



STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 71 (2015)

Supporting information for article:

**Charge Density & Optical Properties of Multicomponent Crystals
Containing Active Pharmaceutical Ingredients or their Analogues**

Marlena Gryl

Cif files for crystal structures of **Cubar** CCDC 1042366 and **lid** CCDC 1042367 are deposited in CSD database.

S1. Synthesis and crystallisation of Cubar

The title compound triaqua-bis(2,4,6-trioxohexahydropyrimidin-5-ide) copper(II) coded **Cubar** was synthesized by mixing saturated ethanol solutions of copper acetate tetrahydrate and barbituric acid at temperature ca. 323K. The solution remained at that temperature for 2h, and next it was left for crystallization at ambient temperature. The green plate-shaped crystals suitable for X-ray diffraction experiment were obtained after two days. In the previously reported synthesis (Xiong *et al.*,2003) a mixture of sodium barbiturate and copper (II) sulfate was stirred for 2h at room temperature and than the solution was left for crystallisation. According to the Authors green crystals appeared after 2 days.

Table S1 Hydrogen bond geometry for **lidbar** (\AA / $^\circ$).

D-H...A	d(D-H)	d(H...A)	d(D...A)	\angle (DHA)
N(1A)-H(1A)...O(4A)#1	0.89(1)	1.86(1)	2.750(2)	175(2)
N(3A)-H(3A)...O(6A)#2	0.89(1)	1.86(1)	2.745(2)	172(2)
N(1B)-H(1B)...O(4B)#3	0.89(1)	1.95(1)	2.833(1)	174(2)
N(3B)-H(3B)...O(6B)#4	0.89(1)	1.93(1)	2.813(1)	177(2)
N(1)-H(1)...O(6A)	0.90(1)	1.90(2)	2.697(2)	149(2)
N(3)-H(3)...O(6B)#4	0.89(1)	1.90(1)	2.792(2)	177(2)
C(5)-H(5C)...O(2B)	0.98(2)	2.45(2)	3.231(2)	137(1)
C(7)-H(7A)...O(2B)	0.99(3)	2.32(3)	3.153(2)	141(2)
C(7)-H(7B)...O(1)	0.94(3)	2.46(3)	3.081(3)	124(2)
N(2)-H(2)...O(4B)	0.89(1)	1.90(1)	2.728(2)	152(2)
N(4)-H(4)...O(4A)#5	0.89(1)	1.90(1)	2.797(2)	177(2)
C(6)-H(6A)...O(2A)#6	0.96(3)	2.40(3)	3.268(2)	150(2)
C(8)-H(8A)...O(2)	0.97(3)	2.56(3)	3.168(2)	120(1)
C(8)-H(8B)...O(2A)#6	0.97(3)	2.32(3)	3.139(2)	142(2)
C(20)-H(20)...O(2)#5	0.94(3)	2.44(3)	3.305(2)	153(3)
C(19)-H(19)...O(1)#7	1.00(3)	2.39(3)	3.197(3)	137(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y-1/2,-z+1 #2 -x+1,y+1/2,-z+1 #3 -x+2,y-1/2,-z+2
#4 -x+2,y+1/2,-z+2 #5 -x+1,y-1/2,-z+2 #6 x,y,z+1
#7 -x+2,y+1/2,-z+1

Table S2 Populations of the Cu(II) d-orbitals in **Cubar** with the d cross terms and the overall sum of the refined monopole (tot d-pop) population.

z^2	1.895
xz	1.957
yz	1.807
x^2-y^2	1.795
xy	1.853
z^2/xz	0.000
z^2/yz	0.000
z^2/x^2-y^2	0.160
z^2/xy	0.000
xz/yz	0.000
xz/x^2-y^2	0.000
xz/xy	0.000
yz/x^2-y^2	0.000
yz/xy	0.000
x^2-y^2/xy	0.000
tot d-pop	9.308

Table S3 Topological analysis of intermolecular interactions in CP (3,-1) for **Cubar**. $\rho(\mathbf{r}) / \text{e}\text{\AA}^{-3}$ – charge density, Laplacian – $\nabla^2\rho(\mathbf{r}) / \text{e}\text{\AA}^{-5}$ and eigenvalues of Hessian – $\lambda_1, \lambda_2, \lambda_3 / \text{e}\text{\AA}^{-5}$. R_{ij} – internuclear separations (\AA), d_1, d_2 – distance between BCPs and atom 1, 2 respectively (\AA), ε – ellipticity. $G(\mathbf{r}_{\text{CP}}) / \text{Hartrees } \text{\AA}^{-3}$, $V(\mathbf{r}_{\text{CP}}) / \text{Hartrees } \text{\AA}^{-3}$ local kinetic and local potential energy density, respectively and $E(\mathbf{r}_{\text{CP}}) / \text{Hartrees } \text{\AA}^{-3}$ – local energy density of the electrons.

