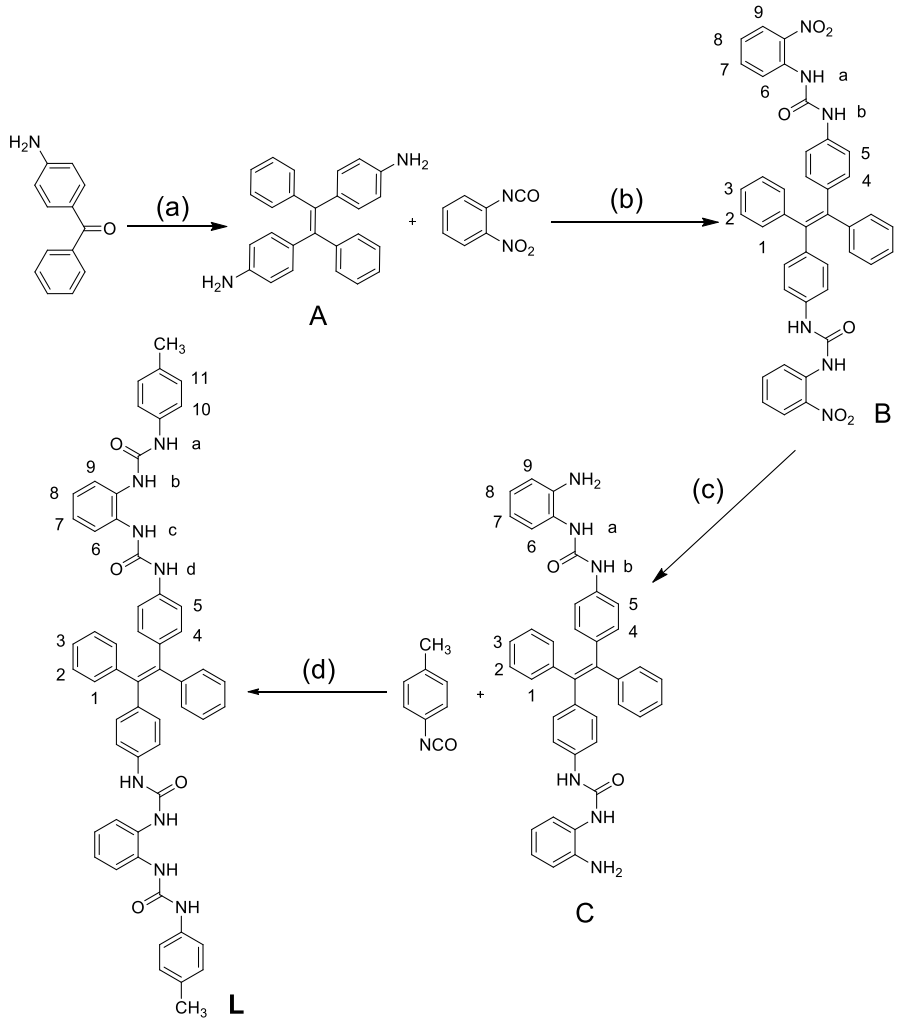
Experimental Procedures

S1. General considerations

o-Nitrophenylisocyanate, *p*-tolyl isocyanate isocyanate and 4-Aminobenzophenone were purchased from Alfa Aesar. All solvents and other reagents were of reagent grade quality and purchased commercially. All NMR spectra were recorded on a Varian unity INOVA-400 or Bruker AVANCE III-400 MHz spectrometer. Mass spectra were performed with a Bruker micrOTOF-Q II (Germany). Fluorescence spectra were recorded by a Hitachi F-4500 (Tokyo, Japan).



Scheme S1 Synthesis of ligand **L**. (a) zinc powder, $TiCl_4$, THF, reflux; (b) 2-nitrophenyl isocyanate, CH_2Cl_2, reflux; (c) $NH_2NH_2{\cdot}H_2O$, Pd/C 10% cat., EtOH, reflux; (d) p-tolyl isocyanate, THF/DMF, reflux.

S2. Synthesis of ligands L and complex 1

S2.1 Compound A

Compound A were synthesized according to the literature procedures.[1]

S2.2 Compound B

CH_2Cl_2 solution (30 mL) of compound **A** (1.09 g, 3.0 mmol) was added to a CH_2Cl_2 solution (20 mL) of *o*-nitrophenylisocyanate (1.20 g, 7.5 mmol). After refluxing under intense stirring for 3 h, the formed precipitate was filtered off and washed several times with CH_2Cl_2 and diethyl ether, and then dried in vacuum to yield analytically pure **B** as an orange-yellow solid (1.78 g, 86%). ^{1}H NMR (400 MHz, [D_6]DMSO, ppm): δ 9.79 (s, 2H, NHa), 9.56 (s, 2H, NHb), 8.25 (d, J = 8.0 Hz, 2H, H9), 8.08 (d, J = 8.0 Hz, 2H, H6), 7.68 (t, 2H, H8), 7.25 (d, J = 8.0 Hz, 4H, H5), 7.12-7.21 (8H, H3/H4/H7), 7.01 (d, J = 8.0 Hz, 4H, H2), 6.87 (d, J = 8.0 Hz, 4H, H1). ^{13}C NMR (100 MHz, [D_6]DMSO): 151.6 (CO), 143.6, 139.7, 137.6, 137.5, 135.0, 134.8, 131.4, 130.8, 127.9, 126.5, 125.4, 122.6, 122.3, 117.8. ESI-MS: *m/z* 713.2 $[M+Na]^+$.

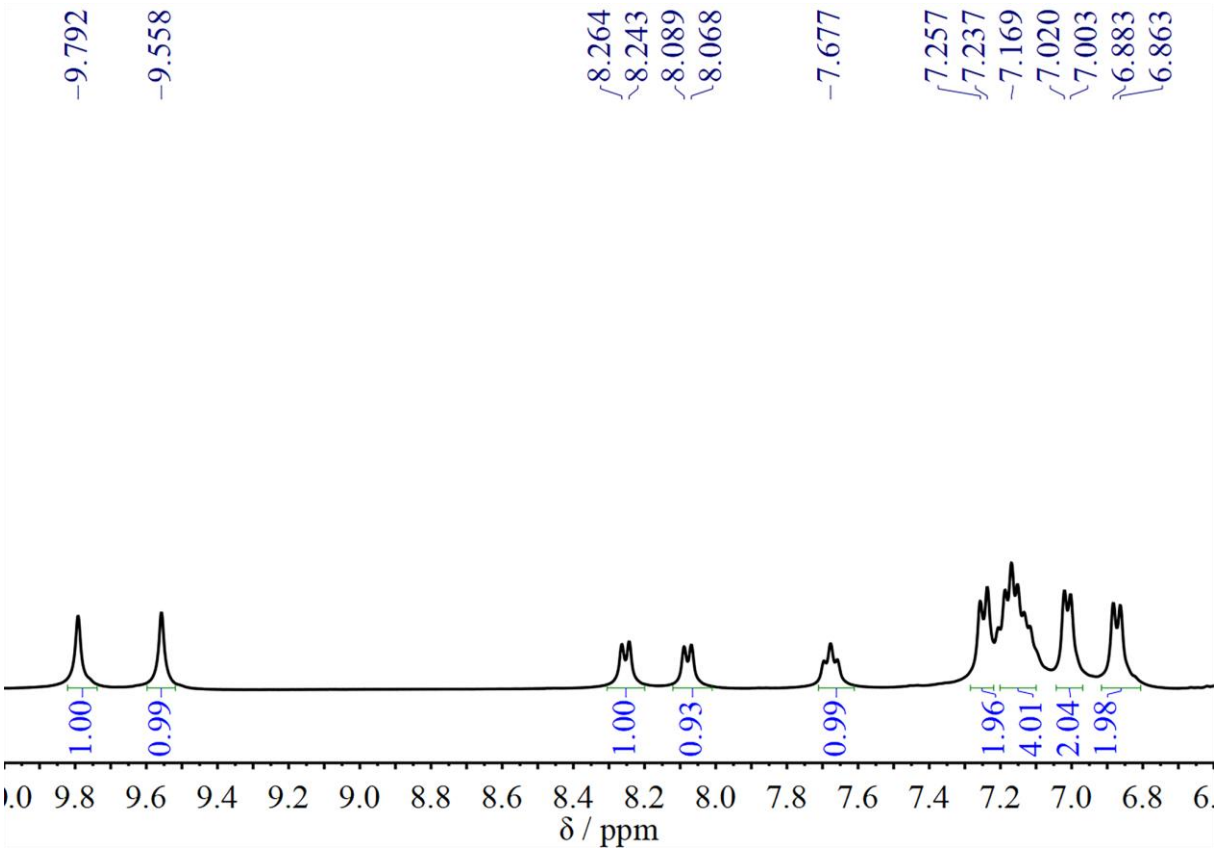


Fig. S1 ^{1}H NMR spectra of compound **B**.

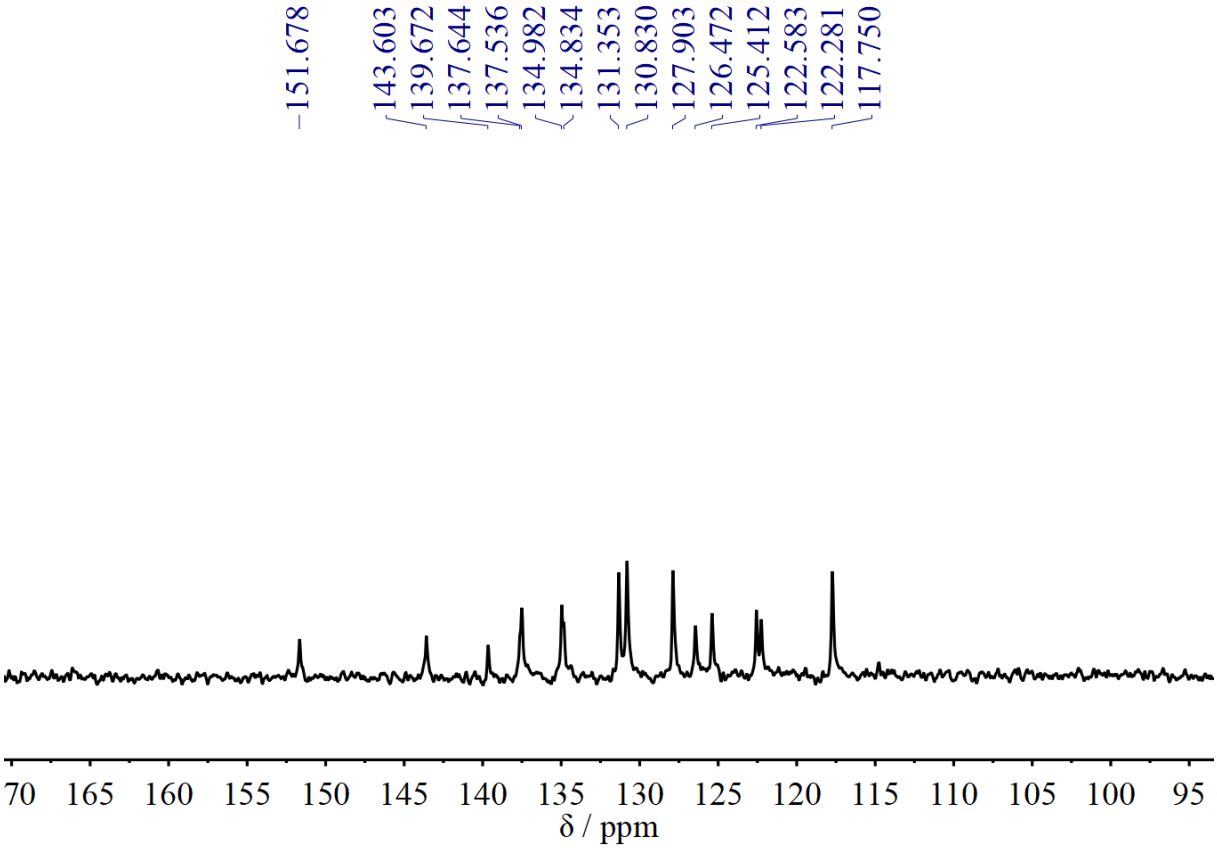


Fig. S2 ^{13}C NMR spectra of compound **B**.

S2.3 Compound C

Ethanol solution (5 mL) of hydrazine monohydrate (0.53 mL) was added dropwise to the suspension of **B** (0.60 g, 0.87 mmol) and Pd/C 10% (0.06 g, cat.) in ethanol (30 mL). After refluxing under intense stirring for 24 h, the solid was filtered off via suction filtration and then dissolved in DMF (5 mL) and filtered through Celite to remove Pd/C. The DMF solution was poured in water (200 mL), and the precipitate thus obtained was filtered off, washed several times with diethyl ether and dried over vacuum to give analytically pure **C** as a yellowish white solid (0.42 g, 77 %). ^{1}H NMR (400 MHz, [D_6]DMSO, ppm): δ 8.71 (s, 2H, NHb), 7.68 (s, 2H, NHa), 7.30 (d, J = 8.0 Hz, 2H, H6), 7.11-7.21 (10H, H4/5/7), 7.01 (d, J = 4.0 Hz, 4H, H2), 6.83 (6H, H1/H3), 6.73 (d, J = 4.0 Hz, 2H, H9), 6.56 (t, 2H, H8), 4.76 (s, 4H, NH_2).^{13}C NMR (100 MHz, [D_6]DMSO): 153.0 (CO), 143.8, 141.0, 139.5, 138.4, 136.5, 131.3, 130.8, 127.8, 126.4, 124.6, 124.5, 123.8, 117.1, 116.8, 115.9.

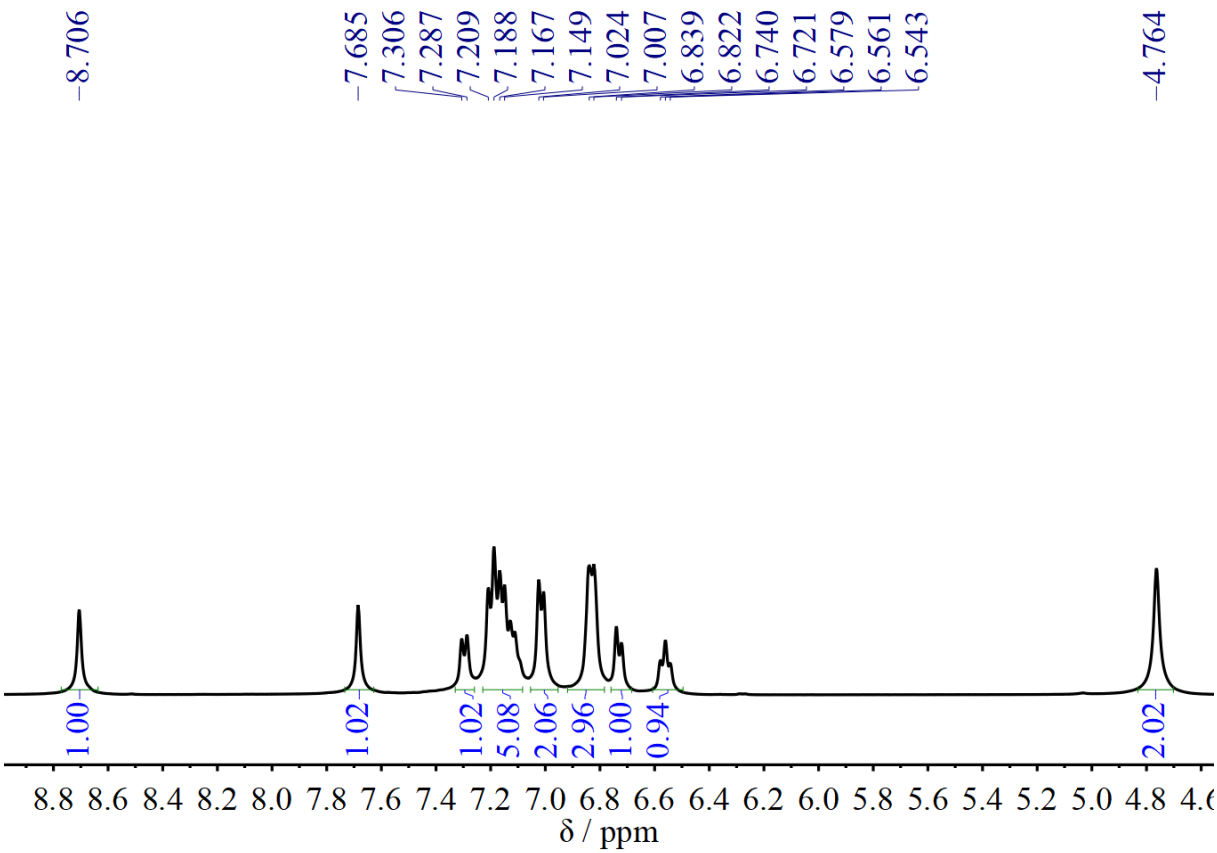


Fig. S3 ^{1}H NMR spectra of compound **C**.

