

Supporting Information for "Structure and Photophysics of β -Octafluoro-*meso*-tetraarylporphyrins"

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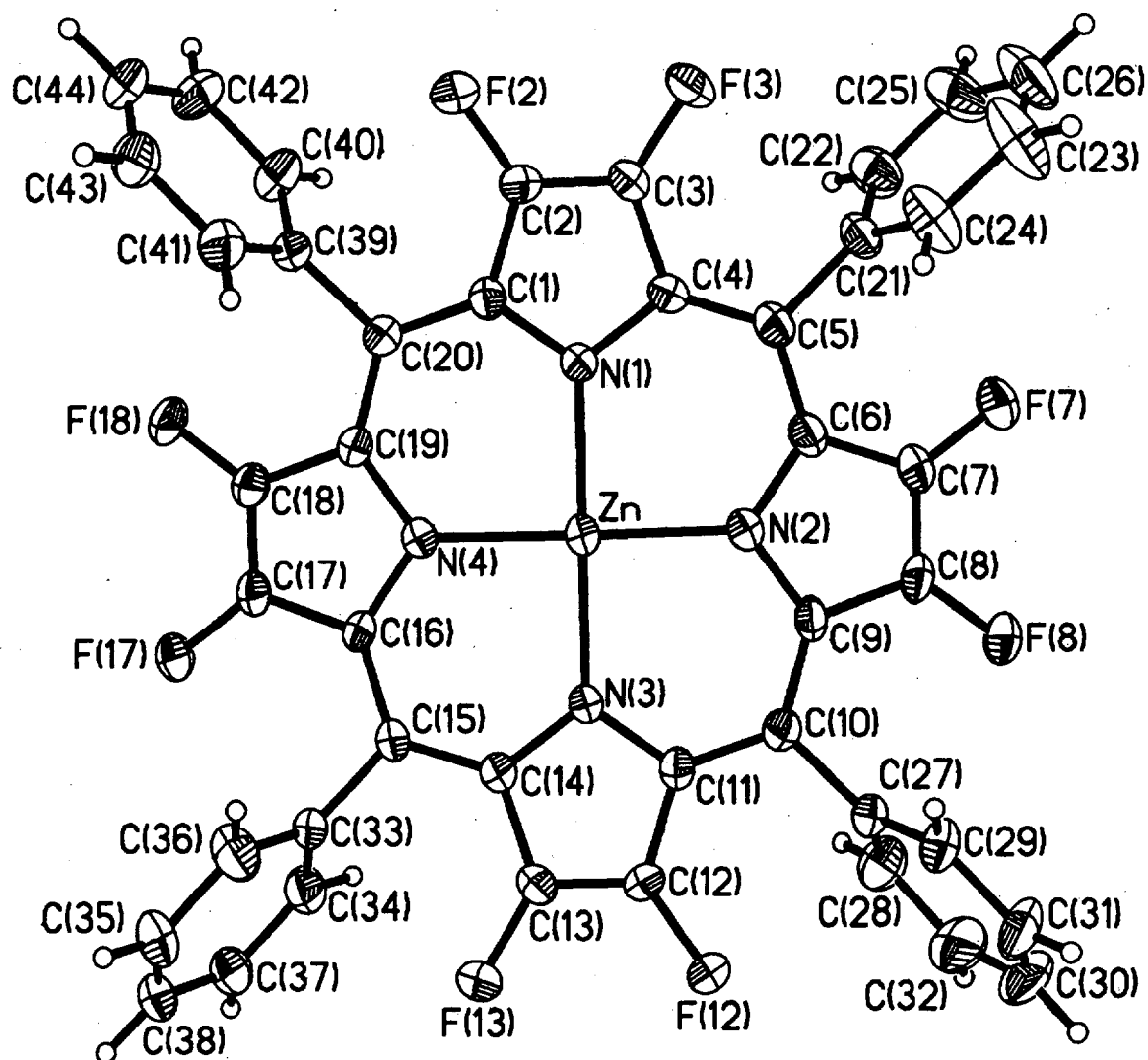


Table 1. Crystal data and structure refinement for Zn(F₈TPP)•THF.

Identification code	ni248
Empirical formula	C ₄₈ H ₂₈ F ₈ N ₄ O Zn
Formula weight	894.11
Temperature	293(2) K
Wavelength	0.56080 Å
Crystal system, space group	Monoclinic P, P2 ₁ /(n)
Unit cell dimensions	a = 14.246(3) Å alpha = 90 deg b = 18.602(4) Å beta = 100.20(3) deg c = 15.209(3) Å gamma = 90 deg
Volume	3966.7(14) Å ³
Z, Calculated density	4, 1.497 Mg/m ³
Absorption coefficient	0.376 mm ⁻¹
F(000)	1816
Crystal size	0.4 x 0.4 x 0.2 mm
Theta range for data collection	3.22 to 17.79 deg
Index ranges	0 ≤ h ≤ 15, 0 ≤ k ≤ 20, -16 ≤ l ≤ 16
Reflections collected / unique	19694 / 5298 [R(int) = 0.0438]
Completeness to 2theta = 17.79	94.9%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5298 / 0 / 560
Goodness-of-fit on F ²	1.185
Final R indices [I > 2sigma(I)]	R1 = 0.0693, wR2 = 0.1701
R indices (all data)	R1 = 0.0781, wR2 = 0.1755
Extinction coefficient	0.0097(11)
Largest diff. peak and hole	1.110 and -0.303 e/Å ³

**Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Zn}(\text{F}_8\text{TPP})\cdot\text{THF}$.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.**

	x	y	z	$U(\text{eq})$
Zn	1054 (1)	6178 (1)	4512 (1)	41 (1)
N1	1680 (3)	6147 (2)	5847 (3)	42 (1)
N2	2381 (3)	6074 (2)	4172 (3)	43 (1)
N3	439 (3)	6012 (3)	3193 (3)	43 (1)
N4	-259 (3)	6013 (3)	4869 (3)	44 (1)
C1	1186 (4)	6265 (3)	6539 (4)	41 (1)
C2	1863 (4)	6494 (3)	7304 (4)	49 (2)
C3	2725 (4)	6493 (4)	7084 (4)	51 (2)
C4	2641 (4)	6271 (3)	6160 (4)	42 (1)
C5	3374 (4)	6198 (3)	5680 (4)	47 (1)
C6	3246 (4)	6072 (3)	4759 (4)	47 (1)
C7	3992 (4)	5974 (4)	4241 (4)	56 (2)
C8	3589 (4)	5950 (4)	3385 (4)	56 (2)
C9	2572 (4)	6014 (3)	3324 (4)	44 (1)
C10	1905 (4)	6043 (3)	2530 (4)	45 (1)
C11	917 (4)	6071 (3)	2479 (4)	44 (1)
C12	219 (4)	6162 (3)	1689 (4)	50 (2)
C13	-643 (4)	6161 (3)	1922 (4)	50 (1)
C14	-526 (4)	6048 (3)	2865 (4)	42 (1)
C15	-1253 (4)	5954 (3)	3358 (4)	43 (1)
C16	-1106 (4)	5885 (3)	4289 (4)	42 (1)
C17	-1819 (4)	5731 (3)	4829 (4)	49 (2)
C18	-1422 (4)	5793 (4)	5677 (4)	53 (2)
C19	-430 (4)	5982 (3)	5728 (4)	44 (1)
C20	212 (4)	6160 (3)	6504 (4)	43 (1)
C21	4381 (4)	6286 (3)	6156 (4)	51 (2)
C22	4860 (5)	5749 (4)	6651 (5)	67 (2)
C23	5794 (6)	7005 (5)	6476 (8)	113 (4)
C24	4856 (5)	6916 (4)	6077 (6)	84 (2)
C25	5804 (6)	5838 (5)	7058 (6)	92 (3)
C26	6255 (6)	6466 (6)	6964 (7)	107 (3)
C27	2277 (4)	6057 (3)	1654 (4)	50 (2)
C28	2252 (5)	5446 (4)	1142 (5)	73 (2)
C29	2648 (5)	6681 (4)	1363 (5)	65 (2)
C30	2907 (7)	6106 (7)	36 (5)	95 (3)
C31	2962 (6)	6710 (6)	554 (6)	88 (3)
C32	2557 (7)	5483 (6)	315 (6)	95 (3)
C33	-2257 (4)	5938 (3)	2862 (4)	46 (1)
C34	-2604 (4)	5364 (4)	2331 (4)	59 (2)
C35	-3783 (5)	6503 (5)	2437 (5)	79 (2)
C36	-2856 (5)	6513 (4)	2906 (5)	71 (2)
C37	-3530 (5)	5363 (5)	1870 (5)	74 (2)
C38	-4120 (5)	5922 (5)	1918 (5)	79 (2)
C39	-184 (4)	6263 (3)	7346 (4)	44 (1)
C40	-13 (5)	5769 (4)	8028 (4)	62 (2)
C41	-686 (5)	6871 (4)	7463 (5)	62 (2)

C42	-352 (6)	5884 (4)	8814 (4)	74 (2)
C43	-1024 (5)	6983 (4)	8258 (5)	69 (2)
C44	-856 (5)	6482 (5)	8938 (5)	71 (2)
F2	1670 (3)	6692 (2)	8105 (2)	70 (1)
F3	3533 (2)	6676 (3)	7635 (3)	80 (1)
F7	4920 (2)	5906 (3)	4551 (3)	82 (1)
F8	4062 (3)	5875 (3)	2705 (3)	80 (1)
F12	390 (2)	6260 (2)	858 (2)	69 (1)
F13	-1457 (2)	6257 (2)	1339 (2)	71 (1)
F17	-2729 (2)	5545 (2)	4516 (2)	67 (1)
F18	-1853 (2)	5663 (2)	6380 (2)	68 (1)
O1S	997 (3)	7331 (2)	4468 (3)	60 (1)
C1S	1771 (6)	7783 (4)	4807 (10)	142 (5)
C2S	1485 (6)	8523 (4)	4622 (6)	90 (3)
C3S	201 (6)	7758 (5)	4164 (10)	144 (5)
C4S	414 (6)	8506 (5)	4370 (6)	90 (3)

Table 4. Bond lengths [Å] and angles [deg] for Zn(F₈TPP)•THF.

