Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

1. Experimental data for all molecules investigated

2. Gas phase ground state B3LYP/6-31+G(d) optimised geometries for molecules in the test subset

3. Tuned range-separation parameters for all molecules

4. Basis set effect on vertical excitation energies

5. Effect of spectral HWHM on the calculated fluorescence lifetimes

6. Charge-transfer diagnostics for VI

7. Fluorescence lifetime calculations for all functionals and molecules investigated

8. Ground and excited state optimised geometries for all molecules using the LC-BLYP* functional

9. Dependence of the range-separation parameter on the basis set and molecular geometry

1. Experimental data for all molecules investigated

Table S1: Experimental quantum yields and fluorescence lifetimes (in ns) of all molecules investigated in this study, as taken from the literature.

	Solvent	ϕ_f	τ_f	**Ref.**
I	Cyclohexane	0.92	12.7	[1]
II	Cyclohexane	0.87	11.5	[2, 3]
III	Acetonitrile	0.98	5.5	[4]
IV	MethylCyclohexane	0.97	6.2	[4]
V	Cyclohexane	1.00	7.5	[1]
VI	Ethanol	0.97	10.5	[5]
VII	Ethanol	0.98	10.6	[5]
VIII	Ethanol	0.99	10.7	[5]
IX	Cyclohexane	0.94	1.36	[1]
X	Methanol	0.85	1.17	[1]
XI	1,4-dioxane	0.90	0.64	[6]
XII	Cyclohexane	0.82	0.87	[7]
XIII	1,4-dioxane	0.92	7.4	[8]
XIV	1,4-dioxane	0.97	9.8	[8]
XV	1,4-dioxane	1.00	17.0	[8]
XVI	1,4-dioxane	1.00	10.7	[8]
XVII	1,4-dioxane	0.90	12.3	[8]
XVIII	1,4-dioxane	0.78	9.0	[8]
XIX	Acetonitrile	0.92	5.2	[9]
XX	Acetonitrile	0.80	3.5	[9]
XXI	Ethyl Acetate	0.99	3.1	[9]
XXII	Cyclohexane	1.00	4.1	[9]
XXIII	Ethanol	0.93	5.4	[9]
XXIV	Toluene	0.90	3.3	[10]

Table S2: Experimental absorption (λ_{abs}), emission (λ_{emi}) and Stokes shift of all molecules in solvent investigated in this study, as taken from the literature. All values are in eV

	Solvent	λ_{abs}	λ_{emi}	Stokes shift	Ref.
I	Cyclohexane	3.271	3.084	0.187	[1]
II	Cyclohexane	2.959	2.938	0.021	[2]
III	Acetonitrile	2.863	2.837	0.026	[4]
IV	MethylCyclohexane	2.837	2.799	0.038	[4]
V	Cyclohexane	3.324	3.061	0.263	[1]
VI	Ethanol	3.116	3.002	0.114	[5]
VII	Ethanol	3.080	2.931	0.149	[5]
VIII	Ethanol	3.123	2.994	0.129	[5]
IX	Cyclohexane	4.092	3.473	0.619	[1]
X	Methanol	4.476	3.690	0.786	[1]
XI	1,4-dioxane	3.875	3.573	0.301	[6]
XII	Cyclohexane	4.240	3.397	0.843	[7]
XIII	1,4-dioxane	3.408	3.174	0.234	[8]
XIV	1,4-dioxane	3.495	3.196	0.299	[8]
XV	1,4-dioxane	3.647	2.871	0.776	[8]
XVI	1,4-dioxane	3.369	2.888	0.481	[8]
XVII	1,4-dioxane	3.447	2.944	0.503	[8]
XVIII	1,4-dioxane	4.003	2.862	1.140	[8]
XIX	Acetonitrile	3.397	2.666	0.731	[9]
XX	Acetonitrile	3.502	2.952	0.550	[9]
XXI	Ethyl Acetate	3.434	2.980	0.454	[9]
XXII	Cyclohexane	3.297	2.863	0.434	[9]
XXIII	Ethanol	3.031	2.475	0.557	[9]
XXIV	Toluene	3.289	2.792	0.496	[10]

Table S3: Refractive index (n) of all solvents used in the calculation of fluorescence lifetimes. All values were taken from the CRC Handbook of Chemistry and Physics.[11]

Solvent	n
1,4-dioxane	1.4224
Acetonitrile	1.3442
Cyclohexane	1.4235
Ethanol	1.3611
Ethyl Acetate	1.3723
Methanol	1.3288
MethylCyclohexane	1.4231
Toluene	1.4941

2. Gas phase ground state B3LYP/6-31+G(d) optimised geometries for molecules in the test set

I

C -9.640514 -1.130303 -0.002846

C -8.269467 -1.111809 0.000707

C -7.551194 0.125649 0.003561

C -8.293358 1.362565 0.002645

C -9.720486 1.302363 -0.001096

C -10.371540 0.093228 -0.003745

C -6.150884 0.163675 0.007213

C -7.575368 2.585300 0.005484

C -6.157870 2.618744 0.009168

C -5.437244 1.369145 0.010017

C -4.006734 1.395718 0.013725

H -3.471414 0.449067 0.014350

C -3.324322 2.585027 0.016418

C -4.038598 3.818392 0.015573

C -5.411713 3.836853 0.012067

H -5.598948 -0.774501 0.007891

H -10.175991 -2.075787 -0.004998

H -7.702012 -2.039568 0.001419

H -10.286661 2.229171 -0.001815

H -11.457919 0.066525 -0.006558

H -2.237776 2.593641 0.019200

H -3.487473 4.754986 0.017743

H -5.946600 4.782062 0.011456

C -8.300969 3.818681 0.004623

N -8.891911 4.823125 0.003924

VI

C -7.688542 -5.356115 -0.065777

C -6.303897 -5.387261 0.000062

C -5.549260 -4.199142 -0.012249

C -6.225081 -2.960229 -0.093340

C -7.632994 -2.929316 -0.160393

C -8.350396 -4.116187 -0.146237

C -4.073100 -4.250911 0.058865

C -4.120228 -1.739483 -0.044134

C -3.383328 -2.942978 0.038202

C -1.978638 -2.878966 0.100659

H -1.438076 -3.818496 0.163540

C -1.316566 -1.660807 0.082334

C -2.061292 -0.468905 0.000217

C -3.446413 -0.501213 -0.062506

H -8.260684 -6.279305 -0.055396

H -5.759151 -6.324371 0.063061

H -8.149527 -1.973493 -0.223117

H -9.435676 -4.082586 -0.197958

H -0.232136 -1.623259 0.130664

H -1.550201 0.490369 -0.014715

H -4.017456 0.422997 -0.126064

N -5.499774 -1.784310 -0.106516

H -6.005219 -0.910365 -0.166635

O -3.455781 -5.318284 0.130834

IX

C -7.233047 0.816458 -1.080443

C -7.239141 0.809780 1.106539

C -8.003272 -0.216742 0.617344

H -8.560002 -0.964802 1.163741

C -6.882760 1.288651 2.434371

C -6.042744 2.404340 2.605189

C -7.379261 0.634220 3.578686

C -5.710600 2.849881 3.885043

H -5.652261 2.918638 1.732929

C -7.043839 1.083800 4.853615

H -8.029879 -0.229193 3.469206

C -6.207639 2.194363 5.014682

H -5.060312 3.713537 3.998533

H -7.436587 0.566012 5.724883

H -5.947420 2.543635 6.010271

C -6.876069 1.294515 -2.411857

C -6.042239 2.411882 -2.589766

C -7.378425 0.620738 -3.539840

C -5.718032 2.845568 -3.875470

H -5.651334 2.935745 -1.723200

C -7.049839 1.060183 -4.820369

H -8.021698 -0.241405 -3.394912

C -6.219256 2.173277 -4.994113

H -5.072533 3.710666 -4.003262

H -7.442658 0.533316 -5.686100

H -5.964888 2.513736 -5.994472

O -6.740819 1.478074 0.008952

N -7.990146 -0.200002 -0.761366

XIII

C -1.255828 -1.346022 -0.182851

C -0.022441 -2.130289 0.000937

C 1.042626 -1.290890 -0.041310

C 1.044062 1.287450 -0.086706

C -0.020065 2.129010 -0.074103

C -1.254328 1.340145 -0.230277

N 0.607083 -0.005501 -0.292505

N -0.770350 -0.006371 -0.385161

O -2.422537 -1.675799 -0.188381

O -2.420664 1.670832 -0.247481

H 2.104260 1.482699 0.008541

H 2.102612 -1.483890 0.060664

H -0.011433 -3.201805 0.134577

H -0.007863 3.204555 0.021716

XIX

C -7.278096 -2.321418 -0.048780

C -5.878242 -2.279564 0.012173

C -5.225888 -1.052105 0.023848

C -5.923945 0.176255 -0.021729

C -7.334821 0.109344 -0.083475

C -7.998024 -1.102434 -0.097094

H -5.284406 -3.188044 0.045578

C -5.124265 1.378600 0.000278

H -7.915803 1.023497 -0.119881

H -9.083358 -1.123068 -0.151176

C -3.769146 1.317471 0.062379

C -3.064986 0.043530 0.109819

H -3.145488 2.201687 0.079804

N -7.947005 -3.528812 -0.112461

H -7.450442 -4.359552 0.180854

H -8.929782 -3.534296 0.125352

C -5.798470 2.734491 -0.049187

F -6.650598 2.904584 0.994498

F -4.918870 3.755850 -0.010306

F -6.529911 2.883036 -1.183304

O -3.861170 -1.097731 0.086290

O -1.864636 -0.101635 0.167281

3. Tuned range-separation parameters for all molecules

Table S4. Tuned range separation parameter γ ($Bohr^{-1}$) for all molecules with the LC-BLYP* and ωB97X* functionals. The default values for LC-BLYP and ωB97X are 0.4700 $Bohr^{-1}$ and 0.3000 $Bohr^{-1}$ respectively. R^2 refers to the coefficient of determination for the fit.

	LC-BLYP*		**ωB97X***	
	γ	R^2	γ	R^2
I	0.2216	0.9997	0.1900	0.9996
II	0.2159	0.9997	0.1850	0.9995
III	0.2098	0.9994	0.1797	0.9990
IV	0.2151	0.9996	0.1841	0.9992
V	0.1831	0.9993	0.1373	0.9994
VI	0.2333	0.9998	0.1974	0.9997
VII	0.2230	0.9997	0.1886	0.9995
VIII	0.2052	0.9998	0.1730	0.9997
IX	0.2143	0.9999	0.1833	0.9997
X	0.2066	0.9998	0.1770	0.9997
XI	0.1933	0.9998	0.1649	0.9999
XII	0.1911	0.9997	0.1646	0.9998
XIII	0.2829	0.9999	0.2398	0.9999
XIV	0.2592	0.9999	0.2194	0.9999
XV	0.2652	1.0000	0.2256	0.9999
XVI	0.2399	0.9999	0.2035	0.9998
XVII	0.2393	0.9999	0.2028	0.9998
XVIII	0.2429	1.0000	0.2059	0.9999
XIX	0.2468	0.9999	0.2106	0.9999
XX	0.2249	1.0000	0.1907	0.9999
XXI	0.2220	0.9999	0.1858	1.0000
XXII	0.2200	1.0000	0.1854	0.9998
XXIII	0.2120	1.0000	0.1785	0.9998
XXIV	0.2101	1.0000	0.1782	0.9998

4. Basis set effect on vertical excitation energies

The geometries used here are those from Section 2 of the Supporting Information

Table S5. Basis set effect on the gas phase vertical excitation energies (in eV) of **I** calculated using TD-DFT. Oscillator strengths are given in parentheses.

	6-31+G*	**6-311+G***	**def2TZVP**	**aug-cc-pVDZ**	**aug-cc-pVTZ**
B3LYP	3.0320 (0.0963)	3.0111 (0.0923)	2.9955 (0.0864)	2.9903 (0.0857)	2.9833 (0.0854)
BMK	3.3087 (0.1239)	3.2877 (0.1188)	3.2661 (0.1117)	3.2582 (0.1087)	3.2514 (0.1089)
CAM-B3LYP	3.3484 (0.1376)	3.3209 (0.1314)	3.2965 (0.1216)	3.2907 (0.1200)	3.2817 (0.1195)
LC-BLYP	3.6388 (0.1781)	3.6037 (0.1691)	3.5681 (0.1547)	3.5637 (0.1521)	3.5516 (0.1510)
M06	3.0175 (0.1027)	3.0062 (0.0982)	2.9925 (0.0932)	2.9701 (0.0908)	2.9849 (0.0911)
M06-2X	3.3813 (0.1314)	3.3477 (0.1259)	3.3345 (0.1176)	3.3200 (0.1139)	3.3087 (0.1144)
M11	3.5354 (0.1598)	3.4807 (0.1530)	3.4632 (0.1431)	3.4711 (0.1387)	3.4356 (0.1380)
PBE0	3.1138 (0.1033)	3.0918 (0.0992)	3.0718 (0.0923)	3.0670 (0.0912)	3.0596 (0.0908)
ωB97	3.5894 (0.1702)	3.5582 (0.1623)	3.5187 (0.1497)	3.5186 (0.1459)	3.5057 (0.1457)
ωB97X	3.5124 (0.1615)	3.4826 (0.1541)	3.4489 (0.1423)	3.4454 (0.1393)	3.4363 (0.1391)
LC-BLYP*	3.2655 (0.1281)	3.2398 (0.1223)	3.2163 (0.1127)	3.2091 (0.1119)	3.2010 (0.1112)
ωB97X*	3.3107 (0.1335)	3.2858 (0.1280)	3.2607 (0.1193)	3.2556 (0.1169)	3.2503 (0.1169)

Table S6. Basis set effect on the gas phase vertical excitation energies (in eV) of **VI** calculated using TD-DFT. Oscillator strengths are given in parentheses.

	6-31+G*	**6-311+G***	**def2TZVP**	**aug-cc-pVDZ**	**aug-cc-pVTZ**
B3LYP	3.5521 (0.0786)	3.5215 (0.0752)	3.5100 (0.0689)	3.4823 (0.0684)	3.4847 (0.0679)
BMK	3.8923 (0.1062)	3.8620 (0.1023)	3.8387 (0.0946)	3.8082 (0.0914)	3.8098 (0.0922)
CAM-B3LYP	3.9494 (0.1152)	3.9142 (0.1101)	3.8927 (0.0996)	3.8586 (0.0988)	3.8614 (0.0982)
LC-BLYP	4.2986 (0.1483)	4.2580 (0.1413)	4.2243 (0.1267)	4.1864 (0.1250)	4.1891 (0.1241)
M06	3.6433 (0.0830)	3.6069 (0.0798)	3.6054 (0.0742)	3.5722 (0.0723)	3.5638 (0.0727)
M06-2X	3.9435 (0.1148)	3.9159 (0.1106)	3.8930 (0.1010)	3.8477 (0.0975)	3.8639 (0.0980)
M11	4.0959 (0.1333)	4.0695 (0.1285)	4.0531 (0.1182)	3.9916 (0.1130)	4.0190 (0.1143)
PBE0	3.6569 (0.0856)	3.6259 (0.0823)	3.6058 (0.0001)	3.5795 (0.0740)	3.5824 (0.0736)
ωB97	4.2301 (0.1396)	4.1887 (0.1339)	4.1574 (0.1213)	4.1188 (0.1182)	4.1231 (0.1181)
ωB97X	4.1427 (0.1326)	4.1039 (0.1272)	4.0736 (0.1151)	4.0394 (0.1130)	4.0418 (0.1129)
LC-BLYP*	3.7893 (0.1059)	3.7556 (0.1010)	3.7333 (0.0902)	3.6988 (0.0904)	3.7008 (0.0897)
ωB97X*	3.9031 (0.1107)	3.8683 (0.1065)	3.8444 (0.0970)	3.8137 (0.0953)	3.8167 (0.0954)

Table S7. Basis set effect on the gas phase vertical excitation energies (in eV) of **IX** calculated using TD-DFT. Oscillator strengths are given in parentheses.

