Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

A supramolecular dual-host based ion-pair induced formation of 1D coordination polymer

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Characterization of the dual-host complex, [$2L_1 2L_C(2K^+)(CO_3^{2-})$] :

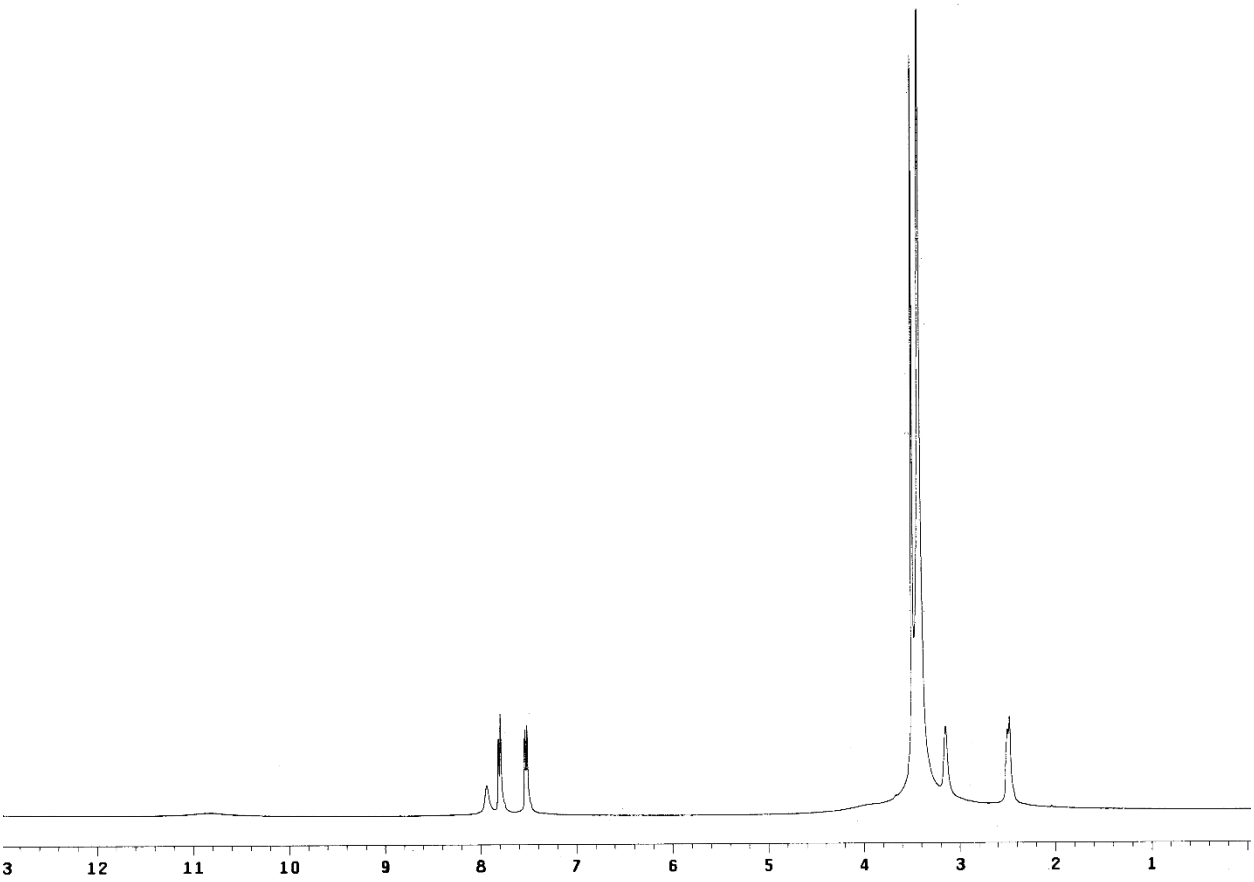

Fig. S1: ^{1}H NMR spectrum of the dual-host complex in DMSO-d_6 (Varian-400 MHz) at 298 K. δ (ppm) 2.47-2.51(t, 12H, NCH_2), 3.14(t, 12H, $NHCH_2$), 3.50 (s, 48H, Crown-ether-CH_2), 7.53 (d, 12H, ArCH), 7.80 (d, 12H, ArCH), 7.94 (s, 6H, urea–NH_a), 10.88 (s, 6H, urea–NH_b).

