



Synthesis, Crystal Structure and Hirshfeld Study of 3,3'-dinitrobenzophenone

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ABSTRACT

The compound 3, 3'-dinitrobenzophenone is prepared by nitrating benzophenone. The structure was confirmed by ¹H NMR, FT-IR, Differential Scanning Calorimetry (DSC), X-ray diffraction. X-ray diffraction study reveals that the compound crystallizes in the triclinic crystal system, in space group $P\bar{1}$. The unit cell parameters are $a=7.6180(5)$ Å, $b=8.0341(6)$ Å, $c=10.8056(8)$ Å, $\alpha=74.358(4)^\circ$, $\beta=82.516(4)^\circ$, $\gamma=68.607(5)^\circ$, $Z=2$, and $V=592.60(8)$ Å³. The compound exhibits intermolecular interaction of the type C–H...O with symmetry code $1+x, y, 1+z$.

Keywords: Benzophenone, Hirshfeld surface analysis, Fingerprint plot, American contact dermatitis society.