	6-31+G*	**6-311+G***	**def2TZVP**	**aug-cc-pVDZ**	**aug-cc-pVTZ**
B3LYP	3.7743 (0.8382)	3.7574 (0.8380)	3.7617 (0.8487)	3.7376 (0.8319)	3.7255 (0.8293)
BMK	4.1078 (0.9043)	4.0900 (0.9031)	4.0869 (0.9132)	4.0626 (0.9026)	4.0549 (0.8968)
CAM-B3LYP	4.1254 (0.8694)	4.1039 (0.8710)	4.1040 (0.8889)	4.0806 (0.8701)	4.0671 (0.8668)
LC-BLYP	4.4362 (0.8512)	4.4083 (0.8534)	4.3989 (0.8743)	4.3803 (0.8590)	4.3649 (0.8548)
M06	3.7625 (0.8047)	3.7590 (0.8083)	3.7728 (0.8334)	3.7261 (0.8068)	3.7361 (0.8008)
M06-2X	4.1714 (0.8863)	4.1451 (0.8864)	4.1580 (0.9108)	4.1255 (0.8888)	4.1096 (0.8847)
M11	4.3621 (0.8801)	4.3144 (0.8768)	4.3273 (0.9209)	4.3151 (0.8901)	4.2732 (0.8821)
PBE0	3.8760 (0.8604)	3.8576 (0.8611)	3.8569 (0.8734)	3.8357 (0.8571)	3.8235 (0.8547)
ωB97	4.4027 (0.8630)	4.3764 (0.8653)	4.3565 (0.8780)	4.3494 (0.8717)	4.3309 (0.8654)
ωB97X	4.3189 (0.8745)	4.2943 (0.8761)	4.2807 (0.8903)	4.2682 (0.8803)	4.2536 (0.8762)
LC-BLYP*	4.0378 (0.8598)	4.0197 (0.8612)	4.0253 (0.8790)	3.9965 (0.8572)	3.9850 (0.8548)
ωB97X*	4.0980 (0.8805)	4.0782 (0.8820)	4.0712 (0.8937)	4.0557 (0.8811)	4.0448 (0.8796)

Table S8. Basis set effect on the gas phase vertical excitation energies (in eV) of **XIII** calculated using TD-DFT. Oscillator strengths are given in parentheses.

	6-31+G*	**6-311+G***	**def2TZVP**	**aug-cc-pVDZ**	**aug-cc-pVTZ**
B3LYP	3.8052 (0.1986)	3.7963 (0.1935)	3.7881 (0.1871)	3.7571 (0.1819)	3.7628 (0.1813)
BMK	4.0057 (0.2318)	4.0047 (0.2261)	3.9844 (0.2184)	3.9586 (0.2107)	3.9634 (0.2099)
CAM-B3LYP	4.0090 (0.2355)	4.0024 (0.2288)	3.9893 (0.2194)	3.9557 (0.2133)	3.9632 (0.2120)
LC-BLYP	4.2255 (0.2744)	4.2226 (0.2655)	4.2041 (0.2530)	4.1683 (0.2461)	4.1773 (0.2442)
M06	3.8400 (0.1985)	3.8274 (0.1941)	3.8182 (0.1920)	3.7962 (0.1821)	3.7868 (0.1826)
M06-2X	4.0015 (0.2371)	3.9993 (0.2302)	3.9825 (0.2193)	3.9457 (0.2144)	3.9637 (0.2118)
M11	4.0239 (0.2476)	4.0232 (0.2433)	4.0053 (0.2302)	3.9681 (0.2230)	3.9785 (0.2241)
PBE0	3.8798 (0.2082)	3.8717 (0.2026)	3.8581 (0.1949)	3.8289 (0.1890)	3.8343 (0.1886)
ωB97	4.1662 (0.2646)	4.1598 (0.2578)	4.1409 (0.2469)	4.1111 (0.2383)	4.1156 (0.2373)
ωB97X	4.1098 (0.2540)	4.1034 (0.2476)	4.0842 (0.2373)	4.0556 (0.2292)	4.0597 (0.2285)
LC-BLYP*	3.9265 (0.2327)	3.9214 (0.2261)	3.9072 (0.2160)	3.8726 (0.2102)	3.8791 (0.2088)
ωB97X*	4.0193 (0.2390)	4.0123 (0.2335)	3.9940 (0.2243)	3.9670 (0.2165)	3.9699 (0.2162)

Table S9. Basis set effect on the gas phase vertical excitation energies (in eV) of **XIX** calculated using TD-DFT. Oscillator strengths are given in parentheses.

	6-31+G*	**6-311+G***	**def2TZVP**	**aug-cc-pVDZ**	**aug-cc-pVTZ**
B3LYP	3.6583 (0.3209)	3.6331 (0.3157)	3.6659 (0.3105)	3.6449 (0.3133)	3.6454 (0.3147)
BMK	3.9800 (0.3961)	3.9570 (0.3913)	3.9799 (0.3833)	3.9599 (0.3831)	3.9576 (0.3860)
CAM-B3LYP	4.0017 (0.3963)	3.9742 (0.3915)	3.9952 (0.3786)	3.9750 (0.3827)	3.9723 (0.3828)
LC-BLYP	4.2823 (0.4417)	4.2508 (0.4369)	4.2628 (0.4209)	4.2436 (0.4243)	4.2384 (0.4238)
M06	3.7229 (0.3367)	3.6989 (0.3328)	3.7387 (0.3300)	3.7120 (0.3290)	3.7117 (0.3311)
M06-2X	4.0241 (0.4067)	3.9996 (0.4019)	4.0225 (0.3910)	3.9959 (0.3912)	4.0015 (0.3936)
M11	4.1495 (0.4245)	4.1224 (0.4201)	4.1467 (0.4107)	4.1224 (0.4087)	4.1236 (0.4095)
PBE0	3.7642 (0.3440)	3.7392 (0.3392)	3.7680 (0.3322)	3.7475 (0.3349)	3.7488 (0.3360)
ωB97	4.2391 (0.4260)	4.2101 (0.4225)	4.2190 (0.4083)	4.2041 (0.4103)	4.1986 (0.4103)
ωB97X	4.1656 (0.4169)	4.1380 (0.4131)	4.1498 (0.3993)	4.1335 (0.4020)	4.1299 (0.4023)
LC-BLYP*	3.9095 (0.3656)	3.8837 (0.3616)	3.9037 (0.3466)	3.8812 (0.3524)	3.8779 (0.3528)
ωB97X*	4.0047 (0.3862)	3.9800 (0.3829)	3.9971 (0.3710)	3.9791 (0.3735)	3.9784 (0.3747)

Table S10. Basis set effect on the gas phase vertical excitation energies (in eV) calculated using correlated wave function methods. Oscillator strengths are given in parentheses where available.

	CIS(D)		CC2		EOM-CCSD	
	6-31+G(d)	6-311+G(d)	6-31+G(d)	6-311+G(d)	6-31+G(d)	6-311+G(d)
I	3.82	3.77	3.59 (0.1384)	3.54 (0.1309)	3.90 (0.1682)	3.85 (0.1610)
VI	4.65	4.60	4.46 (0.9718)	4.41 (0.9740)	4.67 (0.9082)	4.62 (0.9202)
IX	3.79	3.75	3.76 (0.1217)	3.71 (0.1155)	3.97 (0.1304)	3.94 (0.1252)
XIII	3.84	3.83	3.83 (0.3205)	3.82 (0.3137)	4.02 (0.3237)	4.01 (0.3156)
XIX	4.18	4.13	3.96 (0.4312)	3.91 (0.4264)	4.20 (0.4091)	4.16 (0.4118)

The basis set effect on the TD-DFT vertical excitation energies and oscillator strengths were then investigated using the test set. The results obtained using the 6-31+G(d),[12-15] 6-311+G(d),[15, 16] def2TZVP,[17] aug-cc-pVDZ basis sets[18-20] were compared to those using the aug-cc-pVTZ basis set.[18-20] The results are given in Tables S5 to S9. The aug-cc-pVDZ results were found to match the aug-cc-pVTZ results very closely, with their excitation energies and oscillator strengths within 0.02 eV and 0.01 of each other respectively. The def2TZVP results were slightly poorer, while the 6-31+G(d) and 6-311+G(d) basis sets returned excitation energies and oscillator strengths that were noticeable higher than the aug-cc-pVTZ values.

5. Effect of spectral HWHM on the calculated fluorescence lifetimes

Santoro and co-workers have proposed the use of PCM solvation in conjunction with the state-specific method as an *ab initio* approach towards calculating the solvent inhomogeneous broadening for an electronic transition.[21, 22] This is in turn used as the value of the half width at half-maximum (HWHM) of the Gaussian functions used to convolute the simulated vibronic spectra. However, the cited approach is known to underestimate the actual experimental width in the case of non-polar solvents. We have carried out the relevant calculations for the test set (**I**, **VI**, **IX**, **XIV**, **XIX**), and our findings agree with their work (Table S11). However, our set of experimental data consists of a mixture of polar and non-polar solvents. As it would not be desirable to only calculate the HWHM for molecules in polar solvents, we chose to keep the value of the HWHM constant throughout.

Table S11: The computed non-equilibrium and equilibrium vertical emission energy (ν_{emi}), solvation reorganisation energy for emission (λ), and HWHM for the convoluting function used in simulating the emission spectra for the molecules in the test set. All values are in cm^{-1}. The calculations were carried out using PBE0/aug-cc-pVDZ and assuming a temperature of $T = 298\,K$. For further details of the use of the state-specific method to estimate the band width, refer to Ferrer *et al*.[22]

	Solvent	ν_{emi} (non-eq.)	ν_{emi} (eq.)	λ	HWHM
I	Cyclohexane	21560	21560	~0	~0
VI	Cyclohexane	26510	26510	~0	~0
IX	Ethanol	25380	25300	80	220
XIII	1,4-dioxane	27520	27520	~0	~0
XIX	Acetonitrile	22160	21700	450	510

We then investigated the effect of varying the HWHM on the calculated fluorescence lifetimes. The value of the HWHM of the convoluting Gaussian function only affects the results obtained using Scheme C through the $\frac{1}{<\tilde{\nu}_f^{-3}>}$ term (see Table 1 in main paper).

Table S12 summarises the effect of varying the value of HWHM on the $\frac{1}{<\tilde{\nu}_f^{-3}>}$ term and resultant fluorescence lifetime.

Table S12: Effect of changing the HWHM (cm^{-1}) of each band in the simulated vibronic spectra on $\frac{1}{<\tilde{\nu}_f^{-3}>}(\times 10^{-13})$ and fluorescence lifetime, τ_f (ns) for the molecules in the test set, as calculated using the PBE0 functional.

	I		**VI**		**IX**		**XIII**		**XIX**	
HWHM	$\frac{1}{<\tilde{\nu}_f^{-3}>}$	τ_f	$\frac{1}{<\tilde{\nu}_f^{-3}>}$	τ_f	$\frac{1}{<\tilde{\nu}_f^{-3}>}$	τ_f	$\frac{1}{<\tilde{\nu}_f^{-3}>}$	τ_f	$\frac{1}{<\tilde{\nu}_f^{-3}>}$	τ_f
100	1.12	18.02	0.74	19.71	0.72	1.44	0.66	8.88	1.42	9.47
135 (Default)	1.12	18.02	0.74	19.71	0.72	1.44	0.66	8.88	1.42	9.47
200	1.12	18.03	0.74	19.71	0.72	1.44	0.66	8.88	1.42	9.47
300	1.12	18.04	0.74	19.72	0.72	1.44	0.66	8.88	1.42	9.48
400	1.12	18.05	0.74	19.73	0.72	1.44	0.66	8.89	1.43	9.49
500	1.12	18.08	0.74	19.76	0.72	1.45	0.66	8.90	1.43	9.50
600	1.12	18.14	0.74	19.81	0.72	1.45	0.66	8.91	1.43	9.52
700	1.13	18.23	0.75	19.87	0.73	1.45	0.66	8.94	1.44	9.55
800	1.14	18.33	0.75	19.96	0.73	1.46	0.67	8.97	1.44	9.59
900	1.14	18.46	0.75	20.06	0.73	1.46	0.67	9.01	1.45	9.63
1000	1.15	18.60	0.76	20.17	0.73	1.47	0.67	9.06	1.46	9.68

6. Charge-transfer diagnostics for VI

The charge-transfer criteria suggested by Autschbach and co-workers have been evaluated for the π-π* electronic transition of **VI** (Table S13).[23, 24] $O_{\pi\pi^*} = \left\langle \left|\phi_\pi(r)\right\| \phi_{\pi^*}(r) \right\rangle = \int \left|\phi_\pi(r)\phi_{\pi^*}(r)\right| dr$ refers to the spatial overlap integral between the transition orbitals, and $\frac{1}{2}\langle|\Delta\rho|\rangle$ measures the extent of charge transfer between "spatially disjointed" regions with $|\Delta\rho| = \left|\phi_\pi^2 - \phi_{\pi*}^2\right|$. Single point calculations for **VI** in the gas phase with two sets of functionals (BLYP and LC-BLYP*) were carried out and the resultant .fchk files saved for the following evaluation of the charge-transfer criteria. The cubegen and cubeman utilities of Gaussian09 were used in conjunction with the bash command ("sed –i 's/-\([0-9]\.[0-9]\+\)E/ \1E/g'") to obtain .cube files corresponding to $|\phi_{HOMO}||\phi_{LUMO}|$ and $|\Delta\rho|$, while numerical integration over grid points were performed with Gabedit.[25] The default "Medium" option was used as the parameters for the grid used to generate the .cube files in cubegen. Using this set of parameters, the integral of the SCF density of **VI** was found to be 101.8, close to the actual number of electrons in **VI** (102). The values of the calculated charge-transfer criteria is given in Table S12.

Table S13: CT criteria for the π-π* transition of **VI**. and $\frac{1}{2}\langle|\Delta\rho|\rangle$ were found to ~0.7 and ~0.6 respectively for the rhodamines studied in *ChemistryOpen*, 2017, **6**, 385-392. The calculations were carried out in the gas phase.

	O	$\frac{1}{2}\langle\|\Delta\rho\|\rangle$
BLYP	0.72	0.55
LC-BLYP*	0.71	0.57

Moore II *et al.*[23, 24] have suggested that large values for both the overlap integral O as well as the density change criteria $\frac{1}{2}\langle|\Delta\rho|\rangle$ may indicate differential electron correlation between the ground and excited state. In their study of the electronic excitations of

rhodamines, the values of O and $\frac{1}{2}\langle|\Delta\rho|\rangle$ were found to ~0.7 and ~0.6 respectively, which is similar to what we observed for **VI**. As a result, the problem in the results for acridones can similarly be attributed to differential electron correlation between the ground and excited state being treated poorly by TD-DFT.

7. Fluorescence lifetime calculations for all functionals and molecules investigated

Table S14: Vertical energies (in cm^{-1}) and oscillator strengths for the calculation of fluorescence lifetimes using Scheme A. The results were obtained at the ground state optimised geometries in solvent using the state-specific solvation method.