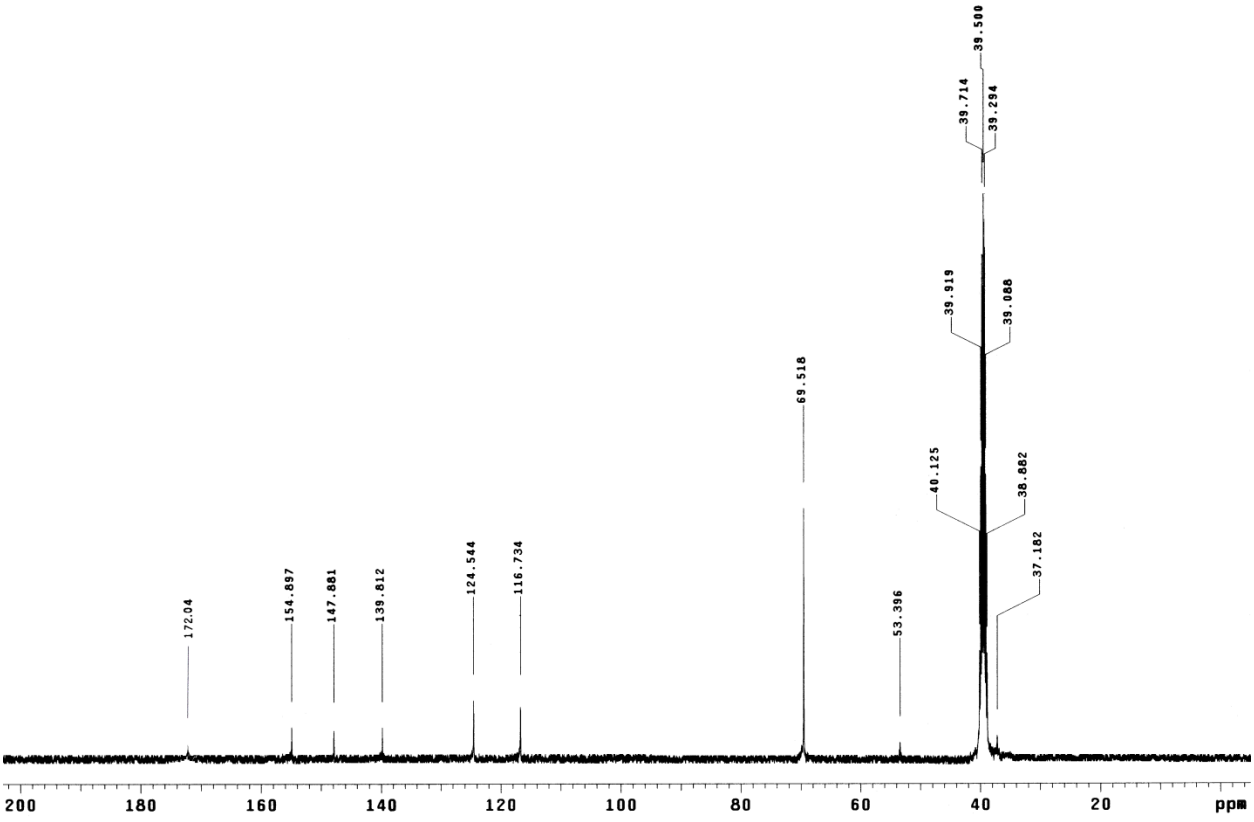

Fig. S2: ^{13}C NMR spectrum of the dual-host complex in DMSO-d_6 (Varian-100 MHz) at 298 K. δ (ppm) 37.18 (×6C, –NCH_2), 53.39 (×6C, −$NHCH_2$), 69.51 (×24C, crown-ether −CH_2), 116.73 (×12C, Ar CC−NH), 124.5 (×12C, Ar CC−NO_2), 139.8 (×6C Ar C−NH), 147.88 (×6C Ar C−NO_2), 154.9 (×6C, −C=O), 172.04 (CO_3^{2-}).

