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Supplementary Information

Photophysical Tuning of the Aggregation-Induced Emission of a Series of *para*-Substituted Bis(imino)acenaphthene Zinc Complexes

By

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1) Fluorescence Spectroscopy

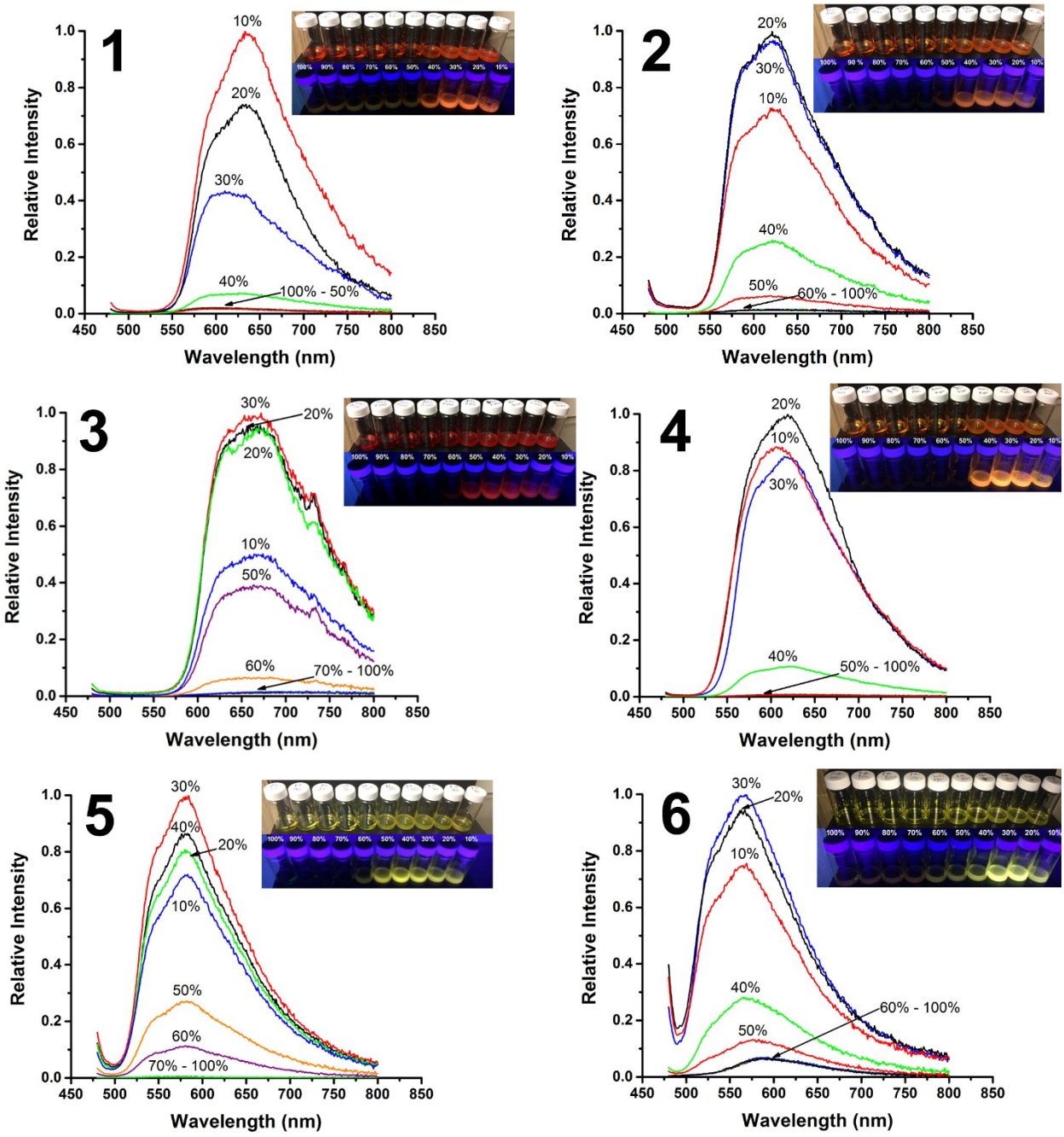

Figure S1. AIE experiment for DCM solutions (~10^{-4}-10^{-3} M) of complexes **1-6** with images of each DCM/hexanes volumetric fraction in ambient light and under UV irradiation (the percentage values above are relative to the DCM content).

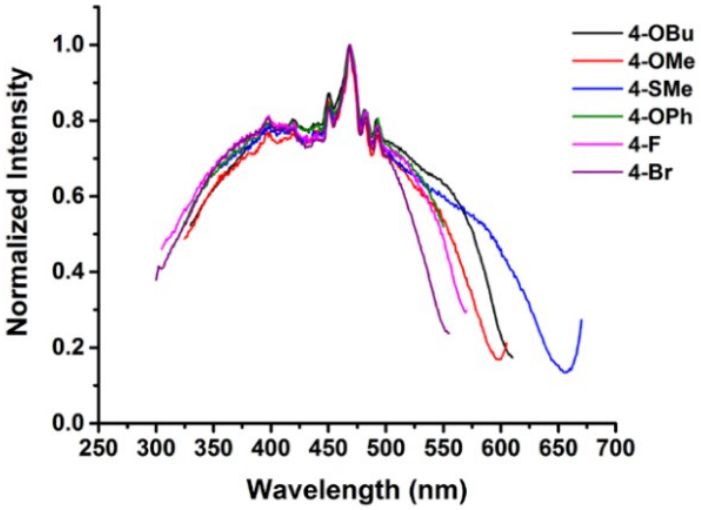

Figure S2. Excitation spectra for complexes **1-6**.

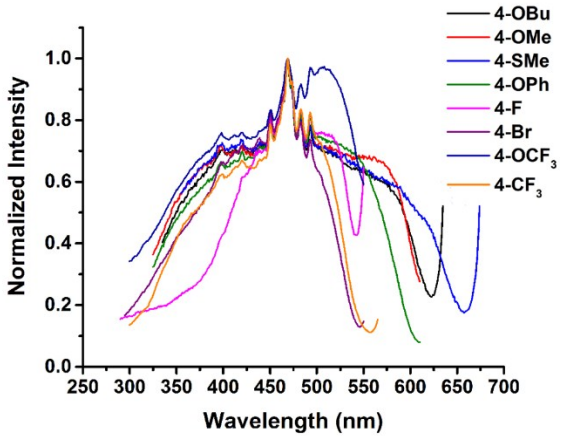

Figure S3. Excitation spectra for solvatomorphs **1-DCM-8-DCM**.

