Vibronic effects accelerate the intersystem crossing processes of the through-space charge transfer states in the triptycene bridged acridine–triazine donor–acceptor molecule TpAT-tFFO

Jeremy M. Kaminski, Angela Rodríguez-Serrano, Fabian Dinkelbach, Hector Miranda-Salinas, Andrew P. Monkman and Christel M. Marian

Department of Theoretical and Computational Chemistry, Heinrich-Heine-University Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany, E-mail: christel.marian@hhu.de

OEM research group, Dept. of Physics, Durham University, Durham, United Kingdom, DH1 3LE, E-mail: a.p.monkman@durham.ac.uk

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Figure S1: Vibrational mode 1 at the $S_0$($\text{Me}$→$\text{N}$) geometry in vacuo.

Figure S2: Scan along vibrational mode 1: (a) Relative DFT/MRCI ground state energy differences w.r.t. the undistorted $S_0$($\text{Me}$→$\text{N}$) geometry, (b) DFT/MRCI excitation energies w.r.t. the ground state energy at the undistorted $S_0$($\text{Me}$→$\text{N}$) geometry, (c) oscillator strengths for the $S_0$ → $S_1$ and $S_0$ → $S_2$ absorption processes, (d) sum of the squared SOCMEs for transitions discussed in this study.
Table S1: DFT/MRCI-R2016 vertical excitation energies and characterization of low-lying singlet and triplet states of TpAT-tFFO calculated at the $S_0$(Me→N) geometry.

| State | ∆E [eV] | f(L) | Transition | Character | % | µ [D] |
|-------|---------|------|------------|-----------|---|-------|
| $S_0$ | 0.02    |      | GS         |           | 96| 0.61  |
| $S_1$ | 3.25    | 0.005| H → L      | CT        | 68| 16.24 |
|       |         |      | H → L+1    |           | 21|       |
| $S_2$ | 3.30    | 0.007| H → L+1    | CT′       | 67| 16.42 |
|       |         |      | H → L      |           | 21|       |
| $T_1$ | 3.14    |      | H → L      | CT        | 70| 15.37 |
|       |         |      | H → L+1    |           | 16|       |
| $T_2$ | 3.19    |      | H → L+1    | CT′       | 67| 14.43 |
|       |         |      | H → L      |           | 14|       |
| $T_3$ | 3.24    |      | H-5 → L    | LE        | 25| 0.39  |
|       |         |      | H-6 → L    |           | 13|       |

Figure S3: BH-LYP molecular orbitals (cutoff 0.03) at the $S_0$(Me→N) geometry in vacuo.
Figure S4: Difference densities (± 0.001) of the excited states at the S₀(Me→N) geometry in vacuo. Areas losing electron density in comparison to the electronic ground state are shown in red, areas gaining electron density in yellow.

Figure S5: Fragment-based analysis for the vertical singlet and triplet state DFT/MRCI-R2016 wavefunctions at the S₀(Me→N) geometry in vacuo.
Table S2: DFT/MRCI-R2016 vertical excitation energies and characterization of low-lying singlet and triplet states of TpAT-tFFO calculated at the $S_0$(Me→Ph) geometry.

| State | $\Delta E$ [eV] | $f(L)$ | Transition | Character | %  | $\mu$ [D] |
|-------|------------------|--------|------------|-----------|----|-----------|
| $S_0$ | 0.00             |        | GS         |           | 96 | 0.65      |
| $S_1$ | 3.27             | 0.002  | H $\rightarrow$ L+1 | CT       | 49 | 16.72     |
|       |                   |        | H $\rightarrow$ L  |           | 39 |           |
| $S_2$ | 3.33             | 0.000  | H $\rightarrow$ L  | CT$'$    | 48 | 18.50     |
|       |                   |        | H $\rightarrow$ L+1 |           | 39 |           |
| $T_1$ | 3.17             |        | H $\rightarrow$ L  | CT       | 71 | 14.41     |
| $T_2$ | 3.17             |        | H $\rightarrow$ L+1 | CT$'$    | 56 | 9.93      |
|       |                   |        | H-5 $\rightarrow$ L+1 |       | 10 |           |
| $T_3$ | 3.29             |        | H $\rightarrow$ L+1 | LE/CT    | 29 | 6.93      |
|       |                   |        | H-6 $\rightarrow$ L  |           | 17 |           |
|       |                   |        | H-4 $\rightarrow$ L  |           | 10 |           |

