

Supporting Information for JP9936852, Castner, Kennedy, and Cave, "Solvent as electron donor: Donor/acceptor coupling as a dynamical variable"

Table 1S: H_{DA} Data for C152-DMA pairs (Nearest Neighbors) for the Minimized Structure.^a

DMA	$\Delta E_{\text{adiabatic}} (\text{cm}^{-1})$	$R_{DA} (\text{\AA})$	$H_{DA} (\text{cm}^{-1})$
1	5270	9.3	16
2	6380	9.2	11
3	2030	5.8	205
4	4280	5.6	29
5	8310	6.7	14
6	10380	6.3	55
7	12830	8.7	61
8	12830	7.6	130
9	9180	5.4	98
10	8560	7.0	15
11	6230	7.7	20
12	8470	7.8	1
13	7300	8.9	1
14	7440	9.0	6
15	8660	7.6	34

^a The values correspond to the various DMA in Figure 10a. For details on the calculation, see Theoretical Methods Section.

Supplementary Material: Castner, Kennedy, and Cave

Table 2S: H_{DA} Data for C152-DMA pairs (Nearest Neighbors) for the 5 ps Frame.^a

DMA	$\Delta E_{\text{adiabatic}} (\text{cm}^{-1})$	$R_{DA} (\text{\AA})$	$H_{DA} (\text{cm}^{-1})$
1	5610	7.7	21
2	11400	8.6	7.2
3	1580	3.8	384
4	8660	6.7	92
5	13200	7.4	106
6	11500	6.3	139
7	13100	8.7	68
8	6940	5.3	82
9	7270	5.8	221
10	7090	6.4	1.6
11	7040	7.6	86
12	6000	9.3	15
13	7500	8.8	2.3
14	1770	7.3	433

^aThe values correspond to the various DMA in Figure 10b. For details on the calculation, see Theoretical Methods Section.

Supplementary Material: Castner, Kennedy, and Cave

Table 3S: H_{DA} Data for C152-DMA pairs (Nearest Neighbors) for the 10 ps Frame.^a

DMA	$\Delta E_{\text{adiabatic}} (\text{cm}^{-1})$	$R_{DA} (\text{\AA})$	$H_{DA} (\text{cm}^{-1})$
1	8560	11.1	0.1
2	4610	6.9	5.4
3	9300	8.4	3.9
4	9990	6.6	47
5	2090	3.1	1024
6	11900	6.8	241
7	14400	10.5	0.8
8	8130	3.5	80
9	8360	6.0	62
10	6360	6.6	147
11	5870	9.0	62
12	6330	8.2	14
13	1700	7.7	19

^a The values correspond to the various DMA in Figure 10c. For details on the calculation, see Theoretical Methods Section.

Supplementary Material: Castner, Kennedy, and Cave

Table 4S: H_{DA} Data for C152-DMA pairs (Nearest Neighbors) for the 20 ps Frame.^a

DMA	$\Delta E_{\text{adiabatic}} (\text{cm}^{-1})$	$R_{DA} (\text{\AA})$	$H_{DA} (\text{cm}^{-1})$
1	8440	10.8	0.2
2	8370	8.9	6.2
3	9070	8.0	30
4	7690	7.4	8.1
5	7810	6.4	84
6	11800	5.4	1828
7	10000	9.4	38
8	8770	6.2	489
9	7500	6.8	23
10	2500	3.4	1013
11	4400	6.2	57
12	4120	8.5	27
13	5720	9.1	0.5
14	16000	3.6	2013
15	4570	6.9	67
16	6120	8.0	5.5

^a The values correspond to the various DMA in Figure 10d. For details on the calculation, see Theoretical Methods Section.

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Table 5S: H_{DA} Data for C152-DMA pairs (Nearest Neighbors) for the 30 ps Frame.^a

DMA	$\Delta E_{\text{adiabatic}} (\text{cm}^{-1})$	$R_{DA} (\text{\AA})$	$H_{DA} (\text{cm}^{-1})$
1	7120	11.0	0.2
2	8440	10.2	1.6
3	3110	6.9	64
4	9030	8.8	5.3
5	9440	7.1	25
6	730	4.1	156
7	9240	6.7	42
8	9630	7.2	172
9	13200	9.3	89
10	6090	5.1	292
11	7890	6.5	115
12	3260	6.7	31
13	2050	8.9	62
14	7340	7.4	2
15	1170	7.5	547
16	4540	8.8	21

^a The values correspond to the various DMA in Figure 10e. For details on the calculation, see Theoretical Methods Section.

Supplementary Material: Castner, Kennedy, and Cave

Table 6S: H_{DA} Data for C152-DMA pairs (Nearest Neighbors) for the 45 ps Frame.^a

DMA	$\Delta E_{\text{adiabatic}} (\text{cm}^{-1})$	$R_{DA} (\text{\AA})$	$H_{DA} (\text{cm}^{-1})$
1	8120	11.4	0.04
2	6230	9.5	0.4
3	2470	7.6	27
4	5450	8.3	5.4
5	5820	7.2	47
6	1630	2.6	176
7	8870	6.2	25
8	7870	5.8	302
9	10700	10.0	20
10	2060	5.4	237
11	4940	5.0	265
12	4210	7.2	6.9
13	538	7.9	0.8
14	2300	7.3	422
15	4860	9.0	3.3

^a The values correspond to the various DMA in Figure 10f. For details on the calculation, see Theoretical Methods Section.

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Table 7S. Coumarin 152 Absorption/Emission spectra in electron-donating solvents:

Solvent	Absorption λ_{max} (nm)	Excitation wavelength (nm)	Observed wavelength (nm)
DMA	398	394	475
DMOT	388	394	475
DMMT		394	475
TMA	394	396	500
DMPT	395	394	475
o-anisid.	404	396	500
TEA	378	396	500
TPA/Bz	398 (shoulder)	396	475
DMP	398	394	475

Table 8S. Emission lifetimes of six coumarins in toluene solution

Coumarin	Lifetime (ns)
C 151	3.87
C 152	4.27
C 153	4.51
C 120	2.41
C 343	3.36
C 500	3.31
C 503	4.04