# Electronic Supplementary Information

# Halo-phenyl based linear dipodal receptors for entrapment of anions/anionic associations within neutral non-cooperative self-assemblies

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## *Characterization of free receptors $L_1$ and $L_2$:*

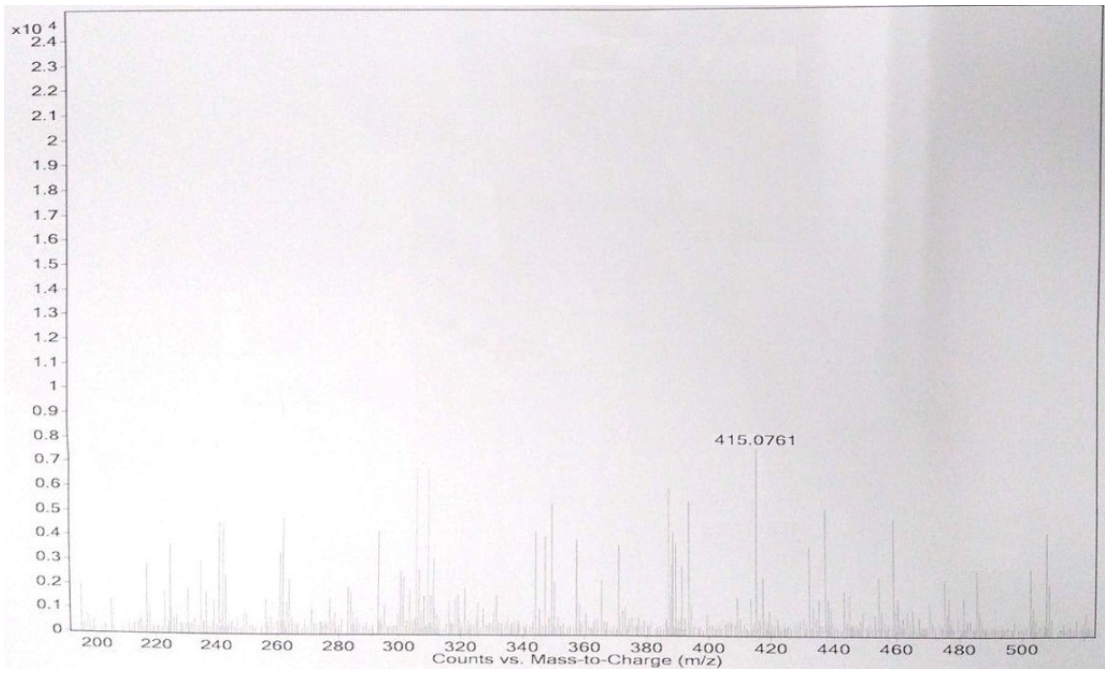


**Figure S1**: ESI-Mass spectrum of *para*-chlorophenyl functionalized *para*-phenylenediamine based bis-urea receptor **$L_1$.**

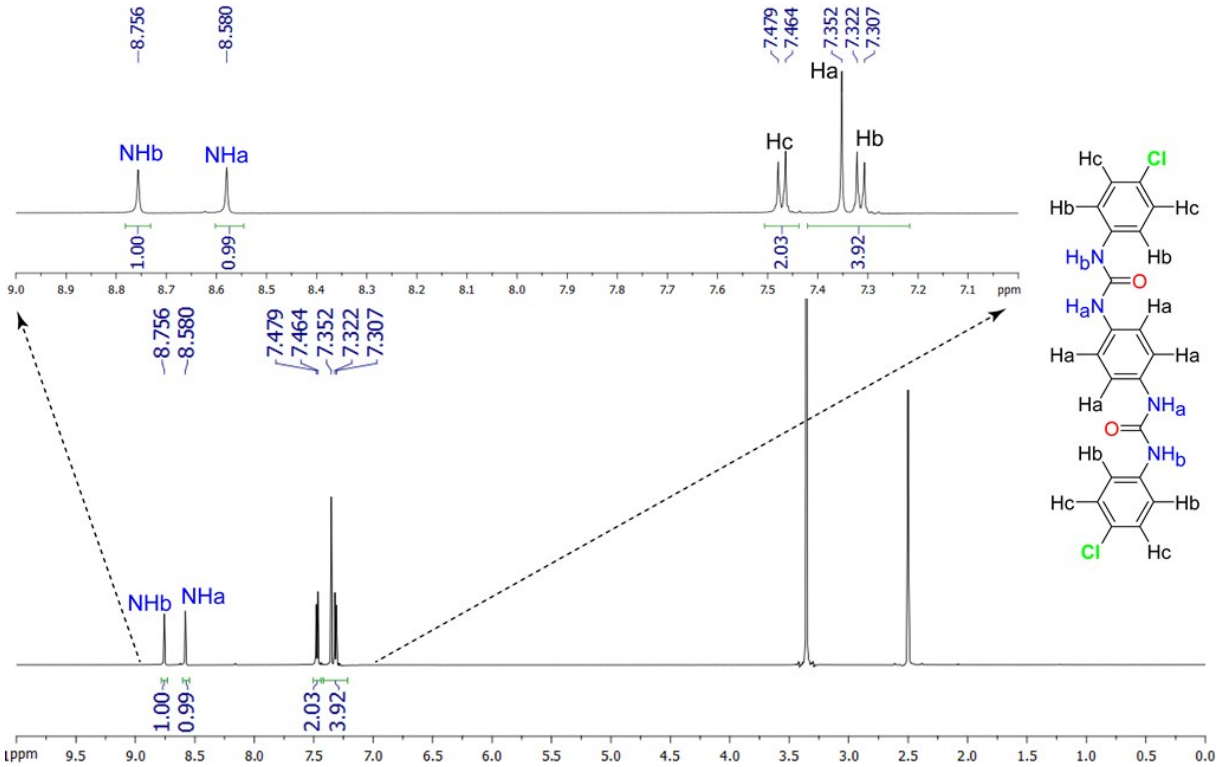


**Figure S2:** Integrated $^1$H-NMR spectrum (full as well as expanded) and interpretation of all hydrogen atoms of free dipodal bis-urea *para*-chloro isomer **$L_1$** in DMSO-$d_6$ at 25ºC.

