Electronic Supplementary Material for CrystEngComm

Crystal-to-Crystal Phase Transformation that Achieves Halogen Bonding: Structures of Dimorphs of Racemic 2,4-di-*O*- (*p*-halo benzoyl)-*myo*-inositol 1,3,5-orthoformates

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The supporting Information consist of

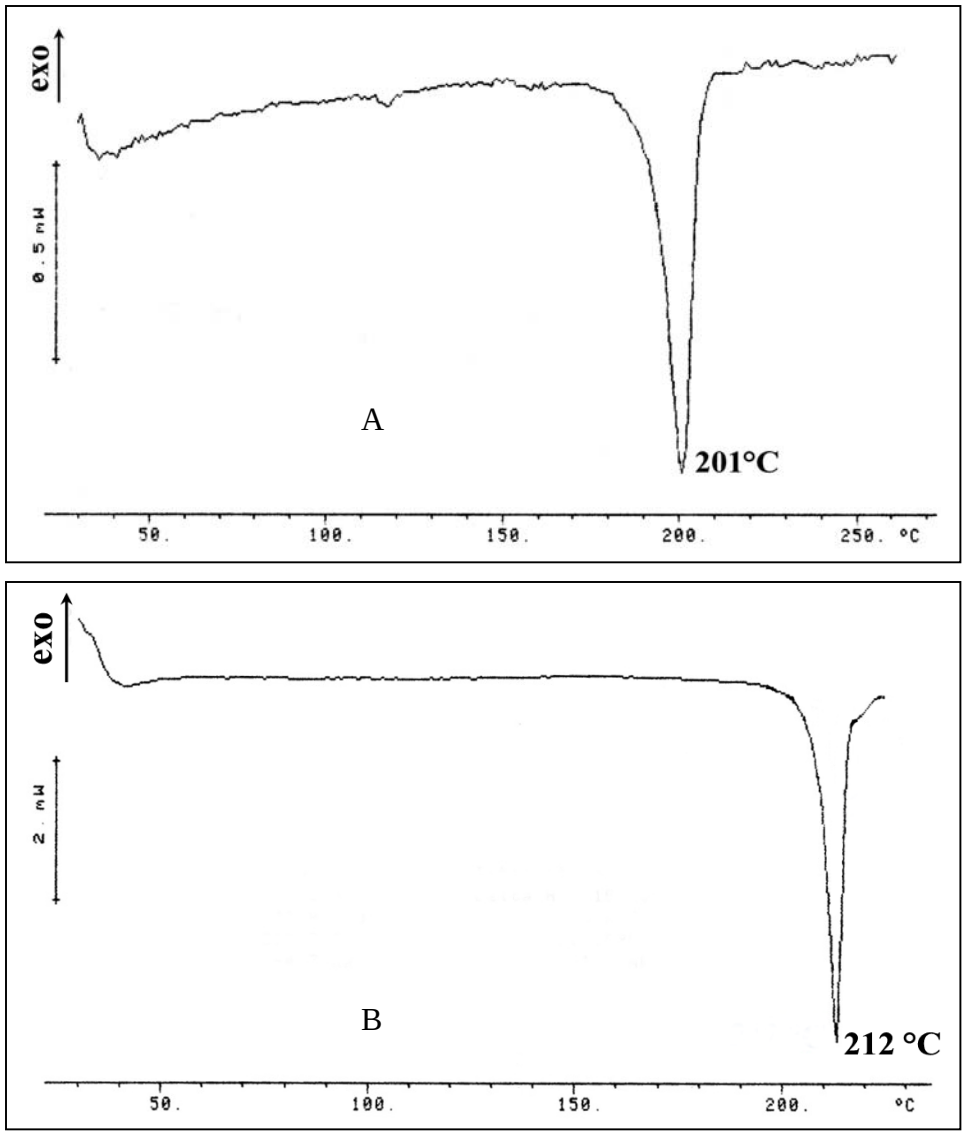
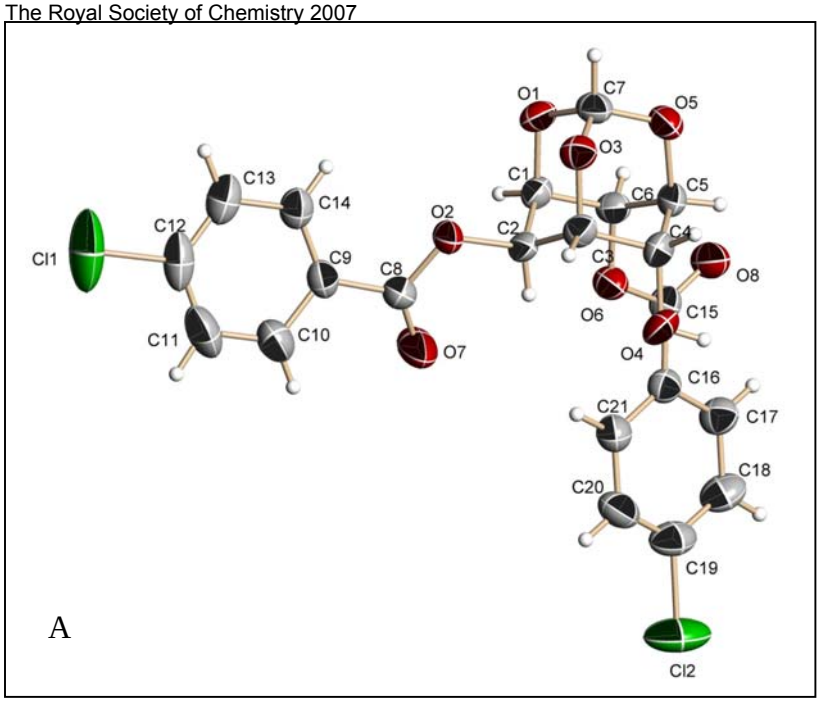