Zn-N2	2.056 (4)
Zn-N4	2.061 (4)
Zn-N1	2.068 (4)
Zn-N3	2.066 (4)
Zn-O1S	2.147 (4)
N1-C1	1.384 (7)
N1-C4	1.387 (7)
N2-C9	1.368 (7)
N2-C6	1.388 (7)
N3-C14	1.379 (7)
N3-C11	1.385 (7)
N4-C19	1.371 (7)
N4-C16	1.383 (7)
C1-C20	1.393 (8)
C1-C2	1.438 (8)
C2-C3	1.329 (8)
C2-F2	1.347 (7)
C3-F3	1.341 (6)
C3-C4	1.450 (8)
C4-C5	1.382 (8)
C5-C6	1.400 (8)
C5-C21	1.496 (8)
C6-C7	1.442 (8)
C7-C8	1.327 (9)
C7-F7	1.329 (7)
C8-F8	1.338 (7)
C8-C9	1.441 (8)
C9-C10	1.399 (8)
C10-C11	1.397 (8)
C10-C27	1.518 (8)
C11-C12	1.427 (8)
C12-C13	1.337 (8)
C12-F12	1.341 (6)
C13-F13	1.341 (6)
C13-C14	1.429 (8)
C14-C15	1.392 (7)
C15-C16	1.401 (8)
C15-C33	1.495 (7)
C16-C17	1.443 (7)
C17-C18	1.320 (8)
C17-F17	1.345 (6)
C18-F18	1.344 (6)
C18-C19	1.446 (8)
C19-C20	1.399 (8)
C20-C39	1.500 (8)
C21-C22	1.360 (9)
C21-C24	1.369 (9)
C22-C25	1.388 (10)
C23-C26	1.347 (13)
C23-C24	1.376 (10)
C25-C26	1.353 (13)
C27-C28	1.376 (9)

C27-C29	1.379(9)
C28-C32	1.403(11)
C29-C31	1.384(10)
C30-C32	1.359(13)
C30-C31	1.367(13)
C33-C34	1.376(9)
C33-C36	1.377(9)
C34-C37	1.381(9)
C35-C38	1.374(11)
C35-C36	1.385(10)
C37-C38	1.348(11)
C39-C41	1.367(9)
C39-C40	1.374(8)
C40-C42	1.383(9)
C41-C43	1.393(9)
C42-C44	1.356(10)
C43-C44	1.381(10)
O1S-C3S	1.394(9)
O1S-C1S	1.409(9)
C1S-C2S	1.449(11)
C2S-C4S	1.506(11)
C3S-C4S	1.448(12)

N2-Zn-N4	166.00(19)
N2-Zn-N1	89.34(17)
N4-Zn-N1	89.49(17)
N2-Zn-N3	89.53(17)
N4-Zn-N3	89.15(17)
N1-Zn-N3	169.76(19)
N2-Zn-O1S	96.73(17)
N4-Zn-O1S	97.27(17)
N1-Zn-O1S	93.81(17)
N3-Zn-O1S	96.43(18)
C1-N1-C4	108.4(4)
C1-N1-Zn	123.6(3)
C4-N1-Zn	124.1(3)
C9-N2-C6	107.8(4)
C9-N2-Zn	126.1(4)
C6-N2-Zn	126.1(4)
C14-N3-C11	108.0(4)
C14-N3-Zn	124.6(3)
C11-N3-Zn	124.5(3)
C19-N4-C16	108.6(4)
C19-N4-Zn	125.4(3)
C16-N4-Zn	125.9(3)
N1-C1-C20	125.9(5)
N1-C1-C2	107.7(5)
C20-C1-C2	126.4(5)
C3-C2-F2	125.1(5)
C3-C2-C1	108.3(5)
F2-C2-C1	126.6(5)
C2-C3-F3	124.9(5)
C2-C3-C4	108.9(5)
F3-C3-C4	126.3(5)
C5-C4-N1	126.5(5)
C5-C4-C3	126.8(5)
N1-C4-C3	106.7(5)

C4-C5-C6	124.6(5)
C4-C5-C21	118.9(5)
C6-C5-C21	116.5(5)
N2-C6-C5	126.0(5)
N2-C6-C7	107.8(5)
C5-C6-C7	126.1(5)
C8-C7-F7	125.1(6)
C8-C7-C6	107.9(5)
F7-C7-C6	127.0(6)
C7-C8-F8	124.9(5)
C7-C8-C9	108.4(5)
F8-C8-C9	126.6(6)
N2-C9-C10	126.4(5)
N2-C9-C8	108.1(5)
C10-C9-C8	125.5(5)
C11-C10-C9	124.9(5)
C11-C10-C27	117.1(5)
C9-C10-C27	118.0(5)
N3-C11-C10	125.7(5)
N3-C11-C12	107.7(5)
C10-C11-C12	126.6(5)
C13-C12-F12	125.4(5)
C13-C12-C11	108.2(5)
F12-C12-C11	126.4(5)
C12-C13-F13	123.4(5)
C12-C13-C14	108.5(5)
F13-C13-C14	128.1(5)
N3-C14-C15	126.0(5)
N3-C14-C13	107.6(5)
C15-C14-C13	126.4(5)
C14-C15-C16	124.3(5)
C14-C15-C33	117.9(5)
C16-C15-C33	117.8(5)
N4-C16-C15	125.9(5)
N4-C16-C17	107.1(5)
C15-C16-C17	126.8(5)
C18-C17-F17	126.0(5)
C18-C17-C16	108.4(5)
F17-C17-C16	125.6(5)
C17-C18-F18	125.8(5)
C17-C18-C19	108.6(5)
F18-C18-C19	125.5(5)
N4-C19-C20	126.5(5)
N4-C19-C18	107.3(5)
C20-C19-C18	126.1(5)
C1-C20-C19	124.3(5)
C1-C20-C39	118.1(5)
C19-C20-C39	117.6(5)
C22-C21-C24	118.0(6)
C22-C21-C5	122.1(6)
C24-C21-C5	119.8(6)
C21-C22-C25	120.8(7)
C26-C23-C24	119.6(9)
C21-C24-C23	121.4(8)
C26-C25-C22	119.7(8)
C25-C26-C23	120.5(7)
C28-C27-C29	119.1(6)

C28-C27-C10	120.3(6)
C29-C27-C10	120.6(6)
C27-C28-C32	119.1(8)
C31-C29-C27	121.4(8)
C32-C30-C31	120.5(7)
C30-C31-C29	119.1(8)
C30-C32-C28	120.7(8)
C34-C33-C36	118.0(6)
C34-C33-C15	121.6(5)
C36-C33-C15	120.4(6)
C33-C34-C37	120.7(7)
C38-C35-C36	120.8(7)
C33-C36-C35	120.4(7)
C38-C37-C34	121.4(8)
C37-C38-C35	118.7(7)
C41-C39-C40	118.8(6)
C41-C39-C20	120.0(5)
C40-C39-C20	121.1(5)
C39-C40-C42	120.4(6)
C39-C41-C43	120.4(6)
C44-C42-C40	121.5(7)
C44-C43-C41	120.6(6)
C42-C44-C43	118.3(6)
C3S-O1S-C1S	108.6(6)
C3S-O1S-Zn	127.1(4)
C1S-O1S-Zn	124.2(4)
O1S-C1S-C2S	108.7(7)
C1S-C2S-C4S	105.5(7)
O1S-C3S-C4S	110.4(7)
C3S-C4S-C2S	103.8(7)

**Table 5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Zn}(\text{F}_8\text{TPP}) \cdot \text{THF}$.
The anisotropic displacement factor exponent takes the form:
 $-2\pi^2 [(h a^*)^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$**