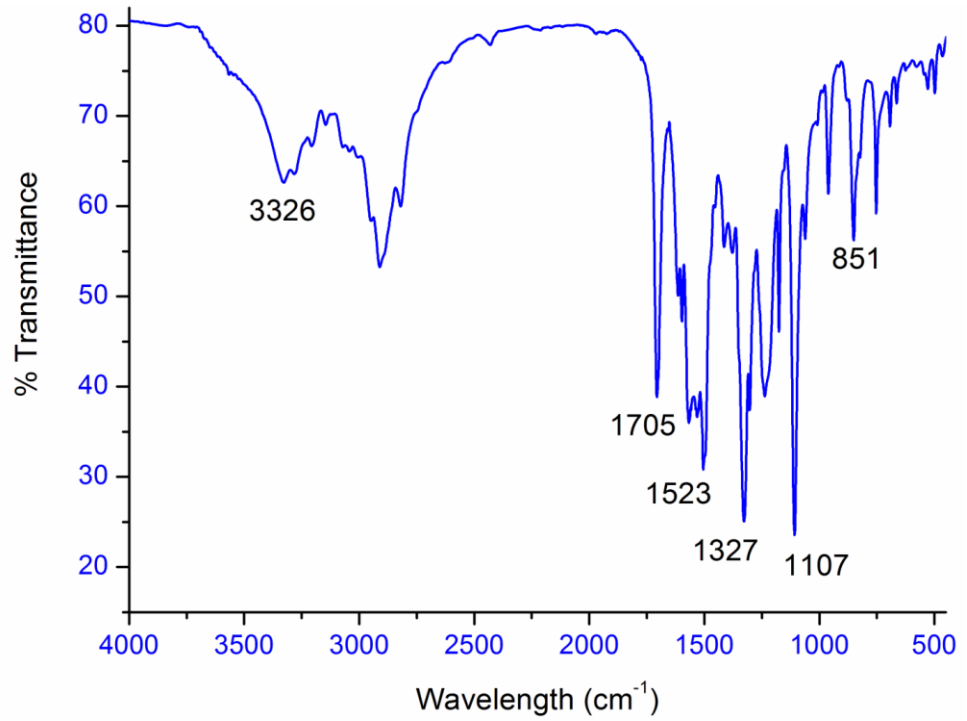

Fig. S3 FT-IR spectrum of the dual-host complex recorded in KBr pellet. υ cm-1: 851 (δ OCO;CO_3^{2-}), 1107 (υ C−O), 1237 (C−N), 1327 (NO2 sym.), 1523 (NO_2 asym.), 1705 (−C=O), 3326 (N−H).