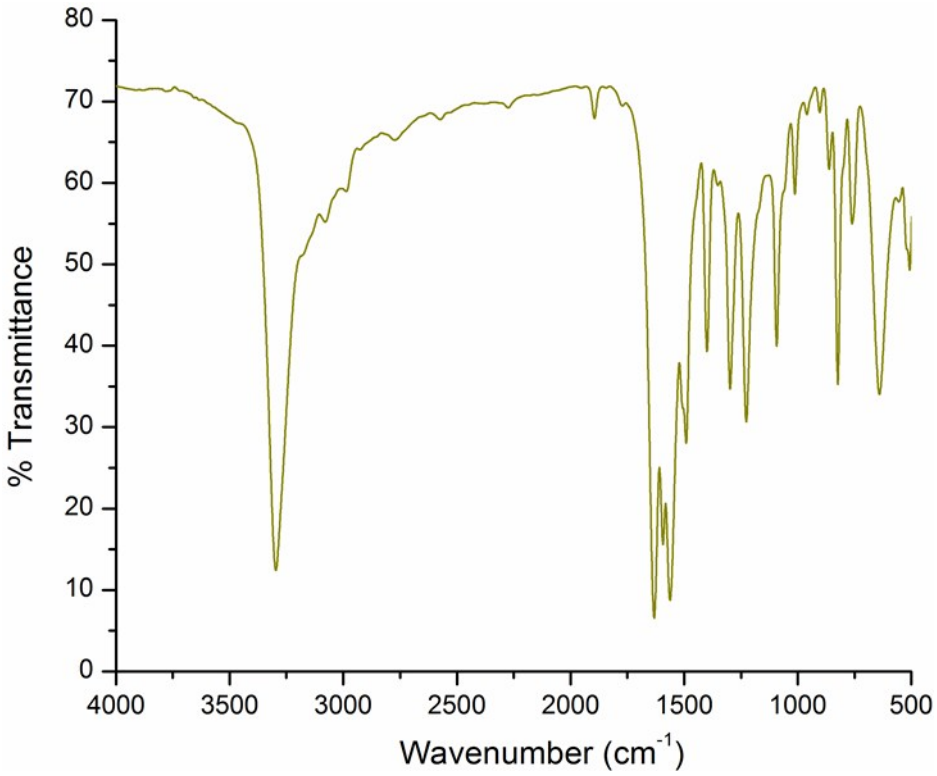


**Figure S3:** FT-IR spectrum of $\mathbf{L_1}$ recorded in KBr pellet.

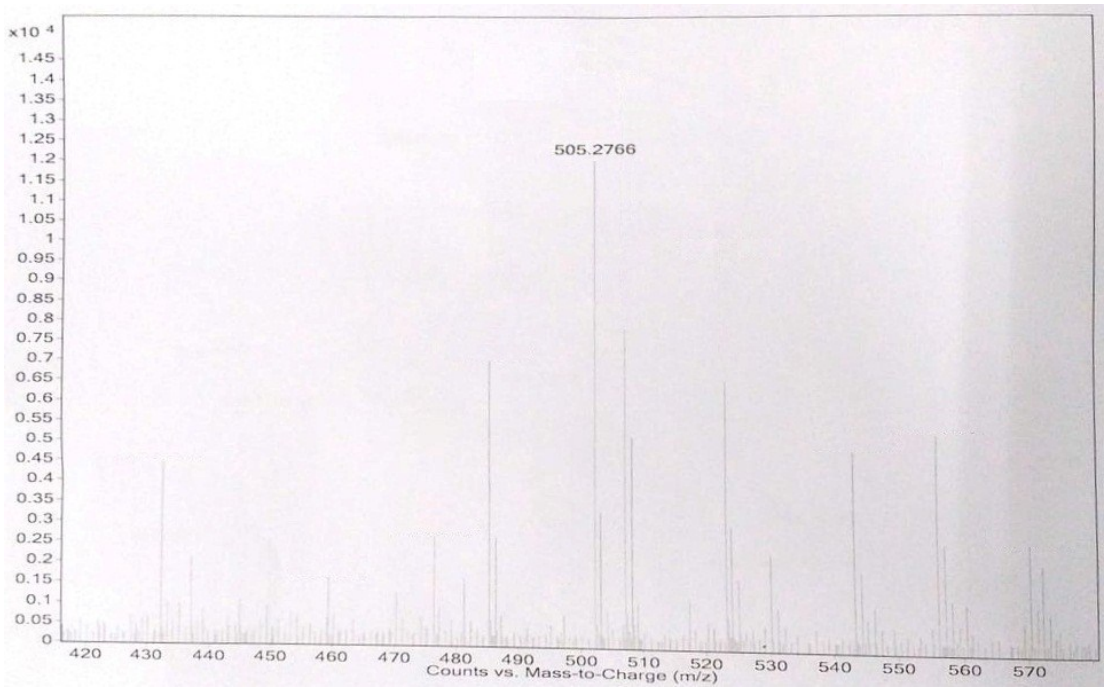


**Figure S4:** ESI-Mass spectrum of *para*-bromophenyl functionalized *para*-phenylenediamine based bis-urea receptor $\mathbf{L_2}$.

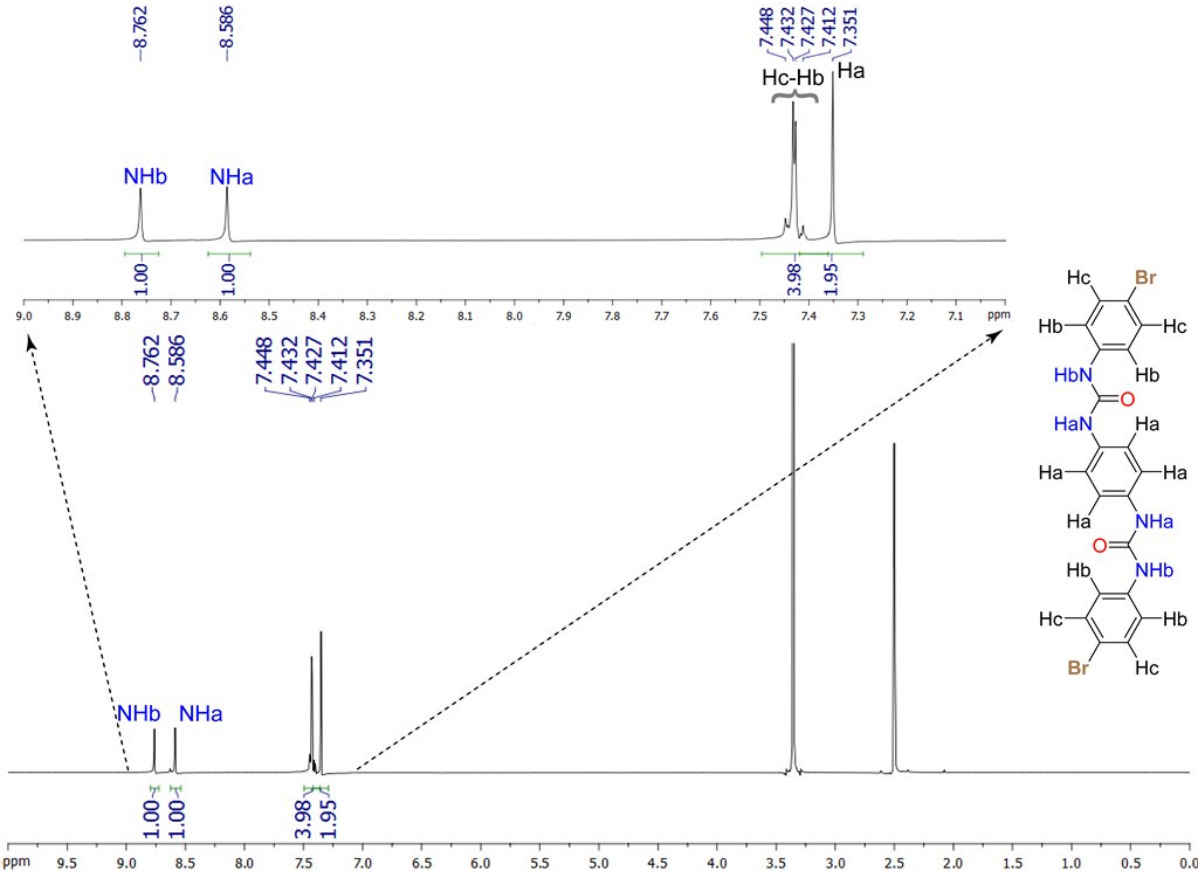


**Figure S5:** Integrated $^{1}$H-NMR spectrum (full as well as expanded) and interpretation of all hydrogen atoms of free dipodal bis-urea *para*-bromoisomer $\mathbf{L_2}$ in DMSO-$d_6$ at 25ºC.