Figure S6: BH-LYP molecular orbitals (cutoff 0.03) at the $S_0$(Me→Ph) geometry in vacuo.
Figure S7: Difference densities (± 0.001) of the excited states at the S_0(Me→Ph) geometry in vacuo. Areas losing electron density in comparison to the electronic ground state are shown in red, areas gaining electron density in yellow.

Figure S8: Fragment-based analysis for the vertical singlet and triplet state DFT/MRCI-R2016 wavefunctions at the S_0(Me→Ph) geometry in vacuo.
Table S3: DFT/MRCI-R2016 vertical excitation energies and characterization of low-lying singlet and triplet states of TpAT-tFFO calculated at the $S_1$ geometry.

| State | $\Delta E$ [eV] | Transition | Character | % | $\mu$ [D] |
|-------|-----------------|------------|-----------|---|------------|
| $S_0$ | 0.41            | GS         |           | 96| 0.45       |
| $S_1$ | 2.97            | H $\rightarrow$ L | CT        | 90| 15.65      |
| $S_2$ | 3.51            | H $\rightarrow$ L+1 | CT'       | 88| 15.65      |
| $T_1$ | 2.89            | H $\rightarrow$ L | CT        | 89| 15.40      |
| $T_2$ | 3.29            | H-5 $\rightarrow$ L | LE        | 25| 1.49       |
|       |                 | H-2 $\rightarrow$ L |          | 15|            |
|       |                 | H-9 $\rightarrow$ L |          | 14|            |
| $T_2$ | 3.42            | H $\rightarrow$ L+1 | CT'       | 83| 14.41      |

Figure S9: BH-LYP molecular orbitals (cutoff 0.03) at the $S_1$ geometry in vacuo.
Figure S10: Difference densities (± 0.001) of the excited states at the $S_1$ geometry in vacuo. Areas losing electron density in comparison to the electronic ground state are shown in red, areas gaining electron density in yellow.

Figure S11: Fragment-based analysis for the vertical singlet and triplet state DFT/MRCI-R2016 wavefunctions at the $S_1$ geometry in vacuo.
Table S4: DFT/MRCI-R2016 vertical excitation energies and characterization of low-lying singlet and triplet states of TpAT-tFFO calculated at the S₂ geometry.

| State | ∆E [eV] | Transition | Character | % | μ [D] |
|-------|---------|------------|-----------|---|-------|
| S₀    | 0.38    | GS         |           | 96 | 1.08  |
| S₂    | 2.98    | H → L      | CT'       | 88 | 18.39 |
| S₁    | 3.47    | H → L+1    | CT        | 88 | 14.92 |
| T₂    | 2.86    | H → L      | CT'       | 83 | 16.77 |
| T₃    | 3.30    | H-6 → L    | LE        | 32 | 2.00  |
|       |         | H-9 → L    |           | 16 |       |
| T₁    | 3.38    | H → L+1    | CT        | 76 | 12.63 |

Figure S12: BH-LYP molecular orbitals (cutoff 0.03) at the S₂ geometry in vacuo.
Figure S13: Difference densities ($\pm$ 0.001) of the excited states at the $S_2$ geometry in vacuo. Areas losing electron density in comparison to the electronic ground state are shown in red, areas gaining electron density in yellow.

