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Synthesis, Crystal Structure and Hirshfeld Surface analysis of a benzoxazole derivative [2-[2-(4-Methylphenyl)ethenyl]-1,3-benzoxazole]

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Abstract

Benzoxazole nucleus is one of the most important heterocyclic compounds exhibiting remarkable pharmacological activities such as antibacterial activity, antifungal activity, Anticonvulsant activity, etc., In view of the importance of benzoxazole derivative we synthesized one benzoxazole derivative, their structural and Hirshfeld Surface were analyzed. The Single crystal x-ray diffraction analysis reveals that the compound 2-[2-(4-Methylphenyl)ethenyl]-1,3-benzoxazole crystallizes in monoclinic system with space group $P2_1/n$. The oxazole and the toluene rings are almost in planar conformation. The dihedral angle between the oxazole ring and toluene ring is 9.49(6)°. The crystal packing is stabilized by intramolecular C—H...O type of hydrogen bonds. In Additional to that, the crystal packing is stabilized by van der Waals forces.

Keywords: Heterocyclic compound; oxazole ring; toluene ring; Hirshfeld Surface; hydrogen bonds.

Specifications Table

Subject area	Organic Chemistry
Compounds	2-[2-(4-Methylphenyl)ethenyl]-1,3-benzoxazole