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# Characteristics of the different S=O, S-O, N---H, O---H and Na---O bonds into the powerful laxative sodium picosulphate drug and their effects on the properties

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In this work, the influence of the different S=O, S-O, N...H, O...H, Na...O bonds present in the structures of the powerful laxative drug, sodium picosulphate in gas and aqueous solution phases were studied combining the density functional theory (DFT) calculations with the experimental available infrared, 1H-NMR and UV-visible spectra. The structural, topological, electronic and vibrational properties were investigated in both media by using the hybrid B3LYP/6-31G* method and the integral equation formalism variant polarised continuum model (IEFPCM). Here, the characteristics of the S=O, S-O, N...H, O...H, Na...O bonds were completely revealed by using atomic charges, natural bond orbital (NBO) and atoms in molecules (AIM) studies. The infrared, 1H-NMR, 13C-NMR and UV-visible spectra are in reasonable concordance with those experimental available in the literature. The following reactivity order it is observed when picosulphate is compared with other potential antimicrobial and antiviral drugs: thione > brincidofovir > sodium picosulfate > thiol > cidofovir. The vibrational analysis of sodium picosulphate was performed considering C3V symmetries for both SO42- groups and the complete assignments of the 126 vibration modes were reported in gas phase and aqueous solution together with their corresponding force fields. In addition, the reactivities of sodium picosulfate increase in solution due to their ionic characteristic which probably justifies their behaviour as a stimulant cathartic and their easy metabolic conversion, as reported in the literature.

## Biography

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