Figure S14: Fragment-based analysis for the vertical singlet and triplet state DFT/MRCI-R2016 wavefunctions at the $S_2$ geometry in vacuo.
Table S5: DFT/MRCI-R2016 vertical excitation energies and characterization of low-lying singlet and triplet states of TpAT-tFFO calculated at the T₁ geometry.

| State | ΔE [eV] | Transition | Character | % | μ [D] |
|-------|---------|------------|-----------|---|-------|
| S₀    | 0.40    | GS         |           | 96 | 0.43  |
| S₁    | 2.96    | H → L      | CT        | 90 | 15.40 |
| S₂    | 3.48    | H → L+1    | CT’       | 88 | 15.45 |
| T₁    | 2.88    | H → L      | CT        | 89 | 15.11 |
| T₃    | 3.29    | H-5 → L    | LE        | 27 | 1.51  |
|       |         | H-2 → L    |           | 20 |       |
|       |         | H-9 → L    |           | 14 |       |
| T₂    | 3.38    | H → L+1    | CT’       | 83 | 14.18 |

(a) HOMO-9  (b) HOMO-5  (c) HOMO-2  
(d) HOMO  (e) LUMO  (f) LUMO+1

Figure S15: BH-LYP molecular orbitals (cutoff 0.03) at the T₁ geometry in vacuo.
Figure S16: Difference densities (± 0.001) of the excited states at the T₁ geometry in vacuo. Areas losing electron density in comparison to the electronic ground state are shown in red, areas gaining electron density in yellow.

Figure S17: Fragment-based analysis for the vertical singlet and triplet state DFT/MRCI-R2016 wavefunctions at the T₁ geometry in vacuo.
Table S6: DFT/MRCI-R2016 vertical excitation energies and characterization of low-lying singlet and triplet states of TpAT-tFFo calculated at the CI geometry.

| State | ∆E [eV] | Transition | Character | %  | μ [D] |
|-------|---------|------------|-----------|----|-------|
| S<sub>0</sub> | 0.24 | GS | 96 | 0.87 |
| S<sub>2</sub> | 3.08 | H → L+1 | CT | 67 | 14.54 |
|        |       | H → L   |   | 21 |
| S<sub>1</sub> | 3.10 | H → L   | CT′ | 67 | 16.49 |
|        |       | H → L+1 |   | 22 |
| T<sub>2</sub> | 2.99 | H → L+1 | CT | 69 | 13.80 |
|        |       | H → L   |   | 17 |
| T<sub>1</sub> | 2.99 | H → L   | CT′ | 67 | 15.58 |
|        |       | H → L+1 |   | 18 |
| T<sub>3</sub> | 3.36 | H-5 → L+1 | LE | 25 | 0.33 |
|        |       | H-6 → L |   | 20 |
|        |       | H-2 → L+1 |   | 13 |

(a) HOMO-6  
(b) HOMO-5  
(c) HOMO-2  
(d) HOMO  
(e) LUMO  
(f) LUMO+1

Figure S18: BH-LYP molecular orbitals (cutoff 0.03) at the CI geometry in vacuo.
Figure S19: Difference densities (± 0.001) of the excited states at the CI geometry in vacuo. Areas losing electron density in comparison to the electronic ground state are shown in red, areas gaining electron density in yellow.

Figure S20: Fragment-based analysis for the vertical singlet and triplet state DFT/MRCI-R2016 wavefunctions at the CI geometry in vacuo.
Table S7: DFT/MRCI-R2016 vertical excitation energies and characterization of low-lying singlet and triplet states of TpAT-tFFO calculated at the T\textsubscript{2} geometry.

