Experimental Electron Density of Melamine

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Melamine is a precursor for polymeric Carbon Nitride (p-CN) materials showing great promise in a variety of different applications including electro- and photo catalysis [1]. The structure consists of layers of extended graphite-like CN with stoichiometry close to C_3N_4 including only a small amount of hydrogen. Insight into the electronic properties of precursor materials could be valuable for understanding the catalytic properties of p-CNs. The 2,4,5-triamino-s-triazine molecule (melamine) crystalizes in the $P2_1/n$ space group and is an archetypical example of an organic molecular crystal.

This study presents the ongoing work of benchmarking synchrotron radiation (with a wavelength of ~0.25 Å) against state of the art in house diffractometers, using respectively Mo (0.71 Å) and Ag (0.56 Å) radiation. Preliminary results show no significant deviation between the three different methods, and the electron density models obtained from the data analysis are for all practical purposes the same. The experimental electron density of melamine crystals is analyzed in terms of chemical interactions. In particular Bader topology and energy frameworks are used to study the chemical importance of the inter-molecular interactions in crystal formation of melamine. Future work includes studies of other p-CN materials with structures that are even closer to the catalytically active p-CN, e.g to gain insight into the chemical effects responsible for the layer forming mechanism.

[1] Larsen, F. K., Mamakhel, A., Overgaard, J., Jørgensen, J. E., Kato, K. and Iversen, B. B. (2019). *Acta Cryst*. B75, 621–633

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