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Polymorphism, Intermolecular Interactions, and spectroscopic properties in Crystal Structures of Sulfonamides

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ABSTRACT

The antibiotics family of sulfonamides has been used worldwide intensively in human therapeutics and farm livestock during decades. Intermolecular interactions of these sulfamides are important to understand their bioactivity and biodegradation. These interactions are also responsible for their supramolecular structures. The intermolecular interactions in the crystal polymorphs of the sulfonamides, sulfamethoxypyridazine and sulfamethoxydiazine, as models of sulfonamides, have been studied by using quantum mechanical calculations. Different conformations in the sulphonamide molecules have been detected in the crystal polymorphs. Several intermolecular patterns have been studied in order to understand the molecular packing behaviour in these antibiotics. Strong intermolecular hydrogen bonds and π-π interactions are the main driving forces for crystal packing in these sulfonamides. Different stability between polymorphs can explain the