Title:	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 and 146 °C. In situ Raman spectra of pyrazinamide between 145 and 146 °C show the conversion of α → γ form by the shift in Cdouble bondO stretching vibration accompanied by several other changes. The phase change is characterized by the breaking of two linear Nsingle bondH ··· O type hydrogen bonds associated with Cdouble bondO stretching vibration in α dimer and formation of one linear Nsingle bondH ··· N type hydrogen bond along with a weak intramolecular Csingle bondH ··· O type hydrogen bond in the γ dimer.
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