CHEMISTRY
A European Journal

Supporting Information

Photophysical and Photoacoustic Properties of Quadrupolar Borondifluoride Curcuminoid Dyes

Stephanie Bellinger,[a] Maryam Hatamimoslehabadi,[b] Seema Bag,[a] Farha Mithila,[a] Jeffrey La,[b] Mathieu Frenette,[a] Samir Laoui,[b] David J. Szalda,[c] Chandra Yelleswarapu,*[b] and Jonathan Rochford*[a]

chem_201704423_sm_miscellaneous_information.pdf

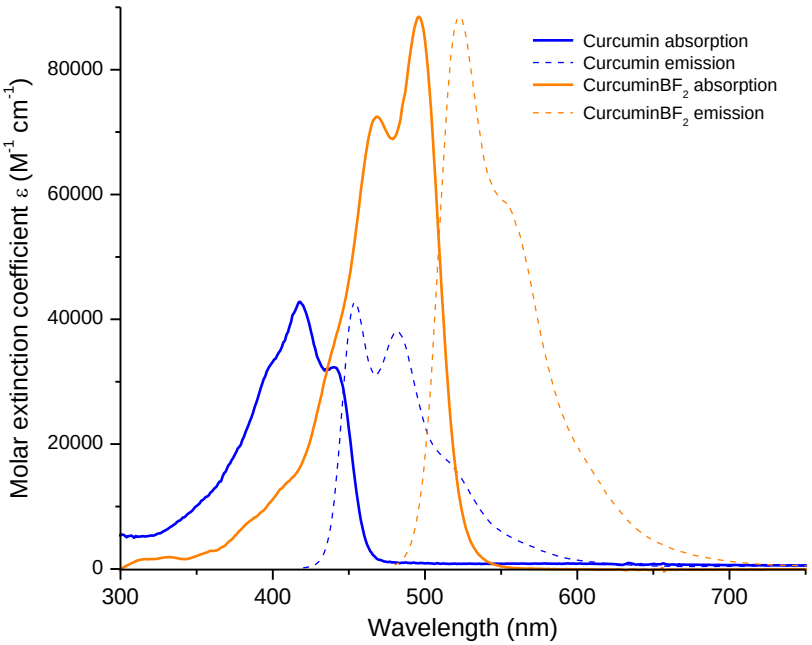

Fig. S1. Overlay of absorption and normalized emission spectra for free acid curcumin and curcuminBF_2 recorded in toluene at room temperature.

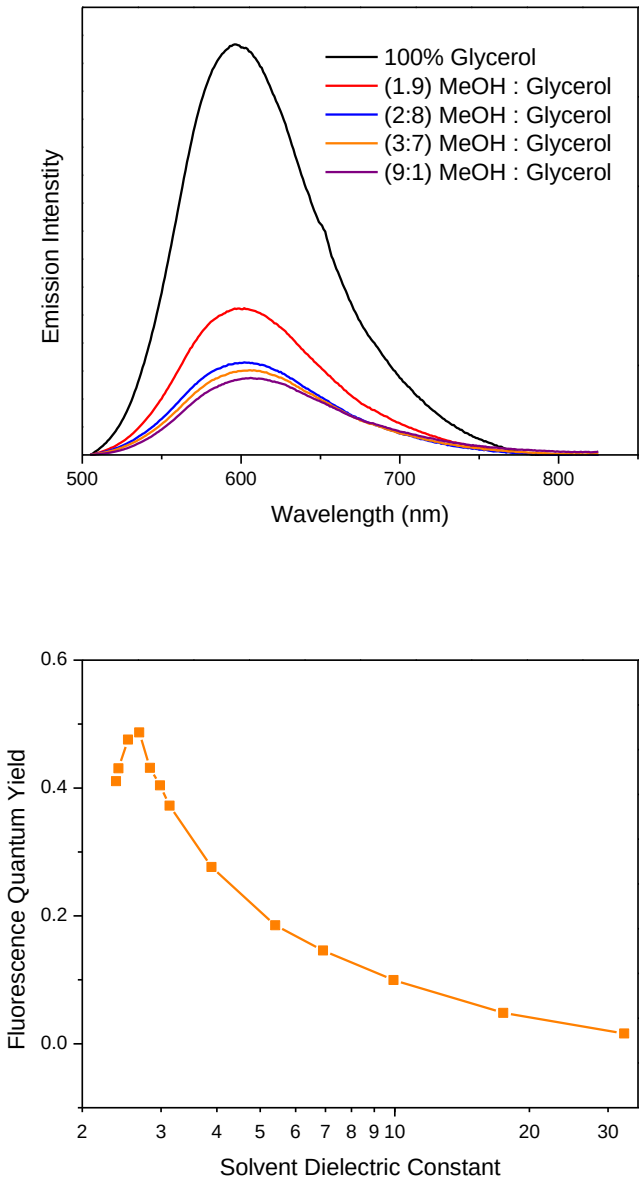

Fig. S2. (Top) Fluorescence spectra of curcuminBF$_2$ (**1**) in various methanol glycerol mixtures indicative of molecular rotor behavior via a TICT state. (Bottom) Polarity dependent of curcuminBF$_2$ (**1**) fluorescence quantum yield on solvent polarity in various toluene-methanol mixtures. An initial increase in fluorescence quantum yield is observed upon addition of < 5% methanol due to hydrogen bonding.

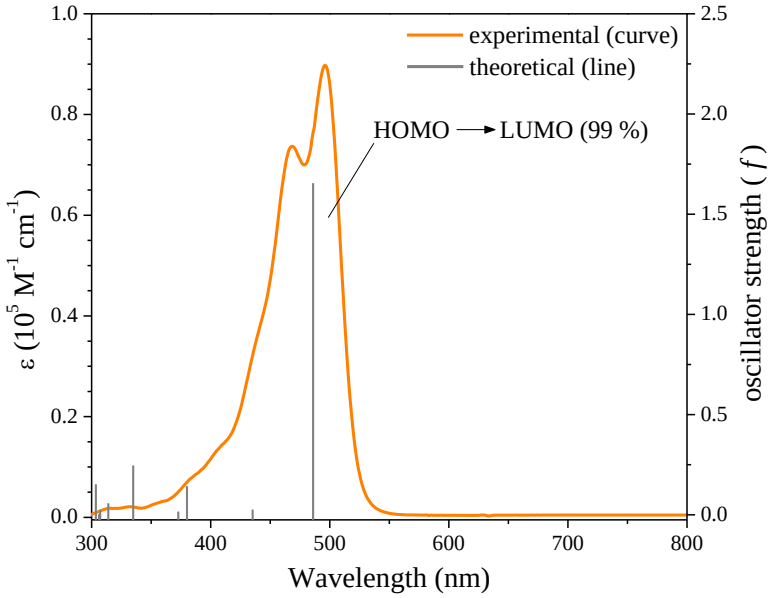

Fig. S3. Overlay of experimental UV-Vis spectrum of **1** recorded in toluene with a TDDFT line spectrum calculated using the CAM-B3LYP/6-311g(d,p)/toluene PCM functional/basis set/solvent model with the configurational interaction keyword cis(d).