2) X-ray Crystallographic Data

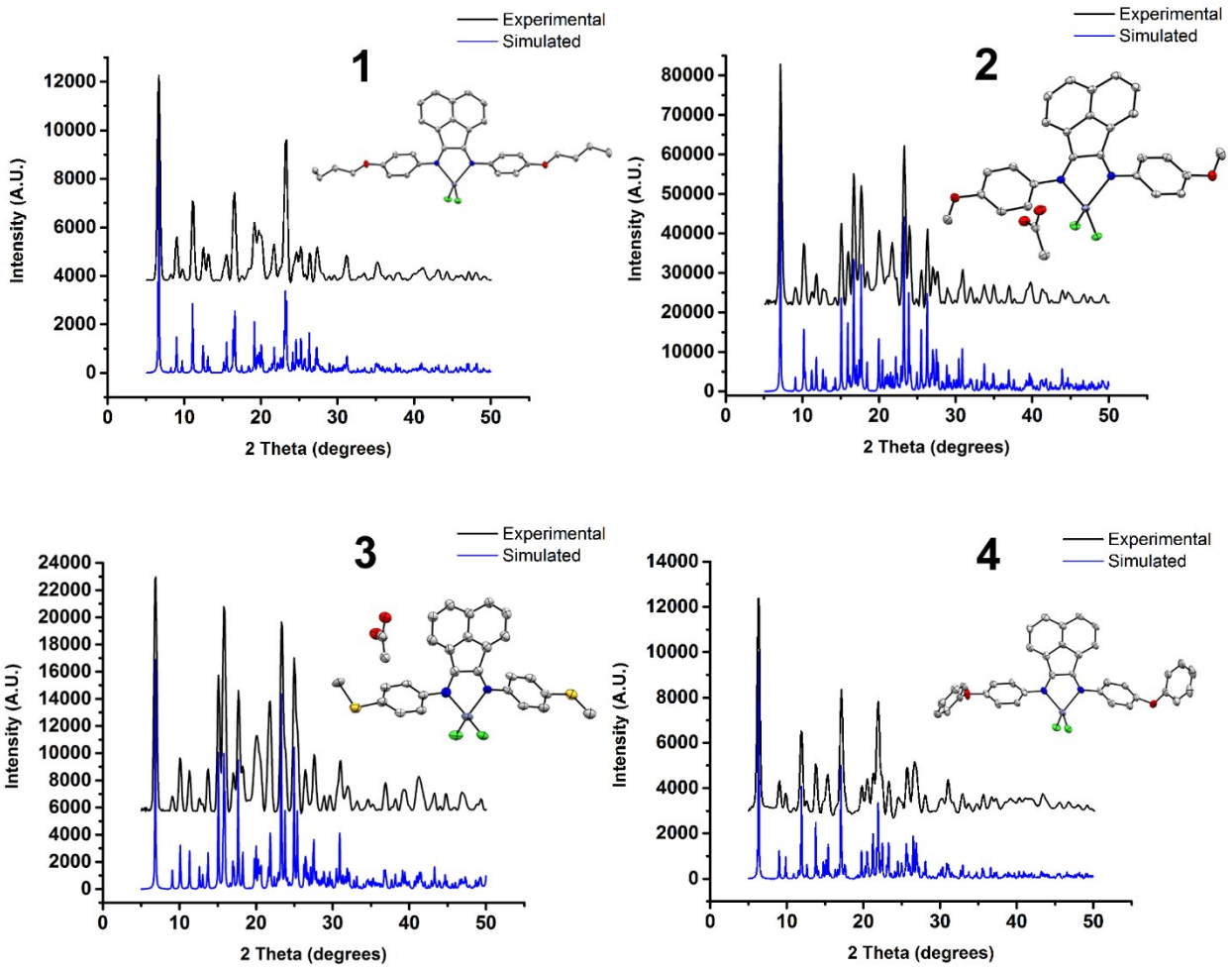

Figure S4. Experimental (black) and simulated (blue) powder X-ray crystallography patterns for complexes **1-4**. All experimental spectra were background corrected using the Eva program.[1]

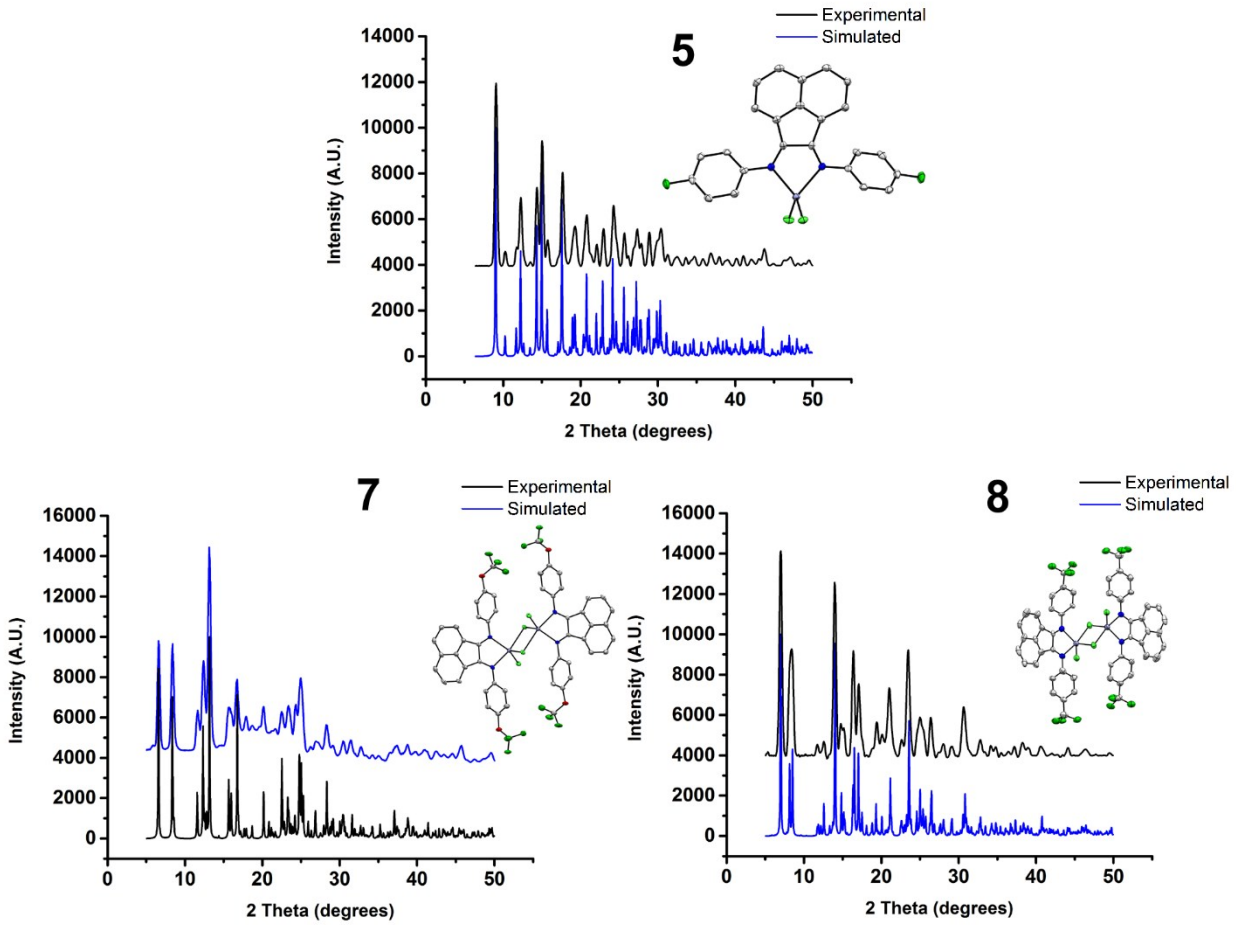

Figure S5. Experimental (black) and simulated (blue) powder X-ray crystallography patterns for complexes **5**, **7**, and **8**. All experimental spectra were background corrected using the Eva program.[1]