	U11	U22	U33	U23	U13	U12
Zn	30 (1)	53 (1)	40 (1)	0 (1)	7 (1)	-1 (1)
N1	35 (2)	52 (3)	38 (2)	3 (2)	6 (2)	1 (2)
N2	32 (2)	54 (3)	42 (3)	0 (2)	5 (2)	2 (2)
N3	30 (2)	61 (3)	39 (3)	-1 (2)	7 (2)	0 (2)
N4	32 (2)	60 (3)	38 (3)	0 (2)	6 (2)	-5 (2)
C1	36 (3)	48 (3)	40 (3)	3 (3)	8 (2)	-1 (2)
C2	47 (4)	64 (4)	37 (3)	-3 (3)	4 (3)	4 (3)
C3	35 (3)	69 (4)	47 (3)	-5 (3)	0 (3)	-1 (3)
C4	38 (3)	49 (3)	38 (3)	0 (2)	0 (2)	0 (2)
C5	36 (3)	50 (3)	54 (4)	-2 (3)	3 (3)	4 (3)
C6	33 (3)	55 (4)	53 (4)	-1 (3)	6 (3)	1 (3)
C7	31 (3)	75 (4)	61 (4)	3 (3)	8 (3)	6 (3)
C8	39 (3)	78 (4)	58 (4)	4 (3)	25 (3)	5 (3)
C9	29 (3)	56 (3)	50 (3)	-4 (3)	13 (3)	-3 (2)
C10	43 (3)	51 (3)	44 (3)	-3 (3)	13 (3)	1 (3)
C11	35 (3)	55 (3)	44 (3)	-2 (3)	11 (2)	-4 (3)
C12	48 (3)	68 (4)	33 (3)	6 (3)	9 (3)	-5 (3)
C13	35 (3)	65 (4)	47 (3)	6 (3)	1 (3)	-2 (3)
C14	35 (3)	52 (3)	39 (3)	-1 (3)	6 (2)	-1 (2)
C15	30 (3)	52 (3)	47 (3)	1 (3)	10 (2)	-1 (2)
C16	37 (3)	53 (3)	39 (3)	5 (3)	15 (2)	-2 (2)
C17	33 (3)	67 (4)	50 (4)	-2 (3)	14 (3)	-9 (3)
C18	44 (3)	72 (4)	45 (4)	4 (3)	15 (3)	-12 (3)
C19	37 (3)	59 (4)	36 (3)	-1 (3)	11 (2)	-4 (3)
C20	42 (3)	49 (3)	39 (3)	0 (3)	10 (2)	1 (3)
C21	35 (3)	59 (4)	57 (4)	-9 (3)	2 (3)	1 (3)
C22	57 (4)	66 (4)	74 (5)	-4 (4)	-1 (4)	11 (3)
C23	49 (5)	81 (6)	195 (11)	-13 (7)	-15 (6)	-8 (4)
C24	50 (4)	66 (5)	125 (7)	2 (5)	-11 (4)	-4 (4)
C25	61 (5)	98 (6)	103 (6)	-15 (5)	-26 (5)	32 (5)
C26	41 (4)	128 (8)	140 (9)	-56 (7)	-15 (5)	7 (5)
C27	37 (3)	72 (4)	44 (3)	-1 (3)	14 (3)	3 (3)
C28	78 (5)	80 (5)	67 (5)	-14 (4)	30 (4)	9 (4)
C29	51 (4)	91 (5)	60 (4)	2 (4)	28 (3)	4 (4)
C30	97 (6)	146 (9)	53 (5)	8 (6)	40 (4)	26 (6)
C31	77 (5)	123 (7)	76 (5)	25 (5)	46 (4)	2 (5)
C32	103 (7)	125 (8)	63 (5)	-26 (5)	33 (5)	27 (6)
C33	34 (3)	64 (4)	40 (3)	4 (3)	11 (2)	-1 (3)
C34	46 (4)	71 (4)	61 (4)	-7 (3)	10 (3)	-5 (3)
C35	46 (4)	110 (6)	82 (5)	7 (5)	12 (4)	25 (4)
C36	52 (4)	76 (5)	82 (5)	-8 (4)	4 (4)	3 (4)
C37	42 (4)	115 (6)	62 (4)	-4 (4)	6 (3)	-20 (4)
C38	34 (4)	143 (8)	59 (4)	17 (5)	7 (3)	-1 (5)
C39	42 (3)	51 (3)	38 (3)	-5 (3)	8 (2)	-3 (3)
C40	78 (5)	59 (4)	55 (4)	2 (3)	28 (3)	12 (3)
C41	57 (4)	71 (4)	59 (4)	1 (3)	12 (3)	6 (3)
C42	87 (5)	92 (5)	47 (4)	9 (4)	27 (4)	-1 (4)

C43	63(4)	77(5)	70(5)	-18(4)	16(4)	16(4)
C44	66(4)	101(6)	50(4)	-18(4)	25(3)	5(4)
F2	61(2)	103(3)	46(2)	-20(2)	7(2)	-4(2)
F3	43(2)	127(4)	63(2)	-29(2)	-8(2)	-5(2)
F7	35(2)	138(4)	73(3)	-1(3)	8(2)	15(2)
F8	43(2)	139(4)	65(2)	2(2)	26(2)	15(2)
F12	53(2)	120(3)	37(2)	9(2)	11(2)	2(2)
F13	46(2)	117(3)	46(2)	16(2)	0(2)	2(2)
F17	36(2)	104(3)	62(2)	-2(2)	11(2)	-23(2)
F18	53(2)	106(3)	52(2)	-3(2)	27(2)	-19(2)
O1S	47(2)	49(2)	80(3)	1(2)	3(2)	-1(2)
C1S	64(5)	57(5)	282(15)	2(7)	-30(7)	-15(4)
C2S	94(6)	65(5)	105(7)	-1(4)	1(5)	-12(4)
C3S	60(5)	62(5)	287(16)	18(7)	-29(7)	14(4)
C4S	79(6)	79(5)	110(7)	-3(5)	12(5)	24(4)

Table 6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Zn}(\text{F}_8\text{TPP})\cdot\text{THF}$.

	x	y	z	U(eq)
H22	4551	5318	6718	81
H23	6107	7435	6410	135
H24	4538	7292	5746	100
H25	6126	5467	7395	111
H26	6887	6526	7238	128
H28	2036	5014	1341	87
H29	2688	7090	1719	78
H30	3112	6121	-512	114
H31	3207	7135	365	106
H32	2519	5077	-46	114
H34	-2210	4973	2283	71
H35	-4181	6894	2474	95
H36	-2637	6911	3253	85
H37	-3752	4967	1520	88
H38	-4744	5915	1605	94
H40	332	5354	7960	75
H41	-804	7211	7009	75
H42	-231	5544	9268	88
H43	-1365	7398	8331	83
H44	-1084	6554	9468	85
H1AS	2314	7669	4526	170
H1BS	1956	7712	5446	170
H2AS	1768	8712	4135	108
H2BS	1681	8821	5146	108
H3AS	-326	7605	4445	173
H3BS	12	7700	3523	173
H4AS	117	8666	4862	108
H4BS	196	8809	3855	108

Table 8. Torsion angles [deg] for Zn(F₈TPP)•THF.

N2-Zn-N1-C1	173.3(4)
N4-Zn-N1-C1	-20.7(4)
N3-Zn-N1-C1	-103.0(10)
O1S-Zn-N1-C1	76.6(4)
N2-Zn-N1-C4	18.1(4)
N4-Zn-N1-C4	-175.8(4)
N3-Zn-N1-C4	101.8(10)
O1S-Zn-N1-C4	-78.6(4)
N4-Zn-N2-C9	91.4(8)
N1-Zn-N2-C9	176.6(5)
N3-Zn-N2-C9	6.8(5)
O1S-Zn-N2-C9	-89.6(5)
N4-Zn-N2-C6	-90.6(8)
N1-Zn-N2-C6	-5.4(5)
N3-Zn-N2-C6	-175.2(5)
O1S-Zn-N2-C6	88.4(5)
N2-Zn-N3-C14	-175.9(5)
N4-Zn-N3-C14	18.0(4)
N1-Zn-N3-C14	100.4(10)
O1S-Zn-N3-C14	-79.2(4)
N2-Zn-N3-C11	-17.1(5)
N4-Zn-N3-C11	176.8(5)
N1-Zn-N3-C11	-100.8(10)
O1S-Zn-N3-C11	79.6(5)
N2-Zn-N4-C19	89.9(8)
N1-Zn-N4-C19	4.7(5)
N3-Zn-N4-C19	174.5(5)
O1S-Zn-N4-C19	-89.1(5)
N2-Zn-N4-C16	-87.1(8)
N1-Zn-N4-C16	-172.3(5)
N3-Zn-N4-C16	-2.5(5)
O1S-Zn-N4-C16	93.9(5)
C4-N1-C1-C20	-176.4(5)
Zn-N1-C1-C20	25.1(8)
C4-N1-C1-C2	1.9(6)
Zn-N1-C1-C2	-156.6(4)
N1-C1-C2-C3	-1.6(7)
C20-C1-C2-C3	176.8(6)
N1-C1-C2-F2	177.1(5)
C20-C1-C2-F2	-4.6(10)
F2-C2-C3-F3	1.5(11)
C1-C2-C3-F3	-179.8(6)
F2-C2-C3-C4	-178.1(6)
C1-C2-C3-C4	0.6(7)
C1-N1-C4-C5	178.7(5)
Zn-N1-C4-C5	-22.9(8)
C1-N1-C4-C3	-1.5(6)
Zn-N1-C4-C3	156.9(4)
C2-C3-C4-C5	-179.7(6)
F3-C3-C4-C5	0.7(10)
C2-C3-C4-N1	0.6(7)
F3-C3-C4-N1	-179.0(6)
N1-C4-C5-C6	8.4(10)

