Supplementary Material (ESI) for Journal of Materials Chemistry

A Comparative Theoretical Study of Exciton-Dissociation and Charge-Recombination Processes in Oligothiophene/Fullerene and Oligothiophene/Perylenediimide Complexes for Organic Solar Cells

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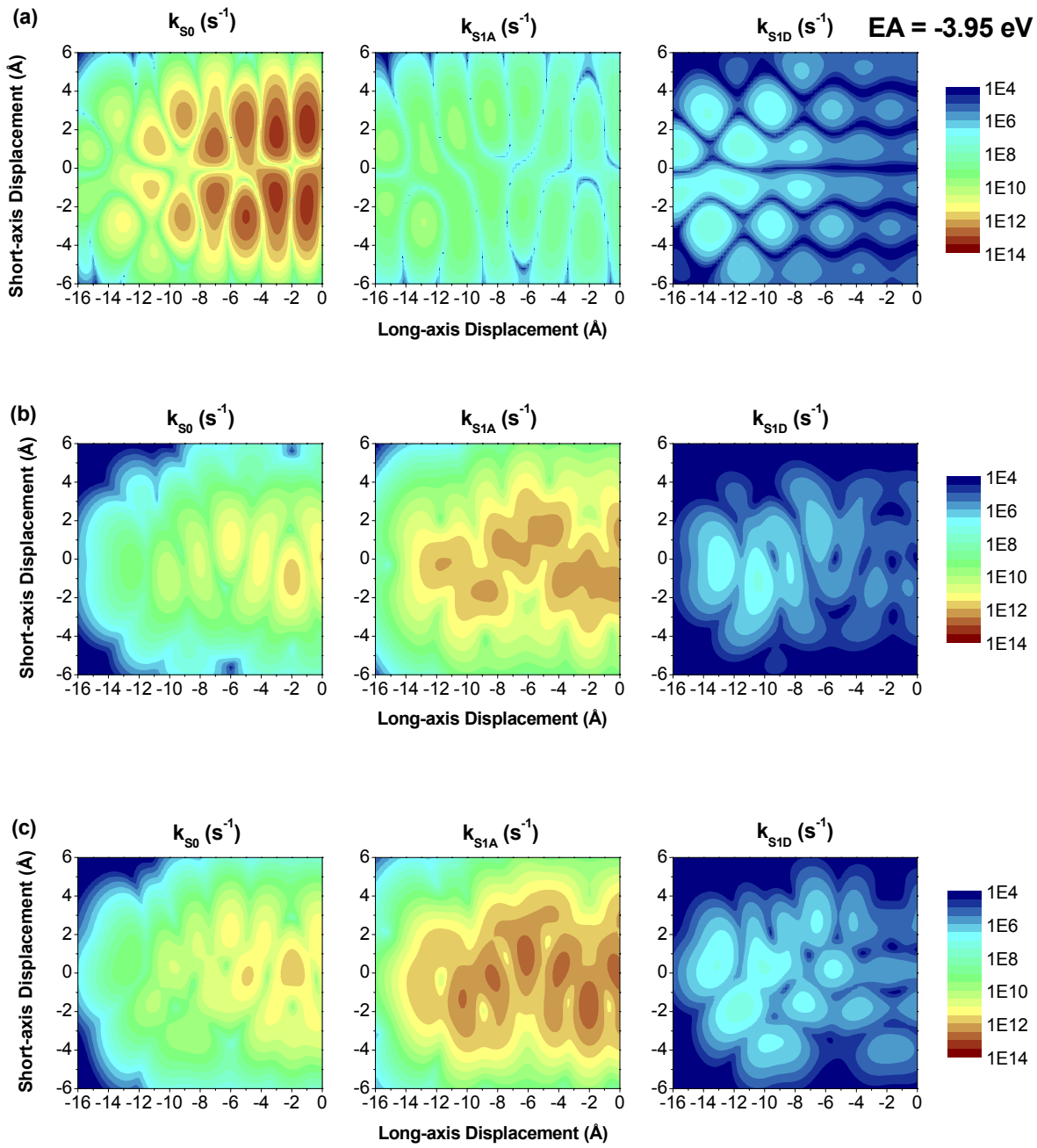
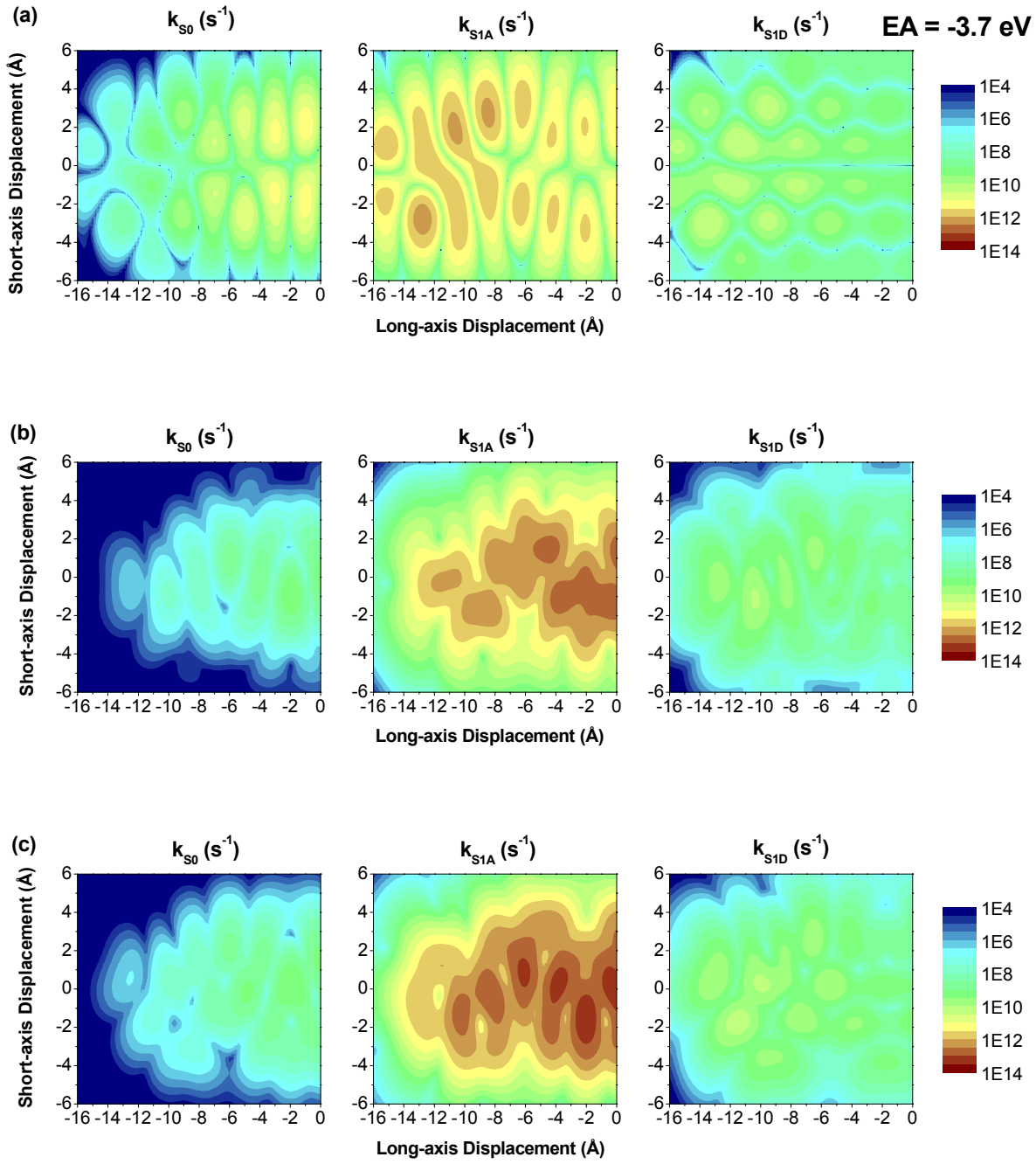
SUPPLEMENTARY INFORMATION:

Calculated electron-transfer rates for configurations a, b, and c using EA values of -3.95, -3.7, and -3.5 eV; calculated Coulomb energies, electronic couplings, and electron-transfer rates for intermolecular orientations generated by rotating the PDI and 6T molecules along the long molecular axis and the central carbon-carbon single bond, respectively.


(a)
k_{S0} (s^{-1})
k_{S1A} (s^{-1})
k_{S1D} (s^{-1})
EA = -3.95 eV
Short-axis Displacement (Å)
Long-axis Displacement (Å)
1E4
1E6
1E8
1E10
1E12
1E14
(b)
k_{S0} (s^{-1})
k_{S1A} (s^{-1})
k_{S1D} (s^{-1})
Short-axis Displacement (Å)
Long-axis Displacement (Å)
1E4
1E6
1E8
1E10
1E12
1E14
(c)
k_{S0} (s^{-1})
k_{S1A} (s^{-1})
k_{S1D} (s^{-1})
Short-axis Displacement (Å)
Long-axis Displacement (Å)
1E4
1E6
1E8
1E10
1E12
1E14


(a)
k_{S0} (s^{-1})
k_{S1A} (s^{-1})
k_{S1D} (s^{-1})
EA = -3.7 eV
Short-axis Displacement (Å)
Long-axis Displacement (Å)
1E4
1E6
1E8
1E10
1E12
1E14
(b)
k_{S0} (s^{-1})
k_{S1A} (s^{-1})
k_{S1D} (s^{-1})
Short-axis Displacement (Å)
Long-axis Displacement (Å)
1E4
1E6
1E8
1E10
1E12
1E14
(c)
k_{S0} (s^{-1})
k_{S1A} (s^{-1})
k_{S1D} (s^{-1})
Short-axis Displacement (Å)
Long-axis Displacement (Å)
1E4
1E6
1E8
1E10
1E12
1E14

