materials

MDPI

Supplementary Materials

New Benzotrithiophene-Based Molecule as Organic P-type Semiconductor for Small-Molecule Organic Solar Cells

1. Graphical representations of electronic excitation monomer for DCVT-BTT

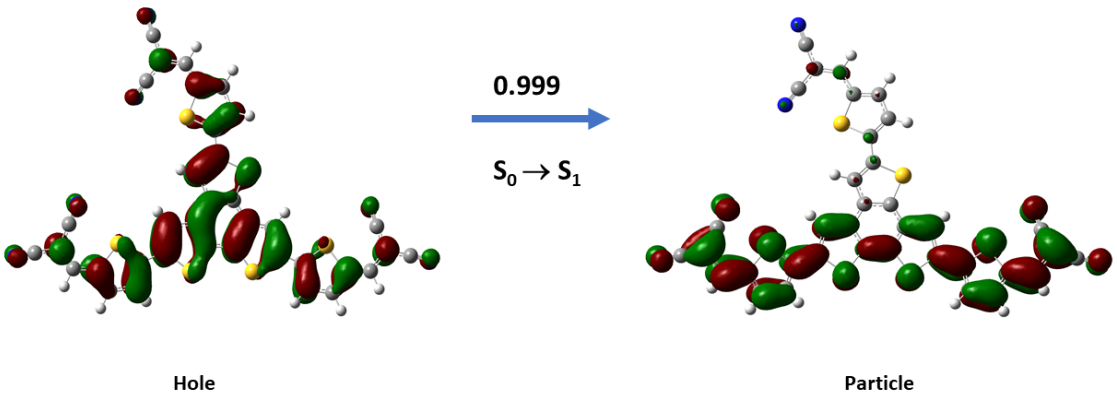


Figure S1. Natural transition orbitals (NTOs) of the first singlet excited-state of DCVT-BTT monomer and its eigenvalue.

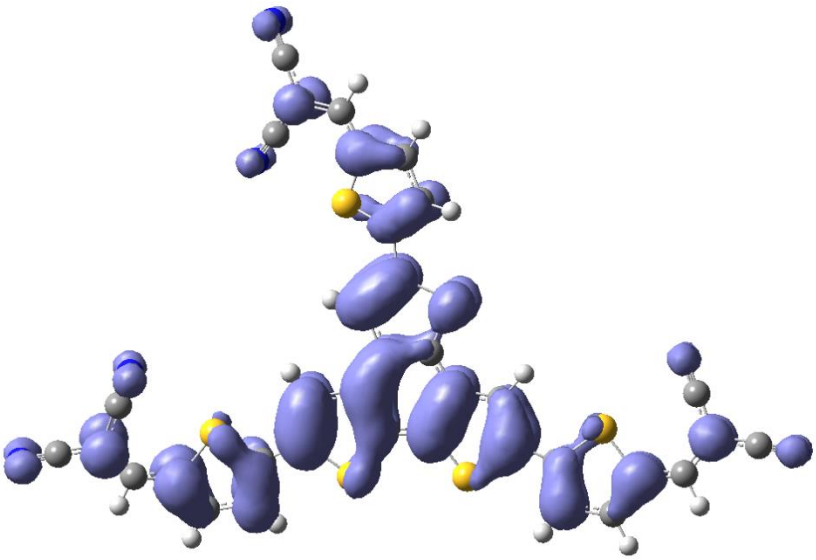


Figure S2. Hole distribution in DCVT-BTT monomer for the excitation $S_0 \rightarrow S_1$.

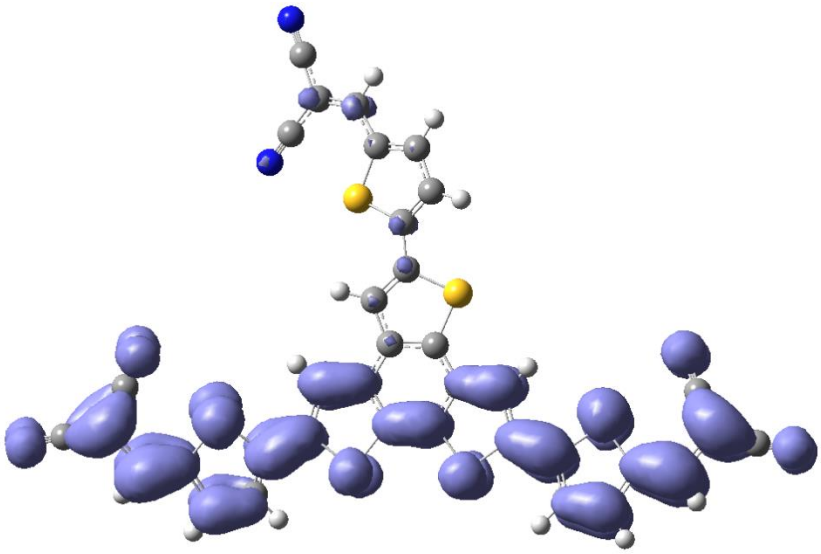


Figure S3. Electron distribution in DCVT-BTT monomer for the excitation $S_0 \rightarrow S_1$.

