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Vibrational Spectroscopic Studies and DFT Calculations of 4-Fluoro-*N*-(2-Hydroxy-4-Nitrophenyl)Benzamide

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Fourier transform infrared (FT-IR) and FT-Raman spectra of 4-fluoro-*N*-(2-hydroxy-4-nitrophenyl)benzamide were recorded and analyzed. The vibrational wavenumbers and corresponding vibrational assignments were examined theoretically using the Gaussian03 set of quantum chemistry codes. The red-shift of the NH-stretching wavenumber in the infrared (IR) spectrum from the computed wavenumber indicates the weakening of the NH bond resulting in proton transfer to the neighboring oxygen atom. The simultaneous IR and Raman activation of the C O-stretching mode gives the charge transfer interaction through a p-conjugated path.

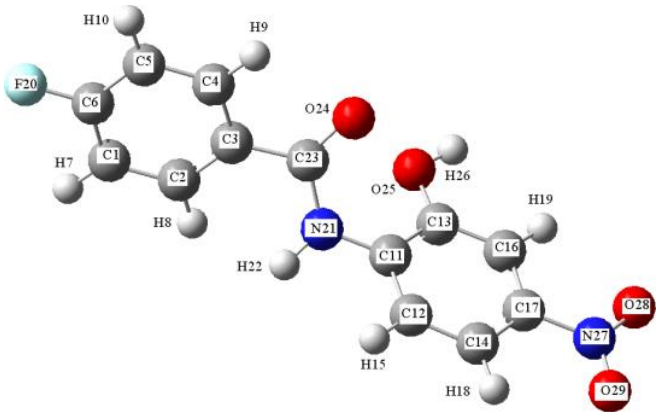

Fig. **Optimized geometry of 4-fluoro-N-(2-hydroxy-4-nitrophenyl)benzamide.**

References

[1] L. Ushakumari, H.T.Varghese, C.Y. Panicker, T. Ertan, I. Yıldız. "Vibrational spectroscopic studies and DFT calculations f 4-fluoro-N-(2-hydroxy-4-nitrophenyl)benzamide", Journal of Raman Spectroscopy, 39, 1832-1839, (2008).