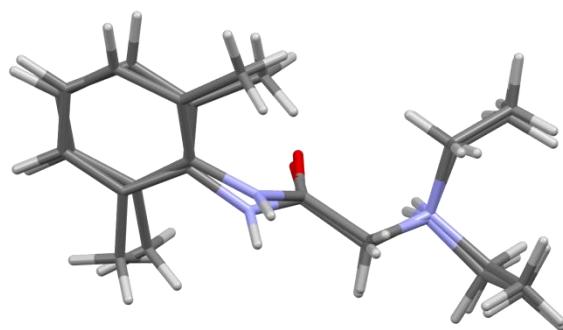


Figure S1 The overlay of lidocaine ions (a and b) from the structure of **lidbar** showing conformational changes.

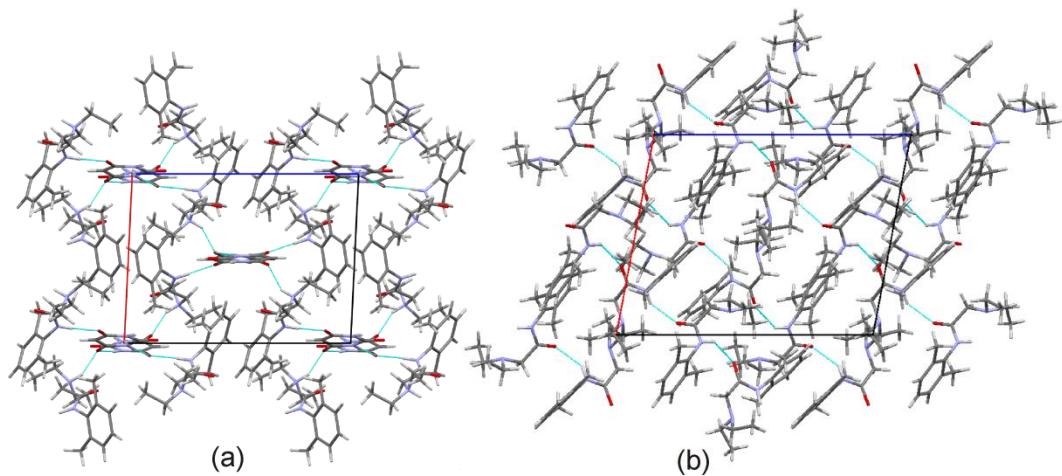


Figure S2 Packing of the structural components in the structures of (a) **lidbar** and (b) **lid** viewed in [010] direction.

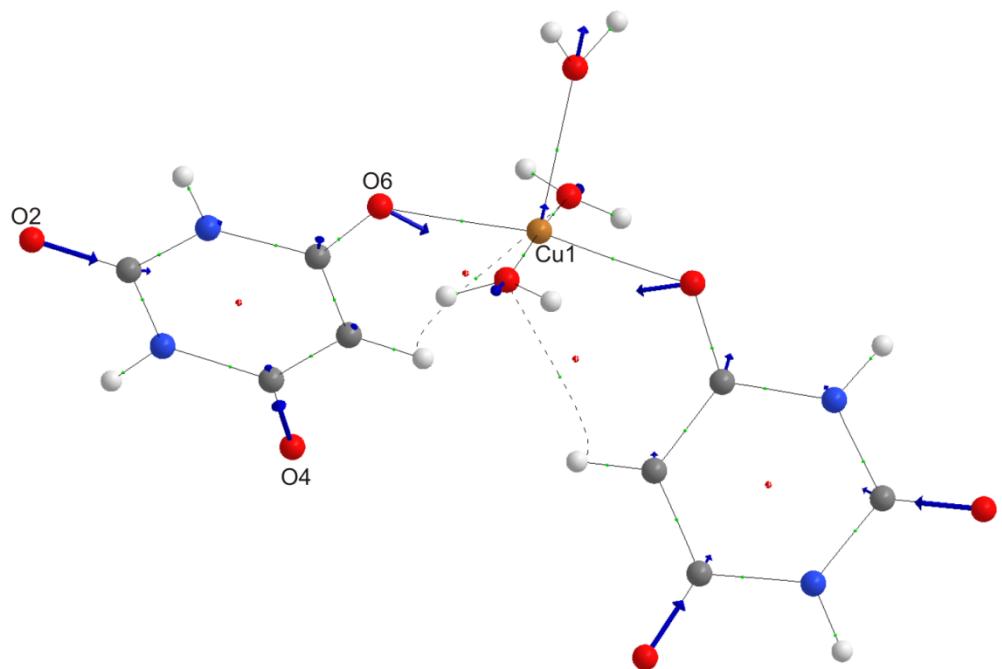


Figure S3 Total dipole moment contributions of atoms building **Cubar** unit calculated by QTAIM method using AIMALL program and B3LYP/TZVP basis set.