C3-C4-C5-C6	-171.3(6)
N1-C4-C5-C21	-174.1(5)
C3-C4-C5-C21	6.2(9)
C9-N2-C6-C5	172.9(6)
Zn-N2-C6-C5	-5.4(8)
C9-N2-C6-C7	-2.7(6)
Zn-N2-C6-C7	179.0(4)
C4-C5-C6-N2	7.0(10)
C21-C5-C6-N2	-170.5(5)
C4-C5-C6-C7	-178.2(6)
C21-C5-C6-C7	4.2(9)
N2-C6-C7-C8	2.5(7)
C5-C6-C7-C8	-173.1(6)
N2-C6-C7-F7	-176.4(6)
C5-C6-C7-F7	8.1(11)
F7-C7-C8-F8	-2.1(12)
C6-C7-C8-F8	179.0(6)
F7-C7-C8-C9	177.6(6)
C6-C7-C8-C9	-1.3(8)
C6-N2-C9-C10	-175.4(6)
Zn-N2-C9-C10	2.9(8)
C6-N2-C9-C8	1.9(6)
Zn-N2-C9-C8	-179.8(4)
C7-C8-C9-N2	-0.3(7)
F8-C8-C9-N2	179.4(6)
C7-C8-C9-C10	177.0(6)
F8-C8-C9-C10	-3.3(11)
N2-C9-C10-C11	-6.3(10)
C8-C9-C10-C11	176.8(6)
N2-C9-C10-C27	172.7(5)
C8-C9-C10-C27	-4.2(9)
C14-N3-C11-C10	-178.5(5)
Zn-N3-C11-C10	19.7(8)
C14-N3-C11-C12	1.2(6)
Zn-N3-C11-C12	-160.5(4)
C9-C10-C11-N3	-6.0(9)
C27-C10-C11-N3	175.0(5)
C9-C10-C11-C12	174.3(6)
C27-C10-C11-C12	-4.7(9)
N3-C11-C12-C13	0.3(7)
C10-C11-C12-C13	-179.9(6)
N3-C11-C12-F12	178.1(6)
C10-C11-C12-F12	-2.2(10)
F12-C12-C13-F13	0.2(11)
C11-C12-C13-F13	178.0(6)
F12-C12-C13-C14	-179.5(6)
C11-C12-C13-C14	-1.7(7)
C11-N3-C14-C15	174.8(5)
Zn-N3-C14-C15	-23.5(8)
C11-N3-C14-C13	-2.2(6)
Zn-N3-C14-C13	159.5(4)
C12-C13-C14-N3	2.5(7)
F13-C13-C14-N3	-177.2(6)
C12-C13-C14-C15	-174.6(6)
F13-C13-C14-C15	5.8(10)
N3-C14-C15-C16	7.2(9)
C13-C14-C15-C16	-176.3(6)

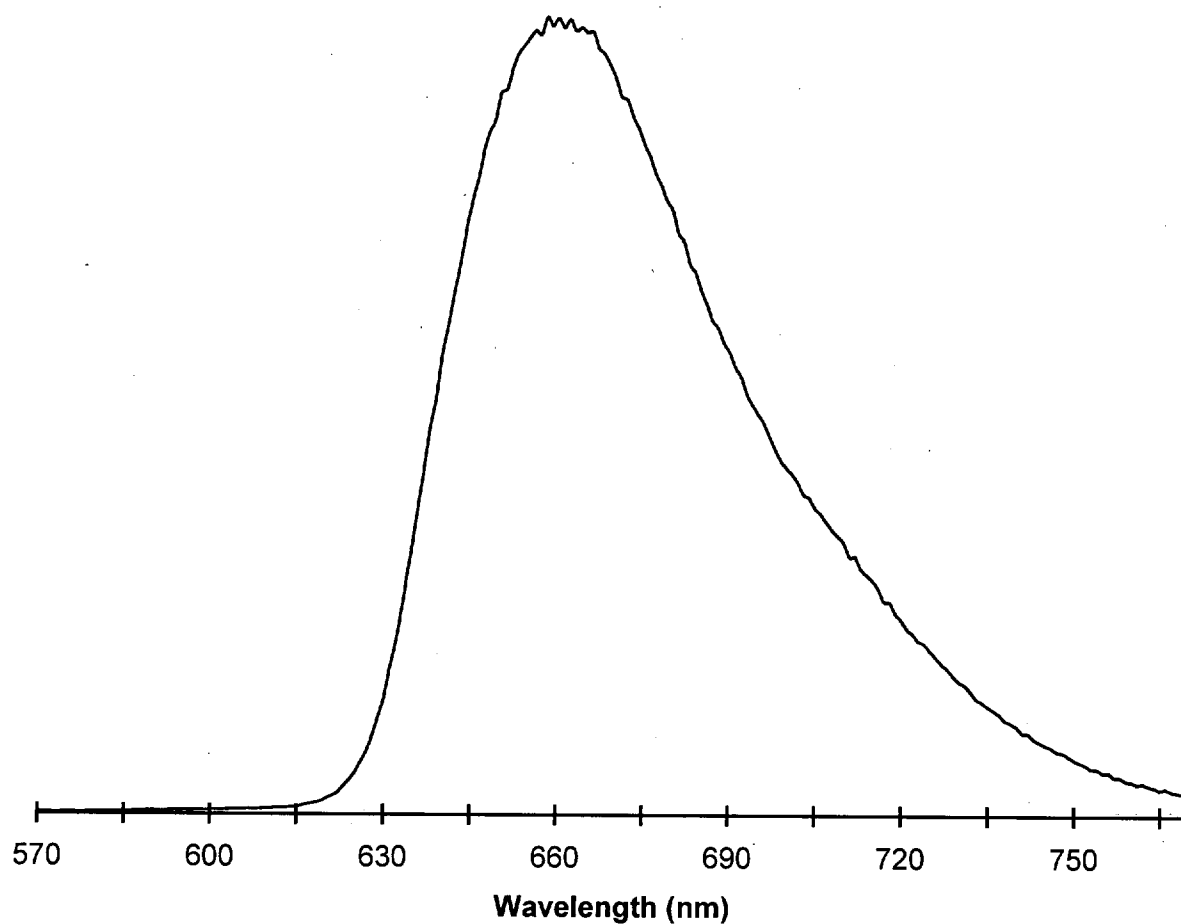
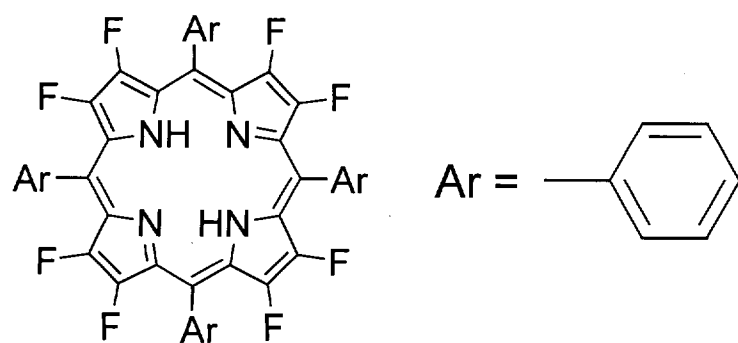
N3-C14-C15-C33	-173.7(5)
C13-C14-C15-C33	2.8(9)
C19-N4-C16-C15	171.9(6)
Zn-N4-C16-C15	-10.6(8)
C19-N4-C16-C17	-3.0(6)
Zn-N4-C16-C17	174.4(4)
C14-C15-C16-N4	11.3(9)
C33-C15-C16-N4	-167.8(5)
C14-C15-C16-C17	-174.7(6)
C33-C15-C16-C17	6.2(9)
N4-C16-C17-C18	2.3(7)
C15-C16-C17-C18	-172.6(6)
N4-C16-C17-F17	-176.8(6)
C15-C16-C17-F17	8.3(10)
F17-C17-C18-F18	1.9(11)
C16-C17-C18-F18	-177.2(6)
F17-C17-C18-C19	178.4(6)
C16-C17-C18-C19	-0.7(7)
C16-N4-C19-C20	-172.3(6)
Zn-N4-C19-C20	10.3(8)
C16-N4-C19-C18	2.6(6)
Zn-N4-C19-C18	-174.8(4)
C17-C18-C19-N4	-1.2(7)
F18-C18-C19-N4	175.3(6)
C17-C18-C19-C20	173.7(6)
F18-C18-C19-C20	-9.8(10)
N1-C1-C20-C19	-6.3(9)
C2-C1-C20-C19	175.7(6)
N1-C1-C20-C39	175.3(5)
C2-C1-C20-C39	-2.7(9)
N4-C19-C20-C1	-13.1(10)
C18-C19-C20-C1	172.9(6)
N4-C19-C20-C39	165.3(5)
C18-C19-C20-C39	-8.7(9)
C4-C5-C21-C22	80.3(8)
C6-C5-C21-C22	-102.0(7)
C4-C5-C21-C24	-101.7(8)
C6-C5-C21-C24	76.0(8)
C24-C21-C22-C25	-0.4(11)
C5-C21-C22-C25	177.7(7)
C22-C21-C24-C23	0.7(13)
C5-C21-C24-C23	-177.4(8)
C26-C23-C24-C21	-0.7(16)
C21-C22-C25-C26	0.1(13)
C22-C25-C26-C23	-0.2(15)
C24-C23-C26-C25	0.5(16)
C11-C10-C27-C28	-78.4(8)
C9-C10-C27-C28	102.5(7)
C11-C10-C27-C29	102.0(7)
C9-C10-C27-C29	-77.1(8)
C29-C27-C28-C32	-3.4(10)
C10-C27-C28-C32	176.9(6)
C28-C27-C29-C31	2.4(10)
C10-C27-C29-C31	-177.9(6)
C32-C30-C31-C29	-0.6(14)
C27-C29-C31-C30	-0.4(12)
C31-C30-C32-C28	-0.5(14)

