

# Characteristics of the dye structure based on triphenylamine moiety

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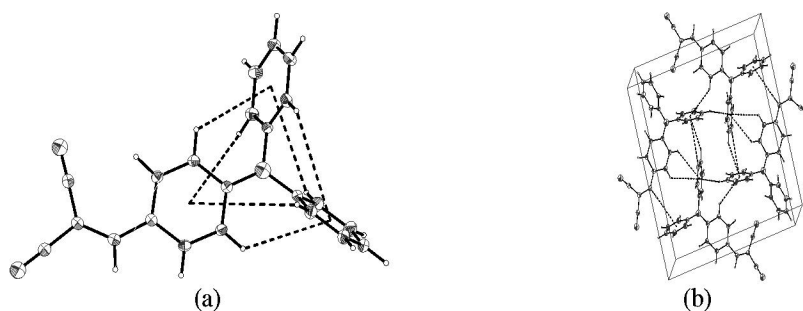
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The popularity of triphenylamine as building blocks is rapidly growing in material chemistry. It is used for the synthesis of many materials, with various applications<sup>1-4</sup>. Cyanovinylene-triphenylamine is one of the so called dicyanomethylene (DCM)-type dye. In the past few years, several groups have developed hybrid systems obtained by fixations of conjugated chains or electron-pull groups on a TPA core as active materials for the fabrication of solar cells and data storage devices<sup>5,6</sup>.

The synthesis of cyanovinylene-triphenylamine and single crystal structure was presented. The crystal structure was determined by <sup>1</sup>H NMR, <sup>13</sup>C NMR and X-ray diffraction. The title compound crystallizes in a P21/c with  $a=6.9070(14)$  Å,  $b=15.666(3)$  Å,  $c=16.101(3)$  Å,  $\alpha=90^\circ$ ,  $\beta=95.13(3)^\circ$ ,  $\gamma=90^\circ$ ,  $M_r=325.4$ ,  $V=1735.2(6)$  Å<sup>3</sup> and  $Z=4$ . Intramolecular C-H $\cdots\pi$  interactions twisted three phenyl rings of the molecule like the blades of a propeller. And the dihedral angle between the mean planes of them are  $70.04(3)^\circ$ ,  $72.66(3)^\circ$  and  $74.16(3)^\circ$ , respectively. Each molecule is chiral because the direction of helicity. Identical number of right-hand helicity and left-hand helicity packing together make the whole crystal achiral. In the unit cell, four molecular were connected to be head-to-tail by weak C-H $\cdots\pi$  interactions. In addition, C-H $\cdots\pi$ , C=C $\cdots\pi$  and C $\equiv$ N $\cdots\pi$  interactions join the molecules in layers(Fig.1). It is interesting that the molecule does not establish any H-bond. The crystal is luminescent when irradiated with 254nm light.



**Fig. 1.** Partial packing diagram of the title compound with C-H $\cdots\pi$  drawn as dashed lines: a) intramolecular C-H $\cdots\pi$  b) intermolecular C-H $\cdots\pi$ .

In conclusion, Cyanovinylene-triphenylamine was synthesized by Knoevenagel condensation and demonstrated by NMR and single crystal. The detailed interactions between molecules are reported. Some less obvious interactions, such as  $C=C\cdots\pi$  and  $C\equiv N\cdots\pi$  interactions, were observed.

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