

*Exploring the structural landscape by chloro-methyl exchange*

Shaunak Chakraborty<sup>1</sup>, Sumy Joseph<sup>1</sup>, Gautam R. Desiraju<sup>1</sup>

<sup>1</sup>*Solid State And Structural Chemistry Unit, Indian Institute Of Science, Bangalore, India*

E-mail: shaunak\_chakraborty@outlook.com

The crystal structure landscape is a mapping of the various dynamic events occurring during the process of crystallization, and these correspond to multitudes of structural and energetic transformations. Polymorphism and solvation being recurrent issues in organic crystal engineering, the relevance of the idea of the crystal structure landscape– in both the academic and the industrial contexts– is undeniable. Experimentally, fluorine substitution augmented by computational crystal structure prediction has proven to be a handy technique in the exploration of the crystal structure landscape of benzoic acid and the benzoic acid-isonicotinamide cocrystal. The device of fluoro substitution works well in the study of the crystal structure landscape of the unsubstituted compound because of the closeness in the sizes of the fluorine atom and the hydrogen atom. The relationship between the chlorine atom and the methyl group are somewhat similar to that between the fluorine and hydrogen atoms, in that both sets of atoms have similar volumes, and both sets of atoms are exchangeable in crystal structures of compounds that are analogous in terms of molecular structure, because the interactions they participate in are largely isotropic. The current work explores this possibility using chlorinated aromatic acids and their methyl analogues, and attempts to chart the crystal structure landscape of the subject compound.

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