C27-C28-C32-C30	2.6(13)
C14-C15-C33-C34	71.5(7)
C16-C15-C33-C34	-109.4(7)
C14-C15-C33-C36	-106.7(7)
C16-C15-C33-C36	72.4(8)
C36-C33-C34-C37	-1.0(10)
C15-C33-C34-C37	-179.3(6)
C34-C33-C36-C35	0.8(10)
C15-C33-C36-C35	179.1(6)
C38-C35-C36-C33	-0.2(12)
C33-C34-C37-C38	0.6(11)
C34-C37-C38-C35	0.1(11)
C36-C35-C38-C37	-0.3(12)
C1-C20-C39-C41	104.0(7)
C19-C20-C39-C41	-74.5(7)
C1-C20-C39-C40	-73.0(8)
C19-C20-C39-C40	108.5(7)
C41-C39-C40-C42	0.5(10)
C20-C39-C40-C42	177.5(6)
C40-C39-C41-C43	-0.4(10)
C20-C39-C41-C43	-177.5(6)
C39-C40-C42-C44	-0.1(12)
C39-C41-C43-C44	0.0(11)
C40-C42-C44-C43	-0.4(12)
C41-C43-C44-C42	0.4(11)
N2-Zn-O1S-C3S	142.6(9)
N4-Zn-O1S-C3S	-37.6(9)
N1-Zn-O1S-C3S	-127.6(9)
N3-Zn-O1S-C3S	52.3(9)
N2-Zn-O1S-C1S	-41.8(8)
N4-Zn-O1S-C1S	137.9(8)
N1-Zn-O1S-C1S	47.9(8)
N3-Zn-O1S-C1S	-132.1(8)
C3S-O1S-C1S-C2S	-6.4(13)
Zn-O1S-C1S-C2S	177.3(6)
O1S-C1S-C2S-C4S	14.8(13)
C1S-O1S-C3S-C4S	-5.1(13)
Zn-O1S-C3S-C4S	171.0(6)
O1S-C3S-C4S-C2S	13.8(13)
C1S-C2S-C4S-C3S	-17.0(13)

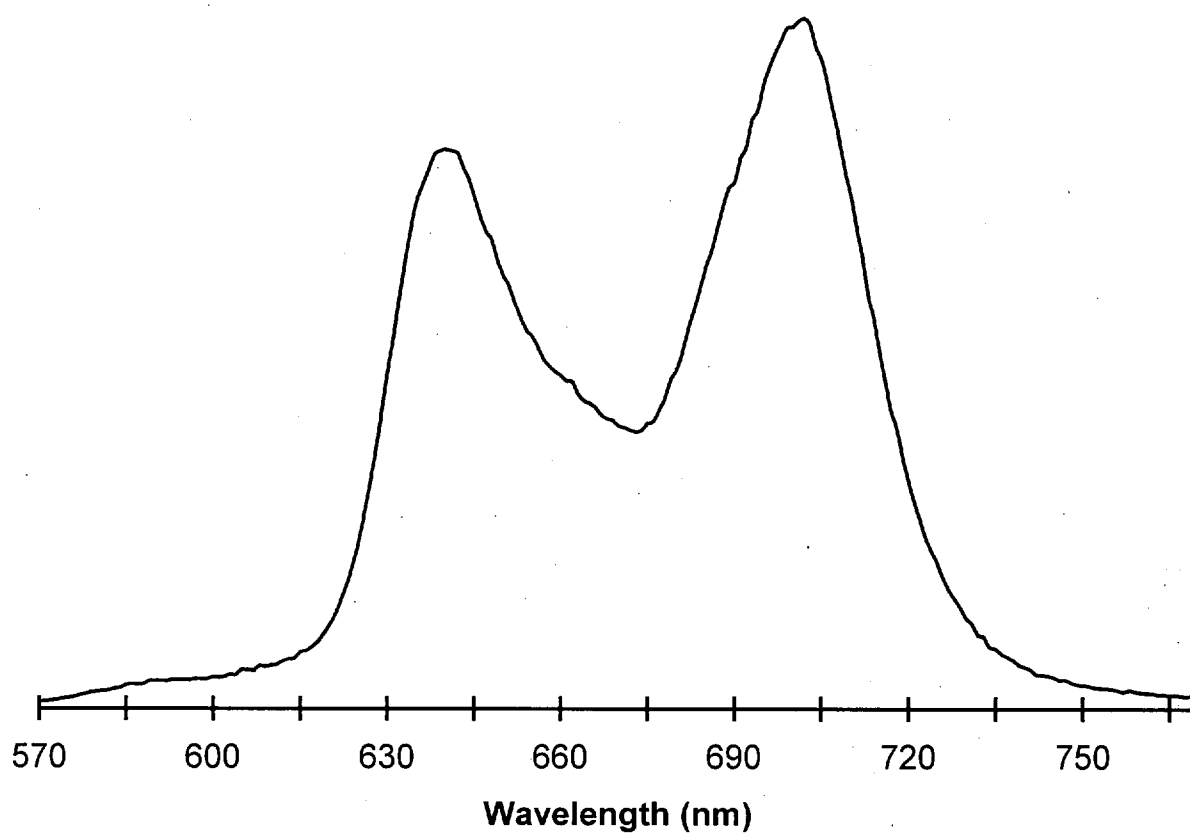
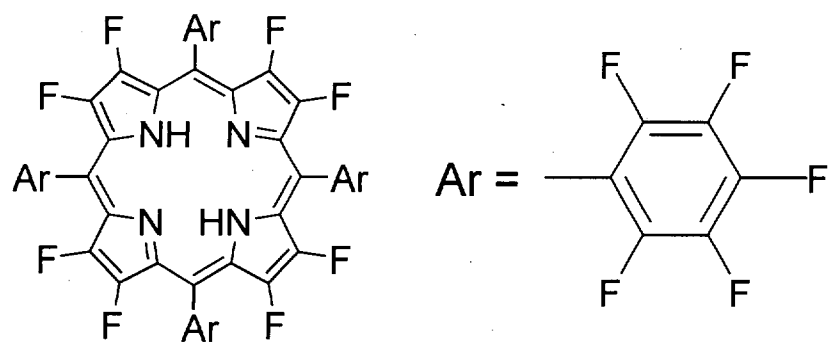
	KBr pellet	Benzonitrile		
	Absorbance, λ_{\max}	Absorbance, λ_{\max}	Emission, λ_{\max}	Stokes shift, cm^{-1}
H ₂ (F ₈ TPP)	406, 507, 540, 588, 645	409, 502, 535, 584, 639	662	544
H ₂ (F ₂₈ TPP)	397, 496, --, 582, --	399, 498, 534, 579, 632	640, 702	198
H ₂ (TPP)	430, 524, 561, 598, 657	422, 516, 552, 592, 649	652, 716	71
Zn(F ₈ TPP)	417, 544, 581	417, 547, 585	610, 639	700
Zn(F ₂₈ TPP)	414, 540, --	416, 544, 585	592, 637	202
Zn(TPP)	434, 561, 600	429, 560, 600	607, 658	192

	KBr pellet	Methylene Chloride		
	Absorbance, λ_{\max}	Absorbance, λ_{\max}	Emission, λ_{\max}	Stokes shift, cm^{-1}
H ₂ (F ₈ TPP)	406, 507, 540, 588, 645	403, 500, 533, 582, 638	663	591
H ₂ (F ₂₈ TPP)	397, 496, --, 582, --	392, 494, 578, 632	641, 702	222
H ₂ (TPP)	430, 524, 561, 598, 657	418, 514, 549, 590, 646	650, 711	95
Zn(F ₈ TPP)	417, 544, 581	407, 499, 534, 572	601, 625	844
Zn(F ₂₈ TPP)	414, 540, --	408, 498, 535, 567	576, 628	276
Zn(TPP)	434, 561, 600	419, 511, 547, 586	595, 642	258

