Crystal Structure Prediction of Nitrobenzene Derivatives

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The main methods of crystal structure prediction base on searching crystal structures corresponding to global minimum in the lattice energy. An intermolecular force field is required to calculate intermolecular energy, which consists of coulombic, polarisation, dispersion and repulsion terms [1]. The lattice energy is calculated as a sum of interactions using the atom-atom potential approach [2].

In this work prediction of crystal structures for selected single-substituted nitrobenzene derivatives was carried out using Monte Carlo simulated annealing [3, 4]. The prediction has been performed for nitrobenzenes with a following second substituent: hydroxyl, amino, nitro or methyl group or chlor, brom, iod atom. The calculations have been carried out for a standard choice of space groups. The *Polymorph Predictor*, module of *Cerius*^{2} program was used [5].

The predicted structures are compared with our experimental results or with crystal structures retrieved from CSD [6]. The polymorph structures are analysed in terms of molecular interactions that influence nucleation, crystallisation and stability of polymorphs.

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