| State | \(\Delta E\) [eV] | Transition | Character | % | \(\mu\) [D] |
|-------|-------------------|------------|-----------|---|-----------|
| \(S_0\) | 0.39 | GS | | 96 | 1.00 |
| \(S_2\) | 2.97 | H \rightarrow L | CT' | 88 | 17.77 |
| \(S_1\) | 3.45 | H \rightarrow L+1 | CT | 88 | 14.47 |
| \(T_2\) | 2.83 | H \rightarrow L | CT' | 82 | 15.77 |
| \(T_1'\) | 3.32 | H \rightarrow L+1 | LE/CT | 30 | 4.78 |
| | | H-6 \rightarrow L | | 20 | |
| | | H-9 \rightarrow L | | 10 | |
| \(T_1''\) | 3.36 | H \rightarrow L+1 | CT/LE | 53 | 8.62 |
| | | H-6 \rightarrow L | | 12 | |
| | | H-9 \rightarrow L | | 7 | |

Figure S21: BH-LYP molecular orbitals (cutoff 0.03) at the T\textsubscript{2} geometry in vacuo.
Figure S22: Difference densities (± 0.001) of the excited states at the T₂ geometry in vacuo. Areas losing electron density in comparison to the electronic ground state are shown in red, areas gaining electron density in yellow.

Figure S23: Fragment-based analysis for the vertical singlet and triplet state DFT/MRCI-R2016 wavefunctions at the T₂ geometry in vacuo.
Table S8: DFT/MRCI-R2016 vertical excitation energies and characterization of low-lying singlet and triplet states of TpAT-tFFO calculated at the T₃ geometry.

| State | ∆E [eV] | Transition | Character | %    | μ [D] |
|-------|---------|------------|-----------|------|-------|
| S₀    | 0.32    | GS         |           | 96   | 0.46  |
| S₁    | 3.17    | H → L      | CT        | 89   | 15.88 |
| S₂    | 3.58    | H → L+1    | CT'       | 87   | 16.00 |
| T₃    | 2.99    | H-2 → L    | LE        | 35   | 2.26  |
|       |         | H-4 → L    |           | 20   |       |
| T₁    | 3.08    | H → L      | CT        | 78   | 14.09 |
| T₂    | 3.44    | H → L+1    | CT'       | 78   | 13.50 |

Figure S24: BH-LYP molecular orbitals (cutoff 0.03) at the T₃ geometry in vacuo.
Figure S25: Difference densities (± 0.001) of the excited states at the T₃ geometry in vacuo. Areas losing electron density in comparison to the electronic ground state are shown in red, areas gaining electron density in yellow.

Figure S26: Fragment-based analysis for the vertical singlet and triplet state DFT/MRCI-R2016 wavefunctions at the T₃ geometry in vacuo.
Figure S27: DFT/MRCI excitation energies ($\Delta E$, eV) at optimized geometries. CI designates the conical intersection between the $T_1$ and $T_2$ PESs. The $S_0$ energy of the slightly more stable (Me→Ph) conformer has been chosen as common origin.
Figure S28: DFT/MRCI energy profiles along linear interpolated pathways (LIPs) between target electronic state minima. Dashed lines correspond to triplet state PESs while solid lines correspond to singlet states.
Figure S29: Scan along vibrational mode 9: (a) Relative DFT/MRCI ground state energy differences w.r.t. the undistorted $S_0$(Me$\rightarrow$N) geometry, (b) DFT/MRCI excitation energies w.r.t. the ground state energy at the undistorted $S_0$(Me$\rightarrow$N) geometry, (c) oscillator strengths for the $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ absorption processes, (d) sum of the squared SOCMEs for transitions discussed in this study.
Figure S30: Scan along vibrational mode 12: (a) Relative DFT/MRCI ground state energy differences w.r.t. the undistorted $S_0(\text{Me}$→$N)$ geometry, (b) DFT/MRCI excitation energies w.r.t. the ground state energy at the undistorted $S_0(\text{Me}$→$N)$ geometry, (c) oscillator strengths for the $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ absorption processes, (d) sum of the squared SOCMEs for transitions discussed in this study.
Table S9: PBE0/def2-SV(P) TDDFT vertical excitation energies (including TDA approximation for triplet states) and characterization of low-lying singlet and triplet states of TpAT-tFFO calculated at the $S_0$(Me→N) geometry.