Figure S1: DSC profiles of A) Form I crystals and B) Form II crystals of **2**.



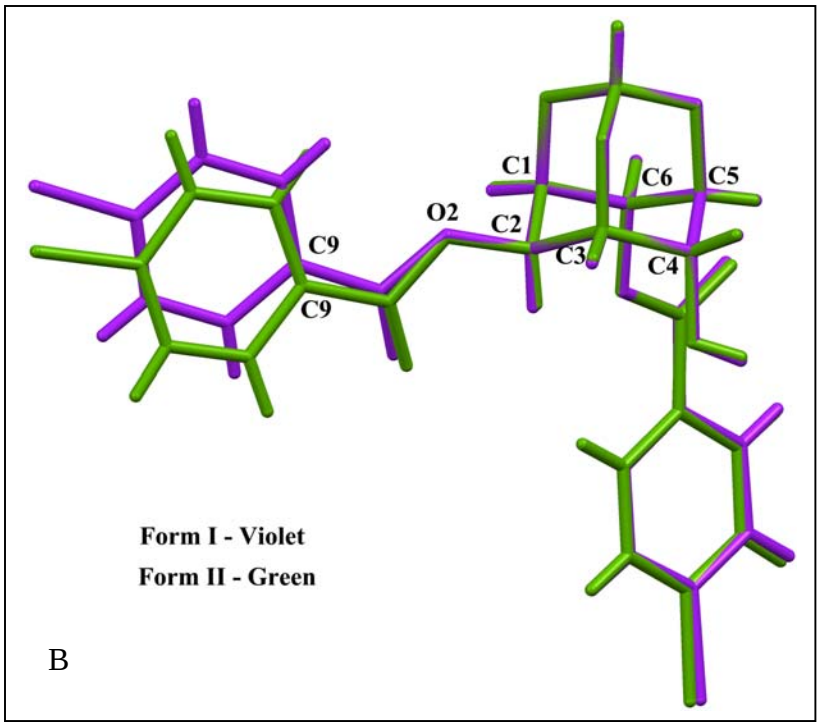


Figure S2: A) ORTEP view Form II crystals of **2** and B) overlap of Form I and Form II crystals of **2**.