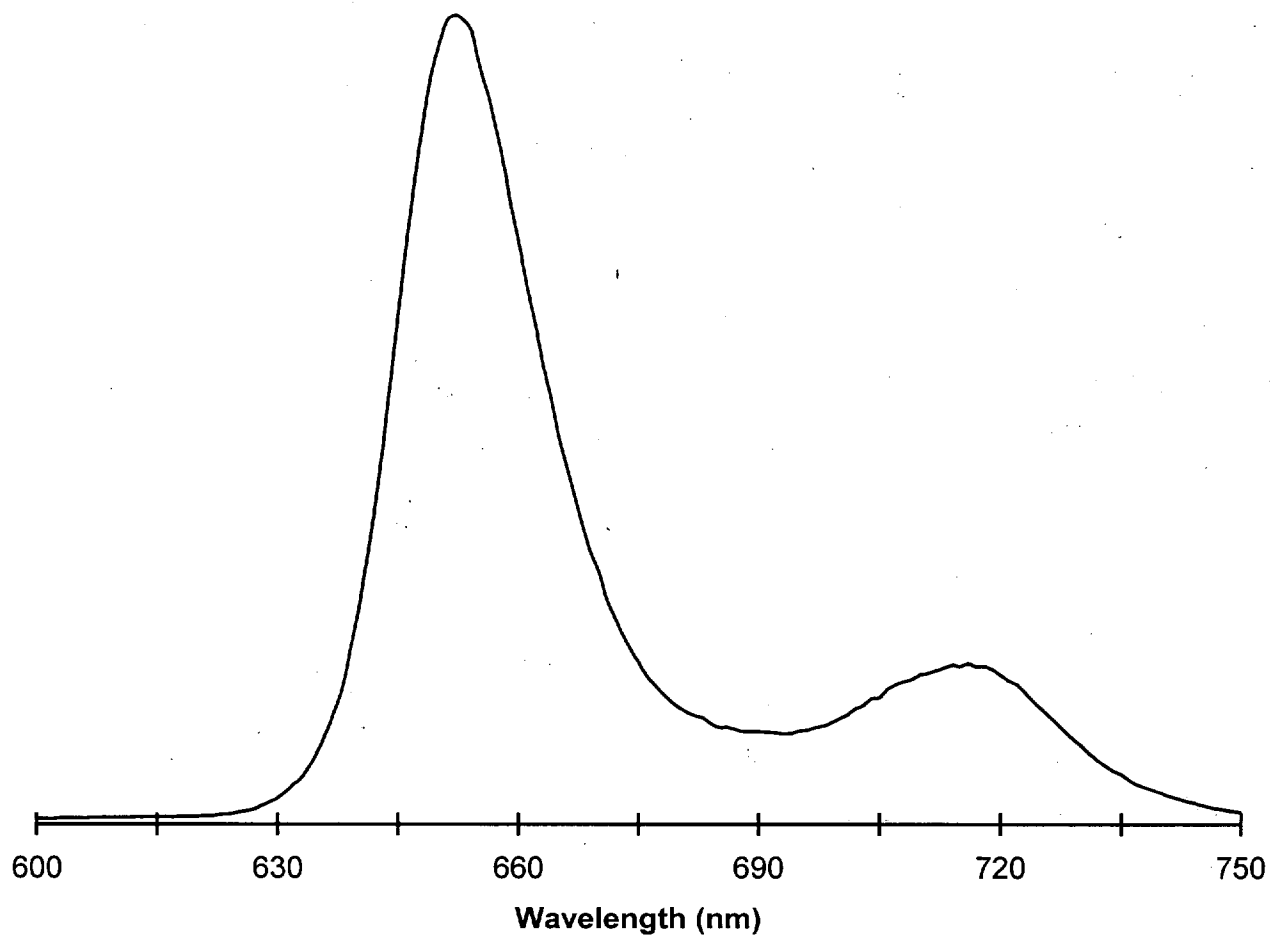
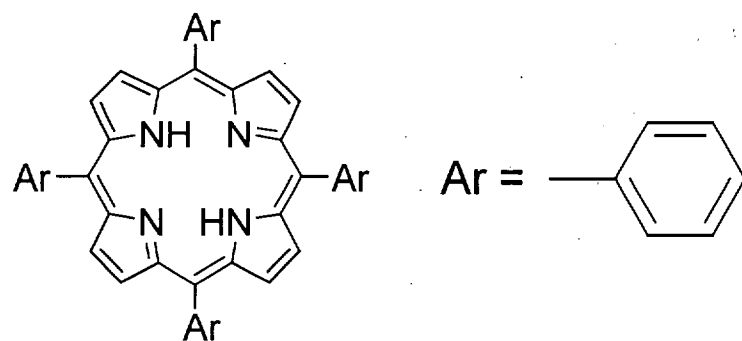
Emission spectrum of $\text{H}_2(\text{F}_8\text{TPP})$ in benzonitrile. Excitation frequency was set to 409 nm.



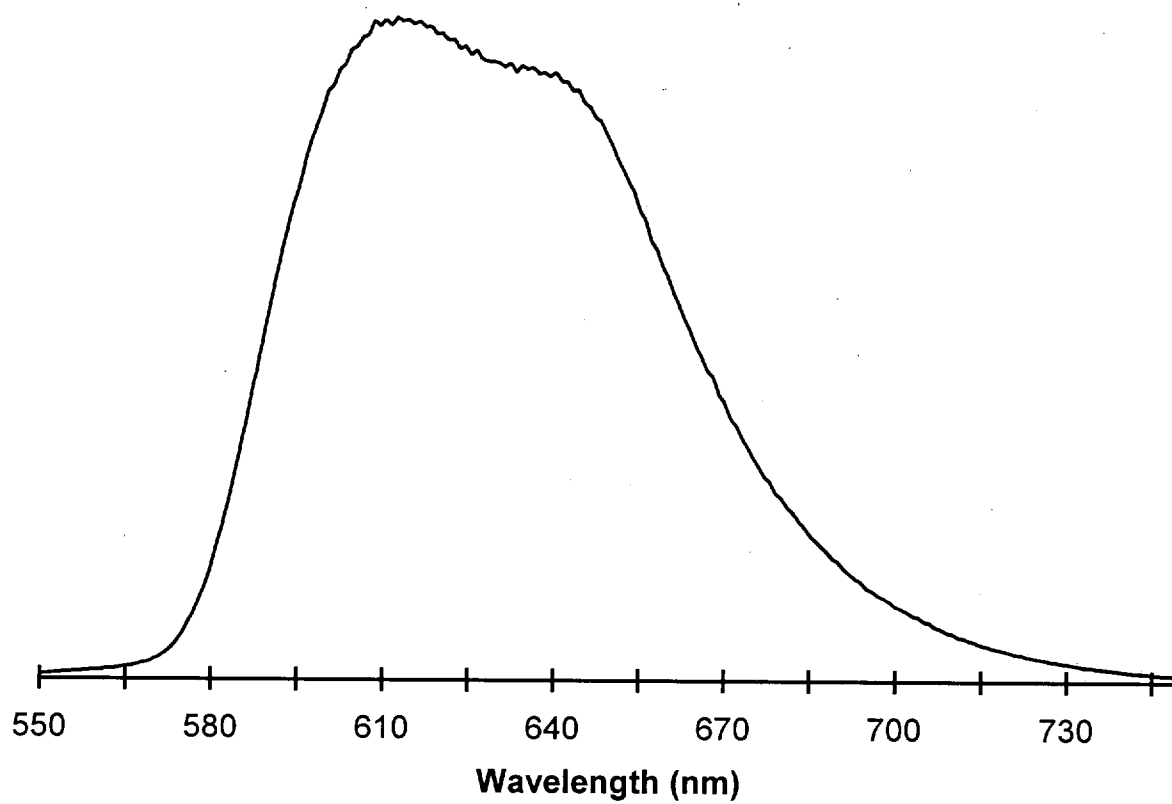
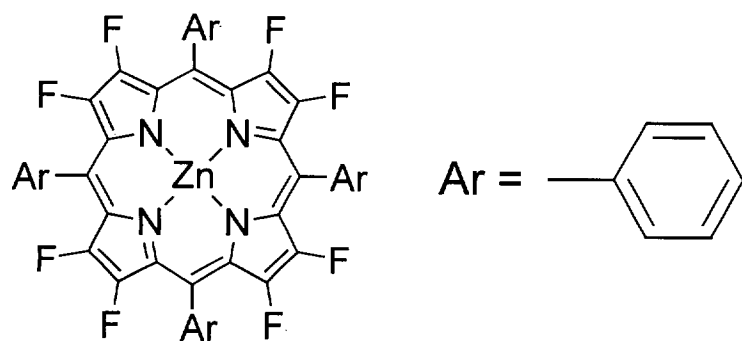
Emission spectrum of **H₂(F₂₈TPP)** in benzonitrile. Excitation frequency was set to 400 nm.



