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Temperature dependent polymorphism of pyrazinamide: An *in situ* Raman and DFT study

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Abstract

The α and γ polymorphs of drug pyrazinamide have been detected with the help of temperature dependent Raman spectroscopic technique. Pyrazinamide is a very useful drug used for the treatment of tuberculosis (TB) and plays a significant role in destroying the dormant tubercle bacilli which are not destroyed by other common TB drugs. Temperature dependent Raman spectra suggest polymorphic phase change from α → γ form of pyrazinamide between 145 - 146 °C. *In situ* Raman spectra of pyrazinamide between 145 - 146 °C show the conversion of α → γ form by the shift in C=O stretching vibration accompanied by several other changes. The phase change is characterized by the breaking of two linear N-H···O type hydrogen bonds associated with C=O stretching vibration in α dimer and formation of one linear N-H···N type hydrogen bond along with a weak intramolecular C-H···O type hydrogen bond in the γ dimer.

Keywords: *pyrazinamide; tuberculosis; hydrogen bonding; Raman Spectroscopy; DFT.*

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