Supplementary information

Fast Estimation of Intersystem Crossings Rate Constant of Radical Pairs

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Table S1. Root mean squared error (RMSE), Coefficient of determination (R^2), total Mean average error (MAE) and MAE for each of the 10 considered dimers for the energies of S_1, S_2, S_3 and S_4 calculated on **CASSCF** and **CASPT2** level.

	$E(T_1\text{-}S_1)$, cm^{-1}	$E(T_1\text{-}S_2)$, cm^{-1}	$E(T_1\text{-}S_3)$, cm^{-1}	$E(T_1\text{-}S_4)$, cm^{-1}
MAE(ButO-ButO)	2.05	19.13	15.93	34.05
MAE(MeO-MeO	3.50	34.55	26.96	58.51
MAE(ButO-MeO	3.19	28.29	15.07	41.55
MAE(AcO-MeO	1.37	27.87	13.43	39.98
MAE(HOBuO-MeO	0.91	30.21	11.93	41.16
MAE(AcO-ButO	1.15	22.05	12.32	33.24
MAE(ButO-HOBuO	0.79	19.60	9.96	28.95
MAE(AcO-AcO	0.98	26.34	15.48	41.15
MAE(AcO-HOBuO	0.51	24.94	12.62	37.27
MAE(HOBuO-HOBuO)	0.74	23.44	11.73	34.59
MAE	1.27	25.13	13.37	37.52
RMSE	5.76	31.67	17.04	43.54
R^2	1.00	1.00	1.00	1.00

Table S2. Root mean squared error (RMSE), Coefficient of determination (R^2), total Mean average error (MAE) and MAE for each of the 10 considered dimers for the SOC between T_1 state and each of the 4 singlet states (S_1, S_2, S_3 and S_4) calculated on **CASPT2** level and with analytical expression on **CASSCF** level.

	$SOC(T_1\text{-}S_1)$, cm^{-1}	$SOC(T_1\text{-}S_2)$, cm^{-1}	$SOC(T_1\text{-}S_3)$, cm^{-1}	$SOC(T_1\text{-}S_4)$, cm^{-1}
MAE(ButO-ButO)	1.82	11.12	8.76	1.10
MAE(MeO-MeO	1.49	12.07	14.01	1.25
MAE(ButO-MeO	1.91	11.70	9.31	1.38
MAE(AcO-MeO	0.77	11.65	11.00	0.65
MAE(HOBuO-MeO	0.70	12.24	10.47	0.50
MAE(AcO-ButO	0.85	10.56	8.70	0.60
MAE(ButO-HOBuO	0.58	11.24	8.75	0.49
MAE(AcO-AcO	0.76	10.55	9.41	0.59
MAE(AcO-HOBuO	0.41	10.79	9.55	0.36
MAE(HOBuO-HOBuO)	0.58	10.92	9.56	0.48
MAE	0.86	11.23	9.79	0.65
RMSE	3.58	12.86	12.96	2.20
R^2	0.97	0.56	0.55	0.99

Table S3. Root mean squared error (RMSE), Coefficient of determination (R^2), total Mean average error (MAE) and MAE for each of the 10 considered dimers for the order of magnitude of k_{ISC} from T_1 state to each of the 4 singlet states (S_1, S_2, S_3 and S_4) calculated on **CASPT2** and **CASSCF** level.

	$k_{ISC}(T_1 \rightarrow S_1)$, s^{-1}	$k_{ISC}(T_1 \rightarrow S_2)$, s^{-1}	$k_{ISC}(T_1 \rightarrow S_3)$, s^{-1}	$k_{ISC}(T_1 \rightarrow S_4)$, s^{-1}	$k_{ISC}(T_1 \rightarrow S_n)$, s^{-1}
MAE(ButO-ButO)	0.16	0.24	0.24	0.23	0.24
MAE(MeO-MeO	0.11	0.22	0.20	0.29	0.22
MAE(ButO-MeO	0.15	0.22	0.22	0.20	0.22
MAE(AcO-MeO	0.14	0.22	0.21	0.20	0.22
MAE(HOBuO-MeO	0.11	0.22	0.19	0.18	0.23
MAE(AcO-ButO	0.16	0.24	0.23	0.21	0.24
MAE(ButO-HOBuO	0.11	0.24	0.21	0.13	0.24
MAE(AcO-AcO	0.17	0.25	0.22	0.26	0.25
MAE(AcO-HOBuO	0.12	0.24	0.22	0.20	0.25
MAE(HOBuO-HOBuO)	0.12	0.24	0.21	0.17	0.24
MAE	0.13	0.23	0.21	0.19	0.24
RMSE	0.19	0.25	0.23	0.25	0.25
R^2	1.00	0.98	0.99	0.99	0.98