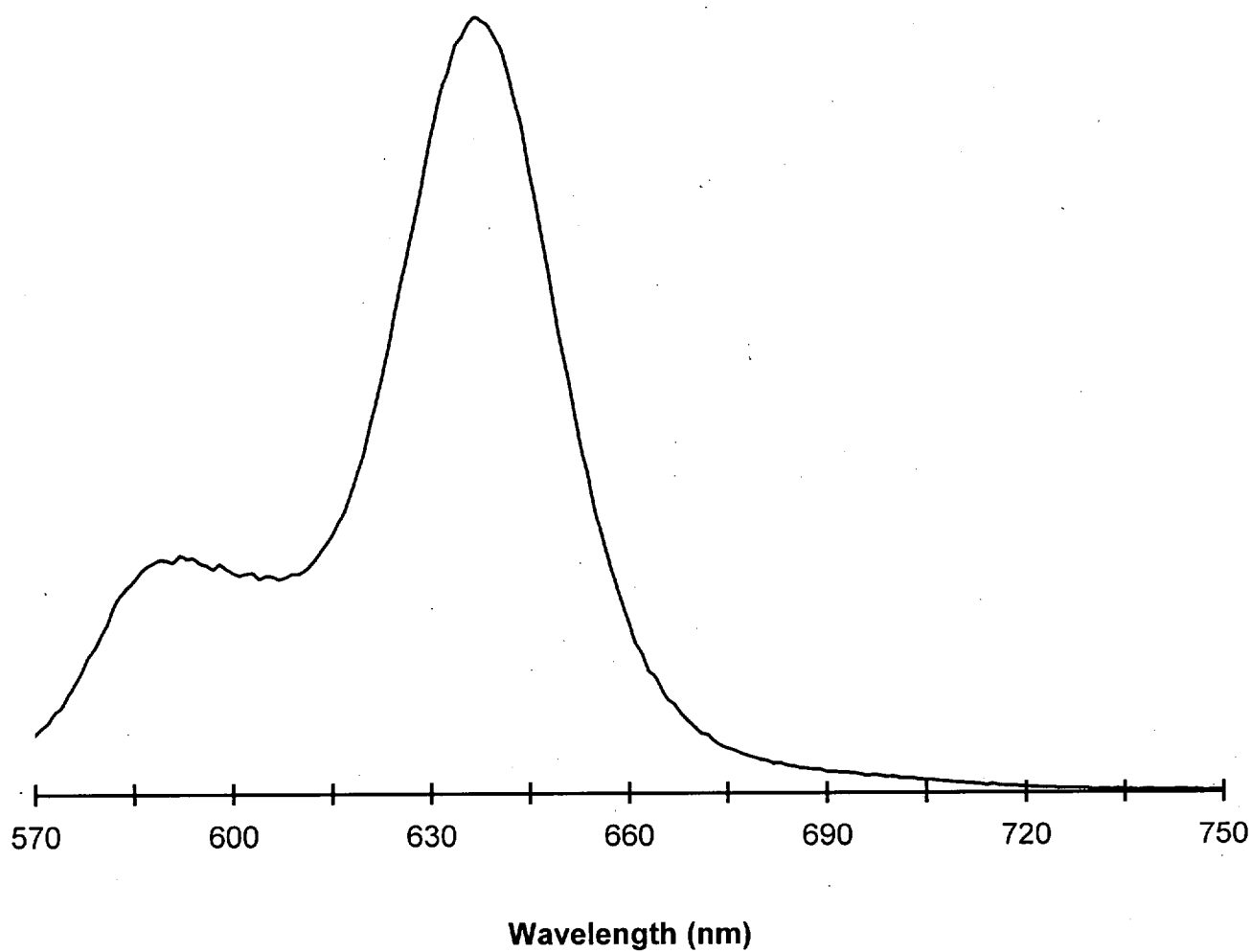
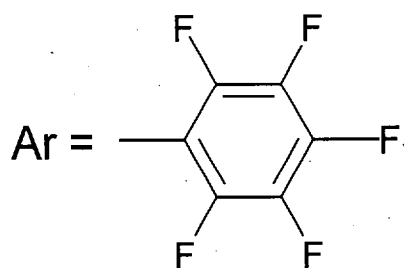
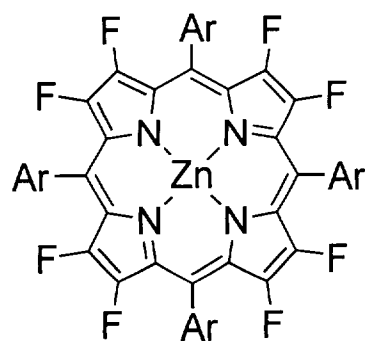
Emission spectrum of **H₂(TPP)** in benzonitrile. Excitation frequency was set to 500 nm.



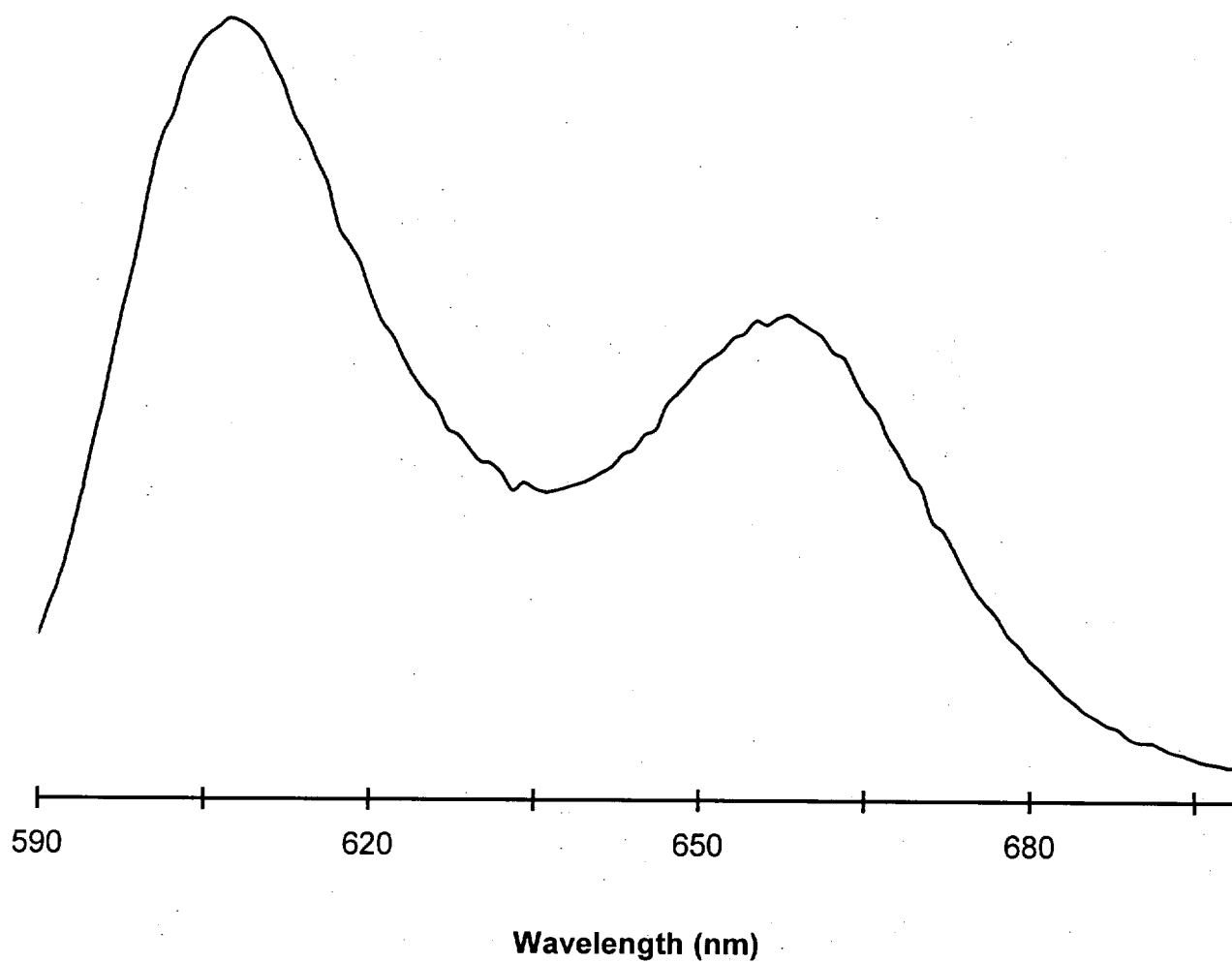
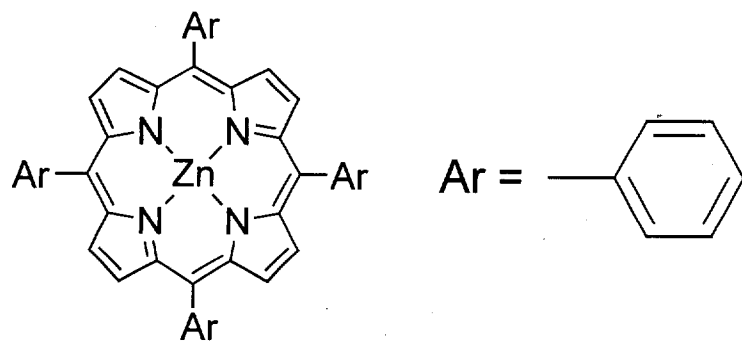
Emission spectrum of **Zn(F₈TPP)** in benzonitrile. Excitation frequency was set to 429 nm.