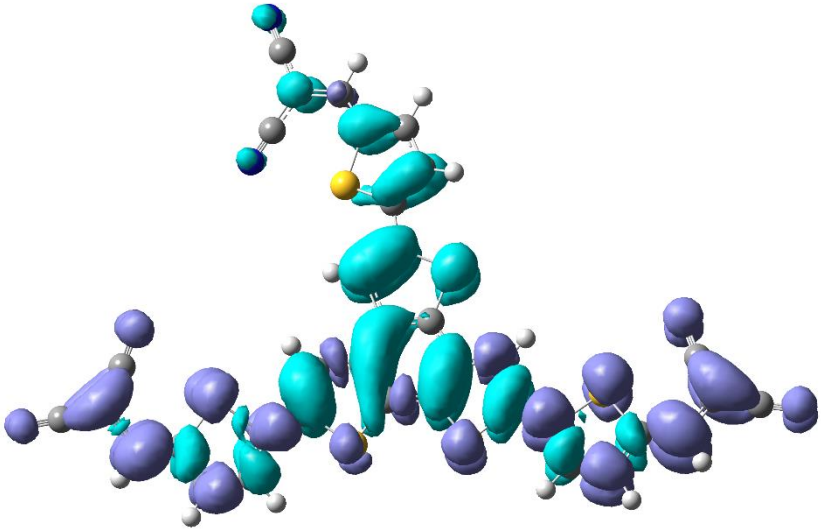


Figure S4. The charge difference densities for DCVT-BTT monomer on the electronic state transition from the ground state.

2. Graphical representations of electronic excitation for DCVT-BTT dimer

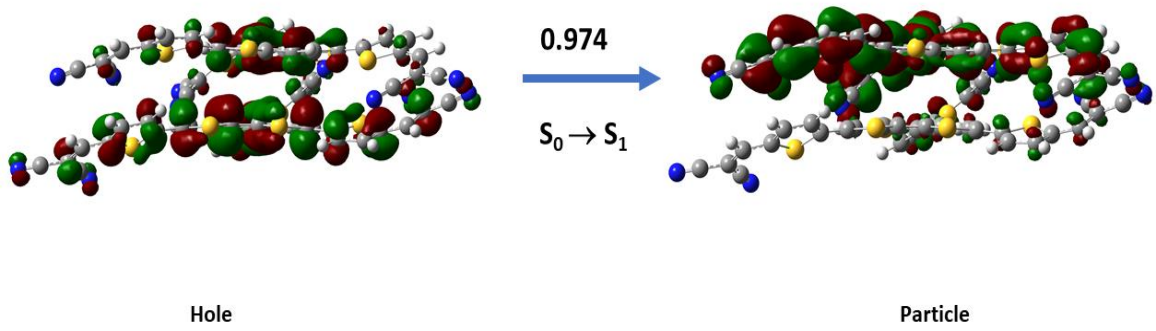


Figure S5. Natural transition orbitals (NTOs) of the first singlet excited-state of DCVT-BTT dimer and its eigenvalue.

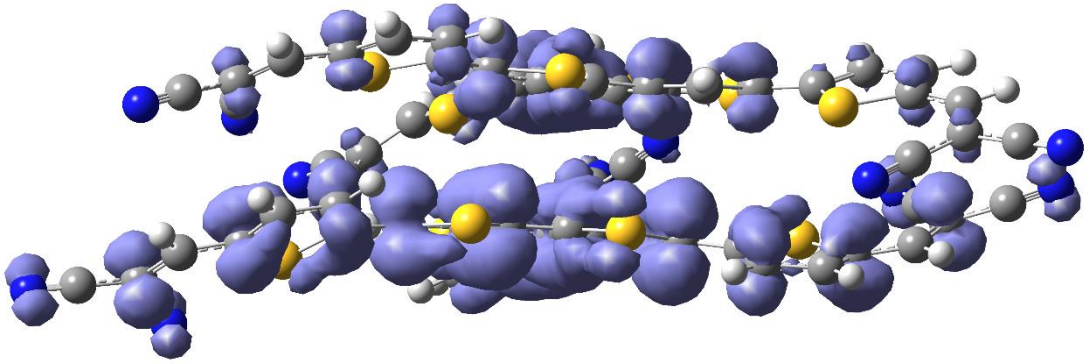


Figure S6. Hole distribution in DCVT-BTT dimer for the excitation $S_0 \rightarrow S_1$.

