Poster Presentation

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Crystal structure of 2-amino-9-{[(1,3-dihydroxypropan-2-yl)oxy]methyl}-1,9-dihydro-6H-purin-6-one

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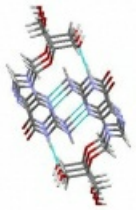
2-amino-9-{[(1,3-dihydroxypropan-2-yl)oxy]methyl}-1,9-dihydro-6H-purin-6-one or commonly known as Ganciclovir is an acyclic guanine nucleoside analog which is a well-known anti-viral agent that inhibits replication of herpes virus. Four polymorphic forms of Ganciclovir have been reported out of which two hydrates and two anhydrous [1,2]. The present study deals with the crystal structure of Ganciclovir Form-I and its comparison of crystal properties with the previously reported Ganciclovir Form-II [3]. The twinned acicular bundle of Ganciclovir Form-I crystals were obtained upon slow evaporation of DMSO solvent which exists as monoclinic having the space group as P21/c with cell parameters a=4.663, b=15.650, c=14.157 and β=91.788. The monoclinic crystal system with β very close to 90° and closeness of b and c appears to be a pseudo-merohedry type of twinned crystal. The uniqueness of the polymorph lies in the primary and secondary amine groups in the pyrimidone ring of the guanine moiety forming a two-point synthon through N-H...N and N…H-N intermolecular hydrogen bonding leading to the formation of six membered ring. The compound is stabilized further by the inter-molecular N1….O2 and O2…N2 forming a 10-membered ring inside the crystal lattice which is observed like a lacuna. The intermolecular hydrogen bonding between the alternate O1…O2 and O2…O1 type of two-point synthon between the diols leads to the formation of a ten membered ring inside the lattice along the a-axis. It is published on Mylan Publication number: IPR/PR/2017/01

[1] U.S. Patent application number 4,642,346, Assignee Syntex (USA) Inc.
[2] Ruchira M. Sarbajna, et al. (2011). Mol. Cryst. Liq. Cryst, 537, 141-154.
[3] Kawamura, T., & Hirayama, N. (2009). X-ray Structure Analysis Online, 25, 51-52.



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