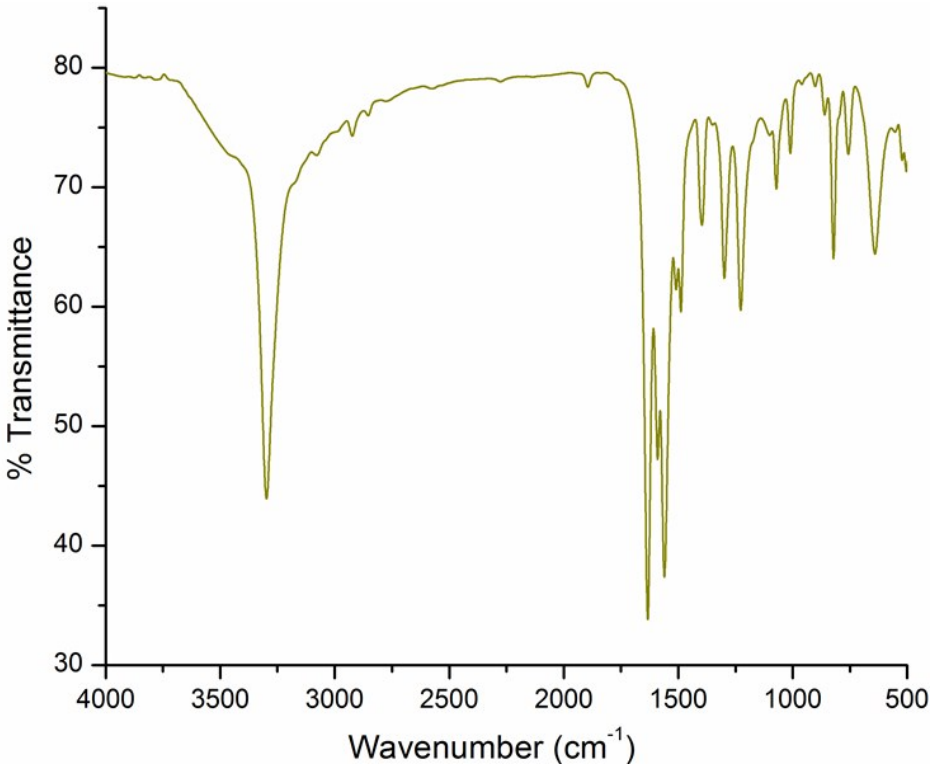


**Figure S6:** FT-IR spectrum of $\mathbf{L_2}$ recorded in KBr pellet.

## *Characterization of neutral anion complexes of receptors:*

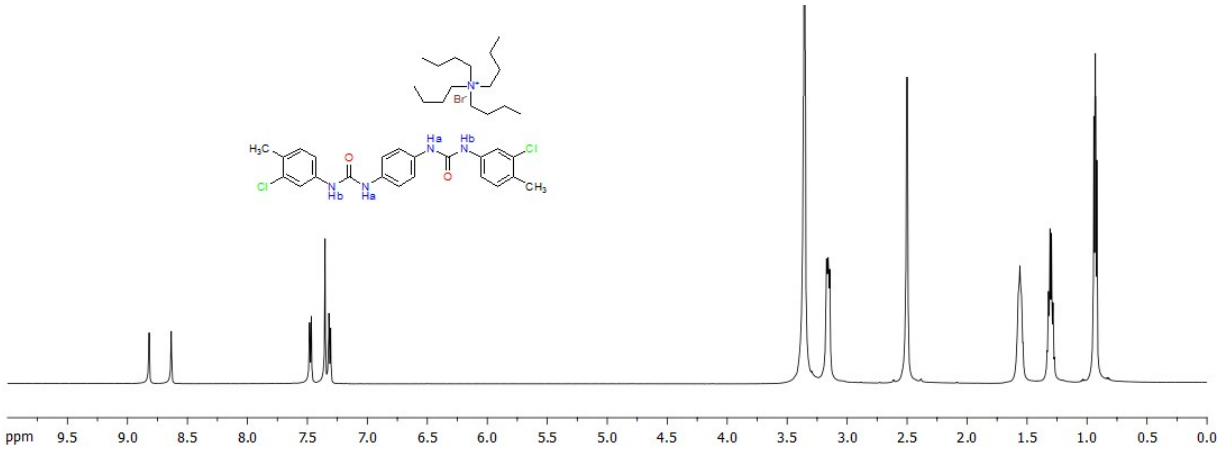


**Figure S7:** $^{1}$H NMR full and expanded spectrum of bromide complex **1a** of $\mathbf{L_1}$ as recorded in DMSO-$d_6$ at 298 K.

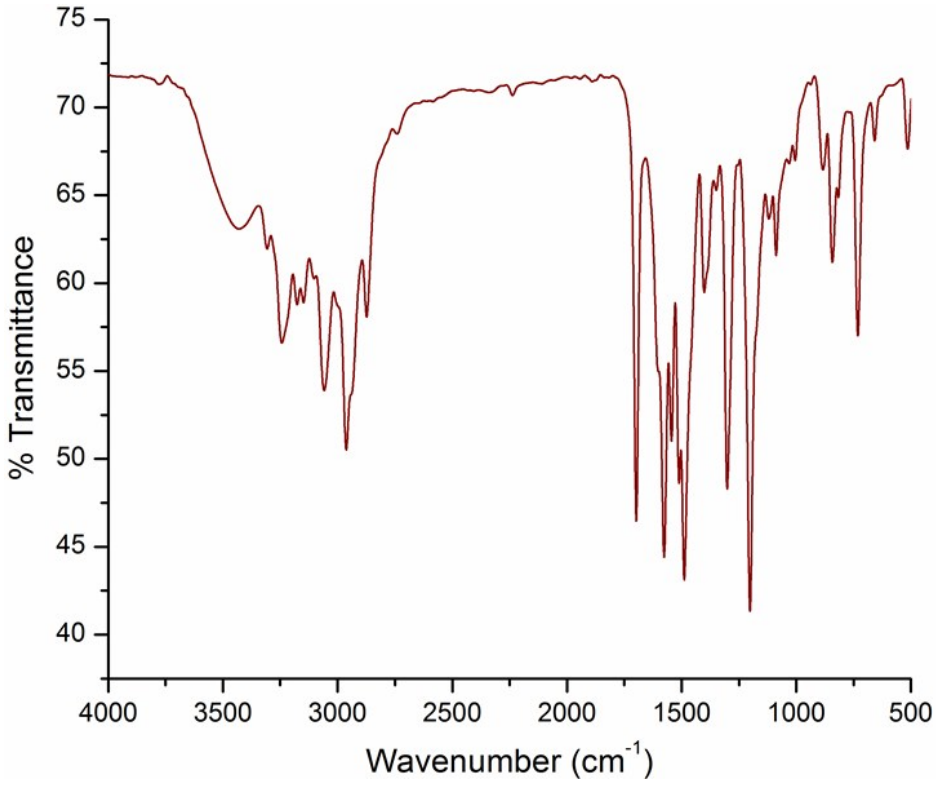


**Figure S8**: FT-IR spectrum of complex **1a** of $\mathbf{L_1}$ recorded in KBr pellet.

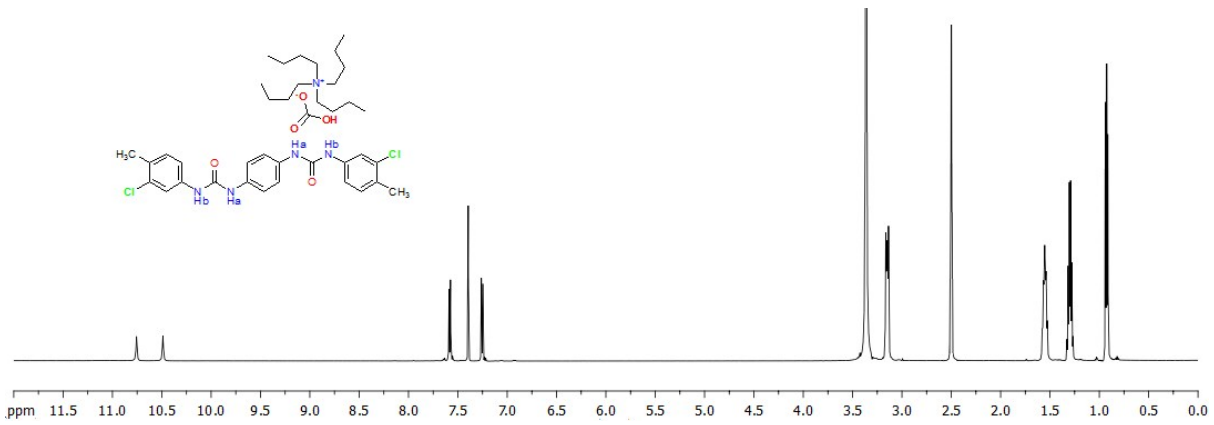


**Figure S9**: $^{1}$H NMR full and expanded spectrum of hydroxide induced hydrogencarbonate dimer entrapped complex **1b** of $\mathbf{L_1}$ as recorded in DMSO-$d_6$ at 298 K.

