Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

An approach to networks based on coordination of alkyl-substituted cucurbit[5]urils and metal ions

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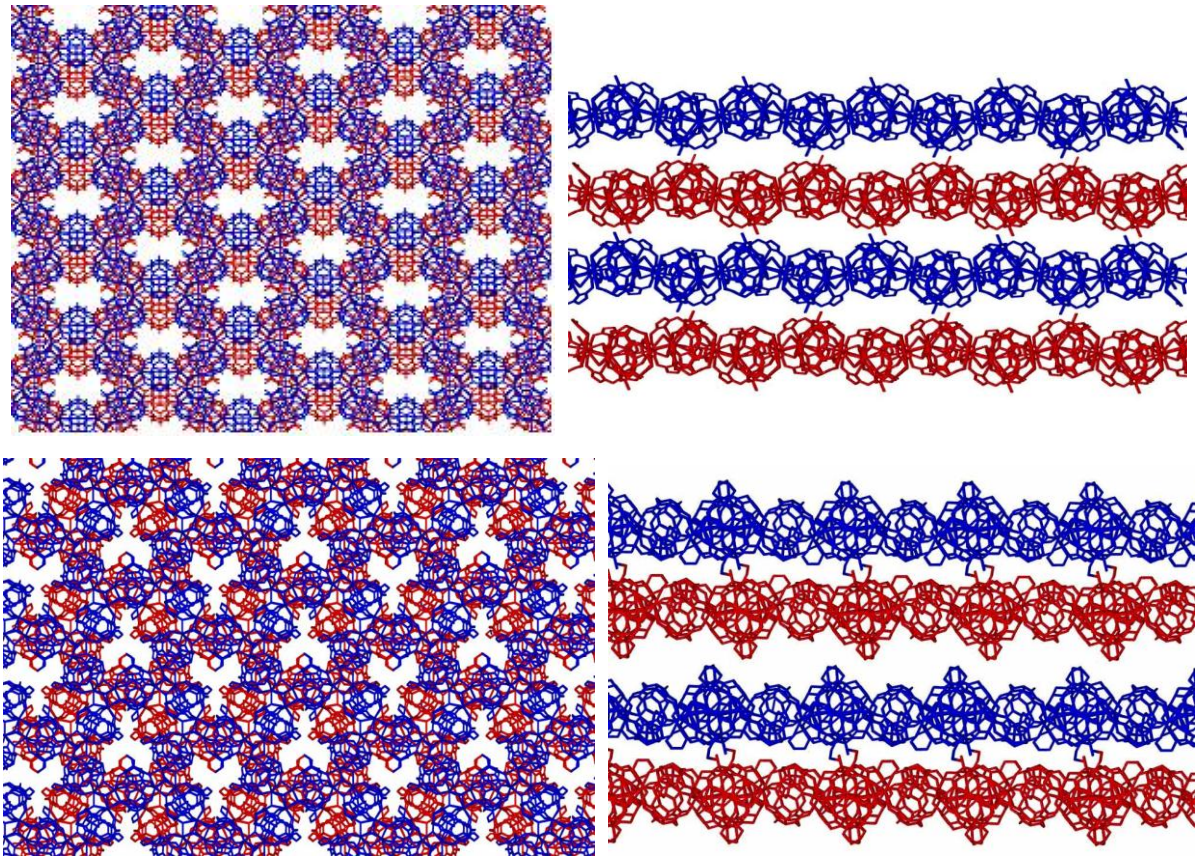
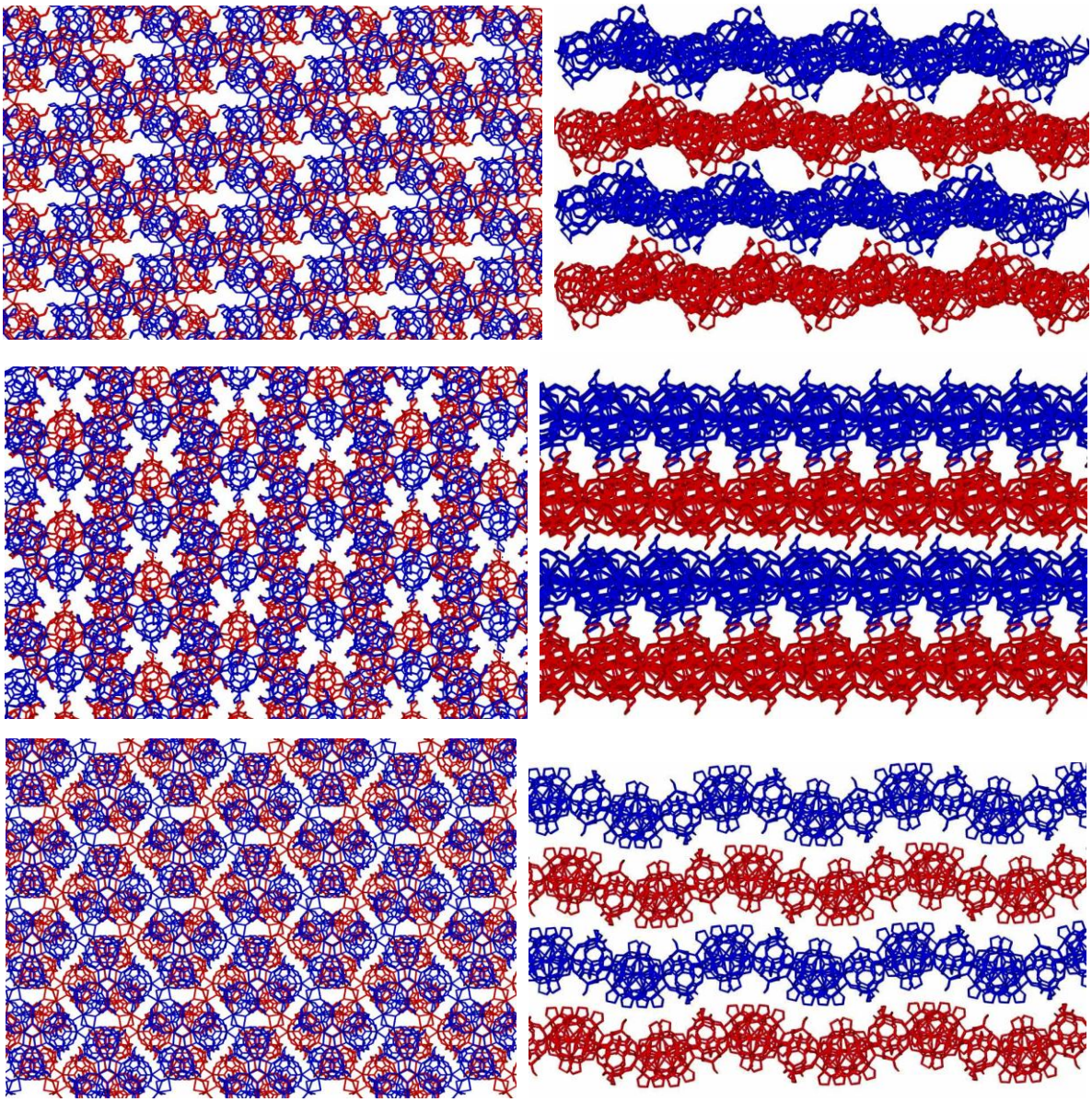
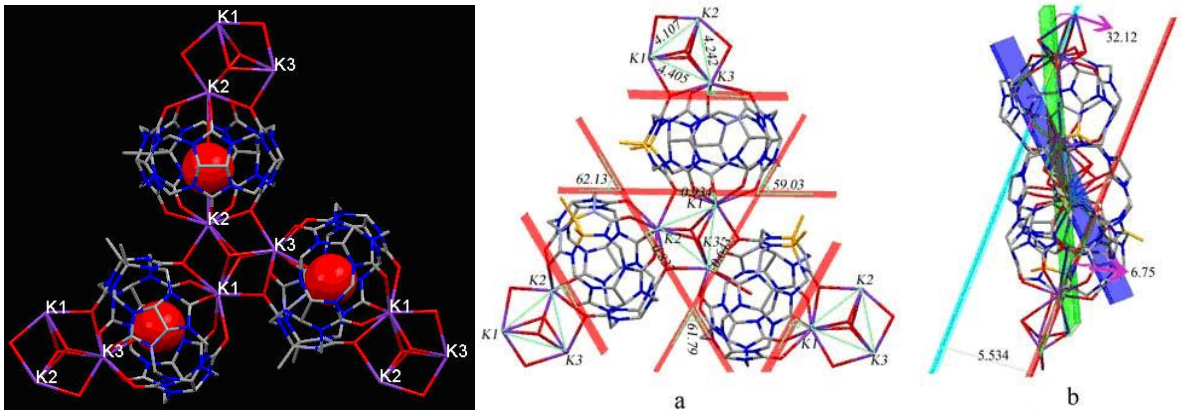
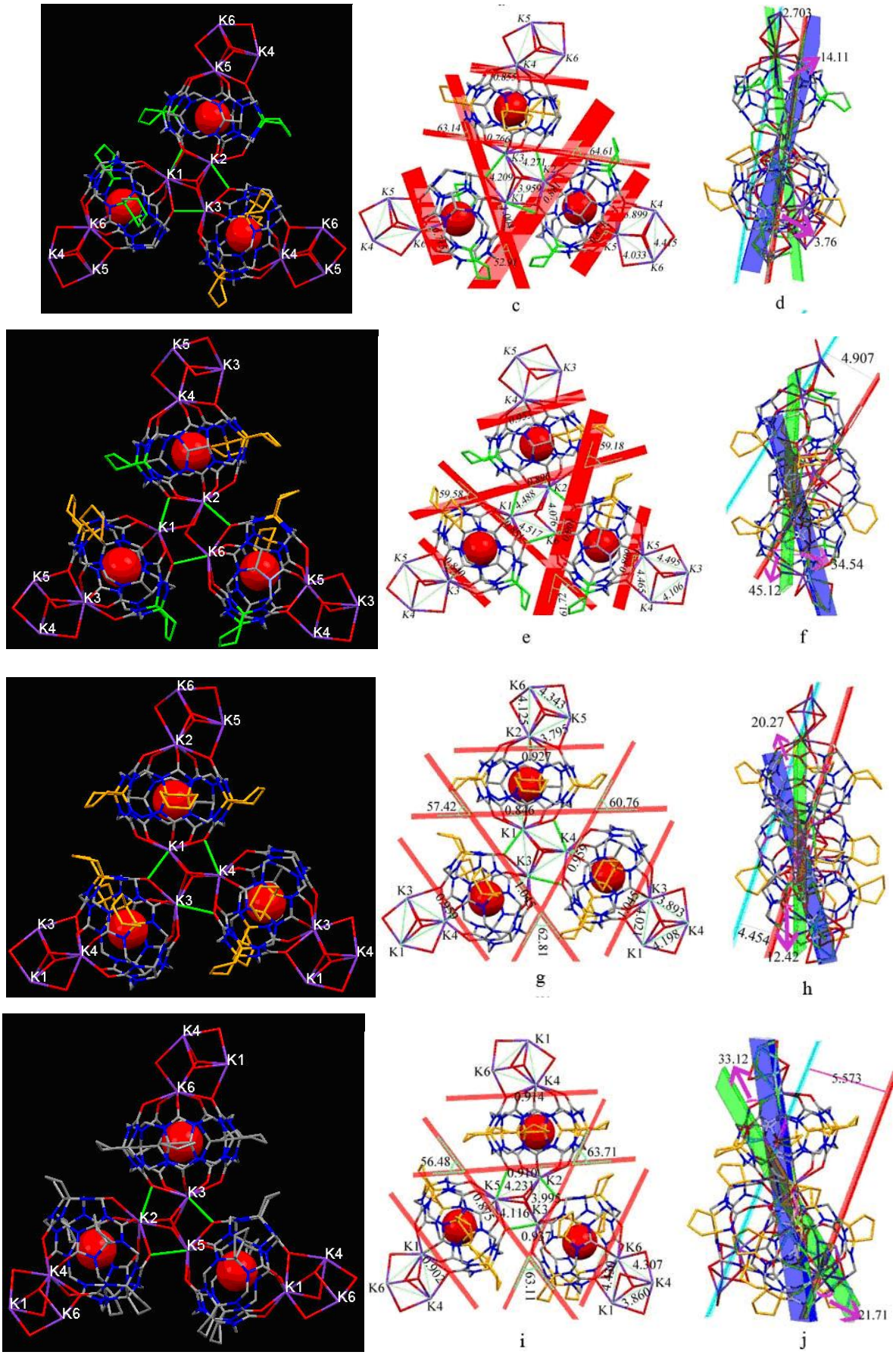