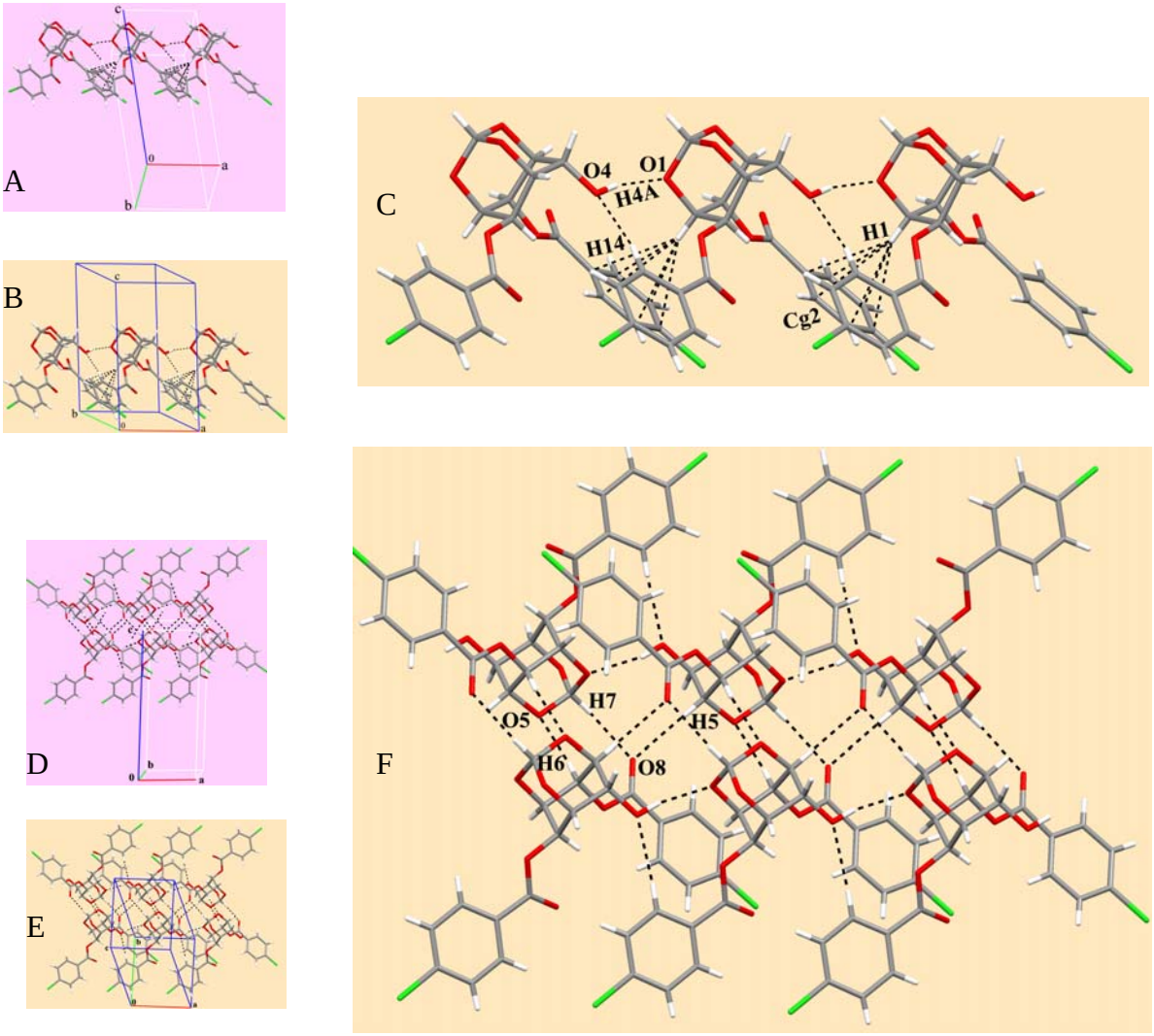


Figure S3: View of identical molecular string linked via O4-H4A···O1, C14-H14···O4 and C1-H1···π (Cg2) contacts showing one-dimensional isostructurality in dimorphs of **2** along a-axis, A) in Form I, B) in Form II and C) a closer view of these interactions in Form II; View of bilayer formed via centrosymmetric C-H···O bridging of these strings along the same axis in crystals of **2**, D) Form I, E) Form II and F) closer view of these interactions in Form II.