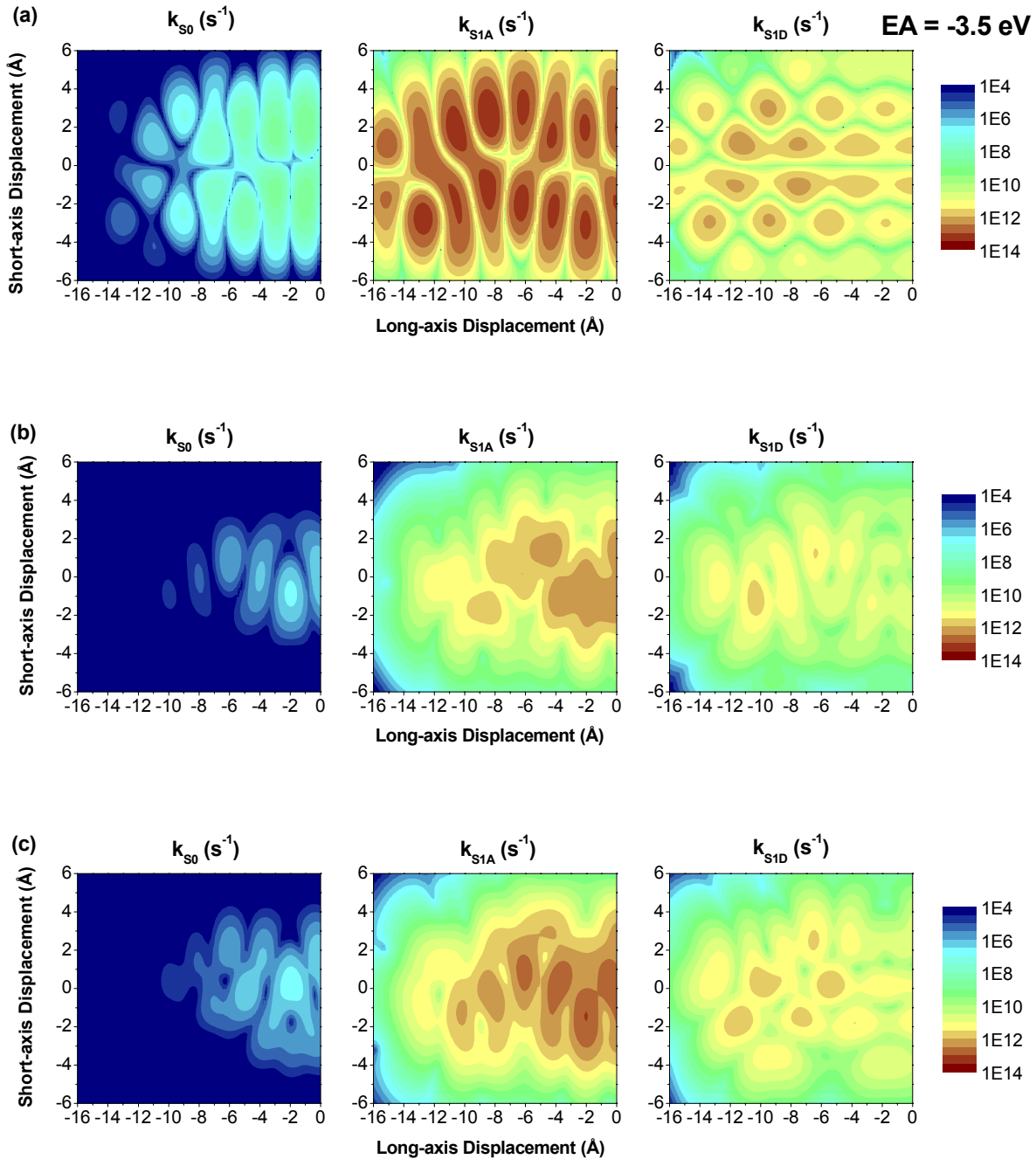


Figure S1. Evolution of the CR rate from the lowest CT state to the ground state (k_{S0}) and of the CT rates from the lowest singlet state on PDI or C_{60} (k_{S1A}) and on 6T (k_{S1D}) to the lowest CT state, as a function of the displacements of 6T along the long and short axes, for complexes 6T/PDI (configuration a) and 6T/C_{60} (configurations b and c). From top to bottom, EA = -3.95, -3.7, and -3.5 eV, respectively.

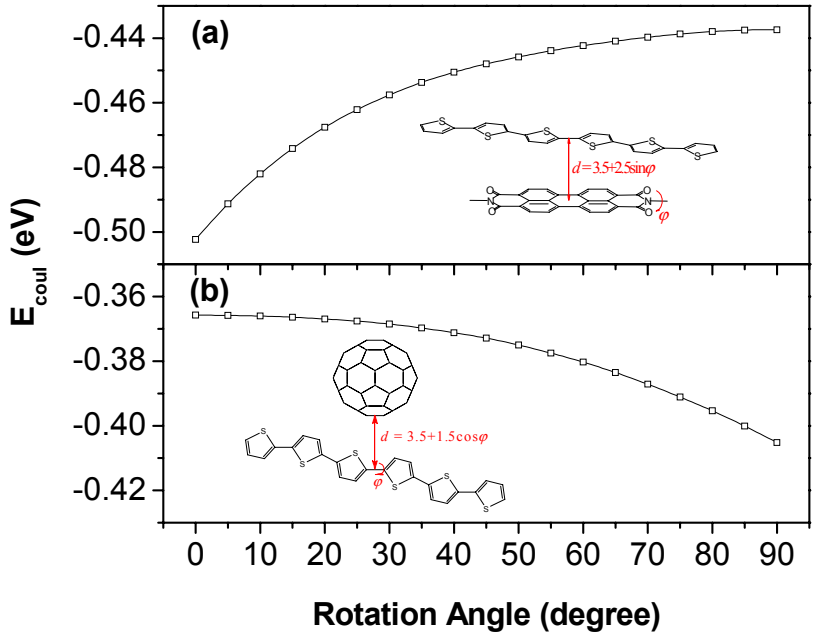


Figure S2. Calculated Coulomb energy of the lowest CT state as a function of the rotation angles along the long axis of PDI and the central carbon-carbon single bond of 6T for complexes 6T/PDI and 6T/C_{60}, respectively.