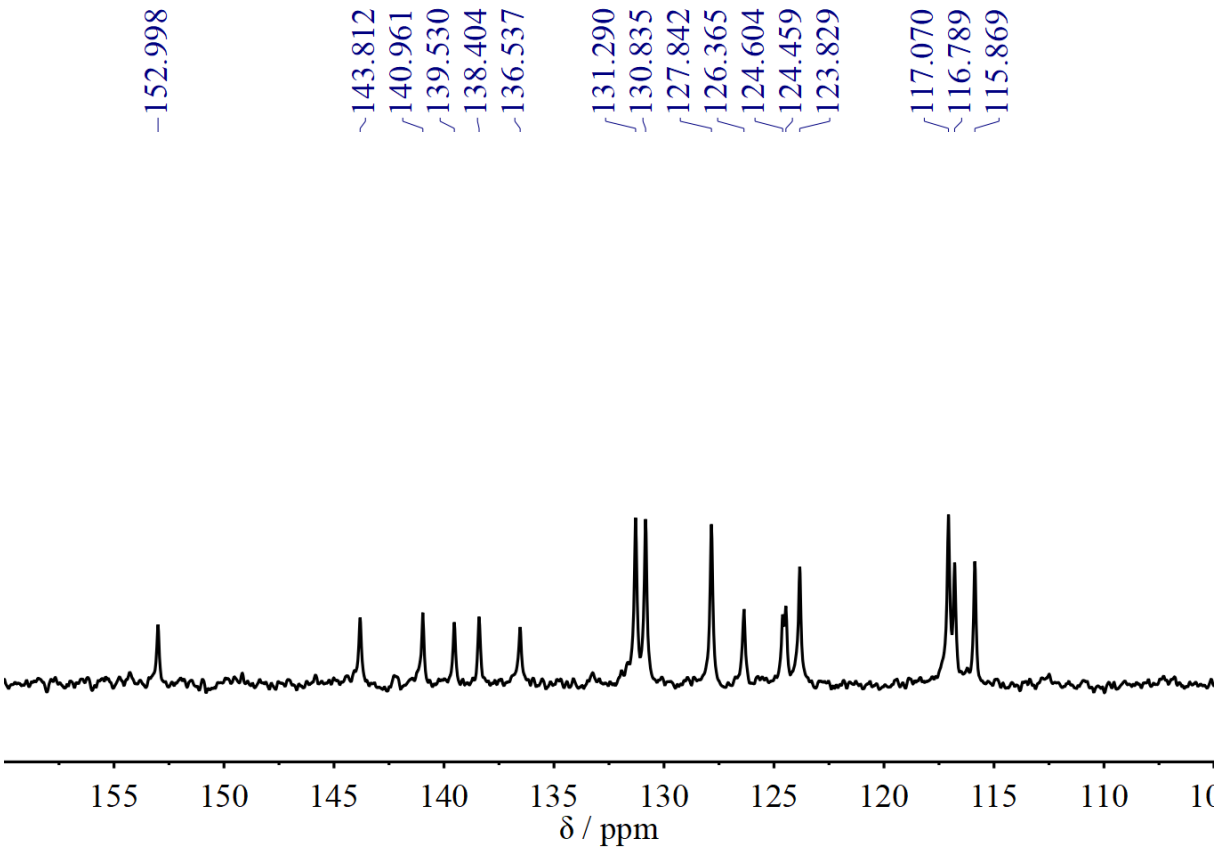


Fig. S4 ^{13}C NMR spectra of compound **C**.

S2.4 L

Compound **C** (0.76 g, 1.2 mmol) was dissolved in 10 mL DMF and the solution was added dropwise into 10 mL refluxing THF solution of p-tolyl isocyanate (454 ul, 3.6 mmol). The mixture was refluxed for 12 h, and the solvent was removed under reduced pressure and poured into 100 mL toluene. The precipitate was filtered off and washed several times with diethyl ether and then dried over vacuum to give **L** as a yellow solid (0.88 g, 82%). ^{1}H NMR (400 MHz, [D$_6$]DMSO, ppm): δ9.02 (s, 2H, NHd), 8.96 (s, 2H, NHc), 8.02 (s, 2H, NHb), 7.98 (s, 2H, NHa), 7.58 (d, J = 8.0 Hz, 2H, H6), 7.52 (d, J = 8.0 Hz, 2H, H9), 7.34 (d, J = 8.0 Hz, 4H, H5), 7.21 (d, J = 8.0 Hz, 4H, H10), 7.05-7.16 (14H, H1/ H2/ H3/ H7/ H8), 7.01 (d, J = 8.0 Hz, 4H, H4), 6.82 (d, J = 8.0 Hz, 4H, H11), 2.23 (s, 6H, CH$_3$). ^{13}C NMR (100 MHz, [D$_6$]DMSO): 153.3 (CO), 153.2 (CO), 143.8, 139.6, 138.2, 137.3, 136.8, 131.6, 131.3, 131.0, 130.9, 130.7, 129.3, 127.9, 126.5, 124.3, 124.2, 123.9, 118.4, 117.4, 20.4 (CH$_3$).

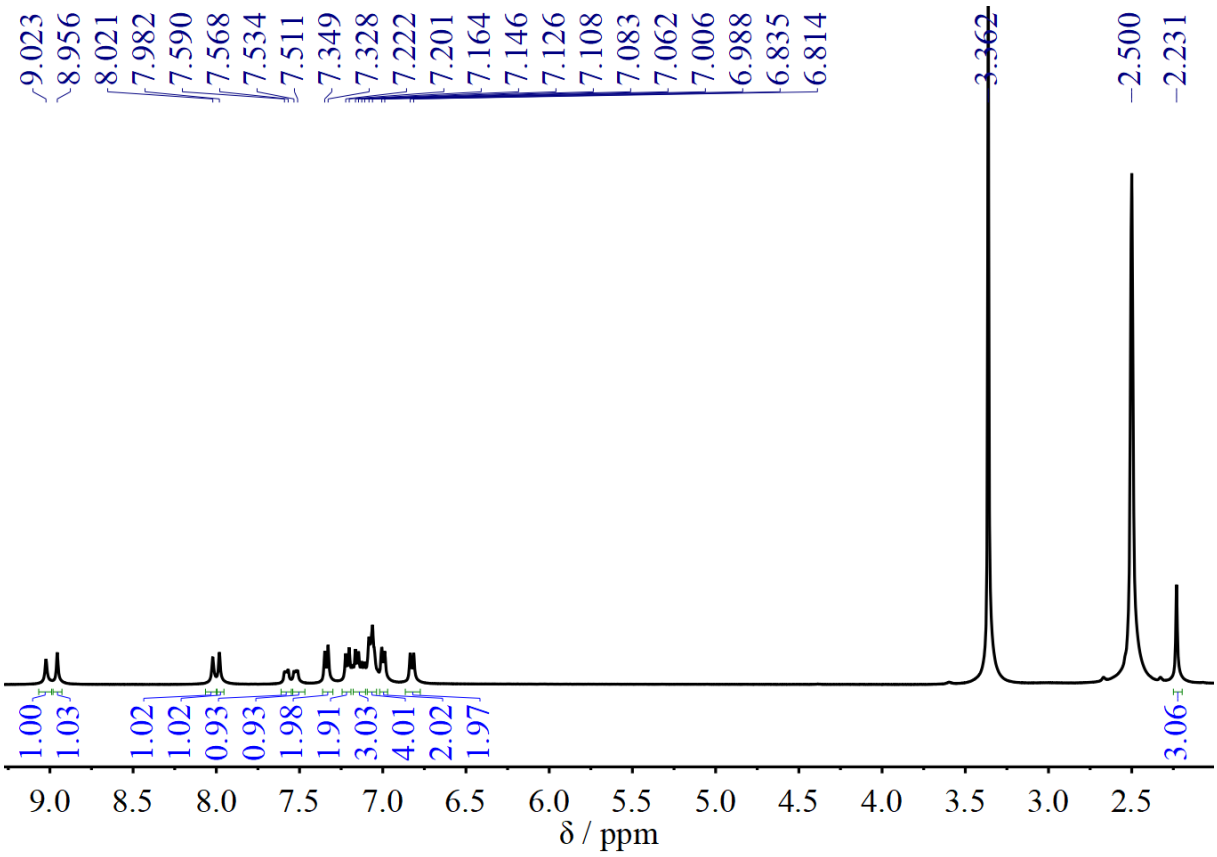


Fig. S5 ^{1}H NMR spectra of compound **L**.

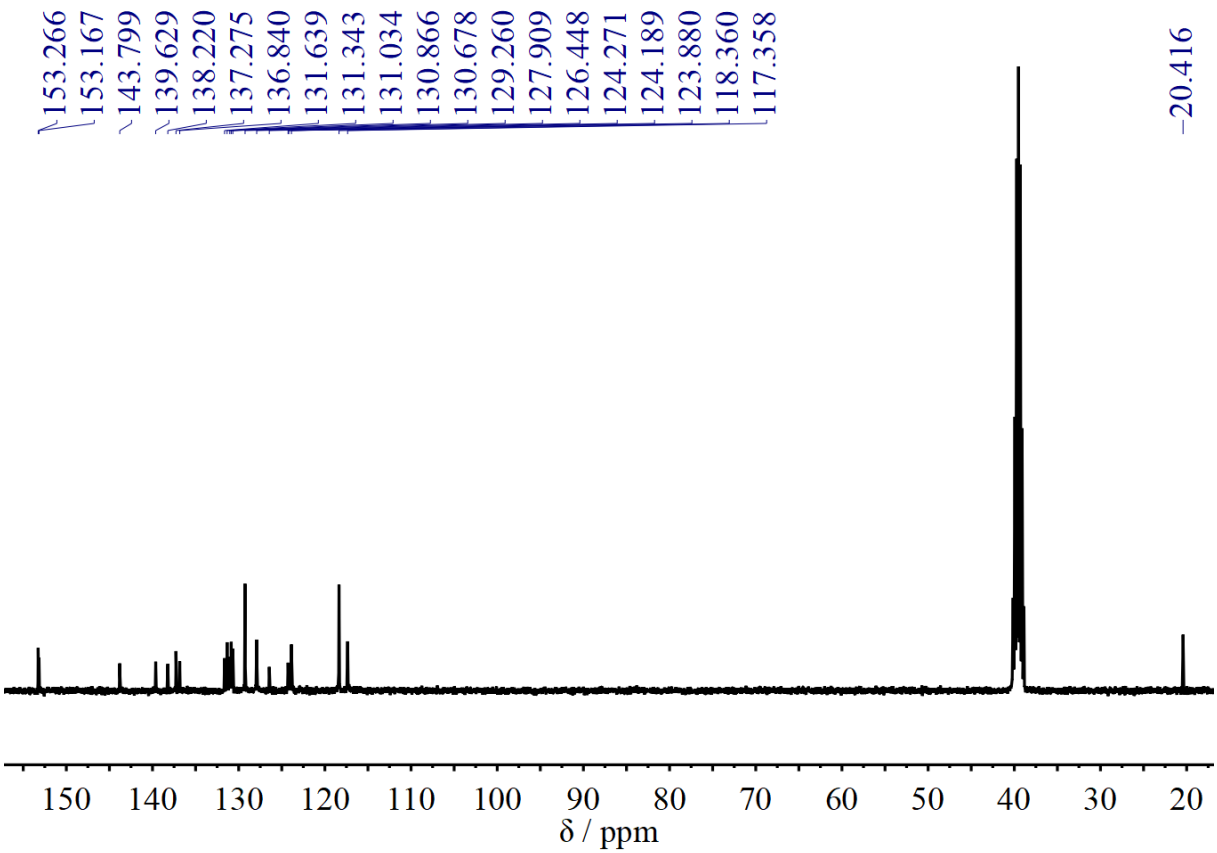


Fig. S6 ^{13}C NMR spectra of compound **L**.

S2.5 [K([18]crown-6)]$_4$[(HPO$_4$)$_2$(L)$_2$] (complex 1)

22 μL PO_4^{3-} (0.5 mol/L, generated in situ by mixing K_3PO_4, and [18]crown-6 in water was added to a solution of **L** (10 mg, 0.011 mmol) in acetone (1 mL). After stirring overnight at room temperature, a clear light yellow solution was obtained. Slow vapor diffusion of diethyl ether into this solution afforded light-yellow crystals of complex **1** within two weeks. ^{1}H NMR (400 MHz, [D$_6$]DMSO, ppm): δ11.05 (s, 2H, NHd), 10.90 (s, 4H, NHb/c), 10.17 (s, 2H, NHa), 7.85 (d, 4H, H6/9), 7.36 (d, 8H, H5/10), 7.16-7.04 (m, 10H, H1/2/3), 6.92 (d, 4H, H7/8), 6.68 (d, 8H, H4/11) 2.13 (S, 6H, CH_3).

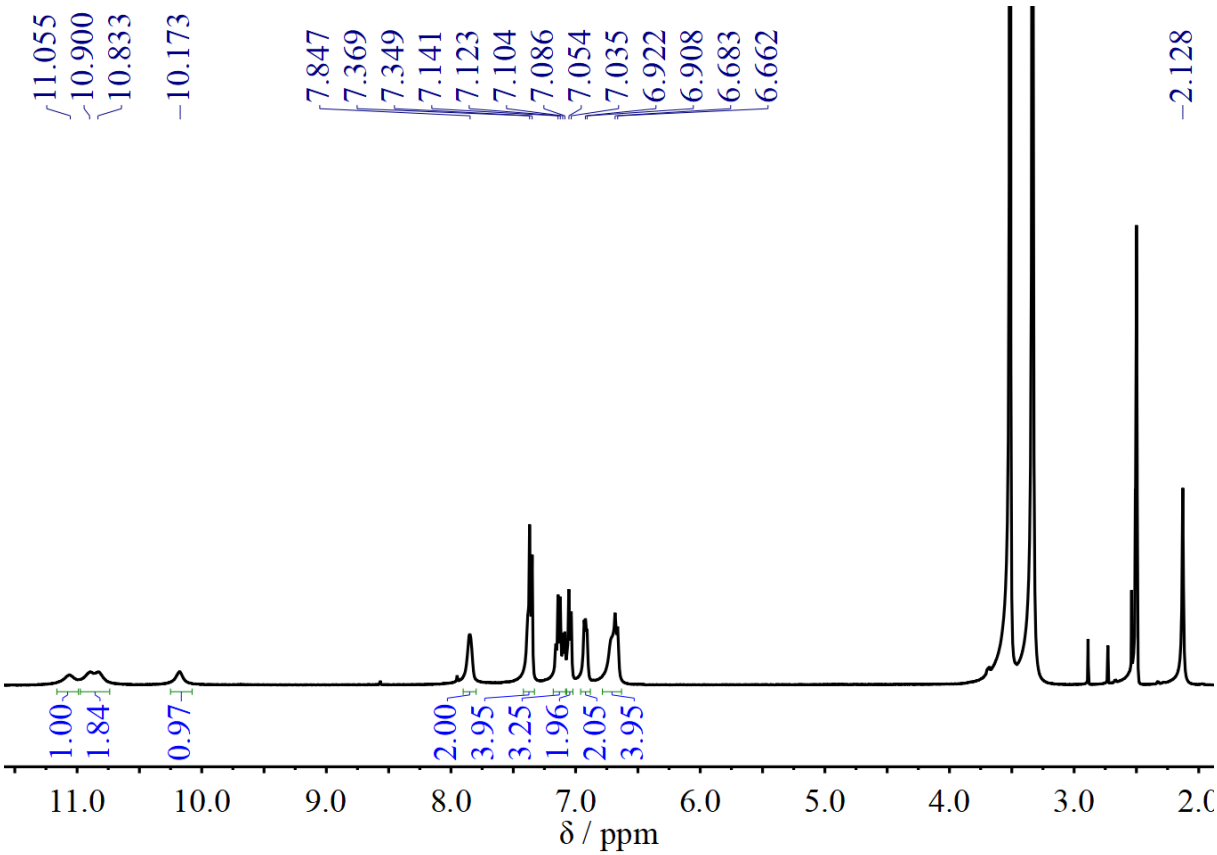


Fig. S7 ^{1}H NMR spectra of complex **1**.

S2.6 [(TBA)$_4$[(SO$_4$)$_2$(L)$_2$] (complex 2)

13 µL (TBA)$_2$SO$_4$ (aqueous solution, w/w 50%) was added to a solution of **L** (10 mg, 0.011 mmol) in acetone (1 mL). After stirring overnight at room temperature, a clear light yellow solution was obtained. Slow vapor diffusion of diethyl ether into this solution afforded light-yellow crystals of complex **2** within two weeks. ^{1}H NMR (400 MHz, [D$_6$]DMSO, ppm): δ9.74 (s, 4H, NHd/c), 9.56 (s, 2H, NHb), 9.15 (s, 2H, NHa), 7.95 (d, 2H, H6), 7.78 (d, 2H, H9), 7.35 (d, 4H, H5), 7.29 (d, 4H, H10), 7.15 (t, 4H, H7/8), 7.08 (t, 2H, H3), 7.00 (m, 8H, H1/2), 6.76 (d, 4H, H4), 6.72 (d, 4H, H11), 2.13 (S, 6H, CH$_3$).

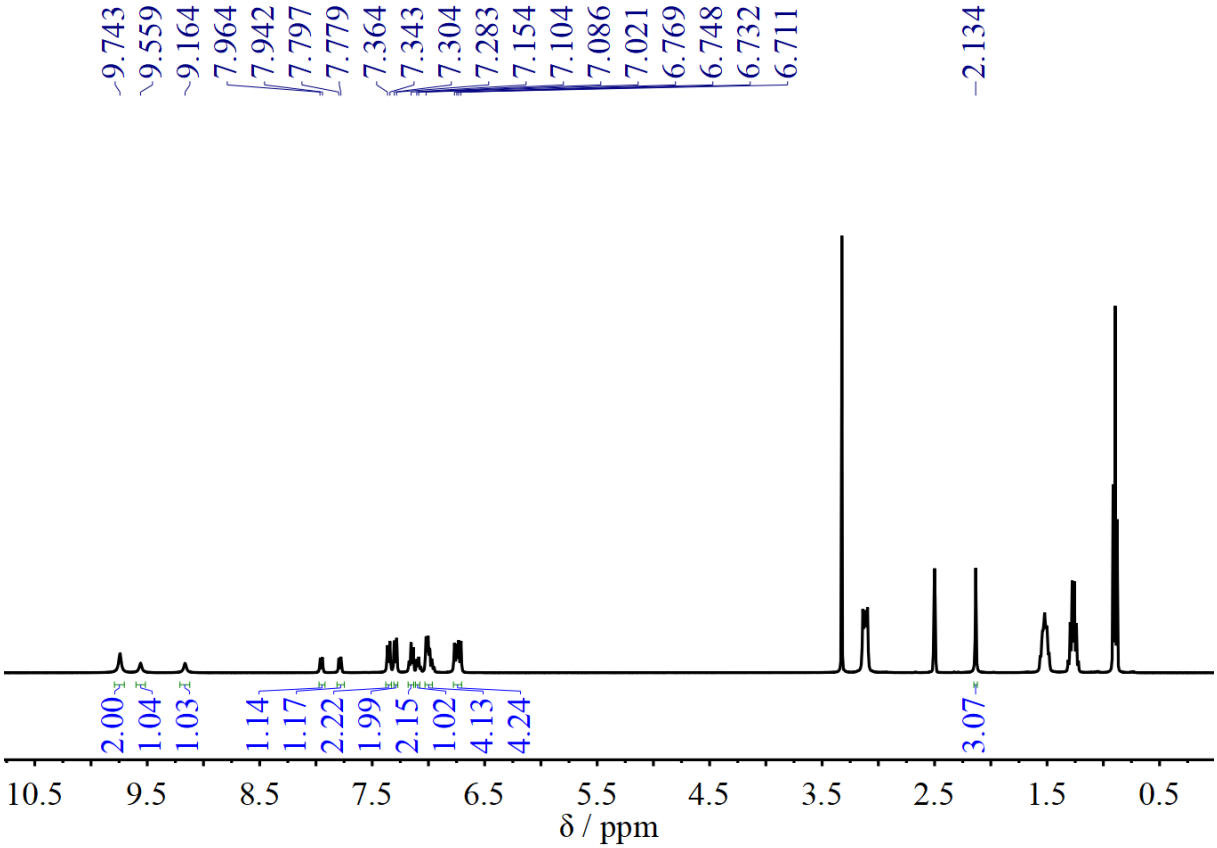


Fig. S8 ^{1}H NMR spectra of complex **2**.

