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Theoretical (DFT) and experimental (FT-IR & FT Raman) approach to investigate the molecular geometry and vibrational properties of 2,5- and 2,6-dihydroxytoluenes

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ABSTRACT

Fourier Transform infrared spectra were measured for 2, 5- dihydroxytoluene (5DHT) and 2, 6- dihydroxytoluene (6DHT), in the spectral range 4000–400 cm^{-1}. Fourier Transform Raman spectra were also recorded for the same molecules, in the spectral region 3500–100 cm^{-1}. Torsional potential energy scans were attempted around ring – ortho hydroxyl C-O bonds, and ring-methyl C-C bond, for the two molecules. Barrier heights were computed for the above bonds for both the target molecules. Optimized molecular geometry, general valence force constants, vibrational wave numbers (harmonic), infrared intensities, and Raman scattering intensities were calculated, employing density functional theory and using B3LYP/6-311++G(d,p) level of formalism. Observed and measured frequencies agreed with an rms error 8.6 and 8.3 cm^{-1}, for 5DHT and 6DHT, respectively, on scaling. In addition, experimental infrared and Raman spectra agreed with their simulated counterparts with good accuracy. Using potential energy distribution (PED) and eigenvectors, all fundamentals were assigned unambiguously for both molecules. Geometry optimization was made for trimers of the two molecules at the same level of theory as used for the monomers. Existence of inter-molecular hydrogen bond was predicted.

1. Introduction

Dihydroxytoluenes are known for their use in medicinal applications, production of plastic resins and as reagents in chemical testing of carbohydrates. For example 3, 5-dihydroxytoluene (5-methyl resorcinol or orcinal) has been in use as a reagent for sucrose, arabinose, saccharose, pentose and lignin in chemical tests; it is the parent substance of the natural dye orcien; it is also used as an external antiseptic in different kinds of skin diseases [1–4]. In addition, due to its antidepresent activity, it has found utility in the preparation of medicine and functional food for treating or preventing depression [5]. Further, the interaction between 3,5-dihydroxytoluene and bovine serum albumin [6] was investigated, in order to understand ligand/drug displacement interactions, which is an important research field in life sciences and clinical medicine [7–11]. Moreover, 5-alkylresorcinols (5-methyl- resorcinol is a member), exhibit fungicidal and bactericidal activities against many pathogens [12]. Their derivatives, such as siccanin [13,14], grifolin [15] are effective antibiotics. It was also found that these compounds, at high concentrations, can cleave DNA in the presence of copper (II) chloride and oxygen [16,17]. It was demonstrated that cytotoxicity of 2, 5 – dihydroxytoluene (5DHT), variously known as toluquinol or 2- methyl- hydroquinone or 2-methyl-1,4-benzenediol, arises from its methyl group [18]. This compound was known to induce thiol-specific response in *Bacillus subtilis*, which is a soil-dwelling bacterium [19]. Further, efficacy of 5DHT to induce proliferactive lesions of the forestomach in Syrian golden hamsters was investigated [20]. Subchronic toxicity [21], along with teratologic and dominant lethal [22] studies were conducted for 2, 6- dihydroxy toluene (6DHT, also called 2-methylresorcinol), in rats. Both 6DHT and 5DHT were studied, along with 3, 5- dihydroxytoluene, in order to understand antithyroid effects of coal-derived pollutants [23]. The structure of trimer of 6DHT, as determined from X-ray analysis, is also available [24]. Recent experimental and theoretical work on octopamine [25,26], 3–1(1-m-toluidinoethylidene)-Chromane-2,4-dione and its palladium (II) complex [27] and Vanillylmandelic acid and its carboxylate anion [28] are also note-worthy. However, to the best of

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