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Study of polymorphism in 2, 2'-diseleno bis(3-pyridinol)

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Abstract

2,2'-Diselenobis(3-pyridinol), $[2-C_5H_3N(3-OH)Se]_2$ (DISPOL) (1) and 3hydroxypyridine-2-(1H) selone (2) were synthesized and characterized by microanalyses, NMR (¹H, ¹³C{¹H}, and ⁷⁷Se{¹H}) spectroscopy. The 1 on recrystallization from various organic and aqueous solutions resulted in different polymorphs which were unambiguously characterized by single crystal X-ray diffraction analyses at room as well as low temperatures. Differential scanning calorimetry (DSC), thermogravimetric analysis (TGA) and differential thermal analysis (DTA) of 1 confirmed the existence of two polymorphs. The bulk 1 and its polymorphs exhibited potent cytotoxicity against A549 human lung carcinoma cells (IC₅₀ values \approx 10 µM). The compound is thermodynamically stable and is a promising candidate for further pharmacological studies as a cytotoxic agent.

1. Introduction

The chemistry of organoselnium compounds has made a great stride in diverse areas during the last two decades or so. These compounds find numerous applications in organic synthesis [1, 2], coordination chemistry [3-5], materials science [4, 6], pharmacy [7] and biology [8, 9]. Selenium is an essential micronutrient for animals and humans and exists in the form of selenocysteine which constitutes an active site of several selenoenzymes [10]. Glutathione peroxidases (GPx), a sub-family of selenoenzymes, have been recognized as

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