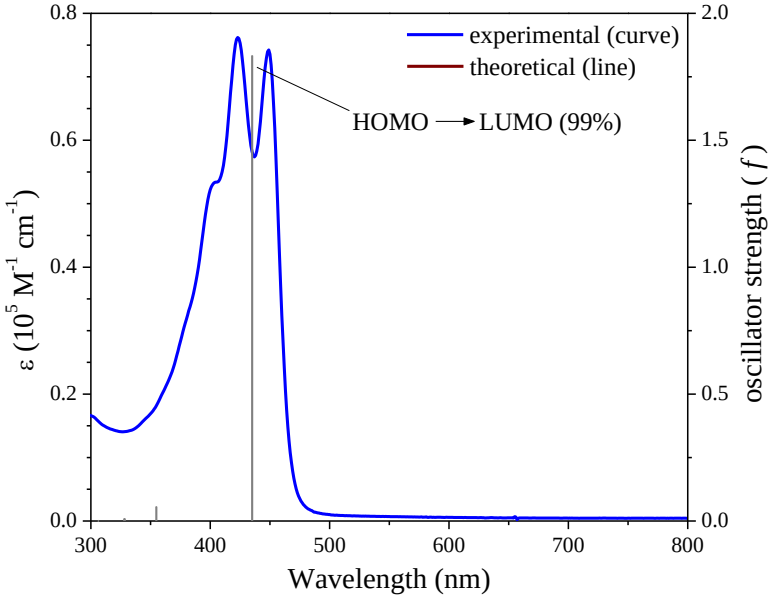

Fig. S4. Overlay of experimental UV-Vis spectrum of **2** recorded in toluene with a TDDFT line spectrum calculated using the B3LYP/6-311g(d,p)/toluene PCM functional/basis set/solvent model.

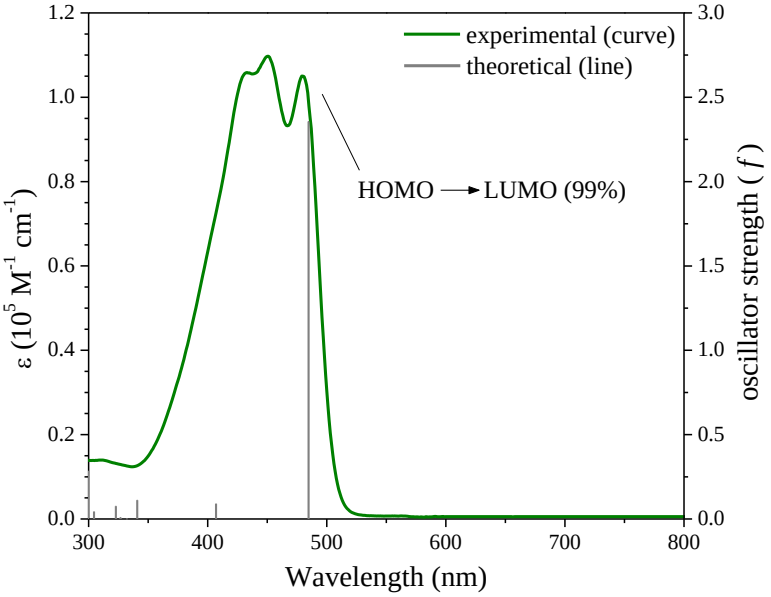

Fig. S5. Overlay of experimental UV-Vis spectrum of **3** recorded in toluene with a TDDFT line spectrum calculated using the B3LYP/6-311g(d,p)/toluene PCM functional/basis set/solvent model.

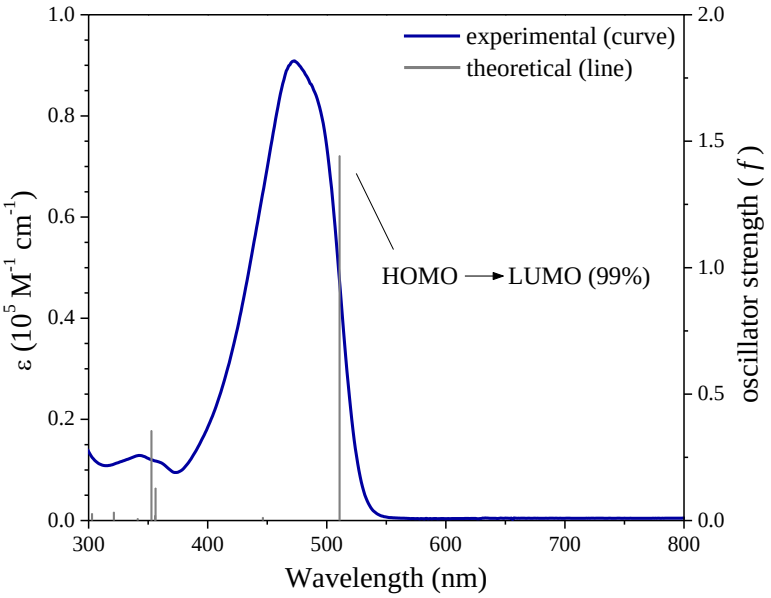

Fig. S6. Overlay of experimental UV-Vis spectrum of **4** recorded in toluene with a TDDFT line spectrum calculated using the B3LYP/6-311g(d,p)/toluene PCM functional/basis set/solvent model.

