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Towards a better comprehension of interactions in the crystalline N-acetylbenzylamine and its sulphur analogue N-benzyl-ethanethioamide. IR, Raman, DFT studies and Hirshfeld surfaces analysis

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ABSTRACT

This paper presents the investigation results of the polarized IR spectra of the hydrogen bond in crystals of N-acetylbenzylamine and its sulphur analogue N-benzyl-ethanethioamide. The spectra were measured at 298 and 77 K by a transmission method, with the use of polarized light. The Raman spectroscopy, Hirshfeld surfaces analysis and DFT studies have been also reported. Theoretical calculations of the isolated molecule were performed by using density functional theory (DFT) method at B3LYP/6-311(d,p), B3LYP/6-311++G(d,p) and B3LYP/6-311++G(3df,2pd) basis set levels. The geometrical parameters of analyzed compounds are in good agreement with the XRD experiment. The vibrational frequencies were calculated and subsequently values have been compared with the experimental Infrared and Raman spectra. It has been shown that the observed and calculated frequencies are found to be in good agreement, as well as the analysis of the Hirshfeld surface has been well correlated to the spectroscopic studies. Additionally, the highest occupied molecular orbital energy (E_{HOMO}), lowest unoccupied molecular orbital energy (E_{LUMO}), the energy gap between E_{HOMO} and E_{LUMO} ($\Delta E_{HOMO–LUMO}$), molecular electrostatic potential and global reactivity descriptors *viz.* chemical potential, global hardness and electrophilicity have been calculated. In N-acetylbenzylamine the presence of the N-benzylamide fragment is essential for activity.

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