	B3LYP	**BMK**	**CAM-B3LYP**	**LC-BLYP**	**M06**	**M06-2X**	**M11**	**PBE0**	**ωB97**	**ωB97X**	**LC-BLYP***	**ωB97X***
I	23974 (0.0862)	26432 (0.1071)	27026 (0.1198)	30832 (0.1774)	24033 (0.0917)	27244 (0.1130)	28740 (0.1374)	24722 (0.0919)	29389 (0.1448)	28581 (0.1387)	25922 (0.1123)	26381 (0.1167)
II	21723 (0.1129)	24251 (0.1404)	24832 (0.1587)	28218 (0.2037)	21899 (0.1208)	25173 (0.1499)	26650 (0.1823)	22472 (0.1210)	27345 (0.1950)	26459 (0.1851)	23504 (0.1459)	24013 (0.1516)
III	22256 (0.3247)	24637 (0.3791)	25363 (0.3927)	28672 (0.4495)	22324 (0.3296)	25445 (0.3850)	27324 (0.4260)	23008 (0.3399)	28018 (0.4427)	27211 (0.4307)	24197 (0.3595)	24789 (0.3809)
IV	22614 (0.3424)	25179 (0.4031)	25813 (0.4158)	29295 (0.4808)	22797 (0.3546)	26006 (0.4103)	27770 (0.4510)	23343 (0.3587)	28447 (0.4655)	27617 (0.4527)	24669 (0.3798)	25160 (0.3991)
V	24609 (0.1311)	26800 (0.1836)	27656 (0.1871)	30815 (0.2396)	24412 (0.1485)	27646 (0.1875)	29124 (0.2362)	25250 (0.1460)	29929 (0.2344)	29182 (0.2218)	25228 (0.1748)	26274 (0.1677)
VI	26770 (0.0722)	29400 (0.0944)	29930 (0.1045)	32983 (0.1347)	27665 (0.0756)	29898 (0.1023)	31041 (0.1193)	27731 (0.0780)	32086 (0.1256)	31430 (0.1196)	29177 (0.1128)	29999 (0.1162)
VII	26057 (0.0827)	28605 (0.1058)	29169 (0.1181)	32185 (0.1514)	26943 (0.0862)	29047 (0.1152)	30134 (0.1348)	26977 (0.0888)	31296 (0.1404)	30652 (0.1339)	27481 (0.1068)	28416 (0.1101)
VIII	26592 (0.1009)	29229 (0.1314)	29783 (0.1464)	32840 (0.1887)	27478 (0.1060)	29695 (0.1429)	30773 (0.1676)	27556 (0.1088)	31928 (0.1758)	31291 (0.1674)	27600 (0.1254)	28677 (0.1321)

	B3LYP	BMK	CAM-B3LYP	LC-BLYP	M06	M06-2X	M11	PBE0	ωB97	ωB97X	LC-BLYP*	ωB97X*
IX	29659 (0.7983)	32998 (0.8887)	33676 (0.8557)	37210 (0.8426)	30038 (0.7856)	33957 (0.8693)	35833 (0.8739)	30784 (0.8321)	36349 (0.8489)	35659 (0.8615)	32400 (0.8340)	33136 (0.8630)
X	27241 (1.8994)	30127 (1.9951)	31296 (1.9309)	34855 (1.8462)	27629 (1.7950)	31579 (2.0016)	33642 (2.0034)	28196 (1.9493)	34044 (1.8627)	33290 (1.9026)	29576 (1.9429)	30296 (1.9550)
XI	34280 (0.9074)	37109 (1.0009)	38169 (0.9497)	41038 (0.9049)	33926 (0.8246)	38241 (0.9995)	39694 (0.9685)	35351 (0.9340)	40491 (0.9295)	40089 (0.9513)	36606 (0.9721)	38117 (0.9612)
XII	31693 (1.2896)	35052 (1.5185)	36420 (1.4811)	39569 (1.4468)	31723 (1.2646)	36251 (1.5209)	37909 (1.5031)	32963 (1.3766)	38970 (1.4780)	38536 (1.5011)	34175 (1.4746)	36002 (1.4861)
XIII	29334 (0.1586)	31036 (0.1811)	31694 (0.1882)	33940 (0.2209)	30480 (0.1621)	31982 (0.1927)	30802 (0.2028)	29993 (0.1690)	34251 (0.2082)	33429 (0.2016)	30774 (0.1845)	32294 (0.1898)
XIV	29724 (0.1371)	31677 (0.1589)	32364 (0.1672)	34675 (0.2005)	31301 (0.1414)	32777 (0.1733)	31542 (0.1835)	30488 (0.1469)	34887 (0.1905)	34078 (0.1828)	31064 (0.1599)	32477 (0.1664)
XV	28952 (0.0877)	31365 (0.1037)	31876 (0.1145)	34643 (0.1453)	30352 (0.0892)	32683 (0.1177)	31662 (0.1273)	29780 (0.0938)	34598 (0.1367)	33660 (0.1283)	30410 (0.1071)	31980 (0.1136)
XVI	27244 (0.1403)	27244 (0.1742)	27244 (0.1857)	27244 (0.2360)	27244 (0.1494)	27244 (0.1891)	27244 (0.2065)	27244 (0.1518)	27244 (0.2203)	27244 (0.2085)	27244 (0.1622)	27244 (0.1769)

	B3LYP	BMK	CAM-B3LYP	LC-BLYP	M06	M06-2X	M11	PBE0	ωB97	ωB97X	LC-BLYP*	ωB97X*
XVII	28329 (0.1347)	28329 (0.1594)	28329 (0.1692)	28329 (0.2079)	28329 (0.1401)	28329 (0.1761)	28329 (0.1879)	28329 (0.1455)	28329 (0.1982)	28329 (0.1878)	28329 (0.1512)	28329 (0.1631)
XVIII	32012 (0.1274)	35254 (0.1456)	35332 (0.1570)	38768 (0.1880)	33769 (0.1240)	36036 (0.1473)	35677 (0.1680)	33128 (0.1372)	38087 (0.1700)	37120 (0.1667)	33161 (0.1426)	34779 (0.1486)
XIX	25204 (0.2978)	28488 (0.3852)	29049 (0.3940)	32480 (0.4620)	26557 (0.3276)	29412 (0.4033)	30469 (0.4367)	26453 (0.3262)	31995 (0.4309)	31180 (0.4222)	27832 (0.3694)	29155 (0.3838)
XX	26746 (0.3846)	29709 (0.4690)	30484 (0.4717)	33609 (0.5282)	28166 (0.3990)	30587 (0.4766)	31626 (0.5036)	27829 (0.4116)	33209 (0.4944)	32487 (0.4896)	28917 (0.4293)	30169 (0.4483)
XXI	25913 (0.3833)	29164 (0.4849)	30168 (0.5067)	33541 (0.5712)	27511 (0.4080)	29996 (0.5123)	31302 (0.5299)	27112 (0.4119)	32832 (0.5452)	31993 (0.5340)	28349 (0.4408)	29321 (0.4725)
XXII	24293 (0.3508)	27624 (0.4621)	28402 (0.4770)	32120 (0.5650)	25778 (0.3875)	28428 (0.4908)	29972 (0.5332)	25540 (0.3825)	31155 (0.5367)	30462 (0.5208)	26726 (0.4220)	27688 (0.4480)
XXIII	24504 (0.3380)	27670 (0.4266)	28582 (0.4385)	32174 (0.4901)	25947 (0.3499)	28623 (0.4379)	30012 (0.4556)	25585 (0.3632)	31580 (0.4692)	30781 (0.4640)	26491 (0.3807)	27705 (0.4127)
XXIV	24665 (0.5212)	27515 (0.6323)	28439 (0.6474)	31874 (0.7376)	25936 (0.5421)	28308 (0.6529)	29749 (0.6920)	25703 (0.5554)	31006 (0.7044)	30306 (0.6888)	26257 (0.5625)	27569 (0.6088)

Table S15: Fluorescence lifetimes (in ns) of all molecules investigated in this study calculated using Scheme A. All results are in solvent

	B3LYP	BMK	CAM-B3LYP	LC-BLYP	M06	M06-2X	M11	PBE0	ωB97	ωB97X	LC-BLYP*	ωB97X*
I	13.77	9.12	7.80	4.05	12.87	8.13	6.01	12.15	5.45	6.02	9.04	8.40
II	12.23	7.87	6.64	3.99	11.23	6.83	5.01	10.65	4.44	5.01	8.07	7.44
III	5.04	3.52	3.21	2.19	4.93	3.25	2.54	4.50	2.33	2.54	3.85	3.46
IV	4.11	2.82	2.60	1.74	3.91	2.59	2.07	3.68	1.91	2.08	3.11	2.85
V	9.32	5.61	5.17	3.25	8.36	5.16	3.69	7.95	3.52	3.92	6.65	6.39
VI	15.53	9.84	8.58	5.48	13.89	8.78	6.98	13.38	6.20	6.79	8.46	7.77
VII	14.53	9.42	8.12	5.19	13.04	8.39	6.66	12.62	5.92	6.48	10.10	9.17
VIII	11.50	7.30	6.32	4.02	10.25	6.50	5.16	9.92	4.57	5.00	8.58	7.54
IX	1.00	0.72	0.72	0.60	0.98	0.69	0.62	0.89	0.62	0.64	0.80	0.73
X	0.47	0.37	0.35	0.30	0.49	0.33	0.29	0.43	0.31	0.32	0.39	0.37
XI	0.67	0.52	0.52	0.47	0.76	0.49	0.47	0.62	0.47	0.47	0.55	0.52
XII	0.47	0.32	0.31	0.27	0.48	0.30	0.28	0.41	0.27	0.27	0.35	0.31

	B3LYP	BMK	CAM-B3LYP	LC-BLYP	M06	M06-2X	M11	PBE0	ωB97	ωB97X	LC-BLYP*	ωB97X*
XIII	5.06	3.96	3.64	2.71	4.57	3.49	3.59	4.53	2.81	3.05	3.94	3.47
XIV	6.01	4.57	4.15	3.01	5.23	3.90	3.99	5.32	3.13	3.41	4.71	4.13
XV	10.22	7.37	6.45	4.31	9.12	5.97	5.89	9.03	4.58	5.16	7.59	6.46
XVI	7.22	4.87	4.36	2.88	6.18	4.10	4.07	6.33	3.06	3.42	5.67	4.65
XVII	6.28	4.62	4.11	2.83	5.50	3.79	3.86	5.51	2.93	3.28	5.18	4.32
XVIII	4.45	3.21	2.96	2.06	4.09	3.03	2.72	3.86	2.35	2.53	3.70	3.23
XIX	4.34	2.60	2.43	1.64	3.52	2.31	1.99	3.58	1.81	1.95	2.83	2.47
XX	2.56	1.68	1.58	1.15	2.19	1.55	1.37	2.20	1.25	1.33	1.93	1.69
XXI	3.25	2.00	1.78	1.26	2.67	1.78	1.57	2.75	1.38	1.49	2.32	2.02
XXII	3.74	2.18	1.99	1.31	2.99	1.94	1.60	3.10	1.46	1.58	2.55	2.23
XXIII	3.97	2.44	2.20	1.54	3.36	2.20	1.91	3.37	1.66	1.78	2.97	2.50
XXIV	1.97	1.30	1.18	0.82	1.71	1.19	1.01	1.70	0.91	0.98	1.60	1.34

Table S16: Vertical energies (in cm^{-1}) and oscillator strengths for the calculation of fluorescence lifetimes using Schemes B and C. The results were obtained at the excited state optimised geometries in solvent using the state-specific solvation method.

	B3LYP	**BMK**	**CAM-B3LYP**	**LC-BLYP**	**M06**	**M06-2X**	**M11**	**PBE0**	**ωB97**	**ωB97X**	**LC-BLYP***	**ωB97X***
I	20950 (0.0856)	22539 (0.1061)	22891 (0.1189)	25157 (0.1764)	20851 (0.0909)	23011 (0.1112)	23959 (0.1348)	21557 (0.0910)	23990 (0.1440)	23706 (0.1374)	22386 (0.1110)	22571 (0.1156)
II	18943 (0.1086)	20651 (0.1359)	20980 (0.1542)	22736 (0.1972)	18963 (0.1167)	21244 (0.1446)	22158 (0.1758)	19556 (0.1165)	22226 (0.1892)	21880 (0.1800)	20291 (0.1417)	20521 (0.1474)
III	19440 (0.3224)	20876 (0.3777)	21182 (0.3923)	22836 (0.4539)	19332 (0.3286)	21309 (0.3826)	22426 (0.4247)	20049 (0.3377)	22493 (0.4456)	22159 (0.4312)	20585 (0.3569)	20908 (0.3797)
IV	19858 (0.3414)	21410 (0.4032)	21687 (0.4167)	23479 (0.4847)	19848 (0.3542)	21863 (0.4101)	22912 (0.4520)	20439 (0.3576)	22978 (0.4697)	22646 (0.4546)	21087 (0.3793)	21325 (0.3999)
V	20516 (0.1877)	21984 (0.2280)	22505 (0.2308)	24119 (0.2733)	20277 (0.1993)	22355 (0.2369)	23414 (0.2705)	20971 (0.2057)	23534 (0.2735)	23326 (0.2590)	21132 (0.2188)	21728 (0.2147)
VI	24372 (0.0710)	26732 (0.0943)	27275 (0.1054)	29938 (0.1388)	25165 (0.0750)	27230 (0.1035)	28350 (0.1215)	25297 (0.0773)	29191 (0.1296)	28670 (0.1225)	26815 (0.1137)	27446 (0.1169)
VII	23446 (0.0777)	25865 (0.1021)	26453 (0.1151)	29292 (0.1529)	24318 (0.0818)	26299 (0.1127)	27411 (0.1331)	24330 (0.0842)	28470 (0.1416)	27896 (0.1337)	24911 (0.1026)	25709 (0.1063)
VIII	24292 (0.0973)	26719 (0.1289)	27293 (0.1449)	30033 (0.1906)	25105 (0.1029)	27194 (0.1417)	28273 (0.1675)	25219 (0.1056)	29264 (0.1778)	28740 (0.1684)	25430 (0.1230)	26333 (0.1300)

	B3LYP	BMK	CAM-B3LYP	LC-BLYP	M06	M06-2X	M11	PBE0	ωB97	ωB97X	LC-BLYP*	ωB97X*
IX	25692 (0.8993)	27487 (0.9665)	27445 (0.9205)	29303 (0.9117)	25621 (0.8708)	27820 (0.9356)	28937 (0.9258)	26509 (0.9226)	28699 (0.9106)	28391 (0.9189)	26912 (0.8791)	27175 (0.9201)
X	24172 (2.0368)	26019 (2.0944)	26707 (2.0118)	29186 (1.9134)	24260 (1.9082)	27049 (2.0749)	28576 (2.0386)	24921 (2.0738)	28580 (1.9269)	28094 (1.9627)	25721 (2.0035)	25718 (2.0247)
XI	26859 (1.1282)	28500 (1.1802)	28646 (1.1317)	30278 (1.0997)	26575 (1.0495)	29027 (1.1544)	30151 (1.1268)	27705 (1.1534)	29882 (1.1146)	29669 (1.1268)	28240 (1.0982)	28537 (1.1440)
XII	24741 (1.6331)	26657 (1.7145)	27205 (1.6449)	29194 (1.5809)	24664 (1.5485)	27397 (1.6694)	28959 (1.6144)	25650 (1.6711)	28804 (1.6000)	28558 (1.6206)	26466 (1.6032)	27060 (1.6567)
XIII	26640 (0.1293)	28113 (0.1527)	28636 (0.1662)	30508 (0.2047)	27372 (0.1379)	28559 (0.1745)	28794 (0.1829)	27517 (0.1414)	29883 (0.1993)	29550 (0.1880)	28068 (0.1644)	28760 (0.1722)
XIV	26806 (0.1037)	28510 (0.1260)	29095 (0.1374)	31348 (0.1755)	27757 (0.1122)	28993 (0.1475)	29279 (0.1555)	27722 (0.1146)	30633 (0.1719)	30199 (0.1596)	28076 (0.1291)	28902 (0.1377)
XV	22578 (0.0615)	24071 (0.0756)	25018 (0.0839)	27487 (0.1145)	23573 (0.0663)	24896 (0.0889)	25150 (0.0943)	23253 (0.0666)	26561 (0.1076)	26060 (0.0976)	23735 (0.0745)	24698 (0.0822)
XVI	22530 (0.1099)	24709 (0.1390)	25328 (0.1484)	28085 (0.1967)	23338 (0.1224)	25091 (0.1541)	25643 (0.1640)	23281 (0.1191)	27224 (0.1845)	26634 (0.1707)	23614 (0.1231)	24734 (0.1390)

