Electronic Supplementary Material (ESI) for Photochemical and Photobiological Science

Electronic Supplementary Information

Quantum mechanical study of the solvent-dependence of electronic energy transfer rates in a Bodipy closely-spaced dyad

Stefano Caprasecca, Carles Curutchet and Benedetta Mennucci

Table 1 Electronic couplings (in meV) and solvent screening factors derived from PCM-EET calculations

Solvent	B3LYP			CAM-B3LYP		
	V_s	V_{TOT}	s	V_s	V_{TOT}	s
Dioxane	9.81	5.73	0.58	11.84	7.00	0.59
$(C_4H_9)_2O$	9.53	5.75	0.60	11.57	7.07	0.61
C_6H_5Cl	9.93	5.15	0.52	11.98	6.30	0.53
$CHCl_3$	9.74	5.49	0.56	11.79	6.74	0.57
$(C_2H_5)_2O$	9.38	5.93	0.63	11.43	7.31	0.64
EtOAc	9.31	5.77	0.62	11.36	7.13	0.63
MTHF	9.37	5.57	0.60	11.41	6.87	0.60
THF	9.45	5.58	0.59	11.51	6.88	0.60
CH_2Cl_2	9.65	5.54	0.57	11.72	6.82	0.58
C_4H_9CN	9.21	5.52	0.60	11.26	6.83	0.61
DMF	9.47	5.42	0.57	11.56	6.71	0.58
C_3H_7CN	9.10	5.53	0.61	11.16	6.85	0.61
PC	9.28	5.40	0.58	11.34	6.68	0.59
C_2H_5CN	9.15	5.66	0.62	11.23	7.03	0.63
CH_3CN	9.00	5.72	0.64	11.06	7.10	0.64

Table 2 Transition dipole moments (in a.u.) derived from PCM-EET calculations

Solvent	Acceptor		Donor	
	B3LYP	CAM-B3LYP	B3LYP	CAM-B3LYP
Dioxane	5.124	5.122	3.020	3.299
$(C_4H_9)_2O$	5.121	5.120	2.984	3.273
C_6H_5Cl	5.253	5.242	3.048	3.330
$CHCl_3$	5.208	5.199	3.005	3.294
$(C_2H_5)_2O$	5.110	5.109	2.940	3.240
EtOAc	5.137	5.135	2.940	3.244
MTHF	5.173	5.168	2.961	3.261
THF	5.198	5.190	2.962	3.263
CH_2Cl_2	5.252	5.236	2.974	3.273
C_4H_9CN	5.195	5.188	2.937	3.246
DMF	5.242	5.231	2.954	3.263
C_3H_7CN	5.190	5.184	2.922	3.236
PC	5.228	5.218	2.944	3.255
C_2H_5CN	5.185	5.179	2.909	3.225
CH_3CN	5.194	5.185	2.888	3.209

Table 3 Distance between donor and acceptor centres of mass R_{DA} (in a.u.), and orientation factors κ, derived from geometries and transition dipole moments determined in each solvent

Solvent	R_{DA}	κ	
		B3LYP	CAM-B3LYP
Dioxane	38.26	1.5150	1.5167
$(C_4H_9)_2O$	38.32	1.5126	1.5145
C_6H_5Cl	38.38	1.5132	1.5150
$CHCl_3$	38.34	1.5178	1.5196
$(C_2H_5)_2O$	38.23	1.5143	1.5162
EtOAc	38.34	1.5144	1.5164
MTHF	38.42	1.5129	1.5149
THF	38.39	1.5165	1.5184
CH_2Cl_2	38.36	1.5232	1.5251
C_4H_9CN	38.44	1.5087	1.5107
DMF	38.55	1.5401	1.5414
C_3H_7CN	38.50	1.5101	1.5121
PC	38.43	1.5084	1.5104
C_2H_5CN	38.57	1.5358	1.5371
CH_3CN	38.52	1.5198	1.5217