S3. X-ray crystallography

Diffraction data for complexes **1** and **2** were collected on a Bruker SMART APEX II diffractometer at 298 K (complex **1**) and 100 K (complex **2**) with graphite-monochromated Mo *Kα* radiation (λ = 0.71073 Å). And complex **4** was collected with Bruker D8 Venture photon II, at low temperature (149.96 K) with Mo *Kα* radiation (λ = 0.71073 Å). An empirical absorption correction using SADABS was applied for all data.[2] The structures were solved by direct methods using the SHELXS program. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares on F^2 using the SHELXL program and OLEX2 1.2.[3]

In complex **1**, severely disordered solvent molecules in the crystal lattice (about three diethyl ether, one acetone and two H_2O molecules per formula, Z = 2), and the SQUEEZE command was employed in the refinement of the structure. Approximately 347 electron equivalents were removed from unit cell. In complex **4**, severely disordered solvent molecules in the crystal lattice (about one diethyl ether molecules per formula, Z = 4), and the SQUEEZE command was employed in the refinement of the structure. Approximately 194 electron equivalents were removed from unit cell. Crystallographic data and refinement details for complex **1**, **2** and **4** are given in Table S1. CCDC 2025857 for [K([18]crown-6)]$_4$[(HPO$_4$)$_2$(**L**)$_2$] (**1**), 2025855 for

$[TBA]_4[(SO_4)_2(\mathbf{L})_2]$ (**2**) and 2025856 for $[(MV)\mathbf{L}SO_4]_2$ (**4**). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystal data and structure refinement of complexes **1**, **2** and **4**.

Complex	**1**	**2**	**4**
Empirical formula	$C_{80}H_{97}K_2N_8O_{20}P$	$C_{91}H_{126}N_{10}O_9S$	$C_{74}H_{74}N_{10}O_{10}S_2$
*F*w	1599.83	1536.07	1327.55
Crystal color	light-yellow	yellow	red
T /K	296	100.15	149.96
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	*P-1*	*P-1*	$P2_1/n$
a /Å	12.111(2)	18.519(3)	9.5514(17)
b /Å	17.685(3)	20.485(4)	29.487(6)
c /Å	25.349(5)	23.872(4)	25.410(5)
α /°	74.055(4)	75.864(4)	90
β /°	88.954(5)	78.757(4)	95.276(5)
γ /°	74.796(4)	83.012(4)	90
V /Å^3	5029.0(16)	8587(3)	7126(2)
Z	2	4	4
D_{calc} /g cm^{-3}	1.057	1.188	1.237
F (000)	1692.0	3320	2800
μ /mm^{-1}	0.171	0.100	0.139
Crystal size (mm^3)	0.30×0.20×0.20	0.20×0.15×0.10	0.05×0.03×0.01
θ range (°)	1.29–27.47	1.12–25.38	2.21–25.41
Reflections collected	74883	61573	79206
Independent reflections	22165	31146	13116
Observed reflections [$I > 2\sigma(I)$]	8067	10342	7096
R_{int}	0.1305	0.1332	0.0886

Refined parameters	993	2043	842
Goodness of fit on F^2	1.043	1.005	1.116
$R1$ [$I > 2\sigma(I)$]	0.0994	0.1172	0.1099
$wR2$ (all data)	0.2412	0.2923	0.3059

Table S2. Hydrogen bonds around the HPO_4^{2-} ions in complex **1**.

HPO_4	D−H···A	d(D−H)	d(H···A)	d(D···A)	∠(DHA)
P1	N5−H5···O5	0.860	1.956	2.767	157
	N6−H6A···O5	0.860	1.980	2.754	149
	N3−H3A···O6	0.860	1.948	2.748	154
	N4−H4A···O6	0.860	1.994	2.794	154
	N7−H7A···O8	0.860	2.150	2.921	149
	N8−H8···O8	0.860	2.036	2.827	153
	N1−H1···O8	0.860	2.052	2.882	162
	N2−H2···O8	0.860	2.234	2.974	144

The structure of the dimer complex **1** possesses a *P-1* symmetry. Each HPO_4^{2-} moiety receives 8 N−H···O hydrogen bonds from the two bis(urea) subunits, in which HPO_4^{2-} ion itself interacts with four urea groups (N···O distances in the range 2.748−2.974 Å, average 2.833 Å; the N−H···O angles from 144° and 162°, average 152°). Four $[K([18]crown-6)]^+$ counter cations situate around complex **1** and form weak C−H···π interactions with the dangling phenyl rings of TPE (3.556-3.776 Å, Fig. S6b), contributing to restriction of the intramolecular rotation of TPE and fluorescence enhancement. Two of them coordinate to O atoms of urea groups and the other two interact with the O atoms of HPO_4^{2-}. The phenyl···phenyl separation between the two TPE cores within one A_2L_2 complex **1** is 4.105 Å (C18···C41; Fig. S6a).

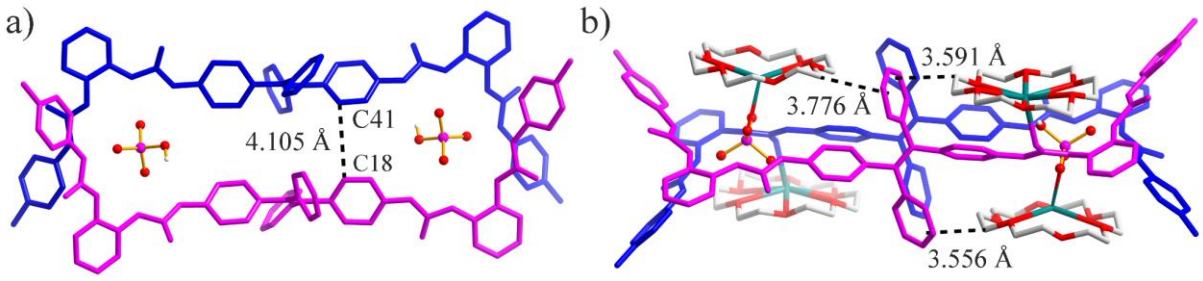


Fig. S9 a) Intermolecular phenyl···phenyl separations of the non-free TPE cores in the A_2L_2 complex **1**; b) C−H···π interactions between the free TPE phenyl and $[K([18]crown-6)]^+$ in complex **1**.

Table S3. Hydrogen bonds around the SO_4^{2-} ions in complex **2**.

SO_4	D−H···A	*d*(D−H)	*d*(H···A)	*d*(D···A)	∠(DHA)
S1	N9−H9···O10	0.880	2.241	3.023	148
	N10−H10A···O10	0.880	2.042	2.883	160
	N11−H11D···O9	0.880	2.101	2.920	155
	N12−H12A···O9	0.880	2.066	2.892	156
	N13−H13A···O12	0.880	1.995	2.857	166
	N14−H14A···O11	0.880	1.926	2.782	168
	N15−H15···O11	0.880	1.973	2.830	165
	N16−H16A···O10	0.880	2.094	2.850	143
S2	N1−H1···O14	0.880	2.150	2.938	149
	N2−H2···O13	0.880	2.022	2.853	157
	N3−H3···O13	0.880	2.081	2.943	167
	N4−H4A···O15	0.880	1.962	2.773	153
	N5−H5A···O14	0.880	2.105	2.974	174
	N6−H6A···O16	0.880	1.956	2.800	162
	N7−H7A···O16	0.880	2.053	2.825	146
	N8−H8A···O13	0.880	2.114	2.894	148

The structure of the dimer complex **2** possesses a *P-1* symmetry and the structure is the analogue of complex **1**. Two SO_4^{2-} moiety receives 8 N−H···O hydrogen bonds respectively, and the hydrogen bonds of SO_4^{2-} (S1) bonds with four urea groups (N···O distances in the range 2.782−3.023 Å, average 2.879 Å; the N−H···O angles from 143° and 168°, average 158°); SO_4^{2-} (S2) bonds with four urea groups (N···O distances in the range 2.773−2.974 Å, average 2.875 Å; the N−H···O angles from 146° and 174°, average 157°) Four TBA^+ counter-cations are located around the $[(SO_4)_2(\mathbf{L})_2]^{4-}$ moiety and two of them interact with phenyl rings of TPE cores through cation-π interactions (Fig. 1b). The shortest phenyl···phenyl separation between the two TPE cores within one $A_2\mathbf{L}_2$ complex **2** is 3.562 Å (C19···C38) and 3.585 Å (C64···C69; Fig. S10).

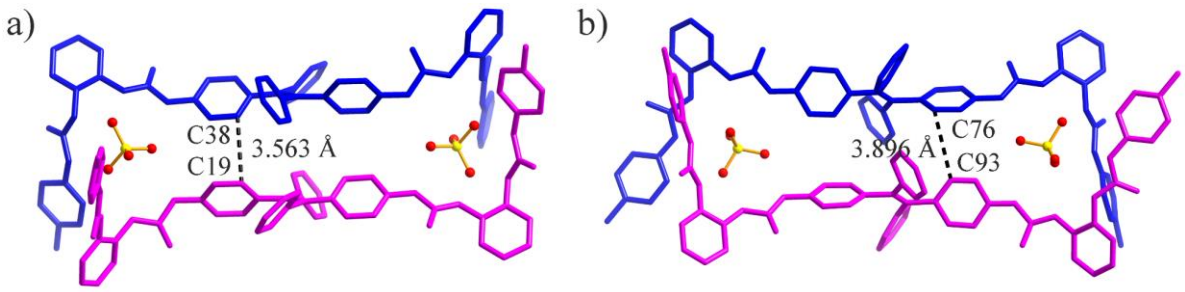


Fig. S10 Intermolecular phenyl···phenyl separations of the non-free TPE cores in the $A_2\mathbf{L}_2$ complex **2**: a) 3.563 Å (C19···C38) and b) 3.896 Å (C76···C93).

Table S4. Hydrogen bonds around the SO_4^{2-} ions in complex **4**.

SO_4	D−H···A	*d*(D−H)	*d*(H···A)	*d*(D···A)	∠(DHA)
S1	N1−H1···O8	0.880	2.076	2.892	155
	N2−H2···O8	0.880	2.232	3.035	152
	N3−H3···O5	0.880	1.928	2.800	173
	N5−H5···O7	0.880	2.034	2.889	164
	N6−H6···O6	0.880	1.930	2.800	170
	N7−H7···O6	0.880	2.022	2.887	169
	N8−H8···O5	0.880	2.036	2.793	145

The structure of the complex **4** possesses a $P2_1/n$ symmetry. Each SO_4^{2-} moiety receives 7 N−H···O hydrogen bonds from the two bis(urea) subunits, in which SO_4^{2-} ion itself interacts with four urea groups (N···O distances in the range 2.793−3.035 Å, average 2.871 Å; the N−H···O angles from 145° and 173°, average 161°). The shortest phenyl···phenyl separation between the two TPE cores within one $A_2\mathbf{L}_2$ complex **4** is 3.771 Å (C21···C38, Fig. S11). Compared with the structure of complex **2** (single sulfate complex) that the distance of phenyl···phenyl is relatively long which indicated that the non-covalent interactions between $A_2\mathbf{L}_2$ and MV^{2+} makes the distance between two ligands bigger.

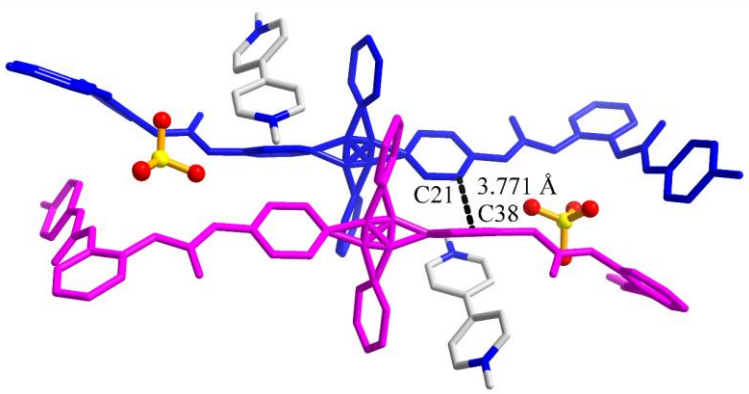


Fig. S11 Intermolecular phenyl···phenyl separations of the non-free TPE cores in the complex **4**.

S4. NMR spectroscopy

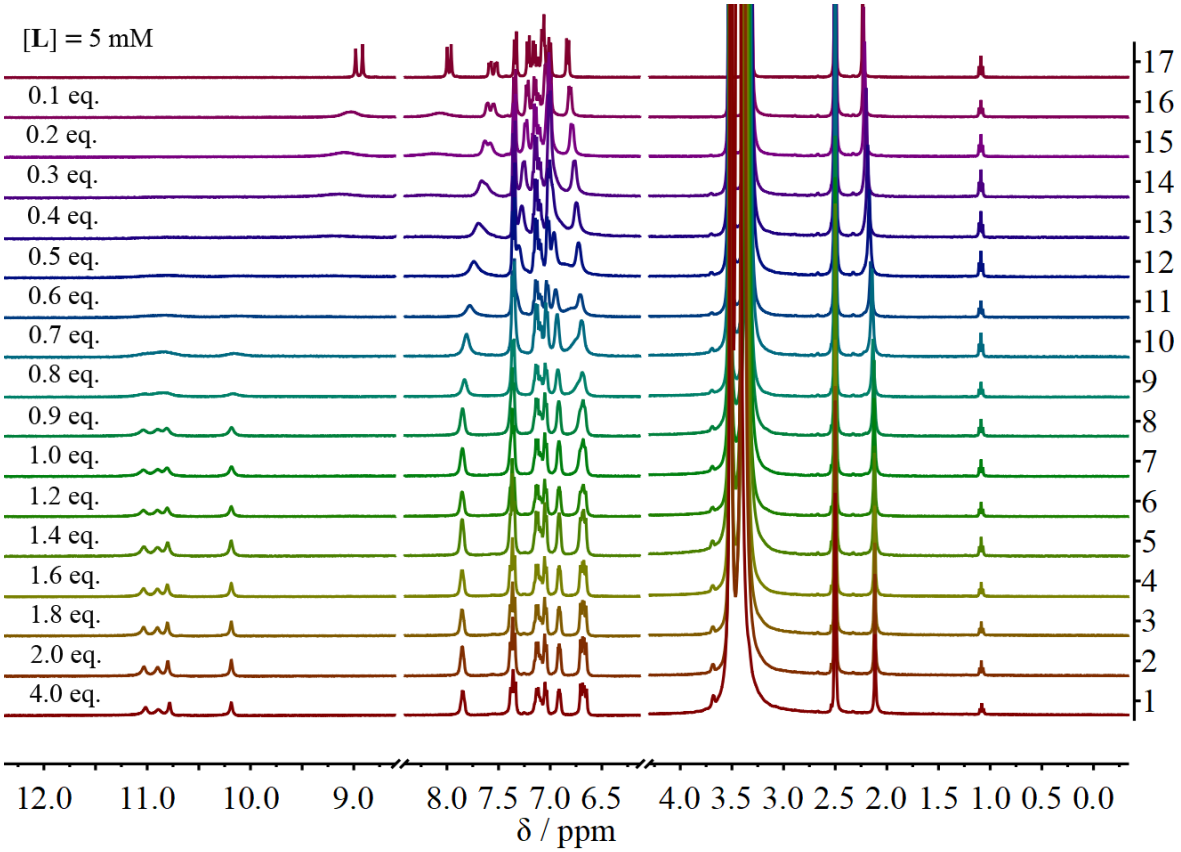


Fig. S12 ^{1}H NMR spectra (400 MHz, [D_6]DMSO) of **L** (5 mM) in presence of various equivalents of HPO_4^{2-} ions (added as $[K([18]crown-6)]^+$ salt).

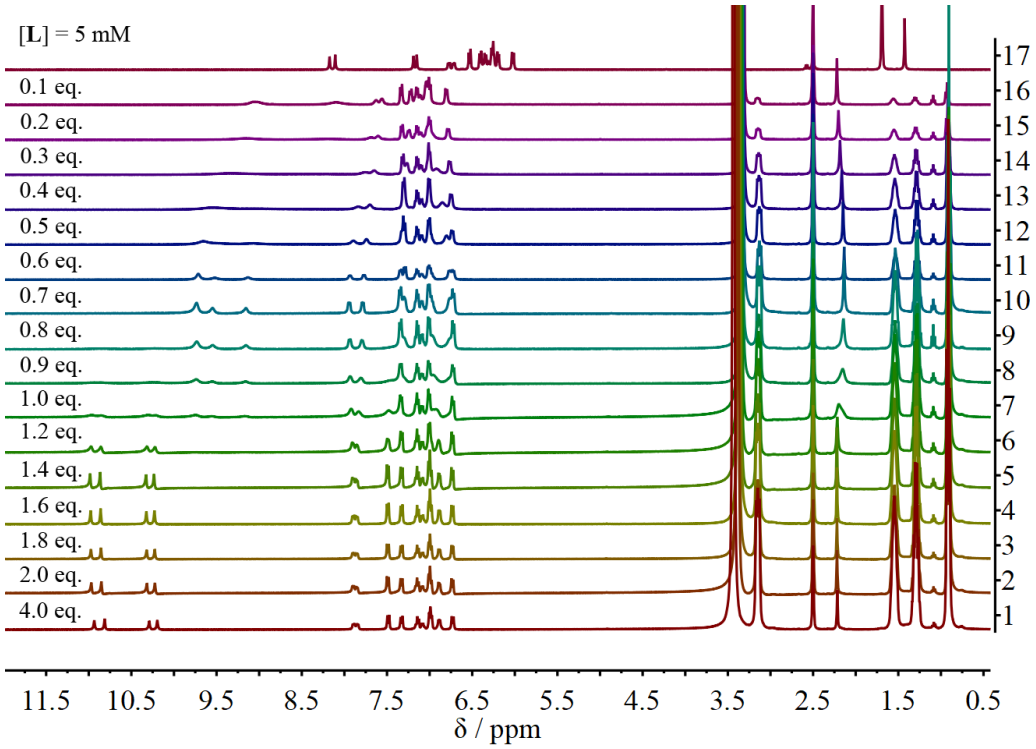


Fig. S13 ^{1}H NMR spectra (400 MHz, [D$_6$]DMSO) of **L** (5 mM) in presence of various equivalents of SO_4^{2-} ions (added as TBA^+ salt).