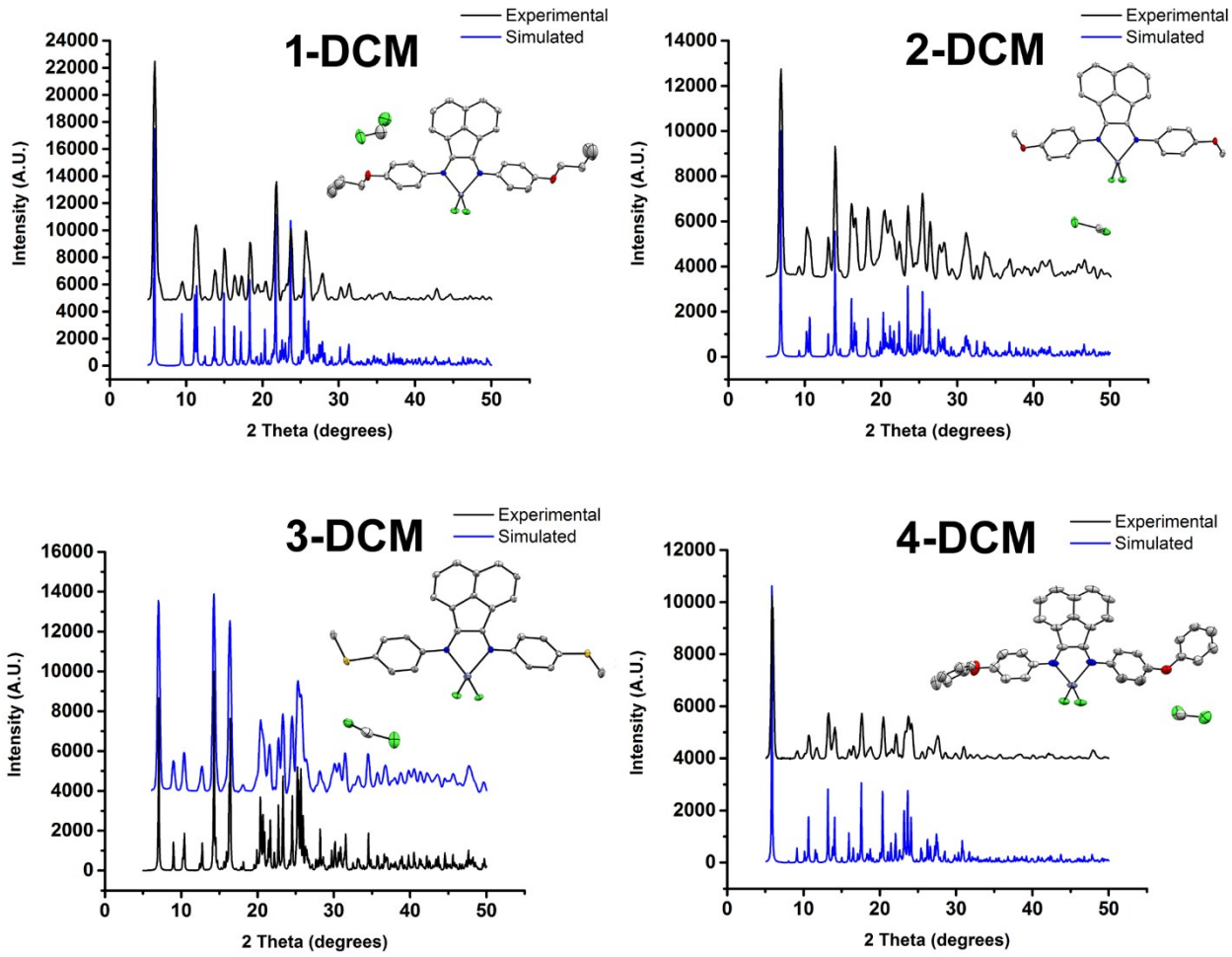

Figure S6. Experimental (black) and simulated (blue) powder X-ray crystallography patterns for complexes **1-DCM-4-DCM**. All experimental spectra were background corrected using the Eva program.[1]

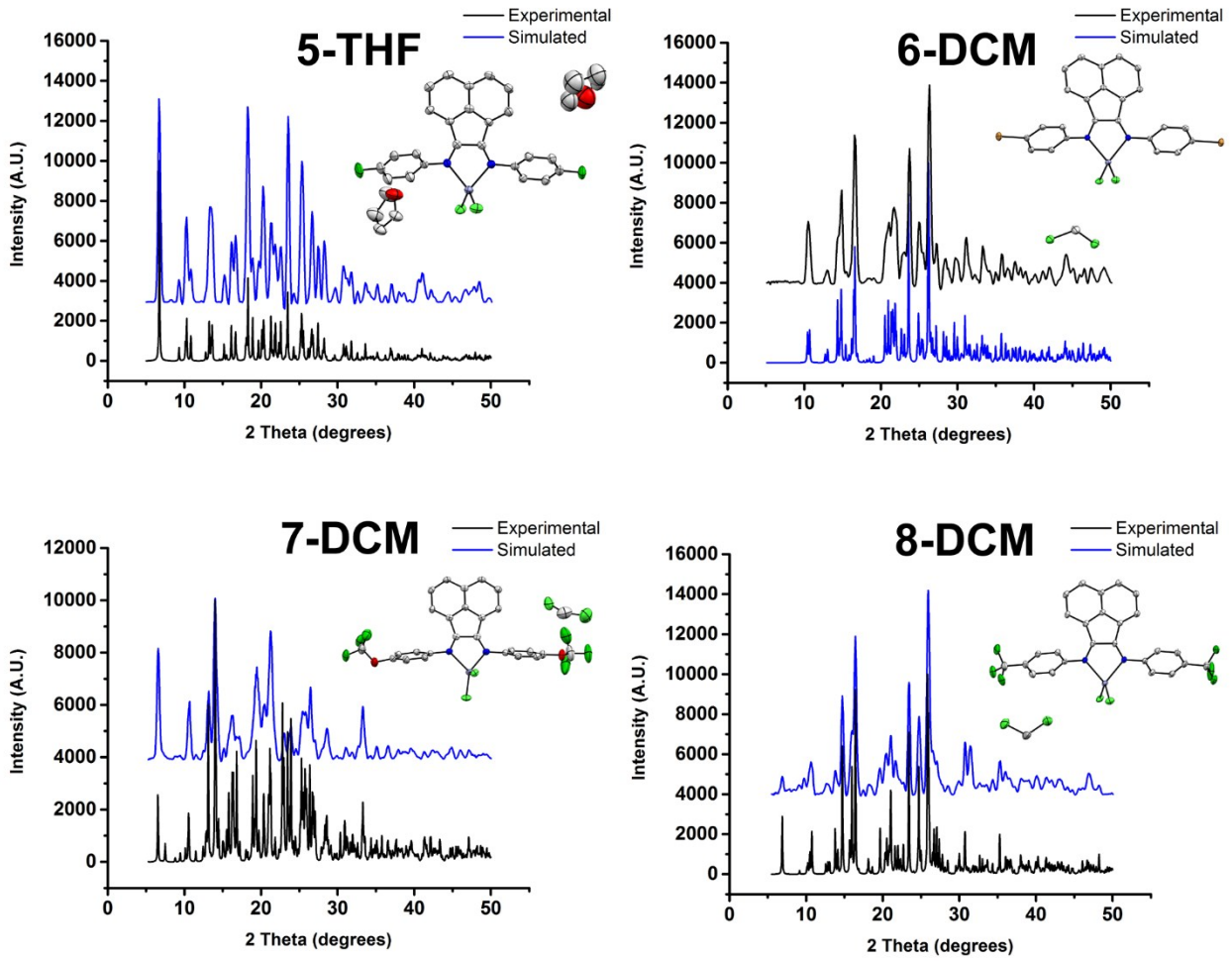

Figure S7. Experimental (black) and simulated (blue) powder X-ray crystallography patterns for complexes **5-THF-8-DCM**. All experimental spectra were background corrected using the Eva program.[1]

3) Single Crystal X-ray Crystallographic Data

Table 1. Crystal data and structure refinement for **1**.