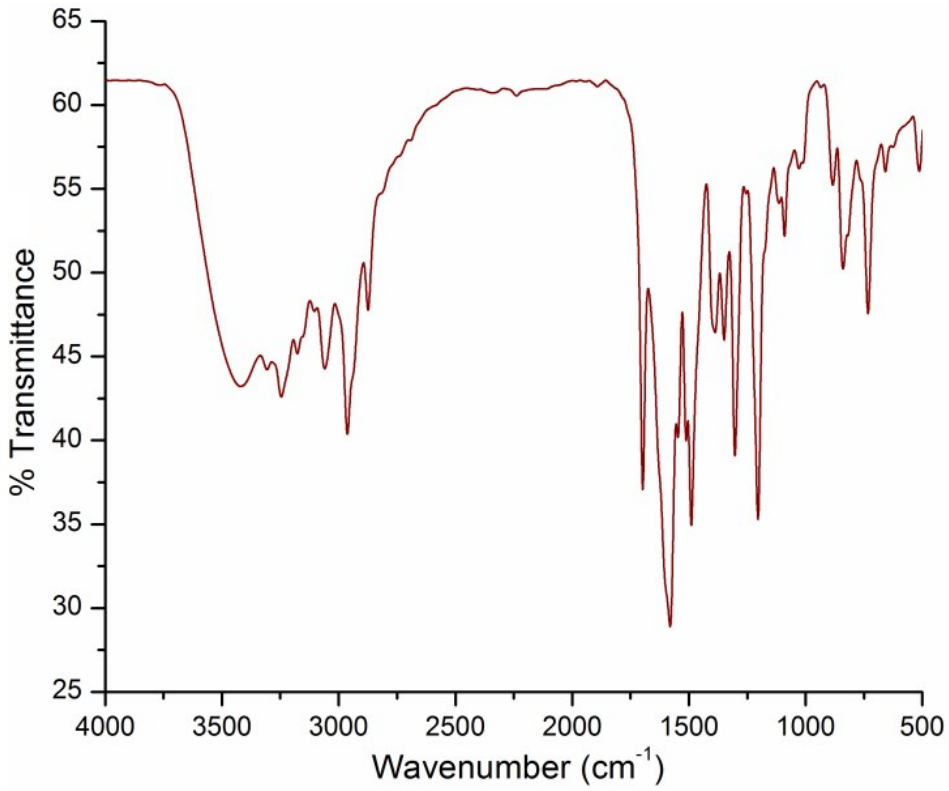


**Figure S10**: FT-IR spectrum of complex **1b** of $\mathbf{L_1}$ recorded in KBr pellet.

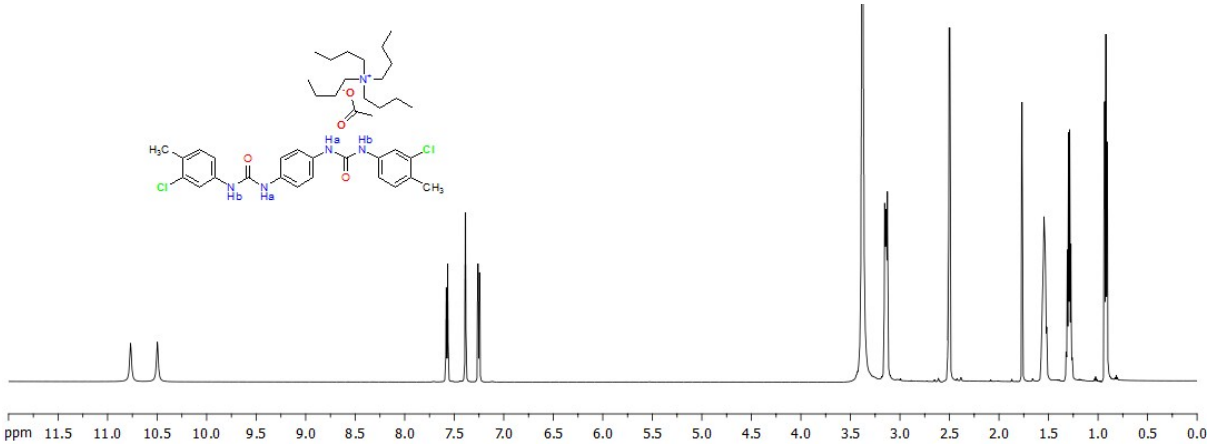


**Figure S11**: $^{1}$H NMR full and expanded spectrum of acetate entrapped complex **1c** of $\mathbf{L_1}$ as recorded in DMSO-$d_6$ at 298 K.

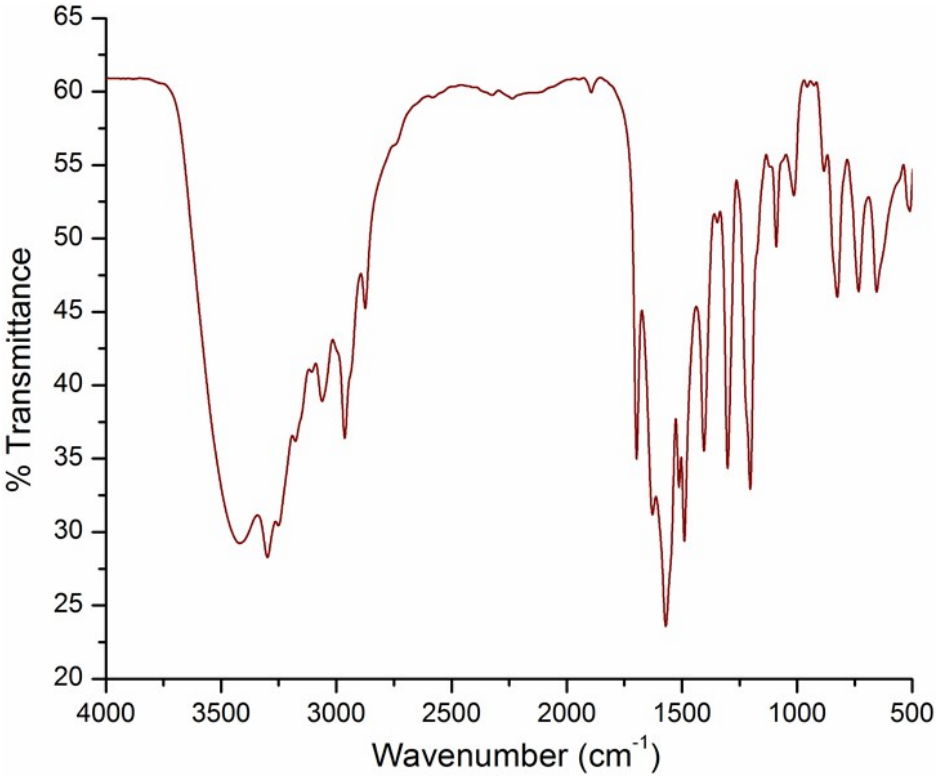


**Figure S12:** FT-IR spectrum of complex **1c** of $\mathbf{L_1}$ recorded in KBr pellet.

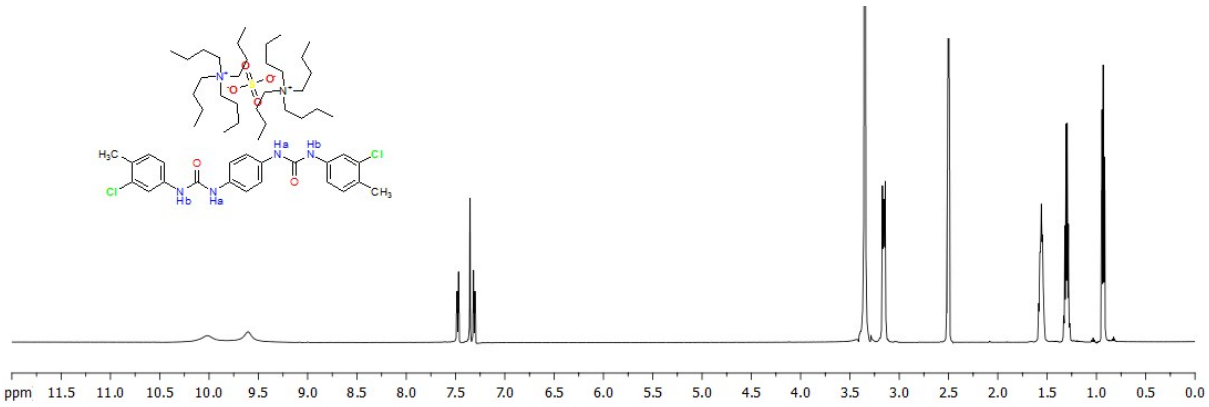


**Figure S13**: $^{1}$H NMR full and expanded spectrum of divalent sulphate complex **1d** of $\mathbf{L_1}$ as recorded in DMSO-$d_6$ at 298 K.