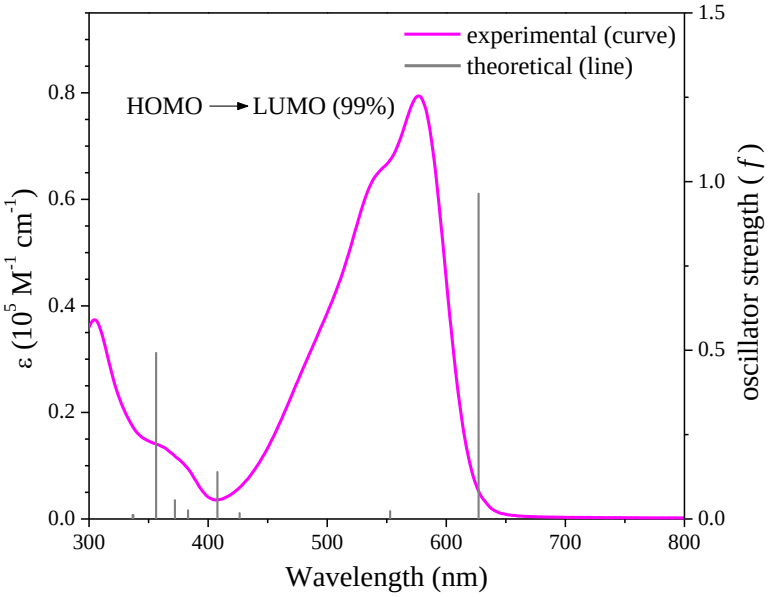

Fig. S7. Overlay of experimental UV-Vis spectrum of **5** recorded in toluene with a TDDFT line spectrum calculated using the B3LYP/6-311g(d,p)/toluene PCM functional/basis set/solvent model.

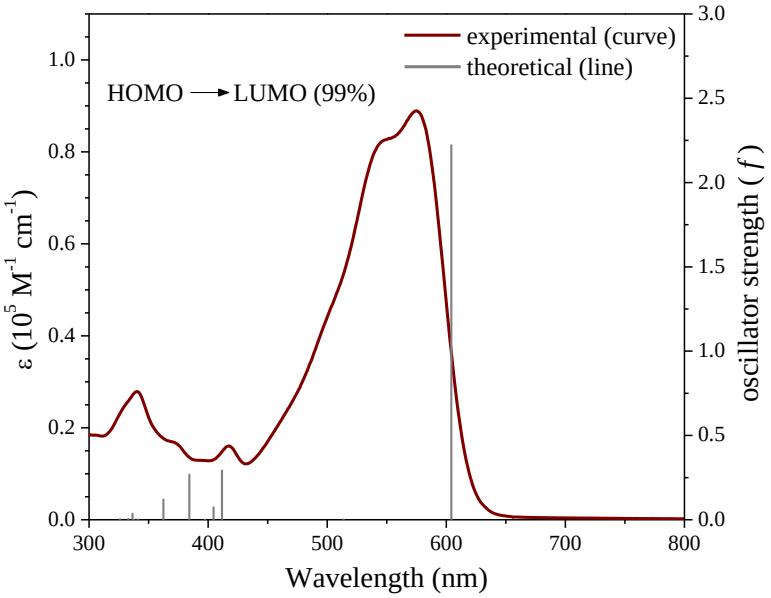

Fig. S8. Overlay of experimental UV-Vis spectrum of **6** recorded in toluene with a TDDFT line spectrum calculated using the B3LYP/6-311g(d,p)/toluene PCM functional/basis set/solvent model.

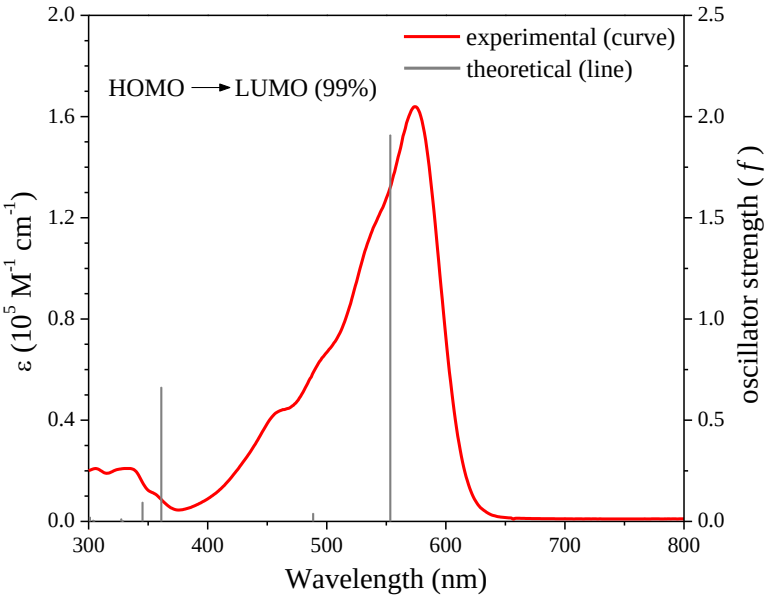

Fig. S9. Overlay of experimental UV-Vis spectrum of **7** recorded in toluene with a TDDFT line spectrum calculated using the CAM-B3LYP/6-311g(d,p)/toluene PCM functional/basis set/solvent model with the configurational interaction keyword cis(d).

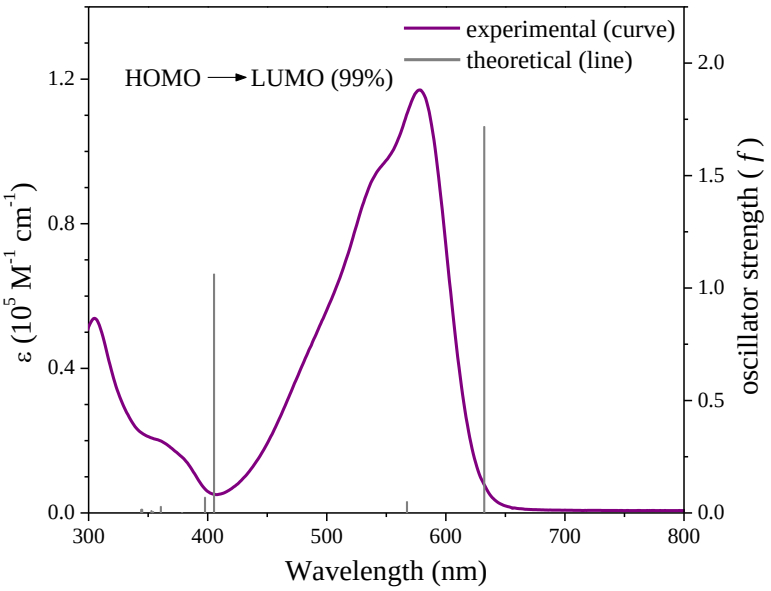

Fig. S10. Overlay of experimental UV-Vis spectrum of **8** recorded in toluene with a TDDFT line spectrum calculated using the CAM-B3LYP/6-311g(d,p)/toluene PCM functional/basis set/solvent model with the configurational interaction keyword cis(d).

