Supporting Information for manuscript:

On the importance of non covalent interactions in the structure of coordination Cu(II) and Co(II) complexes of pyrazine- and pyridine-dicarboxylic acid derivatives: Experimental and theoretical views

Masoud Mirzaei[a,*], Hossein Eshtiagh-Hosseini[a], Antonio Bauzá[b], Sara Zarghami[a], Pablo Ballester[c], Joel T. Mague[d] and Antonio Frontera[b,*]

[a] Department of Chemistry, Ferdowsi University of Mashhad, Mashhad 917751436, Iran, E-mail: mirzaeesh@um.ac.ir
[b] Departament de Quimica, Universitat de les Illes Balears, Palma de Mallorca (Baleares), Spain
[c] Institute of Chemical Research of Catalonia (ICIQ), Avgda. Països Catalans 16, 43007 Tarragona, Spain and Catalan Institution for Research and Advanced Studies (ICREA), Passeig Lluís Companys, 23, 08018, Barcelona, Spain.
[d] Department of Chemistry, Tulane University, New Orleans, LA 70118, USA

Table of contents:

1. Figures S1-S5

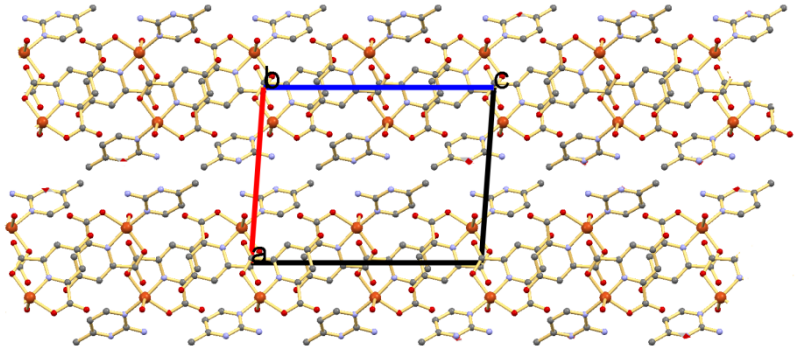

Fig. S1. Packing diagram of complex **1**.

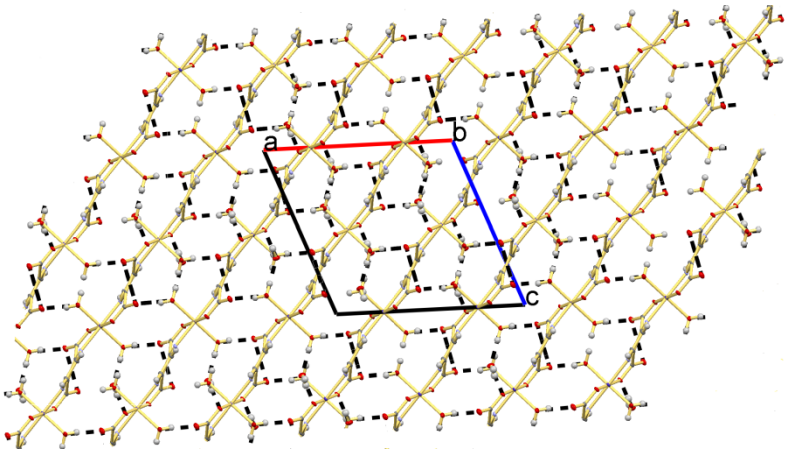

Fig. S2 Packing diagram of **2**. Dashed lines show H-bonding in the structure.

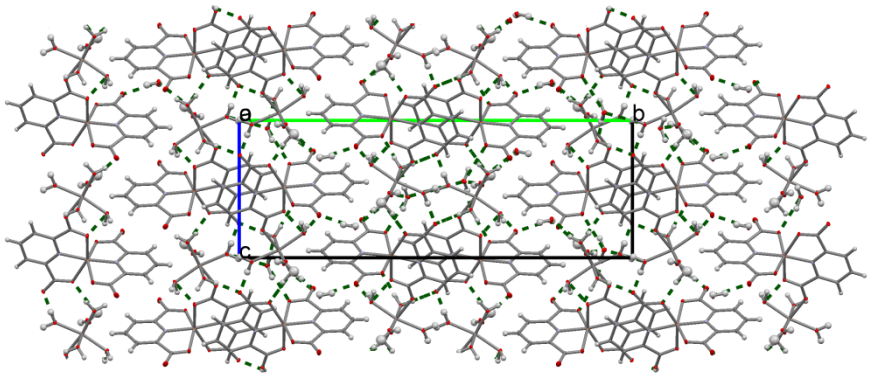

Fig. S4 Packing diagram of **3** viewed down the *a* axis. Hydrogen bonds are shown in dashed lines.

