MS34-02 | Towards Crystal Structure Solution of Organic Compounds by fit to the Pair Distribution Function without Prior Knowledge of Space Group and Lattice Parameters

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Local structures in crystalline, nanocrystalline and amorphous compounds can be investigated using pair distribution functions (PDFs). However, the fit of structural models to the PDF curve has rarely been done for organic compounds. In our previous research, the method developments for structure determination from PDF were successful with determination of molecular position and orientation starting from random values [1]. Experimental lattice parameters and space group have been given as an input. For many nanocrystalline organic compounds the space group and lattice parameters are unknown. Therefore, a global procedure in which the lattice parameters, the space group, the molecular position and orientation are determined from PDF-Data has been developed [2]. The calculations initiate with a large set of random starting structures in various space groups using FIDEL Software [3]. The space groups have been chosen according to the space group frequency [4]. The optimisation of lattice parameters starts from random values within the sensible range. The ranges are chosen depending on the size of the investigated molecule and space group in which the calculations are performed. The optimisation calculations have been carried out using TOPAS Software [5].

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[5] A. A. Coelho, *J. Appl. Cryst.*, 2018, 51, 210.