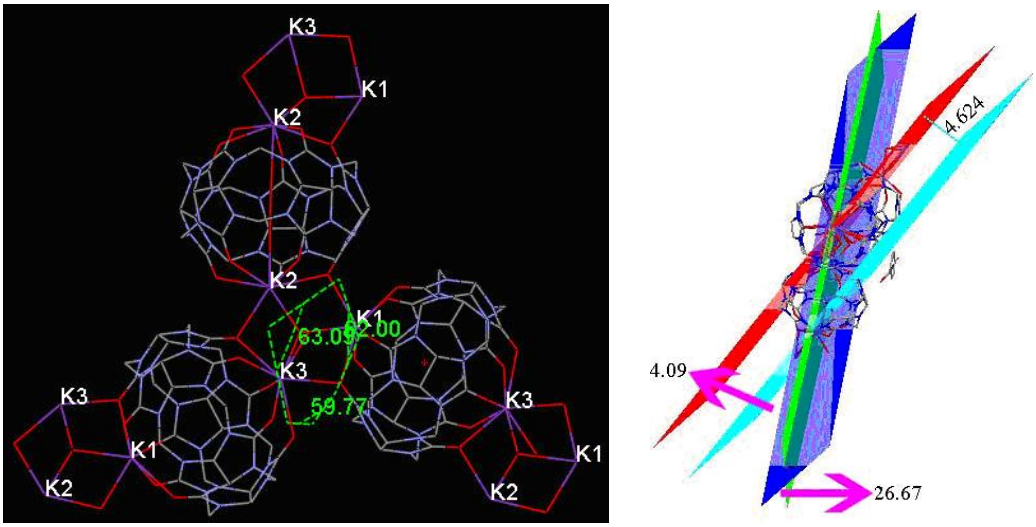


SI-Figure 1 the first row) the structures of the related five SQ[5]s (top view) in the compound **A-E** respectively; the second row) the corresponding trigonal planar branches constructed of SQ[5]s with K^+ ions; the third row) the corresponding 6-membered "bracelets" fused by the trigonal planar branches; the fourth row) 2D networks based on coordination of alkyl-substituted cucurbit[5]urils and potassium cations