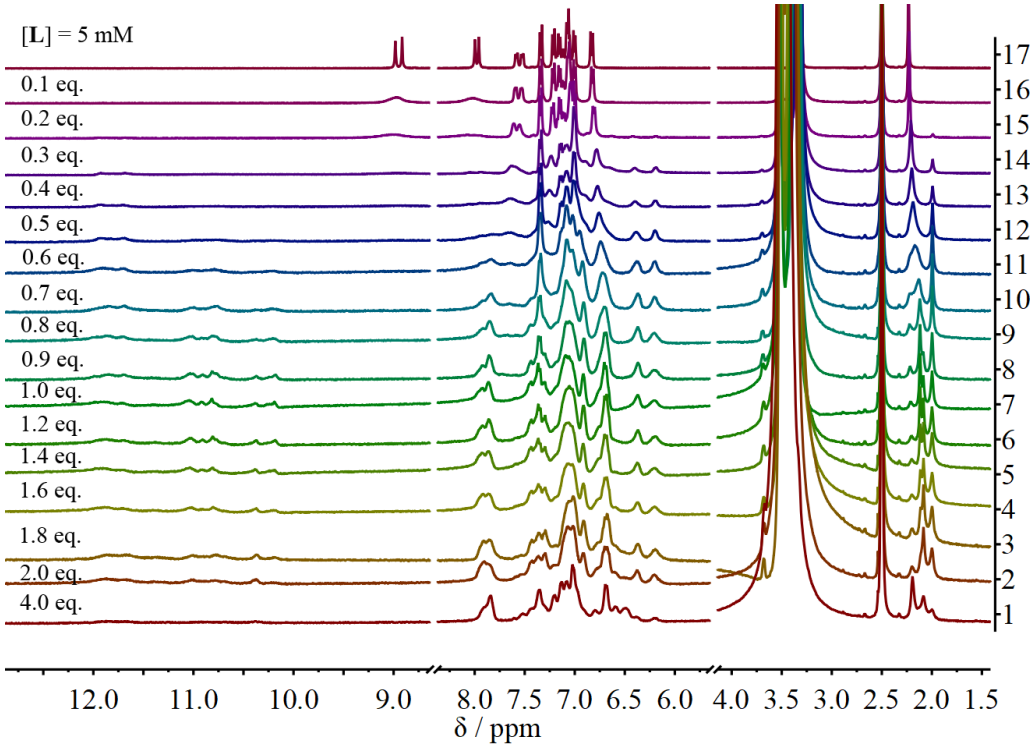


Fig. S14 ^{1}H NMR spectra (400 MHz, [D$_6$]DMSO) of **L** (5 mM) in presence of various equivalents of PO_4^{3-} ions (added as $[K([18]crown-6)]^+$ salt).

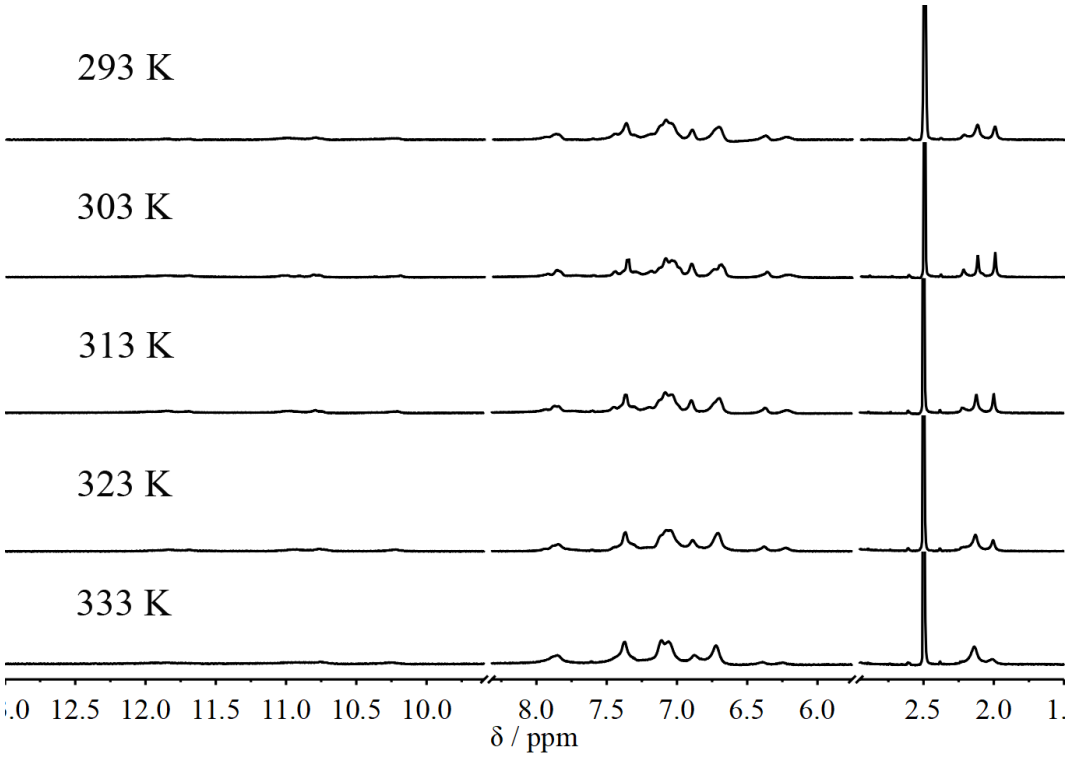


Fig. S15 ^{1}H NMR spectra (400 MHz, [D_6]DMSO) of **L** with 1.0 equiv of [K([18]crown-6)]$_3$$PO_4$ in different temperatures:293 K, 303 K, 313 K, 323 K, 333K.

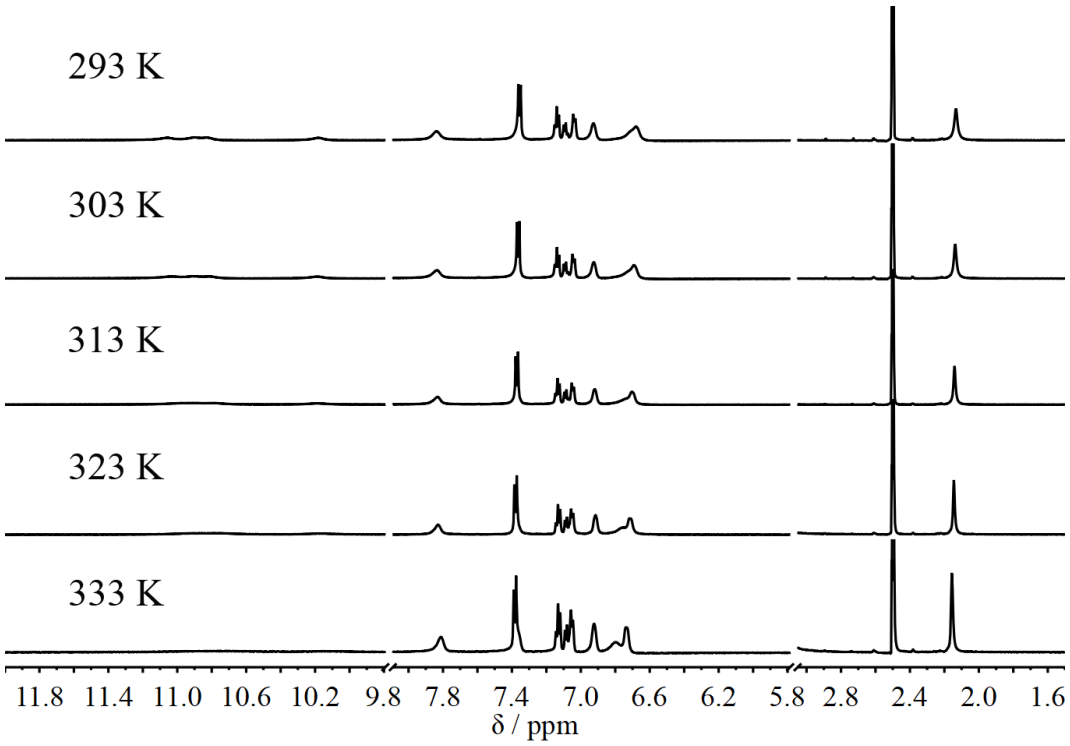


Fig. S16 ^{1}H NMR spectra (400 MHz, [D_6]DMSO) of **L** with 1.0 equiv of [K([18]crown-6)]$_2$$HPO_4$ in different temperatures:293 K, 303 K, 313 K, 323 K, 333K.

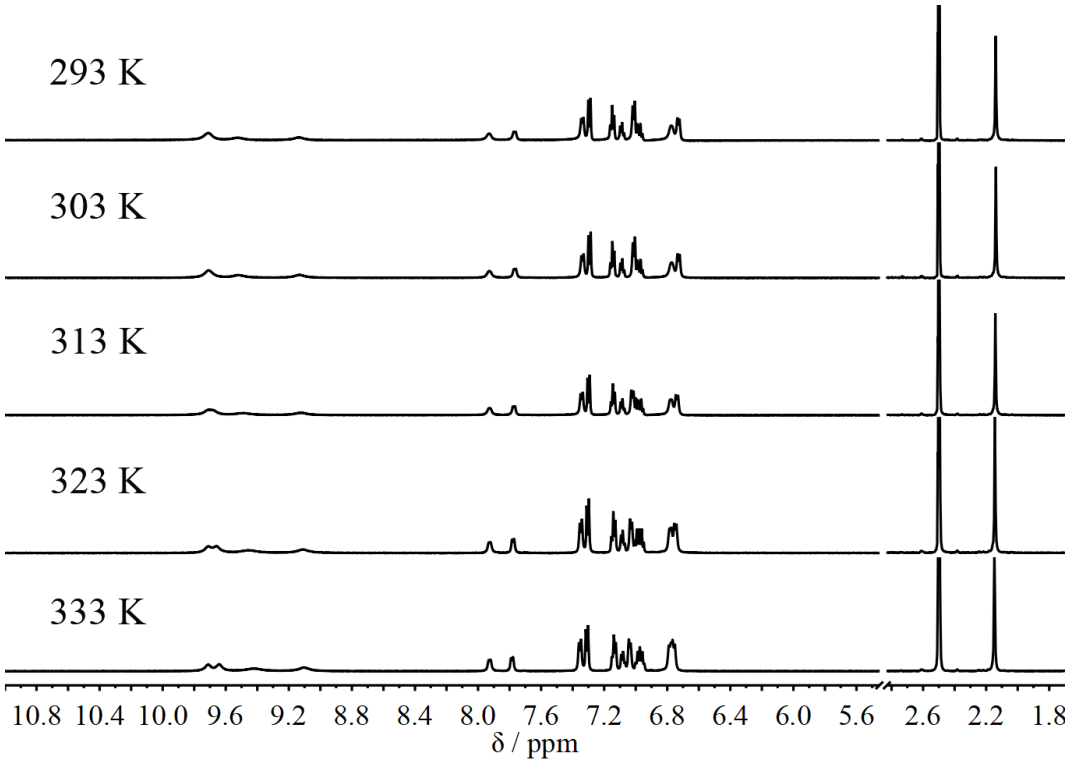


Fig. S17 ^{1}H NMR spectra (400 MHz, [D_6]DMSO) of **L** with 1.0 equiv of TBA_2SO_4 in different temperatures:293 K, 303 K, 313 K, 323 K, 333K.

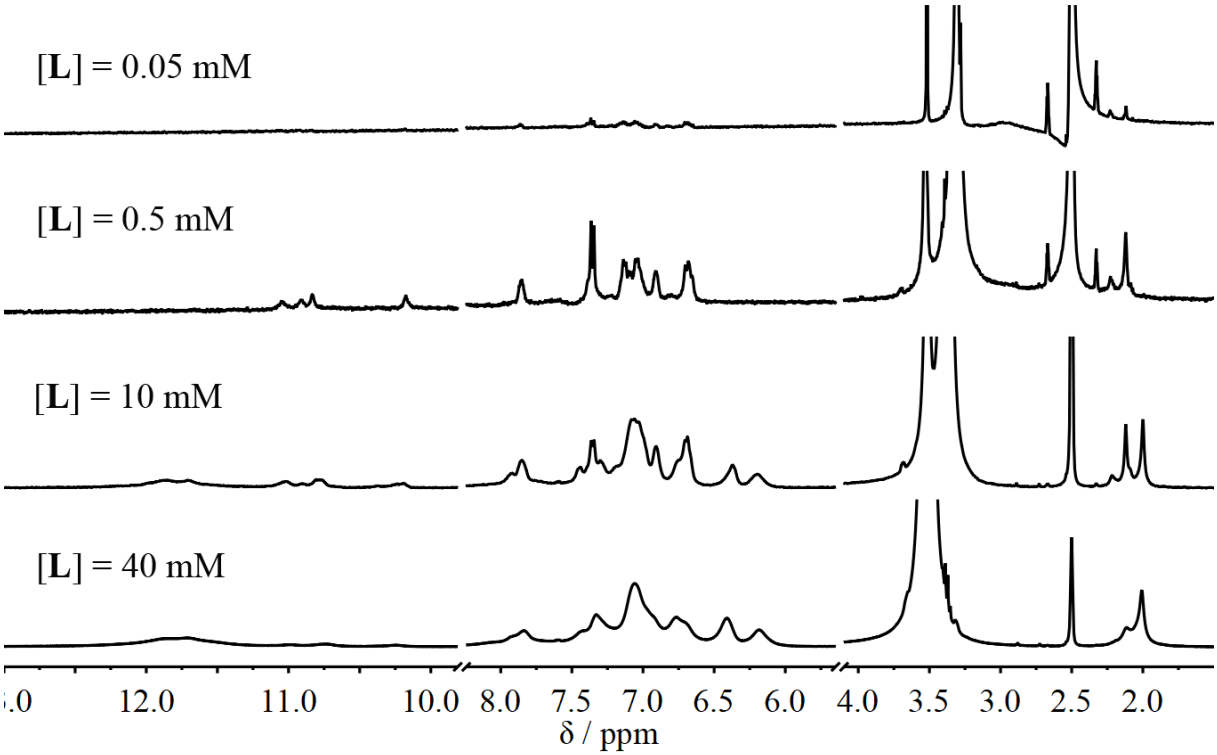


Fig. S18 ^{1}H NMR spectra (400 MHz, [D_6]DMSO) of **L** with 1.0 equiv of $[K([18]crown-6)]_3PO_4$ in different concentrations : [L] = 0.05, 0.5, 10, 40 mM.

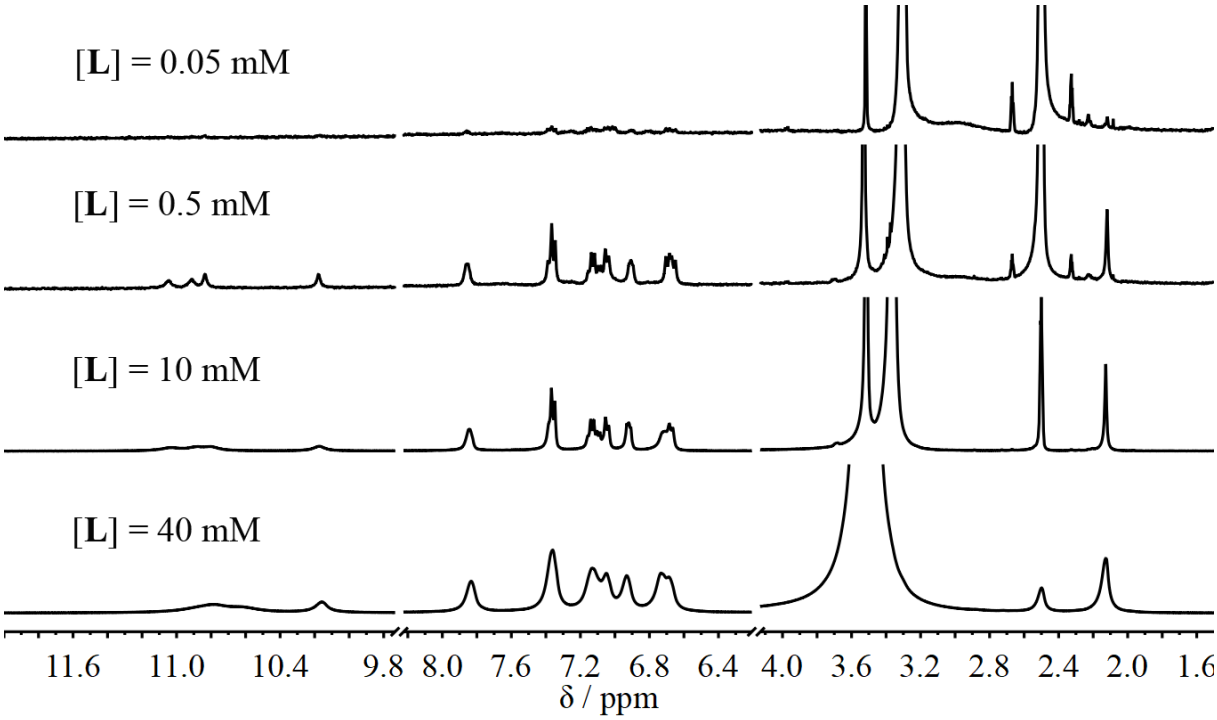


Fig. S19 ^{1}H NMR spectra (400 MHz, [D_6]DMSO) of **L** with 1.0 equiv of [K([18]crown-6)]$_2$HPO$_4$ in different concentrations : [L] = 0.05, 0.5, 10, 40 mM.

