Polymorphism in Halo Derivatives (Cl, Br, I) of Lawsone: Combined Molecular and DFT Correlations

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Here we present various polymorphic forms of lawsone, its haloderivative by herishfield surface analysis prior to crystallographic and DFT correlations i.e. 2- hydroxy-1,4-napthoquinone; (LW), Chlorolawsone; ClLw (2-choloro-3-hydroxy,1-4-napthoquinone); Bromolawsone, BrLw; (2-bromo-3-hydroxy,1-4,napthoquinone), Iodolawsone; ILw, (2-iodo-3-hydroxy,1-4-naphthoquinono). Molecular structures were obtained by wB97X based denisty functional theory. Neighboring group associations were discussed by single crystal x-ray. These halo derivatives show variable oxidation state and suspect to various oxidation forms with varied bond angles, bond distances, and crystallizes in various polymorphic forms with varied solvation. Commonly observed molecular interactions are via. O-H…O, C-H…O, π-π stacking of quinonoid and benzenoid rings.

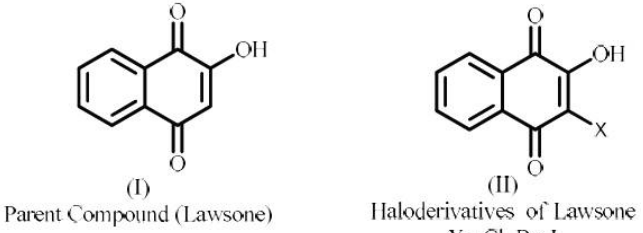

Fig. 1: Molecular Structure of parent Compound (I) Lawsone and its halo derivatives (II)

Keywords: Lawsone, C (3) derivatives, Crystallography, Herishfield, DFT, NLO

References

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