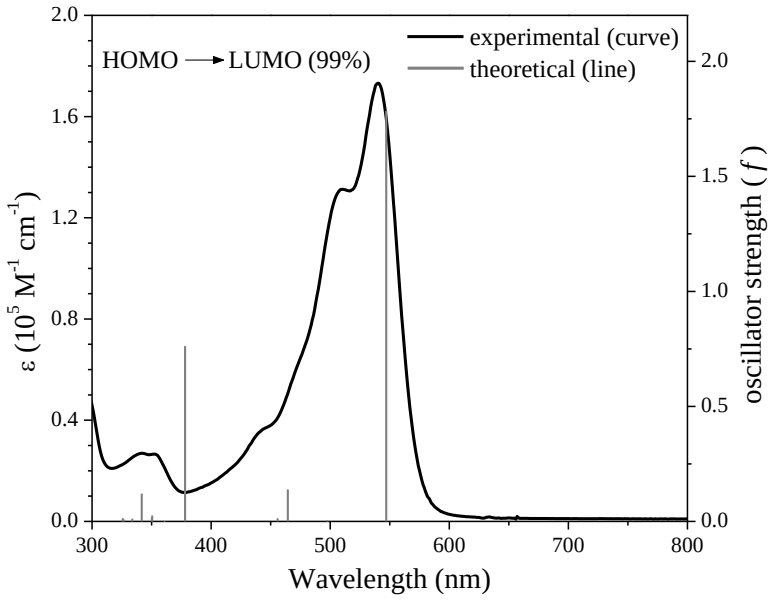

Fig. S11. Overlay of experimental UV-Vis spectrum of **9** recorded in toluene with a TDDFT line spectrum calculated using the CAM-B3LYP/6-311g(d,p)/toluene PCM functional/basis set/solvent model with the configurational interaction keyword cis(d).

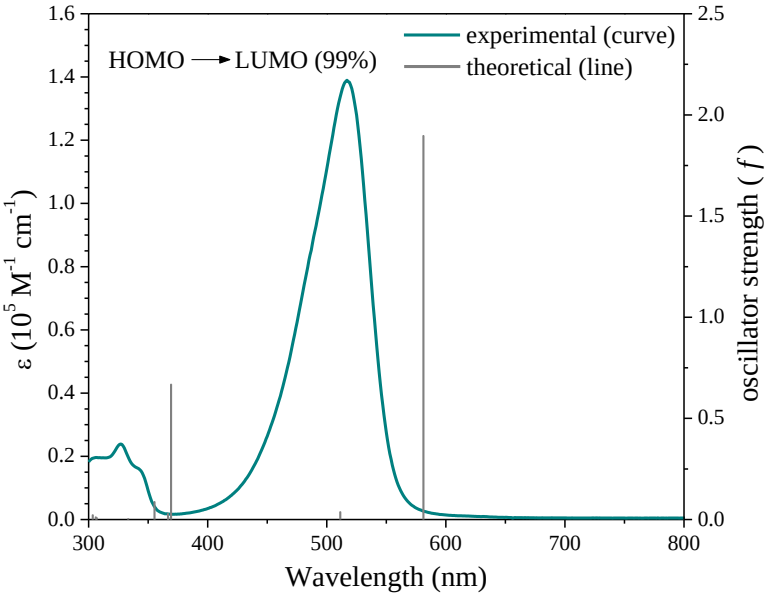

Fig. S12. Overlay of experimental UV-Vis spectrum of **10** recorded in toluene with a TDDFT line spectrum calculated using the CAM-B3LYP/6-311g(d,p)/toluene PCM functional/basis set/solvent model with the configurational interaction keyword cis(d).

Table S1. Collective UV-Vis absorption and emission data recorded in toluene, dichloromethane (DCM), acetonitrile (ACN), and methanol (MeOH) including fluorescence lifetimes, radiative and non-radiative rate constants.

	solvent	λ_{abs} (nm)	ε (10^4 M^{-1} cm^{-1})	λ_{em} (nm)	Φ_{fl}	$^1\tau$ (ns)	k_r (10^8 s^{-1})	k_{nr} (10^8 s^{-1})	Stokes shift (cm^{-1})
1	Toluene	495	8.85	522	0.42	1.36	3.07	4.29	1,077
	DCM	498	9.8	558	0.52	1.73	3.01	2.78	2159
	ACN	498	9.4	588	0.05	1.83	0.26	5.20	3074
	MeOH	500	10.1	588	0.02	~	~	~	2993
2	Toluene	449	7.38	465	0.29	1.15	2.50	6.21	720
	DCM	449	8.0	473	0.22	0.90	2.42	8.64	1130
	ACN	446	7.6	473	0.23	0.95	2.44	8.14	1280
	MeOH	444	7.4	473	0.23	~	~	~	1381
3	Toluene	480	10.48	506	0.32	0.93	3.45	7.28	1,109
	DCM	450	11.4	536	0.23	1.34	1.68	5.77	3566
	ACN	474	10.4	548	0.37	1.67	2.21	3.77	2849
	MeOH	447	11.2	548	0.46	~	~	~	4123
4	Toluene	479	8.13	532	0.53	1.69	3.12	2.79	1,576
	DCM	479	10.0	563	0.44	2.06	2.16	2.70	3115
	ACN	474	9.0	584	0.33	3.71	0.89	1.81	3974
	MeOH	474	5.6	580	0.27	~	~	~	3856
5	Toluene	577	7.94	644	0.28	1.82	1.56	3.95	2,353
	DCM	556	8.3	707	0.05	~	~	~	3841
	ACN	539	8.2	748	0.003	0.48	0.06	20.64	5184
	MeOH	543	4.3	708	0.00	~	~	~	4292
6	Toluene	574	8.91	616	0.23	1.03	2.22	7.54	1,214
	DCM	574	8.4	645	0.09	1.47	0.58	6.22	1918
	ACN	559	8.7	667	0.01	0.002	36.19	5801.52	2897

