Poster Presentation

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Polymorphic nature of two organic zwitterions

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A series of zwitterions has previously been prepared in our group in a straightforward manner using simple starting materials [1]. What makes these organic molecules unusual is that they are stable zwitterions, despite the fact that many zwitterions tend to be highly reactive and difficult to isolate [2]. They also have interesting shapes, as well as the potential to form hydrogen bonds. A detailed investigation of one of the zwitterions in the series has been reported [3] and revealed some very interesting solid-state chemistry. Further studies have thus been carried out on two of the other zwitterions in the series, (2Z)-3-carboxy-1-hydroxy-2-pyridinium-1-ylprop-2-en-1-olate (1) and (2Z)-3-carboxy-2-(4-cyanopyridinium-1-yl)-1-hydroxyprop-2-en-1-olate (2), in order to further investigate their solid-state structures. These results will be presented.

Zwitterions 1 and 2 can be formed by reacting acetylenedicarboxylic acid (ADC) with pyridine or 4-cyanopyridine respectively. The possible solid-state products were explored by systematically varying the solvent and temperature of the synthesis as well as the crystallisation conditions. These products were usually crystalline and thus could be identified using single-crystal X-ray diffraction. Mechanochemical synthesis was also attempted. Furthermore, we attempted to form co-crystals by combining each zwitterion (in solution as well as mechanochemically) with numerous other organic molecules chosen based on known supramolecular synthons.

Two polymorphs of each zwitterion were identified. The reaction to produce zwitterion 1 also sometimes results in the formation of an unreacted salt of the starting materials. This salt seems to be the kinetic product of the reaction. No co-crystals or solvates were obtained for either zwitterion. An in-depth study of the relationship between the different forms of each zwitterion was therefore carried out using thermal analysis, solvent-immersion and -slurry experiments, as well as mechanical grinding in order to obtain data about polymorph stability and control.

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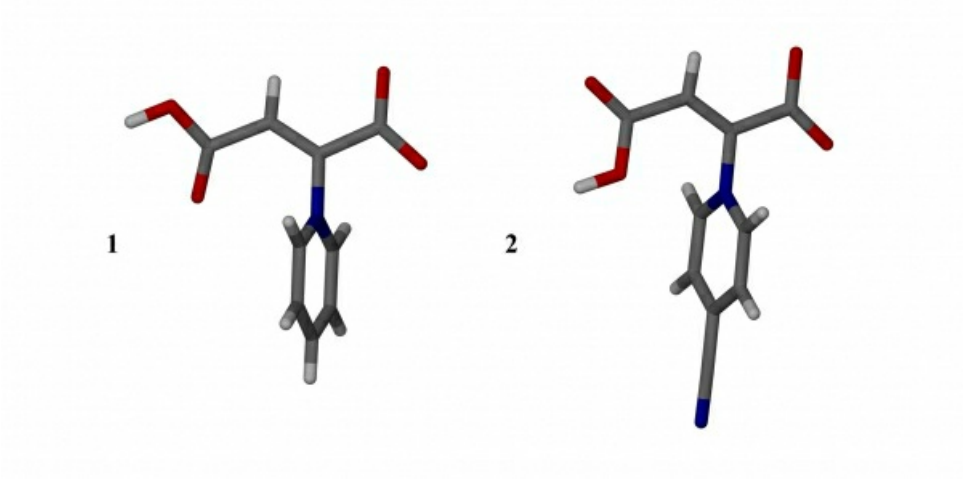
[3] Loots, L, et al. (2015). Cryst. Growth Des. 15, 5849-5857.



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