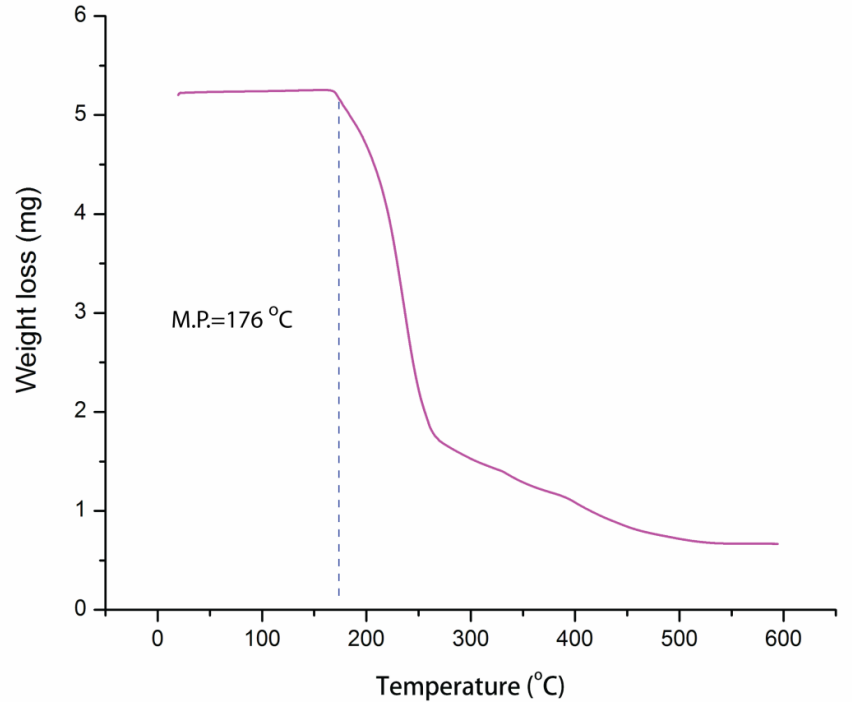

Fig. S4 Thermo gravimetric (TGA) curve of the complex obtained at a heating rate of 5°C/min in N_2 atmosphere.

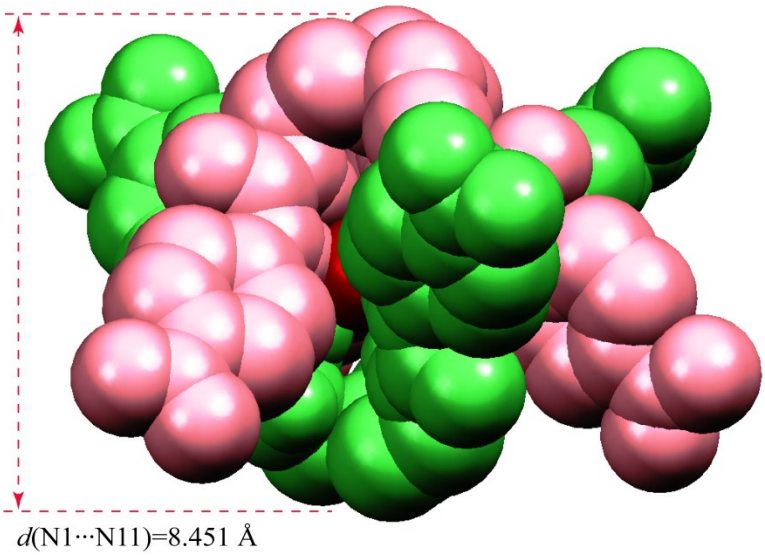

Fig. S5 Spacefill representation depicting full encapsulation of the CO_3^{2-} anion and capsule size.

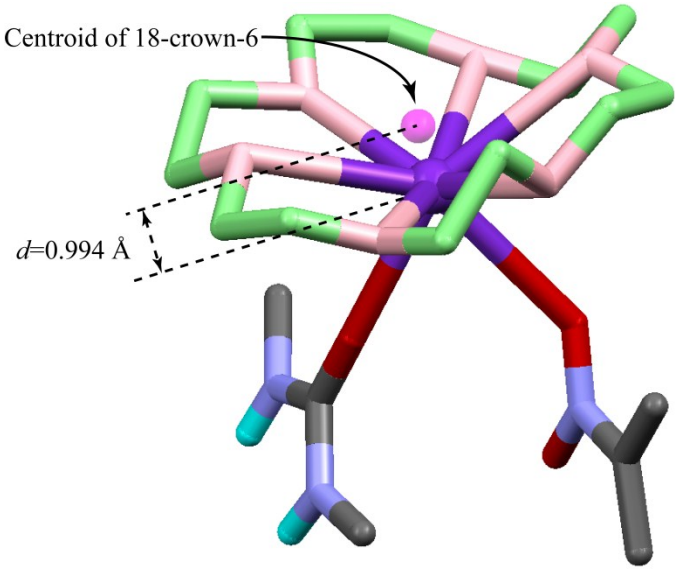

Fig. S5 Ball and stick representation depicting the doming out of K^+_2 from the crown-ether plane.