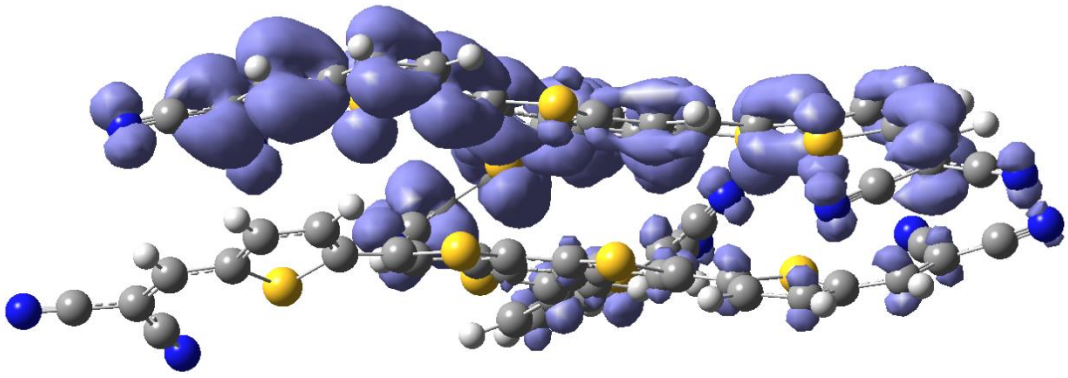


Figure S7. Electron distribution in DCVT-BTT dimer for the excitation $S_0 \rightarrow S_1$.

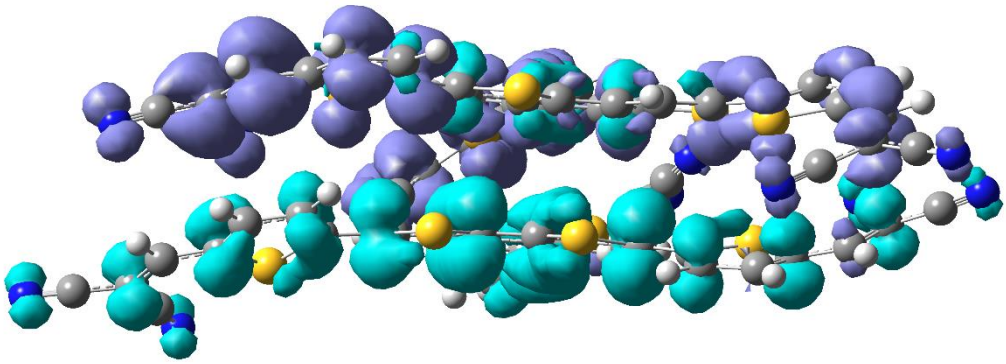


Figure S8. The charge difference densities for DCVT-BTT dimer on the electronic state transition from the ground state.