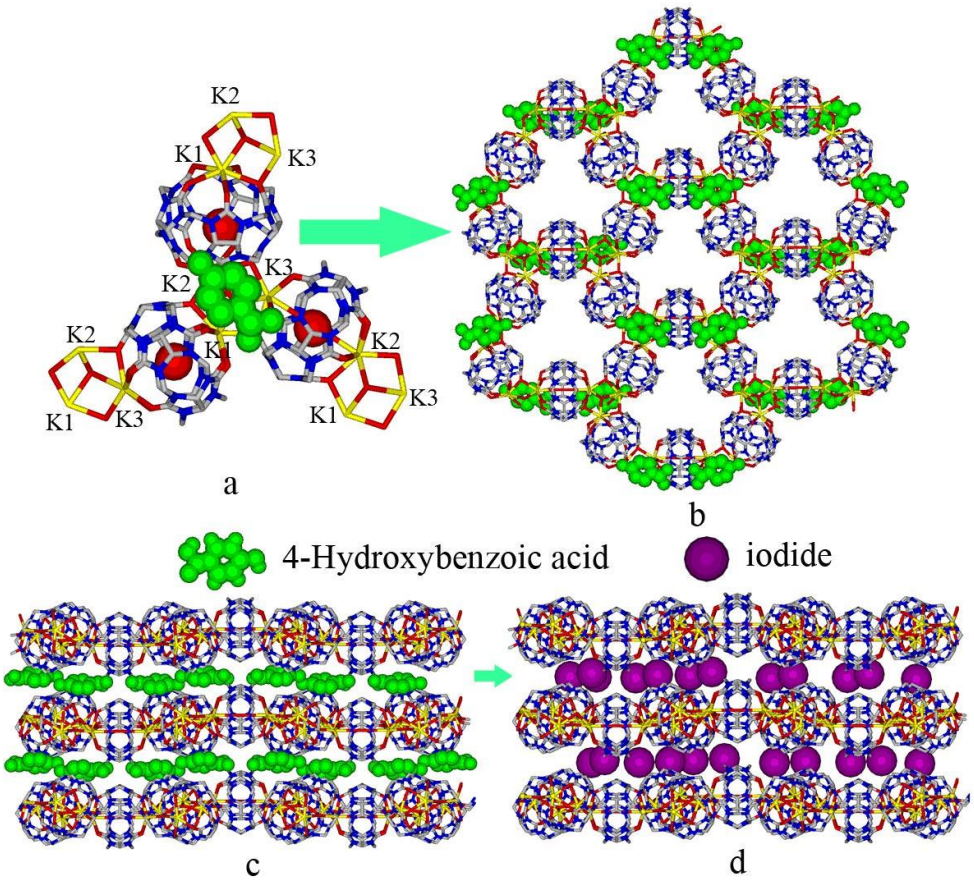




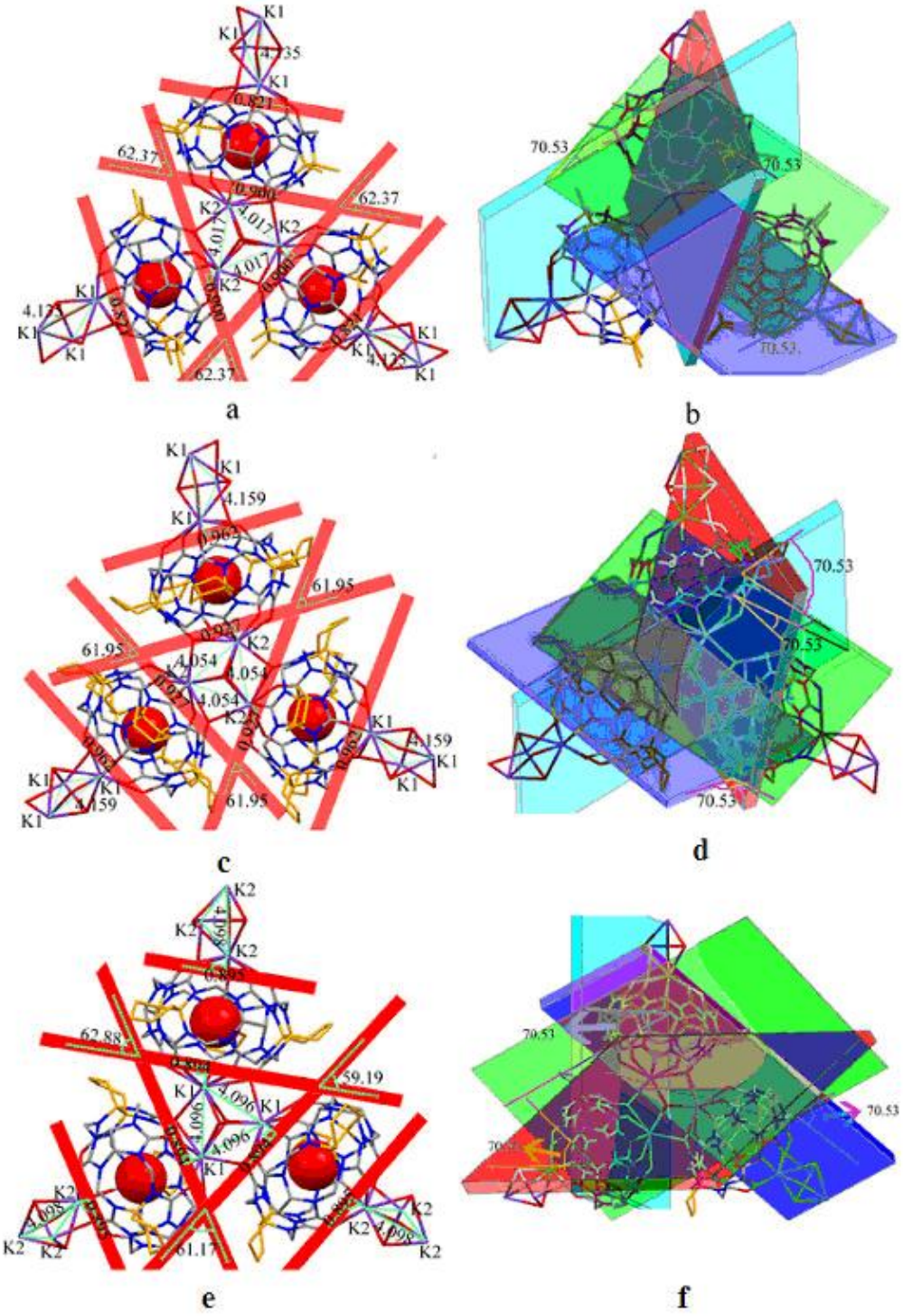
SI-Figure 2 the structural details of the trigonal planar branch a,b) in the compound **A**; c,d) in the compound **B**; e,f) in the compound **C**; g,h) in the compound **D**; i,j) in the compound **E**



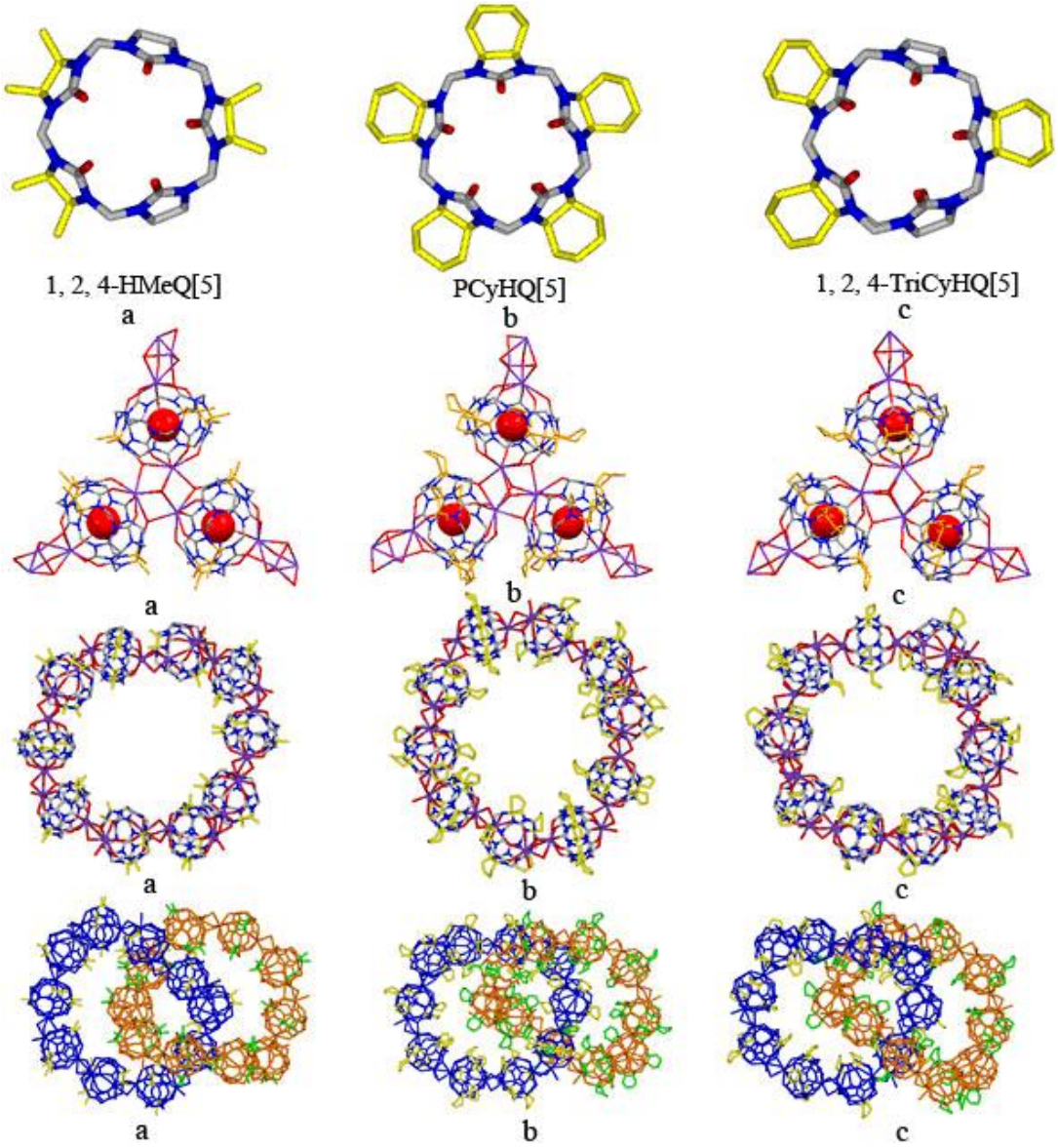
SI-Figure 3 the structural details of the trigonal planar branch in the compound **F**



