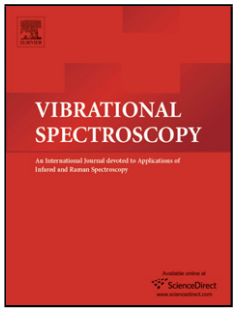

Title: Vibrational (FT-IR and FT-Raman), electronic (UV-Vis) and quantum chemical investigations on pyrogallol: A study on benzenetriol dimers

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Vibrational (FT-IR and FT-Raman), electronic (UV-Vis) and quantum chemical investigations on pyrogallol: A study on benzenetriol dimers

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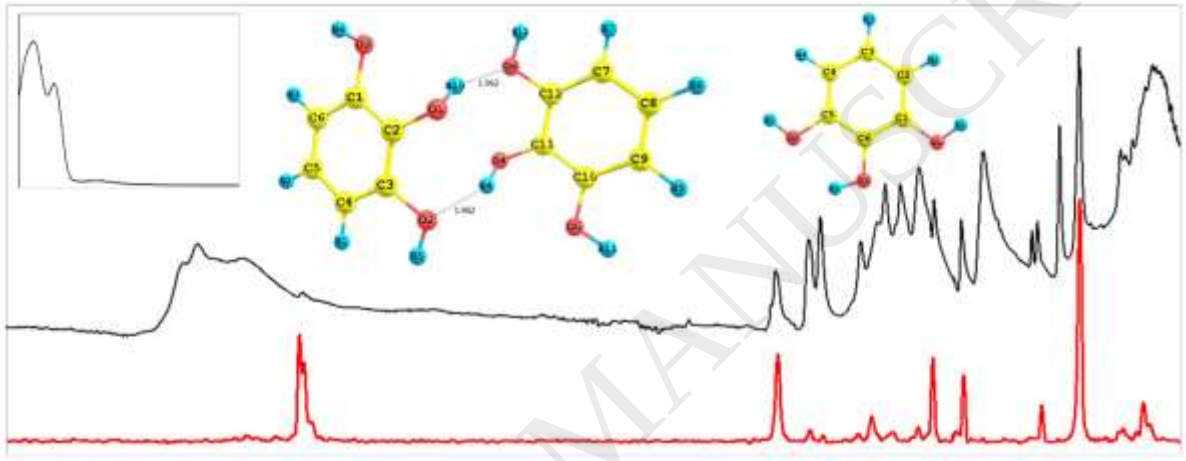
Graphical Abstract



HIGHLIGHTS

- Spectroscopic properties of pyrogallol were analyzed experimentally and theoretically.
- Vibrational and electronic spectra of pyrogallol were compared with its isomers (phloroglucinol and hydroxyquinol).
- HOMO-LUMO energy gaps were predicted for isomeric benzenetriols.
- Optimized monomer and dimer structure of benzenetriols were investigated.
- Experimental and theoretical FT-IR, FT-Raman and UV-Vis spectra show good agreement.

Abstract

Pyrogallol was identified for the first time from the natural extract of Abrus precatorius Linn seeds using GC-MS technique. The vibrational analysis of pyrogallol was investigated in solid phase by FT-IR and FT-Raman spectroscopic techniques in the region 4000-400 cm^{-1} and 4000-40 cm^{-1}, respectively. The optimized molecular geometry, wave number and intensity of the vibrational bands of pyrogallol and its isomers were obtained by DFT method with different basis sets. The electronic transition energy and intensities, HOMO-LUMO energy gap have been computed with the ZINDO, CIS, TDDFT theory for isomers and the differences were compared with UV-Vis absorption spectra. The observed wave numbers in FT-IR, FT-Raman