Quantification of intercontacts of 2-Nitrobenzyl Methanesulfonate Crystal Structure using Hirshfeld Surfaces Computational Studies

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Abstract

The coordinates of the title compound, 2-Nitrobenzyl methanesulfonate obtained from single crystal X-ray diffraction method is used to analyze the short contacts through Hishfeld surfaces computational method. The intercontcts of the crystal structure are quantified and reveals C...C, C...H, H...H, N...C, N...H, O...C, O...H, O...N and O...O types. The major intercontacts of them are O...H, H...H and C...H with 50.6%, 25.7 %, and 10.6, respectively. The 2D finger print plots for the corresponding intercontacts are visualized and plotted.

Keywords Nitroalkanes, Intercontacts, Hirshfeld surfaces, 2D - Fingerprint plots.

Introduction

One of the organic molecules, nitro alkanes shows high-electron withdrawing power of the nitro group promising an improvement in the hydrogen activity [1]. The Michael addition of nitro alkanes to a variety of nitriles can be achieved with task-specific ionic liquid [2]. The crystal structure studies of nitrobenzene derivatives are reported from our research group; 2-Nitrobenzyl methanesulfonate and 4-Chloro-1-[2-(2-chlorophenyl)ethyl]-2-nitrobenzene[3-4.The title compound shows C---H...O intermolecular hydrogen bonds [4].The Hirshfeld surface analysis computational method is a graphical tool for visualization and understanding of intermolecular interactions [5-7].

With the importance of the analysis and quantification of intercontacts in the crystal structure, here we present the Hirshfeld surface analysis of the title compound, 2-Nitrobenzyl methanesulfonate [3].

Materials and Methods

The program Crystal Explorer 3.0 [5] was used to perform Hirshfeld surfaces computational analysis and to quantify the intermolecular interactions in terms of surface contribution and generating graphical representations (Figure 1), plotting 2D fingerprint plots (Figures 2) [8]. Crystallographic data of the title compound is retrieved from the supplementary file hb7217 with doi: 10.1107/S160053681400899X.

Results and discussion

The Hirshfeld surfaces analyses performed to the molecule and is as shown in Figure 1 and 2. The red spots over the surface indicate the intercontacts involved in hydrogen bond. The dark-red spots on the dnorm surface arise as a result of the short interatomic contacts, i.e., strong hydrogen bonds, while the other intermolecular interactions appear as light-red spots. The 2D Finger print plots over the Hirshfeld surfaces shows the presence of intercontacts and are C…C – 0.8 %, (b) C…H – 10.6 %, (c) H…H – 25.7 %, (d) N…C – 1.9 %, (e) N…H – 0.1 %, (f) O…C – 5.1 %, (g) O…H – 50.6 %, (h) O…N – 1.6 %, (i) O…O – 3.7 % and (j) full.

The outline of the full fingerprint is shown in gray. This is the closest internal distance from a given point on the Hirshfeld surface and de is the closest external contacts. The major contributions for the Hirshfeld surfaces are from H…H and O…H when compared to other intercontacts.

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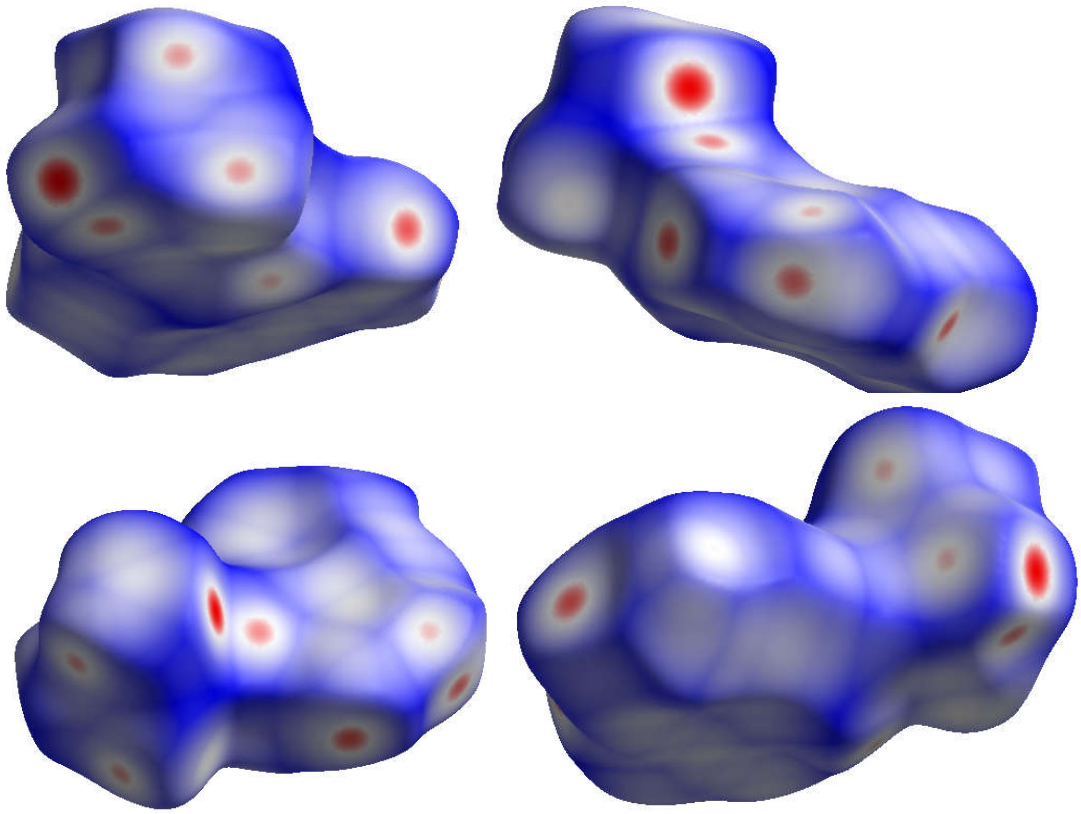