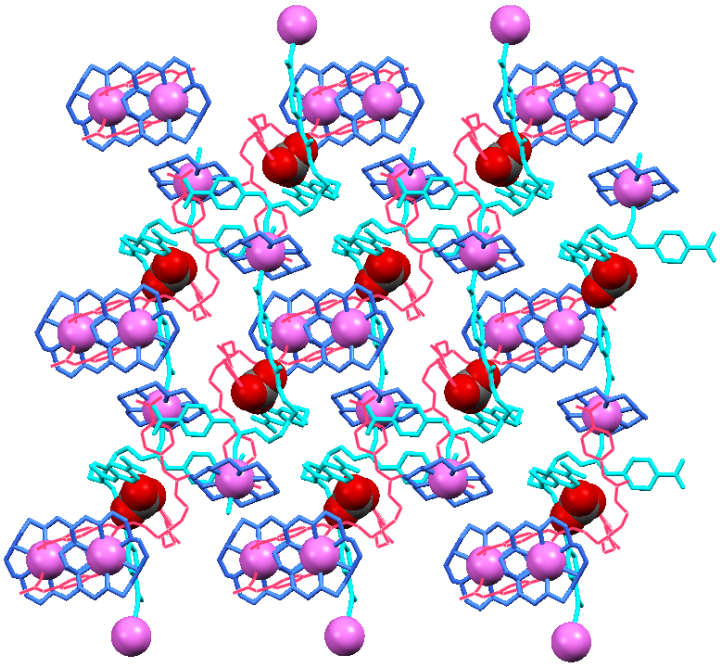

Fig. S6 Packing diagram of the coordination polymeric complex along *a*-axis.

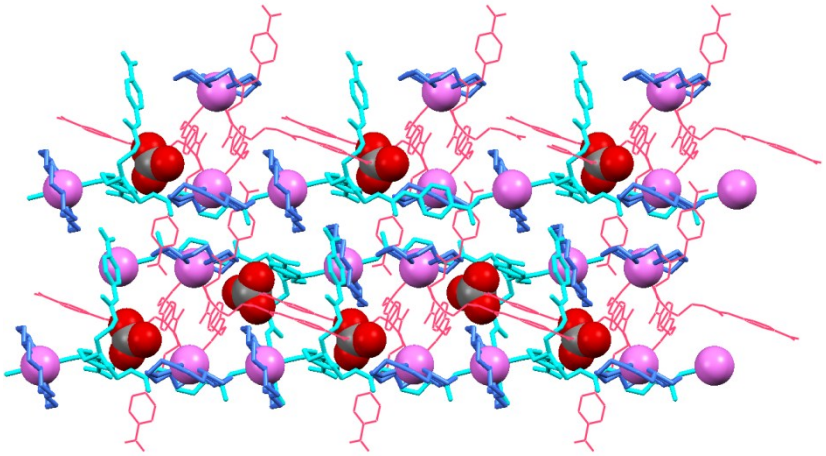

Fig. S7 Packing diagram of the coordination polymeric complex along *b*-axis.

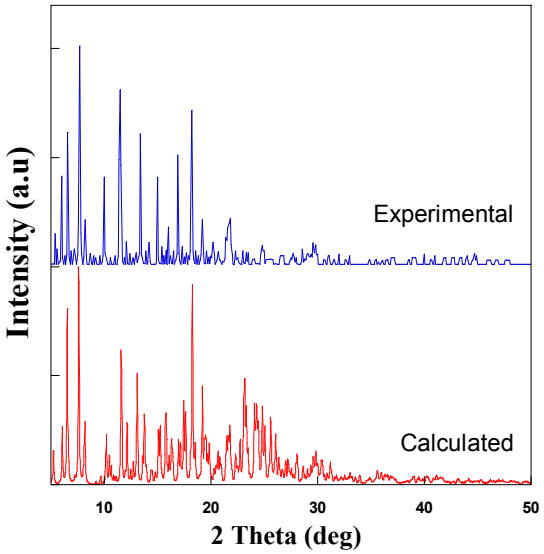

Fig. S8 Theoretical and experimental PXRD pattern of the complex.