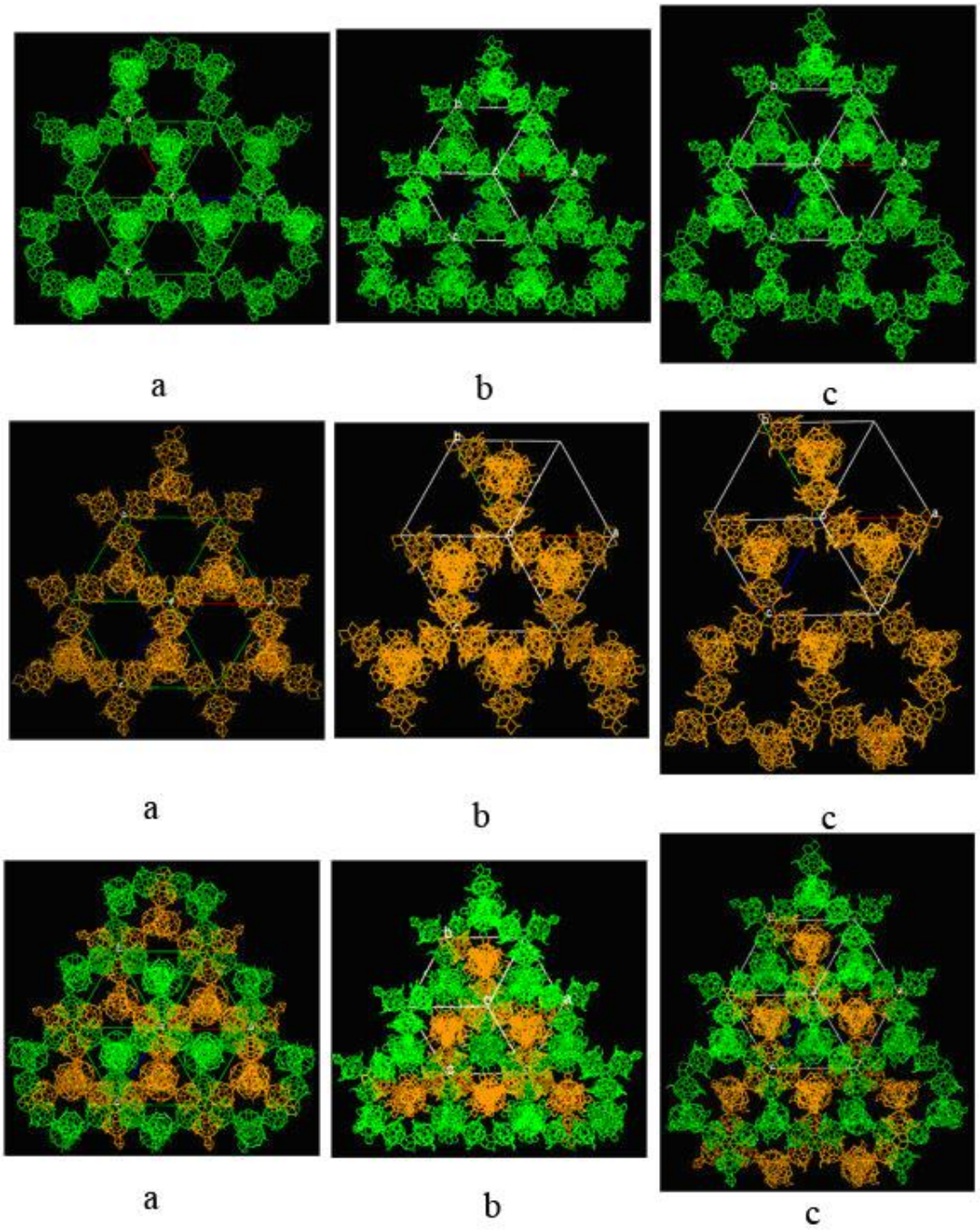
SI-Figure 4 a) Trigonal junctions of three Q[5] coordinated to potassium ions (yellow). b) 6-membered Q[5] 'beaded' rings in a single layer with molecules of *p*-hydroxybenzoic acid (green) centred over each junction. H_2O found in the channels has been omitted for clarity. c) A view of the template molecules, *p*-hydroxybenzoic acid (green), between the layers. d) The location of the I^- ions between the netting layers of Q[5] 'beaded' ring.



SI-Figure 5. Structural details for the trigonal planar branches (a) and (b) in **A**; (c) and (d) in the **B**; (e) and (f) in **C**.

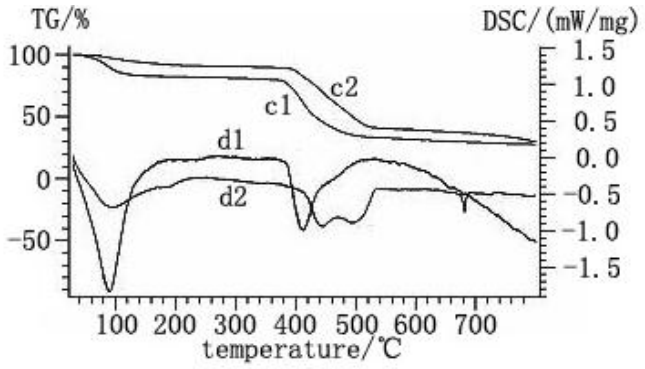


SI-Figure 6 (Part 1). The first row: the structures of the related three SQ[5]s (top view) in **A-C** respectively; the second row: the corresponding trigonal planar branches constructed of SQ[5]s with K^+ ions; the third row: the corresponding 10-membered "bracelets" fused by the trigonal planar branches; the fourth row: the catenane structures based on the interlocked 10-membered bracelets; the fifth and sixth rows: two isolated 3D networks based on coordination of alkyl-substituted cucurbit[5]urils and potassium cations; the seventh row: the combination of the two isolated 3D networks. ***(Figure and caption continued below).***



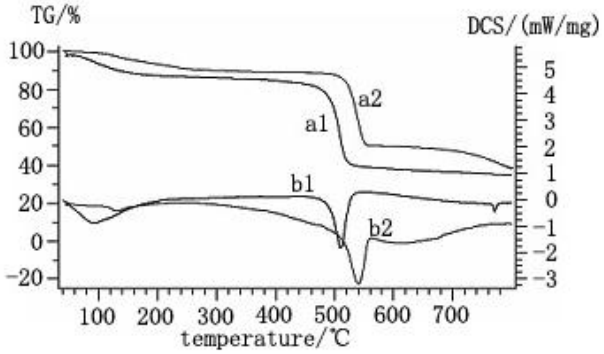
SI-Figure 6 (Part 2). Figure and caption continued from **SI-Figure 1 (Part 1)** above**.** The fifth and sixth rows: two isolated 3D networks based on coordination of alkyl-substituted cucurbit[5]urils and potassium cations; the seventh row: the combination of the two isolated 3D networks.