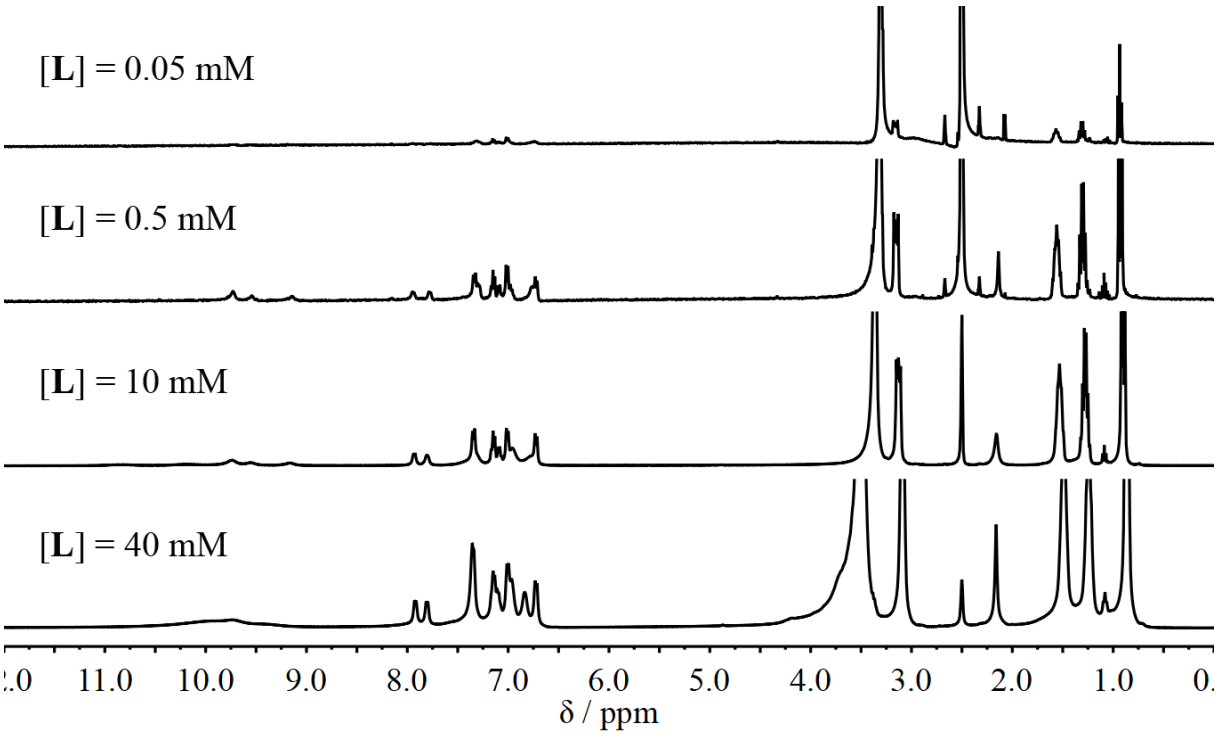


Fig. S20 ^{1}H NMR spectra (400 MHz, [D_6]DMSO) of **L** with 1.0 equiv of TBA$_2$SO$_4$ in different concentrations : [L] = 0.05, 0.5, 10, 40 mM.

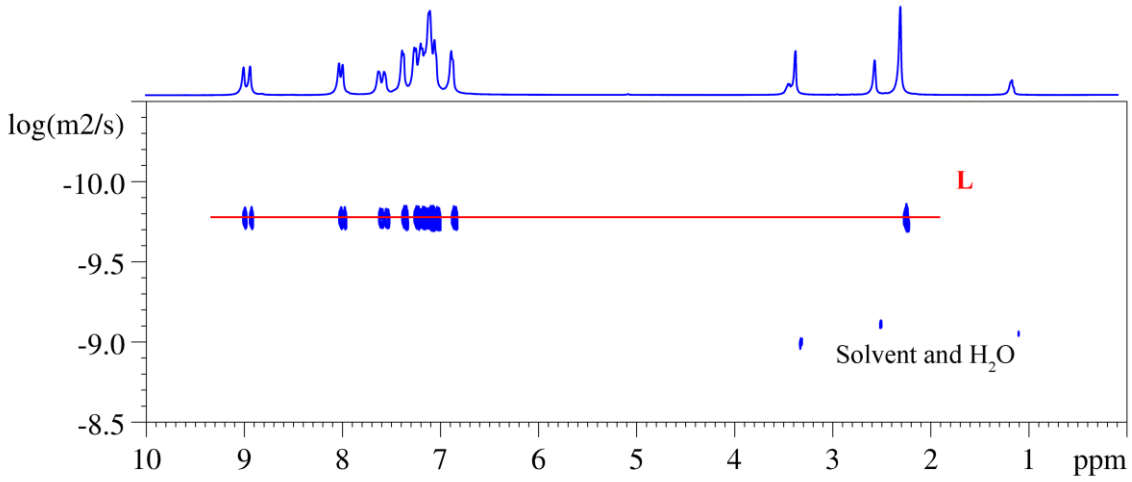


Fig. S21 ^{1}H-^{1}H DOSY spectrum of **L** (40mM) (400 MHz, [D$_6$]DMSO, 303 K).

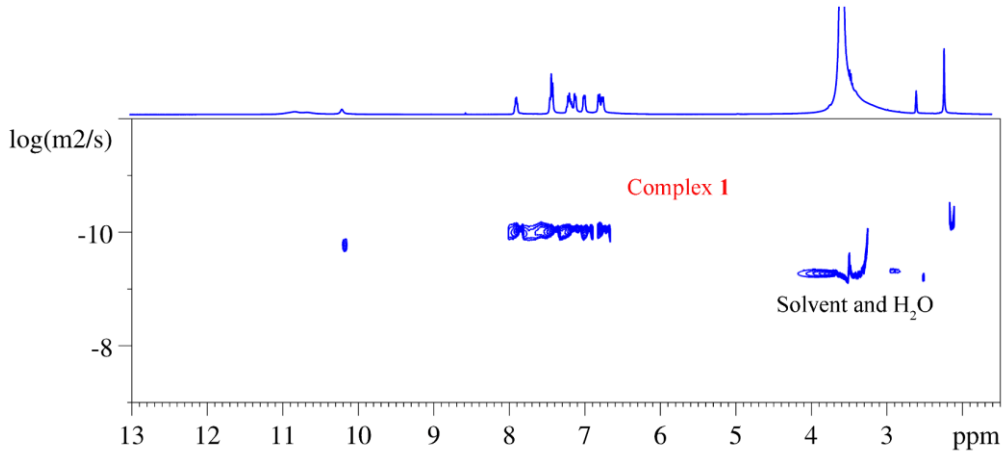


Fig. S22 ^{1}H-^{1}H DOSY spectrum of **L** (40mM) with 1.0 equiv of [K([18]crown-6)]$_2$HPO$_4$ (400 MHz, [D$_6$]DMSO, 303 K).

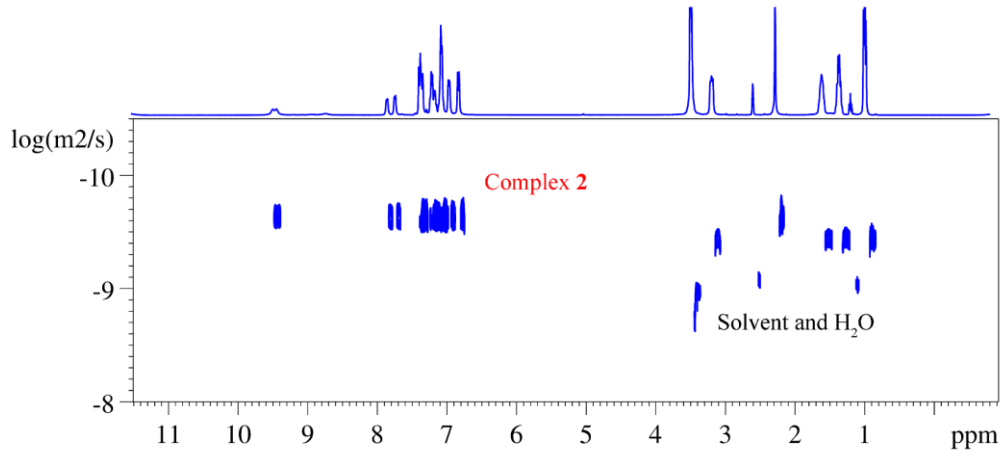


Fig. S23 ^{1}H-^{1}H DOSY spectrum of **L** (40mM) with 1.0 equiv of TBA$_2$SO$_4$ (400 MHz, [D$_6$]DMSO, 303 K).

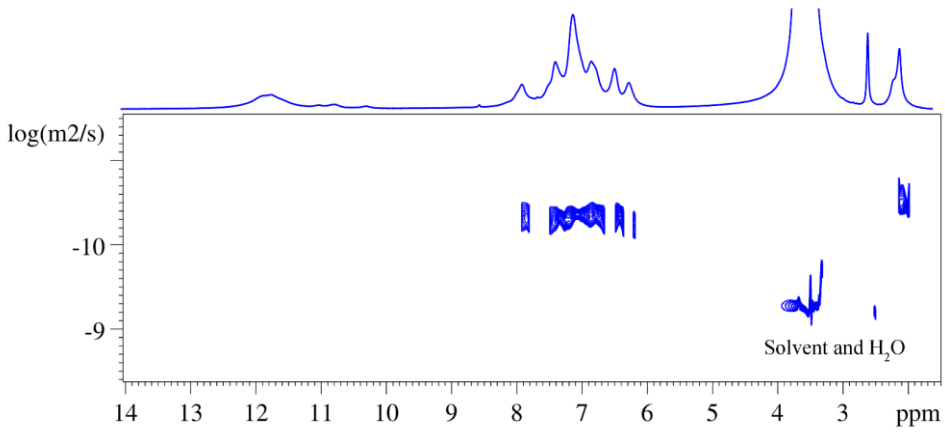


Fig. S24 ^{1}H-^{1}H DOSY spectrum of **L** (40mM) with 1.0 equiv of [K([18]crown-6)]$_3$PO$_4$ (400 MHz, [D$_6$]DMSO, 303 K).

Two forms of urea hydrogen were observed when 1.0 equiv phosphate anions (generated in situ from K$_3$PO$_4$, and [18]crown-6) was added to the [D$_6$]DMSO solution of **L** (Figure S1), one owes to PO_4^{3-} ions (11.70 ppm to 11.97 ppm) and the other one belongs to HPO_4^{2-} ions (10.19 ppm to 11.02 ppm) based on our previous work.[4] However, the ^{1}H NMR spectrum of the complex becomes to a single form after MVCl$_2$ added to the above solution, which is the same with the ^{1}H NMR spectrum of complex **1**. Namely, the complex will become the assemble with HPO_4^{2-} ions after adding MVCl$_2$. What is more, four ^{1}H NMR signals (9.10 ppm, 8.85 ppm, 8.56 ppm and 7.99 ppm) which should belong to some impurity from MVCl$_2$ due to the alkaline environment.

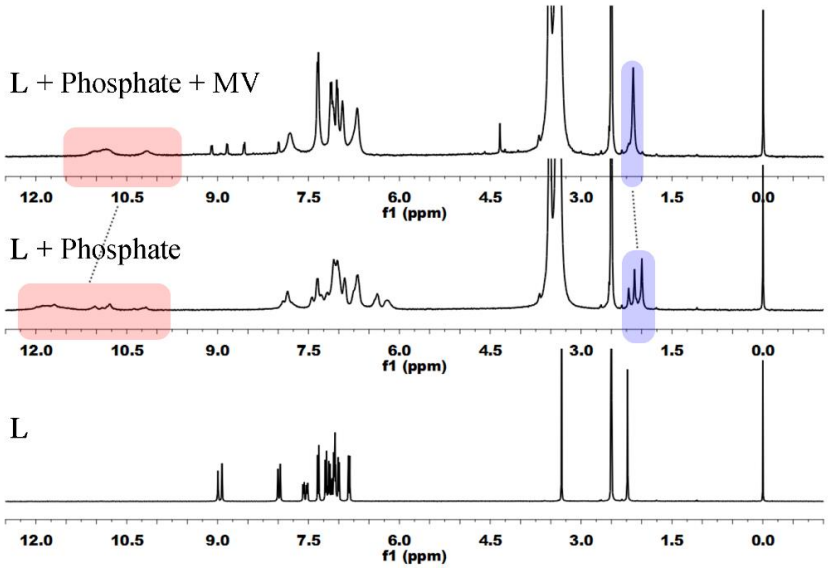


Fig. S25 ^{1}H NMR spectra (400 MHz, 298 K, [D$_6$]DMSO) of **L**, **L** with 1.0 equiv phosphate anions and **L** with 1.0 equiv phosphate anions and MVCl$_2$. The read areas are the signals of urea hydrogen and the blue areas are the signals of methyl groups.

S5. High-resolution MS studies

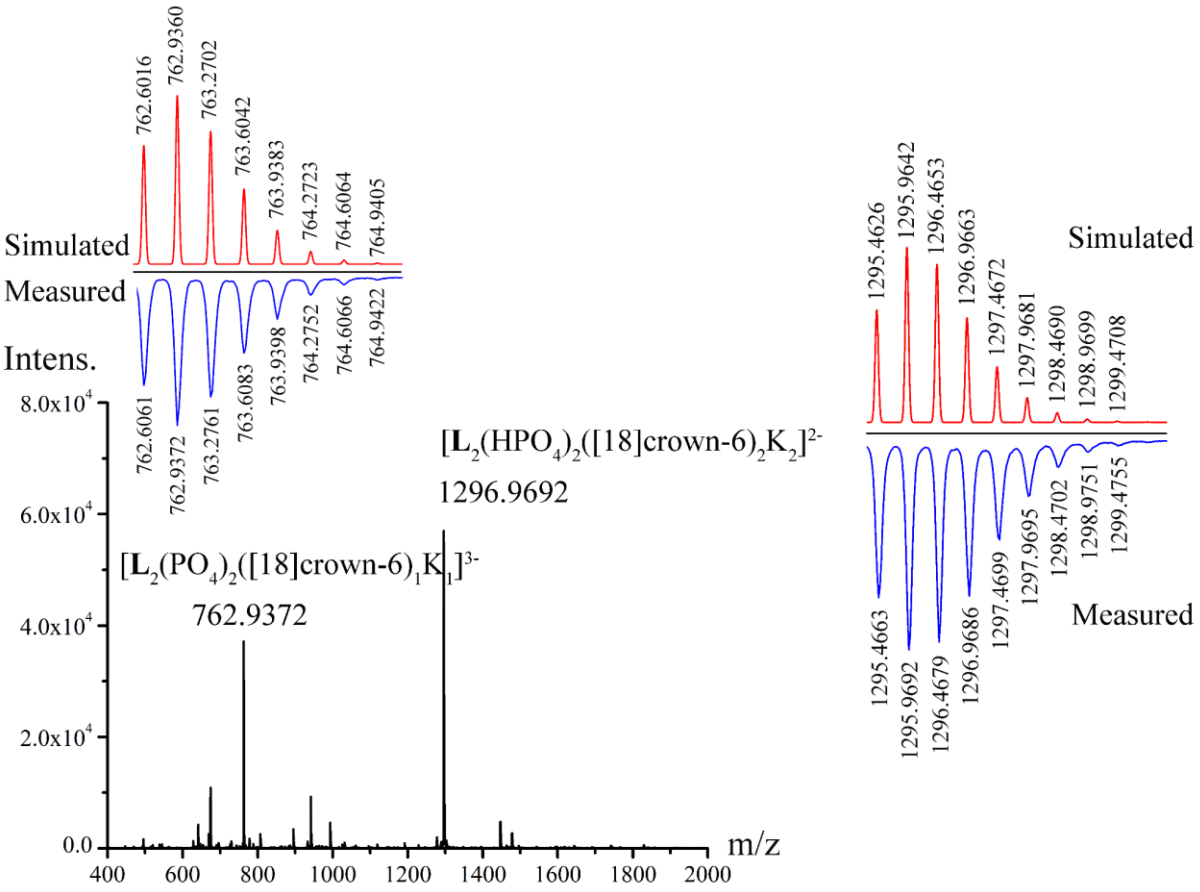


Fig. S26 High-resolution ESI-mass spectra of phosphate complex **1**.

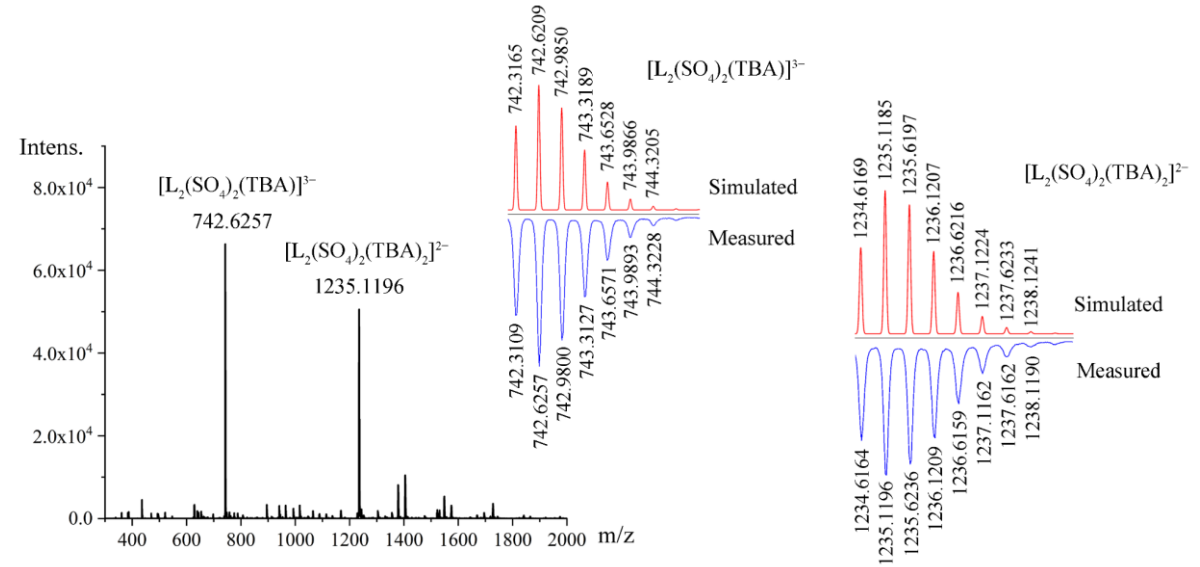


Fig. S27 High-resolution ESI-mass spectra of sulfate complex **2**.

