Abstract

The determination of the distribution of electron density of ***4-methoxulbenzencarbothioamide (4-MBCA)*** *with chemical formula* ***C8H9NOS*** *was investigated by single from a spectrum of high-resolution X-ray diffraction on single crystal. This determination requires first a record of high quality diffraction spectrum of materials studied, followed by appropriate treatment of these intensities. The* ***4-MBCA*** *appears in orthorhombic form of the structure which has a noncentrosymmetric structure with the space group* $P2_12_12_1$.

High resolution single crystal diffraction experiment was performed at low temperature (173) with MoKα radiation. We used the formalism of blessing for reducing these intensities taking into account the different experimental errors that may affect measurement. The crystal structure was refined using the multipolar model of Hansen and Coppens (1978). The molecular electron charge density distribution is described accurately. The molecular dipole moment has been estimated experimentally.

The study reveals the nature of inter-molecular interactions including charge transfer and hydrogen bonds in the title compound. In this crystal, the molecules form dimmers via intermolecular N-H….S intermolecular hydrogen bonds. The dimmers are further linked by C-H….O hydrogen bonds into chains along the c axis.

Finally, our results could be analyzed in more detail, ***4-methoxulbenzencarbothioamide compounds****, if they were completed by quantum chemistry calculations: the Semi-empirical and Ab initio calculations.*