	B3LYP	BMK	CAM-	LC-	M06	M06-2X	M11	PBE0	ωB97	ωB97X	LC-	ωB97X*

			B3LYP	BLYP						BLYP*		
XVII	23415 (0.1054)	25393 (0.1229)	25760 (0.1368)	28012 (0.1746)	24435 (0.1104)	25620 (0.1447)	25985 (0.1501)	24206 (0.1150)	27397 (0.1683)	26897 (0.1558)	24174 (0.1153)	25296 (0.1295)
XVIII	24499 (0.1417)	25582 (0.1675)	26399 (0.1775)	28215 (0.2160)	25254 (0.1481)	26223 (0.1826)	26108 (0.1907)	24889 (0.1541)	27734 (0.2053)	27359 (0.1949)	25066 (0.1560)	26110 (0.1687)
XIX	20126 (0.2346)	23992 (0.3776)	24218 (0.4019)	25850 (0.4907)	22065 (0.2926)	24473 (0.4115)	24961 (0.4496)	21705 (0.2794)	25283 (0.4629)	25210 (0.4472)	23223 (0.3689)	24056 (0.3920)
XX	23816 (0.3843)	26774 (0.4981)	27071 (0.5096)	28432 (0.5723)	25439 (0.4191)	26786 (0.5133)	27323 (0.5412)	25020 (0.4213)	27859 (0.5481)	27815 (0.5374)	25771 (0.4598)	26609 (0.4863)
XXI	22539 (0.3466)	26480 (0.5172)	27122 (0.5450)	28743 (0.6219)	25022 (0.4154)	26656 (0.5481)	27428 (0.5797)	23979 (0.3958)	28125 (0.5964)	28045 (0.5827)	25661 (0.4772)	26525 (0.5118)
XXII	20701 (0.2548)	24991 (0.4318)	25637 (0.4676)	27534 (0.5718)	22564 (0.3148)	25779 (0.4829)	26522 (0.5323)	22390 (0.3039)	26899 (0.5408)	26782 (0.5238)	24147 (0.4011)	25011 (0.4329)
XXIII	21128 (0.3086)	24566 (0.4614)	25232 (0.4947)	26891 (0.5818)	22892 (0.3581)	24901 (0.4949)	25579 (0.5320)	22345 (0.3503)	26388 (0.5592)	26235 (0.5428)	23360 (0.4148)	24412 (0.4553)
XXIV	22708 (0.5003)	24880 (0.6364)	25157 (0.6486)	26345 (0.7105)	23795 (0.5424)	25024 (0.6517)	25433 (0.6755)	23655 (0.5450)	25821 (0.6817)	25755 (0.6732)	23651 (0.5595)	24568 (0.6088)

Table S17: Fluorescence lifetimes (in ns) of all molecules investigated in this study calculated using Scheme B. All results are in solvent

	B3LYP	BMK	CAM-B3LYP	LC-BLYP	M06	M06-2X	M11	PBE0	ωB97	ωB97X	LC-BLYP*	ωB97X*
I	18.15	12.65	10.94	6.11	17.24	11.58	8.81	16.12	8.22	8.83	12.26	11.58
II	16.74	11.23	9.58	6.36	15.52	9.96	7.52	14.63	6.94	7.53	11.16	10.48
III	6.65	4.92	4.61	3.43	6.60	4.67	3.79	5.97	3.60	3.83	5.36	4.88
IV	5.35	3.89	3.67	2.69	5.16	3.67	3.03	4.82	2.90	3.09	4.27	3.96
V	9.37	6.72	6.33	4.65	9.03	6.25	4.98	8.18	4.89	5.25	7.57	7.30
VI	19.30	12.07	10.39	6.54	17.16	10.60	8.33	16.44	7.36	8.08	10.05	9.36
VII	19.43	12.14	10.30	6.30	17.18	10.64	8.28	16.64	7.21	7.96	13.01	11.81
VIII	14.48	9.03	7.70	4.82	12.82	7.92	6.19	12.36	5.44	5.96	10.42	9.21
IX	1.17	0.95	1.00	0.89	1.22	0.96	0.90	1.07	0.93	0.94	1.09	1.02
X	0.56	0.47	0.46	0.41	0.59	0.44	0.40	0.52	0.42	0.43	0.50	0.50
XI	0.88	0.75	0.77	0.71	0.97	0.74	0.70	0.81	0.72	0.72	0.82	0.77
XII	0.61	0.50	0.50	0.45	0.64	0.48	0.45	0.55	0.46	0.46	0.54	0.50

	B3LYP	BMK	CAM-B3LYP	LC-BLYP	M06	M06-2X	M11	PBE0	ωB97	ωB97X	LC-BLYP*	ωB97X*
XIII	7.57	5.75	5.08	3.62	6.70	4.86	4.56	6.47	3.87	4.20	5.35	4.85
XIV	9.84	7.16	6.28	4.22	8.43	5.89	5.48	8.30	4.51	5.00	7.19	6.35
XV	24.29	17.38	14.46	8.75	20.58	13.78	12.74	21.12	9.97	11.43	18.14	15.14
XVI	13.59	8.90	7.92	4.84	11.32	7.78	7.00	11.73	5.49	6.21	11.03	8.87
XVII	11.87	8.66	7.52	4.97	10.37	7.19	6.74	10.16	5.39	6.04	10.17	8.24
XVIII	6.92	5.37	4.74	3.40	6.20	4.67	4.52	6.15	3.70	4.01	5.99	5.10
XIX	9.13	3.85	3.52	2.49	5.96	3.36	2.94	6.51	2.76	2.88	4.19	3.65
XX	3.32	1.97	1.87	1.49	2.61	1.90	1.72	2.72	1.62	1.66	2.30	2.03
XXI	4.91	2.30	2.06	1.59	3.23	2.13	1.88	3.76	1.73	1.78	2.64	2.30
XXII	7.17	2.85	2.49	1.75	4.84	2.38	2.03	5.11	1.94	2.02	3.28	2.83
XXIII	6.10	2.92	2.55	1.88	4.38	2.62	2.30	4.76	2.03	2.12	3.60	2.98
XXIV	2.42	1.57	1.50	1.25	2.02	1.51	1.41	2.04	1.35	1.38	1.97	1.68

Table S18: Computed value of $\frac{1}{<\tilde{\nu}_f^{-3}>}(\times 10^{13})$ for all molecules for the calculation of fluorescence lifetimes using Scheme C. All results are in solvent

	B3LYP	BMK	CAM-B3LYP	LC-BLYP	M06	M06-2X	M11	PBE0	ωB97	ωB97X	LC-BLYP*	ωB97X*
I	0.821	1.018	0.854	1.382	0.809	0.861	0.959	0.896	1.200	1.168	1.085	0.993
II	0.604	0.640	0.663	1.020	0.607	0.684	0.766	0.666	0.961	0.922	0.833	0.739
III	0.540	0.630	0.656	1.021	0.539	0.670	0.763	0.600	0.716	0.711	0.676	0.777
IV	0.589	0.726	0.720	0.838	0.582	0.731	0.824	0.642	0.797	0.782	0.735	0.761
V	0.776	0.944	1.019	1.223	0.745	0.999	1.131	0.831	1.143	1.122	1.036	0.842
VI	1.199	1.654	1.766	2.343	1.330	1.742	1.986	1.350	2.151	2.046	1.794	1.668
VII	1.100	1.475	1.624	2.176	1.223	1.521	1.796	1.232	1.974	1.892	1.644	1.302
VIII	1.135	1.700	1.805	2.412	1.395	1.733	2.034	1.373	2.234	2.126	1.868	1.372
IX	1.266	1.469	1.447	1.664	1.260	1.497	1.655	1.388	1.471	1.459	1.401	1.391
X	1.079	1.296	1.355	1.710	1.078	1.426	1.637	1.177	1.600	1.537	1.411	1.378
XI	1.731	2.053	2.035	2.350	1.528	2.079	2.395	1.871	2.263	2.203	2.121	1.978

XII	1.353	1.677	1.752	2.145	1.340	1.799	2.095	1.506	2.058	1.990	1.869	1.636

	B3LYP	**BMK**	**CAM-B3LYP**	**LC-BLYP**	**M06**	**M06-2X**	**M11**	**PBE0**	**ωB97**	**ωB97X**	**LC-BLYP***	**ωB97X***
XIII	1.398	1.903	1.990	2.489	1.552	1.914	2.089	1.520	2.249	2.188	1.980	1.829
XIV	1.506	1.993	2.084	2.644	1.677	1.928	2.123	1.725	2.416	2.282	2.016	1.750
XV	0.868	1.127	1.205	1.626	0.935	1.214	1.268	0.961	1.469	1.357	1.223	1.019
XVI	0.949	1.277	1.344	1.860	1.043	1.262	1.423	1.013	1.729	1.373	1.386	1.058
XVII	1.030	1.347	1.438	1.844	1.081	1.335	1.501	1.164	1.725	1.625	1.449	1.152
XVIII	1.116	1.318	1.459	1.836	1.220	1.457	1.388	1.130	1.474	1.503	1.466	1.207
XIX	0.532	1.008	0.952	1.095	0.791	0.961	1.044	0.702	0.951	0.986	1.296	0.909
XX	1.059	1.526	1.523	1.683	1.285	1.444	1.548	1.258	1.452	1.562	1.528	1.328
XXI	0.805	1.478	1.781	1.750	1.246	1.675	1.581	0.987	1.980	1.666	1.602	1.327
XXII	0.642	1.174	1.317	1.535	1.023	1.330	1.426	0.810	1.444	1.462	1.406	1.061
XXIII	0.737	1.183	1.259	1.367	0.951	1.207	1.276	0.884	1.301	1.377	1.310	1.128
XXIV	0.866	1.202	1.168	1.243	0.990	1.159	1.180	0.997	1.204	1.228	1.244	1.047

Table S19: Fluorescence lifetimes (in ns) of all molecules investigated in this study calculated using Scheme C. All results are in solvent.

	B3LYP	**BMK**	**CAM-B3LYP**	**LC-BLYP**	**M06**	**M06-2X**	**M11**	**PBE0**	**ωB97**	**ωB97X**	**LC-BLYP***	**ωB97X***
I	20.34	14.22	15.36	7.03	19.32	16.38	12.64	18.02	9.46	10.07	13.85	13.03
II	18.83	15.45	13.34	7.33	17.44	13.96	10.68	16.42	7.93	8.56	12.62	11.78
III	9.06	7.12	6.67	4.00	8.86	6.74	5.60	8.02	5.71	5.86	6.02	6.16
IV	7.11	5.26	5.20	4.16	6.93	5.25	4.43	6.41	4.42	4.59	5.26	4.93
V	10.42	7.56	7.08	5.34	10.11	6.99	5.66	9.08	5.57	5.94	8.49	8.11
VI	23.30	13.95	11.94	7.49	20.57	12.28	9.55	19.71	8.51	9.31	11.62	10.88
VII	22.77	14.25	11.74	7.28	20.20	12.72	9.49	19.45	8.42	9.13	15.45	14.42
VIII	18.29	10.13	8.67	5.42	14.55	9.19	6.88	14.45	6.10	6.66	12.49	10.34
IX	1.57	1.35	1.43	1.34	1.63	1.38	1.31	1.44	1.49	1.47	1.53	1.53
X	0.73	0.64	0.65	0.59	0.78	0.61	0.57	0.68	0.62	0.62	0.62	0.63
XI	0.99	0.84	0.89	0.84	1.19	0.87	0.80	0.92	0.85	0.86	0.93	0.90

XII	0.68	0.56	0.57	0.52	0.72	0.55	0.52	0.62	0.53	0.54	0.61	0.57

	B3LYP	**BMK**	**CAM-B3LYP**	**LC-BLYP**	**M06**	**M06-2X**	**M11**	**PBE0**	**ωB97**	**ωB97X**	**LC-BLYP***	**ωB97X***
XIII	10.24	6.72	5.99	4.13	8.85	5.91	5.21	8.88	4.60	4.96	6.46	5.85
XIV	12.58	8.32	7.42	4.92	10.76	7.44	6.48	10.26	5.37	6.04	9.09	7.94
XV	32.20	21.52	18.79	11.17	28.85	17.52	15.99	27.63	12.72	14.91	23.81	19.30
XVI	16.38	10.52	9.58	5.77	13.80	9.74	8.29	14.61	6.41	8.55	13.73	10.79
XVII	14.79	10.52	8.94	5.93	13.99	9.06	7.88	12.38	6.42	7.24	12.47	9.85
XVIII	9.12	6.82	5.97	4.16	8.19	5.78	5.79	8.39	5.36	5.46	7.81	6.81
XIX	13.99	5.27	5.25	3.93	8.09	5.13	4.39	9.47	4.69	4.68	5.77	5.72
XX	4.23	2.48	2.43	2.04	3.34	2.53	2.27	3.38	2.42	2.29	2.96	2.21
XXI	6.99	2.89	2.30	2.15	4.06	2.41	2.46	5.25	1.94	2.36	3.36	2.84
XXII	9.90	3.79	3.18	2.38	5.44	3.07	2.66	7.08	2.61	2.65	4.36	3.62
XXIII	7.80	3.66	3.25	2.67	5.52	3.36	3.01	6.01	2.87	2.79	4.07	3.40
XXIV	3.27	2.01	2.05	1.83	2.74	2.04	1.97	2.71	1.93	1.91	2.50	2.20

8. Ground and excited state optimised geometries for all molecules for the LC-BLYP* functional

I

Ground state optimised structure	Excited state optimised structure
C -9.638675 -1.125724 -0.002854	C -9.678733 -1.126941 -0.002904
C -8.269291 -1.110586 0.000668	C -8.273235 -1.097651 0.000641
C -7.550096 0.127156 0.003554	C -7.563788 0.118187 0.003467
C -8.288065 1.358646 0.002666	C -8.307438 1.346862 0.002591
C -9.716167 1.306017 -0.001027	C -9.708062 1.296727 -0.000944
C -10.368437 0.100034 -0.003694	C -10.394650 0.065813 -0.003679
C -6.150732 0.163530 0.007205	C -6.147695 0.158413 0.007121
C -7.570031 2.576178 0.005486	C -7.575692 2.585971 0.005414
C -6.156992 2.612267 0.009147	C -6.137143 2.623506 0.009218
C -5.439119 1.368973 0.010015	C -5.424557 1.376591 0.010021
C -4.007849 1.396202 0.013747	C -4.017162 1.405903 0.013687
H -3.470382 0.442050 0.014407	H -3.472210 0.455839 0.014299
C -3.329168 2.585634 0.016437	C -3.308499 2.619971 0.016547
C -4.046024 3.818967 0.015542	C -4.003202 3.825204 0.015785
C -5.417026 3.834855 0.012013	C -5.412668 3.823236 0.012139
H -5.594695 -0.781540 0.007887	H -5.591880 -0.786254 0.007762
H -10.179963 -2.076189 -0.005049	H -10.201241 -2.087571 -0.005033
H -7.696521 -2.044017 0.001340	H -7.707741 -2.035691 0.001249
H -10.279581 2.244350 -0.001691	H -10.274597 2.233664 -0.001564
H -11.462135 0.074583 -0.006509	H -11.487913 0.058210 -0.006403
H -2.235433 2.596874 0.019283	H -2.215007 2.609816 0.019358
H -3.492412 4.762537 0.017713	H -3.465391 4.777061 0.018000
H -5.963331 4.783259 0.011335	H -5.956199 4.773712 0.011553
C -8.296091 3.810282 0.004609	C -8.292910 3.804627 0.004355
N -8.888751 4.817612 0.003897	N -8.889353 4.816745 0.003448

