SUPPORTING INFORMATION

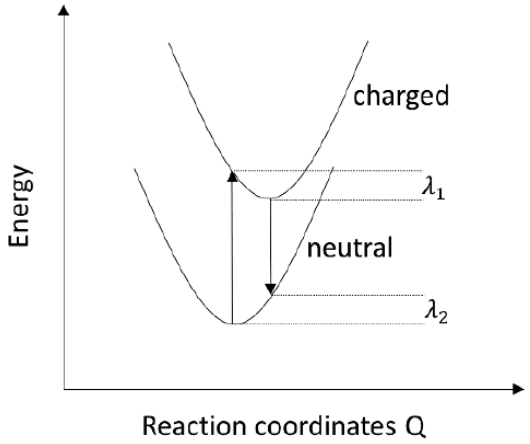

Figure S1: Reorganization energies corresponding to structural relaxation of ionic and neutral states of molecules during charge transfer

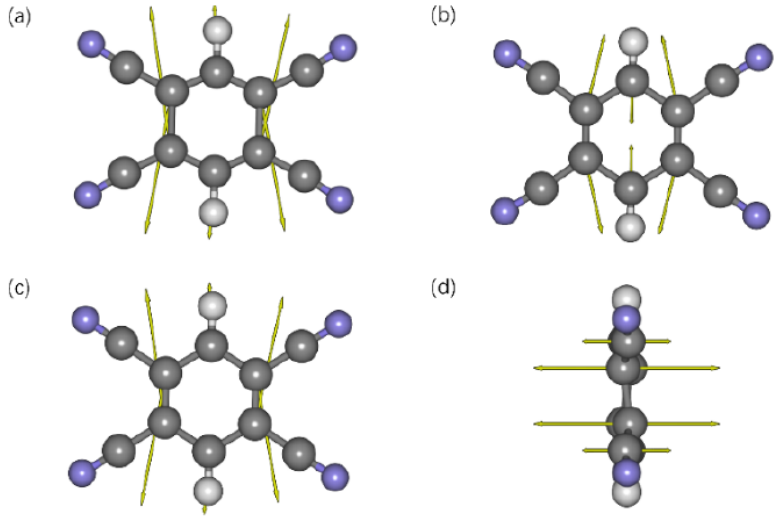

Figure S2: Vibrational diagram of the highest value of electron reorganization energy in PCNTC-O in the ground (**a**) and excited states (**b**) and hole reorganization energy in the ground (**c**) and excited states (**d**).

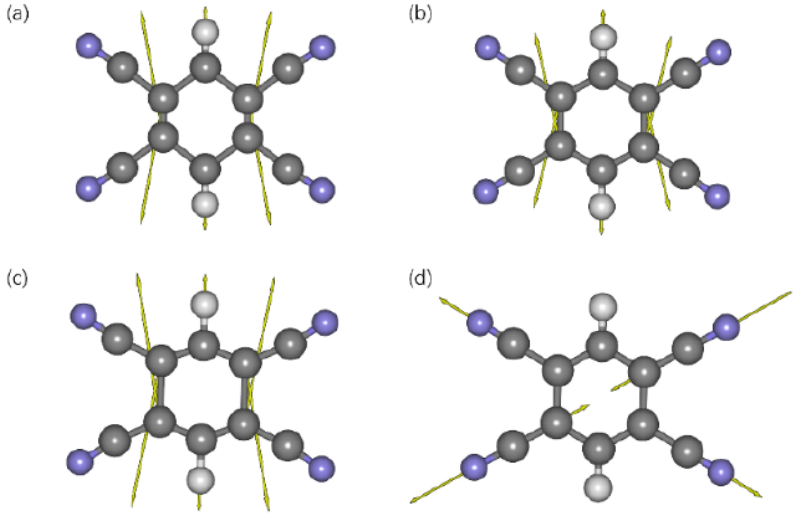

Figure S3: Vibrational diagram of the highest value of electron reorganization energy in PCNTC-R in the ground (**a**) and excited states (**b**) and hole reorganization energy in the ground (**c**) and excited states (**d**).