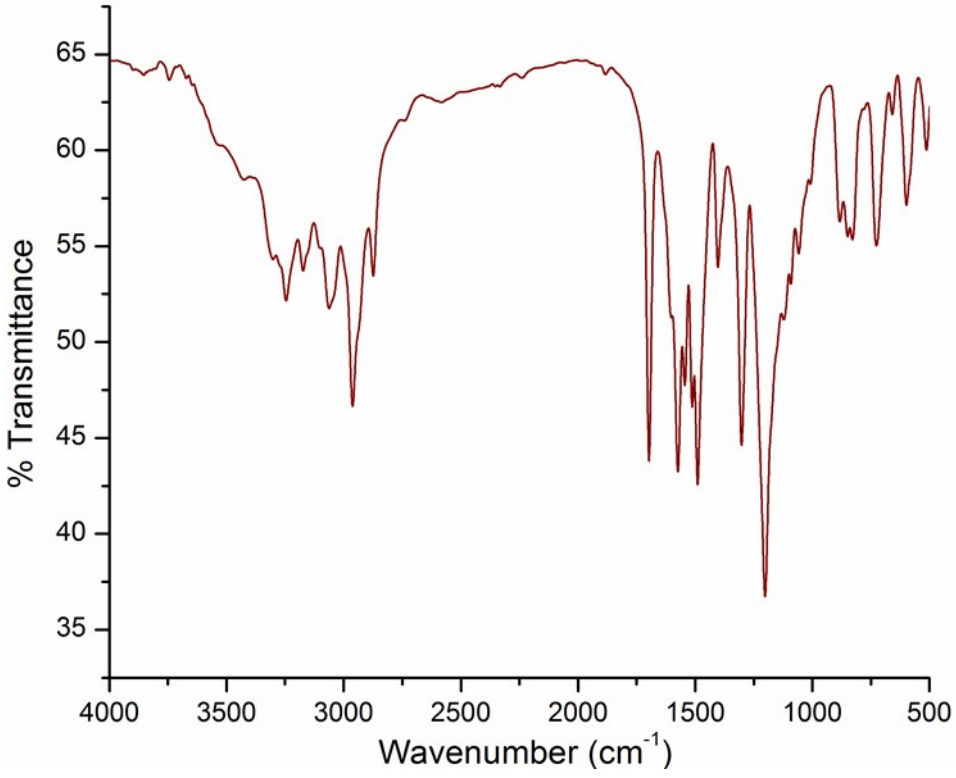


**Figure S14**: FT-IR spectrum of complex **1d** of $\mathbf{L_1}$ recorded in KBr pellet.

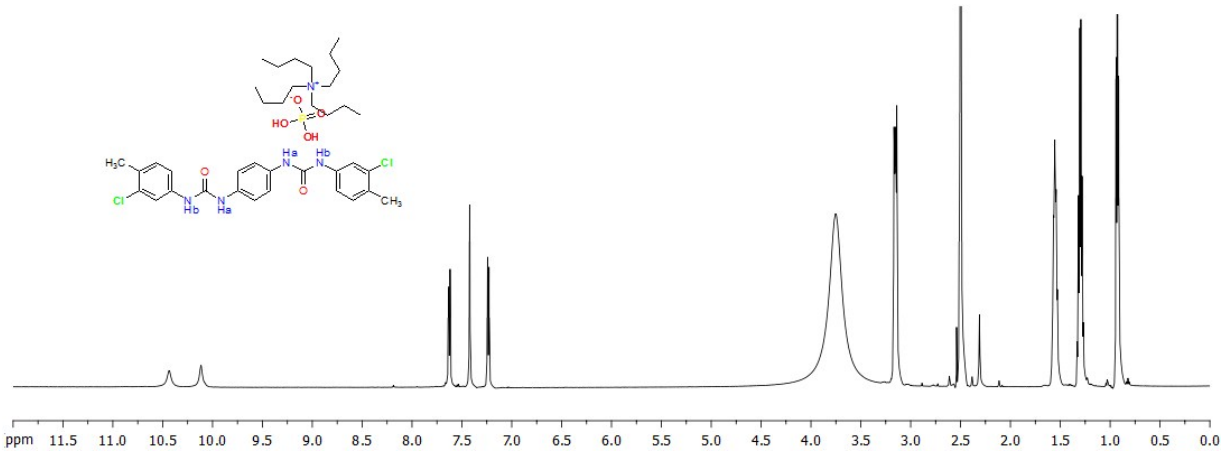


**Figure S15**: $^{1}$H NMR full and expanded spectrum of dihydrogenphosphate polymer trapped complex **1e** of $\mathbf{L_1}$ as recorded in DMSO-$d_6$ at 298 K.

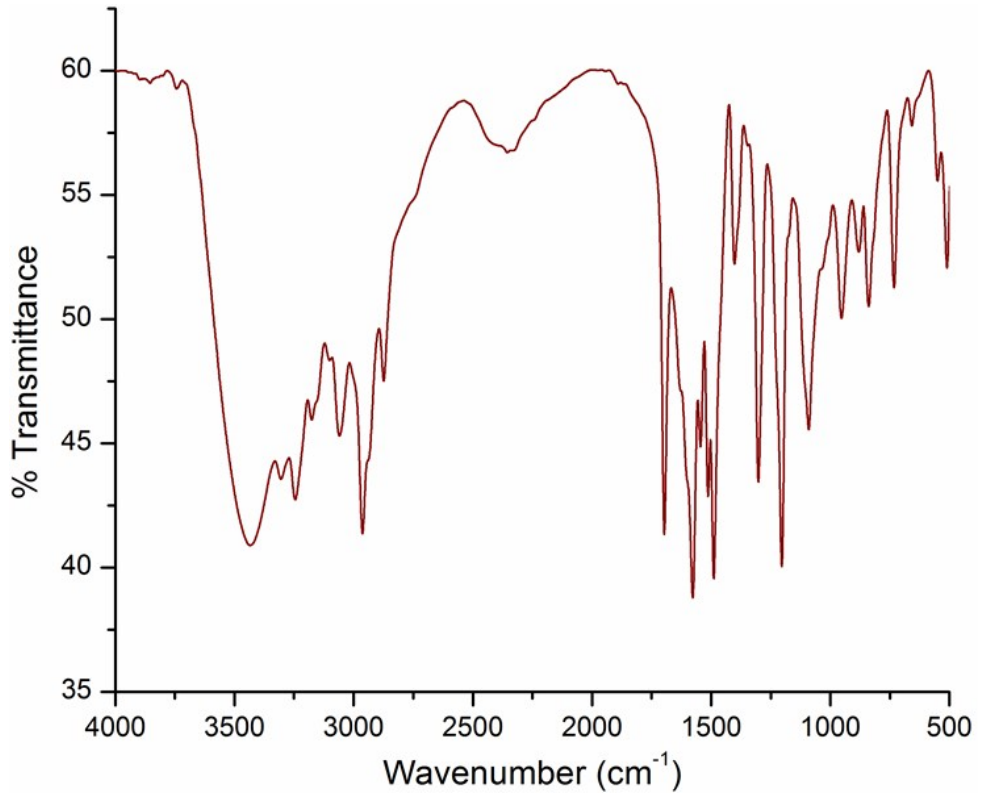


**Figure S16:** FT-IR spectrum of complex **1e** of $\mathbf{L_1}$ recorded in KBr pellet.

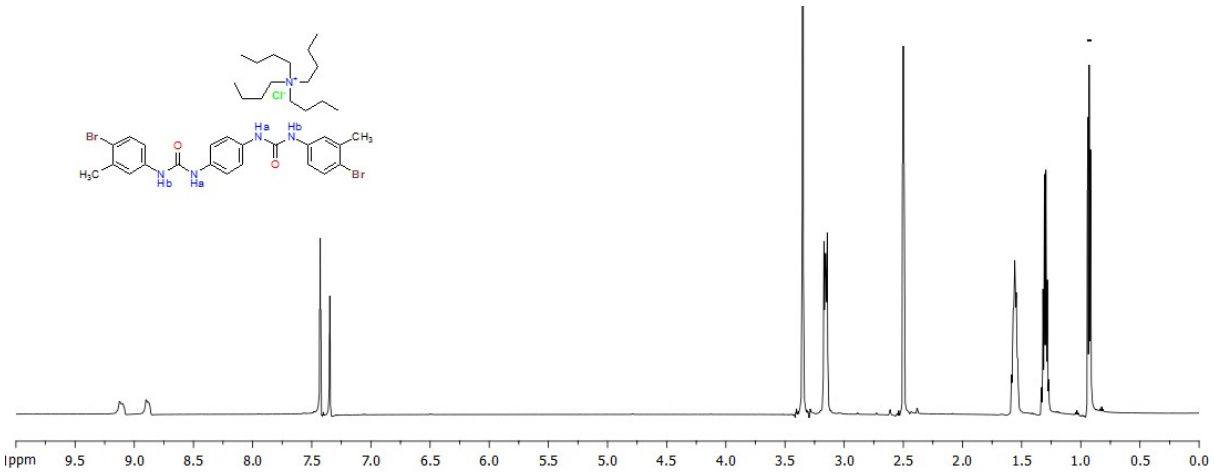


**Figure S17**: $^{1}$H NMR full and expanded spectrum of chloride complex **2a** of $\mathbf{L_2}$ as recorded in DMSO-$d_6$ at 298 K.