Empirical formula	$C_{32}H_{32}Cl_2N_2O_2Zn$	
Formula weight	612.87	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	I2/a	
Unit cell dimensions	a = 18.3252(3) Å	α = 90°.
	b = 11.6963(2) Å	β = 97.0670(10)°.
	c = 26.7400(4) Å	γ = 90°.
Volume	5687.83(16) $Å^3$	
Z	8	
Density (calculated)	1.431 Mg/m^3	
Absorption coefficient	3.182 mm^{-1}	
F(000)	2544	
Crystal size	0.03 x 0.05 x 0.38 mm^3	
Theta range for data collection	3.33 to 76.26°.	
Index ranges	-22<=h<=22, -14<=k<=13, -33<=l<=33	
Reflections collected	27764	
Independent reflections	5871 [R(int) = 0.0342]	
Completeness to theta = 76.26°	98.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.49341	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5871 / 0 / 354	
Goodness-of-fit on F^2	1.055	
Final R indices [I>2sigma(I)]	R1 = 0.0335, wR2 = 0.0889	
R indices (all data)	R1 = 0.0365, wR2 = 0.0918	
Largest diff. peak and hole	0.466 and -0.521	

Table 2. Crystal data and structure refinement for **2**.

Empirical formula	$C_{28}H_{24}Cl_2N_2O_4Zn$	
Formula weight	588.76	
Temperature	153(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.4510(3) Å	α = 90°.
	b = 11.7454(3) Å	β = 95.969(2)°.
	c = 17.4508(4) Å	γ = 90°.
Volume	2538.20(11) $Å^3$	
Z	4	
Density (calculated)	1.541 Mg/m^3	
Absorption coefficient	3.603 mm^{-1}	
F(000)	1208	
Crystal size	0.14 x 0.09 x 0.07 mm^3	
Theta range for data collection	3.57 to 74.33°.	
Index ranges	-12<=h<=15, -12<=k<=14, -19<=l<=21	
Reflections collected	9920	
Independent reflections	5030 [R(int) = 0.0284]	
Completeness to theta = 74.33°	97.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.74906	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5030 / 0 / 341	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I)]	R1 = 0.0320, wR2 = 0.0837	
R indices (all data)	R1 = 0.0365, wR2 = 0.0872	
Largest diff. peak and hole	0.476 and -0.425 e.$Å^{-3}$	

Table 3. Crystal data and structure refinement for **3**.

Empirical formula	$C_{28}H_{24}Cl_2N_2O_2S_2Zn$	
Formula weight	620.88	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.036(3) Å	α= 90°.
	b = 11.7210(15) Å	β= 98.657(16)°.
	c = 17.716(2) Å	γ= 90°.
Volume	2676.1(8) $Å^3$	
Z	4	
Density (calculated)	1.541 Mg/m^3	
Absorption coefficient	4.813 mm^{-1}	
F(000)	1272	
Crystal size	0.070 x 0.030 x 0.010 mm^3	
Theta range for data collection	3.429 to 67.484°.	
Index ranges	-15<=h<=15, -10<=k<=14, -21<=l<=20	
Reflections collected	16148	
Independent reflections	16148 [R(int) = 0.0000]	
Completeness to theta = 67.684°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.60099	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16148 / 528 / 338	
Goodness-of-fit on F^2	1.088	
Final R indices [I>2sigma(I)]	R1 = 0.1556, wR2 = 0.3454	
R indices (all data)	R1 = 0.3689, wR2 = 0.3854	
Largest diff. peak and hole	0.690 and -0.858 e.$Å^{-3}$	

Table 4. Crystal data and structure refinement for **4**.

Empirical formula	$C_{36}H_{24}Cl_2N_2O_2Zn$	
Formula weight	652.84	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 14.0015(9) Å	α = 90°.
	b = 11.7228(9) Å	β = 91.996(6)°.
	c = 17.9471(12) Å	γ = 90°.
Volume	2944.0(4) $Å^3$	
Z	4	
Density (calculated)	1.473 Mg/m^3	
Absorption coefficient	3.122 mm^{-1}	
F(000)	1336	
Crystal size	0.10 x 0.03 x 0.02 mm^3	
Theta range for data collection	4.506 to 76.612°.	
Index ranges	-17<=h<=17, -14<=k<=14, -22<=l<=21	
Reflections collected	33186	
Independent reflections	6070 [R(int) = 0.1948]	
Completeness to theta = 67.684°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.89282	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6070 / 0 / 388	
Goodness-of-fit on F^2	1.409	
Final R indices [I>2sigma(I)]	R1 = 0.1160, wR2 = 0.3155	
R indices (all data)	R1 = 0.2048, wR2 = 0.3473	
Largest diff. peak and hole	0.512 and -0.877 $e.Å^{-3}$	

Table 5. Crystal data and structure refinement for **5**.

Empirical formula	$C_{24}H_{14}Cl_2F_2N_2Zn$	
Formula weight	504.64	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 9.984(3) Å	α = 90°.
	b = 11.965(4) Å	β = 101.504(5)°.
	c = 17.609(7) Å	γ = 90°.
Volume	2061.3(13) $Å^3$	
Z	4	
Density (calculated)	1.626 Mg/m^3	
Absorption coefficient	1.483 mm^{-1}	
F(000)	1016	
Crystal size	0.110 x 0.090 x 0.050 mm^3	
Theta range for data collection	2.071 to 24.999°.	
Index ranges	-9<=h<=11, -14<=k<=14, -20<=l<=20	
Reflections collected	21742	
Independent reflections	3627 [R(int) = 0.0626]	
Completeness to theta = 24.999°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.7659	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3627 / 0 / 280	
Goodness-of-fit on F^2	1.245	
Final R indices [I>2sigma(I)]	R1 = 0.0506, wR2 = 0.0868	
R indices (all data)	R1 = 0.0539, wR2 = 0.0881	
Largest diff. peak and hole	0.444 and -0.516 $e.Å^{-3}$	

Table 6. Crystal data and structure refinement for **7**.

Empirical formula	$C_{26}H_{14}Cl_2F_6N_2O_2Zn$	
Formula weight	636.66	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.1932(8) Å	α = 112.425(13)°.
	b = 12.0306(16) Å	β = 91.392(9)°.
	c = 14.760(2) Å	γ = 109.799(10)°.
Volume	1245.5(3) $Å^3$	
Z	2	
Density (calculated)	1.698 Mg/m^3	
Absorption coefficient	4.024 mm^{-1}	
F(000)	636	
Crystal size	0.080 x 0.040 x 0.030 mm^3	
Theta range for data collection	4.189 to 76.579°.	
Index ranges	-10<=h<=10, -15<=k<=10, -12<=l<=18	
Reflections collected	9457	
Independent reflections	4945 [R(int) = 0.0417]	
Completeness to theta = 67.684°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.90542	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4945 / 0 / 352	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0480, wR2 = 0.0984	
R indices (all data)	R1 = 0.0672, wR2 = 0.1062	
Largest diff. peak and hole	0.597 and -0.599 e.$Å^{-3}$	

Table 7. Crystal data and structure refinement for **8**.

