

## Microsymposium

MS25.O05

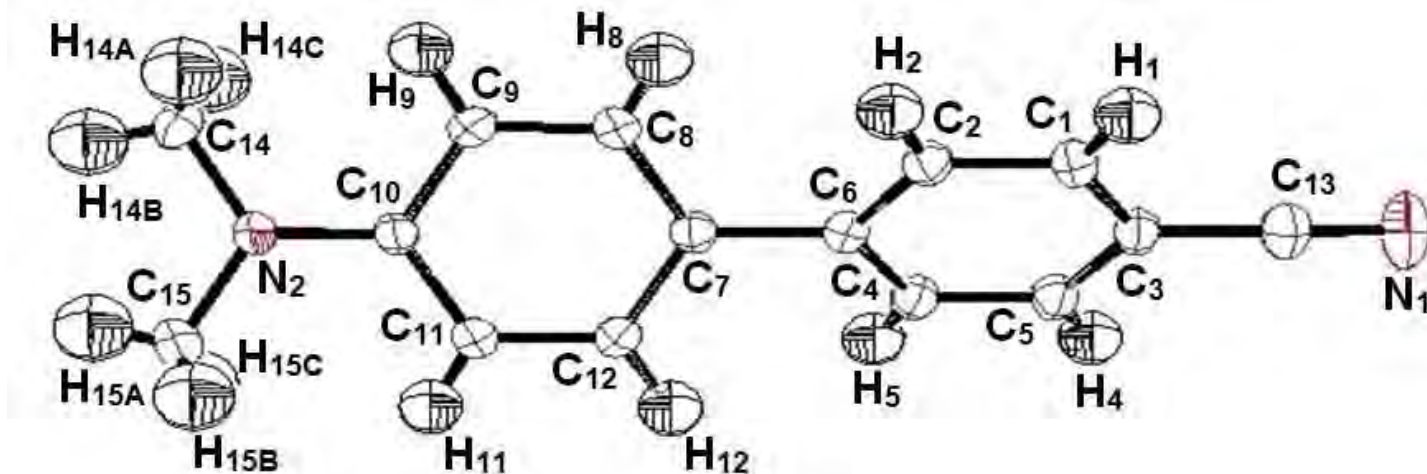
*The electron charge density distribution in a non linear optical compound*

H. Fodil<sup>1</sup>, C. Abdelkader<sup>1</sup>

<sup>1</sup>University of Mostaganem, Laboratoire LTPS, Mostaganem, Algeria

The 4,4 dimethyl amino-cyanobiphenyl crystal (DMACB) is characterized by its nonlinear optical properties. The intra molecular charge transfer of this molecule (figure-1) results mainly from the electronic transmission of the electro-acceptor (Cyano) and the electro-donor (Di-Methyl-Amino) groups [1]. An accurate electron charge density distribution around the molecule has been calculated from a high-resolution X-ray diffraction study. The data were collected at 123 K using graphite-monochromated Mo-K $\alpha$  radiation. The crystal structure has been validated and deposited at the Cambridge Crystallographic Data Centre with the deposition number CCDC 876507. The refinement was carried using the multipolar model of Hansen and Coppens [2]. We have explored systematically the main molecule planes. The different sections show clearly the accumulation of the electron charge density along the chemical bonding. The oxygen lone pairs have been perfectly localized. The charge density function has been used for the calculation of the molecular dipole moment and the electrostatic potential around the molecule [3]. The obtained results show clearly the nature of electron charge transfer in the DMACB compound.

[1] Andraud, C.; Zabulon, T.; Collet, A.; Zyss, J. *Nonlinear optical properties of poly octupoles: a multipolar tensorial quantum analysis. Chemical Physics* 245 (1999) 243–261, [2] Hansen, N.K.; Coppens, P. *Testing aspherical atom refinements on small-molecule data sets. Acta Cryst. A* 1978, 34, 909-921, [3] Boubegra N.; Chouaih A; Drissi M.; Hamzaoui F. *Structural and electron charge density studies of a nonlinear optical compound 4,4 dimethyl amino cyano biphenyl. Chin. Phys. B* 2014, Vol. 23(1): 016103



**Keywords:** Electron charge density, Non Linear Optical properties, High resolution X-ray data