| State | $\Delta E$ [eV] | Transition | Character | % |
|-------|----------------|------------|-----------|---|
| $S_1$ | 2.78           | $H \rightarrow L$ | CT($A \rightarrow T$) | 89 |
|       |                 | $H \rightarrow L+1$ | CT($A \rightarrow T/\text{Tp}$) | 11 |
| $S_2$ | 2.83           | $H \rightarrow L+1$ | CT($A \rightarrow T/\text{Tp}$) | 89 |
|       |                 | $H \rightarrow L$ | CT($A \rightarrow T$) | 11 |
| $T_1$ | 2.76           | $H \rightarrow L$ | CT($A \rightarrow T$) | 91 |
| $T_2$ | 2.81           | $H \rightarrow L+1$ | CT($A \rightarrow T/\text{Tp}$) | 91 |
| $T_3$ | 3.33           | $H-6\rightarrow L$ | LE($T/\text{Tp}$) | 22 |
|       |                 | $H-5\rightarrow L$ | LE($T/\text{Tp}$) | 19 |
|       |                 | $H-5\rightarrow L+1$ | LE($T/\text{Tp}$) | 11 |

Figure S31: PBE0 molecular orbitals (cutoff 0.03) at the $S_0$(Me→N) geometry in vacuo.
Table S10: LC-ωPBE/6-31+G(d) (ω = 0.1664) TDDFT vertical excitation energies (including TDA approximation for triplet states) and characterization of low-lying singlet and triplet states of TpAT-tFFO calculated at the S0(Me→N) geometry.

| State | ∆E [eV] | Transition | Character | %   |
|-------|---------|------------|-----------|-----|
| S₁    | 2.96    | H →L      | CT (A→T)  | 56  |
|       |         | H →L+1    | CT (A→T/TP) | 42  |
| S₂    | 3.03    | H →L+1    | CT (A→T/TP) | 55  |
|       |         | H →L      | CT (A→T)  | 40  |
| T₁    | 2.93    | H →L      | CT (A→T)  | 62  |
|       |         | H →L+1    | CT (A→T/TP) | 34  |
| T₂    | 3.00    | H →L+1    | CT (A→T/TP) | 61  |
|       |         | H →L      | CT (A→T)  | 32  |
| T₃    | 3.33    | H-5→L    | LE(A/TP)  | 21  |
|       |         | H-6→L    | LE(A/TP)  | 20  |

Figure S32: LC-ωPBE (ω = 0.1664) molecular orbitals (cutoff 0.03) at the S0(Me→N) geometry in vacuo.
Table S11: PBE0/def2-SV(P) TDDFT vertical excitation energies (including TDA approximation for triplet states) and characterization of low-lying singlet and triplet states of **TpAT-tFFO** calculated at the S₀(Me→Ph) geometry.

| State | ∆E [eV] | Transition | Character | %  |
|-------|---------|------------|-----------|----|
| S₁    | 2.83    | H →L+1    | CT(A→T/Tp) | 53 |
|       |         | H →L      | CT(A→T)   | 46 |
| S₂    | 2.87    | H →L      | CT(A→T)   | 53 |
|       |         | H →L+1    | CT(A→T/Tp)| 46 |
| T₁    | 2.81    | H →L      | CT(A→T)   | 63 |
|       |         | H →L+1    | CT(A→T/Tp)| 35 |
| T₂    | 2.84    | H →L+1    | CT(A→T/Tp)| 63 |
|       |         | H →L      | CT(A→T)   | 34 |
| T₃    | 3.34    | H-6→L     | LE(A/Tp)  | 30 |
|       |         | H-5→L+1   | LE(A/Tp)  | 30 |
|       |         | H-4→L     | CT(A→T)   | 10 |

Figure S33: PBE0 molecular orbitals (cutoff 0.03) at the S₀(Me→Ph) geometry in vacuo.

