We present here preliminary results of our efforts to build a machine learning model that is able to distinguish whether a compound will form a crystal under certain conditions. Our aim is to train this model on our in-house data and then use it to predict optimal crystallization conditions for previously unseen compounds.

**Keywords:** crystallisation, statistical analysis, crystallisation database, machine learning

# MS15-P2 Substituent effects in nitro derivatives of carbazole investigated by XRD studies and DFT calculations

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Carbazole and its derivatives have attracted significant attention owing to their applications in pharmacy. These compounds are considered also to be potential candidates for electronic applications such as colour displays, organic semiconductors, laser and solar cells as they demonstrate electroactivity and luminenscence. In the last years, cross-linked polycarbazole have been widely employed as electron donors in materials for organo-electronic applications as organic light emitting diodes (OLEDs) [1]. The crystal structure of 9*H*-carbazole (I, Fig. 1a), has been re-determined at low temperature for use as a reference structure in a comparative study with the structures of 1-nitro-9*H*-carbazole (II, Fig. 1b), and 9-nitrocarbazole (III, Fig. 1c). All three solid-state structures are slightly nonplanar, the dihedral angles between the planes of the arene and pyrrole rings ranking from 0.40(7)° in (III) to 1.8(2)° in (II). Nevertheless, a density functional theory (DFT) study predicts completely planar conformations for the isolated molecules. To estimate the influence of nitro-group substitution on aromaticity, the HOMA (Harmonic Oscillator Model of Aromaticity) [2,3] descriptor of π-electron delocalization has been calculated. The HOMA indices for the isolated and solid-state molecules are relatively consistent and decrease in value for aromatic rings that are substituted with a π-electron-withdrawing nitro group. Substitution of the arene ring influences the π-electron delocalization in the ring only weakly, showing strong resistance to a perturbation of its geometry, contrary to what is observed for nitro substitution of the five-membered heterocyclic pyrrole ring. In (II), the molecules are arranged in near-planar dimers connected to each other by strong N-HO hydrogen bonds that stack parallel to the crystallographic *b* axis. A similar stacking arrangement is observed in (III), although here the stacked structure is formed by stand-alone molecules [4]. References: [1] Shirota Y, Kageyama H, (2007) Chem. Rev. 107, 953–1010 [2] Krygowski TM (1993) J. Chem. Inf. Comput. Sci. 33, 70-78 [3] Krygowski TM, Cyrański MK (1996) Tetrahedron 52, 10255-10264 [4] Gajda K, Zarychta B, Kopka K, Daszkiewicz Z, Ejsmont K (2014) *Acta Cryst.* C70, 987-991.

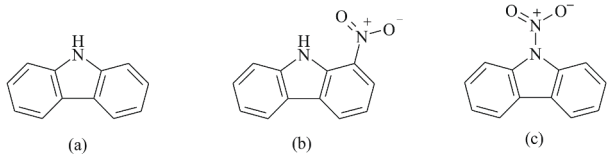


**Figure 1.** The chemical schemes of nitro derivatives of carbazole

**Keywords:** carbazole, substituent effect, DFT calaculations, HOMA index