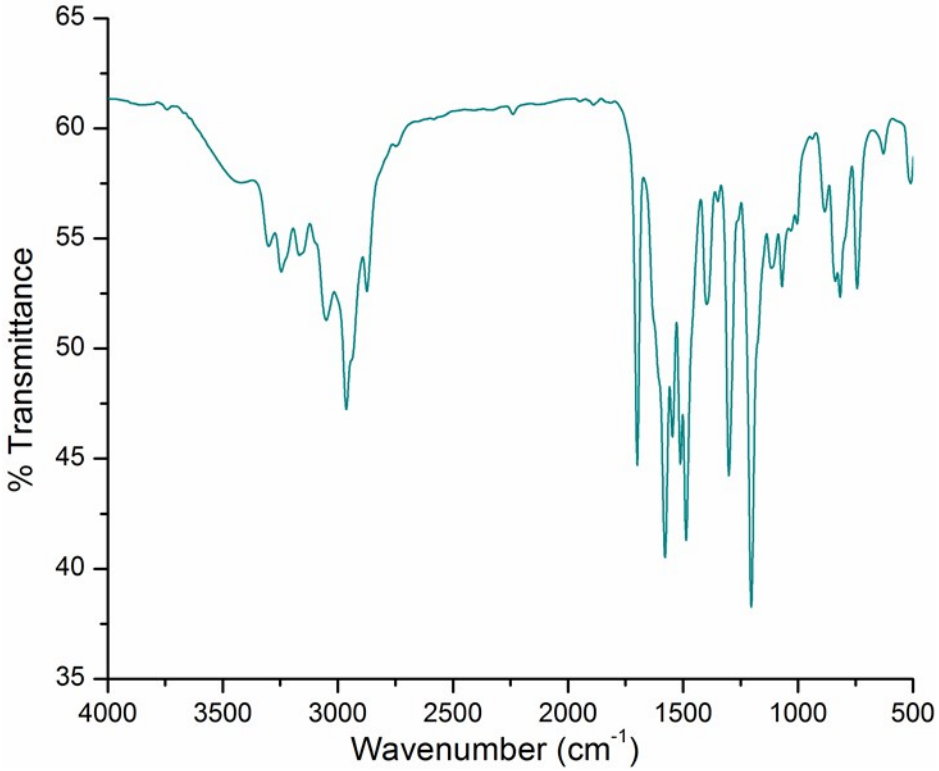


**Figure S18**: FT-IR spectrum hydrated-acetate complex **2a** of $\mathbf{L_2}$ recorded in KBr pellet.

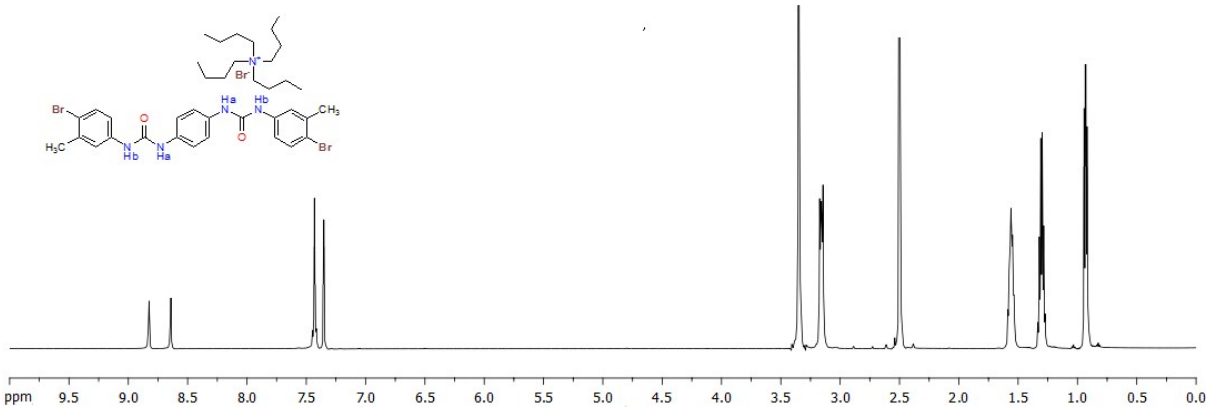


**Figure S19**: $^{1}$H NMR full and expanded spectrum of bromide entrapped complex **2b of $L_2$** as recorded in DMSO-$d_6$ at 298 K.

