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Gas Phase Electronic Structure of the DTDCTB Small-Molecule Donor for Vacuum-Processed Organic Photovoltaics Compared to Its Constituent Building Blocks

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C 1s ionization energies for α, β, γ carbons in the BTD building block molecule

The origin of the different C1s ionization energies of the C_α, C_β, and C_γ atoms of the BTD molecule, are due to their chemically inequivalence, *i.e.*, the different chemical enviroment that these Carbon atoms experience. Figure S1(a) provides the calculated C 1s XPS spectrum for the BTD building block molecule. The core binding energies (BEs) were calculated as the total energy difference between the molecule with a full core hole (FCH) on a specific C atom and the ground state (GS) molecule in a ΔKohn-Sham approach. The GS and FCH energies were calculated using the StoBe software package and the same functional and basis sets as described in the Computational Details section of the manuscript. The BE for C_α is calculated at 290.73 eV, while the BEs for C_β, and C_γ are quite close to each other and are calculated at about 289.69 eV and 289.65 eV, respectively. The energy shift between the C_α and C_β, C_γ 1s BEs (XPS peaks) is equal to 1.05 eV and is very similar to the shift between the experimental NEXAFS peaks A (C_β, and C_γ) and B (C_α) of BTD that is about 0.91 eV (Figure S1(b)). The C1s XPS of DPTA (Figure S2) and DTDCTB (Figure S3) are provided for completeness.

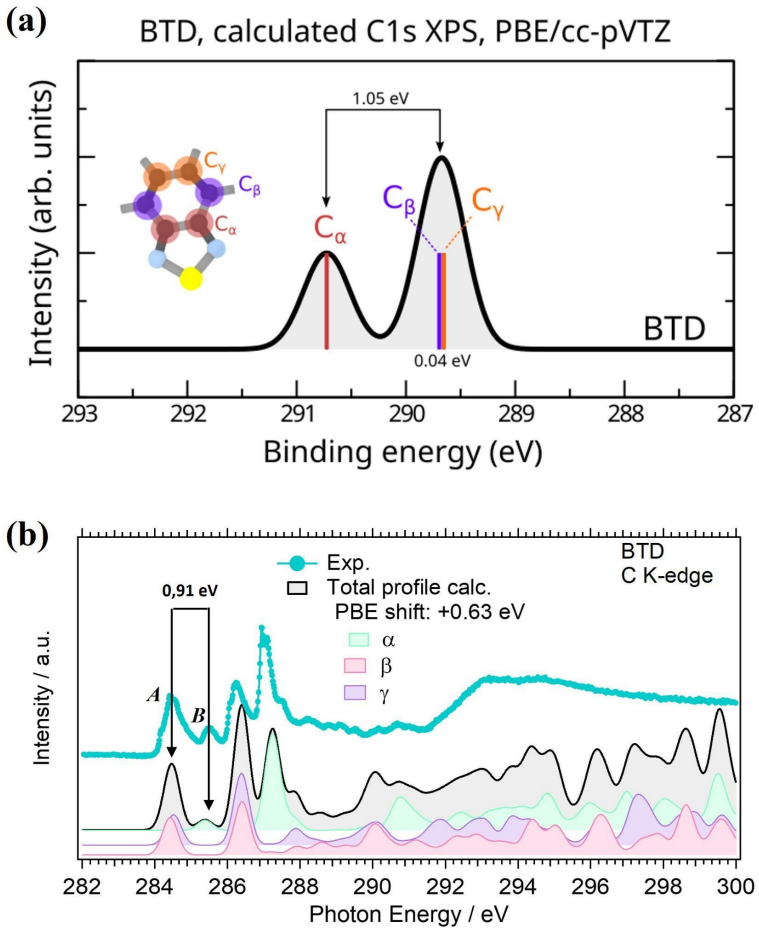

Figure S1: (a) Calculated (PBE/cc-pVTZ) C 1s XPS spectrum and **(b)** experimental C K-edge NEXAFS of BTD building block molecule.