Empirical formula	$C_{52}H_{28}Cl_4F_{12}N_4Zn_2$	
Formula weight	1209.32	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.9861(17) Å	α = 99.188(9)°.
	b = 14.4270(17) Å	β = 102.008(11)°.
	c = 16.0295(14) Å	γ = 114.266(13)°.
Volume	2376.4(5) $Å^3$	
Z	2	
Density (calculated)	1.690 Mg/m^3	
Absorption coefficient	4.116 mm^{-1}	
F(000)	1208	
Crystal size	0.10 x 0.04 x 0.03 mm^3	
Theta range for data collection	2.931 to 67.498°.	
Index ranges	-14<=h<=14, -17<=k<=12, -19<=l<=19	
Reflections collected	17656	
Independent reflections	8564 [R(int) = 0.1294]	
Completeness to theta = 67.498°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.44297	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8564 / 0 / 667	
Goodness-of-fit on F^2	1.082	
Final R indices [I>2sigma(I)]	R1 = 0.1127, wR2 = 0.2856	
R indices (all data)	R1 = 0.1975, wR2 = 0.3387	
Largest diff. peak and hole	0.851 and -1.056 e.$Å^{-3}$	

Table 8. Crystal data and structure refinement for **1-DCM**.

Empirical formula	$C_{33}H_{34}Cl_4N_2O_2Zn$	
Formula weight	697.79	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 17.490(3) Å	α = 90°.
	b = 11.6120(17) Å	β = 117.505(3)°.
	c = 17.926(3) Å	γ = 90°.
Volume	3229.2(8) $Å^3$	
Z	4	
Density (calculated)	1.435 Mg/m^3	
Absorption coefficient	1.124 mm^{-1}	
F(000)	1440	
Crystal size	0.560 x 0.220 x 0.200 mm^3	
Theta range for data collection	3.105 to 24.996°.	
Index ranges	-20<=h<=20, -13<=k<=13, -21<=l<=21	
Reflections collected	27165	
Independent reflections	5671 [R(int) = 0.0660]	
Completeness to theta = 25.242°	97.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.7151	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5671 / 93 / 409	
Goodness-of-fit on F^2	1.000	
Final R indices [I>2sigma(I)]	R1 = 0.0761, wR2 = 0.1944	
R indices (all data)	R1 = 0.0826, wR2 = 0.2013	
Largest diff. peak and hole	2.068 and -2.158 e.$Å^{-3}$	

Table 9. Crystal data and structure refinement for **2-DCM**.

Empirical formula	$C_{27}H_{22}Cl_4N_2O_2Zn$	
Formula weight	613.63	
Temperature	153(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.840(5) Å	α = 90°.
	b = 11.647(4) Å	β = 111.446(4)°.
	c = 17.844(6) Å	γ = 90°.
Volume	2677.2(15) $Å^3$	
Z	4	
Density (calculated)	1.522 Mg/m^3	
Absorption coefficient	1.345 mm^{-1}	
F(000)	1248	
Crystal size	0.140 x 0.090 x 0.070 mm^3	
Theta range for data collection	2.136 to 27.474°.	
Index ranges	-17<=h<=17, -13<=k<=15, -22<=l<=23	
Reflections collected	20087	
Independent reflections	6116 [R(int) = 0.0522]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.5110	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6116 / 0 / 327	
Goodness-of-fit on F^2	1.045	
Final R indices [I>2sigma(I)]	R1 = 0.0348, wR2 = 0.0888	
R indices (all data)	R1 = 0.0389, wR2 = 0.0918	
Largest diff. peak and hole	0.688 and -0.649 $e.Å^{-3}$	

Table 10. Crystal data and structure refinement for **3-DCM**.

Empirical formula	$C_{27}H_{22}Cl_4N_2S_2Zn$	
Formula weight	645.75	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.2610(2) Å	α = 90°.
	b = 12.02200(10) Å	β = 109.1270(10)°.
	c = 18.1350(2) Å	γ = 90°.
Volume	2731.54(6) $Å^3$	
Z	4	
Density (calculated)	1.570 Mg/m^3	
Absorption coefficient	1.464 mm^{-1}	
F(000)	1312	
Crystal size	0.180 x 0.170 x 0.050 mm^3	
Theta range for data collection	1.625 to 26.554°.	
Index ranges	-16<=h<=16, -14<=k<=14, -22<=l<=22	
Reflections collected	16166	
Independent reflections	5505 [R(int) = 0.0318]	
Completeness to theta = 25.242°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.77049	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5505 / 294 / 356	
Goodness-of-fit on F^2	1.237	
Final R indices [I>2sigma(I)]	R1 = 0.0711, wR2 = 0.1747	
R indices (all data)	R1 = 0.0718, wR2 = 0.1750	
Largest diff. peak and hole	0.543 and -0.945 $e.Å^{-3}$	

Table 11. Crystal data and structure refinement for **4-DCM**.

Empirical formula	$C_{36.37}H_{24.74}Cl_{2.74}N_2O_2Zn$	
Formula weight	1369.38	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	I2/a	
Unit cell dimensions	a = 17.442(7) Å	α = 90°.
	b = 11.790(5) Å	β = 104.238(7)°.
	c = 31.054(15) Å	γ = 90°.
Volume	6190(5) $Å^3$	
Z	4	
Density (calculated)	1.469 Mg/m^3	
Absorption coefficient	1.068 mm^{-1}	
F(000)	2798	
Crystal size	0.05 x 0.21 x 0.27 mm^3	
Theta range for data collection	1.855 to 24.998°.	
Index ranges	-20<=h<=20, -14<=k<=13, -36<=l<=36	
Reflections collected	39380	
Independent reflections	5446 [R(int) = 0.0481]	
Completeness to theta = 25.242°	97.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.7810	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5446 / 879 / 527	
Goodness-of-fit on F^2	1.225	
Final R indices [I>2sigma(I)]	R1 = 0.0637, wR2 = 0.1751	
R indices (all data)	R1 = 0.0675, wR2 = 0.1788	
Largest diff. peak and hole	1.510 and -0.574 $e.Å^{-3}$	

Table 12. Crystal data and structure refinement for **5-THF**.

Empirical formula	$C_{30}H_{26}Cl_2F_2N_2O_{1.5}Zn$	
Formula weight	1225.59	
Temperature	153(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 14.3180(15) Å	α = 90°.
	b = 11.7050(8) Å	β = 112.958(4)°.
	c = 17.7720(18) Å	γ = 90°.
Volume	2742.5(4) $Å^3$	
Z	2	
Density (calculated)	1.484 Mg/m^3	
Absorption coefficient	1.133 mm^{-1}	
F(000)	1256	
Crystal size	0.230 x 0.110 x 0.090 mm^3	
Theta range for data collection	2.139 to 27.500°.	
Index ranges	-18<=h<=18, -15<=k<=15, -23<=l<=22	
Reflections collected	28653	
Independent reflections	6289 [R(int) = 0.0641]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.7994	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6289 / 672 / 417	
Goodness-of-fit on F^2	1.070	
Final R indices [I>2sigma(I)]	R1 = 0.0518, wR2 = 0.1089	
R indices (all data)	R1 = 0.0732, wR2 = 0.1248	
Largest diff. peak and hole	0.448 and -0.494 e.$Å^{-3}$	

Table 13. Crystal data and structure refinement for **6-DCM**.