	MeOH	543	6.6	690	0.05	~	~	~	3923
7	Toluene	572	16.30	612	0.77	1.32	5.80	1.75	1,188
	DCM	597	13.9	682	0.67	1.49	4.50	2.22	2088
	ACN	596	13.9	705	0.22	0.74	2.95	10.58	2594
	MeOH	581	10.6	705	0.01	~	~	~	3027
8	Toluene	578	11.71	628	0.49	1.73	2.85	2.92	1,377
	DCM	592	12.3	733	0.08	1.48	0.51	6.23	3249
	ACN	581	12.8	770	0.01	1.53	0.03	6.51	4225
	MeOH	577	11.7	733	0.01	~	~	~	3688
9	Toluene	540	17.30	570	0.76	1.69	4.49	1.43	944
	DCM	547	15.9	629	0.74	2.71	2.74	0.95	2383
	ACN	546	16.2	645	0.34	2.01	1.67	3.30	2811
	MeOH	540	17.0	645	0.32	~	~	~	3015
10	Toluene	517	13.95	555	0.33	2.00	1.63	3.36	1,292
	DCM	537	13.7	600	0.015	n/a	n/a	n/a	1955
	ACN	536	12.3	612	0.005	3.05	0.01	3.27	2317
	MeOH	530	12.6	600	0.01	~	~	~	2201

Lippert-Mataga Analysis

This excited state solvatochromism has been evaluated using the Lippert-Mataga equation (Eq. S1) which provides a framework for discerning non-specific solvent effects on the Stokes shift [1-3]

$$\bar{\nu}_A - \bar{\nu}_F = \frac{2\Delta f}{hc} \frac{(\mu_E - \mu_G)^2}{\alpha^3} + constant \qquad \text{(S1)}$$

where $\bar{\nu}_A - \bar{\nu}_F$ ($\Delta\nu$) is equal to the Stokes shift, h is Planck's constant, c is the speed of light, μ_e-μ_g is the difference in dipole moment between the excited and ground state dipoles, a is the molecular cavity radius (assumed spherical), and Δf is the solvent polarizability. Δf is a measure of the effect of solvent reorganization and is expressed as

$$\Delta f = \left(\frac{\varepsilon-1}{2\varepsilon+1} - \frac{n^2-1}{2n^2+1}\right) \qquad \text{(S2)}$$

where ε is the dielectric constant of the solvent and n is its refractive index. As anticipated from Eq. S1, a linear relationship between Δf and $\Delta\nu$ is expected using this model. Figure S13 shows the experimentally determined Stokes shift plotted as a function of solvent polarity (Δf), also known as a Lippert-Mataga (L-M) plot.

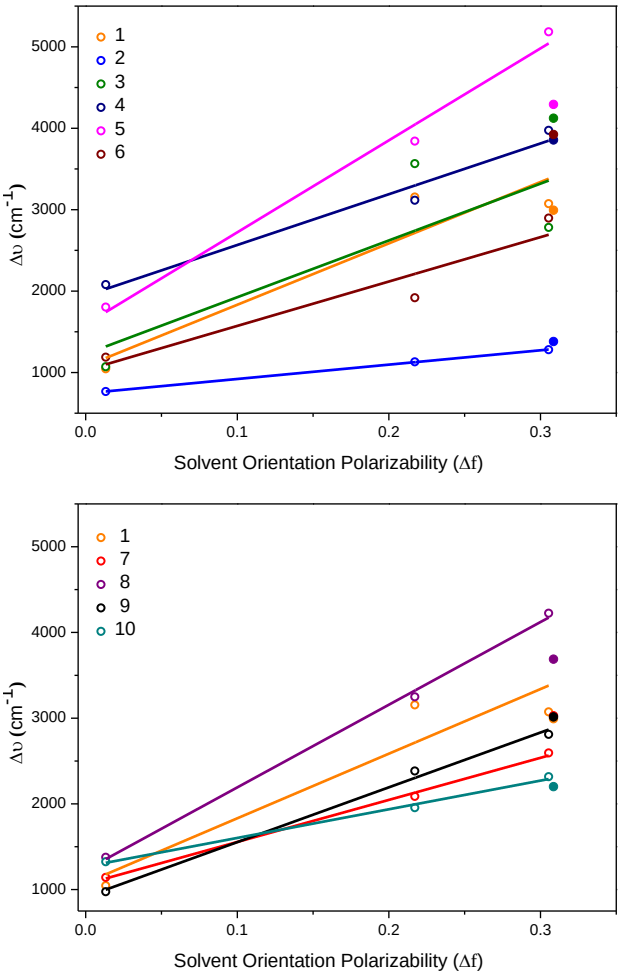

Figure S13. Lippert-Mataga plots for all molecules showing the variation in Stokes shift ($\Delta\nu$) as a function of solvent orientation polarizability. Data points collected in methanol are shown as filled circle and not considered for calculated L-M slope.

Kamlet-Taft analysis

Due to the potential for hydrogen bonding in these molecules, a more in-depth evaluation of specific solvatochromic properties through Kamlet-Taft analysis has been conducted. Kamlet-Taft analysis utilizes empirically derived values for a solvents capacity to serve as a Brönsted acid (α), Brönsted base (β) and its polarity and polarizability (π) for the determination of specific solute-solvent interactions. The Kamlet-Taft equation is given as

$$XYZ = XYZ_O + s\pi^* + a\alpha + b\beta \qquad \text{(eqn. S3)}$$

where XYZ is the molecular parameter being explored, XYZ_0 is the value in the absence of solvent, π*, α, and β are the Kamlet-Taft solvent parameters as stated above, s, a, and b are the molecules susceptibility to these parameters. Table S2 shows the calculated susceptibilities a, b, and s for **1** - **10** determined through multiple linear regression of the experimentally determined emission maxima in toluene, dichloromethane, methanol, and acetonitrile.

Table S2. Calculated susceptibilities to α, β, and π* Kamlet-Taft solvent parameters determined through multiple linear regression of λ_{em} in toluene, dichloromethane, methanol, and acetonitrile.

	Intercept	s	a	b
1	22.22	-4.80	0.49	-4.27
2	22.20	-1.24	-0.15	-0.26
3	22.12	-3.95	-0.17	-2.03
4	21.31	-4.01	0.43	-3.15
5	19.05	-5.67	1.25	-4.16
6	17.83	-2.51	-0.38	-2.21
7	19.92	-6.02	-0.17	-2.97
8	21.04	-8.59	0.62	-4.31
9	21.00	-5.86	-0.25	-2.63
10	20.98	-5.01	0.22	-2.30

Table S3. Crystal data and structure refinement for **5**·$CHCl_3$.