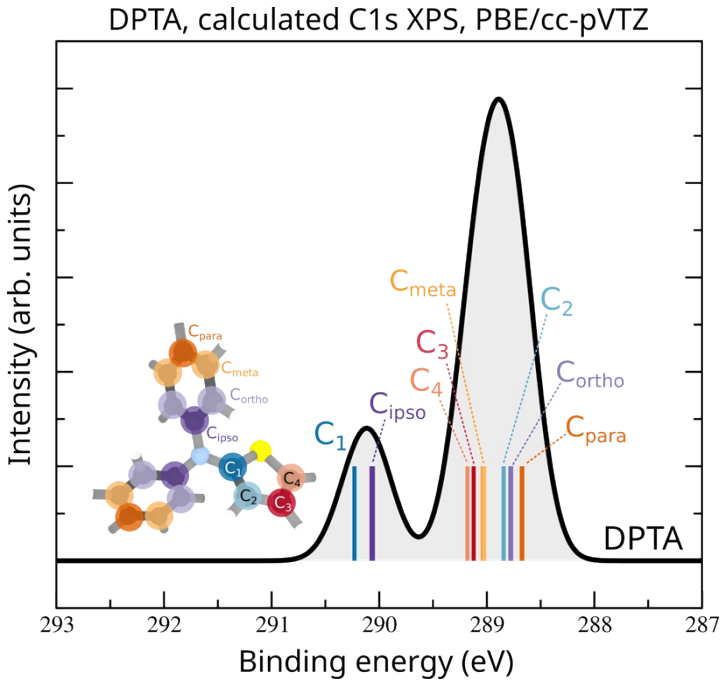

Figure S2: Calculated C 1s XPS spectrum of DPTA.

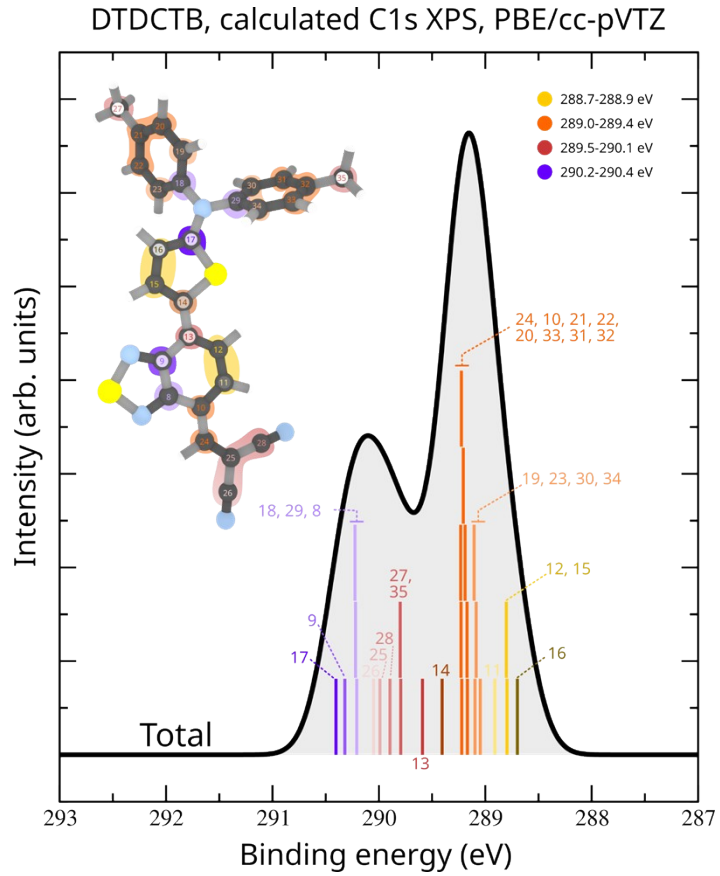

Figure S3: Calculated C 1s XPS spectrum of DTDCTB.