Empirical formula	$C_{25}H_{16}Br_2Cl_4N_2Zn$	
Formula weight	711.39	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.10500(10) Å	α = 90°.
	b = 11.84230(10) Å	β = 110.0250(10)°.
	c = 17.5235(2) Å	γ = 90°.
Volume	2555.12(4) $Å^3$	
Z	4	
Density (calculated)	1.849 Mg/m^3	
Absorption coefficient	8.994 mm^{-1}	
F(000)	1392	
Crystal size	0.140 x 0.060 x 0.030 mm^3	
Theta range for data collection	3.590 to 76.359°.	
Index ranges	-16<=h<=16, -14<=k<=13, -21<=l<=21	
Reflections collected	25415	
Independent reflections	5292 [R(int) = 0.0273]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.59098	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5292 / 0 / 307	
Goodness-of-fit on F^2	1.086	
Final R indices [I>2sigma(I)]	R1 = 0.0250, wR2 = 0.0682	
R indices (all data)	R1 = 0.0260, wR2 = 0.0691	
Largest diff. peak and hole	0.511 and -0.432 e.$Å^{-3}$	

Table 14. Crystal data and structure refinement for **7-DCM**.

Empirical formula	$C_{27}H_{16}Cl_4F_6N_2O_2Zn$	
Formula weight	721.59	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.8689(6) Å	α= 107.262(7)°.
	b = 14.1948(11) Å	β= 92.978(5)°.
	c = 17.6232(16) Å	γ = 94.504(5)°.
Volume	2817.8(4) $Å^3$	
Z	4	
Density (calculated)	1.701 Mg/m^3	
Absorption coefficient	5.342 mm^{-1}	
F(000)	1440	
Crystal size	0.10 x 0.25 x 0.38 mm^3	
Theta range for data collection	3.530 to 76.980°.	
Index ranges	-14<=h<=12, -17<=k<=17, -21<=l<=21	
Reflections collected	17297	
Independent reflections	17297 [R(int) = 0.0000]	
Completeness to theta = 67.684°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.45025	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	17297 / 702 / 758	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0877, wR2 = 0.2289	
R indices (all data)	R1 = 0.1073, wR2 = 0.2449	
Largest diff. peak and hole	2.192 and -1.217 $e.Å^{-3}$	

Table 15. Crystal data and structure refinement for **8-DCM**.

Empirical formula	$C_{27}H_{16}Cl_4F_6N_2Zn$	
Formula weight	689.59	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.7395(5) Å	α = 90°.
	b = 11.9489(3) Å	β = 111.023(4)°.
	c = 17.6137(5) Å	γ = 90°.
Volume	2699.19(16) $Å^3$	
Z	4	
Density (calculated)	1.697 Mg/m^3	
Absorption coefficient	5.486 mm^{-1}	
F(000)	1376	
Crystal size	0.420 x 0.090 x 0.080 mm^3	
Theta range for data collection	4.575 to 76.256°.	
Index ranges	-17<=h<=11, -13<=k<=14, -15<=l<=21	
Reflections collected	10491	
Independent reflections	5421 [R(int) = 0.0313]	
Completeness to theta = 67.684°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.50168	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5421 / 366 / 390	
Goodness-of-fit on F^2	0.980	
Final R indices [I>2sigma(I)]	R1 = 0.0415, wR2 = 0.1110	
R indices (all data)	R1 = 0.0458, wR2 = 0.1160	
Largest diff. peak and hole	0.434 and -0.688 $e.Å^{-3}$	

4) TD-DFT Calculated Excitations

4-OMe (2)

```
   Number of loops in Davidson routine     =   26
   Number of matrix-vector multiplications = 1050
   Type of excitations = SINGLET-SINGLET


Symmetry A

Excitation energies E in a.u. and eV, dE wrt prev. cycle,
oscillator strengths f in a.u.

no.  E/a.u.        E/eV      f           dE/a.u.
-----------------------------------------------------
  1 0.69882E-01  1.9016     0.15468      0.23E-09
  2 0.70159E-01  1.9091     0.74517E-01  0.31E-09
  3 0.73685E-01  2.0051     0.20537E-01  0.10E-10
  4 0.73877E-01  2.0103     0.58340E-02  0.14E-09
  5 0.80127E-01  2.1804     0.12078E-01  0.78E-10
  6 0.82517E-01  2.2454     0.13986E-01  0.10E-09
  7 0.88003E-01  2.3947     0.13135E-01  0.58E-11
  8 0.90943E-01  2.4747     0.86997E-01  0.91E-09
  9 0.91775E-01  2.4973     0.25968E-01  0.21E-09
 10 0.92919E-01  2.5285     0.44400E-04  0.23E-10
 11 0.97532E-01  2.6540     0.13177E-01  0.47E-09
 12 0.10139      2.7591     0.34997E-01  0.48E-10
 13 0.10182      2.7706     0.11352E-01  0.99E-10
 14 0.10690      2.9089     0.10860E-02  0.11E-09
 15 0.10778      2.9330     0.10902E-01  0.11E-09
 16 0.10887      2.9625     0.67617E-01  0.11E-08
 17 0.11844      3.2230     0.21566E-02  0.69E-09
 18 0.12054      3.2799     0.14280E-01  0.23E-09
 19 0.12450      3.3877     0.12075E-02  0.66E-09
 20 0.12489      3.3985     0.12931E-01  0.71E-09
 21 0.12504      3.4026     0.33070E-02  0.63E-10
 22 0.12715      3.4600     0.66715E-02  0.15E-09
 23 0.12771      3.4752     0.40331E-01  0.28E-08
 24 0.13666      3.7186     0.17285E-04  0.45E-09
 25 0.13759      3.7440     0.48803E-03  0.95E-10
 26 0.14034      3.8190     0.20054E-03  0.26E-09
 27 0.14062      3.8264     0.28036E-01  0.14E-08
 28 0.14182      3.8590     0.93906E-04  0.11E-10
 29 0.14526      3.9527     0.54086E-02  0.52E-10
 30 0.14586      3.9691     0.55303E-02  0.32E-09
 31 0.14700      4.0002     0.14494E-01  0.72E-09
 32 0.15000      4.0816     0.18668E-02  0.17E-09
 33 0.15119      4.1141     0.68900E-02  0.24E-09
 34 0.15237      4.1463     0.74877E-03  0.98E-10
 35 0.15315      4.1675     0.98616E-01  0.20E-09
 36 0.15380      4.1851     0.12729      0.34E-09
 37 0.15631      4.2534     0.10323E-02  0.93E-10
 38 0.15675      4.2654     0.10288E-02  0.11E-09
 39 0.15735      4.2817     0.19519E-01  0.14E-08
 40 0.15743      4.2838     0.25590E-01  0.17E-08
 41 0.15758      4.2880     0.10730E-01  0.10E-08
 42 0.15838      4.3097     0.14567E-01  0.67E-09
 43 0.16236      4.4181     0.55033E-01  0.71E-09
 44 0.16282      4.4306     0.38170E-01  0.49E-09
 45 0.16305      4.4367     0.41826E-02  0.37E-09
 46 0.16447      4.4755     0.17241E-02  0.19E-08
 47 0.16543      4.5015     0.71855E-05  0.24E-07
```