Identification code	**5**·$CHCl_3$
Empirical formula	C36 H24 B Cl3 F2 O2
Formula weight	643.71
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 7.3937(4) A alpha = 84.631(4) deg. b = 12.7776(8) A beta = 88.516(4) deg. c = 15.8112(9) A gamma = 80.334(4) deg.
Volume	1466.00(15) A^3
Z, Calculated density	2, 1.458 Mg/m^3
Absorption coefficient	0.360 mm^-1
F(000)	660
Crystal size	0.50 x 0.10 x 0.03 mm
Theta range for data collection	2.17 to 25.00 deg.
Limiting indices	-8<=h<=8, -15<=k<=15, -18<=l<=18
Reflections collected / unique	19570 / 5116 [R(int) = 0.0877]
Completeness to theta = 25.00	99.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.6085
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5116 / 0 / 407
Goodness-of-fit on F^2	0.983

Final R indices [I>2sigma(I)]	R1 = 0.0702, wR2 = 0.1521
R indices (all data)	R1 = 0.1518, wR2 = 0.1739
Largest diff. peak and hole	0.668 and -0.568 e.A^-3

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5**·$CHCl_3$. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
B(11)	1672(7)	6250(4)	5859(3)	31(1)
F(11)	3244(3)	6591(2)	6114(2)	40(1)
F(12)	191(4)	6623(2)	6322(2)	45(1)
O(11)	1350(4)	6623(2)	4952(2)	29(1)
O(16)	2020(4)	5061(2)	5976(2)	28(1)
C(12)	2079(5)	6035(3)	4353(3)	24(1)
C(13)	2910(5)	4993(3)	4549(2)	23(1)
C(14)	2805(5)	4508(3)	5371(2)	22(1)
C(121)	1880(5)	6488(3)	3488(3)	25(1)
C(122)	865(5)	7437(3)	3267(3)	25(1)
C(131)	339(5)	7958(3)	2430(2)	22(1)
C(132)	164(5)	9083(3)	2291(2)	23(1)
C(133)	-500(5)	9629(3)	1498(2)	22(1)
C(134)	-895(5)	9035(3)	863(3)	28(1)
C(135)	-708(5)	7928(3)	965(3)	26(1)
C(136)	-123(5)	7365(3)	1760(3)	24(1)
C(143)	657(5)	9725(3)	2917(2)	26(1)
C(144)	431(6)	10805(3)	2786(3)	32(1)
C(145)	-256(6)	11326(4)	2010(3)	32(1)
C(146)	-706(5)	10765(3)	1386(3)	28(1)
C(151)	-152(6)	6253(3)	1857(3)	32(1)
C(152)	-599(6)	5741(4)	1192(3)	38(1)
C(153)	-1089(6)	6287(4)	405(3)	39(1)
C(154)	-1165(6)	7355(4)	290(3)	33(1)
C(155)	3443(5)	3394(3)	5580(2)	23(1)
C(156)	3338(5)	2930(3)	6370(2)	23(1)

C(161)	3845(5)	1817(3)	6703(2)	20(1)
C(162)	3530(5)	967(3)	6250(2)	21(1)
C(163)	4044(5)	-111(3)	6623(3)	23(1)
C(164)	4778(5)	-290(3)	7428(3)	28(1)
C(165)	5017(5)	529(3)	7913(2)	25(1)
C(166)	4575(5)	1606(3)	7540(2)	23(1)
C(173)	2603(5)	1101(3)	5458(2)	26(1)
C(174)	2291(6)	249(3)	5065(3)	33(1)
C(175)	2890(6)	-808(3)	5407(3)	33(1)
C(176)	3741(6)	-972(3)	6166(3)	30(1)
C(181)	4924(5)	2421(3)	8037(3)	27(1)
C(182)	5565(6)	2207(4)	8836(3)	32(1)
C(183)	5934(6)	1145(4)	9205(3)	34(1)
C(184)	5689(6)	334(4)	8750(3)	32(1)
C(9)	5036(7)	3543(4)	1960(3)	53(1)
Cl(91)	2972(2)	3429(1)	2505(1)	60(1)
Cl(92)	5191(2)	2898(1)	1042(1)	73(1)
Cl(9A)	5670(40)	4696(18)	1896(6)	79(5)
Cl(9B)	4850(50)	4963(12)	1590(30)	123(9)

Table S5. Bond lengths [A] and angles [deg] for **5**·$CHCl_3$.

B(11)-F(12)	1.345(6)
B(11)-F(11)	1.390(5)
B(11)-O(11)	1.481(5)
B(11)-O(16)	1.492(6)
O(11)-C(12)	1.312(5)
O(16)-C(14)	1.309(5)
C(12)-C(13)	1.380(5)
C(12)-C(121)	1.435(5)
C(13)-C(14)	1.394(5)
C(13)-H(13)	0.9500
C(14)-C(155)	1.433(5)
C(121)-C(122)	1.336(5)
C(121)-H(121)	0.9500
C(122)-C(131)	1.456(5)
C(122)-H(122)	0.9500
C(131)-C(132)	1.419(5)
C(131)-C(136)	1.438(5)
C(132)-C(133)	1.433(5)
C(132)-C(143)	1.434(5)
C(133)-C(134)	1.378(6)

C(133)-C(146)	1.428(6)
C(134)-C(135)	1.393(6)
C(134)-H(134)	0.9500
C(135)-C(154)	1.427(6)
C(135)-C(136)	1.428(5)
C(136)-C(151)	1.419(6)
C(143)-C(144)	1.359(6)
C(143)-H(143)	0.9500
C(144)-C(145)	1.405(6)
C(144)-H(144)	0.9500
C(145)-C(146)	1.351(6)
C(145)-H(145)	0.9500
C(146)-H(146)	0.9500
C(151)-C(152)	1.365(6)
C(151)-H(151)	0.9500
C(152)-C(153)	1.393(6)
C(152)-H(152)	0.9500
C(153)-C(154)	1.351(6)
C(153)-H(153)	0.9500
C(154)-H(154)	0.9500
C(155)-C(156)	1.337(5)
C(155)-H(155)	0.9500
C(156)-C(161)	1.459(5)
C(156)-H(156)	0.9500
C(161)-C(162)	1.409(5)
C(161)-C(166)	1.428(5)
C(162)-C(173)	1.425(5)
C(162)-C(163)	1.441(5)
C(163)-C(164)	1.381(5)
C(163)-C(176)	1.422(5)
C(164)-C(165)	1.390(5)
C(164)-H(164)	0.9500
C(165)-C(184)	1.412(5)
C(165)-C(166)	1.434(5)
C(166)-C(181)	1.421(5)
C(173)-C(174)	1.357(6)
C(173)-H(173)	0.9500
C(174)-C(175)	1.410(6)
C(174)-H(174)	0.9500
C(175)-C(176)	1.351(5)
C(175)-H(175)	0.9500
C(176)-H(176)	0.9500
C(181)-C(182)	1.349(5)
C(181)-H(181)	0.9500
C(182)-C(183)	1.411(6)
C(182)-H(182)	0.9500

