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Density functional study of electronic, charge density, and chemical bonding properties of 9-methyl-3-Thiophen-2-YI-Thieno [3,2-e] [1, 2, 4] Thriazolo [4,3-c] pyrimidine-8-Carboxylic acid ethyl ester crystals

Abstract

A comprehensive theoretical density functional investigation of the electronic crystal structure, chemical bonding, and the electron charge densities of 9-Methyl-3-Thiophen-2-YI-Thieno [3, 2-e] [1, 2, 4] Thriazolo [4,3-c] Pyrimidine-8-Carboxylic Acid Ethyl Ester ($C_{15}H_{12}N_4O_2S_2$) is performed. The density of states at Fermi level equal to 5.50 (3.45) states/Ry cell, and the calculated bare electronic specific heat coefficient is found to be 0.95 (0.59) mJ/mole-K2 for the local density approximation (Engel–Vosko generalized gradient approximation). The electronic charge density space distribution contours in (1 0 0) and (1 1 0) planes were calculated. We find that there are two independent molecules (A and B) in the asymmetric unit exhibit intramolecular C–H…O, C–H…N interactions. This intramolecular interaction is different in molecules A and B, where A molecule show C–H…O interaction while B molecule exhibit C–H…N interaction. We should emphasis that there is π–π interaction between the pyrimidine rings of the two neighbors B molecules gives extra strengths and stabilizations to the superamolecular structure. The calculated distance between the two neighbors pyrimidine rings found to be 3.345 Å, in good agreement with the measured one (3.424(1) Å).

Keywords

Applied organic compound; Structural material; Electronic structure; Electrochemical property; Crystal structure