Synthesis, Crystal Structure, and DFT Study of *N*-[2-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-ethanesulfonamide

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Received November 28, 2021; revised December 16, 2021; accepted December 16, 2021

Abstract—*N*-[2-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]ethanesulfonamide has been synthesized by the Miyaura borylation and sulfonylation reactions, and its structure has been identified by FT-IR, ^{1}H NMR, and mass spectroscopy. Crystal structure of the compounds has been studied by X-ray diffraction and conformational analysis. The molecular structure has been further calculated by density functional theory (DFT). The calculated data are consistent with the results of X-ray diffraction. DFT has been used to calculate and analyze electrostatic potential of molecules as well as molecular frontier orbitals for further analysis of physical and chemical properties of the compound. Based on the calculated Hirshfeld surface and two-dimensional fingerprint of the molecules, hydrogen bonds in the cells and input of various forces have been approached.

Keywords: ethanesulfonamide, X-ray crystallography analysis, DFT, synthesis, Hirshfeld surface

DOI: 10.1134/S1070363222010170