Thermal Properties of the compound **C**



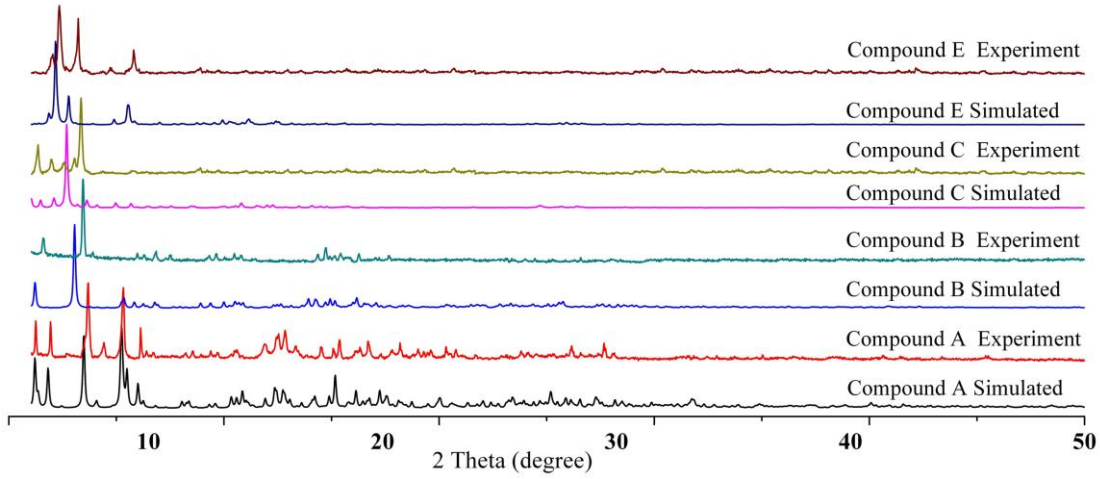
c1) TG curve of 1,2,4-triCyHQ[5], c2) TG curve of the crystals of the compound **B**; d1) DCS curve of 1,2,4-triCyHQ[5], d2) DCS curve of the crystals of the compound **B**

Thermal Properties of the compound **C**



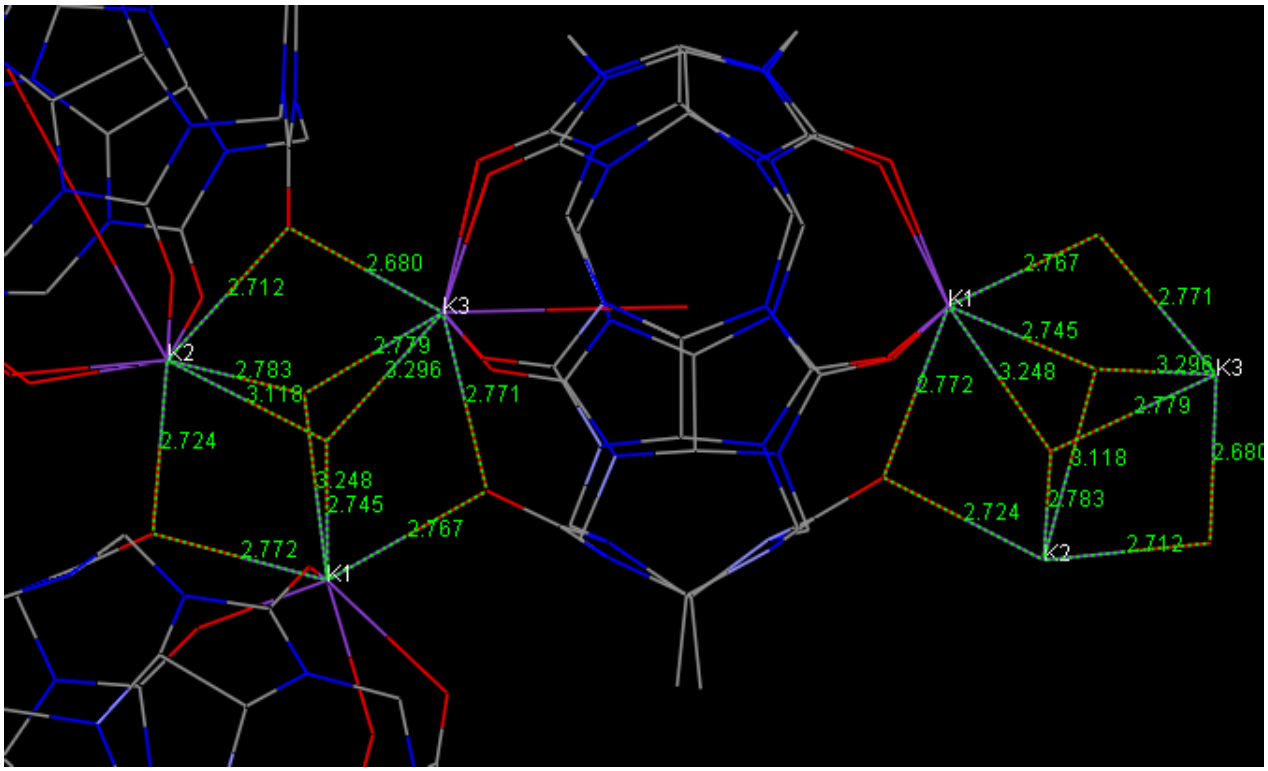
a1) TG curve of 1,2,3-triCyHQ[5], a2) TG curve of the crystals of the compound **C**; b1) DCS curve of 1,2,3-triCyHQ[5], b2) DCS curve of the crystals of the compound **C**

SI-Figure 7 The thermal Properties of the compounds **B** and **C**

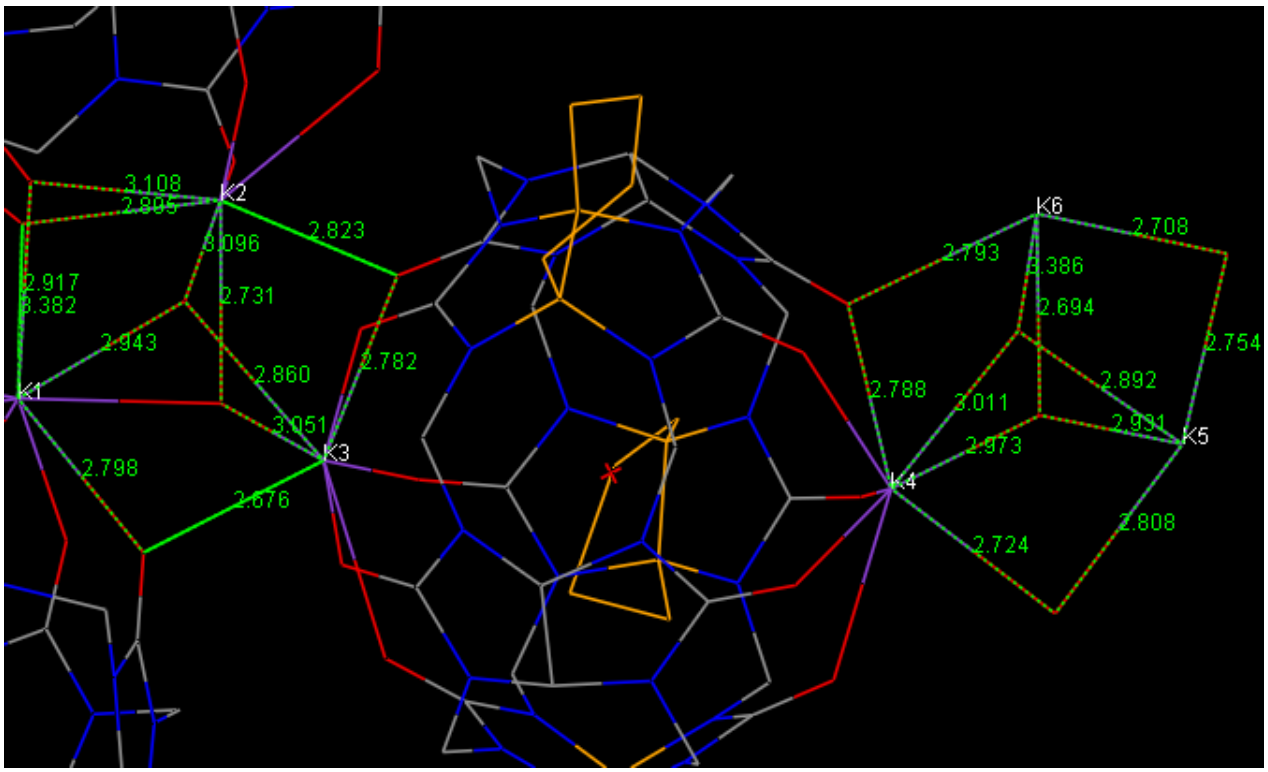


SI-Figure 8 Powder X-ray diffraction (PXRD) of the related compounds and comparison with simulation show that the corresponding samples

