

THE PNICTOGEN BONDING BETWEEN NITRO-GROUPS IN CRYSTALS

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Having an objective view of the details of the chemical bonds formation and structure-forming non-covalent interactions on the electronic level, we are able to predict the physical, chemical, thermal and thermodynamic properties of substances and to develop functional materials with desired properties. One of these important non-covalent interactions is the pnictogen bond.

The pnictogen bonding is the type of non-covalent interaction in which the covalently bonded pnictogens (N, P, As) acts as the acceptor of the electron density. The nitrogen atom of the nitro group, for example, has the region of increased positive values of electrostatic potential, called " π -hole" [1], through nitrogen atom of the nitro group guided by electrostatic interactions with the oxygen atom of the neighboring nitro group.

The objects of our study are the pnictogen bonds in crystals. Some molecules can form the infinite chain through interactions between the nitrogen atom of one nitro group with the oxygen atom of another one (Figure 1).

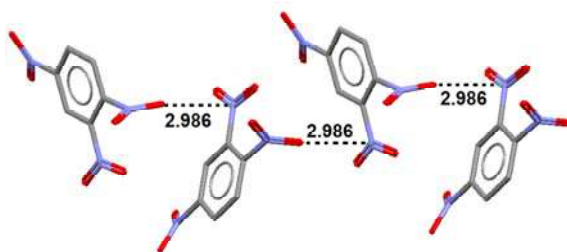


Figure 1. Chained motive with pnictogen bonds in the crystal of 1,2,4-trinitrobenzene (BEYDOY).

Analysis of the Cambridge Structural Database [2] showed that it contains more than four thousand crystal structures, which includes the pnictogen bond between two neighboring nitro groups. The diapason of these bond lengths in our sample varies from 1.76 to 3.17 Å. The centrosymmetric structures are prevail among the considered crystals.

Reference

- [1] J.S. Murray, P. Lane, T. Clark, K.E. Riley, P. Politzer *J. Mol. Model.* 2012, 18 541.
- [2] F.H. Allen. *Acta Crystallogr. B* 2002, 58, 380.

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