(a) HOMO-6  
(b) HOMO-5  
(c) HOMO-4  
(d) HOMO  
(e) LUMO  
(f) LUMO+1
Table S12: LC-ωPBE/6-31+G(d) (ω = 0.1664) TDDFT vertical excitation energies (including TDA approximation for triplet states) and characterization of low-lying singlet and triplet states of TpAT-tFFO calculated at the S0(Me→Ph) geometry.

| State | ∆E [eV] | Transition | Character | %  |
|-------|---------|------------|-----------|----|
| S1    | 3.01    | H →L+1    | CT (A→T/Tp) | 55 |
|       |         | H →L      | CT (A→T)   | 41 |
| S2    | 3.12    | H →L      | CT (A→T)   | 52 |
|       |         | H →L+1    | CT (A→T/Tp)| 41 |
| T1    | 2.99    | H →L      | CT (A→T)   | 47 |
|       |         | H →L+1    | CT (A→T/Tp)| 46 |
| T2    | 3.07    | H →L+1    | CT (A→T/Tp)| 45 |
|       |         | H →L      | CT (A→T)   | 40 |
| T3    | 3.35    | H-5→L+1   | LE(A/Tp)   | 28 |
|       |         | H-6→L     | LE(A/Tp)   | 21 |

Figure S34: LC-ωPBE (ω = 0.1664) molecular orbitals (cutoff 0.03) at the S0(Me→Ph) geometry in vacuo.
Table S13: PBE0/def2-SV(P) Adiabatic TDDFT excitation energies of low-lying singlet and triplet states of TpAT-tFFO (including TDA approximation for triplet states). Zero-point vibrational energy corrections were computed at the (TD)DFT level of theory.

| State | ∆E [eV] | Transition | Character | %  | ZPVE |
|-------|---------|------------|-----------|----|------|
| S₁    | 2.47    | H →L       | CT        | 99.8 | -0.11 |
| S₂    | 2.49    | H →L+1     | CT'       | 99.1 | -0.12 |
| T₁    | 2.45    | H →L       | CT        | 99.4 | -0.11 |
| T₂    | 2.45    | H →L+1     | CT'       | 97.3 | -0.12 |
| T₃    | 3.09    | H-2→L      | LE        | 38.3 | +0.04 |

Table S14: FC rate constants (direct ISC/rISC, s⁻¹) between low-lying singlet and triplet state minima of TpAT-tFFO. Values smaller than 1 s⁻¹ have been omitted.

| State          | ISC (20 K) | ISC (300 K) | rISC (20 K) | rISC (300 K) |
|----------------|------------|-------------|-------------|--------------|
| S₁(CT)~~~T₁(CT)| 9.8×10⁴   | 8.7×10⁴     | —           | 5.2×10³      |
| S₁(CT)~~~T₂(CT')| 3.0×10²   | 2.9×10⁵     | —           | 9.1×10²      |
| S₁(CT)~~~T₃(LE)| —         | 9.5×10⁴     | 5.0×10⁶     | 2.2×10⁶      |
| S₂(CT')~~~T₁(CT)| —         | 8.6×10³     | —           | 4.2×10³      |
| S₂(CT')~~~T₂(CT')| 1.3×10⁵ | 5.3×10⁵     | —           | 2.6×10⁴      |
| S₂(CT')~~~T₃(LE)| —         | 3.5×10⁴     | 7.3×10⁴     | 1.2×10⁵      |
Figure S35: Important coupling vibrational normal modes calculated at the $S_1$ minimum of $\text{TpAT-tFFO}$. 
Figure S36: Important coupling vibrational normal modes calculated at the S$_2$ minimum of TpAT-tFFO.
Figure S37: Important coupling vibrational normal modes calculated at the T₁ minimum of TpAT-tFFO.
Figure S38: Important coupling vibrational normal modes calculated at the T₂ minimum of TpAT-ťFFO.
Figure S39: Important coupling vibrational normal modes calculated at the T₃ minimum of TpAT-tFFO.
Table S15: FC-HT rate constants (direct and vibronic ISC, s$^{-1}$) at 300 K with shifted potentials in the range of 20 and 170 meV between low-lying singlet and triplet state minima of TpAT-tFFO.