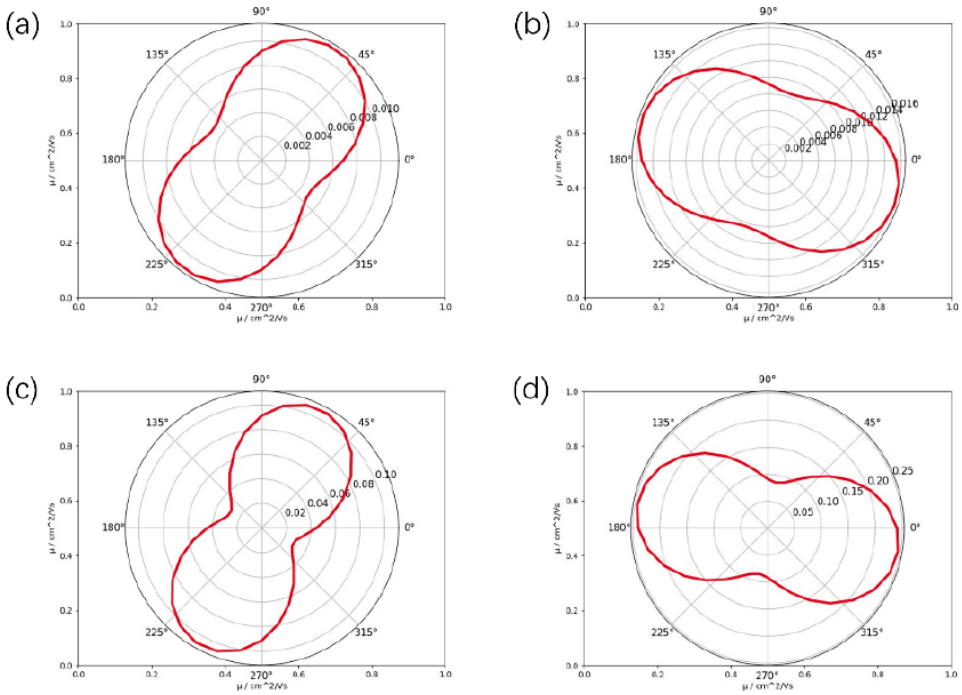

Figure S4: Mobility of electrons in the (**a**) xz, (**b**) yz planes and holes in the (**c**) xz, (**d**) yz planes in PCNTC-O cocrystal.

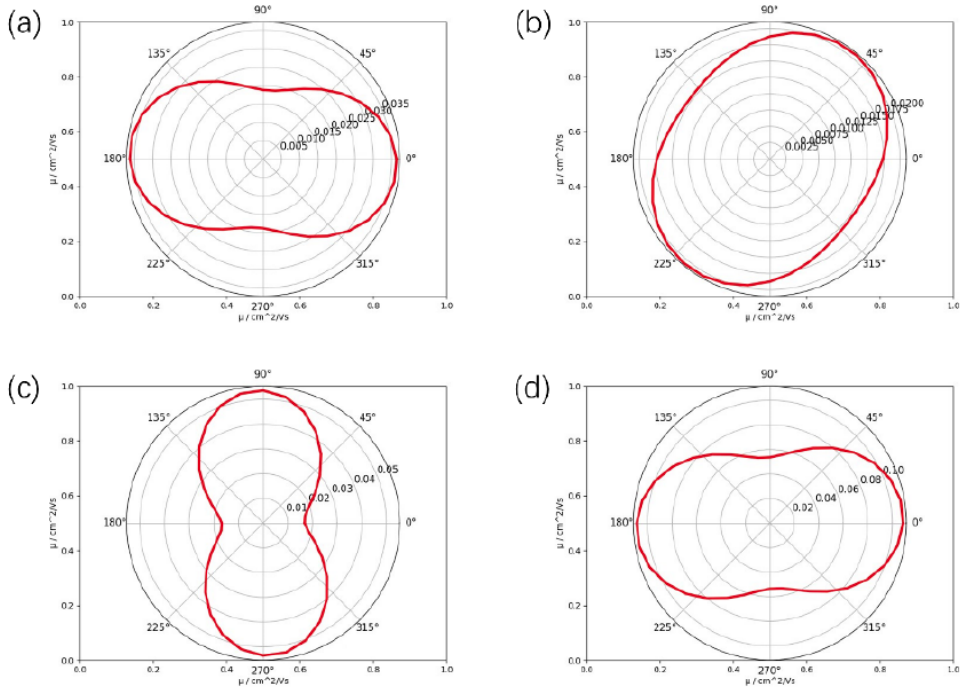

Figure S5: Mobility of electrons in the (**a**) xz, (**b**) yz planes and holes in the (**c**) xz, (**d**) yz planes in PCNTC-R cocrystal.