IUCrJ

Volume 4 (2017)

Supporting information for article:

Charge-transport properties of 4-(1,2,2-triphenylvinyl)aniline salicylaldehyde hydrazone: tight-packing induced molecular `hardening'

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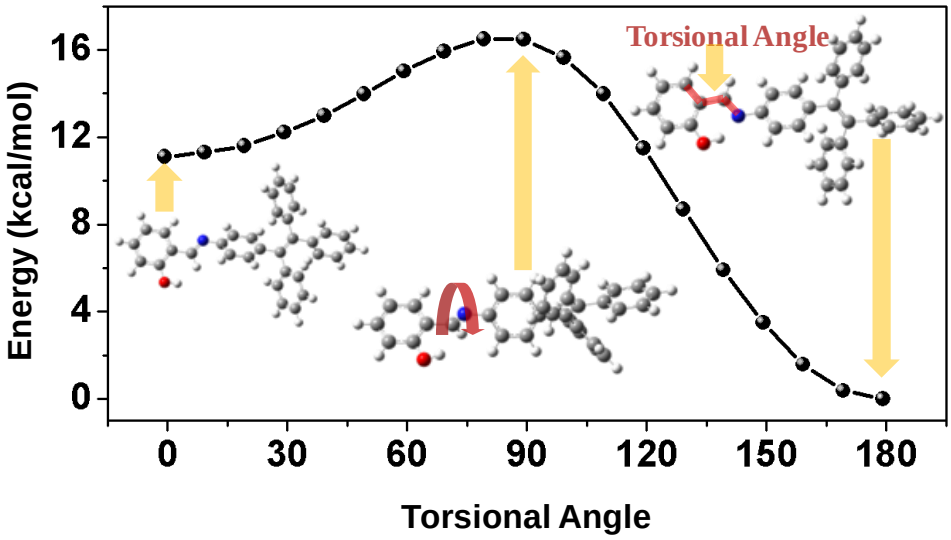

Figure S1. Variation of energy of molecule ***A*** as a function of rotation of the torsional angle between edge benzene ring and the other part of molecule ***A***.

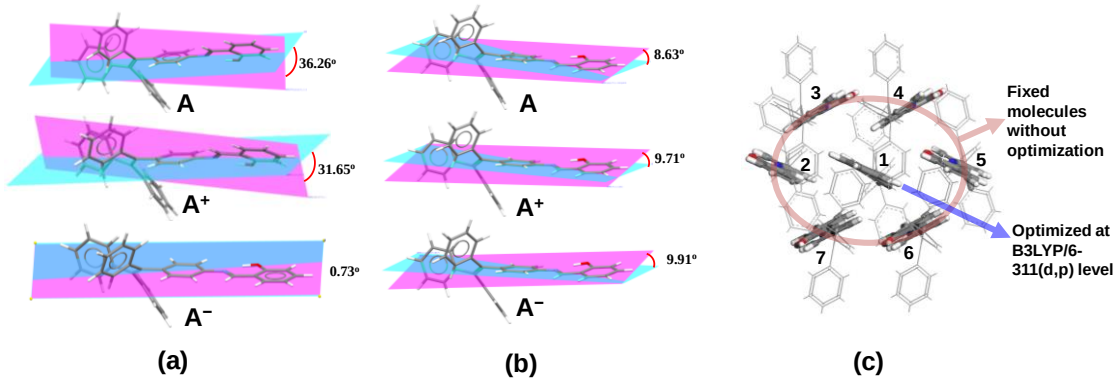

Figure S2. Dihedral angles between conjugate planes for ***A***, A^+, and A^- in gas phase (a); and dihedral angles between conjugate planes for ***A***, A^+, and A^- carved out of (b); (c) the computational model of the molecule ***A*** confined in the organic crystal. During structural optimization, the central molecule ***A*** (**1**) in the model is relaxed at b3lyp/6-311g(d,p), and the surrounding molecules ***A*** (**2**, **3**, **4**, **5**, **6**, and **7**) are fixed without optimization.

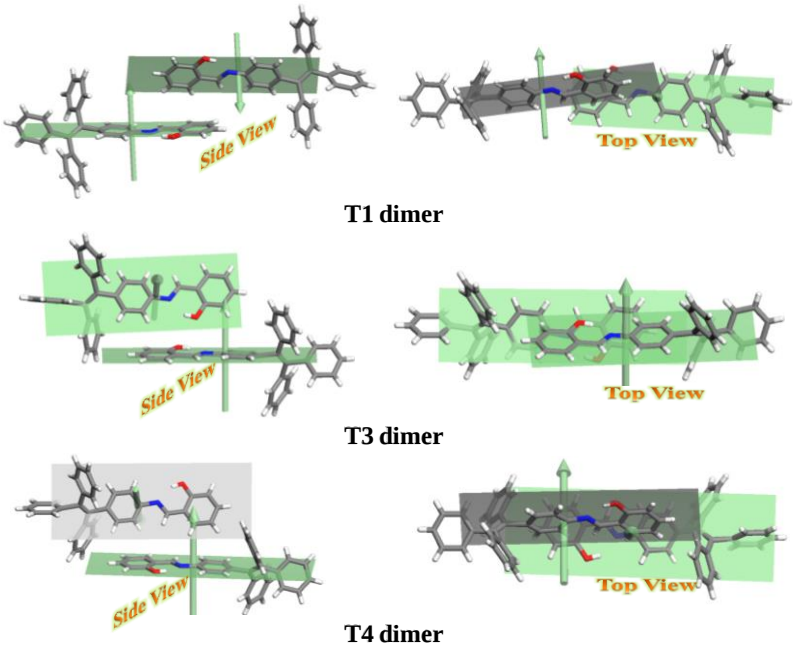

Figure S3. The relative positions of two interacting ***A*** in T1 dimer, T3 dimer, and T4 dimer in top view and in side view.