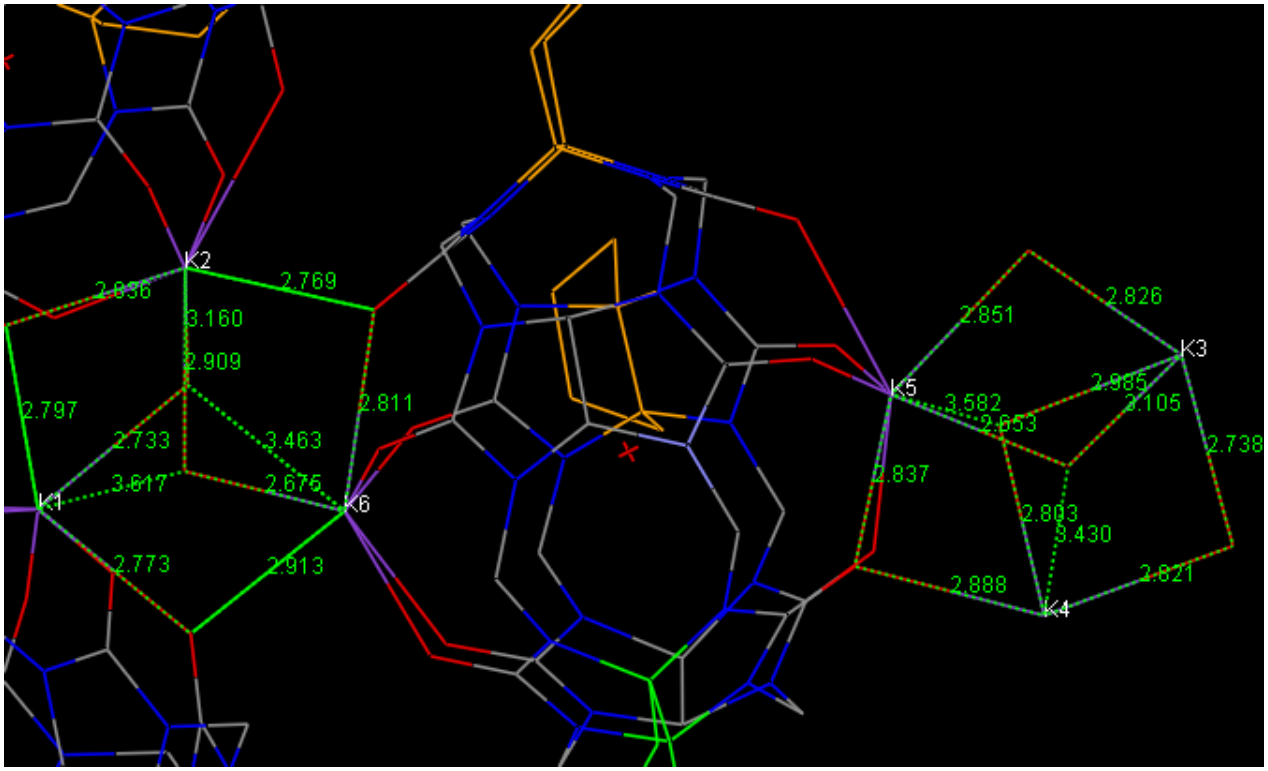
The structural information about the K_3O_2 junctions



