Intermolecular interactions in uric acid cluster

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The formation of uric acid crystals has received little attention from the scientific community. The form in which the uric acid crystallizes is called lactam and from all forms of tautomers, the lactam form has the most stable form. In this way, the structural stability and the charge transfer effects were investigated using DFT and MP2(DLPNO-SCS-MP2) methods. For the DFT method, the functional wB97X-D3 together with the def2-TZVP basis set were chosen, while for the MP2 theory the DLPNO-SCS-MP2 method provide accurate results for our systems. The stacking-type dimers and the cyclic-hydrogen bonds have been identified. Also, the nature of the intermolecular interaction energy has been studied. In the case of experimentally obtained crystalline structures [1], the nature of the intermolecular interaction energy has been investigated between the crystalline units.

References

[1] Mechanical Properties of Anhydrous and Hydrated Uric Acid Crystals, Chem. Mater. 30, (2018), 3798−3805, DOI: 10.1021/acs.chemmater.8b00939