# CHANGES IN THE VIBRATIONAL CHARACTERISTICS OF SUBSTITUTED 1,2,4,5-TETRAZINES AFTER COMPLEXATION WITH 1,2,3-BENZOTRIAZOLE: A THEORETICAL STUDY

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The complexation of 3,6-substituted 1,2,4,5-tetrazines with benzotriazole was studied theoretically based on the vibrational spectra. For model complexes, the energy was minimized by the geometrical parameters, and the spectral characteristics were calculated by the PM3 method. The shift of the bond vibration frequencies of the atoms involved in complexation after the formation of different various intermolecular contacts was determined. This made it possible to determine the type of intermolecular interaction and suggest the structures of the complexes.

**Keywords:** 1,2,4,5-tetrazines, IR spectroscopy, stretching vibration frequencies, molecular co-crystals, hydrogen bond.