In the vanadium-boron system the binary phases V_3B_2, VB, V_5B_6, V_2B_3, V_3B_4, and VB_2 have been reported so far. However, there is a lack of systematical and complete structure information. In most cases, crystal structures were not determined, but only the structure type was assigned and unit cell parameters were refined, except for V_2B_3 and V_3B_2 [1, 2]. Accounting for the similar environment of atoms, characteristic bond lengths in the boron substructure are expected (~1.75 Å). However, one of the published B-B bond distances in V_3B_4 is extraordinarily short (1.495 Å), although no crystal chemical reason is obvious [3]. The crystal structures of VB_2, VB, V_5B_6, V_2B_3 and V_3B_4 were reinvestigated using high resolution single-crystal X-ray diffraction data. Topological aspects of the crystal structures as well as electron densities are analysed on basis of the precise crystallographic information.

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Keywords: vanadium borides; crystal structure; electron density

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Electron Charge Density Distribution in an Organic Compound : The 4,4 DiMethyl Cyano Biphenyl (DMACB).

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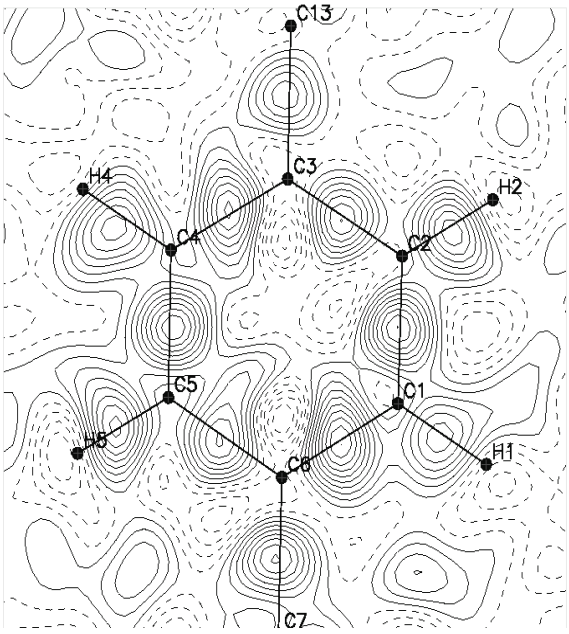
At room temperature, the 4,4 dimethylamino-cyanobiphenyl (DMACB) appears in two polymorphic structures: orthorhombic and monoclinic forms. In the present work, we shall focus on the monoclinic form of this compound which has a centrosymmetric structure with the space group Cc. The molecular dipole moment has been estimated experimentally [1].
High resolution single crystal diffraction experiment was performed at low temperature with MoKα radiation. The crystal structure was refined using the multipolar model of Hansen and Coppens (1978) [2]. The molecular electron charge density distribution is described accurately. The study reveals the nature of inter-molecular interactions including charge transfer. The results could be analyzed in more detail, if they were complemented by a quantum chemistry calculation. The electronic structure of this molecule has been investigated theoretically by the Semi-empirical and Ab initio calculations. The agreement between the experimental and theoretical results such as: atomic net charge, molecular dipole moment, electrostatic potential and electron density was satisfactory. All these results will be presented in the meeting. The figure below gives the charge density distribution in the phenyl plane.



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