Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Applied Dispersion Correction

We computed the dimer energies applied Grimme's dispersion corrections.[41] Because we contrasted the energies of the dimer systems estimated almost equal magnitude of the dispersion forces in this paper, the dispersion interaction does not make a difference to the charge-recombination factors and the parameters for Marcus-Hush equation. However, the van der Waals interaction is important in the intermolecular interactions for large π-systems, we obtained the charge-recombination factors and the four-states energies with Grimme's dispersion correction as a function of the acceptor rotation angle or the donor rotation angle.

angle [°]	$\log_{10}(\square\ [s^{-1}])$	(1)	(2)	(3)	(4)
A15	–4.13	–1698.33803	–1698.37914	–1698.32908	–1698.38889
A30	–0.30	–1698.34295	–1698.37973	–1698.33412	–1698.38972
A45	2.20	–1698.34591	–1698.37872	–1698.33766	–1698.38869
A60	0.33	–1698.34704	–1698.37967	–1698.33883	–1698.38939
A75	3.97	–1698.35233	–1698.38114	–1698.34578	–1698.39110

A90		7.73	−1698.35579	−1698.38162	−1698.35009	−1698.39168