Conformational Dynamics of Semiflexibly Bridged Donor-Acceptor Systems Studied with a Streak Camera and Spectrotemporal Parametrization of Fluorescence

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Supporting Information

Table S1. Estimated spectral parameters[a] of **1** in various solvents at room temperature.

		ECT			CCT		
Solvent	Δf	ν_{max}	$\Delta\nu$	b	ν_{max}	$\Delta\nu$	b
n-hexane	0.092	24.67	4.19	-0.232	20.56	4.26	-0.519
cyclohexane	0.100	24.52	4.94	0.194	20.26	4.22	-0.245
trans-decalin	0.110	24.18	4.12	0.066	20.24	4.16	-0.266
di-*n*-pentylether	0.171	21.83	4.48	-0.101	20.17	4.10	-0.171
benzene	0.116[b]	20.32	4.60	-0.148	18.86	4.43	-0.034
diisopropylether	0.237	19.57	4.48	0.037	18.89	4.46	-0.105
diethylether	0.251	19.14	4.57	-0.07	18.81	4.48	-0.101
ethylacetate	0.292	16.77	4.73	-0.012	-	-	-
tetrahydrofuran	0.308	16.88	4.70	-0.034	-	-	-

[a] emission maximum ν_{max} (10^3 cm^{-1}), spectral width $\Delta\nu$ (10^3 cm^{-1}) and skewness b are defined in equation (2). [b] benzene is known to behave as more polar than expected based on its Δf value and is not included in the Lippert-Mataga analyses.

Table S2. Estimated spectral parameters[a] of **2** in various solvents at room temperature.

		ECT			CCT		
Solvent	Δf	ν_{max}	$\Delta\nu$	b	ν_{max}	$\Delta\nu$	b
n-hexane	0.092	23.92	5.74	-0.174	20.52	4.29	-0.149
cyclohexane	0.100	23.85	4.68	0.078	20.38	4.18	-0.247
trans-decalin	0.110	23.56	3.93	0.172	20.29	4.11	-0.262
di-*n*-pentylether	0.171	20.91	4.50	-0.112	19.44	4.32	-0.152
benzene	0.116[b]	20.06	4.27	-0.113	18.90	4.40	-0.063
diisopropylether	0.237	19.35	4.64	-0.051	18.92	4.33	-0.117
diethylether	0.251	19.02	4.46	-0.078	18.78	4.38	-0.161
ethylacetate	0.292	16.67	4.69	0.026	-	-	-
tetrahydrofuran	0.308	16.78	4.73	-0.033	-	-	-

[a] emission maximum ν_{max} (10^3 cm^{-1}), spectral width $\Delta\nu$ (10^3 cm^{-1}) and skewness b are defined in equation (2). [b] benzene is known to behave as more polar than expected based on its Δf value and is not included in the Lippert-Mataga analyses.

Table S3. Estimated spectral parameters[a] of **3** in various solvents at room temperature.

		ECT			CCT		
Solvent	Δf	ν_{max}	$\Delta\nu$	b	ν_{max}	$\Delta\nu$	b
n-hexane	0.092	25.08	5.15	0.276	20.98	3.84	-0.220
cyclohexane	0.100	24.66	4.06	-0.072	20.89	3.78	-0.282
trans-decalin	0.110	24.42	4.06	-0.075	20.62	3.70	-0.291
di-*n*-pentylether	0.171	20.78	4.62	-0.129	19.67	3.86	-0.203
benzene	0.116[b]	20.21	4.24	-0.075	19.03	3.98	-0.084
diisopropylether	0.237	19.35	4.45	-0.019	19.13	4.07	-0.135
diethylether	0.251	19.04	4.23	-0.067	18.90	4.18	-0.105
ethylacetate	0.292	16.64	4.42	0.016	-	-	-
tetrahydrofuran	0.308	16.71	4.41	-0.020	-	-	-

[a] emission maximum ν_{max} (10^3 cm^{-1}), spectral width $\Delta\nu$ (10^3 cm^{-1}) and skewness b are defined in equation (2). [b] benzene is known to behave as more polar than expected based on its Δf value and is not included in the Lippert-Mataga analyses.

Table S4. Estimated spectral parameters[a] of **4** in various solvents at room temperature.

		ECT			CCT		
Solvent	Δf	ν_{max}	$\Delta\nu$	b	ν_{max}	$\Delta\nu$	b
n-hexane	0.092	25.84	8.53	-0.160	21.89	3.89	-0.240
cyclohexane	0.100	25.22	6.24	-0.006	21.80	3.83	-0.245
trans-decalin	0.110	25.58	4.29	0.079	21.53	3.78	-0.257
di-*n*-pentylether	0.171	21.44	4.65	-0.080	20.52	3.88	-0.163
benzene	0.116[b]	20.92	4.33	-0.098	19.89	4.08	-0.086
diisopropylether	0.237	19.98	4.62	-0.052	19.75	4.32	-0.138
diethylether	0.251	19.83	4.39	-0.096	19.69	4.29	-0.107
ethylacetate	0.292	17.28	4.61	-0.002	-	-	-
tetrahydrofuran	0.308	17.37	4.51	-0.010	-	-	-

[a] emission maximum ν_{max} (10^3 cm^{-1}), spectral width $\Delta\nu$ (10^3 cm^{-1}) and skewness b are defined in equation (2). [b] benzene is known to behave as more polar than expected based on its Δf value and is not included in the Lippert-Mataga analyses.

Table S5. Fluorescence quantum yields of the ECT species and product of the fluorescence quantum yield and the quantum yield of folding for the CCT species of **1**, **2**, **3** and **4** in various solvents.

Solvent	**1**		**2**		**3**		**4**	
	Φ_{ECT}	$\Phi_{fold}\cdot\Phi_{CCT}$	Φ_{ECT}	$\Phi_{fold}\cdot\Phi_{CCT}$	Φ_{ECT}	$\Phi_{fold}\cdot\Phi_{CCT}$	Φ_{ECT}	$\Phi_{fold}\cdot\Phi_{CCT}$
n-hexane	0.005	0.045	0.007	0.063	0.001	0.059	-	-
cyclohexane	0.008	0.072	0.008	0.062	0.003	0.127	0.005	0.195
trans-decalin	0.017	0.083	0.012	0.078	-	-	-	-
di-*n*-pentylether	0.015	0.035	0.013	0.037	0.015	0.065	-	-
benzene	-	-	0.008	0.042	-	-	0.006	0.047
diisopropylether	0.008	0.022	0.009	0.021	0.007	0.023	-	-
diethylether	0.005	0.015	0.007	0.023	0.006	0.024	-	-