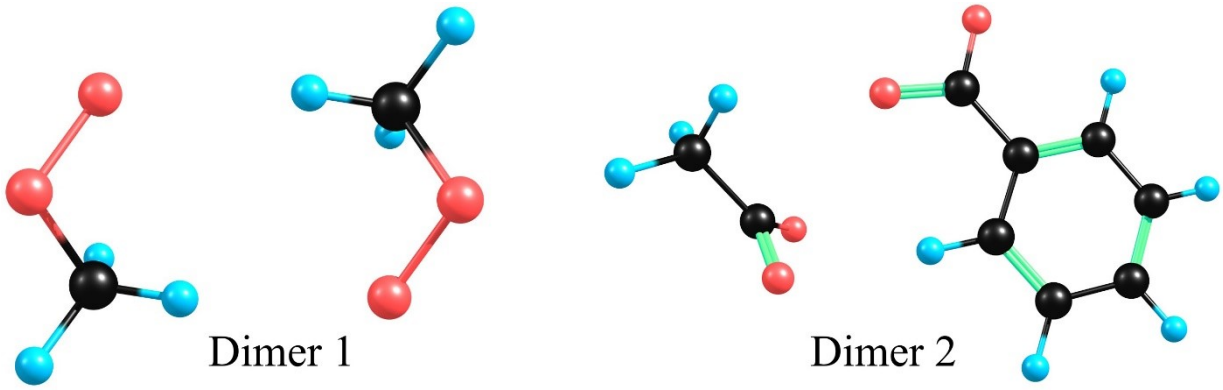

Figure S1. Structures of dimers **Dimer 1** and **Dimer 2** for test calculation

Table S4. Energy gap (E), spin-orbit coupling matrix element (SOC) and intersystem crossing rate constant (k_{ISC}) for transitions $T_1 \rightarrow S_n$, (n=1-4) calculated on **CASSCF** and **CASPT2** levels of theory for **Dimer 1** and **Dimer 2**

	Dimer 1, **CASSCF**	Dimer 1, **CASPT2**	Dimer 2, **CASSCF**	Dimer 2, **CASPT2**
$E(T_1\text{-}S_1)$, cm^{-1}	-16.56	-39.46	0.28	-6.51
$E(T_1\text{-}S_2)$, cm^{-1}	4168.52	7427.71	4831.73	4449.06
$E(T_1\text{-}S_3)$, cm^{-1}	4187.37	7437.48	5479.87	4832.53
$E(T_1\text{-}S_4)$, cm^{-1}	8423.96	14900.44	10345.47	9296.20
$SOC(T_1\text{-}S_1)$, cm^{-1}	0.76	0.77	0.01	0.01
$SOC(T_1\text{-}S_2)$, cm^{-1}	56.51	39.70	110.52	90.81
$SOC(T_1\text{-}S_3)$, cm^{-1}	167.25	160.38	11.48	89.78
$SOC(T_1\text{-}S_4)$, cm^{-1}	0.30	0.69	0.07	0.08
$k_{ISC}(T_1 \rightarrow S_1)$, s^{-1}	$6.78 \cdot 10^{8}$	$6.90 \cdot 10^{8}$	$7.81 \cdot 10^{4}$	$1.15 \cdot 10^{5}$
$k_{ISC}(T_1 \rightarrow S_2)$, s^{-1}	$3.74 \cdot 10^{1}$	$5.22 \cdot 10^{-9}$	$1.80 \cdot 10^{0}$	$1.53 \cdot 10^{1}$
$k_{ISC}(T_1 \rightarrow S_3)$, s^{-1}	$3.00 \cdot 10^{2}$	$7.96 \cdot 10^{-8}$	$2.57 \cdot 10^{-4}$	$7.32 \cdot 10^{-2}$
$k_{ISC}(T_1 \rightarrow S_4)$, s^{-1}	$2.93 \cdot 10^{-16}$	$8.44 \cdot 10^{-36}$	$2.01 \cdot 10^{-23}$	$4.51 \cdot 10^{-20}$
$k_{ISC}(T_1 \rightarrow S_n)$, s^{-1}	$6.78 \cdot 10^{8}$	$6.90 \cdot 10^{8}$	$7.81 \cdot 10^{4}$	$1.15 \cdot 10^{5}$