II

Ground state optimised structure	Excited state optimised structure
C -7.737310 -0.662219 -0.014677	C -7.775489 -0.665419 -0.014857
C -6.366751 -0.664416 -0.009804	C -6.371269 -0.649622 -0.010023
C -5.639508 0.565645 -0.010501	C -5.653336 0.559958 -0.010598
C -6.366431 1.802119 -0.016373	C -6.378125 1.792893 -0.016383
C -7.794916 1.765009 -0.021328	C -7.784219 1.754036 -0.021145
C -8.459636 0.566441 -0.020495	C -8.481087 0.534848 -0.020375
C -4.227713 0.605947 -0.005599	C -4.218703 0.590531 -0.005546
C -5.644648 3.016097 -0.017073	C -5.653657 3.031513 -0.017166
C -4.232853 3.056400 -0.012175	C -4.219024 3.062086 -0.012116
C -3.505930 1.819926 -0.006314	C -3.494236 1.829151 -0.006331
C -2.077445 1.857035 -0.001403	C -2.088141 1.868008 -0.001571
H -1.526067 0.911898 0.003030	H -1.532804 0.924507 0.002789
C -1.412724 3.055603 -0.002273	C -1.391273 3.087196 -0.002343
C -2.135050 4.284263 -0.008060	C -2.096871 4.287464 -0.007859
C -3.505609 4.286460 -0.012877	C -3.501091 4.271666 -0.012691
H -8.283784 -1.609534 -0.014101	H -8.304742 -1.621962 -0.014237
H -5.809187 -1.605918 -0.005302	H -5.817108 -1.593811 -0.005677
H -8.346294 2.710146 -0.025776	H -8.339557 2.697537 -0.025505
H -9.553143 0.549667 -0.024303	H -9.574280 0.537635 -0.024127
H -0.319217 3.072377 0.001500	H -0.298081 3.084410 0.001408
H -1.588577 5.231579 -0.008664	H -1.567618 5.244006 -0.008480
H -4.063173 5.227963 -0.017355	H -4.055252 5.215855 -0.017036
C -3.501246 -0.629555 0.000306	C -3.501156 -0.629540 0.000495
N -2.909123 -1.636683 0.005097	N -2.905432 -1.641397 0.005490
C -6.371114 4.251600 -0.022985	C -6.371204 4.251585 -0.023205
N -6.963235 5.258729 -0.027783	N -6.966929 5.263442 -0.028198

III

Ground state optimised structure	Excited state optimised structure
C -8.482140 -8.819602 0.075783	C -8.470245 -8.802608 0.075663
C -7.062821 -8.856863 0.024633	C -7.056358 -8.846183 0.024510
C -6.321507 -7.632871 0.010788	C -6.311410 -7.616210 0.010553
C -7.027255 -6.385722 0.048576	C -7.010112 -6.371008 0.048054
C -8.415050 -6.403686 0.097658	C -8.438286 -6.383870 0.098673
C -9.143339 -7.612553 0.111524	C -9.144778 -7.578938 0.112019
C -4.889735 -7.681170 -0.040601	C -4.884623 -7.659216 -0.040553
C -6.259947 -5.119062 0.034242	C -6.265069 -5.141020 0.034161
C -4.828169 -5.167372 -0.017123	C -4.838280 -5.184027 -0.016885
C -4.122433 -6.414524 -0.054892	C -4.139576 -6.429229 -0.054325
C -4.086864 -3.943377 -0.030965	C -4.093332 -3.954054 -0.030845
C -4.776957 -2.702046 0.006503	C -4.786491 -2.720459 0.006639
C -6.152580 -2.674690 0.055624	C -6.183034 -2.688931 0.056524
C -6.886457 -3.880184 0.069233	C -6.914806 -3.868693 0.070276
H -9.033935 -9.765580 0.086180	H -9.028030 -9.745046 0.086435
H -8.977416 -5.467462 0.127070	H -8.993949 -5.445080 0.127825
H -10.236266 -7.579565 0.150867	H -10.238195 -7.560895 0.151231
H -4.194267 -1.774755 -0.004389	H -4.209781 -1.789433 -0.003823
H -6.687879 -1.720881 0.084623	H -6.705243 -1.727721 0.085124
H -7.976297 -3.815152 0.108564	H -8.003825 -3.810877 0.109469
C -2.734634 -6.396546 -0.103899	C -2.711395 -6.416368 -0.104782
H -2.172217 -7.332742 -0.133252	H -2.155729 -7.355159 -0.133847
C -2.006351 -5.187682 -0.117740	C -2.004903 -5.221301 -0.118093
H -0.913421 -5.220672 -0.157013	H -0.911481 -5.239345 -0.157188
C -2.667549 -3.980628 -0.082049	C -2.679440 -3.997629 -0.081867
H -2.115752 -3.034652 -0.092422	H -2.121655 -3.055191 -0.092636
C -4.997126 -10.125541 -0.062081	C -4.966666 -10.111302 -0.063122
H -4.461835 -11.079352 -0.091150	H -4.444462 -11.072511 -0.091844
C -6.372750 -10.098177 -0.012898	C -6.363204 -10.079776 -0.013107
H -6.955438 -11.025470 -0.002022	H -6.939915 -11.010801 -0.002652
C -4.263241 -8.920058 -0.075670	C -4.234893 -8.931541 -0.076836
H -3.173410 -8.985144 -0.115069	H -3.145876 -8.989357 -0.116116

IV

Ground state optimised structure	Excited state optimised structure
C -8.494693 -8.775264 0.076499	C -8.486014 -8.760456 0.076156
C -7.076135 -8.828694 0.025409	C -7.071794 -8.818197 0.025338
C -6.336860 -7.613959 0.011564	C -6.322877 -7.600425 0.011232
C -7.021939 -6.362612 0.048849	C -7.003975 -6.352879 0.048346
C -8.404775 -6.349424 0.098406	C -8.424207 -6.336427 0.099451
C -9.139301 -7.556743 0.112147	C -9.144899 -7.527430 0.112720
C -4.910670 -7.691455 -0.040070	C -4.902985 -7.670562 -0.040101
C -6.239145 -5.109667 0.033732	C -6.246797 -5.130635 0.033762
C -4.812920 -5.187205 -0.017905	C -4.826908 -5.200773 -0.017572
C -4.127840 -6.438538 -0.055190	C -4.145808 -6.448321 -0.054688
C -4.073634 -3.972486 -0.031751	C -4.077991 -3.983001 -0.031680
C -4.805294 -2.757613 0.006767	C -4.813261 -2.778406 0.006787
C -6.180648 -2.804003 0.055238	C -6.212441 -2.825837 0.056014
H -9.061207 -9.712291 0.086913	H -9.055281 -9.695815 0.086250
H -8.914458 -5.382774 0.126644	H -8.920998 -5.363606 0.127557
H -10.232182 -7.517200 0.151588	H -10.237884 -7.498407 0.152094
H -4.278112 -1.798415 -0.002228	H -4.296324 -1.813659 -0.001879
H -6.771416 -1.882236 0.085753	H -6.783714 -1.890219 0.085860
C -2.744990 -6.451753 -0.104752	C -2.725577 -6.464772 -0.105796
H -2.235326 -7.418413 -0.132992	H -2.228785 -7.437592 -0.133902
C -2.010466 -5.244447 -0.118494	C -2.004885 -5.273767 -0.119068
H -0.917586 -5.283986 -0.157938	H -0.911901 -5.302791 -0.158446
C -2.655084 -4.025911 -0.082843	C -2.663770 -4.040742 -0.082502
H -2.088567 -3.088885 -0.093258	H -2.094503 -3.105383 -0.092598
C -4.969115 -9.997244 -0.061577	C -4.937340 -9.975364 -0.062350
H -4.378434 -10.919072 -0.092088	H -4.366071 -10.910984 -0.092194
C -6.344516 -10.043566 -0.013105	C -6.336523 -10.022792 -0.013127
H -6.871729 -11.002744 -0.004109	H -6.853460 -10.987539 -0.004462
N -6.897357 -3.957684 0.068930	N -6.934271 -3.948424 0.070216
N -4.252349 -8.843703 -0.075273	N -4.215506 -8.852781 -0.076552

V

Ground state optimised structure	Excited state optimised structure
C -2.593071 0.271434 0.001989	C -2.628288 0.256680 0.063746
C -1.220345 0.267798 0.021140	C -1.221678 0.275450 0.119777
C -0.470949 1.491704 -0.002302	C -0.486758 1.476433 0.019435
C -1.195236 2.740180 -0.018490	C -1.215976 2.721174 -0.038408
C -2.629492 2.697177 -0.053999	C -2.622677 2.667827 -0.142811
C -3.307760 1.503624 -0.046455	C -3.327215 1.450082 -0.091063
C 0.941961 1.495204 0.001078	C 0.949920 1.493723 -0.001797
C -0.491124 3.965083 -0.009275	C -0.499315 3.966376 -0.011106
C 0.921745 3.968586 0.003352	C 0.937283 3.983796 0.014797
C 1.646143 2.720080 -0.002402	C 1.666675 2.738759 -0.033712
C 3.080710 2.762971 -0.021638	C 3.073710 2.791533 -0.133805
H 3.630554 1.818093 -0.048833	H 3.632272 1.859930 -0.252498
C 3.758900 3.956518 -0.008482	C 3.778093 4.009550 -0.086519
C 3.043749 5.188801 0.029682	C 3.078676 5.203785 0.059391
C 1.670892 5.192511 0.033222	C 1.671888 5.185317 0.110904
H -3.142996 -0.674760 0.021830	H -3.159117 -0.697465 0.134623
H -0.673005 -0.678282 0.055882	H -0.683320 -0.667038 0.245896
H -3.179014 3.641974 -0.089168	H -3.180845 3.598746 -0.268510
H -4.401916 1.495903 -0.075729	H -4.418869 1.453728 -0.164959
H 4.853320 3.964164 -0.025283	H 4.869982 4.005503 -0.156825
H 3.593449 6.135016 0.054191	H 3.609281 6.158310 0.126723
H 1.123263 6.138678 0.060174	H 1.133127 6.128482 0.230044
C 1.691054 0.204366 0.010773	C 1.697157 0.221353 0.010772
C 2.343164 -0.233927 1.174661	C 2.641992 -0.054778 1.022178
C 1.756494 -0.594030 -1.142583	C 1.488879 -0.755469 -0.986211
C 3.043785 -1.444405 1.187048	C 3.343474 -1.261966 1.040609
H 2.295467 0.384842 2.077466	H 2.804655 0.685970 1.812189
C 2.459886 -1.802994 -1.133959	C 2.202328 -1.955898 -0.976503
H 1.249705 -0.257489 -2.053678	H 0.771017 -0.550754 -1.787484
C 3.104711 -2.231829 0.031724	C 3.130248 -2.217077 0.039108
H 3.544518 -1.772955 2.103430	H 4.060381 -1.459139 1.844241
H 2.503485 -2.412538 -2.042266	H 2.033703 -2.691938 -1.769282

H 3.653969 -3.178600 0.039761	H 3.684579 -3.160721 0.050057
C -1.240324 5.255883 -0.010421	C -1.246585 5.238795 -0.008055
C -1.291538 6.052929 -1.165437	C -1.035059 6.210159 -1.009674
C -1.907015 5.695387 1.144723	C -2.194675 5.520436 0.998785
C -1.995285 7.261712 -1.167026	C -1.748506 7.410633 -1.008791
H -0.773364 5.715381 -2.069730	H -0.314607 6.001057 -1.807479
C -2.607999 6.905700 1.146944	C -2.896178 6.727707 1.008389
H -1.870566 5.077636 2.048753	H -2.359890 4.784004 1.792287
C -2.654699 7.691756 -0.009979	C -2.679685 7.677344 0.002396
H -2.027694 7.870167 -2.076531	H -1.577308 8.142342 -1.805017
H -3.120204 7.235209 2.056616	H -3.615674 6.929269 1.808611
H -3.204246 8.638393 -0.009913	H -3.234019 8.621042 0.006409

VI

Ground state optimised structure	Excited state optimised structure
C -7.678410 -5.354807 -0.064701	C -7.705784 -5.331448 -0.066548
C -6.297149 -5.384472 0.000114	C -6.297156 -5.390229 0.000364
C -5.544967 -4.193341 -0.013047	C -5.532549 -4.221772 -0.011704
C -6.219224 -2.956538 -0.093953	C -6.226335 -2.978821 -0.093593
C -7.628072 -2.926883 -0.160212	C -7.622194 -2.915811 -0.160197
C -8.340923 -4.112695 -0.145243	C -8.369536 -4.107677 -0.146357
C -4.078935 -4.240698 0.057012	C -4.073052 -4.251160 0.056755
C -4.126559 -1.742530 -0.044773	C -4.103489 -1.747877 -0.043754
C -3.390633 -2.943668 0.037169	C -3.371981 -2.969015 0.038894
C -1.984532 -2.883328 0.099914	C -1.979333 -2.886236 0.100681
H -1.440969 -3.830375 0.162533	H -1.409483 -3.816410 0.163809
C -1.322717 -1.669003 0.082418	C -1.329394 -1.633516 0.081527
C -2.069043 -0.475466 0.001031	C -2.059274 -0.448128 0.000646
C -3.451026 -0.504287 -0.061780	C -3.463592 -0.504248 -0.062749
H -8.254710 -6.283686 -0.053722	H -8.280125 -6.262383 -0.055129
H -5.747483 -6.327978 0.063503	H -5.774446 -6.347797 0.063094
H -8.144700 -1.963723 -0.222764	H -8.119882 -1.942871 -0.221967
H -9.433262 -4.081044 -0.196682	H -9.459964 -4.067122 -0.197842
H -0.231293 -1.630800 0.131258	H -0.237187 -1.597947 0.131049
H -1.552957 0.489067 -0.012779	H -1.551954 0.519208 -0.013762
H -4.027321 0.424353 -0.124045	H -4.058170 0.412548 -0.125924
N -5.501142 -1.782116 -0.107693	N -5.478909 -1.820322 -0.105904
H -6.011933 -0.900180 -0.169554	H -5.991494 -0.933967 -0.167573
O -3.455458 -5.318419 0.129396	O -3.438139 -5.349616 0.129583

VII

Ground state optimised structure	Excited state optimised structure
C -7.638529 -5.403997 -0.140647	C -7.660114 -5.376568 -0.186742
C -6.270145 -5.388705 0.061367	C -6.279497 -5.384249 0.087321
C -5.545113 -4.182322 0.056267	C -5.540199 -4.197346 0.086701
C -6.217598 -2.952458 -0.144704	C -6.226406 -2.970952 -0.162125
C -7.614606 -2.981100 -0.371408	C -7.596348 -2.969887 -0.456197
C -8.302508 -4.185194 -0.366380	C -8.315915 -4.180192 -0.471153
C -4.093781 -4.223043 0.246803	C -4.102335 -4.211772 0.326025
C -4.128658 -1.741358 -0.096127	C -4.107861 -1.742838 -0.113009
C -3.402150 -2.940004 0.106084	C -3.392607 -2.952752 0.135981
C -1.995944 -2.910352 0.160733	C -1.995988 -2.900663 0.185559
H -1.483496 -3.862790 0.324617	H -1.458947 -3.826584 0.405928
C -1.296940 -1.726651 0.006627	C -1.308669 -1.693265 -0.040495
C -2.017194 -0.540516 -0.220539	C -2.011706 -0.524123 -0.325021
C -3.402890 -0.539119 -0.273775	C -3.419247 -0.547647 -0.358965
H -8.194027 -6.345609 -0.138196	H -8.216265 -6.318753 -0.180027
H -5.703209 -6.309551 0.226292	H -5.748905 -6.313851 0.307868
H -8.164123 -2.062971 -0.581344	H -8.114242 -2.040561 -0.697978
H -9.380842 -4.177261 -0.552038	H -9.383814 -4.168591 -0.701996
H -0.204538 -1.712567 0.047390	H -0.215568 -1.678954 0.003937
H -1.482748 0.402754 -0.368743	H -1.484205 0.412981 -0.518463
H -3.919785 0.397957 -0.482647	H -3.960080 0.368626 -0.600339
N -5.517837 -1.752161 -0.124535	N -5.505171 -1.776181 -0.079308
O -3.483655 -5.285567 0.485516	O -3.483737 -5.291068 0.589192
C -6.250531 -0.488503 -0.149592	C -6.237567 -0.515885 -0.005601
H -6.434007 -0.137496 -1.179757	H -6.442142 -0.117208 -1.015009
H -7.209432 -0.609794 0.369014	H -7.185290 -0.678472 0.521357
H -5.685264 0.274931 0.398772	H -5.646725 0.213307 0.561612