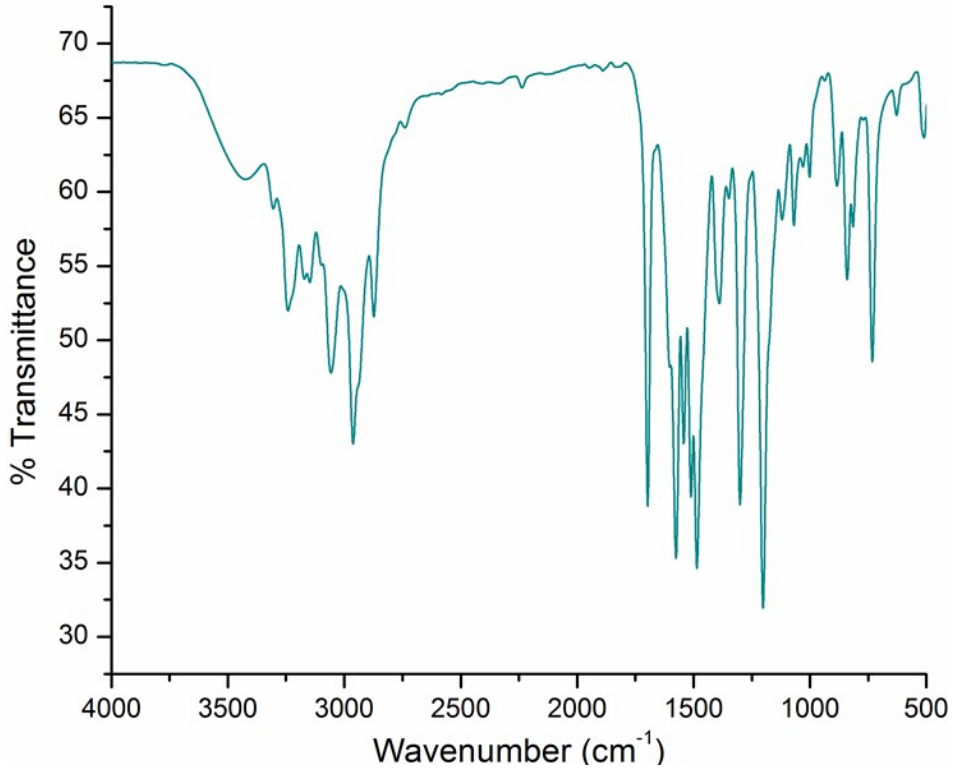


**Figure S20**: FT-IR spectrum of complex **2b** of **$L_2$** recorded in KBr pellet.

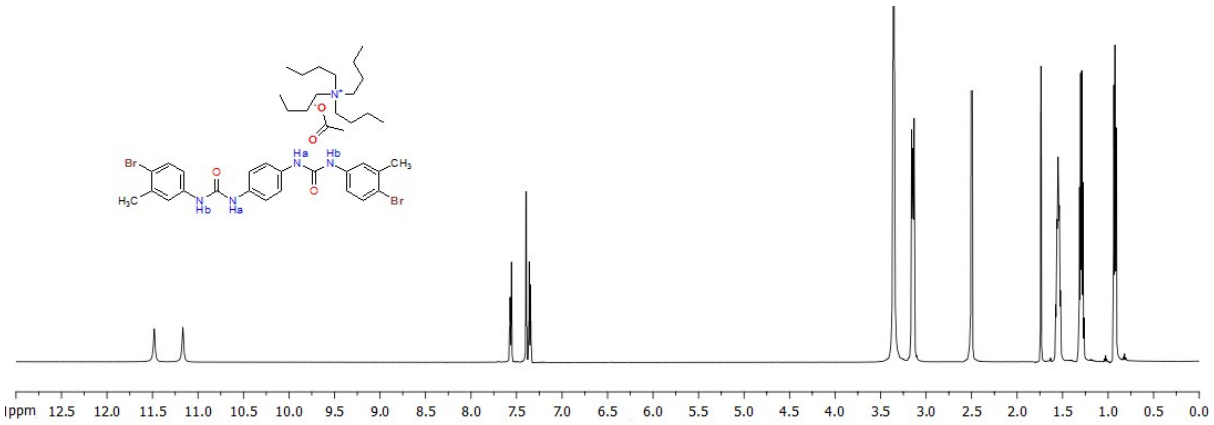


**Figure S21**: $^1$H NMR full and expanded spectrum of acetate entrapped complex **2c of $L_2$** as recorded in DMSO-$d_6$ at 298 K.

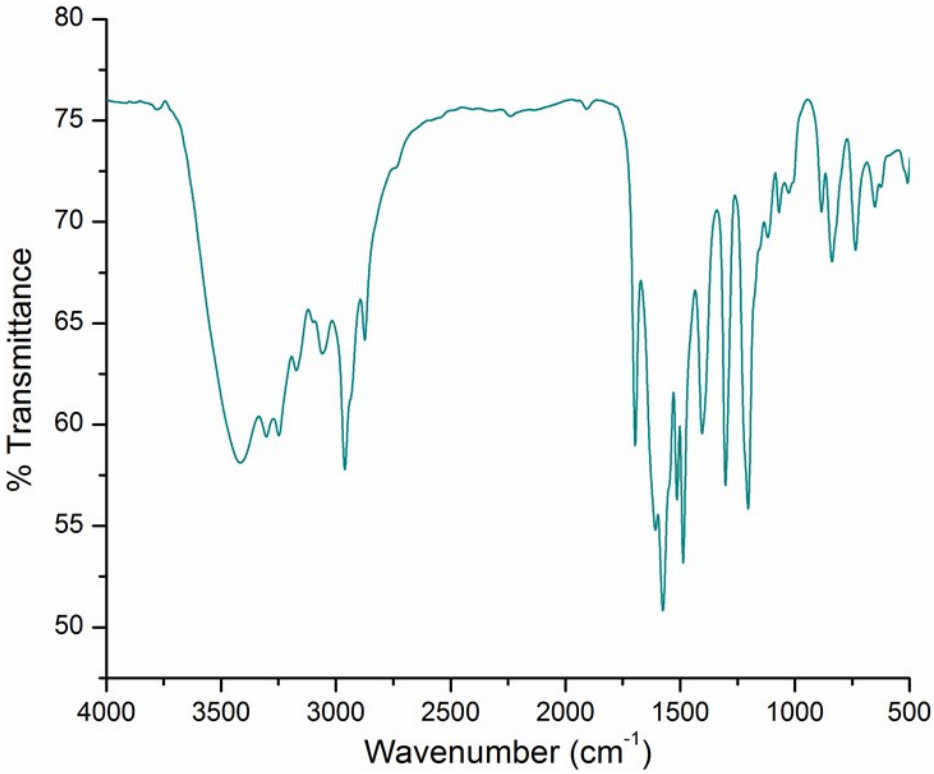


**Figure S22**: FT-IR spectrum of complex **2c** of **$L_2$** recorded in KBr pellet.

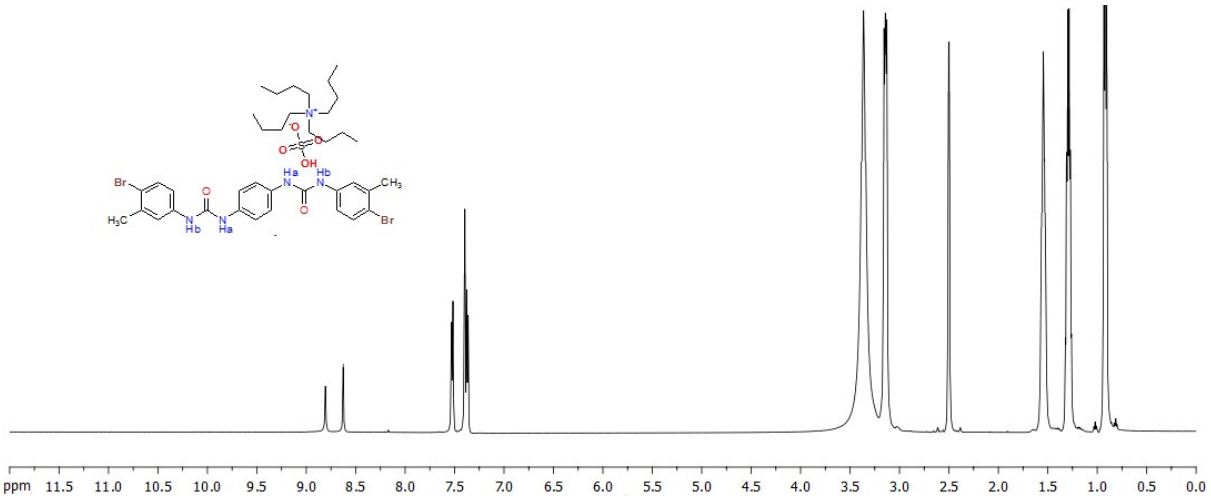


**Figure S23**: $^{1}$H NMR full and expanded spectrum of hydrogensulphate dimer entrapped complex **2d** of $\mathbf{L_2}$ as recorded in DMSO-$d_6$ at 298 K.