48	0.16665	4.5347	0.18969E-01	0.12E-07
49	0.16799	4.5713	0.34943E-01	0.91E-06
50	0.16836	4.5813	0.15508E-01	0.76E-07

4-SMe (3)

```
   Number of loops in Davidson routine     =   16
   Number of matrix-vector multiplications =  650
   Type of excitations = SINGLET-SINGLET


Symmetry A

Excitation energies E in a.u. and eV, dE wrt prev. cycle,
oscillator strengths f in a.u.
```

no.	E/a.u.	E/eV	f	dE/a.u.
1	0.59012E-01	1.6058	0.34922	0.20E-08
2	0.64634E-01	1.7588	0.11738E-01	0.38E-09
3	0.71225E-01	1.9381	0.43356E-02	0.47E-10
4	0.74191E-01	2.0188	0.61286E-02	0.12E-09
5	0.74256E-01	2.0206	0.60564E-01	0.25E-09
6	0.78545E-01	2.1373	0.26957E-01	0.19E-09
7	0.79328E-01	2.1586	0.85101E-01	0.12E-08
8	0.82759E-01	2.2520	0.65061E-02	0.23E-09
9	0.90586E-01	2.4650	0.15342E-02	0.15E-10
10	0.93880E-01	2.5546	0.74074E-03	0.31E-08
11	0.94029E-01	2.5587	0.94880E-03	0.56E-10
12	0.96595E-01	2.6285	0.22097E-02	0.14E-09
13	0.10244	2.7875	0.15069E-02	0.16E-09
14	0.10719	2.9167	0.26941E-02	0.28E-08
15	0.10804	2.9399	0.80050E-02	0.52E-09
16	0.10925	2.9728	0.46795E-01	0.34E-09
17	0.11505	3.1308	0.14797E-02	0.73E-09
18	0.11651	3.1704	0.46495E-04	0.17E-09
19	0.11723	3.1900	0.77722E-02	0.57E-09
20	0.11776	3.2043	0.52604E-02	0.12E-08
21	0.12012	3.2686	0.50020E-01	0.67E-09
22	0.12554	3.4162	0.89526E-03	0.66E-10
23	0.12594	3.4269	0.14989E-02	0.76E-09
24	0.12674	3.4487	0.55326E-03	0.13E-09
25	0.12713	3.4594	0.64807E-03	0.26E-08
26	0.13255	3.6067	0.19997E-02	0.61E-09
27	0.13343	3.6309	0.47697E-02	0.33E-09
28	0.13378	3.6403	0.15334E-02	0.63E-09
29	0.13572	3.6932	0.87127E-01	0.24E-08
30	0.13664	3.7183	0.77600E-01	0.13E-08
31	0.13981	3.8045	0.19707E-03	0.11E-09
32	0.14277	3.8850	0.29021E-01	0.49E-09
33	0.14309	3.8937	0.10369E-01	0.19E-09
34	0.14354	3.9058	0.31648E-01	0.11E-08
35	0.14481	3.9404	0.31313E-01	0.37E-08
36	0.14554	3.9602	0.22668E-01	0.20E-08
37	0.14566	3.9637	0.43479E-02	0.12E-08
38	0.14604	3.9739	0.17334E-01	0.36E-08
39	0.14956	4.0698	0.22140E-01	0.65E-08
40	0.15174	4.1290	0.53361E-02	0.28E-09
41	0.15258	4.1519	0.37347E-03	0.91E-10
42	0.15346	4.1759	0.18159	0.19E-08
43	0.15387	4.1870	0.54142E-02	0.19E-09
44	0.15535	4.2272	0.20217E-01	0.17E-07
45	0.15593	4.2431	0.13497E-02	0.40E-08
46	0.15662	4.2618	0.26698E-01	0.47E-09
47	0.15699	4.2720	0.21237E-02	0.66E-06
48	0.15854	4.3140	0.31555E-01	0.23E-06

49	0.15859	4.3155	0.44198E-01	0.93E-07
50	0.15981	4.3487	0.24116E-02	0.10E-06

4-F (5)

Number of loops in Davidson routine = 13
Number of matrix-vector multiplications = 530
Type of excitations = SINGLET-SINGLET

Symmetry A

Excitation energies E in a.u. and eV, dE wrt prev. cycle, oscillator strengths f in a.u.

no.	E/a.u.	E/eV	f	dE/a.u.
1	0.67092E-01	1.8257	0.41110E-02	0.45E-09
2	0.69496E-01	1.8911	0.25734E-02	0.89E-10
3	0.72281E-01	1.9669	0.22728E-02	0.26E-09
4	0.76963E-01	2.0943	0.71202E-01	0.52E-09
5	0.82119E-01	2.2346	0.74853E-01	0.11E-08
6	0.87293E-01	2.3754	0.28388E-02	0.57E-10
7	0.89676E-01	2.4402	0.38368E-02	0.27E-08
8	0.92210E-01	2.5092	0.36461E-03	0.68E-09
9	0.92260E-01	2.5105	0.33205E-02	0.15E-09
10	0.97455E-01	2.6519	0.23474E-01	0.12E-08
11	0.98331E-01	2.6757	0.41251E-01	0.13E-08
12	0.10212	2.7789	0.16458E-01	0.46E-09
13	0.10665	2.9020	0.71645E-01	0.58E-08
14	0.10804	2.9400	0.26025E-01	0.96E-09
15	0.10855	2.9537	0.10307E-02	0.27E-09
16	0.11179	3.0421	0.28453E-01	0.84E-09
17	0.11660	3.1730	0.26052E-02	0.87E-08
18	0.12106	3.2941	0.30659E-01	0.37E-08
19	0.12417	3.3788	0.28245E-03	0.26E-09
20	0.12648	3.4416	0.27770E-01	0.55E-08
21	0.12803	3.4839	0.23463E-02	0.34E-09
22	0.12966	3.5282	0.30494E-01	0.54E-08
23	0.13630	3.7088	0.19716E-03	0.42E-09
24	0.13732	3.7366	0.17342E-04	0.33E-09
25	0.13937	3.7924	0.23197E-02	0.45E-09
26	0.14095	3.8355	0.67402E-05	0.22E-09
27	0.14117	3.8416	0.33571E-04	0.40E-09
28	0.14729	4.0079	0.11049E-01	0.20E-08
29	0.14753	4.0146	0.75690E-02	0.41E-08
30	0.14874	4.0473	0.28248E-03	0.31E-09
31	0.15033	4.0907	0.19502E-02	0.51E-10
32	0.15075	4.1021	0.38434E-01	0.22E-08
33	0.15118	4.1138	0.87858E-02	0.62E-09
34	0.15263	4.1531	0.17295E-01	0.31E-08
35	0.15279	4.1575	0.12585E-01	0.54E-08
36	0.15332	4.1720	0.27730E-04	0.19E-09
37	0.15584	4.2406	0.96305E-02	0.20E-08
38	0.15658	4.2606	0.27486E-03	0.16E-08
39	0.15855	4.3143	0.24831	0.33E-07
40	0.16074	4.3739	0.29945E-03	0.26E-08
41	0.16132	4.3898	0.40644E-01	0.15E-07
42	0.16208	4.4103	0.68166E-03	0.22E-08
43	0.16213	4.4118	0.54285E-03	0.20E-09
44	0.16371	4.4548	0.80711E-02	0.22E-08
45	0.16554	4.5047	0.65959E-02	0.97E-06
46	0.16609	4.5196	0.13768E-01	0.16E-07
47	0.16654	4.5316	0.24966E-01	0.50E-07
48	0.16668	4.5356	0.42916E-02	0.44E-06
49	0.16753	4.5588	0.12135E-02	0.32E-08

50 0.16800 4.5716 0.97357E-03 0.63E-06

4-Br (6)

Number of loops in Davidson routine = 15
Number of matrix-vector multiplications = 610
Type of excitations = SINGLET-SINGLET

4-CF_3 (8)

Symmetry A

Excitation energies E in a.u. and eV, dE wrt prev. cycle,
oscillator strengths f in a.u.

