

**Unusual C=O...C=O carbonyl interactions in co-crystals of urea and dicarboxylic acids****Anna Krawczuk<sup>1</sup>, Mariusz Mitoraj<sup>2</sup>**<sup>1</sup>*University of Göttingen, Göttingen, Germany;*<sup>2</sup>*Jagiellonian University in Krakow, Krakow, Poland;**anna.krawczuk@uni-goettingen.de*

Carbonyl...carbonyl interactions have been identified in biologically active systems such as small biomolecules, proteins or protein-ligand complexes. Their contribution into molecular assembly was proven to be comparable to moderate hydrogen bonds, thus they can be considered as organic synthons playing crucial role in determining three-dimensional crystal packing or even stabilizing the secondary structure motifs of proteins. In the literature one can find many examples of C=O...C=O interactions between the same molecules, however to the best of our knowledge, only one case where such a pattern was characterized between different molecules (urea and oxalic acid co-crystal) [1].

Here we report a series of co-crystals of urea and dicarboxylic acid, where antiparallel carbonyl...carbonyl motif [2] between heteromolecules is observed and acts as a “glue” between 2D layers built of strong hydrogen bonds. In order to get inside into the nature and mechanism of the synthons, experimental and theoretical electron density studies were engaged as well as ETS-NOCV method (Extended transition state. Natural orbitals for chemical valence) was applied [3]. NCI analysis [4] and interaction energies calculated with EP/MM (Exact Potential and Multipole Method) method [5] indicate a correlation between the strength of carbonyl interactions and the number of carbon atoms in the main chain of the acid molecules.

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