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CRYSTAL STRUCTURE AND NMR SPECTROSCOPIC CHARACTERIZATION OF 1,5-BIS(2-HYDROXY-3-METHOXYBENZYLIDENE)CARBONOHYDRAZIDE

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Abstract. The solid-state structure of a symmetrical carbohydrazone, namely 1,5-bis(2-hydroxy-3-methoxybenzylidene)carbonohydrazide was determined by X-ray single crystal diffraction method. Compound **1** crystallizes in the monoclinic space group $P2_1/n$ with unit cell parameters a= 10.1198(6), b= 22.7847(11), c= 15.1738(10) Å, β= 100.458(6)°, Z= 4, V= 3440.6(3) Å^3, R_1= 0.0540. Crystal structure of **1** is defined by two crystallographic independent molecules, which are bonded *via* N–H···O hydrogen bond. The organic molecules are as keto tautomers with respect to the carbamide fragment, and adopt the *anti* conformation. 1D and 2D NMR experiments have argued on the presence of the title compound in DMSO-d_6 solution mostly as keto tautomer in *syn* conformation, and enol-imino form when considering *o*-vanillin residue.

Keywords: carbohydrazide, *o*-vanillin, *syn-anti* isomer, X-ray diffraction, NMR spectroscopy.

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