Synthesis, crystal structure, vibrational properties and DFT studies of 1-(4-((6-bromopyrido [2, 3-d]pyrimidin-4-yl)oxy)phenyl)-3-(2,4-difluorophenyl)urea

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Abstract

In this present work, the title compound 1-(4-((6-bromopyrido[2,3-d]pyrimidin-4-yl)oxy) phenyl)-3-(2,4-difluorophenyl)urea (1) was synthesized and the structure was characterized by spectroscopy (FT-IR, 1H NMR, 13C NMR and MS). The single crystal of the title compound was confirmed by X-ray diffraction, and the optimized molecular crystal structure was determined based on DFT calculations using B3LYP/6-311G (2d, p) basis set, which was compared with the X-ray diffraction. The results of the conformation analysis indicated that the molecular structure optimized by DFT was consistent with the crystal structure determined by X-ray single crystal diffraction.

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