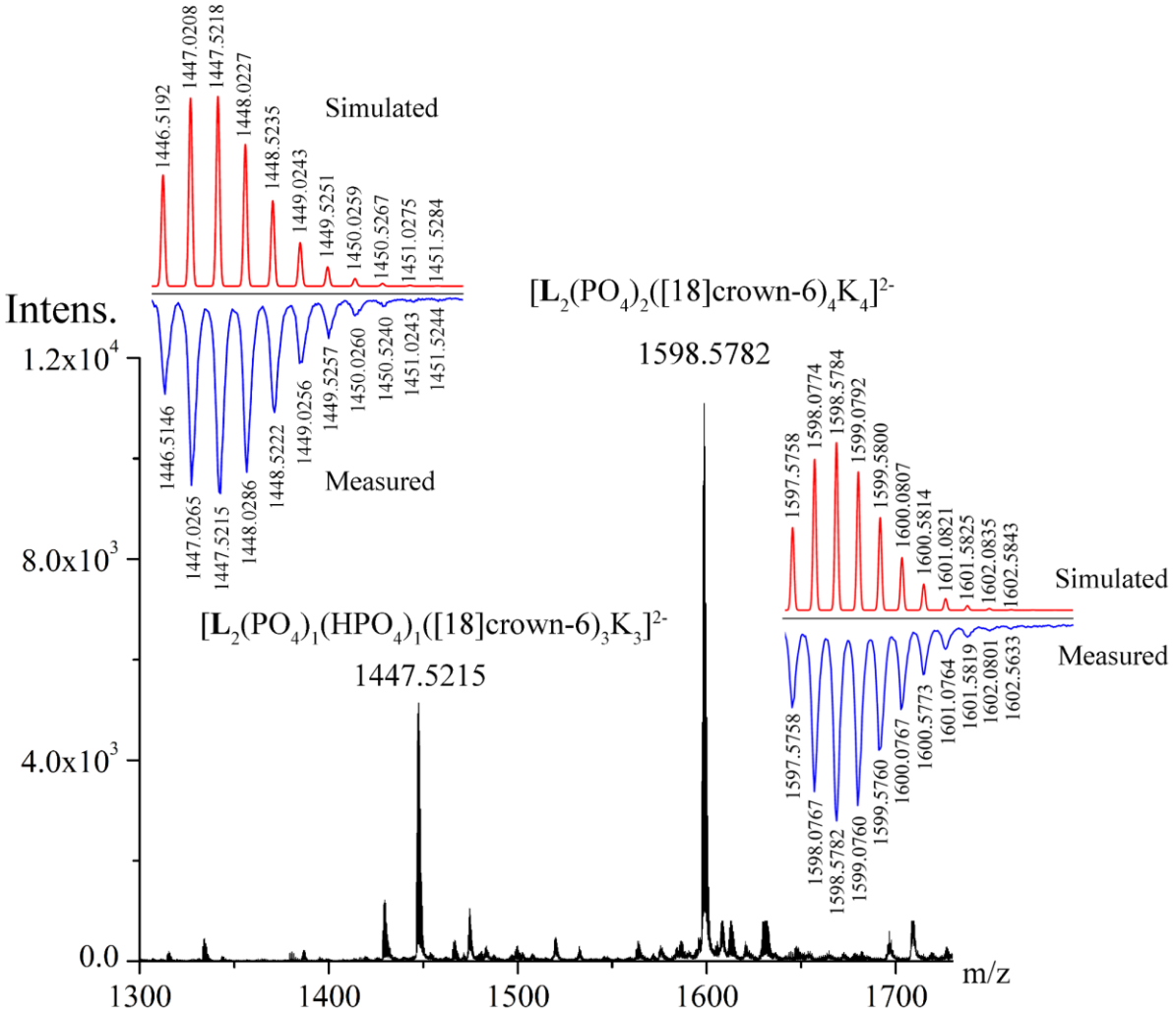


Fig. S28 High-resolution ESI-mass spectra of **L** with 1.0 equiv phosphate anions.

S6. Fluorescence and UV-Vis spectra

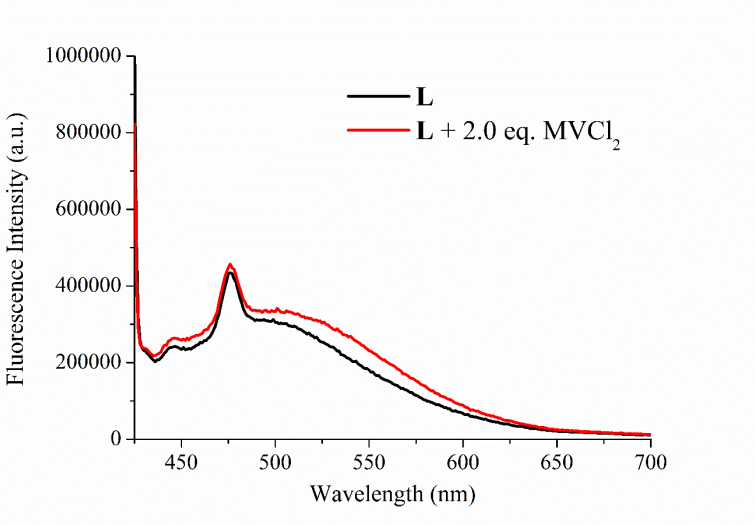


Fig. S29 Fluorescence spectra of **L** (1×10^{-4} M in DMSO) and **L** with 2.0 $MVCl_2$ (λ_{ex} = 415 nm).

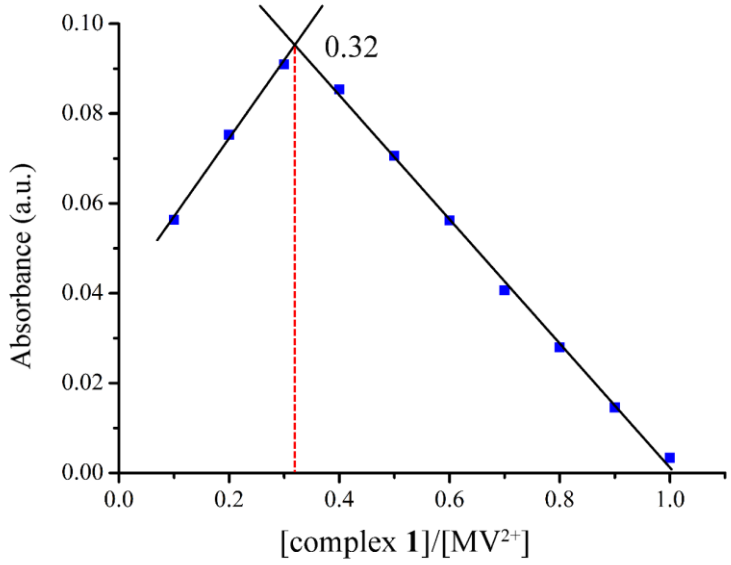


Fig. S30 Job's plot analyses for the complex **1** with MV^{2+} (complex **1** = 1×10^{-4} M in DMSO) and the result shows complex **1** : $MV^{2+} \approx 1 : 2$.

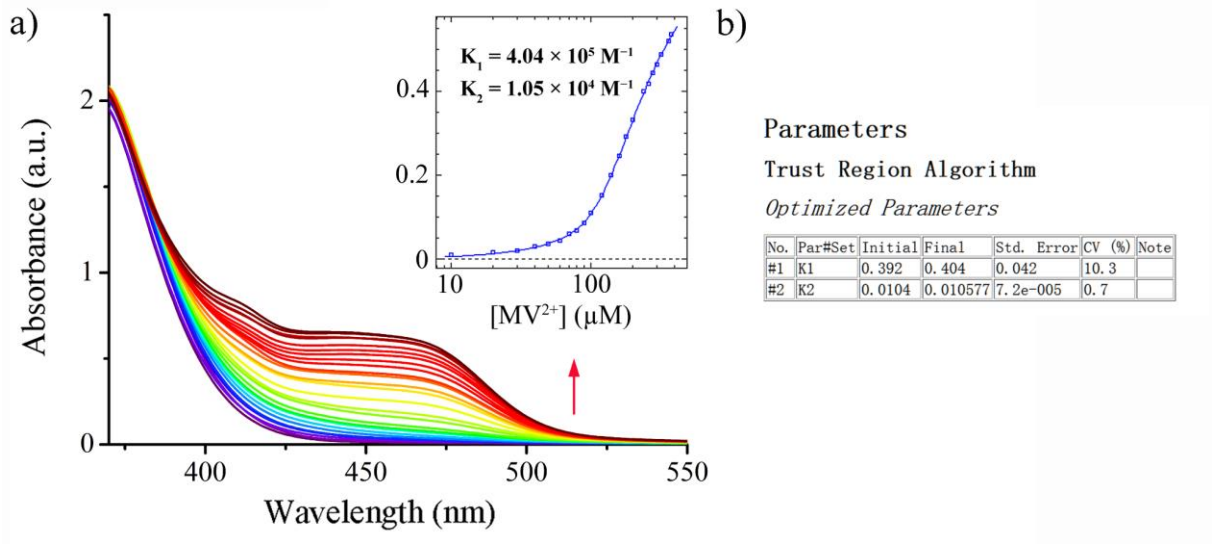


Fig. S31 a) UV-vis titrations of complex **1** (1.0×10^{-4} M in DMSO) upon addition of 0-4.0 equiv $MVCl_2$. Insets show structures of analytes and the corresponding association constants determined by fitting the titration curves at 475 nm (blue dots) to a 1:2 (host : guest) binding mode by the Dynafit program[5], which was further confirmed by the Job's plot (Figure S27); b) parameters of the fitting result (error = 10.3% and 0.7%).

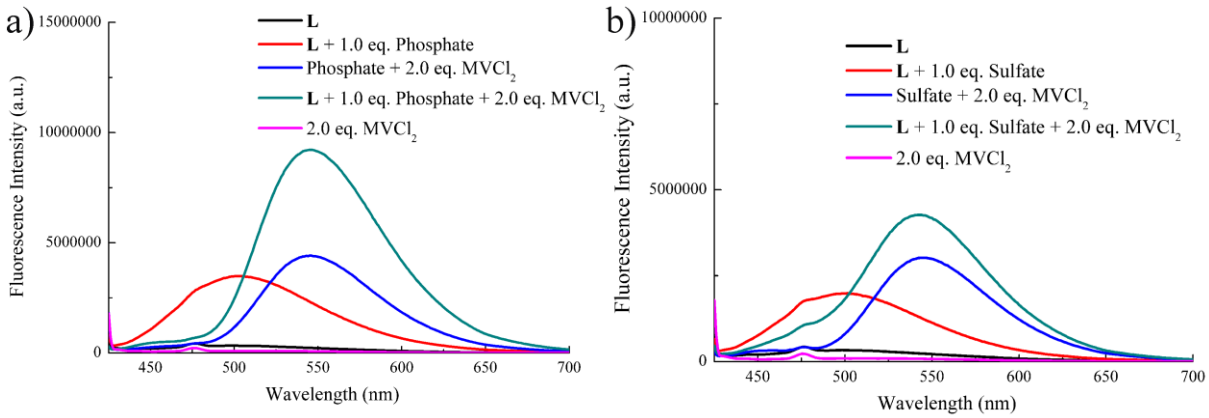


Fig. S32 a) Fluorescence spectra of **L** (1×10^{-4} M in DMSO), **L** with 1.0 equiv phosphate anions, **L** with 1.0 equiv phosphate anions and 2.0 equiv $MVCl_2$, phosphate anions with 2.0 equiv $MVCl_2$; b) Fluorescence spectra of **L** (1×10^{-4} M in DMSO), **L** with 1.0 equiv phosphate anions, **L** with 1.0 equiv sulfate anions and 2.0 equiv $MVCl_2$, sulfate anions with 2.0 equiv $MVCl_2$ (λ_{ex} = 415 nm).

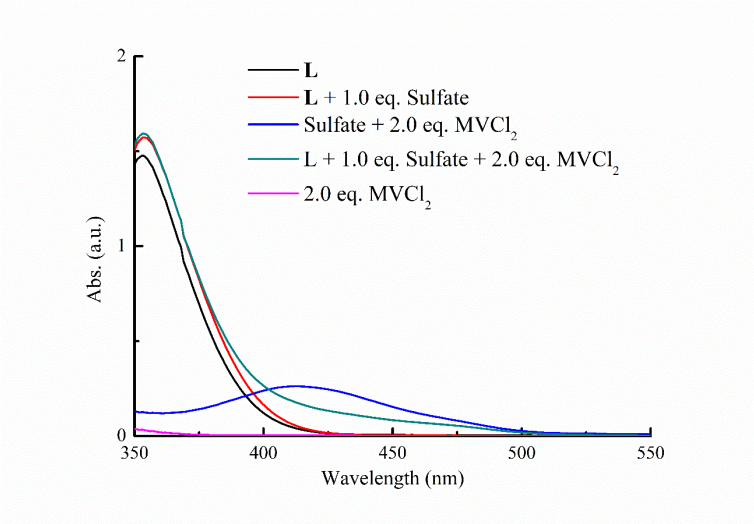


Fig. S33 Absorption spectra of the **L** upon addition of 1.0 equiv. sulfate anions and both 1.0 equiv. sulfate anions and 2.0 equiv. $MVCl_2$, only sulfate anions and 2.0 equiv. $MVCl_2$ (1×10^{-4} M in DMSO).

S7. Density Functional Theory (DFT) computations

The geometries were optimized by the dispersion-corrected semi-empirical PM6 method[6] with implementation of the Gaussian 09 package[7].

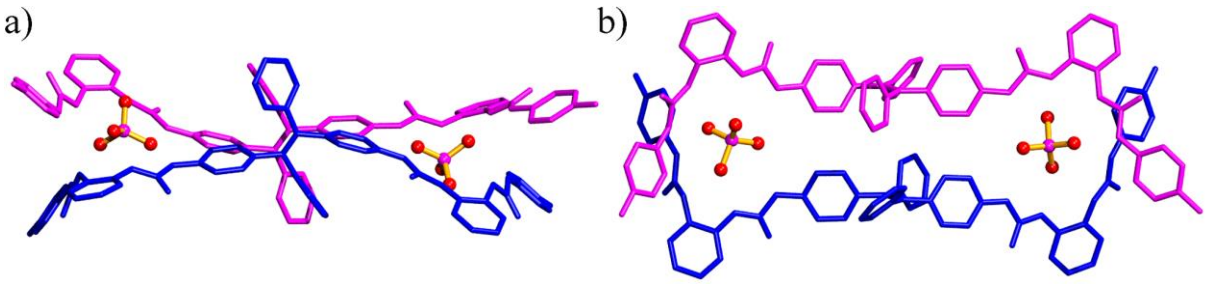


Fig. S34 The structure of $[(PO_4)_2(\mathbf{L})_2]^{6-}$ by PM6 optimization. a) front view; b) top view (non-acidic hydrogen atoms and cations were omitted for clarity).

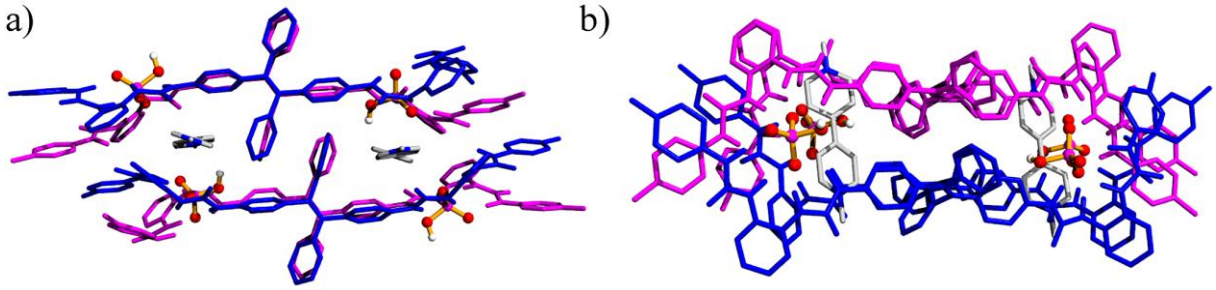


Fig. S35 The structure of $[MV]_2[(HPO_4)_4(\mathbf{L})_4]^{4-}$ by PM6 optimization. a) front view; b) top view (part non-acidic hydrogen atoms were omitted for clarity).

