Polymorphism in an Anti-implantation Agent: A Subtle Interplay of Weak Intermolecular Interactions

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Polymorphism is defined as a solid crystalline phase of a given compound resulting from the possibility of at least two crystalline arrangements of that compound in the solid state. Substituted Indol-4-ones are anti-fertility agents and have been used for the inhibition of implantation activity in rats. Polymorphism in 1-(4-fluorophenyl)-3,6,6-trimethyl-2-phenyl-1, 5, 6, 7-tetrahydro-4H-indol-4-one based on solvent variation and the subsequent changes in intermolecular interactions is discussed.

A complete analysis has been made in terms of morphology, Single Crystal Structure, Powder X-Ray diffraction, Non Linear Optical Activity (NLO) and Differential Scanning Calorimetry. Polymorph **(P1)** crystallizes from a solution in Dichloromethane/Hexane in a monoclinic space group, non-centrosymmetric $P2_1$ (as plates) whereas the second polymorph **(P2)** crystallizes from a solution in EtOH/Acetone in a tetragonal space group, centrosymmetric $P4_2/n$ (as blocks).[1] C-H…O and C-H…π intermolecular interactions forming chains stabilize **P1** while **P2** is stabilized by C-H...O and C-H…π dimers and a not so common F…F intermolecular interaction.

[1] Chopra D., Nagarajan K., Guru Row T.N., *Cryst. Growth & Design*, 2005, *in press*.

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