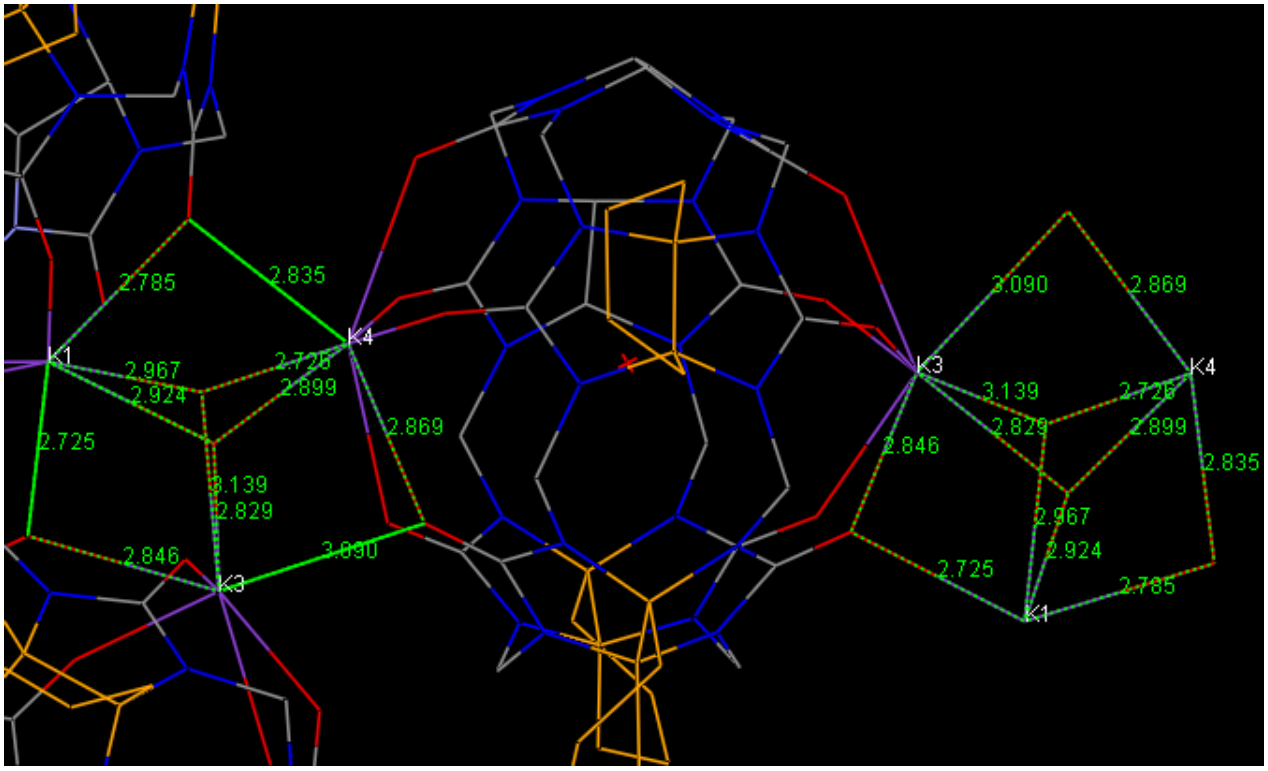
The K_3O_2 junction in the compound A



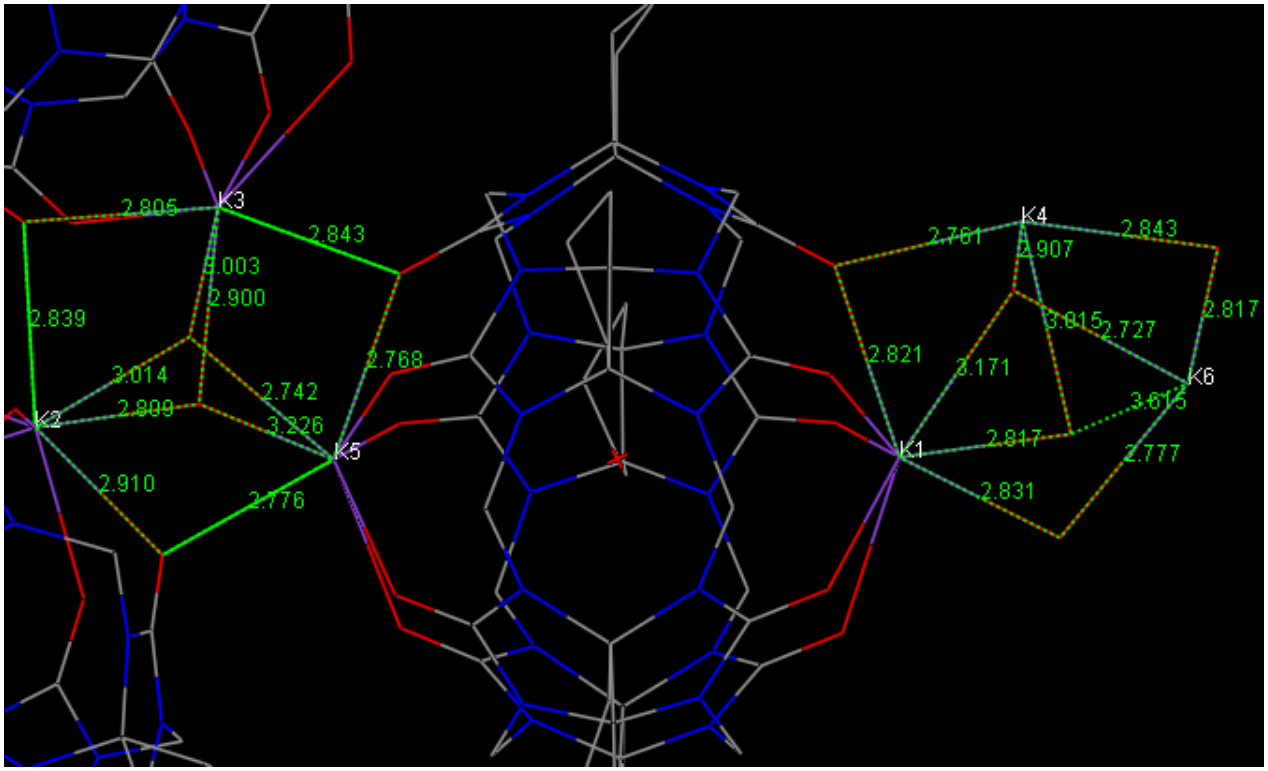
The K_3O_2 junction in the compound B



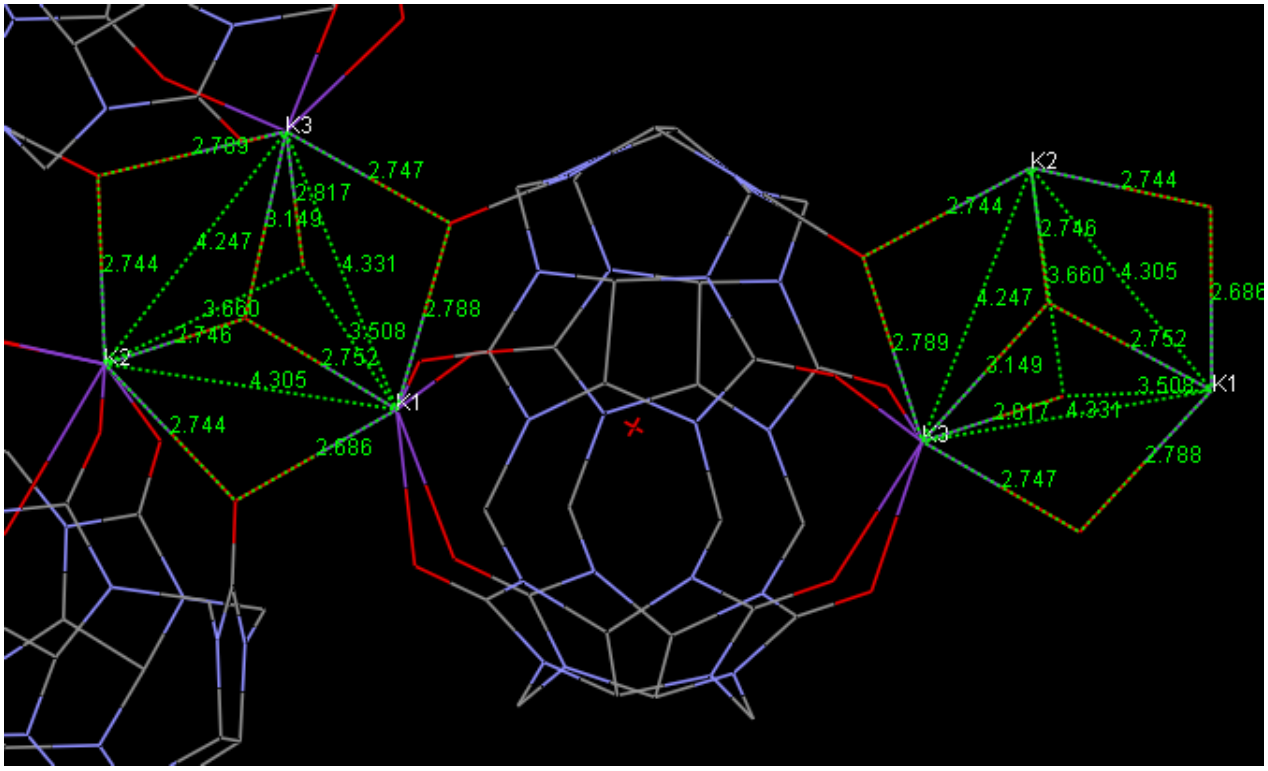
The K_3O_2 junction in the compound C



The K_3O_2 junction in the compound D

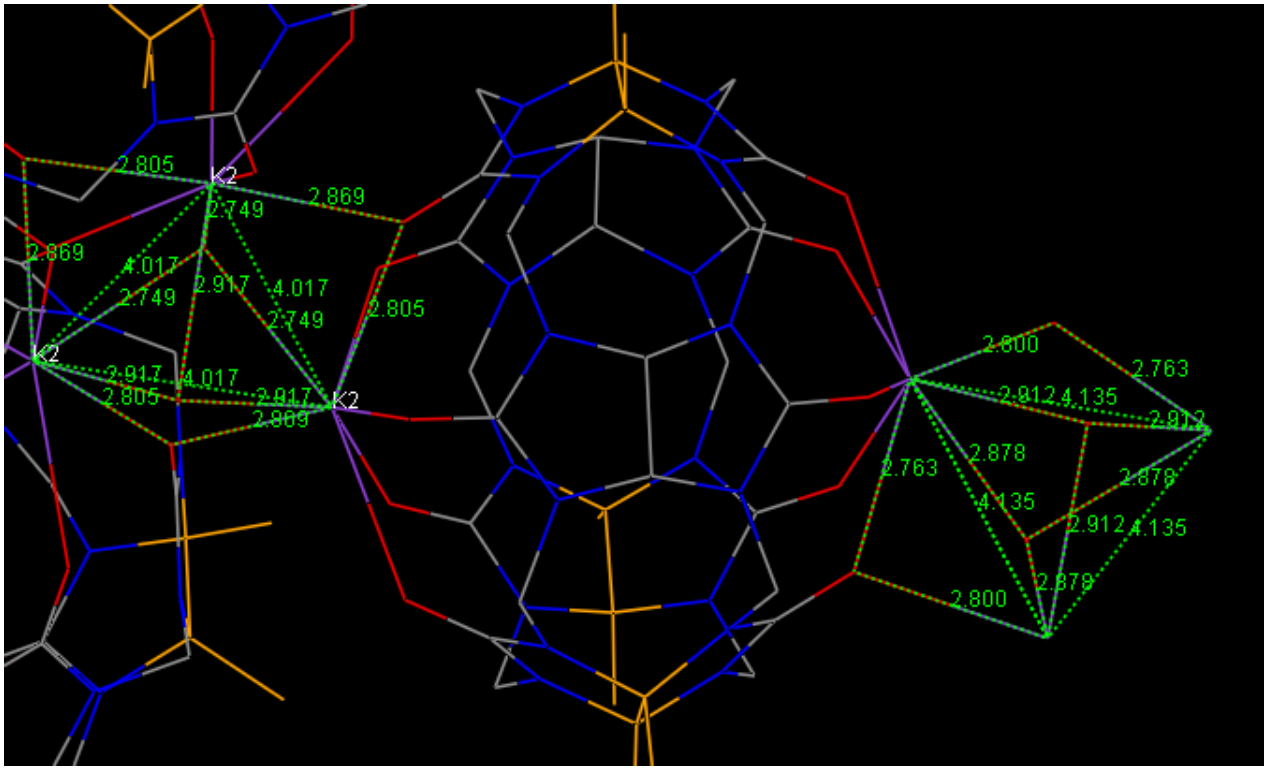


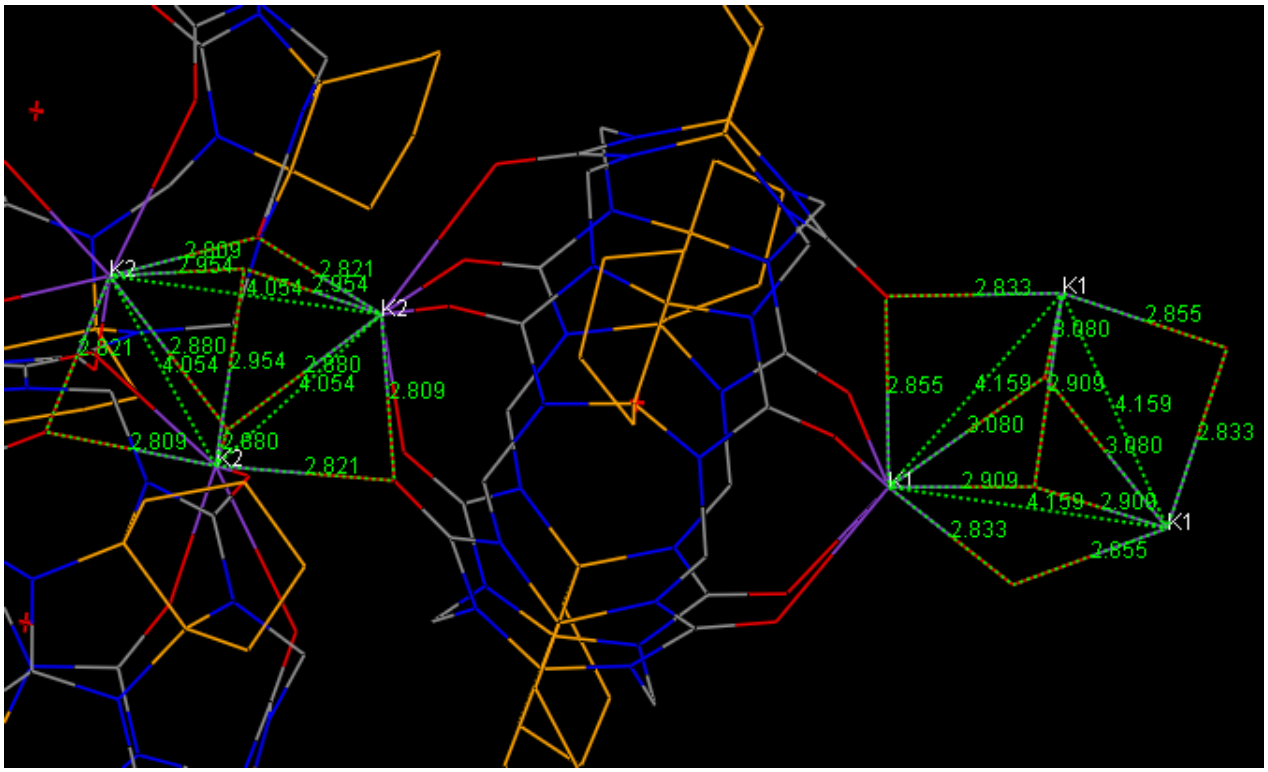
The K_3O_2 junction in the compound E

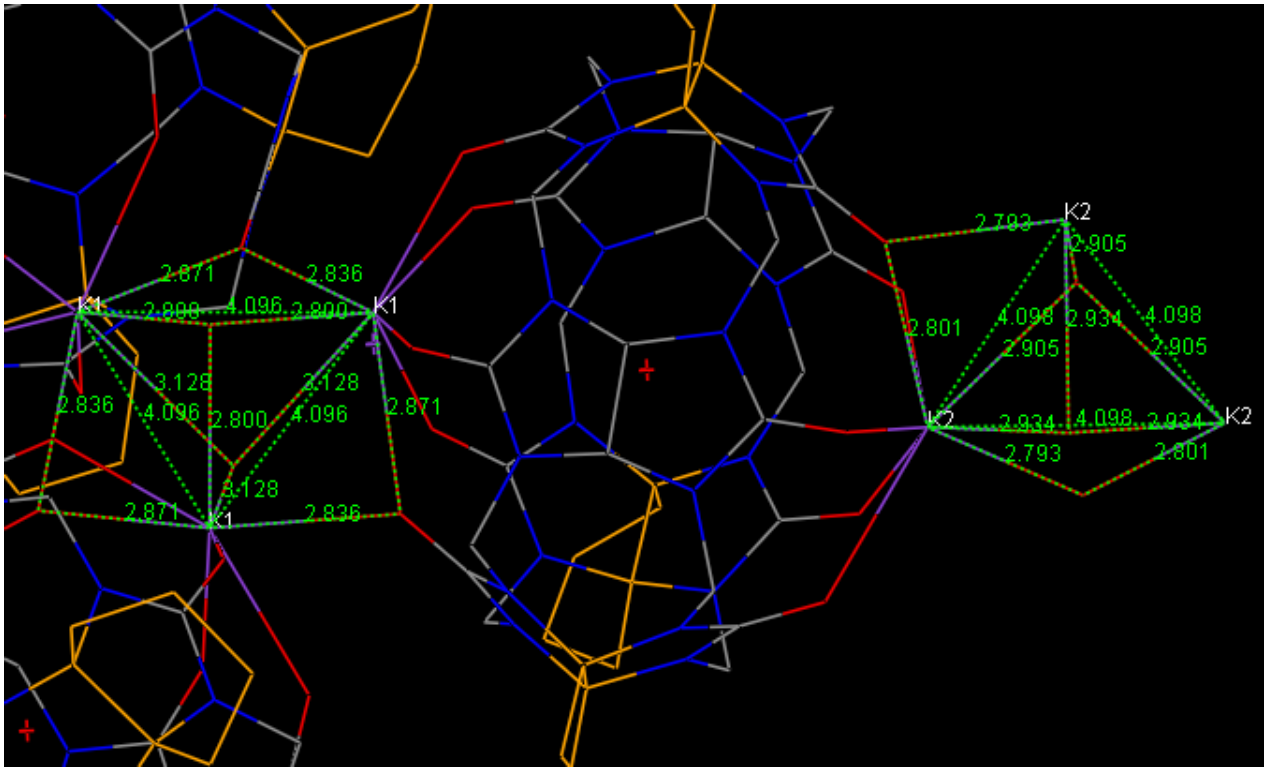


The K_3O_2 junction in the compound K-Q[5] in the presence of hydroxybenzoic acid in the ref. 14

Three compounds in which the formation of 3D fused 10-membered "bracelet" frameworks derived from the alkyl-substituted curcurbit[5]urils (SQ[5]s), 1,2,4-tricyclohexanocucurbit[5]uril (1,2,4-TriCyHQ[5]) (ref. 11), 1,2,4-hexamethylcucurbit[5]uril (1,2,4-HMeQ[5]) and pentacyclopentanocucurbit[5]uril (PCyHQ[5]) (ref. 13) and K^+ ions. The structural information about the K_3O_2 junctions in these three compounds are shown below.







The FT-IR spectra show no significant difference of four compounds compared to the corresponding pure SQ[5] respectively, except the absorption band of portal carbonyl shifts with betwee 13 cm^{-1} for the compound **A** and -4 cm^{-1} for the compound **E**.