

Molecular Structure and Vibrational Spectroscopy investigation of Secnidazole using Density-Functional Theory

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Secnidazole (α , 2-dimethyl-5-nitro-1H-imidazole-1-ethanol) is an antimicrobial drug and is particularly effective in the treatment of amebiasis, giardiasis, trichomoniasis and bacterial vaginosis. Secnidazole crystallizes as a hemihydrate, which belongs to a monoclinic system, space group $P2_1/c$, $a = 12.424 \text{ \AA}$, $b = 12.187 \text{ \AA}$, $c = 6.662 \text{ \AA}$, $\beta = 100.9^\circ$. The optimized geometry of Secnidazole molecule has been determined by Density Functional Theory (DFT) method. Energies have been obtained using DFT method with B3LYP functionals with extended basis sets 4-31G, 6-31G and 6-311++G(d,p) for the three stable conformers of secnidazole. Using the optimized structure, we have determined the infrared and Raman frequencies for the molecule using DFT method. In this work, we also present a detailed vibrational spectroscopy investigation of secnidazole by using infrared and Raman spectroscopies. Based on these results, we discuss the correlation between the vibrational modes and the crystalline structure of the most stable conformer of secnidazole. The resulting frequencies are in excellent agreement with experiment. A complete assignment is provided the fundamental vibrational bands in terms of frequency and potential energy distribution. The calculated Raman spectrum is compared with experimental data obtained in the hemihydrate (30 °C) and anhydrous (90 °C) forms.