

MS32-P16 | INTERPLAY BETWEEN OCCURRENCE FREQUENCIES OF CHARGED AND NEUTRAL BASE PAIRS IN SMALL MOLECULE CRYSTALS

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We searched Cambridge Structural Database for structures containing one of the nucleobases – adenine, guanine, hypoxanthine, thymine, uracil or cytosine – and then made an extensive survey concerning the base pairs they formed. The nucleobases behaved mostly in accordance to their pKa values - hypoxanthine, thymine and uracil did not form any base pairs with protonated molecules, whereas adenine, guanine and cytosine did form charged base pairs. It is interesting that we did not find any statistically important differences between the bonds lengths of charged and neutral base pairs, which suggests that factors like higher-order structure and presence of other molecules in the crystal structure are important enough to outweigh electrostatic repulsion between two cations. The charge of the molecules comes mainly from additional protons located in the molecule ring, which heavily affects their ability to form particular base pairs – it can enable, prevent or not affect the formation at all. It is worth to note that although protonation may enable the formation of new base pair, it does not favor such base pairs. Although there are visible trends in the nucleobases behavior, we found a few structures with base pairs formed from differently protonated molecules or behaving in an unexpected way.