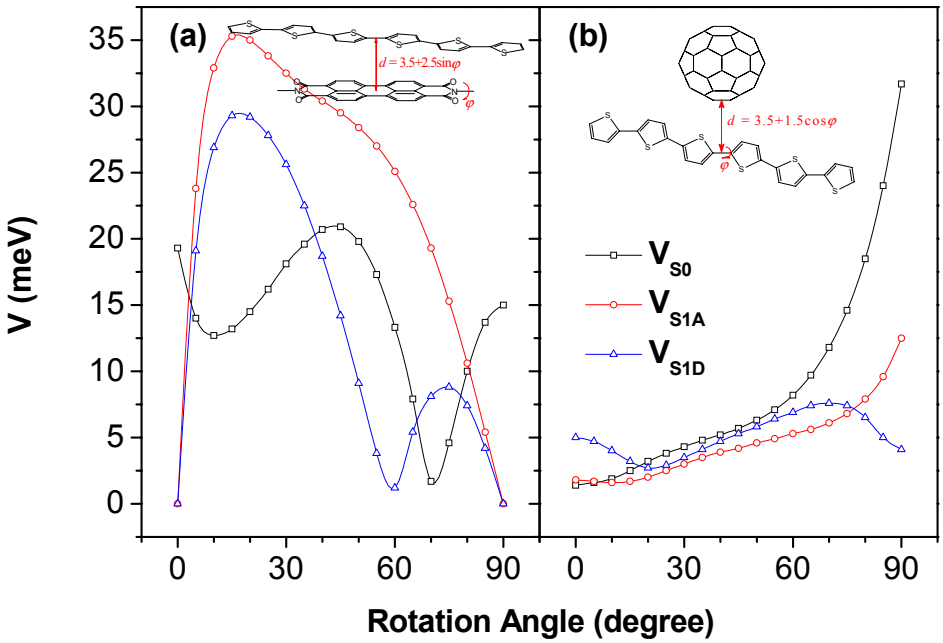
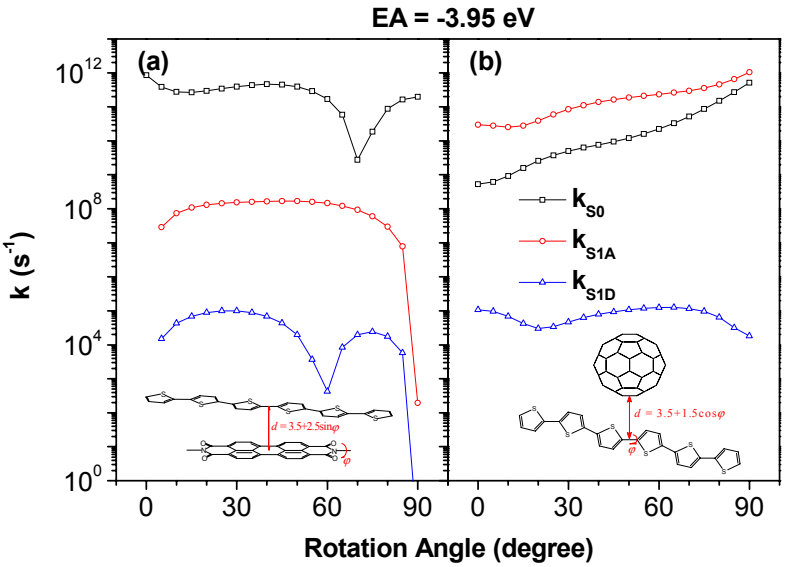
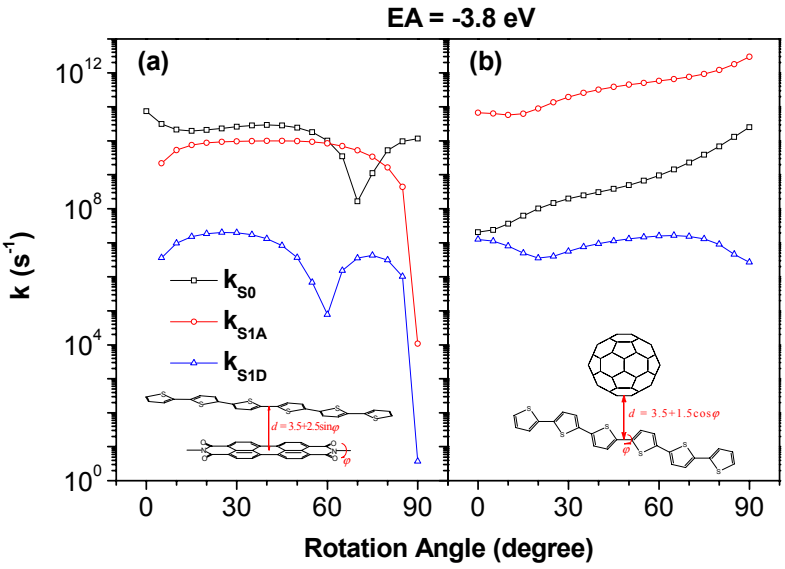


Figure S3. Electronic couplings to the lowest CT state for the ground state (V_{S0}) and for the lowest local-excited singlet state on PDI or C_{60} (V_{S1A}) and on 6T (V_{S1D}), as a function of the rotation angles along the long axis of PDI and the central carbon-carbon single bond of 6T, for complexes 6T/PDI and 6T/C_{60}, respectively.


