**Figure S1:** Reorganization energies corresponding to structural relaxation of ionic and neutral states of molecules during charge transfer.

**Figure S2:** Vibrational diagram of the highest value of electron reorganization energy in PCNTC-O in the ground (a) and excited states (b) and hole reorganization energy in the ground (c) and excited states (d).

**Figure S3:** Vibrational diagram of the highest value of electron reorganization energy in PCNTC-R in the ground (a) and excited states (b) and hole reorganization energy in the ground (c) and excited states (d).
Figure S4: Mobility of electrons in the (a) xz, (b) yz planes and holes in the (c) xz, (d) yz planes in PCNTC-O cocrystal.

Figure S5: Mobility of electrons in the (a) xz, (b) yz planes and holes in the (c) xz, (d) yz planes in PCNTC-R cocrystal.