VIII

Ground state optimised structure	Excited state optimised structure

C -8.207864 -1.130867 0.414447	C -8.239858 -1.103355 0.419313
C -6.831735 -1.123853 0.265011	C -6.837300 -1.118323 0.266195
C -6.120361 0.083959 0.119380	C -6.115686 0.070484 0.119557
C -6.821519 1.312966 0.125624	C -6.837346 1.302131 0.128527
C -8.227581 1.299772 0.278580	C -8.231776 1.316028 0.280432
C -8.900493 0.095559 0.419754	C -8.935875 0.103806 0.426838
C -4.662965 0.048303 -0.036629	C -4.665227 0.051801 -0.038334
C -4.753768 2.550067 -0.169818	C -4.736605 2.558933 -0.173009
C -4.004440 1.349877 -0.184188	C -3.994831 1.339344 -0.186068
C -2.605107 1.404780 -0.342329	C -2.607255 1.412183 -0.343895
H -2.065535 0.453070 -0.348740	H -2.046854 0.473738 -0.353349
C -1.947393 2.614527 -0.483454	C -1.956111 2.655758 -0.486011
C -2.698334 3.806056 -0.467100	C -2.688347 3.841264 -0.471010
C -4.076340 3.783328 -0.313644	C -4.088267 3.794893 -0.313426
H -8.751963 -2.072663 0.526886	H -8.778925 -2.048804 0.532499
H -6.250035 -2.050394 0.254608	H -6.277667 -2.057227 0.258276
H -8.783018 2.239867 0.285064	H -8.773176 2.263852 0.285436
H -9.988497 0.106991 0.536809	H -10.022069 0.122979 0.544902
H -0.861326 2.648088 -0.605915	H -0.869120 2.683242 -0.608348
H -2.193242 4.770632 -0.577100	H -2.190652 4.807976 -0.580219
H -4.640368 4.718265 -0.303757	H -4.665613 4.721190 -0.300966
O -4.022433 -1.024147 -0.043430	O -4.012819 -1.040838 -0.046805
C -6.875282 3.754089 -0.005724	C -6.865522 3.737711 -0.006689
C -7.095388 4.411847 1.206041	C -7.086226 4.386577 1.208678
C -7.358054 4.276417 -1.207186	C -7.340312 4.256489 -1.211803
C -7.810726 5.612465 1.213624	C -7.801759 5.586624 1.213713
H -6.705073 3.979459 2.132730	H -6.699301 3.951803 2.135182
C -8.072856 5.477360 -1.193933	C -8.054870 5.457103 -1.195631
H -7.170356 3.739534 -2.142391	H -7.148867 3.721818 -2.147056
C -8.298882 6.144577 0.015078	C -8.285097 6.120764 0.014337
H -7.986839 6.133488 2.159284	H -7.981175 6.105014 2.159942
H -8.454093 5.892609 -2.131479	H -8.432432 5.874119 -2.133621
H -8.858608 7.084653 0.023310	H -8.844869 7.060579 0.022670
N -6.136632 2.516115 -0.016547	N -6.125295 2.497141 -0.017392

IX

Ground state optimised structure	Excited state optimised structure
C -7.246144 0.804968 -1.078809	C -7.215042 0.848116 -1.093238
C -7.252224 0.799295 1.103872	C -7.206019 0.862060 1.108193
C -8.020515 -0.224629 0.622599	C -8.004822 -0.202225 0.597287
H -8.583072 -0.973482 1.177668	H -8.559107 -0.939998 1.178372
C -6.887742 1.285351 2.429058	C -6.877356 1.299499 2.402110
C -6.049828 2.400930 2.579839	C -6.027417 2.432573 2.594377
C -7.377091 0.633865 3.573309	C -7.386684 0.619017 3.552103
C -5.708683 2.855051 3.854747	C -5.711433 2.852695 3.877929
H -5.667496 2.909947 1.690493	H -5.635398 2.956124 1.718188
C -7.033252 1.091488 4.844006	C -7.056696 1.057921 4.822629
H -8.031408 -0.237205 3.465452	H -8.038407 -0.250575 3.421815
C -6.197564 2.203870 4.990278	C -6.218629 2.175253 4.998764
H -5.054594 3.725960 3.960458	H -5.060045 3.721265 4.016415
H -7.420722 0.575488 5.727703	H -7.451563 0.530405 5.696303
H -5.928683 2.561672 5.988650	H -5.963663 2.514536 6.007096
C -6.881053 1.288712 -2.407752	C -6.881037 1.289676 -2.380989
C -6.044395 2.402965 -2.565146	C -6.029551 2.422618 -2.574236
C -7.379131 0.622302 -3.537353	C -7.394230 0.602914 -3.526028
C -5.709784 2.845576 -3.845479	C -5.715087 2.837005 -3.859867
H -5.658882 2.918694 -1.680963	H -5.635901 2.949357 -1.700567
C -7.040674 1.069946 -4.813234	C -7.063784 1.038715 -4.797192
H -8.030369 -0.244958 -3.395763	H -8.044493 -0.262248 -3.369522
C -6.205861 2.181613 -4.971139	C -6.224315 2.155381 -4.977946
H -5.056733 3.715418 -3.964295	H -5.063068 3.704558 -4.002833
H -7.431004 0.547610 -5.691897	H -7.459361 0.509390 -5.669702
H -5.941766 2.530845 -5.973992	H -5.969538 2.491419 -5.987574
O -6.750465 1.466537 0.008216	O -6.700736 1.534841 0.011180
N -8.007566 -0.208956 -0.761709	N -8.003318 -0.201421 -0.734249

X

Ground state optimised structure	Excited state optimised structure
C -6.039342 3.110295 -1.033165	C -6.050643 3.087937 -1.032921
C -5.194639 3.446344 -2.104849	C -4.725536 3.189342 -1.580869
C -4.484776 4.649597 -2.107059	C -4.031138 4.389247 -1.579579
C -4.608629 5.541564 -1.036766	C -4.604579 5.553299 -1.038218
C -5.447309 5.219067 0.035219	C -5.899216 5.487242 -0.493767
C -6.154526 4.014170 0.036747	C -6.607416 4.295461 -0.486889
C -6.792034 1.829754 -1.031839	C -6.772958 1.858140 -1.031193
C -6.230202 0.659467 -1.568020	C -6.220093 0.637865 -1.576957
C -6.937359 -0.542682 -1.568777	C -6.913273 -0.541631 -1.576559
C -8.232396 -0.621553 -1.030732	C -8.248460 -0.651786 -1.030699
C -8.793698 0.548474 -0.493280	C -8.800692 0.568109 -0.483454
C -8.087609 1.751336 -0.495135	C -8.107519 1.747604 -0.483861
H -5.107824 2.765115 -2.957779	H -4.243340 2.309389 -2.011634
H -3.837348 4.894924 -2.954863	H -3.023874 4.425909 -2.006797
H -4.053583 6.484730 -1.038072	H -4.051314 6.497165 -1.040540
H -5.546038 5.905997 0.881691	H -6.358000 6.385645 -0.068488
H -6.791053 3.761074 0.891110	H -7.609756 4.288021 -0.053841
H -5.216781 0.685844 -1.981624	H -5.216422 0.642529 -2.006818
H -6.477961 -1.434570 -2.007350	H -6.428969 -1.420975 -2.006070
H -9.796438 0.516045 -0.054800	H -9.803809 0.563081 -0.052297
H -8.557583 2.649842 -0.082006	H -8.591235 2.626618 -0.053020
C -8.984663 -1.902475 -1.030443	C -8.971944 -1.880889 -1.031474
C -10.376489 -1.919627 -1.224167	C -10.297637 -1.981789 -0.484861
C -8.321114 -3.126096 -0.836942	C -8.415939 -3.088092 -1.578965
C -11.084686 -3.123923 -1.223705	C -10.993271 -3.180975 -0.488686
H -10.908824 -0.978587 -1.397527	H -10.779304 -1.101998 -0.053160
C -9.027138 -4.331639 -0.838957	C -9.125362 -4.279161 -1.574604
H -7.240109 -3.132173 -0.662590	H -7.413284 -3.080929 -2.011276
C -10.412526 -4.335481 -1.031831	C -10.420537 -4.344753 -1.031389
H -12.167596 -3.115437 -1.382916	H -12.000954 -3.217284 -0.062427
H -8.491753 -5.273088 -0.680304	H -8.667148 -5.177343 -2.000963
H -10.966374 -5.279358 -1.032614	H -10.974778 -5.288049 -1.031066

XI

Ground state optimised structure	Excited state optimised structure
C -5.647292 -0.384370 0.011016	C -5.617967 -0.388224 0.010226
C -4.251911 -0.388986 0.011996	C -4.228282 -0.398727 0.011278
C -3.538534 0.826119 0.000382	C -3.499988 0.826110 0.000436
C -4.251525 2.041441 -0.012200	C -4.227886 2.051172 -0.011413
C -5.646907 2.037249 -0.013113	C -5.617575 2.041099 -0.012301
C -6.348696 0.826546 -0.001525	C -6.321912 0.826547 -0.001533
H -6.191423 -1.333857 0.020119	H -6.165090 -1.336207 0.018619
H -3.698435 -1.332577 0.021770	H -3.675404 -1.342661 0.020372
H -3.697750 2.984864 -0.021221	H -3.674704 2.994934 -0.019734
H -6.190737 2.986902 -0.022957	H -6.164392 2.989252 -0.021459
H -7.443035 0.826713 -0.002268	H -7.416133 0.826716 -0.002301
C -2.108515 0.825903 0.001353	C -2.100869 0.825896 0.001394
C -0.887008 0.825720 0.002184	C -0.856816 0.825712 0.002233
C 0.541413 0.825508 0.003151	C 0.527261 0.825507 0.003160
C 1.258139 -0.388235 0.012969	C 1.268517 -0.411529 0.014897
C 1.258511 2.039039 -0.005697	C 1.268897 2.062326 -0.007590
C 2.649353 -0.388440 0.013910	C 2.638967 -0.411729 0.015818
H 0.707994 -1.333512 0.019852	H 0.712301 -1.353335 0.023047
C 2.649725 2.038834 -0.004758	C 2.639347 2.062122 -0.006691
H 0.708654 2.984479 -0.013325	H 0.712970 3.004295 -0.016481
C 3.366451 0.825091 0.005061	C 3.380601 0.825087 0.005057
H 3.199210 -1.333880 0.021538	H 3.194895 -1.353698 0.024720
H 3.199870 2.984112 -0.011641	H 3.195563 3.003928 -0.014852
C 4.794875 0.824880 0.006028	C 4.764681 0.824883 0.005983
C 6.016382 0.824696 0.006858	C 6.008731 0.824701 0.006820
C 7.446399 0.824480 0.007829	C 7.407856 0.824489 0.007776
C 8.159390 -0.390840 0.020643	C 8.135753 -0.400565 0.020147
C 8.159777 2.039582 -0.004016	C 8.136145 2.049319 -0.003591
C 9.554772 -0.386648 0.021557	C 9.525443 -0.390491 0.021038
H 7.605614 -1.334261 0.029846	H 7.582573 -1.344325 0.028877
C 9.555157 2.034966 -0.003037	C 9.525831 2.038821 -0.002547
H 7.606301 2.983171 -0.013971	H 7.583266 2.993249 -0.013092

C 10.256561 0.824052 0.009737	C 10.229779 0.824057 0.009738
H 10.098601 -1.336299 0.031584	H 10.072261 -1.338639 0.030611
H 10.099289 2.984451 -0.012324	H 10.072953 2.986801 -0.011359
H 11.350900 0.823885 0.010480	H 11.324000 0.823890 0.010504

XII

Ground state optimised structure	Excited state optimised structure
C -6.042685 3.104075 -1.033432	C -6.046228 3.096192 -1.032344
C -4.749118 3.179701 -1.577944	C -4.807593 3.229000 -1.717919
C -4.040151 4.383644 -1.575903	C -4.106362 4.430908 -1.719687
C -4.614027 5.537086 -1.030832	C -4.605979 5.548886 -1.036601
C -5.901500 5.475319 -0.487217	C -5.824468 5.442103 -0.351077
C -6.607570 4.269669 -0.487630	C -6.532472 4.244157 -0.348446
C -6.794252 1.823873 -1.034630	C -6.781958 1.844154 -1.031080
C -6.138250 0.598505 -0.829647	C -6.172581 0.610959 -1.419052
C -6.844461 -0.604424 -0.830450	C -6.862649 -0.578292 -1.416550
C -8.234274 -0.628495 -1.035898	C -8.250790 -0.654721 -1.031439
C -8.890248 0.597053 -1.241152	C -8.859118 0.595108 -0.645481
C -8.183806 1.799813 -1.240669	C -8.155729 1.776558 -0.642675
H -4.303168 2.287164 -2.029542	H -4.406014 2.383701 -2.283179
H -3.036651 4.422515 -2.011630	H -3.160867 4.501246 -2.267127
H -4.059899 6.480903 -1.029718	H -4.052031 6.492556 -1.038341
H -6.356866 6.369969 -0.050567	H -6.222677 6.303465 0.194910
H -7.604754 4.223633 -0.037157	H -7.465317 4.184217 0.218617
H -5.060791 0.590453 -0.634034	H -5.115313 0.596525 -1.697104
H -6.312299 -1.541322 -0.634957	H -6.329246 -1.486107 -1.706706
H -9.967629 0.605580 -1.437107	H -9.911702 0.619341 -0.355215
H -8.715607 2.737008 -1.435784	H -8.682507 2.693327 -0.364399
C -8.985892 -1.907589 -1.035207	C -8.971457 -1.880123 -1.032191
C -10.284505 -1.984102 -0.504313	C -10.359586 -1.956561 -0.647039
C -8.421694 -3.080363 -1.564767	C -8.363139 -3.129944 -1.418192
C -10.991965 -3.186207 -0.504144	C -11.049651 -3.145814 -0.644535