EA = -3.95 eV
(a)
(b)
k (s-1)
Rotation Angle (degree)
kS0
kS1A
kS1D
d = 3.5+2.5sinφ
d = 3.5+1.5cosφ


EA = -3.8 eV
(a)
(b)
k (s-1)
Rotation Angle (degree)
kS0
kS1A
kS1D
d = 3.5+2.5sinφ
d = 3.5+1.5cosφ

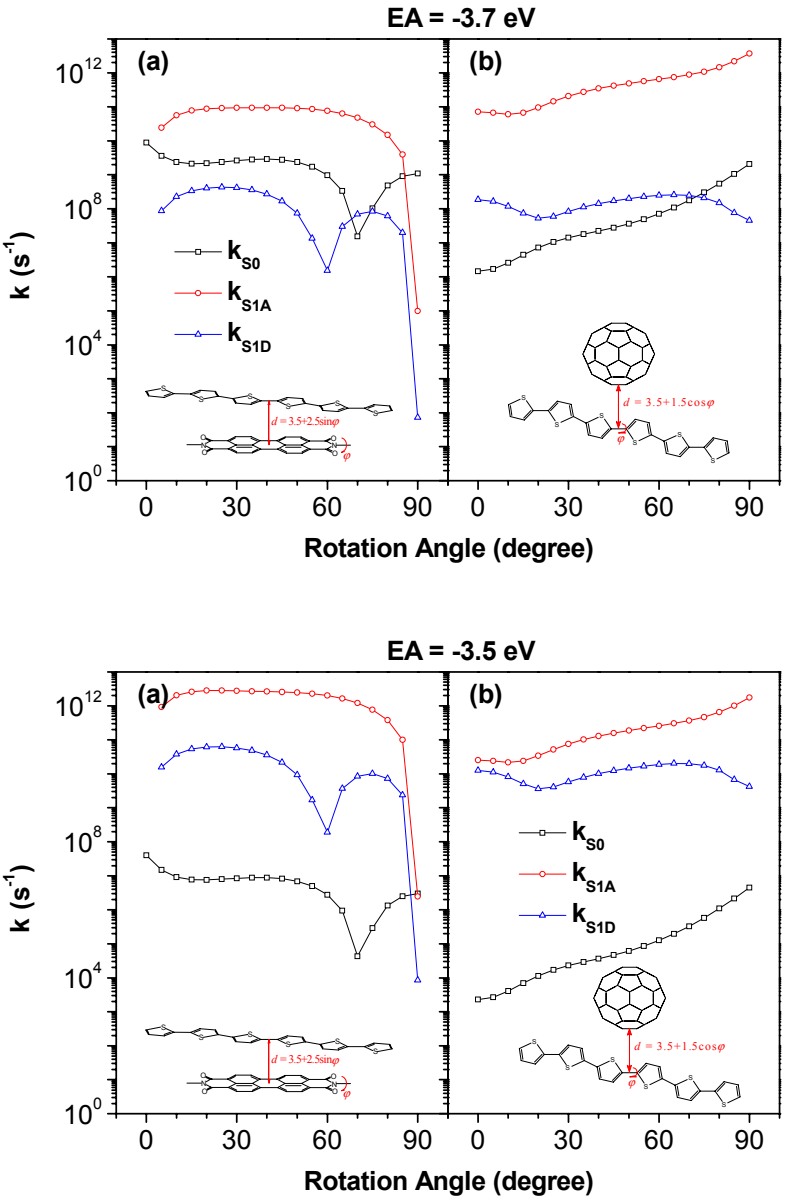


Figure S4. The CR rate from the lowest CT state to the ground state (k_{S0}) and of the CT rates from the lowest local-excited singlet state on PDI or C_{60} (k_{S1A}) and on 6T (k_{S1D}) to the lowest CT state, as a function of the rotation angles along the long axis of PDI and the middle carbon-carbon single bond of 6T, for complexes 6T/PDI and 6T/C_{60}, respectively. From top to bottom, EA = -3.95, -3.8, -3.7, and -3.5 eV, respectively.