C(183)-C(184)	1.354(6)
C(183)-H(183)	0.9500
C(184)-H(184)	0.9500
C(9)-Cl(9A)	1.611(13)
C(9)-Cl(92)	1.727(5)
C(9)-Cl(91)	1.753(5)
C(9)-Cl(9B)	1.84(2)
C(9)-H(9)	1.0000

F(12)-B(11)-F(11)	111.9(4)
F(12)-B(11)-O(11)	109.4(4)
F(11)-B(11)-O(11)	108.6(4)
F(12)-B(11)-O(16)	109.4(4)
F(11)-B(11)-O(16)	107.0(4)
O(11)-B(11)-O(16)	110.4(4)
C(12)-O(11)-B(11)	120.6(3)
C(14)-O(16)-B(11)	120.4(3)
O(11)-C(12)-C(13)	120.7(4)
O(11)-C(12)-C(121)	117.9(4)
C(13)-C(12)-C(121)	121.2(4)
C(12)-C(13)-C(14)	120.4(4)
C(12)-C(13)-H(13)	119.8
C(14)-C(13)-H(13)	119.8
O(16)-C(14)-C(13)	120.0(4)
O(16)-C(14)-C(155)	117.6(3)
C(13)-C(14)-C(155)	122.4(4)
C(122)-C(121)-C(12)	122.9(4)
C(122)-C(121)-H(121)	118.6
C(12)-C(121)-H(121)	118.6
C(121)-C(122)-C(131)	130.1(4)
C(121)-C(122)-H(122)	114.9
C(131)-C(122)-H(122)	114.9
C(132)-C(131)-C(136)	119.3(3)
C(132)-C(131)-C(122)	119.1(4)
C(136)-C(131)-C(122)	121.5(4)
C(131)-C(132)-C(133)	120.5(4)
C(131)-C(132)-C(143)	122.6(3)
C(133)-C(132)-C(143)	116.9(4)
C(134)-C(133)-C(146)	122.2(4)
C(134)-C(133)-C(132)	118.7(4)
C(146)-C(133)-C(132)	119.1(4)
C(133)-C(134)-C(135)	122.8(4)
C(133)-C(134)-H(134)	118.6
C(135)-C(134)-H(134)	118.6
C(134)-C(135)-C(154)	120.4(4)
C(134)-C(135)-C(136)	119.8(4)

C(154)-C(135)-C(136)	119.8(4)
C(151)-C(136)-C(135)	117.3(4)
C(151)-C(136)-C(131)	123.8(4)
C(135)-C(136)-C(131)	118.8(4)
C(144)-C(143)-C(132)	122.0(4)
C(144)-C(143)-H(143)	119.0
C(132)-C(143)-H(143)	119.0
C(143)-C(144)-C(145)	120.1(4)
C(143)-C(144)-H(144)	119.9
C(145)-C(144)-H(144)	119.9
C(146)-C(145)-C(144)	120.8(4)
C(146)-C(145)-H(145)	119.6
C(144)-C(145)-H(145)	119.6
C(145)-C(146)-C(133)	121.1(4)
C(145)-C(146)-H(146)	119.5
C(133)-C(146)-H(146)	119.5
C(152)-C(151)-C(136)	120.6(4)
C(152)-C(151)-H(151)	119.7
C(136)-C(151)-H(151)	119.7
C(151)-C(152)-C(153)	121.8(4)
C(151)-C(152)-H(152)	119.1
C(153)-C(152)-H(152)	119.1
C(154)-C(153)-C(152)	120.0(4)
C(154)-C(153)-H(153)	120.0
C(152)-C(153)-H(153)	120.0
C(153)-C(154)-C(135)	120.4(4)
C(153)-C(154)-H(154)	119.8
C(135)-C(154)-H(154)	119.8
C(156)-C(155)-C(14)	122.2(4)
C(156)-C(155)-H(155)	118.9
C(14)-C(155)-H(155)	118.9
C(155)-C(156)-C(161)	130.5(4)
C(155)-C(156)-H(156)	114.7
C(161)-C(156)-H(156)	114.7
C(162)-C(161)-C(166)	119.9(4)
C(162)-C(161)-C(156)	122.3(3)
C(166)-C(161)-C(156)	117.6(4)
C(161)-C(162)-C(173)	124.1(4)
C(161)-C(162)-C(163)	119.2(4)
C(173)-C(162)-C(163)	116.5(4)
C(164)-C(163)-C(176)	121.1(4)
C(164)-C(163)-C(162)	119.4(4)
C(176)-C(163)-C(162)	119.5(4)
C(163)-C(164)-C(165)	123.0(4)
C(163)-C(164)-H(164)	118.5
C(165)-C(164)-H(164)	118.5

C(164)-C(165)-C(184)	122.3(4)
C(164)-C(165)-C(166)	118.4(4)
C(184)-C(165)-C(166)	119.3(4)
C(181)-C(166)-C(161)	123.1(4)
C(181)-C(166)-C(165)	116.9(4)
C(161)-C(166)-C(165)	119.9(4)
C(174)-C(173)-C(162)	121.3(4)
C(174)-C(173)-H(173)	119.4
C(162)-C(173)-H(173)	119.4
C(173)-C(174)-C(175)	122.1(4)
C(173)-C(174)-H(174)	118.9
C(175)-C(174)-H(174)	118.9
C(176)-C(175)-C(174)	118.6(4)
C(176)-C(175)-H(175)	120.7
C(174)-C(175)-H(175)	120.7
C(175)-C(176)-C(163)	121.8(4)
C(175)-C(176)-H(176)	119.1
C(163)-C(176)-H(176)	119.1
C(182)-C(181)-C(166)	122.2(4)
C(182)-C(181)-H(181)	118.9
C(166)-C(181)-H(181)	118.9
C(181)-C(182)-C(183)	120.3(4)
C(181)-C(182)-H(182)	119.9
C(183)-C(182)-H(182)	119.9
C(184)-C(183)-C(182)	120.1(4)
C(184)-C(183)-H(183)	120.0
C(182)-C(183)-H(183)	120.0
C(183)-C(184)-C(165)	121.2(4)
C(183)-C(184)-H(184)	119.4
C(165)-C(184)-H(184)	119.4
Cl(9A)-C(9)-Cl(92)	116.9(5)
Cl(9A)-C(9)-Cl(91)	116.7(10)
Cl(92)-C(9)-Cl(91)	110.9(3)
Cl(9A)-C(9)-Cl(9B)	25.6(7)
Cl(92)-C(9)-Cl(9B)	104.7(12)
Cl(91)-C(9)-Cl(9B)	105.2(6)
Cl(9A)-C(9)-H(9)	103.3
Cl(92)-C(9)-H(9)	103.3
Cl(91)-C(9)-H(9)	103.3
Cl(9B)-C(9)-H(9)	128.9