no.	E/a.u.	E/eV	f	dE/a.u.
1	0.67512E-01	1.8371	0.52932E-02	0.16E-08
2	0.69793E-01	1.8992	0.37656E-01	0.62E-09
3	0.72296E-01	1.9673	0.29492E-02	0.22E-08
4	0.72958E-01	1.9853	0.17454	0.18E-08
5	0.80817E-01	2.1992	0.22735E-01	0.59E-09
6	0.84188E-01	2.2909	0.15284E-02	0.59E-09
7	0.87502E-01	2.3810	0.62994E-02	0.22E-09
8	0.90285E-01	2.4568	0.62702E-01	0.46E-09
9	0.92150E-01	2.5075	0.91347E-02	0.26E-09
10	0.92293E-01	2.5114	0.59367E-02	0.61E-10
11	0.94892E-01	2.5821	0.76168E-02	0.31E-08
12	0.10184	2.7711	0.39287E-02	0.45E-10
13	0.10309	2.8052	0.29243E-01	0.44E-09
14	0.10600	2.8845	0.15431E-02	0.18E-09
15	0.10656	2.8998	0.93712E-04	0.38E-09
16	0.10731	2.9201	0.63166E-01	0.19E-08
17	0.10921	2.9716	0.41037E-02	0.74E-10
18	0.10933	2.9750	0.70286E-02	0.24E-09
19	0.11612	3.1598	0.30266E-02	0.58E-09
20	0.11629	3.1644	0.56458E-02	0.10E-08
21	0.12407	3.3761	0.29000E-01	0.32E-08
22	0.12517	3.4060	0.77859E-05	0.23E-09
23	0.12626	3.4356	0.81291E-04	0.68E-09
24	0.12637	3.4387	0.16450E-02	0.14E-09
25	0.12708	3.4581	0.10030E-01	0.91E-09
26	0.13047	3.5504	0.22846E-03	0.19E-10
27	0.13049	3.5509	0.78263E-04	0.25E-10
28	0.13432	3.6550	0.58417E-03	0.39E-09
29	0.13594	3.6991	0.29770E-04	0.16E-09
30	0.13659	3.7168	0.41407E-04	0.40E-09
31	0.14116	3.8411	0.17030E-01	0.98E-09
32	0.14127	3.8441	0.91638E-03	0.14E-09
33	0.14138	3.8471	0.11458	0.44E-08
34	0.14601	3.9731	0.10816E-02	0.19E-08
35	0.14636	3.9827	0.25065E-01	0.14E-07
36	0.14826	4.0345	0.18057E-03	0.15E-09
37	0.14860	4.0437	0.24806E-02	0.64E-08
38	0.15092	4.1068	0.52275E-03	0.11E-09
39	0.15111	4.1118	0.83202E-03	0.32E-09
40	0.15152	4.1230	0.17654E-02	0.21E-08
41	0.15233	4.1450	0.10299E-02	0.95E-09
42	0.15385	4.1865	0.97788E-04	0.16E-08
43	0.15434	4.1999	0.69800E-05	0.29E-09
44	0.15488	4.2144	0.42712E-01	0.67E-08
45	0.15596	4.2438	0.99417E-02	0.69E-09
46	0.15613	4.2484	0.86855E-02	0.98E-09
47	0.15644	4.2569	0.41130E-01	0.11E-08
48	0.15685	4.2680	0.23999E-01	0.14E-08
49	0.15859	4.3154	0.65215E-01	0.78E-07
50	0.15913	4.3302	0.11039E-01	0.65E-06

```
   Number of loops in Davidson routine     =   18
   Number of matrix-vector multiplications =  730
   Type of excitations = SINGLET-SINGLET


Symmetry A

Excitation energies E in a.u. and eV, dE wrt prev. cycle,
oscillator strengths f in a.u.

no.  E/a.u.        E/eV      f           dE/a.u.
-----------------------------------------------------
  1 0.67270E-01  1.8305     0.42066E-02  0.96E-10
  2 0.69608E-01  1.8941     0.11157E-02  0.98E-11
  3 0.72124E-01  1.9626     0.16858E-02  0.70E-10
  4 0.77855E-01  2.1186     0.18504E-01  0.65E-10
  5 0.85186E-01  2.3180     0.90765E-01  0.72E-09
  6 0.88362E-01  2.4045     0.39194E-02  0.15E-10
  7 0.91587E-01  2.4922     0.27949E-02  0.75E-10
  8 0.92953E-01  2.5294     0.17040E-02  0.27E-10
  9 0.96792E-01  2.6338     0.21310E-01  0.41E-09
 10 0.97301E-01  2.6477     0.83514E-02  0.26E-09
 11 0.10018      2.7261     0.12241E-01  0.31E-09
 12 0.10244      2.7874     0.37122E-02  0.29E-09
 13 0.10366      2.8208     0.18001E-02  0.11E-09
 14 0.10532      2.8658     0.60726E-02  0.29E-09
 15 0.10824      2.9454     0.10404      0.66E-09
 16 0.11567      3.1476     0.39591E-02  0.11E-08
 17 0.11758      3.1996     0.19225E-01  0.15E-09
 18 0.12230      3.3278     0.76116E-02  0.45E-09
 19 0.12326      3.3541     0.24620E-01  0.53E-09
 20 0.12352      3.3611     0.48562E-02  0.19E-09
 21 0.12626      3.4358     0.89996E-03  0.47E-10
 22 0.12847      3.4958     0.52959E-01  0.34E-08
 23 0.13758      3.7437     0.26405E-03  0.15E-09
 24 0.14015      3.8136     0.19441E-02  0.16E-09
 25 0.14171      3.8562     0.46952E-02  0.10E-08
 26 0.14215      3.8681     0.14613E-04  0.15E-09
 27 0.14408      3.9207     0.38523E-02  0.15E-08
 28 0.14840      4.0381     0.62133E-02  0.36E-09
 29 0.14956      4.0696     0.23217E-02  0.76E-10
 30 0.14980      4.0764     0.23091E-02  0.87E-10
 31 0.15235      4.1457     0.22962E-02  0.36E-09
 32 0.15264      4.1535     0.11767E-01  0.15E-09
 33 0.15312      4.1667     0.56982E-01  0.12E-08
 34 0.15372      4.1830     0.40859E-02  0.39E-10
 35 0.15418      4.1955     0.12607E-02  0.84E-10
 36 0.15443      4.2022     0.26754E-02  0.12E-09
 37 0.15523      4.2241     0.13122E-03  0.46E-10
 38 0.15651      4.2588     0.30910E-01  0.95E-09
 39 0.15661      4.2615     0.85567E-01  0.23E-08
 40 0.15708      4.2742     0.17692      0.35E-08
 41 0.15808      4.3016     0.18180E-02  0.26E-09
 42 0.15861      4.3161     0.43908E-04  0.10E-09
 43 0.15992      4.3516     0.51079E-03  0.10E-09
 44 0.16110      4.3837     0.98189E-01  0.37E-09
 45 0.16184      4.4038     0.10620E-01  0.52E-08
 46 0.16243      4.4200     0.24966E-01  0.41E-08
 47 0.16417      4.4674     0.38689E-02  0.50E-06
 48 0.16459      4.4786     0.14993E-01  0.99E-06
 49 0.16547      4.5027     0.35406E-02  0.30E-06
 50 0.16600      4.5170     0.11283E-02  0.29E-06
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5) References:

(1) Eva, version 15.0.0.0; Bruker-AXS, Madison, WI, USA, 2009.