Supporting information for

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Title: Benign synthesis of the unsymmetrical ligand 8-(2-quinolinecarboxamido) quinoline (Hqcq) and the varied crystal chemistry of its Cu(II), Zn(II), Cd(II) complexes bearing acetate and aqua co-ligands.

Authors: Soraia Meghdadi, Mehdi Amirnasr, S.B. Hoda Moein Sadat, Kurt Mereiter, and Ahmad Amiri

Corresponding author: Mehdi Amirnasr. Department of Chemistry, Isfahan University of Technology, Isfahan 84156-83111, Iran. e-mail: amirnasr@cc.iut.ac.ir

Powder X-ray diffraction

Powder X-ray diffraction patterns (PXRD) of [Cu(qcq)(OAc)(H₂O)] (1), [Zn(qcq)(OAc)(H₂O)] (2), and [Cd(qcq)(OAc)(H₂O)] (3), were measured at $T = 295$ K with a Panalytical X’Pert X-ray powder diffractometer using Bragg-Brentano geometry (flat specimen in reflection mode), instrument radius 200 mm, Ni-filtered Cu-Kα radiation of a long-fine-focus tube operated at 40 kV and 40 mA, $\lambda = 1.5418$ Å, 0.5° fixed divergence, soller slits 0.04 rad, X’Celerator linear detector of 2.55° opening angle. The specimens were finely ground in heptane, distributed as a slurry on non-reflecting monocrystalline Si sample supports, and after drying measured under sample spinning. Fig. S1 to S3 show X-ray powder diffraction patterns thus obtained. In order to verify the identities of the solids, simplified profile fits were carried out with program PowderCell 2.3 (K. Kraus & G. Nolze, 2000; Bundesanstalt f. Materialforschung und –prüfung, Berlin, Germany) using the crystal structure data determined at 100K (space group, unit cell dimensions, and atomic parameters $x$, $y$, $z$, and $U_{eq}$) and adjusting unit cell dimensions for $T = 295$ K. The results are shown in Figs. S4 to S6. The unit cell dimensions applied for $T = 295$ K were $a = 9.94$ Å, $b = 19.85$ Å, $c = 10.04$ Å, $\beta = 105.95^\circ$ for [Cu(qcq)(OAc)(H₂O)], $a = 9.90$ Å, $b = 10.30$ Å, $c = 10.99$ Å, $\alpha = 63.52^\circ$, $\beta = 80.12^\circ$, $\gamma = 72.65^\circ$ for [Zn(qcq)(OAc)(H₂O)], and $a = 10.22$ Å, $b = 10.36$ Å, $c = 10.83$ Å, $\alpha = 62.75^\circ$, $\beta = 80.57^\circ$, $\gamma = 71.44^\circ$ for [Cd(qcq)(OAc)(H₂O)] (crystal system, space group and setting as for $T = 100$ K, see Text and CIF’s). The Figures S4 to S6 show a reasonable match between measured and calculated X-ray powder patterns and verify that the bulk samples of the complexes correspond to the single crystal structures determined at $T = 100$ K and reported in the text. Moreover the patterns indicate that the bulk samples are pure for the Cu and the Cd compound, while for the Zn-compound a small unidentified impurity could be seen, which was visible also under the stereomicroscope in the form of needle-like yellow crystals accompanying in small amounts the rhombus-shaped yellow plates of [Zn(qcq)(OAc)(H₂O)].
Fig. S1. X-ray powder pattern of a specimen of [Cu(qcq)(OAc)(H$_2$O)] (1).

Fig. S2. X-ray powder pattern of a specimen of [Zn(qcq)(OAc)(H$_2$O)] (2).

Fig. S3. X-ray powder pattern of a specimen of [Cd(qcq)(OAc)(H$_2$O)] (3).
Fig. S4. Measured (red) and calculated (blue) X-ray powder pattern of [Cu(qcq)(OAc)(H$_2$O)] (1) for $T = 295$ K. The blue tickmarks give the positions of the Bragg reflections.

Fig. S5. Measured (red) and calculated (blue) X-ray powder pattern of [Zn(qcq)(OAc)(H$_2$O)] (2) for $T = 295$ K. The blue tickmarks give the positions of the Bragg reflections. Crosses mark impurity peaks of a small amount of thin yellow needles accompanying the large yellow rhombi of of [Zn(qcq)(OAc)(H$_2$O)].

Fig. S6. Measured (red) and calculated (blue) X-ray powder pattern of [Cd(qcq)(OAc)(H$_2$O)] (3) for $T = 295$ K. The blue tickmarks give the positions of the Bragg reflections.