Symmetry transformations used to generate equivalent atoms:

Table S6. Anisotropic displacement parameters (A^2 x 10^3) for **5**·$CHCl_3$.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
B(11)	41(3)	26(3)	24(3)	-3(2)	6(3)	-8(3)
F(11)	54(2)	26(2)	45(2)	-3(1)	-11(1)	-16(1)
F(12)	55(2)	36(2)	39(2)	-3(1)	15(1)	2(1)
O(11)	42(2)	20(2)	25(2)	-2(1)	1(1)	-5(1)
O(16)	41(2)	21(2)	23(2)	-1(1)	2(1)	-7(1)
C(12)	22(2)	23(3)	27(2)	0(2)	1(2)	-11(2)
C(13)	28(2)	22(3)	20(2)	-2(2)	2(2)	-7(2)
C(14)	25(2)	23(3)	19(2)	-1(2)	-6(2)	-12(2)
C(121)	28(2)	23(3)	25(2)	1(2)	3(2)	-6(2)
C(122)	28(2)	25(3)	22(2)	1(2)	-2(2)	-9(2)
C(131)	21(2)	26(3)	21(2)	-1(2)	-1(2)	-6(2)
C(132)	25(2)	21(3)	24(2)	0(2)	-2(2)	-7(2)
C(133)	22(2)	25(3)	19(2)	2(2)	2(2)	-6(2)
C(134)	27(2)	29(3)	24(2)	9(2)	-5(2)	-4(2)
C(135)	22(2)	31(3)	27(2)	-6(2)	1(2)	-9(2)
C(136)	20(2)	24(3)	27(2)	-2(2)	1(2)	-4(2)
C(143)	28(2)	30(3)	19(2)	3(2)	-5(2)	-6(2)
C(144)	37(3)	29(3)	32(3)	-5(2)	0(2)	-15(2)
C(145)	38(3)	24(3)	35(3)	4(2)	1(2)	-11(2)
C(146)	31(2)	25(3)	26(2)	7(2)	-4(2)	-7(2)
C(151)	37(3)	28(3)	31(3)	-3(2)	-6(2)	-4(2)
C(152)	44(3)	27(3)	44(3)	-8(2)	-3(2)	-4(2)
C(153)	47(3)	36(3)	36(3)	-17(2)	-4(2)	-9(2)
C(154)	34(3)	39(3)	26(2)	-6(2)	-4(2)	-4(2)
C(155)	27(2)	18(2)	25(2)	-5(2)	-2(2)	-9(2)
C(156)	23(2)	24(3)	24(2)	-5(2)	0(2)	-9(2)
C(161)	21(2)	22(2)	20(2)	1(2)	2(2)	-9(2)
C(162)	22(2)	19(2)	24(2)	-1(2)	4(2)	-8(2)
C(163)	23(2)	17(2)	30(2)	-5(2)	3(2)	-4(2)
C(164)	31(2)	16(2)	37(3)	2(2)	0(2)	-7(2)
C(165)	24(2)	26(3)	24(2)	1(2)	0(2)	-6(2)
C(166)	21(2)	25(3)	23(2)	1(2)	2(2)	-7(2)
C(173)	32(2)	24(3)	23(2)	0(2)	1(2)	-10(2)
C(174)	42(3)	31(3)	27(2)	-4(2)	-4(2)	-11(2)
C(175)	41(3)	27(3)	35(3)	-12(2)	5(2)	-11(2)
C(176)	34(3)	18(3)	39(3)	-2(2)	1(2)	-7(2)

C(181)	29(2)	28(3)	27(2)	-1(2)	0(2)	-13(2)
C(182)	35(3)	39(3)	26(3)	-4(2)	-1(2)	-17(2)
C(183)	28(2)	49(3)	24(2)	4(2)	-8(2)	-9(2)
C(184)	33(3)	34(3)	27(3)	8(2)	-2(2)	-8(2)
C(9)	49(3)	60(4)	55(3)	-19(3)	2(3)	-16(3)
Cl(91)	51(1)	53(1)	76(1)	-5(1)	7(1)	-14(1)
Cl(92)	116(1)	55(1)	48(1)	-15(1)	0(1)	-5(1)
Cl(9A)	96(8)	56(6)	101(6)	-23(3)	17(5)	-50(6)
Cl(9B)	126(12)	50(4)	209(17)	-44(7)	87(13)	-51(6)

Table S7. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5**·$CHCl_3$.

	x	y	z	U(eq)
H(13)	3559	4604	4120	28
H(121)	2496	6095	3054	30
H(122)	415	7836	3729	30
H(134)	-1313	9397	333	33
H(143)	1156	9384	3440	31
H(144)	738	11209	3220	38
H(145)	-406	12081	1922	38
H(146)	-1166	11131	865	33
H(151)	143	5860	2390	38
H(152)	-576	4993	1267	46
H(153)	-1370	5908	-51	46
H(154)	-1526	7727	-244	39
H(155)	3958	2970	5143	27
H(156)	2856	3401	6781	28
H(164)	5137	-1005	7662	33
H(173)	2196	1800	5200	31
H(174)	1649	369	4543	39
H(175)	2698	-1393	5110	40
H(176)	4149	-1682	6400	36
H(181)	4698	3141	7798	33
H(182)	5769	2772	9151	38
H(183)	6355	999	9773	40
H(184)	5975	-379	8999	38
H(9)	5983	3087	2335	64

References

1. Lippert, E., *Z. Elektrochem* **1957,** *61*, 962.
2. Mataga, N.; Kaifu, Y.; Koizumi, M., *Bulletin of the Chemical Society of Japan* **1956,** *29*, 465-470.
3. Lakowicz, J. R., *Principles of Fluorescence Spectroscopy*. Springer US: 2007.