Cartesian coordinates (Å) for the optimized geometries of $[(PO_4)_2(\mathbf{L})_2]^{6-}$

C	14.75274400	-0.36450300	4.14627700	C	5.94841200	-5.40576300	0.75539300
H	14.10615900	-0.34835200	5.03314200	H	5.03889400	-5.79939100	1.25641100
H	15.19880000	0.63496900	4.04581000	H	6.05959900	-5.88402300	-0.23732900
H	15.56956100	-1.06639400	4.34786500	C	8.26388800	-6.14056000	1.00940700
C	13.97770900	-0.72556900	2.91762600	H	8.09337800	-6.61231500	0.02184700
C	14.32423100	-1.84499500	2.14969300	H	8.69746200	-6.88763600	1.70687100
H	15.16951700	-2.46376200	2.43977900	C	9.16496300	-4.92137700	0.86616600
C	13.60145800	-2.17893000	1.00333500	H	10.02372500	-5.13370800	0.19269600
H	13.87524300	-3.05404800	0.40856400	H	8.63674500	-4.01159200	0.48737800
C	12.50273200	-1.38930100	0.61911200	O	9.11837400	0.20719600	0.91629400
C	12.13936100	-0.27142900	1.40107200	O	7.00303900	-0.02443300	-0.56425000
H	11.25428300	0.31907500	1.12862500	O	9.67868900	-4.66374200	2.20146600
C	12.88209600	0.06433300	2.52515000	O	10.27574700	-2.85906300	4.53743800
H	12.60730400	0.94925200	3.09816800	O	8.12463500	-0.85078600	4.07527300
C	11.53036700	-2.96949300	-1.03257900	O	5.26838300	-1.47786000	4.13079200
C	10.05093500	-4.32053800	-2.46693500	O	5.25039400	-3.41442000	1.82735700
C	8.64576800	-4.52728100	-2.62113400	O	6.99801700	-5.84815300	1.64073800
C	8.18594400	-5.75519900	-3.12459500	C	1.89401100	-1.56260500	5.75356300
H	7.11555900	-5.89000700	-3.30295000	N	6.15168700	2.18470500	1.07744800

C	9.08306900	-6.78460900	-3.41143500	H	6.56874200	1.35152900	0.54999400
H	8.70945300	-7.72886000	-3.79764200	N	8.34703300	2.81177700	1.57294900
C	10.45154900	-6.60415400	-3.20044900	H	8.70700100	1.13730100	1.14880700
H	11.14848100	-7.41168200	-3.40463500	H	7.99080500	2.41771600	-1.39516700
C	10.93336000	-5.37937600	-2.73582600	H	10.38225100	1.67579100	0.55244700
H	12.00337700	-5.23307800	-2.56558200	N	10.96323000	1.83825000	-1.87595600
C	6.52979100	-3.27211300	-2.85641600	H	10.42084800	0.95763300	-1.55327100
C	4.45095300	-1.90204200	-2.62830000	C	-10.28994700	3.40180200	-2.31704600
C	3.84074100	-0.88031700	-1.86764300	H	-9.82875000	2.43442700	-2.01593000
H	4.45715300	-0.26945200	-1.18937000	H	-11.09153900	3.65719400	-1.58417000
C	2.47508200	-0.65644300	-1.96836500	C	-10.84729000	3.40904100	-3.73636500
H	2.01111100	0.12451300	-1.36462000	H	-10.94037900	4.44298800	-4.12997700
C	1.69056500	-1.44701800	-2.82288600	H	-11.83950100	2.91429400	-3.76217700
C	2.30991400	-2.40100900	-3.64358400	C	-10.11832000	1.36878400	-4.85842200
H	1.70891200	-2.98217500	-4.34054200	H	-11.18054400	1.08336800	-4.72623400
C	3.68101100	-2.63169700	-3.55520500	H	-9.82174100	1.21477900	-5.91744500
H	4.15873100	-3.38788700	-4.18703400	C	-9.22293400	0.57752900	-3.91001900
C	0.21096900	-1.36796300	-2.75501900	H	-9.56398500	-0.47225800	-3.80553600
C	-0.43224200	-2.00763800	-1.75483200	H	-9.15402200	1.02283700	-2.88512600
C	0.34928400	-2.70023000	-0.69545100	C	-6.95912700	-0.26441500	-3.86689700
C	0.92501000	-3.95525600	-0.94439400	H	-6.91763300	-0.00844900	-2.77780900
H	0.75892100	-4.44340400	-1.90242200	H	-7.29616100	-1.31561500	-3.96207700
C	1.74642000	-4.54783800	0.01794500	C	-5.63175100	-0.02880800	-4.57909400
H	2.22145600	-5.50417200	-0.19008600	H	-5.76297500	0.05423300	-5.67720200
C	1.98436400	-3.90116600	1.23470300	H	-4.91931900	-0.84674200	-4.35019200
H	2.66375900	-4.34228000	1.96405300	C	-4.24542600	1.25702700	-3.04155900
C	1.38075200	-2.66752200	1.49672700	H	-3.50172900	2.05264400	-3.26086300
H	1.55536500	-2.16268400	2.44804900	C	-5.07731000	1.57776700	-1.80242300
C	0.56245900	-2.06585400	0.53806700	H	-4.56445000	1.26051400	-0.86767400
H	0.10599900	-1.09767600	0.74385600	H	-6.08839400	1.10466100	-1.82002900
C	-0.46832100	-0.54872200	-3.78079000	C	-5.75784300	3.53696800	-0.56332100
C	-0.10395500	0.79914300	-3.93290400	H	-6.81084800	3.17150000	-0.43102900
H	0.71733000	1.21207800	-3.33314900	H	-5.14537800	3.16436100	0.28240800
C	-0.77973400	1.61441900	-4.84236900	C	-5.66865100	5.05408000	-0.68843200
H	-0.50503400	2.66262500	-4.93782600	H	-4.70909500	5.37062500	-1.14664200
C	-1.81174200	1.08666000	-5.62456800	H	-5.77952400	5.52974200	0.30492200
H	-2.35721600	1.72537600	-6.31530100	C	-7.91860200	5.93467700	-1.04849200
C	-2.15131200	-0.26457500	-5.50576000	H	-7.77974800	6.41590100	-0.06082700
H	-2.94715200	-0.67866800	-6.12154400	H	-8.29365900	6.68344500	-1.77623000
C	-1.48479300	-1.08132800	-4.58920500	C	-8.86088000	4.74520100	-0.92849500
H	-1.76029600	-2.13022200	-4.49441600	H	-9.75536200	4.99467400	-0.31838000
C	-1.89748900	-2.05732400	-1.58883500	H	-8.37930700	3.83532800	-0.48409500
C	-2.66005600	-3.04727800	-2.22876400	K	-7.15690100	3.37710800	-3.83638600
H	-2.16164300	-3.77989400	-2.86308400	O	-8.32891300	2.13485300	0.43827800

C	-4.04265600	-3.09618500	-2.07909000	O	-6.68226700	0.20666300	0.80351100
H	-4.62926600	-3.84370100	-2.62905300	O	-9.29149700	4.45446400	-2.28627100
C	-4.69077700	-2.15764300	-1.24014600	O	-9.96859100	2.79612200	-4.70482400
C	-3.91612900	-1.15879200	-0.59635200	O	-7.91682300	0.58697600	-4.54832200
H	-4.41664600	-0.41099200	0.04801200	O	-5.03657100	1.24334000	-4.25000200
C	-2.54359100	-1.11306300	-0.77610800	N	-7.54156800	3.44917600	2.55896300
H	-1.96325600	-0.33200600	-0.27995600	H	-7.82017700	2.82372800	1.67266700
C	-7.04160800	-3.04282300	-1.56685700	N	-5.65088800	2.07189100	2.71825300
C	-9.40658900	-3.39096500	-1.82835900	H	-10.67939300	0.86566800	0.81616000
C	-9.39547200	-4.21363900	-2.96637800	O	-6.63283100	5.59920800	-1.61297700
H	-8.47824800	-4.28125800	-3.55259600	N	-10.34610400	3.03263600	2.13018200
C	-10.52203600	-4.95563800	-3.33631500	C	-14.26210400	0.27577700	-4.25123800
H	-10.48204200	-5.58308600	-4.22114000	H	-13.83721000	-0.60684800	-4.74571100
C	-11.68178800	-4.88801500	-2.57129000	H	-15.31283200	0.04379100	-4.03042800
H	-12.56084700	-5.46007500	-2.84918200	H	-14.24566100	1.09901900	-4.97577600
C	-11.72580100	-4.07768100	-1.42903200	C	-13.52101100	0.63479600	-3.00119600
H	-12.64193500	-4.03915600	-0.83059900	C	-13.90341600	1.75691200	-2.25083200
C	-10.61050100	-3.33026800	-1.03974700	H	-14.74791400	2.36167800	-2.57151400
C	-11.62736100	-2.51675100	1.10432800	H	-13.52199000	2.98093600	-0.50482200
C	-12.38818000	-1.13104000	3.05983800	C	-12.12148500	1.33366100	-0.66596900
C	-13.54344500	-1.88063800	3.34834800	C	-11.72709900	0.21016600	-1.42444100
H	-13.73481800	-2.81323400	2.80873100	C	-12.43586900	-0.14370600	-2.56688000
C	-14.44102500	-1.41935000	4.30901900	H	-12.14128600	-1.03737700	-3.11698800
H	-15.33325100	-2.00223200	4.52409600	C	-8.45630500	4.48458200	2.88589600
C	-14.20874600	-0.21675600	4.99377000	C	-8.04284400	5.69215400	3.46831100
C	-13.05690100	0.52930700	4.69719300	H	-6.99954000	5.80317100	3.77901200
H	-12.86798000	1.47106100	5.20938300	C	-8.95177400	6.73519800	3.65753600
C	-12.14986400	0.08465900	3.74002400	H	-8.61183300	7.66470500	4.10623900
H	-11.26822800	0.68246900	3.50820600	C	-10.28328200	6.58967100	3.26743100
C	-15.18731800	0.26519000	6.01974200	H	-10.98438100	7.40914900	3.39192600
H	-16.15765000	0.49108900	5.55801500	C	-10.72700400	5.38062500	2.72412100
H	-14.84618300	1.17914000	6.52082900	H	-11.77024600	5.26035100	2.41907900
H	-15.35291000	-0.49077900	6.79729200	C	-6.31174400	3.23640800	3.19623400
C	-1.95624600	-3.64601600	1.84181800	C	-4.28590200	1.78120600	2.95916300
H	-2.11092700	-2.99550800	0.95508300	H	-4.37653400	0.17261900	1.49262800
H	-0.86962200	-3.73484700	2.04452100	C	-2.37360200	0.45821000	2.26701100
C	-2.69960400	-3.12928900	3.06861700	H	-1.94402600	-0.32518700	1.64137800
H	-2.89532000	-3.92517000	3.81093300	C	-1.54723700	1.20641100	3.12149700
H	-2.11966700	-2.30478500	3.55223700	C	-2.11774600	2.17279800	3.96230200
C	-4.79253600	-2.05094500	3.61881400	H	-1.48584800	2.72035900	4.65895600
H	-4.30691800	-1.13651000	4.01669300	C	-3.47916200	2.46377800	3.88956900
H	-4.91742000	-2.79401400	4.42762200	H	-3.91962900	3.23569100	4.52812100
C	-6.11177800	-1.71848200	2.93396100	C	-0.07007400	1.08744000	3.01785200
H	-6.68838600	-0.96665500	3.50852600	C	0.55187700	1.74889600	2.01669800

H	-5.98207100	-1.32298000	1.89567600	C	-0.26885700	2.43208400	0.97854600
C	-8.13643400	-2.85166400	2.25180900	C	-0.87225500	3.67184700	1.23576900
H	-8.76787200	-2.14220200	2.82526300	H	-0.67989200	4.18043500	2.17793200
H	-8.01118100	-2.45370400	1.22092300	C	-1.76209100	4.21783700	0.30671000
C	-8.72122400	-4.26128700	2.26142700	H	-2.25994100	5.16050200	0.52411500
H	-8.46493300	-4.82303000	3.17881900	H	-2.78457100	3.93157700	-1.57974500
H	-9.82290600	-4.23237900	2.13935500	C	-1.40191800	2.32753900	-1.16040600
C	-8.81673300	-6.11541700	0.69254500	H	-1.61510800	1.79768000	-2.08966500
H	-8.65873800	-6.91646000	1.43716400	C	-0.50647400	1.77774200	-0.24055600
H	-9.89915800	-5.88736000	0.59983100	H	-0.01250900	0.83164200	-0.45983200
C	-8.22534300	-6.46436100	-0.66996900	C	0.60368000	0.21110200	3.99660600
H	-8.92504100	-7.08128800	-1.26284000	C	0.05369900	-1.05590200	4.26461200
H	-7.96784000	-5.55129600	-1.25867800	H	-0.89004900	-1.35159800	3.78949800
C	-6.00819700	-7.09969100	-1.41573200	C	0.69927700	-1.93857600	5.13098800
H	-5.88625800	-6.01633400	-1.67448700	H	0.27271600	-2.92117400	5.31944300
H	-6.31010600	-7.64737700	-2.32720100	H	2.40832200	-2.25401400	6.41630700
C	-4.75342900	-7.69879100	-0.78380700	C	2.43020400	-0.29403700	5.51485200
H	-4.98455600	-8.23263900	0.15858000	H	3.36230700	-0.00134100	5.99617200
H	-4.22702700	-8.38253700	-1.47409400	C	1.79029100	0.59094000	4.64309500
C	-2.69152800	-6.88348400	0.20971300	H	2.22083800	1.57468700	4.45783000
H	-2.09253800	-7.60532600	-0.37735700	C	2.00925800	1.85082300	1.81605900
H	-2.95381700	-7.33243000	1.18720100	C	2.71151200	2.95289900	2.33416800
C	-1.95373600	-5.55537300	0.36798500	H	2.17445600	3.69902900	2.91963300
H	-0.86240700	-5.70729500	0.48947700	C	4.07821300	3.09523000	2.12571500
H	-2.12583400	-4.87184800	-0.48981500	H	4.61646100	3.93827800	2.58069600
K	-5.37855100	-4.44692600	0.83483100	C	4.77559300	2.13572500	1.34901000
N	11.72834300	-1.66354400	-0.54272800	C	4.06480200	1.01835000	0.84405500
H	11.04573100	-0.90467800	-0.86763600	H	4.60383200	0.26884200	0.24211300
N	10.57259300	-3.04885400	-2.07321800	C	2.70499400	0.88071800	1.08070800
H	9.97083800	-2.20559400	-2.24718500	H	2.17313900	0.01156300	0.69022400
N	7.74330600	-3.50905000	-2.20110600	C	7.04405900	3.20602100	1.58311500
H	8.04653900	-2.92020100	-1.30254700	C	9.36081800	3.69912900	1.97400900
N	5.82653300	-2.13349700	-2.37398000	C	9.20680500	4.66373300	2.99244300
H	6.28959700	-1.44772400	-1.71433100	H	8.23751400	4.75458900	3.48451500
N	-6.07498900	-2.11867700	-1.01021100	C	10.25728700	5.51156100	3.34212700
H	-6.43319300	-1.26391600	-0.49938800	H	10.11001400	6.24834100	4.12753300
N	-8.31503700	-2.58223400	-1.45451500	C	11.48642100	5.42809000	2.68629400
H	-8.50711500	-0.78019300	-1.40639300	H	12.29577500	6.10038400	2.94659000
N	-10.63392300	-2.48859100	0.11153800	C	11.67557100	4.46983100	1.68407800
H	-9.82972800	-1.80879200	0.21888700	H	12.62650700	4.40332400	1.15423300
N	-11.40035600	-1.55692800	2.12892900	C	11.15344000	2.91544400	-0.98612800
H	-10.57557400	-0.91035400	2.01760300	C	11.34261300	1.83256500	-3.24417300
O	12.16025900	-3.94890800	-0.63257000	C	12.07168500	2.86640100	-3.85624300
O	6.07865900	-3.99139700	-3.74401600	H	12.38119000	3.73618000	-3.27092400

O	-6.62327800	-4.11124700	-2.06266900	C	12.39463200	2.77131600	-5.21029700
O	-12.55689000	-3.31771900	1.13405900	H	12.95976300	3.57422400	-5.67670600
O	-2.47221600	-4.98059300	1.59400300	C	12.00085400	1.66033200	-5.96806100
O	-3.93958000	-2.58513300	2.56909100	C	11.26990200	0.63009200	-5.34929000
O	-6.85270200	-2.96774800	2.92253800	H	10.95814000	-0.23876000	-5.92559600
O	-8.12069700	-4.92429900	1.12145500	C	10.93782900	0.70818400	-4.00346100
O	-7.05342200	-7.28966500	-0.42910200	C	12.35584400	1.57585900	-7.42069600
O	-3.88861100	-6.56039500	-0.53727700	H	13.44409200	1.59091400	-7.56158300
C	10.63849600	3.60034000	1.33554600	H	11.98057300	0.65626400	-7.88571600
N	10.88787800	2.57369100	0.35912000	H	11.93223200	2.41962800	-7.98001000
H	10.36069900	-0.09010400	-3.51815600	C	1.88508300	3.61646600	-1.44271300
H	-10.86039800	-0.38002000	-1.11659400	H	2.13468800	3.02162000	-0.53849000
C	-9.84077300	4.30882700	2.55430800	H	0.78268100	3.69500100	-1.53471000
H	12.16549200	-2.99189300	3.63977200	C	2.49957500	3.02490300	-2.70611000
H	10.18341000	-2.64700100	1.83480000	H	2.64989400	3.78285900	-3.49750500
H	6.89585800	-3.40406000	0.50433000	H	1.85609800	2.20075000	-3.10179900
H	5.26022200	-3.60259900	-0.25649300	C	4.51637800	1.88860500	-3.40192000
O	9.46893300	-0.40676600	-1.48602900	H	3.99878400	0.96223800	-3.72297700
P	8.41087000	-0.61133800	-0.36711400	H	4.56263100	2.60266800	-4.24504300
O	8.33921900	-2.11332000	0.00344100	C	5.89950300	1.58665600	-2.83707500
K	7.45605000	-3.60605500	3.68011100	H	6.42743700	0.82157100	-3.44111000
H	-3.71152800	0.29147700	-2.92383100	H	5.88584800	1.23080800	-1.77917500
O	-8.22358600	0.20645400	-1.24929300	C	7.97502200	2.77106300	-2.44717900
P	-8.10371000	0.60314400	0.37306600	H	8.53568500	2.04935600	-3.07655600
O	-9.28723800	-0.15376400	1.02168100	C	8.51176200	4.19224000	-2.59327900
C	10.65694600	-3.59075600	2.19490000	H	8.10641800	4.70967300	-3.48274400
H	11.47394200	-3.87108800	1.48945500	H	9.62159300	4.20296000	-2.63866900
C	11.18413500	-3.50826400	3.62255500	C	8.85580300	6.03871400	-1.05318700
H	11.28895300	-4.51526600	4.07697100	H	8.74212900	6.81473600	-1.83043700
C	10.35359000	-1.41755400	4.56345400	H	9.92146900	5.71791500	-0.97900800
H	11.40588600	-1.09473700	4.44244500	C	8.32976200	6.49284600	0.30311200
H	10.01051000	-1.18548500	5.59343300	H	9.08142700	7.10092600	0.83974000
C	9.46163200	-0.75774800	3.51603600	H	8.04002800	5.63142800	0.94567500
H	9.71947000	0.31116600	3.36490900	C	6.21078800	7.32674500	1.12607500
H	9.49879900	-1.25614300	2.51693700	H	6.08966700	6.29063800	1.53485500
C	7.14090200	-0.09359300	3.32648200	H	6.58239400	7.98365000	1.93336100
H	7.00683600	-0.53004100	2.31318500	C	4.91979900	7.86200900	0.50904200
H	7.49997600	0.95207000	3.21923000	H	5.08419700	8.24950900	-0.51511900
C	5.87327700	-0.16748400	4.17328900	H	4.45806400	8.64989800	1.13077600
H	6.09905000	-0.04940800	5.25314600	C	2.75647200	6.97342700	-0.15294400
H	5.14395500	0.60512600	3.85919100	H	2.21336300	7.74243200	0.42837600
C	4.28407200	-1.66709800	3.09613900	H	2.91080200	7.33575900	-1.18776100
H	3.64385000	-0.76293600	3.01914400	C	2.02192800	5.63350100	-0.11964700
H	3.68047700	-2.50365600	3.50717600	H	0.92263000	5.77067100	-0.13870800