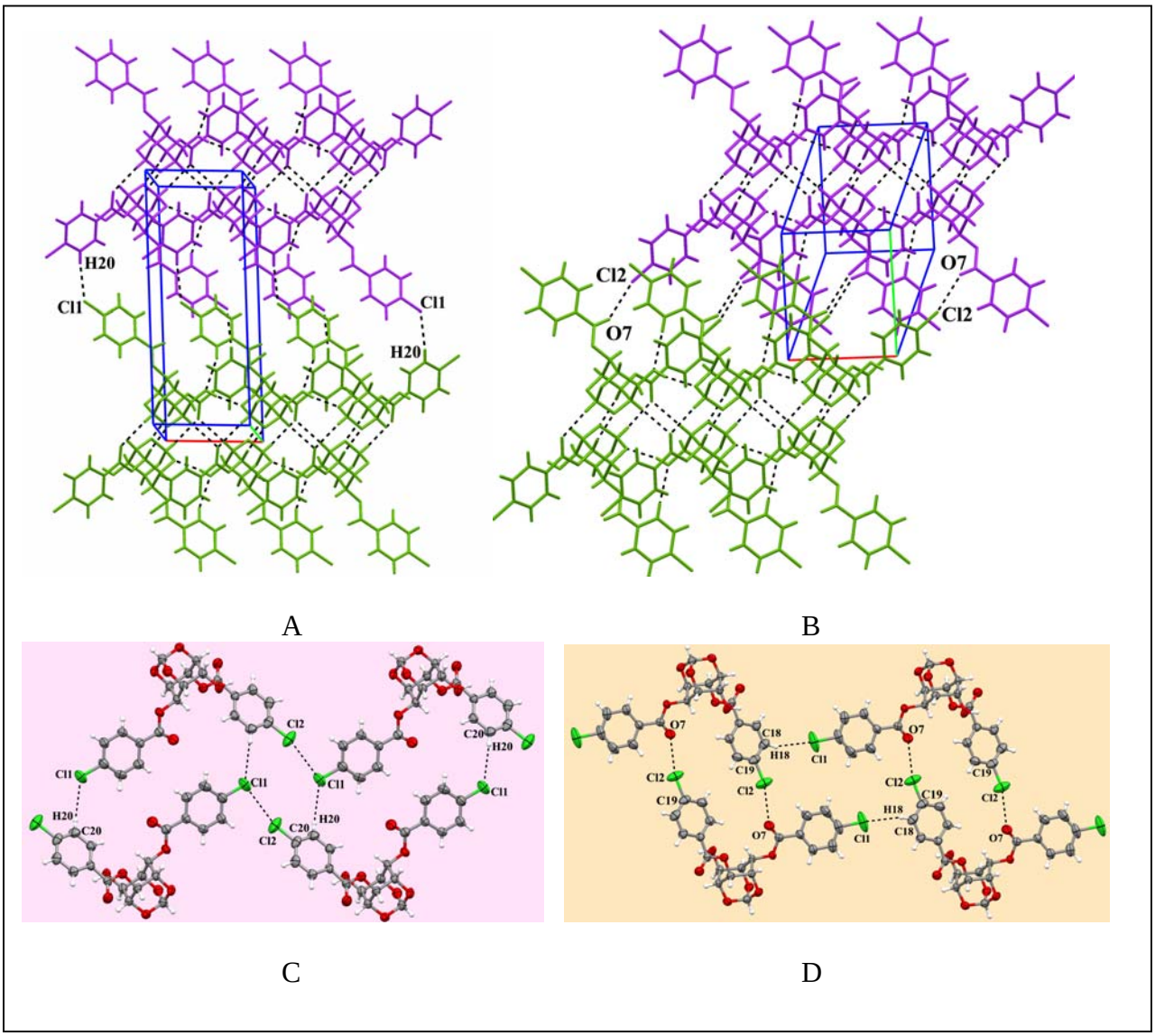


Figure S4. Different adhesions of bilayers in dimorphs of **2**; A) via C-H···Cl contact in Form I and B) through C-Cl···O (halogen bonding) contact in Form II; ORTEP views (C) and (D) shows the interfacing of bilayers in Form I and Form II crystals respectively.

