

Synthesis, characterisation and structure determination of 3-[(1Z)-{2- [bis(2-methylphenyl)methyl]sulfanyl)methylidene]hydrazin-1-ylidene)methyl]benzene-1,2-diol

ABSTRACT

A light-yellow crystalline product (1), which was isolated after one week from the filtrate of the reaction between S-2-methylbenzylthiocarbamate and 2,3-dihydroxybenzaldehyde, was characterised by single crystal X-ray diffraction, FTIR and NMR spectroscopic analyses. The experimental molecular structure of 1 has been established by X-ray crystallography and showed, to a first approximation, a planar C₂N₂S₂ + dihydroxyphenyl region that has an almost orthogonal relationship to the rings of the pendant S-bound benzyl groups. This structure has been verified via density functional theory calculations using the B3LYP/6311G(d,p) level of theory. The molecular packing featured linear supramolecular chains along the b-axis sustained by tolyl-CH...N(imine) and tolyl-CH... π (tolyl) interactions; the importance of these contacts is indicated by a Hirshfeld surface analysis.

Keyword: Dithiocarbamate diester; Single crystal X-ray diffraction analyses; DFT; 2,3-Dihydroxybenzaldehyde