3. Chemical characterization analysis for DCVT-BTT

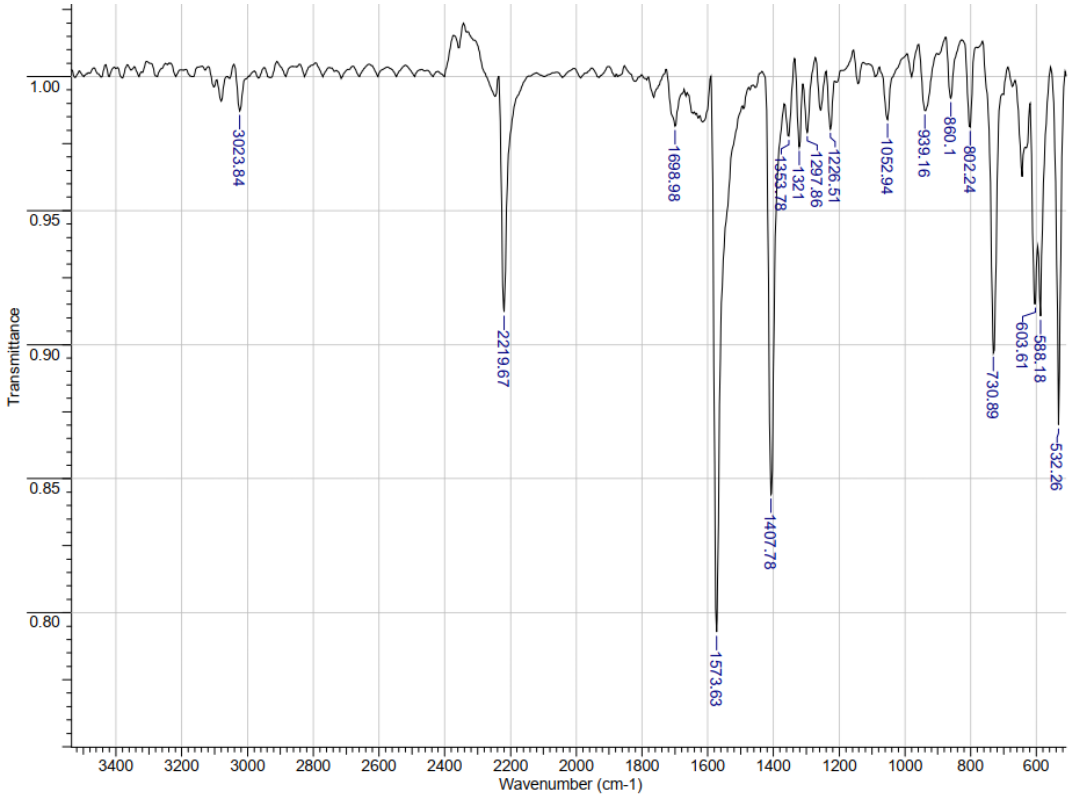


Figure S9. Fourier transform-infrared (FT-IR, cm^{-1}) spectra of **DCVT-BTT.**

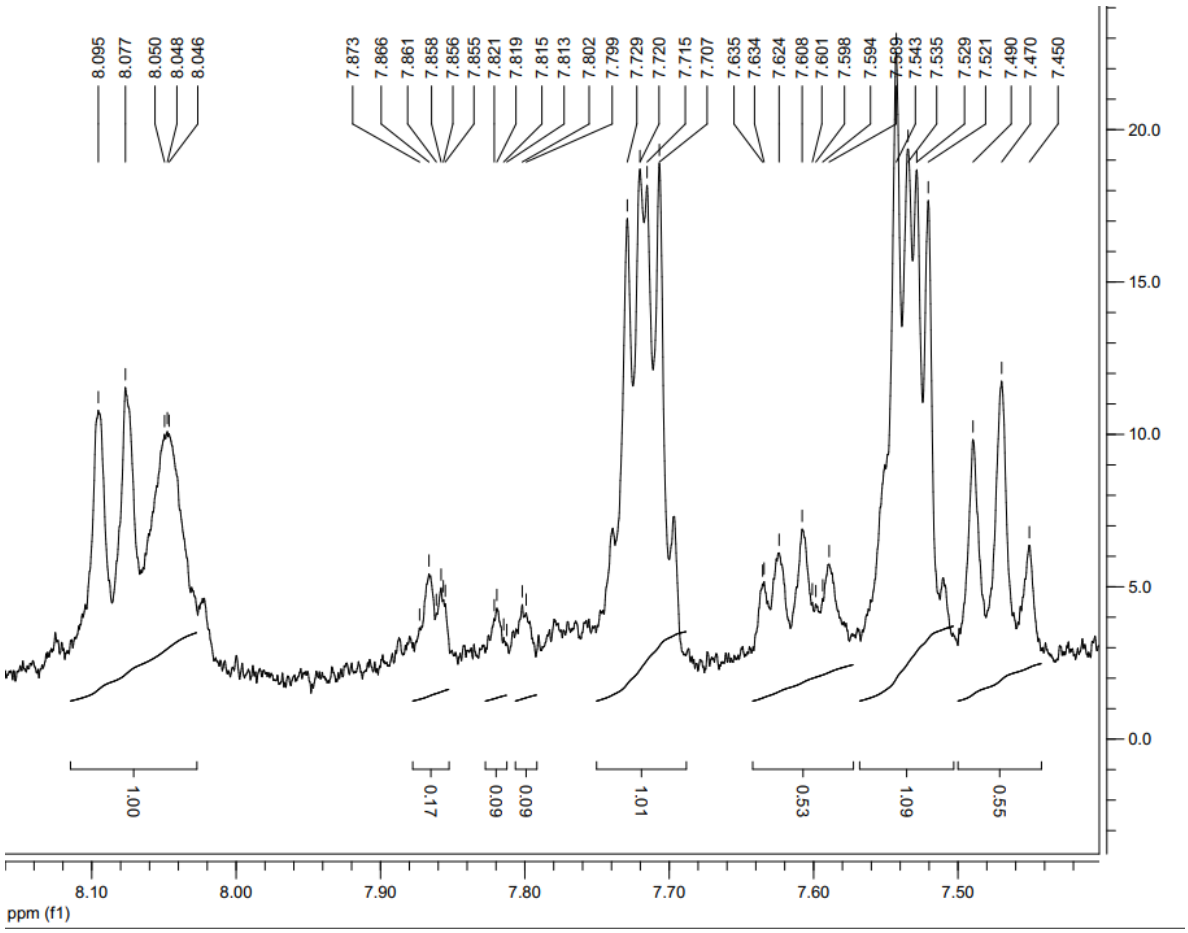


Figure S10. ^{1}H-NMR spectrum of **DCVT-BTT**.