| State          | 20 meV | 50 meV | 80 meV | 110 meV | 140 meV | 170 meV |
|----------------|--------|--------|--------|---------|---------|---------|
| $S_1$(CT)$\rightarrow T_1$(CT) | $4.2\times10^6$ | $1.4\times10^6$ | $1.1\times10^6$ | $7.4\times10^5$ | $9.6\times10^5$ | $8.9\times10^5$ |
| $S_1$(CT)$\rightarrow T_2$(CT$'$) | $6.0\times10^4$ | $1.0\times10^5$ | $1.6\times10^5$ | $2.4\times10^5$ | $3.4\times10^5$ | $4.6\times10^5$ |
| $S_1$(CT)$\rightarrow T_3$(LE) | $8.6\times10^5$ | $4.5\times10^5$ | $2.1\times10^5$ | $9.0\times10^4$ | $3.6\times10^4$ | $1.4\times10^4$ |
| $S_2$(CT$'$)$\rightarrow T_1$(CT) | $4.1\times10^4$ | $6.9\times10^4$ | $1.1\times10^5$ | $1.6\times10^5$ | $2.3\times10^5$ | $3.2\times10^5$ |
| $S_2$(CT$'$)$\rightarrow T_2$(CT$'$) | $2.8\times10^7$ | $9.8\times10^6$ | $5.9\times10^6$ | $1.1\times10^7$ | $7.3\times10^6$ | $4.3\times10^6$ |
| $S_2$(CT$'$)$\rightarrow T_3$(LE) | $8.8\times10^4$ | $4.8\times10^4$ | $2.4\times10^4$ | $1.1\times10^4$ | $3.8\times10^3$ | $5.3\times10^2$ |

Table S16: FC-HT rate constants (direct and vibronic rISC, s$^{-1}$) at 300 K with shifted potentials in the range of 20 and 170 meV between low-lying singlet and triplet state minima of TpAT-tFFO.

| State            | 20 meV | 50 meV | 80 meV | 110 meV | 140 meV | 170 meV |
|------------------|--------|--------|--------|---------|---------|---------|
| $S_1$(CT)$\leftarrow T_1$(CT) | $2.6\times10^6$ | $3.6\times10^6$ | $5.8\times10^4$ | $1.5\times10^4$ | $5.3\times10^3$ | $1.7\times10^3$ |
| $S_1$(CT)$\leftarrow T_3$(CT$'$) | $3.9\times10^4$ | $2.1\times10^4$ | $1.0\times10^4$ | $4.6\times10^3$ | $2.0\times10^3$ | $8.6\times10^2$ |
| $S_1$(CT)$\leftarrow T_3$(LE) | $1.4\times10^6$ | $2.2\times10^6$ | $3.3\times10^6$ | $4.6\times10^6$ | $5.9\times10^6$ | $7.3\times10^6$ |
| $S_2$(CT$'$)$\leftarrow T_1$(CT) | $3.3\times10^4$ | $1.7\times10^4$ | $7.9\times10^3$ | $3.6\times10^3$ | $1.6\times10^3$ | $6.5\times10^2$ |
| $S_2$(CT$'$)$\leftarrow T_2$(CT$'$) | $1.7\times10^7$ | $2.0\times10^6$ | $3.7\times10^5$ | $2.1\times10^5$ | $4.6\times10^4$ | $8.2\times10^3$ |
| $S_2$(CT$'$)$\leftarrow T_3$(LE) | $1.1\times10^5$ | $1.9\times10^5$ | $3.1\times10^5$ | $4.6\times10^5$ | $6.6\times10^5$ | $9.1\times10^5$ |