H -10.743209 -1.089330 -0.070417	H -10.892979 -1.048756 -0.356837
C -9.128240 -4.283094 -1.561972	C -9.066527 -4.311394 -1.421000
H -7.417074 -3.046974 -1.999399	H -7.310569 -3.154166 -1.708510
C -10.427186 -4.359145 -1.032249	C -10.440285 -4.379002 -1.032550
H -12.008854 -3.212895 -0.098640	H -12.106908 -3.131387 -0.366442
H -8.657615 -5.185539 -1.966164	H -8.539757 -5.228154 -1.699321
C -11.179491 -5.638926 -1.029839	C -11.176014 -5.631040 -1.031286
C -11.072239 -6.539416 -2.103745	C -10.689781 -6.779002 -1.715197
C -12.016588 -5.978973 0.046851	C -12.414643 -5.763851 -0.345699
C -11.779628 -7.744310 -2.101398	C -11.397787 -7.976947 -1.712566
H -10.443624 -6.279943 -2.962251	H -9.756941 -6.719062 -2.282270
C -12.726570 -7.182267 0.050059	C -13.115876 -6.965757 -0.343932
H -12.093260 -5.300686 0.903284	H -12.816217 -4.918554 0.219569
C -12.610617 -8.070497 -1.024393	C -12.616268 -8.083732 -1.027030
H -11.687885 -8.428189 -2.951298	H -10.999584 -8.838306 -2.258562
H -13.367281 -7.431297 0.902051	H -14.061367 -7.036096 0.203516
H -13.165728 -9.013743 -1.022398	H -13.170218 -9.027401 -1.025290

XIII

Ground state optimised structure	Excited state optimised structure
C -1.248108 -1.328392 -0.182194	C -1.257103 -1.347525 -0.149604
C -0.025384 -2.122072 0.000604	C -0.033570 -2.128586 -0.067457
C 1.040572 -1.290236 -0.046679	C 1.067642 -1.284490 -0.017562
C 1.041060 1.286228 -0.087680	C 1.068961 1.281937 -0.061440
C -0.024035 2.120401 -0.070755	C -0.031385 2.125017 -0.139575
C -1.246723 1.323074 -0.236503	C -1.255402 1.342760 -0.200679
N 0.610837 -0.005661 -0.304323	N 0.585474 -0.001508 -0.067615
N -0.760974 -0.006681 -0.392221	N -0.790578 -0.002150 -0.147764
O -2.423635 -1.642583 -0.174463	O -2.440230 -1.686526 -0.207360
O -2.421375 1.639956 -0.257266	O -2.437482 1.680560 -0.282228
H 2.106410 1.487598 0.013004	H 2.137136 1.469274 -0.002810
H 2.106032 -1.489738 0.056567	H 2.135601 -1.471085 0.047149
H -0.020939 -3.199198 0.142291	H -0.018589 -3.215977 -0.049072
H -0.018600 3.201428 0.037279	H -0.015339 3.212419 -0.156324

XIV

Ground state optimised structure	Excited state optimised structure
C -1.234738 -1.325595 -0.165666	C -1.255306 -1.342696 -0.159105
C -0.016481 -2.117462 0.003490	C -0.033975 -2.121669 -0.073187
C 1.068406 -1.300468 -0.051748	C 1.086107 -1.291065 -0.005526
C 1.064925 1.298291 -0.091444	C 1.085895 1.289081 -0.052780
C -0.019965 2.117509 -0.083627	C -0.035837 2.116976 -0.126122
C -1.235900 1.320327 -0.240616	C -1.256294 1.335011 -0.195884
N 0.631212 -0.004961 -0.302112	N 0.602022 -0.001576 -0.060422
N -0.745944 -0.007756 -0.387551	N -0.788022 -0.003272 -0.148716
O -2.415188 -1.634591 -0.145153	O -2.442215 -1.684261 -0.214961
O -2.415867 1.631122 -0.265661	O -2.441610 1.673634 -0.290438
H -0.010196 -3.196727 0.137664	H -0.017892 -3.210313 -0.055649
H -0.014410 3.200823 0.012597	H -0.020333 3.205652 -0.140469
C 2.516416 -1.625969 0.061897	C 2.535109 -1.619687 0.036742
H 3.068256 -1.303923 -0.835627	H 3.041471 -1.380793 -0.914737
H 2.976142 -1.139316 0.936709	H 3.062903 -1.092241 0.846638
H 2.636926 -2.712255 0.172291	H 2.646070 -2.699450 0.210043
C 2.509148 1.624410 0.060491	C 2.527633 1.621297 0.089191
H 2.913792 1.218922 1.002111	H 2.908839 1.387573 1.098594
H 3.105252 1.216921 -0.770828	H 3.155510 1.091922 -0.644268
H 2.635785 2.715484 0.078449	H 2.657496 2.700661 -0.073278

XV

Ground state optimised structure	Excited state optimised structure
C -1.240124 -1.293251 -0.218736	C -1.276213 -1.329898 -0.154024
C -0.019702 -2.048236 0.057539	C -0.037143 -2.079873 -0.052995
C 1.084908 -1.278017 -0.062940	C 1.102649 -1.278471 0.001150
C 1.085186 1.271607 -0.118236	C 1.103281 1.276892 -0.051874
C -0.018781 2.047811 -0.034822	C -0.034774 2.075453 -0.159350
C -1.238803 1.284322 -0.289252	C -1.273806 1.322366 -0.234588
N 0.664415 -0.011801 -0.486064	N 0.617907 -0.001402 -0.060374
N -0.727917 -0.013420 -0.574612	N -0.796744 -0.003177 -0.161148
O -2.412577 -1.608113 -0.182350	O -2.450734 -1.702900 -0.221333
O -2.410197 1.605068 -0.288433	O -2.447085 1.692454 -0.332804
C 2.514127 -1.642753 0.109293	C 2.533198 -1.650333 0.130842
H 3.115265 -1.308430 -0.750000	H 3.152457 -1.199665 -0.660227
H 2.937471 -1.198153 1.024262	H 2.950064 -1.358422 1.109052
H 2.599307 -2.735463 0.194239	H 2.617029 -2.743258 0.044213
C 2.514419 1.643783 0.034326	C 2.536812 1.651925 0.026387
H 2.975729 1.143792 0.900254	H 3.034392 1.207760 0.902664
H 3.089751 1.376872 -0.865898	H 3.092710 1.354606 -0.878233
H 2.588308 2.729539 0.188329	H 2.605520 2.745610 0.116852
F -0.037504 -3.355726 0.334302	F -0.002593 -3.399856 -0.018974
F -0.035612 3.365907 0.186049	F 0.000742 3.395526 -0.187985

XVI

Ground state optimised structure	Excited state optimised structure
C -1.245405 -1.296646 -0.215521	C -1.276560 -1.319859 -0.187440
C -0.026809 -2.083874 0.010774	C -0.048342 -2.096975 -0.087227
C 1.075715 -1.289658 -0.068727	C 1.092756 -1.281860 -0.007516
C 1.086139 1.283859 -0.104182	C 1.106169 1.277389 -0.044011
C -0.007619 2.093484 -0.065364	C -0.027899 2.102103 -0.125251
C -1.232080 1.313931 -0.281095	C -1.263572 1.335279 -0.210577
N 0.649301 -0.005206 -0.403018	N 0.617526 -0.000246 -0.063972
N -0.733959 -0.000474 -0.502141	N -0.790684 0.005641 -0.168332
O -2.421059 -1.605982 -0.192766	O -2.456674 -1.670534 -0.263953
O -2.403665 1.638900 -0.297490	O -2.439266 1.695999 -0.305474
C 2.512657 -1.637368 0.072946	C 2.531029 -1.640576 0.065342
H 3.079257 -1.349500 -0.827271	H 3.057739 -1.432321 -0.882669
H 2.969582 -1.136393 0.941778	H 3.053047 -1.106029 0.874795
H 2.608113 -2.723313 0.214173	H 2.613773 -2.719718 0.261964
C 2.522847 1.616991 0.071042	C 2.542413 1.623825 0.096490
H 2.904969 1.244407 1.036344	H 2.920916 1.415818 1.112840
H 3.136676 1.184737 -0.734323	H 3.173574 1.080941 -0.624616
H 2.643782 2.709726 0.059268	H 2.663373 2.701227 -0.089581
Cl -0.064308 -3.773959 0.285925	Cl -0.039353 -3.786855 -0.059368
Cl -0.026462 3.791676 0.156901	Cl -0.002295 3.792088 -0.134196

XVII

Ground state optimised structure	Excited state optimised structure
C -1.186022 -1.310884 -0.277713	C -1.238025 -1.331578 -0.082398
C 0.016561 -2.114948 -0.039371	C -0.018124 -2.126892 -0.008204
C 1.102963 -1.295776 -0.115913	C 1.105894 -1.286004 0.017961
C 1.103053 1.289682 -0.157776	C 1.106316 1.285167 -0.013530
C 0.017246 2.112149 -0.112488	C -0.015117 2.124833 -0.106916
C -1.184439 1.303633 -0.340554	C -1.235051 1.328140 -0.164762
N 0.685414 -0.008493 -0.468196	N 0.632506 -0.000684 -0.023467
N -0.694389 -0.010097 -0.570624	N -0.774292 -0.001459 -0.098973
O -2.367418 -1.627181 -0.257456	O -2.424826 -1.691636 -0.131358
O -2.364232 1.625743 -0.362635	O -2.420656 1.686695 -0.244423
C -0.058456 -3.581725 0.214798	C -0.031756 -3.605581 0.019039
H -0.622965 -3.792244 1.138492	H 0.450439 -4.004082 0.930677
H -0.587963 -4.093161 -0.606624	H -1.073392 -3.959687 -0.011285
H 0.941323 -4.031503 0.314599	H 0.510598 -4.034257 -0.844349
C -0.058512 3.585443 0.100619	C -0.027608 3.603504 -0.134585
H -0.558078 4.079375 -0.749716	H 0.548427 4.002816 -0.989596
H -0.652578 3.819843 0.999755	H -1.066970 3.956492 -0.214849
H 0.939374 4.033743 0.223125	H 0.419054 4.032601 0.781790
C 2.548450 -1.610537 0.057127	C 2.546722 -1.628267 0.151460
H 3.146355 -1.230096 -0.786305	H 3.178570 -1.079826 -0.565026
H 2.951346 -1.172572 0.985652	H 2.930670 -1.426185 1.168114
H 2.686341 -2.699629 0.113976	H 2.674934 -2.704027 -0.041969
C 2.549009 1.609070 0.000968	C 2.553012 1.628537 0.006087
H 2.977893 1.130143 0.896327	H 3.106438 1.079572 0.784444
H 3.130232 1.274636 -0.873697	H 3.041904 1.427685 -0.964762
H 2.679086 2.695390 0.105636	H 2.659926 2.704130 0.212884

XVIII

Ground state optimised structure	Excited state optimised structure
C -1.187001 -1.308979 -0.611868	C -1.281800 -1.373702 -0.333480
C 0.019494 -1.996264 -0.088402	C -0.018078 -2.092370 -0.061081
C 1.060382 -1.144534 -0.254277	C 1.054424 -1.190076 -0.185117
C 1.061765 1.119601 -0.294675	C 1.052485 1.162660 -0.199883
C 0.022267 1.978586 -0.160549	C -0.008161 2.075078 -0.118673
C -1.184007 1.277136 -0.665768	C -1.274205 1.358479 -0.388863
N 0.635412 -0.024625 -0.963173	N 0.469644 -0.016543 -0.521428
N -0.735476 -0.026557 -1.122983	N -0.888190 -0.014438 -0.644903
O -2.348553 -1.671492 -0.598785	O -2.439453 -1.797088 -0.338195
O -2.343582 1.645678 -0.678062	O -2.426823 1.793944 -0.424202
C -0.054273 -3.331217 0.569277	C -0.000979 -3.520369 0.327124
H -0.886150 -3.361315 1.291355	H -1.030612 -3.872854 0.490335
H -0.240980 -4.128162 -0.170485	H 0.455445 -4.141851 -0.466238
H 0.882699 -3.568098 1.097376	H 0.588374 -3.691140 1.245715
C -0.050963 3.334637 0.452714	C 0.011210 3.514200 0.227043
H -0.245087 4.106287 -0.311428	H 0.034209 4.136660 -0.688221
H -0.878039 3.386260 1.179202	H -0.907289 3.786984 0.770652
H 0.888566 3.591319 0.966775	H 0.892784 3.779507 0.832208
C 2.428378 -0.793376 0.277080	C 2.428426 -0.802218 0.324982
H 2.562565 -1.185278 1.296030	H 2.567651 -1.163788 1.358543
H 3.232621 -1.209389 -0.349307	H 3.244813 -1.224712 -0.279429
C 2.429643 0.785775 0.248006	C 2.446975 0.789708 0.255527
H 2.566432 1.214767 1.251482	H 2.679491 1.240697 1.234013
H 3.233354 1.177034 -0.394889	H 3.219126 1.131027 -0.451782

XIX

Ground state optimised structure	Excited state optimised structure
C -7.272475 -2.314223 -0.039032	C -7.278523 -2.304665 -0.001625
C -5.872102 -2.276972 0.022903	C -5.857611 -2.270242 0.053292
C -5.227726 -1.049520 0.029683	C -5.202754 -1.065520 0.049387
C -5.917578 0.174794 -0.020656	C -5.910071 0.185380 -0.008486
C -7.328166 0.116167 -0.081320	C -7.342468 0.119324 -0.063629
C -7.990740 -1.091331 -0.090658	C -8.009141 -1.076387 -0.060896
H -5.279682 -3.194732 0.064450	H -5.279705 -3.196812 0.099425
C -5.119676 1.370747 -0.003048	C -5.147537 1.389063 -0.006683
H -7.907850 1.041228 -0.120346	H -7.911126 1.050051 -0.108465
H -9.082966 -1.115758 -0.139630	H -9.101211 -1.105429 -0.103073
C -3.767373 1.320758 0.059097	C -3.738068 1.295368 0.052218
C -3.076578 0.046011 0.110139	C -3.059511 0.057278 0.108076
H -3.145244 2.215778 0.073533	H -3.116140 2.191891 0.056233
N -7.942635 -3.507246 -0.089111	N -7.928073 -3.479246 0.002401
H -7.450194 -4.363660 0.159288	H -7.425955 -4.366871 0.046363
H -8.945527 -3.516412 0.089150	H -8.947200 -3.522428 -0.034676
C -5.802728 2.712054 -0.054971	C -5.818373 2.698908 -0.067038
F -6.650324 2.876816 0.991672	F -6.689422 2.909998 0.975912
F -4.933255 3.742258 -0.026867	F -4.946748 3.732972 -0.053615
F -6.544236 2.846273 -1.183231	F -6.594623 2.858449 -1.190940
O -3.855234 -1.088170 0.092018	O -3.837585 -1.124410 0.104203
O -1.865064 -0.105178 0.167699	O -1.835504 -0.136986 0.162376

XX

Ground state optimised structure	Excited state optimised structure
C -7.945651 -2.065602 0.029681	C -7.914318 -2.087671 -0.004894
C -5.959221 -0.938807 0.807666	C -5.919424 -0.976369 0.804800
C -6.175180 0.147758 -0.051745	C -6.159256 0.154430 -0.060269
C -7.319986 0.089830 -0.880753	C -7.325039 0.088455 -0.892472
C -5.229708 1.236926 -0.037971	C -5.258422 1.248425 -0.049536
H -7.520124 0.921005 -1.564707	H -7.531604 0.929666 -1.560140
C -4.160126 1.170208 0.808646	C -4.148748 1.156068 0.831231
C -3.942746 0.049881 1.688128	C -3.906188 0.052377 1.676825
H -3.416326 1.968821 0.856250	H -3.417791 1.968031 0.884087
C -5.428740 2.415954 -0.941906	C -5.474471 2.437654 -0.928099
O -4.871773 -0.974637 1.648616	O -4.833836 -1.026540 1.641274
O -3.008616 -0.088524 2.476348	O -2.966558 -0.120943 2.477805
H -5.446691 2.102553 -1.999835	H -5.485540 2.164428 -2.001415
H -4.622994 3.153491 -0.811224	H -4.676371 3.182356 -0.780701
H -6.392730 2.912009 -0.735727	H -6.441872 2.935987 -0.721722
C -6.814417 -2.035000 0.861646	C -6.763042 -2.057149 0.834591
H -6.584903 -2.850316 1.550452	H -6.535956 -2.885970 1.508018
C -8.200089 -0.973823 -0.862366	C -8.192465 -0.984165 -0.887505
N -8.822188 -3.114456 0.072054	N -8.751304 -3.148860 0.021170
H -9.522368 -3.174350 -0.666412	H -9.566095 -3.131141 -0.596420
C -8.579484 -4.323652 0.841888	C -8.590491 -4.323460 0.866475
C -9.709414 -5.318546 0.628025	C -9.728685 -5.302876 0.631658
H -8.505430 -4.060225 1.913194	H -8.564804 -4.005257 1.925589
H -7.609573 -4.774905 0.550542	H -7.616988 -4.799136 0.643367
H -9.531550 -6.229762 1.220045	H -9.597858 -6.187223 1.273831
H -10.676452 -4.888971 0.939355	H -10.702399 -4.845661 0.874854
H -9.783099 -5.612565 -0.433237	H -9.749251 -5.643277 -0.417128
C -9.412550 -1.007617 -1.750779	C -9.403355 -1.021018 -1.772860
H -9.390047 -1.865323 -2.449072	H -9.378135 -1.878610 -2.470437
H -10.346602 -1.087333 -1.164755	H -10.339363 -1.095468 -1.189096
H -9.475451 -0.091370 -2.357793	H -9.464596 -0.104428 -2.378629