C	4.88567100	-2.01356500	1.73656800	H	2.29359100	5.02585400	0.76845600
H	4.13106100	-1.91173200	0.92756700	K	5.36010200	4.44879300	-0.82137400
H	5.77272800	-1.39315400	1.47408100	O	-11.82044800	3.90963200	0.55247400
C	5.88919200	-3.88949100	0.61051800	O	-5.83861800	3.96543000	4.06283400
C	-11.21107100	2.93941700	0.99884700	O	6.55823300	4.29430900	1.95571400
N	-11.38092900	1.62582100	0.51541100	O	11.55317300	4.02701900	-1.32939700
C	-13.21971500	2.10694700	-1.08723400	O	2.41991900	4.96283300	-1.34114400
C	-3.72826900	0.73919000	2.18209200	O	3.76200800	2.45682000	-2.29591800
C	-2.04294700	3.53837200	-0.88275500	O	6.61156400	2.84551600	-2.94415800
H	-6.13323600	1.41867600	2.01292000	O	8.05566300	4.88722500	-1.40671200
H	-9.67351400	2.25282900	2.24282800	O	7.18896700	7.36254000	0.05791100
O	-5.19635100	3.02451300	-1.80081700	O	4.02592200	6.71902400	0.49306200

Cartesian coordinates (Å) for the optimized geometries of $[MV]_2[(HPO_4)_4(\mathbf{L})_4]^{4-}$

O	-7.73725800	-1.59372600	2.21300700	C	-10.17356500	4.43925100	-1.51491800
O	-7.27907100	0.87082200	2.60634800	H	-10.05632000	5.29227200	-0.84908900
O	-8.39059800	0.11973200	0.39180700	C	-10.85893900	-0.37839200	-1.70356900
O	11.42497200	1.70013500	2.24317700	C	-10.63547200	-2.72911300	-1.04972400
O	7.03185700	5.03965800	0.27456800	C	-11.75506500	-3.14926200	-1.78785500
O	-5.80344700	5.00756200	1.60299000	H	-12.42112900	-2.39786100	-2.19120000
O	-11.54875700	1.58716500	1.65913400	C	-12.00382000	-4.49202000	-2.02831600
N	10.61905300	-0.01481400	0.92132900	H	-12.87232900	-4.77433800	-2.61710000
H	9.84897800	-0.16666300	0.24540200	C	-11.16175300	-5.46571000	-1.49490000
N	10.58945500	2.12280500	0.15271800	H	-11.35570100	-6.52184100	-1.65871500
H	10.33259800	1.69663900	-0.73160600	C	-10.08224000	-5.07134100	-0.71969200
N	8.56177400	3.73257400	-0.84372800	H	-9.42326400	-5.81224900	-0.28257100
H	8.61470700	2.81426200	-1.30048200	C	-9.78570000	-3.72042800	-0.50798800
N	6.35335700	3.47933600	-1.28954900	C	-7.44883300	-4.04656700	0.12385400
H	6.74699900	2.67971300	-1.82118800	C	-5.16810800	-3.63981300	0.93322400
N	-5.31417600	2.77050500	1.93834000	C	-4.45903700	-4.27990000	-0.10009100
H	-5.77187300	1.88133000	2.18918900	H	-4.98339700	-4.96873000	-0.74950200
N	-7.46212700	3.44913000	1.98385300	C	-3.10552700	-4.03025800	-0.27035000
H	-7.56502200	2.42183600	2.09785500	H	-2.58180200	-4.51288100	-1.09106400
N	-9.73769700	2.20846100	2.92262200	C	-2.39125500	-3.17042900	0.57628200
H	-8.83822100	1.81325300	3.20572600	C	-3.07690900	-2.64688500	1.68284000
N	-10.43903900	0.01981500	2.91340600	H	-2.54094700	-2.03826800	2.40735200
H	-9.54958200	-0.16506400	3.36452900	C	-4.43319200	-2.87455700	1.86225400
C	11.34972400	-4.77258800	4.02569600	H	-4.94763100	-2.46715100	2.73212500
H	10.45281800	-4.99798400	4.61871100	C	-0.96020800	-2.87180500	0.35551600
H	12.19052400	-4.70200800	4.72340400	C	-0.12174100	-2.88656700	1.58692600
H	11.52703400	-5.63252800	3.37052900	C	0.54469700	-1.73145900	2.01489400
C	11.18651500	-3.50786200	3.22919400	H	0.50204200	-0.83358700	1.40374600
C	11.69506500	-2.28821900	3.67689000	C	1.24226100	-1.71724300	3.22087800

H	12.24095600	-2.25470700	4.61816800	H	1.71460000	-0.79756600	3.55361400
C	11.54350500	-1.10420900	2.95571600	C	1.32211400	-2.87318200	3.99501600
H	11.96816300	-0.17686800	3.31773400	H	1.86662100	-2.86300700	4.93562200
C	10.85577200	-1.12258900	1.73602600	C	0.67858500	-4.03515600	3.56963800
C	10.34900900	-2.34634900	1.27031100	H	0.72592600	-4.93762900	4.17377100
H	9.83524800	-2.36736300	0.31580200	C	-0.05642800	-4.03360200	2.38787800
C	10.51479500	-3.51220000	2.00140200	H	-0.59498200	-4.92519200	2.07695000
H	10.13837000	-4.44589300	1.58600400	C	-0.39387400	-2.61858400	-0.85608200
C	10.93607200	1.28643500	1.18558000	C	-1.14099400	-2.39675800	-2.11957400
C	10.74945600	3.51791800	0.18770500	C	-0.62617900	-2.90533700	-3.32219100
C	11.89236300	4.11118800	0.72701000	H	0.30955300	-3.45568600	-3.30444700
H	12.68006700	3.46877700	1.10036000	C	-1.29262700	-2.72397700	-4.52892100
C	11.99620600	5.49475000	0.80596600	H	-0.87241500	-3.13757200	-5.44153400
H	12.88631600	5.94258900	1.23862100	C	-2.48822400	-2.01505300	-4.56647200
C	10.97100200	6.29883800	0.31226200	H	-3.01325200	-1.86752200	-5.50624300
H	11.05039400	7.38132400	0.35896100	C	-3.00179200	-1.48438200	-3.38416800
C	9.84489300	5.71829000	-0.25846800	H	-3.93113400	-0.92234400	-3.41821200
H	9.03899000	6.33276200	-0.64294500	C	-2.33710800	-1.66340000	-2.17547500
C	9.71433300	4.32825100	-0.31010200	H	-2.73415900	-1.23742100	-1.25663400
C	7.29429500	4.16636400	-0.55625500	C	1.08415300	-2.69020300	-1.01389100
C	4.99031200	3.42458900	-1.05615300	C	1.87454400	-1.59022600	-1.36471100
C	4.31912800	4.11721400	-0.03267000	H	1.41749600	-0.60746900	-1.45971900
H	4.86410400	4.83693200	0.56398600	C	3.23824800	-1.72645300	-1.57377200
C	2.97034200	3.88248500	0.19013900	H	3.84820700	-0.85734300	-1.79172400
H	2.47212500	4.40500100	1.00241000	C	3.86211400	-2.98445900	-1.48473100
C	2.23238100	2.97938400	-0.58573700	C	3.06544800	-4.10174000	-1.18823200
C	2.88439200	2.37412300	-1.66848900	H	3.51738900	-5.08350000	-1.17369300
H	2.32505200	1.72356000	-2.33668600	C	1.70992800	-3.93778700	-0.93244800
C	4.23495700	2.58708300	-1.90025000	H	1.10511900	-4.81126600	-0.69891500
H	4.71830700	2.13388100	-2.76542600	C	6.07028400	-4.08991200	-1.32448800
C	0.80418900	2.70353900	-0.31248000	C	8.51823800	-4.51404000	-1.25167400
C	-0.07809200	2.80133100	-1.50925000	C	8.49228700	-5.77004900	-0.63589500
C	-0.77368300	1.68709800	-1.99300100	H	7.53569300	-6.17596200	-0.33397100
H	-0.71125900	0.74331100	-1.45699100	C	9.66659200	-6.49428700	-0.45358100
C	-1.52221800	1.77287100	-3.16483300	H	9.62363900	-7.47011400	0.02282000
H	-2.01052200	0.88276800	-3.55067800	C	10.87904500	-5.97046300	-0.88678700
C	-1.62267900	2.98420300	-3.84628400	H	11.80219600	-6.52561800	-0.74635800
H	-2.20795400	3.04976500	-4.75983300	C	10.91996400	-4.73306200	-1.51893000
C	-0.94664200	4.10448400	-3.36403800	H	11.85777900	-4.31225500	-1.85498800
H	-1.00846700	5.05056300	-3.89568500	C	9.75305800	-3.98869100	-1.71274700
C	-0.16197400	4.00541300	-2.21945400	C	10.80430500	-1.82894500	-2.29339500
H	0.39919500	4.86641400	-1.86518600	C	11.16152500	0.57632400	-2.80533500
C	0.28148400	2.41805900	0.91029200	C	10.51214200	1.73378800	-3.26808300
C	1.06900200	2.18049900	2.14778200	H	9.48551300	1.66377600	-3.61439900

C	2.34441200	1.58924900	2.14994700	C	11.15064500	2.96452300	-3.22558600
H	2.77425300	1.26104900	1.20721900	H	10.61489800	3.84701400	-3.56973400
C	3.05653500	1.43777200	3.33463900	C	12.45259000	3.09688300	-2.73244100
H	4.05216700	1.00277300	3.31972200	C	13.08636300	1.93709200	-2.28910900
C	2.50837200	1.83709400	4.55265300	H	14.09771500	2.00404700	-1.89309400
H	3.07133400	1.71408300	5.47381100	C	12.46954500	0.68861000	-2.31950200
C	1.23147800	2.38645900	4.57218700	H	12.97760000	-0.19232800	-1.95235100
H	0.78163900	2.69384500	5.51219900	C	13.11394200	4.44396200	-2.66385600
C	0.52370400	2.55400800	3.38684900	H	14.11405400	4.37476300	-2.22457400
H	-0.46882100	2.99193900	3.41679800	H	13.21637500	4.89211000	-3.65994800
C	-1.19432300	2.47769900	1.10397400	H	12.52851900	5.13767600	-2.04877900
C	-1.97349200	1.35532000	1.40511600	N	8.07211600	2.38053800	2.68071800
H	-1.51394400	0.37008100	1.43475000	N	4.87998500	-3.76277300	1.69586200
C	-3.33003800	1.47490400	1.65903700	C	8.78532600	3.64343500	2.92628000
H	-3.93084800	0.59203300	1.84800300	H	9.85553200	3.46036000	2.80536400
C	-3.95702600	2.73447400	1.66769200	H	8.45076500	4.38337500	2.19627000
C	-3.17661100	3.86953600	1.39604500	H	8.56523800	3.98245000	3.94207400
H	-3.63226200	4.84890500	1.44984200	C	6.88633400	2.39105000	2.03937300
C	-1.82655700	3.72429600	1.09968600	H	6.51732300	3.36336600	1.73134500
H	-1.23125500	4.61133200	0.89502100	C	6.22469000	1.21855900	1.75564500
C	-6.16821500	3.85168700	1.83874000	H	5.31818900	1.27164800	1.16851700
C	-8.61174200	4.22489400	2.11218400	C	6.79224600	-0.00764400	2.12100100
C	-8.66573200	5.58987800	1.80605800	C	7.98597000	0.02147600	2.84855200
H	-7.75334000	6.08905300	1.50635700	H	8.48083600	-0.88478200	3.17820100
C	-9.86823400	6.28258800	1.89866200	C	8.61377200	1.22010000	3.09884500
H	-9.89186900	7.34179000	1.65613900	H	9.58995800	1.28103800	3.56630800
C	-11.02929100	5.62696200	2.29765200	C	6.12725800	-1.29740900	1.85013400
H	-11.97174600	6.16254300	2.36364900	C	4.73963000	-1.40231900	1.74502400
C	-10.97772200	4.28019900	2.63728000	H	4.09373400	-0.53545700	1.74465300
H	-11.86907800	3.75551000	2.96091400	C	4.13867500	-2.64240000	1.66937900
C	-9.78261700	3.56595600	2.55510900	H	3.06377100	-2.76270500	1.60934200
C	-10.63686700	1.28555600	2.43220000	C	6.23025300	-3.69214500	1.69521200
C	-11.16985000	-1.12926800	2.56854100	H	6.76337000	-4.63229100	1.61596900
C	-10.61937300	-2.36988900	2.91429000	C	6.87519000	-2.48071400	1.76463500
H	-9.63731400	-2.40379300	3.37573800	H	7.95900700	-2.46112500	1.72576500
C	-11.29943400	-3.54568800	2.62871400	C	4.23539300	-5.07934800	1.73265400
H	-10.84253600	-4.49588800	2.89769800	H	3.16023900	-4.94791600	1.61631500
C	-12.54325700	-3.53532100	1.99413900	H	4.63431700	-5.66747600	0.90487600
C	-13.08304800	-2.29079900	1.66826100	H	4.45040600	-5.54623000	2.69691400
H	-14.05350200	-2.24458600	1.17796200	N	-7.72676300	-2.57134200	-3.00480500
C	-12.42433600	-1.09847700	1.94796200	N	-5.31639300	3.74385300	-1.31147200
H	-12.87009300	-0.14966400	1.68396700	C	-8.25194100	-3.86248300	-3.47215100
C	-13.25048200	-4.81226300	1.63937400	H	-7.99164100	-4.61728400	-2.72749400
H	-14.33758400	-4.67850100	1.62895500	H	-7.81636400	-4.09176200	-4.44841300

H	-13.01510100	-5.61183600	2.35016300	H	-9.33793300	-3.79148700	-3.54300900
H	-12.94981700	-5.15833300	0.64279400	C	-6.53400600	-2.52494400	-2.37358400
O	7.74761800	1.28373300	-2.00705600	H	-6.02601400	-3.46891800	-2.23325300
O	7.34125400	-1.20616800	-2.46031000	C	-6.03923400	-1.33976500	-1.88089400
O	8.17671600	-0.48564000	-0.15006400	H	-5.12344300	-1.36408900	-1.30630700
O	-11.17472600	-0.57495300	-2.88045500	C	-6.75873700	-0.15397800	-2.06647300
				C	-7.96724700	-0.23088000	-2.75713700
O	-7.19517000	-4.87552500	-0.75636200	H	-8.57154500	0.65068600	-2.94607100
O	5.66922900	-5.18633400	-0.92168000	C	-8.44140100	-1.45014300	-3.19345700
O	11.91023600	-2.06959500	-1.83475300	H	-9.42675000	-1.54491300	-3.63922500
N	-10.86389300	0.85962900	-1.12391100	C	-6.24113900	1.16481100	-1.65930700
H	-10.85094600	0.90277700	-0.10599500	C	-4.87588200	1.45488300	-1.71114400
N	-10.40321900	-1.36585200	-0.84731700	H	-4.13219000	0.69633000	-1.92094900
				C	-4.43695200	2.74928000	-1.53196700
H	-9.69917400	-1.03189000	-0.16741400	H	-3.38874200	3.01722800	-1.58688800
N	-8.64063000	-3.37966600	0.23731300	C	-6.63365000	3.47825800	-1.16111700
H	-8.67456400	-2.64223200	0.95550800	H	-7.27845200	4.31436600	-0.91494800
N	-6.54232300	-3.66314300	1.08959500	C	-7.12015300	2.20141500	-1.31887000
H	-6.91676400	-2.92509800	1.72645900	H	-8.17061400	2.00879700	-1.13816100
N	5.23247500	-3.05053400	-1.68876300	C	-4.85700700	5.13620200	-1.25352600
H	5.70477500	-2.19735200	-2.01131100	H	-5.23002200	5.57593000	-0.32638000
N	7.37654400	-3.72195100	-1.42060300	H	-5.23511200	5.66562800	-2.13156800
H	7.50370400	-2.73053900	-1.68743800	H	-3.76738500	5.14470400	-1.25341800
N	9.76435100	-2.74093200	-2.34455800	P	7.39794700	-0.08223400	-1.39888800
H	8.86941600	-2.33488000	-2.62038300	P	-7.45809700	-0.23800600	1.54429800
N	10.43172600	-0.61652700	-2.83713700	O	5.82187200	0.05698900	-0.84211200
H	9.45440100	-0.51260900	-3.09559100	H	5.36964700	0.76174600	-1.32745400
C	-9.62181300	5.92418300	-3.48655500	O	-5.95458100	-0.36694900	0.81722100
H	-9.12630700	5.81397900	-4.45720500	H	-5.41882400	-1.02340000	1.28745600
H	-10.51374400	6.54371900	-3.64575900	C	-10.67450000	2.08127600	-1.77205000
H	-8.95484400	6.49162700	-2.82701100	C	-10.51568300	3.21512600	-0.95958200
C	-9.97998800	4.58968500	-2.89305300	H	-10.66376600	3.12283600	0.11138900
C	-10.18415300	3.46525400	-3.69341700	H	-10.73274100	1.38089500	-3.80767500
H	-10.07471100	3.55339200	-4.77300600				
C	-10.54105900	2.22790400	-3.16073500				

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