A STUDY ON 4-(*E*)-AMINO-3-[(*E*)-4-NITROPHENYLAZO]-3-PENTEN-2-ONE AND OTHER RELATED AZOENAMINONES IN CRYSTALLINE STATE

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Azoenaminones, compounds with potential nonlinear optical properties exist as azoenamine/hidrazimino tautomeric mixtures in solution while their tautomeric composition in crystalline state has not been studied extensively. In this work the nature of 4-nitrophenylazoenaminones, and particularly of 4-(*E*)-amino-3-[(*E*)-4-nitrophenylazo]-3-penten-2-one were studied by *ab initio*, structural chemometric methods. These compounds in free state are planar heteroaromatic systems where tautomerism is coupled with intrinsic π-electron delocalization and intramolecular hydrogen bonds. Bond lengths indicate different tautomeric character for distinct compounds. Intermolecular interactions affect the molecular geometry, especially planarity, and are partically responsible for crystal packing. Some electronic and steric molecular properties exhibit qualitative or quantitative relationship with crystal packing properties like crystal density, coordination number, average atomic volume, and ability to form hydrogen bond networks or □…□ stacks.