XXI

Ground state optimised structure	Excited state optimised structure
C -7.948830 -2.278395 -0.211493	C -7.953464 -2.269604 -0.222341
C -6.224530 -0.983269 0.900827	C -6.219358 -0.995737 0.924672
C -6.127943 -0.066637 -0.159543	C -6.119008 -0.058518 -0.162143
C -6.972088 -0.298562 -1.265023	C -6.975636 -0.301775 -1.288038
C -5.184570 1.020729 -0.052913	C -5.202964 1.020510 -0.071289
H -6.929174 0.381546 -2.120921	H -6.922245 0.378292 -2.141659
C -4.421074 1.119735 1.073011	C -4.414717 1.101687 1.101968
C -4.521016 0.175078 2.160772	C -4.503528 0.184086 2.174028
H -3.693151 1.923539 1.204965	H -3.683737 1.906200 1.221617
C -5.058846 2.016847 -1.166570	C -5.073606 2.011356 -1.182652
O -5.438096 -0.854851 2.020955	O -5.445114 -0.878273 2.045727
O -3.871471 0.194161 3.201141	O -3.864490 0.168323 3.239397
H -4.767635 1.521074 -2.108644	H -4.766810 1.530535 -2.132505
H -4.303057 2.779998 -0.928141	H -4.321906 2.778120 -0.937489
H -6.020938 2.525106 -1.351344	H -6.030425 2.530189 -1.387617
C -7.094797 -2.065756 0.893019	C -7.093435 -2.054440 0.902981
H -7.083675 -2.728808 1.758672	H -7.100381 -2.718344 1.767776
C -7.848856 -1.365139 -1.304394	C -7.859879 -1.360508 -1.320749
H -8.468168 -1.499483 -2.191824	H -8.486806 -1.494477 -2.203048
N -8.850889 -3.313410 -0.228289	N -8.835303 -3.313342 -0.232002
C -8.903943 -4.269207 0.874031	C -8.899257 -4.264368 0.878888
C -7.806390 -5.333753 0.832742	C -7.804696 -5.332902 0.828405
H -9.894266 -4.751084 0.837035	H -9.891798 -4.738284 0.837851
H -8.868656 -3.715202 1.828628	H -8.855153 -3.706786 1.828560
H -7.881134 -5.992639 1.714346	H -7.896154 -5.995330 1.705142
H -7.898172 -5.957292 -0.071590	H -7.894522 -5.949252 -0.080250
H -6.803112 -4.876406 0.830572	H -6.800719 -4.878557 0.840799
C -9.671948 -3.575583 -1.407535	C -9.671525 -3.581247 -1.402778
C -8.932021 -4.290166 -2.539282	C -8.924221 -4.284198 -2.538342
H -10.101612 -2.624269 -1.767532	H -10.106800 -2.629824 -1.753018
H -10.525332 -4.187752 -1.074309	H -10.510968 -4.205135 -1.060837
H -9.602754 -4.431023 -3.403806	H -9.605356 -4.429148 -3.393160
H -8.056240 -3.710078 -2.874552	H -8.061344 -3.689646 -2.879229
H -8.577852 -5.281685 -2.212911	H -8.556916 -5.272239 -2.218561

XXII

Ground state optimised structure	Excited state optimised structure
C -7.765715 -2.204579 0.365412	C -7.775652 -2.194075 0.364177
C -6.505252 -2.113297 0.995243	C -6.509719 -2.099519 1.009013
C -5.680854 -1.025768 0.745756	C -5.670911 -1.030453 0.767233
C -6.031370 0.014930 -0.133888	C -6.026669 0.019505 -0.132113
C -7.284506 -0.093223 -0.775154	C -7.289399 -0.097406 -0.784073
C -8.123361 -1.163744 -0.544816	C -8.138302 -1.156942 -0.552707
H -6.136949 -2.875116 1.682467	H -6.156858 -2.857639 1.708296
C -5.078084 1.079342 -0.299058	C -5.092146 1.100917 -0.313667
H -7.600317 0.684427 -1.475289	H -7.590567 0.681529 -1.488207
H -9.074458 -1.200719 -1.076649	H -9.090047 -1.191526 -1.083250
C -3.894811 1.077859 0.364048	C -3.873785 1.051467 0.383942
C -3.545641 -0.007057 1.267651	C -3.530813 -0.002744 1.273371
H -3.159159 1.875521 0.255266	H -3.128552 1.840388 0.266856
N -8.620177 -3.244544 0.628287	N -8.613624 -3.240724 0.622339
C -5.403586 2.222082 -1.224328	C -5.412933 2.209194 -1.225286
F -6.537428 2.864233 -0.838252	F -6.575926 2.868680 -0.885732
F -4.421378 3.146809 -1.278344	F -4.438259 3.145156 -1.279024
F -5.614754 1.787948 -2.495054	F -5.634456 1.796994 -2.524125
O -4.478732 -1.021867 1.410703	O -4.488328 -1.047698 1.444879
O -2.510631 -0.097844 1.903846	O -2.497713 -0.137888 1.930201
C -9.889435 -3.373866 -0.082934	C -9.893246 -3.373793 -0.076609
H -10.531314 -4.032443 0.524380	H -10.526107 -4.032951 0.537144
H -10.393896 -2.391905 -0.102680	H -10.390196 -2.389598 -0.096408
C -9.756831 -3.938236 -1.498033	C -9.756186 -3.941923 -1.490702
H -9.338499 -4.957902 -1.477317	H -9.338573 -4.961173 -1.470043
H -10.744932 -3.981504 -1.986850	H -10.747889 -3.986220 -1.970483
H -9.093297 -3.313194 -2.118393	H -9.097866 -3.313769 -2.112376
C -8.222564 -4.321881 1.530300	C -8.216562 -4.322059 1.526361
H -9.147771 -4.808639 1.879185	H -9.142458 -4.813048 1.862919
H -7.752691 -3.880021 2.426745	H -7.749931 -3.880784 2.422616
C -7.296132 -5.359916 0.895083	C -7.282725 -5.346699 0.877942
H -7.004414 -6.118091 1.641368	H -7.002371 -6.111880 1.620485
H -7.797042 -5.875605 0.059326	H -7.774293 -5.852557 0.031535
H -6.377164 -4.893314 0.503545	H -6.360081 -4.871885 0.507069

XXIII

Ground state optimised structure	Excited state optimised structure
C -7.609449 -2.268479 0.106804	C -7.587925 -2.280554 0.061739
C -5.663372 -1.046895 0.838289	C -5.634259 -1.068759 0.838440
C -5.954020 0.039349 -0.003860	C -5.936690 0.041066 -0.015208
C -7.112229 -0.069018 -0.800073	C -7.114424 -0.069657 -0.821001
C -7.927660 -1.185402 -0.774261	C -7.920371 -1.192910 -0.811218
C -5.065136 1.174438 -0.004578	C -5.080856 1.177314 -0.013029
H -7.375730 0.753826 -1.473570	H -7.378570 0.762298 -1.480763
C -3.967105 1.154845 0.809158	C -3.971028 1.154428 0.860891
C -3.667224 0.038026 1.667978	C -3.656529 0.059354 1.695550
H -3.264345 1.990704 0.843793	H -3.292603 2.011007 0.914162
N -8.435308 -3.375044 0.177276	N -8.378026 -3.396107 0.113830
C -5.351563 2.352128 -0.887634	C -5.375592 2.353731 -0.887061
O -4.544721 -1.032167 1.644406	O -4.514979 -1.070208 1.638480
O -2.702570 -0.061272 2.426660	O -2.701869 -0.066067 2.489817
C -9.487252 -3.568756 -0.814469	C -9.495458 -3.568497 -0.811209
H -10.208115 -4.289064 -0.392814	H -10.199877 -4.276091 -0.347152
H -9.071255 -4.021777 -1.741430	H -9.115993 -4.038590 -1.744794
C -10.169973 -2.249497 -1.142579	C -10.164547 -2.240733 -1.128303
H -10.971172 -2.419984 -1.880346	H -10.986620 -2.413368 -1.841235
H -10.637651 -1.846201 -0.225915	H -10.603759 -1.822642 -0.204497
C -9.133198 -1.270086 -1.684874	C -9.129111 -1.281790 -1.706801
H -8.812983 -1.608828 -2.689182	H -8.820199 -1.640618 -2.708452
H -9.568651 -0.264959 -1.818906	H -9.555052 -0.274654 -1.852713
C -6.454808 -2.192075 0.924659	C -6.423081 -2.196961 0.912741
H -5.381241 2.051265 -1.949200	H -5.403448 2.076272 -1.959111
H -4.582898 3.130385 -0.768157	H -4.611326 3.137255 -0.761711
H -6.335015 2.793108 -0.649786	H -6.361983 2.803082 -0.656034
C -6.071242 -3.304917 1.871995	C -6.054199 -3.322095 1.841458
H -5.683780 -2.876397 2.811486	H -5.610429 -2.909286 2.761588
H -5.236062 -3.889285 1.439782	H -5.262024 -3.939806 1.372086
C -7.257179 -4.225608 2.148760	C -7.263976 -4.195776 2.154102
H -7.982213 -3.723268 2.814477	H -7.973954 -3.652289 2.803143

H -6.922792 -5.145924 2.655079	H -6.957760 -5.111005 2.685779
C -7.954964 -4.579631 0.843865	C -7.964237 -4.580375 0.861504
H -7.261825 -5.141102 0.179097	H -7.285760 -5.189626 0.224029
H -8.828662 -5.225943 1.029618	H -8.866845 -5.180851 1.052503

XXIV

Ground state optimised structure	Excited state optimised structure
C -5.260236 -0.745136 2.769162	C -5.261274 -0.735028 2.754537
C -4.864683 0.446944 2.177680	C -4.848738 0.430447 2.149678
C -5.761196 1.371956 1.624818	C -5.763828 1.367106 1.571727
C -7.128769 1.038727 1.697108	C -7.148644 1.021119 1.667908
C -7.559781 -0.138088 2.280726	C -7.581662 -0.139773 2.268521
H -4.481484 -1.403189 3.156153	H -4.487811 -1.390125 3.157045
C -5.246863 2.569771 1.025508	C -5.281370 2.539542 0.956833
H -7.863805 1.730388 1.271636	H -7.881194 1.711496 1.237410
H -8.629488 -0.350081 2.298507	H -8.651735 -0.348438 2.299003
C -3.902648 2.789059 0.970007	C -3.873777 2.728632 0.930201
C -2.979708 1.825208 1.587039	C -2.962340 1.805324 1.542028
H -5.963071 3.292112 0.629363	H -5.980032 3.270387 0.555492
O -3.509151 0.698219 2.152317	O -3.491266 0.651342 2.144909
O -1.766627 1.987314 1.633759	O -1.730823 1.945057 1.602843
N -7.065857 -2.211615 3.474489	N -7.062823 -2.203533 3.466147
C -6.104000 -3.169328 4.010656	C -6.098025 -3.149021 4.028072
C -5.466959 -4.077103 2.956066	C -5.468946 -4.076467 2.985622
H -6.637108 -3.779929 4.757864	H -6.632980 -3.741444 4.787147
H -5.324550 -2.618161 4.566770	H -5.318489 -2.583438 4.565998
H -4.717451 -4.738518 3.423203	H -4.726760 -4.733445 3.469510
H -6.227777 -4.709748 2.469444	H -6.232449 -4.712751 2.508950
H -4.963304 -3.488025 2.171615	H -4.957996 -3.501833 2.195726
C -8.479301 -2.576352 3.478838	C -8.476573 -2.579337 3.484603
C -8.976404 -3.175092 2.161448	C -8.968058 -3.180669 2.165949
H -9.080569 -1.690592 3.751825	H -9.078121 -1.694700 3.757440
H -8.620948 -3.302298 4.296223	H -8.604581 -3.306472 4.301719
H -10.054867 -3.399972 2.225583	H -10.042980 -3.417028 2.239488
H -8.819309 -2.479236 1.320360	H -8.824316 -2.479293 1.327718
H -8.442633 -4.111441 1.929147	H -8.426018 -4.110622 1.929310
N -3.210513 3.880507 0.431424	N -3.210112 3.832648 0.416155
C -3.561924 4.840436 -0.493755	C -3.578262 4.858870 -0.438246
H -2.218324 3.902381 0.700473	H -2.211899 3.851593 0.676557

O -2.734380 5.702616 -0.804951	O -2.753167 5.752205 -0.667971
C -4.938301 4.800520 -1.107220	C -4.940092 4.848837 -1.083603
H -4.933566 5.467955 -1.979739	H -4.909098 5.553809 -1.925871
H -5.222371 3.781909 -1.418938	H -5.221317 3.847111 -1.444202
H -5.695875 5.167920 -0.393539	H -5.712842 5.193241 -0.374877
C -6.634264 -1.063047 2.851692	C -6.647666 -1.058356 2.843285

9. Dependence of the range-separation parameter on the basis set and molecular geometry

The effect on the optimal value of γ for different basis sets were explored in earlier studies[26,27] and found to be minimal. In the course of our work, we have also performed a limited study using a few molecules in the test subset. The results are given in Table S20 and we concluded that the basis set effect on the tuned γ is not significant.

Table S20: Tuned range separation parameters ($Bohr^{-1}$) with the LC-BLYP* functional, as determined using the 6-31+G(d) and 6-311+G(d) basis sets. The tuning procedure was carried out in the gas phase.

	6-31+G(d)	**6-311+G(d)**
I	0.2219	0.2261
XIII	0.2829	0.2821
XIX	0.2468	0.2467

In addition, a truly consistent approach for calculations carried out with tuned γ necessitates the use of γ that are re-calculated with changes in molecular geometry. For geometry optimizations carried out with a particular γ, the optimal γ corresponding to the minimum should be re-determined and checked for consistency. Otherwise, geometry optimization should be repeated using the new-found γ and the process repeated till self-consistency is obtained. This is indeed a cumbersome procedure. There is previous work[28] that reports the dependence of γ on the molecular geometry and found it to be small. We have also considered this aspect in the course of our work and carried out studies albeit on a limited scale and arrived at the same conclusion- variation of γ between optimized molecular geometries in the ground and excited state is not significant. The results are summarized in Table S21.

Table S21: Optimally tuned range separation parameters ($Bohr^{-1}$) for LC-BLYP*/6-31+G*, as determined at the ground and excited state optimised geometries. The tuning procedure was carried out in the gas phase.

	Ground state opt. geom.	**Excited state opt. geom.**
I	0.2219	0.2187
XIII	0.2829	0.2801

XIX	0.2468	0.2423

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