CRYSTAL AND MOLECULAR STRUCTURE OF KINETIN-PICRATE: A NOVEL COMPOUND CONTAINING A N(3)H AND N(7)H TAUROMERIC FORM OF PURINE, BY MANUEL SORIANO-GARCIA AND R.A. TOSCANO, INSTITUTO DE QUIMICA, UNIVERSIDAD NACIONAL AUTONOMA DE MEXICO, CIUDAD UNIVERSITARIA, 04510 MEXICO D.F., MEXICO.

6-furfurylaminopurine (Kinetin) is a highly potent growth factor (cytokinin) which is implicated in many aspects of plant growth. It promotes cell division and differentiation. A 1:1 crystal complex of kinetin and picric acid was crystallized and we present its crystal and molecular structure as an appropriate model compound for studying the structural properties of cytokinins in an ionic environment.

The complex, C_{6}H_{10}N_{4}O_{5}, crystallizes in the monoclinic system, space group P2_{1}/n with cell dimensions (at 18±2°C) a = 4.995(1) Å, b = 13.931(3) Å, c = 26.065 Å, β = 90.99(2)°, V = 1.63 g/cm³ and ρ = 4. The structure was solved from diffractometer data by direct methods and refined by a cascade matrix least-squares refinement, using 12040 observed reflections.

The present structure provides the first description of the adenine moiety with the N(3)H and N(7)H tautomers. The molecular geometry of the adenine ring found in this structure differs considerably from the assumed in theoretical calculations on the N(3)H tautomer of purine. The molecular geometry of the adenine ring found in this structure differs considerably from the assumed in theoretical calculations on the N(3)H tautomer of purine.

The kinetin cation assumes a similar conformation from structural studies of the adenine group, C_{5}H_{5}N_{4}, as found in the structures of the adenine cations and adenine·picrate salts. In the crystal, the kinetin cations and the picrate anions are aggregated separately into monoclinic and cubic packing units of the kinetin cations, with the picrate anions being held together in pairs across centers of symmetry by N(3)H···N(7)H hydrogen bonds. The two layers of unlike molecules are interconnected primarily through a specific ion-pair interaction between the N(7) of the tetazaolo ring and the deprotonated oxygen atom of the picrate ion.

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