

out the promise of different complexes with a range of electron acceptors.

Recent x-ray investigations of crystals obtained by cocrystallization of tri-, tetra- and pentamethylene-3,4-dihydroquinazolin-4-one homologues with oxalic acid shows that in the case of first two homologues cocrystal structures is formed without protonation of quinazolin-4-one molecule in the ratio 2:1, in contrast to first crystallization of pentamethylene-3,4-dihydroquinazolin-4-one with oxalic acid gives salt type crystals in the 1:1 ratio. In this case protonation occurs through nitrogen atom of quinazolone molecule and it reflects in changing of some bond lengths in the molecules of quinazoline and oxalic acid.

For comparison to first structures also the crystals of 2,3-pentamethylene-3,4-dihydroquinazolone-4 hydrochloride oxalic acid is obtained and structure is investigated.

Such research of a structure of this cocrystals of biologically active tricyclic derivatives of quinazoline [2] are important in crystal engineering terms since they offer the possibility of designing new materials through control of hydrogen bonding

[1] Desiraji, G.R. *Crys.Engineer. The Design of Organic Solids*, Elsevier: Amsterdam, 1989.

[2] Shakhidoyatov, Kh.M. *Quinazolin-4-one and their application*. Tashkent.1989.

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On the Electronic Structure of Strong O–H···N Hydrogen Bonds [Marc Schmidtman](#)^a, Derek S Middlemiss^a, Louis J Farrugia^a, Chick C Wilson^a
^aWestCHEM, *Department of Chemistry, University of Glasgow, UK*. E-mail: marcsc@chem.gla.ac.uk

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The molecular complex of isonicotinamide (IN) with oxalic acid (OA) crystallises in two polymorphic forms, with a ratio of 2:1 IN:OA. The key difference between the two polymorphs of IN₂/OA is a *cis/trans* isomerism of the OA hydroxyl. Both polymorphs share a repeating ··IN–OA–IN·· hydrogen-bonded chain motif in which short, strong hydrogen bonds (SSHBs) of the type O–H(acid)···N(pyridine) link IN and OA molecules. Enhanced covalency of the H···N bond in combination with the short O···N distance leads to an overlap of N lone-pair density with that for the H and thereby to a strong electronic delocalisation in these type of SSHBs. This makes an assignment regarding the protonation state difficult when based purely on standard X-ray crystallography. We have therefore carried out single crystal neutron diffraction and X-ray charge density studies to clarify this situation. Structural and computational results on this system will be presented.