Fig.1. d_{norm} mapped on Hirshfeld surface for visualizing the intercontacts in different orientations. Color scale in between −0.18 au (blue) to 1.4 au (red)

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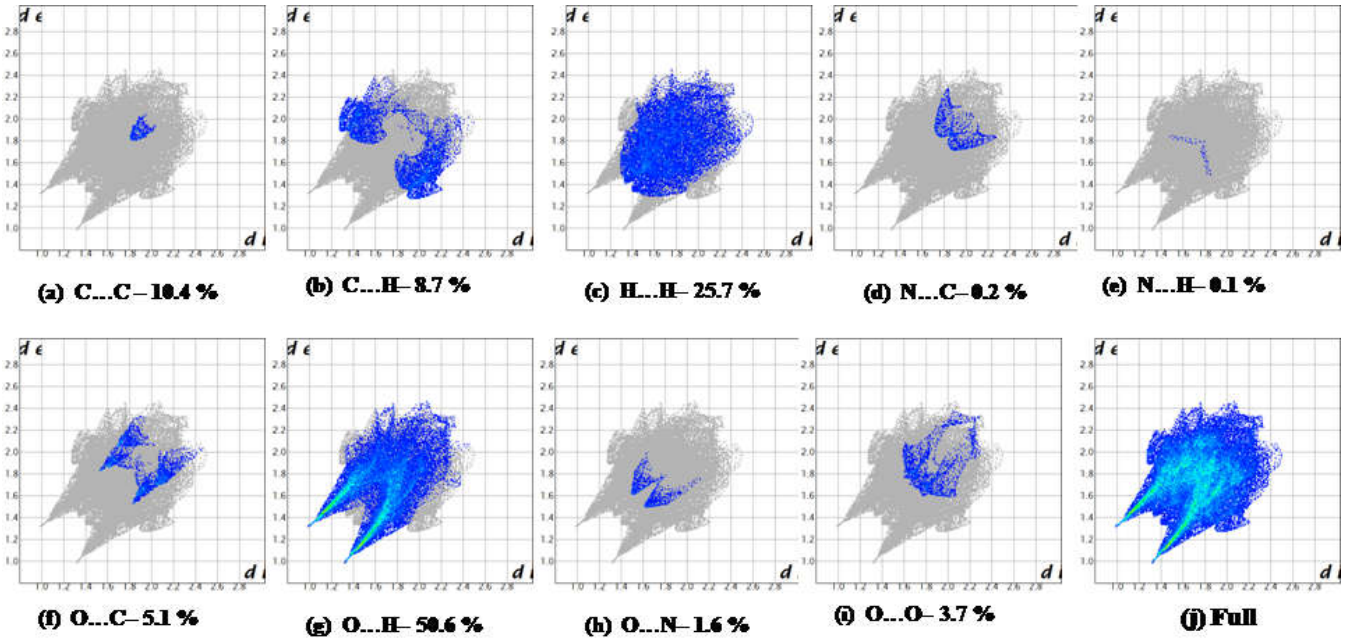

Fig. 2.Fingerprint of the title compound, (a) C…C – 0.8 % (b) C…H – 10.6 %, (c) H…H – 25.7 %, (d) N…C – 1.9 %, (e) N…H – 0.1 %, (f) O…C – 5.1 %, (g) O…H – 50.6 %, (h) O…O – 3.7 %, and (i) full. The outline of the full fingerprint is shown in gray. *dï*s the closest internal distance from a given point on the Hirshfeld surface and *de* is the closest external contacts.

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