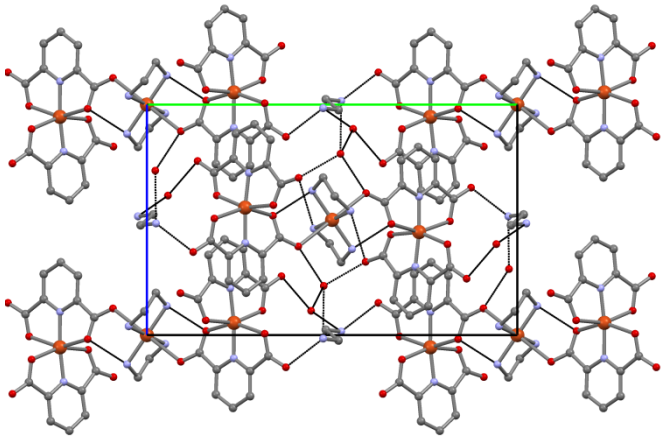

Fig. S5 The crystal packing of **4** showing hydrogen bonds as black lines.

2. CSD searches

We have not found in the literature previous studies devoted to π–hole interactions between coordinated carboxylate groups and Lewis bases by searching in the SciFinder database this research topic.

We have performed two searches in the CSD in order to find X-ray structures exhibiting lp–π–hole contacts. We have used either a hydroxyl group or water as lone pair donor molecules. The fragments used for the searches are shown in Fig. S5. We have retrieved only those hits where the O···C distance is lesser that the sum of van der Waals radii.

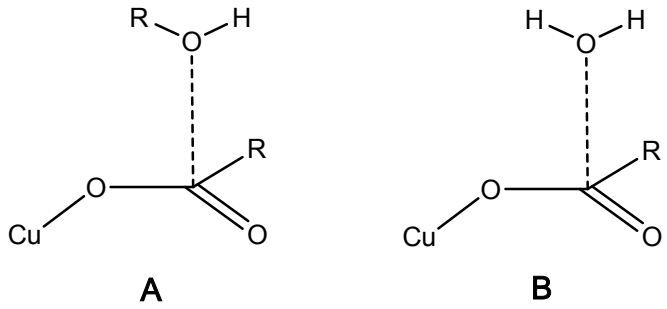

Fig S5. Fragments A and B used in the searches.

The CSD reference codes retrieved from the database for each search are gathered in Table S1. We have found only 6 hits when the donor group is a hydroxyl and 58 hits when the donor molecule is water. A representative example for each series is depicted in Figure S6.

Table S1. Reference codes for searches A and B (see Fig S5).

CSD CODES for search A				
IPUXIB	OHAKAK	OXCUPR	SOHFIF	CIHFEG
NEYXUM				
CSD CODES for search B				
VEXTUP	XIPQAQ	AGOYEA	AYOLOP	BABCOY
BUNREI	CUOXNA10	CUPLUU	DEFZOE	DEGKEF
DOPBUF	DOPBUF01	DOPBUF10	ENIXUU	ETURUH
FELYOM	FERCOV	GAWMAU	GUVBUV	HOWSIW
IBUHIX	IBUHIX01	ITANOG	KOLKUR	LAFYEX
LIQSEK	LIZGUX	LOBYEH	LUTTIE	NAYVEP
NIBDIM	OYEFII	PIGQUS01	PIGQUS02	PIGQUS03
PIZZEE	QAGTEZ	QANMAV	QEZKEM	QONYAT
RISZEZ	ROKMIO	SASXEQ	SCTART10	SIKVAK
TUKQOG	VAZNAM	WAWKAH	WEGXEM	WIGVUE
XOJZAY	XOZVEN	YAQJAD	YEXSAV01	YIDPOR
YILNIR	GEZBUK	WEWHOX		

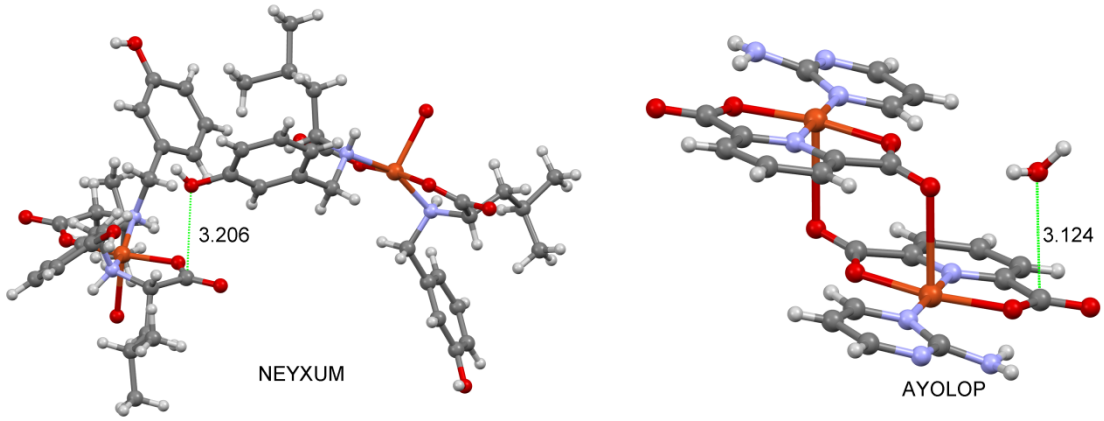

Fig S6. Partial views of the X-ray structures of NEYXUM and AYOLOP. Distances in Å.