Supporting Information

Organic Thin Films with Charge-Carrier Mobility Exceeding that of Single Crystals

Zachary A. Lamport[†], Ruipeng Li[§], Chao Wang[⊥], William Mitchell[‡], David Sparrowe[‡], Detlef-M. Smilgies[§], Cynthia Day[‖], Veaceslav Coropceanu[⊥], and Oana D. Jurchescu*[,†]

[†]Department of Physics, Wake Forest University, Winston-Salem, North Carolina 27109, United States

[‡]Merck Chemicals Ltd., Chilworth Technical Centre, University Parkway, Southampton SO16 7QD, United Kingdom

[§]Cornell High Energy Synchrotron Source, Cornell University, Ithaca, New York 14850, United States

[‖]Department of Chemistry, Wake Forest University, Winston-Salem, North Carolina 27109, United States

[⊥]School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, Georgia 30332, United States

*Corresponding author: Oana D. Jurchescu; E-mail: jurchescu@wfu.edu

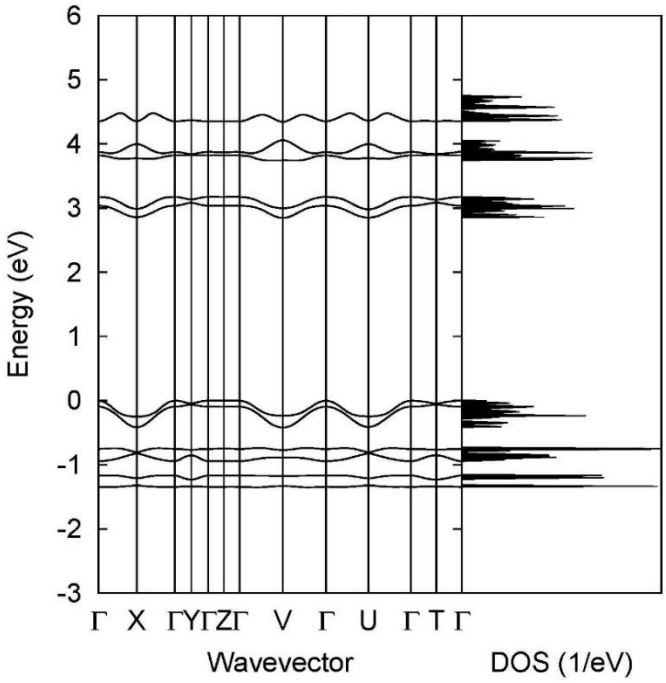

Fig. S1 Electronic band structures and densities of states of TMS-BT. The points of high symmetry in the first Brillouin zone are in crystallographic coordinates: Γ = (0, 0, 0); X = (0.5, 0, 0); Y= (0, 0.5, 0); Z = (0, 0, 0.5); V = (0.5, 0.5, 0); U = (0.5, 0, 0.5); T = (0, 0.5, 0.5).

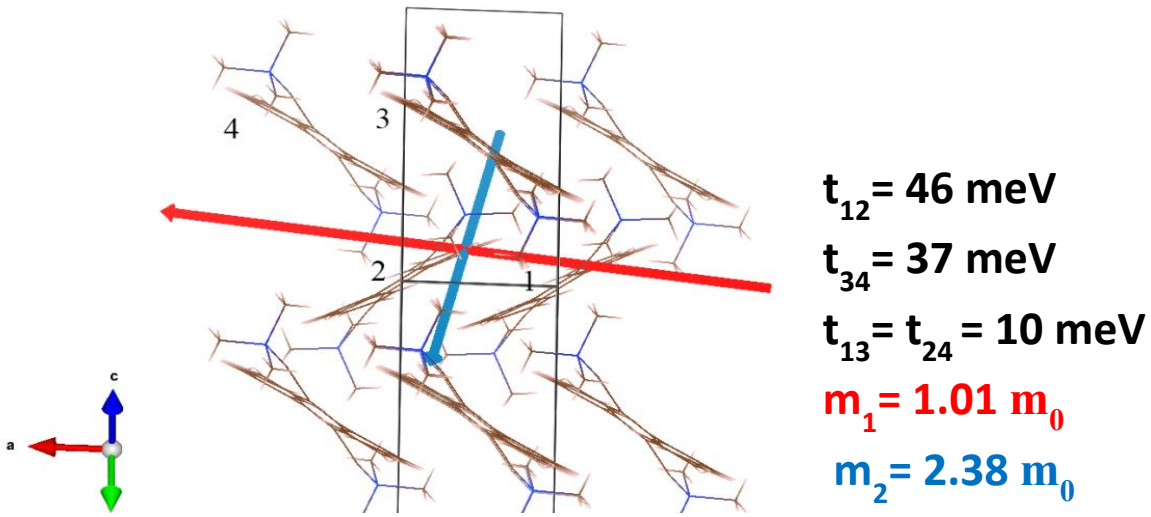

Fig. S2 Illustration of dominant charge transport pathways for holes in TMS-BT crystals. The smallest effective mass is observed along the stacking direction (*a* axis, indicated by a red arrow), and the next smallest effective mass component is along the [210] direction (indicated by a blue arrow). The numbers in the crystal structure label the molecules used for the electronic coupling calculations.