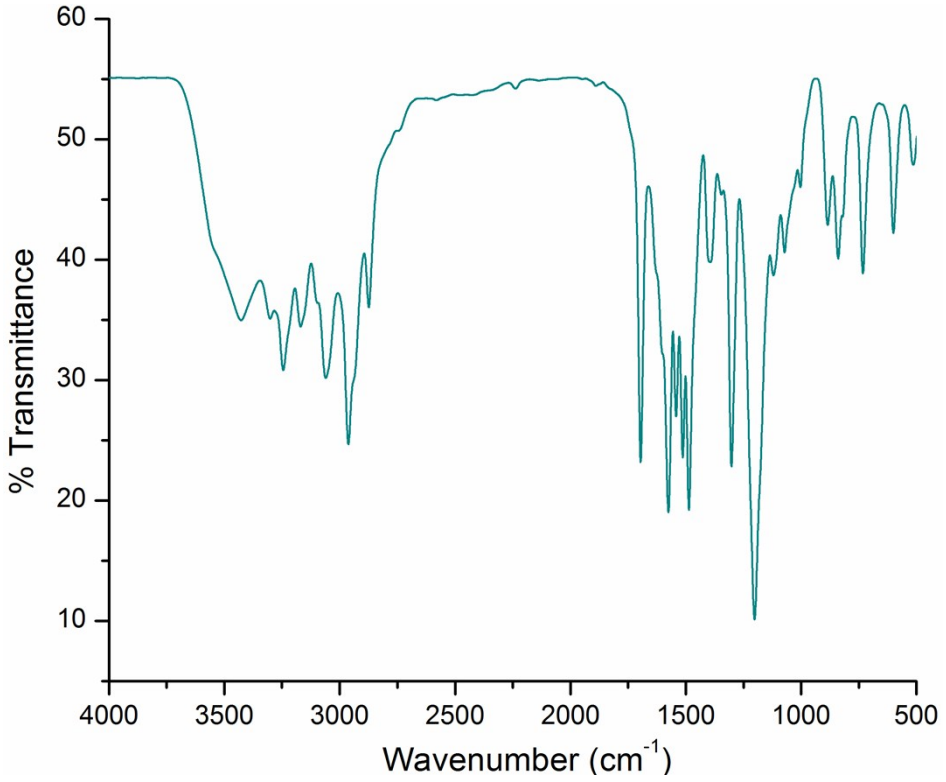


**Figure S24**: FT-IR spectrum of complex **2d** of $\mathbf{L_2}$ recorded in KBr pellet.

**Table S1.** Hydrogen bonding distances (Å) and Bond angles (°) in the neutral anion-receptor complexes:

| Ligand/Complex | D–H···A | *d*(D···H)/Å | *d*(H···A)/Å | *d*(D···A)/Å | <D–H···A/° | Symmetry codes |
|---|---|---|---|---|---|---|
| **1a** | N1-H1N···Br1 | 0.86 | 2.52 | 3.351(5) | 162 | 1/2-x,-1/2+y,1/2-z |
| | N2-H2N···Br1 | 0.86 | 2.50 | 3.332(4) | 163 | 1/2-x,-1/2+y,1/2-z |
| **1b** | N1-H1N···O2 | 0.86 | 1.93 | 2.76(13) | 164 | x,y,z |
| | N2-H2N···O3 | 0.86 | 2.00 | 2.83(13) | 165 | x,y,z |
| | O4-H4O···O3 | 0.82 | 1.83 | 2.64(13) | 169 | 1-x,1-y,-z |
| **1c** | N1-H1N···O3 | 0.86 | 2.00 | 2.834(4) | 163 | x,y,z |
| | N2-H2N···O4 | 0.86 | 1.93 | 2.776(4) | 166 | x,y,z |
| | N3-H3N···O5 | 0.86 | 1.97 | 2.785(4) | 158 | 1-x,-1/2+y,1/2-z |
| | N4-H4N···O6 | 0.86 | 1.96 | 2.809(4) | 167 | 1-x,-1/2+y,1/2-z |
| **1d** | N1-H1N···O4 | 0.86 | 2.00 | 2.833(7) | 162 | x,y,z |
| | N1-H1N···O6 | 0.86 | 2.06 | 2.854(7) | 154 | x,y,z |
| | N2-H2N···O4 | 0.86 | 2.58 | 3.248(6) | 135 | x,y,z |
| | N2-H2N···O5 | 0.86 | 2.17 | 2.927(6) | 147 | x,y,z |
| | N2-H2N···O3 | 0.86 | 1.95 | 2.765(5) | 159 | 1-x,-y,1-z |
| | N3-H3N···O6 | 0.86 | 2.54 | 3.299(6) | 148 | 1-x,1/2+y,1/2-z |
| | N3-H3N···O3 | 0.86 | 2.00 | 2.798(5) | 154 | x,1/2-y,-1/2+z |
| | N3-H3N···O4 | 0.86 | 2.29 | 3.051(6) | 148 | x,1/2-y,-1/2+z |
| | N3-H3N···O5 | 0.86 | 2.51 | 3.233(6) | 142 | x,1/2-y,-1/2+z |
| | N4-H4N···O6 | 0.86 | 2.03 | 2.828(6) | 153 | 1-x,1/2+y,1/2-z |
| | N4-H4N···O5 | 0.86 | 2.00 | 2.835(6) | 163 | x,1/2-y,-1/2+z |
| **1e** | N1-H1N···O5 | 0.86 | 2.13 | 2.923(4) | 153 | x,y,z |
| | N2-H2N···O4 | 0.86 | 2.01 | 2.833(4) | 161 | x,y,z |
| | O2-H2O···O5 | 0.82 | 1.75 | 2.549(4) | 164 | 1-x,-y,1-z |
| | O3-H3O···O4 | 0.82 | 1.76 | 2.558(4) | 166 | -x,-y,1-z |
| **2a** | N1-H1N···Cl1 | 0.86 | 2.35 | 3.181(6) | 161 | 3/2-x,1/2+y,1/2-z |
| | N2-H2N···Cl1 | 0.86 | 2.35 | 3.181(6) | 162 | 3/2-x,1/2+y,1/2-z |
| **2b** | N1-H1N···Br2 | 0.86 | 2.52 | 3.352(6) | 163 | 1/2-x,-1/2+y,1/2-z |
| | N2-H2N···Br2 | 0.86 | 2.49 | 3.319(6) | 163 | 1/2-x,-1/2+y,1/2-z |
| **2c** | N1-H1N···O3 | 0.86 | 1.97 | 2.809(7) | 164 | x,y,z |
| | N2-H2N··· O4 | 0.86 | 1.92 | 2.766(7) | 166 | x,y,z |
| | N3-H3N··· O6 | 0.86 | 1.96 | 2.778(7) | 158 | 1+x,y,z |
| | N4-H4N··· O5 | 0.86 | 1.97 | 2.812(7) | 166 | 1+x,y,z |
| **2d** | N1-H1N···O10 | 0.86 | 2.04 | 2.902(7) | 175 | x,y,z |
| | N2-H2N··· O11 | 0.86 | 2.15 | 2.992(7) | 166 | x,y,z |
| | O8-H8··· O11 | 0.82 | 1.83 | 2.646(6) | 172 | 1-x,1-y,1-z |

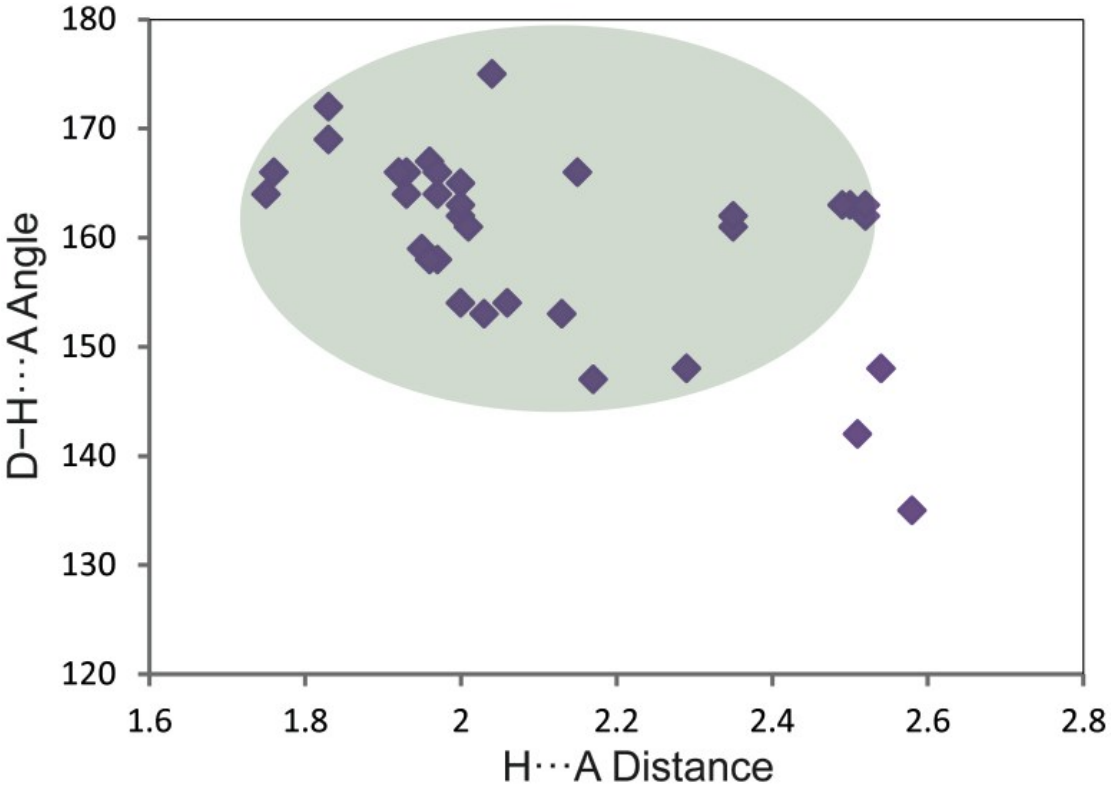


**Figure S25.** The scatter plot of D–H···A angles *vs*. H···A distances of the hydrogen bonds in neutral halide and oxyanion complexes **1a**-**1e**, **2a**-**2d** of receptors $\mathbf{L_1}$ and $\mathbf{L_2}$ and encircled area in the plot representing most of the interactions are present in strong hydrogen-bonding regions.