



STRUCTURAL
CHEMISTRY

Volume 74 (2018)

Supporting information for article:

**Topological study of diverse hydrogen-bonded patterns found
in a system of a nickel(II) complex and the sulfate anion**

**Miguel Angel Harvey, Sebastián Suarez, Pavel N. Zolotarev, Davide M. Proserpio
and Ricardo Baggio**

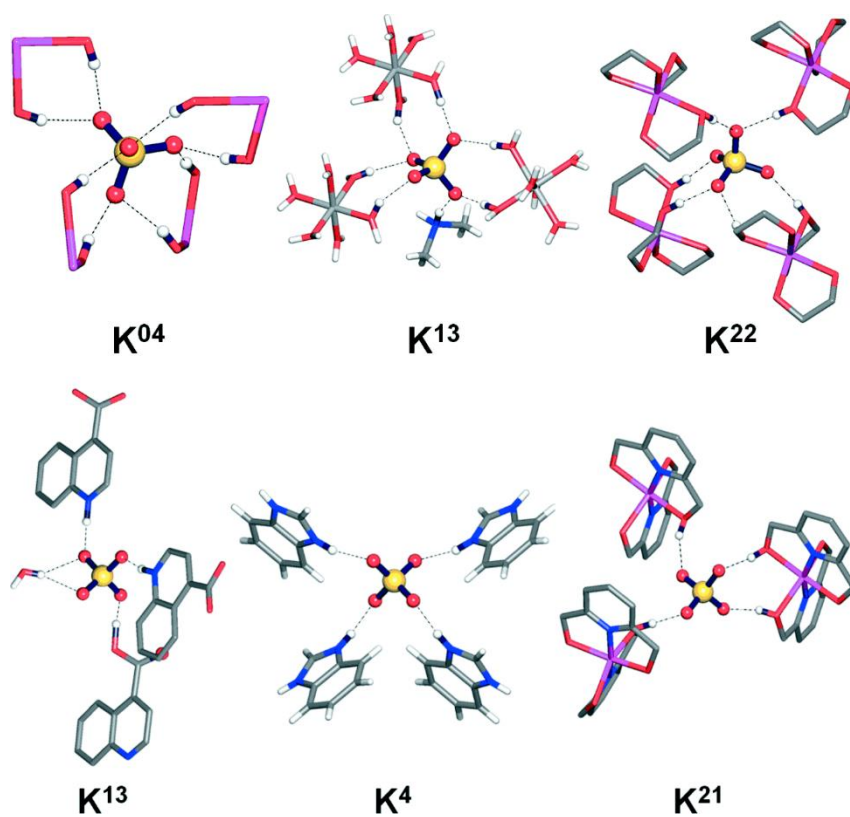
Supplementary document SD1

Discussion of “child” (**I,II,III**) vs. “parent” (**IV**) structural relationships

For the sake of clarity in what follows, we have identified some of the symmetry equivalent $R_4^4(16)$ loops in Fig. 5b with labels C_1 , C_1' , C_2 and C_2' . Now, if we compare Fig.3c (structure **II**) and Fig.5b (structure **IV**) it is apparent that loop B_2 (in **II**) and C_2 , or C_2' (in **IV**) appear in strict geometrical correspondence, being topologically equivalent. On the other side, when considering loop B_1 in **II** it can be seen that it corresponds to the combination of $C_1 + C_1'$ (in **IV**) except that the H-bond separating these two latter $R_4^4(16)$ groups (Fig.5b, highlighted) is not present in B_1 , where it "breaks up" giving rise to a larger $R_6^6(24)$ loop and thus leaving the corresponding donor and acceptor atoms (encircled and marked with arrows in Fig. 3c) free to enter into further interactions.

On the other hand, when comparing the ring scheme in **IV** with rings **A1** in **I** (Fig.3a) or **II** (Fig.3b), it can be seen that a similar process occurs, but now involving both pairs C_1 , C_1' and C_2 , C_2' (Fig 5b), in which the H-bonds serving as a limit between them "break up" to give rise to one single type of $R_6^6(24)$ loop **A1** in **I**, topologically similar to **A1** and **B1** in **II**.

Finally, the relationship between **III** and **IV** is much more straightforward: both structures can be considered as built up from the same columnar arrays (Figures 4a and 5a), with the sole difference that in **III** these columns are not linked to each other into a 2D framework, because the corresponding NH responsible of the job in **IV** is “blocked” in **III** by way of its entering into a H-bonding interaction to a water solvate. Figures 4b and 5b serve to clarify these structural differences, and the steps needed to go from **III** to **IV** are explained with the help of the square inset in Fig. 4b, viz.: (Step 1): by loosing the water solvate O3W and (Step 2) by breaking one of the bifurcated H-bonds, the H5NB donor and the O1 acceptor are ready to enter into new interactions. Thus (Step 3), through the interconnection of both centres through a new H-bond the same 2D supramolecular structure in the unsolvated **IV** (Fig 5b) is replicated.



Supplementary Figure S1

Examples of the connection types of sulfate anions that are hydrogen bonded to neighbouring molecules.