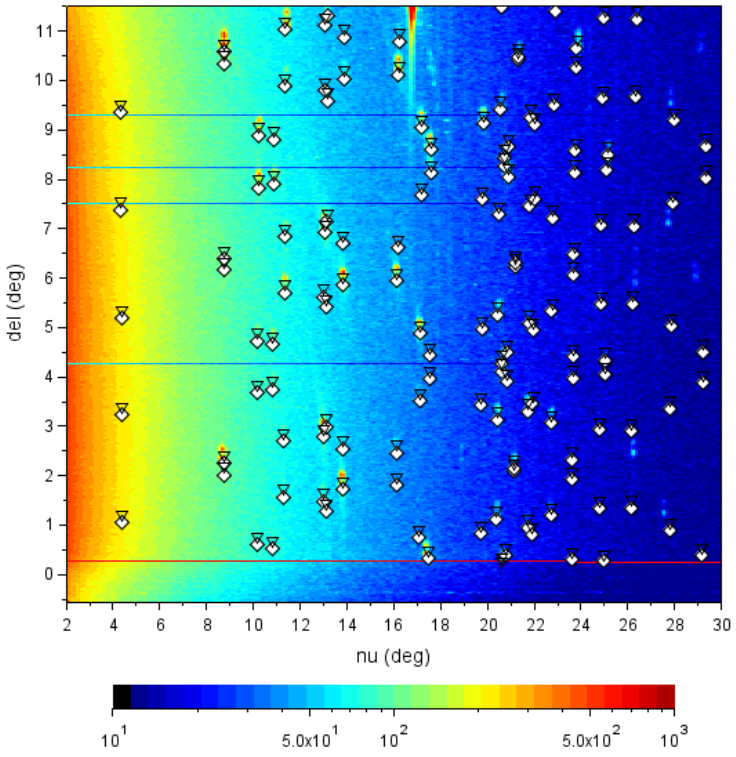

Fig. S3 Indexation of the grazing-incidence diffraction pattern of a single crystal. Laminated single crystals show a predominant (001) texture.

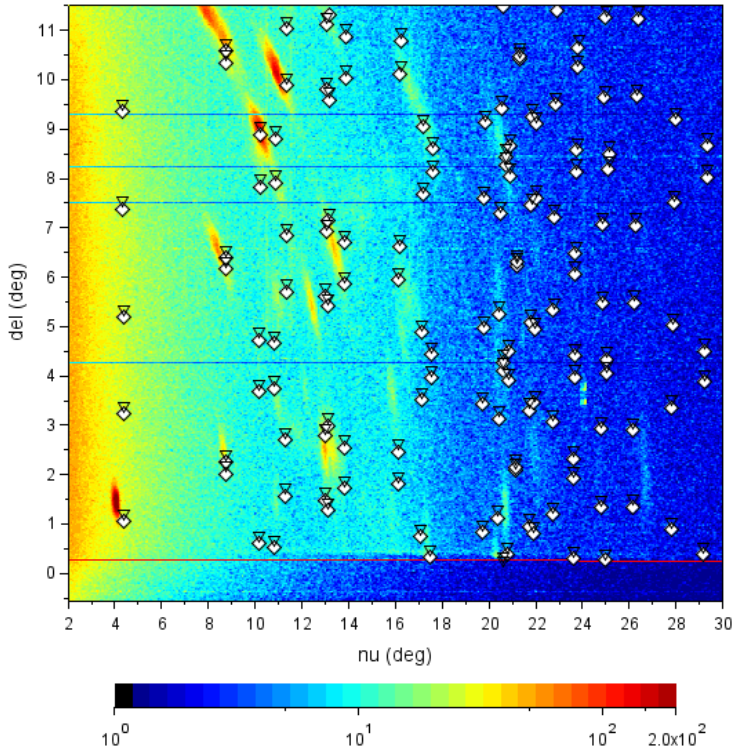

Fig. S4 Indexation of a thin film diffraction pattern assuming the bulk structure and a (001) texture.

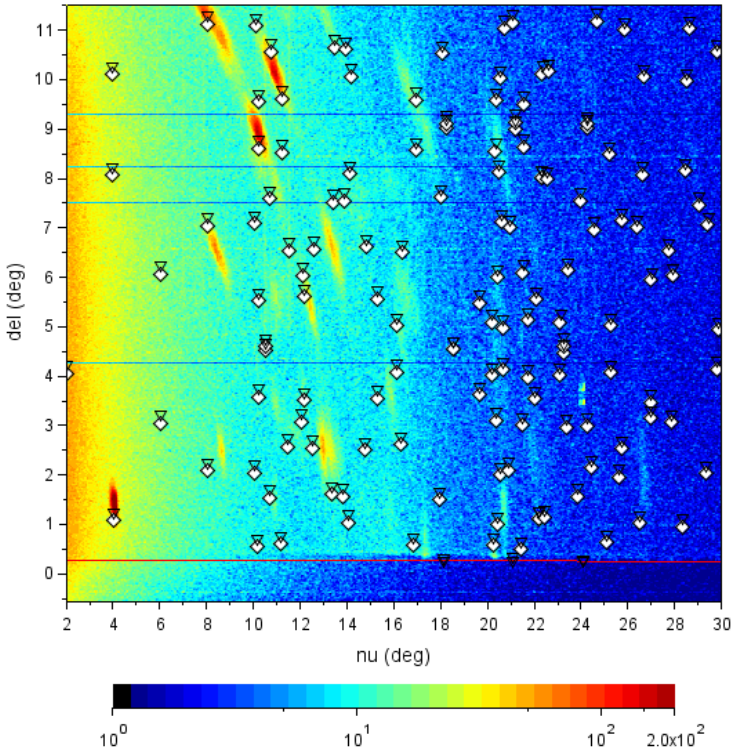

Fig. S5 Indexation of a thin film pattern assuming bulk structure and (02-1) texture.