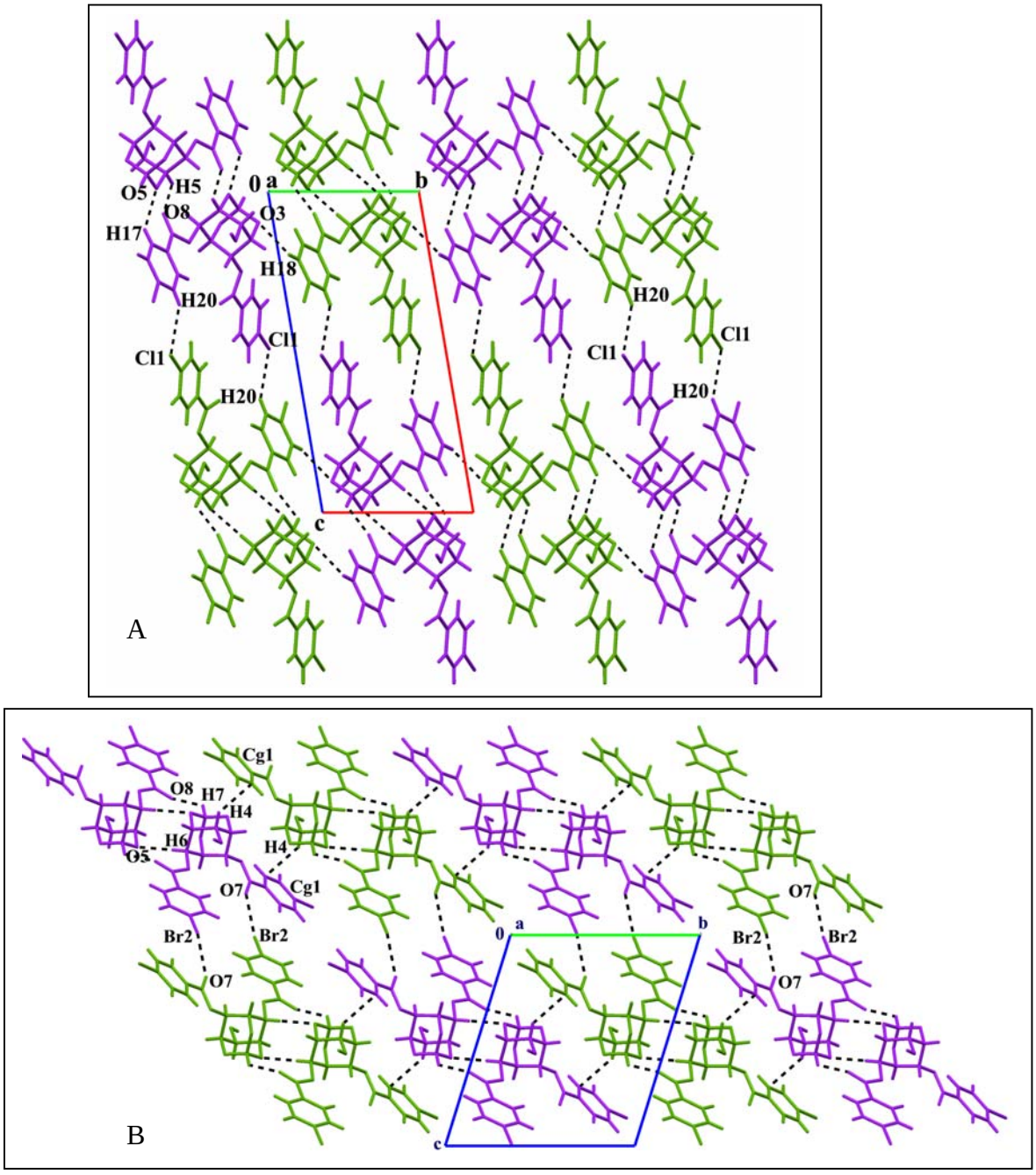


Figure S5. Difference in the organization of (isostructural) bilayers viewed down a-axis in dimorphs of **2**, A) Form I and B) Form II crystals.