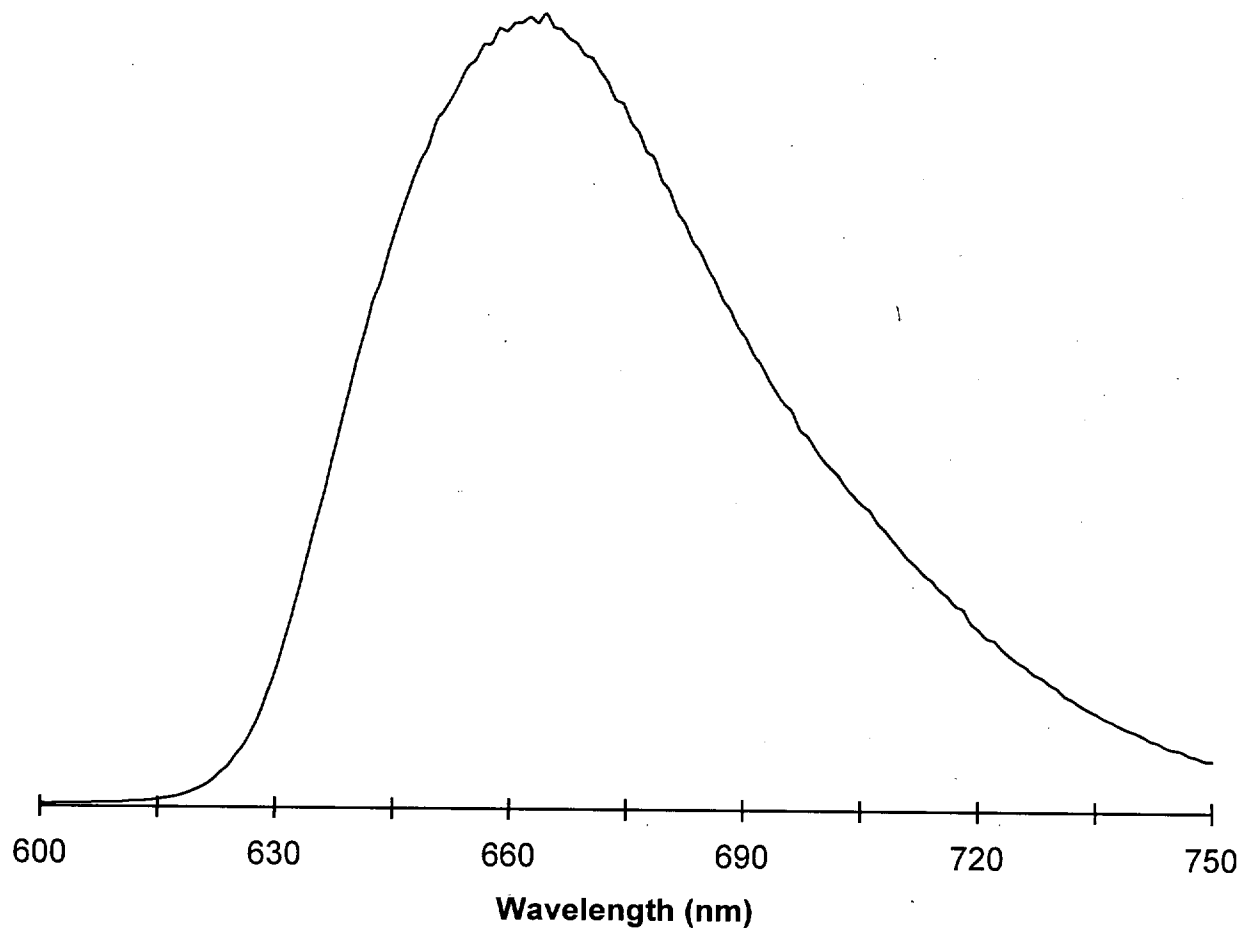
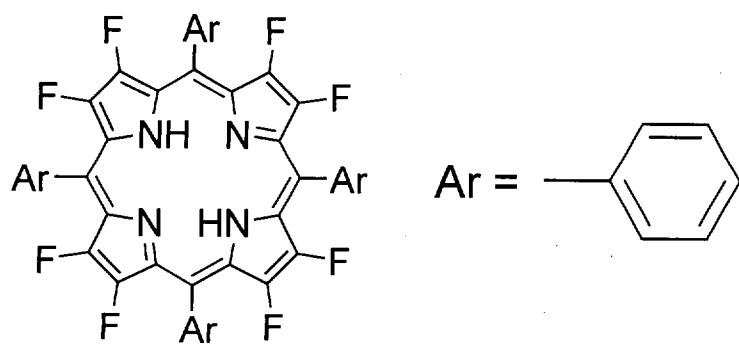
Emission spectrum of **Zn(F₂₈TPP)** in benzonitrile. Excitation frequency was set to 540 nm.



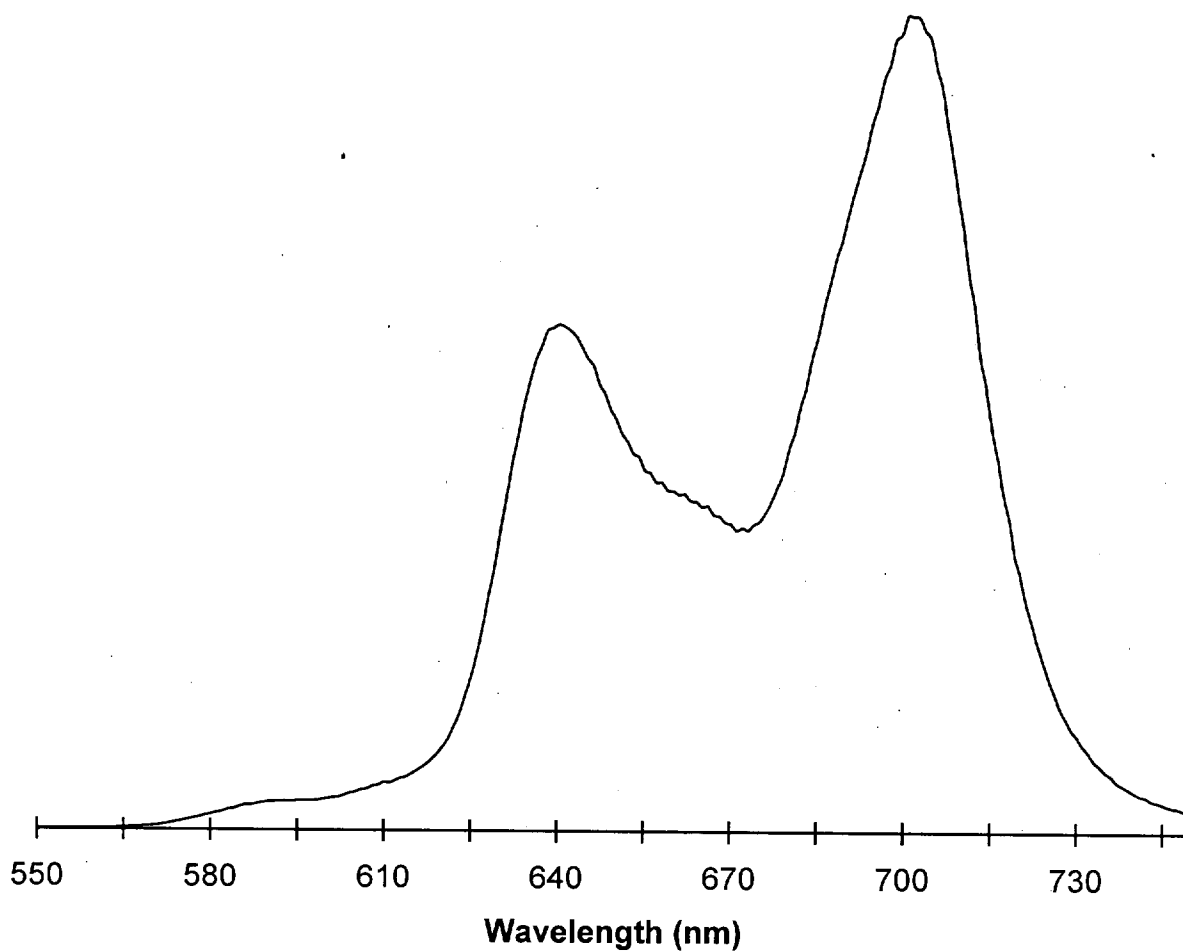
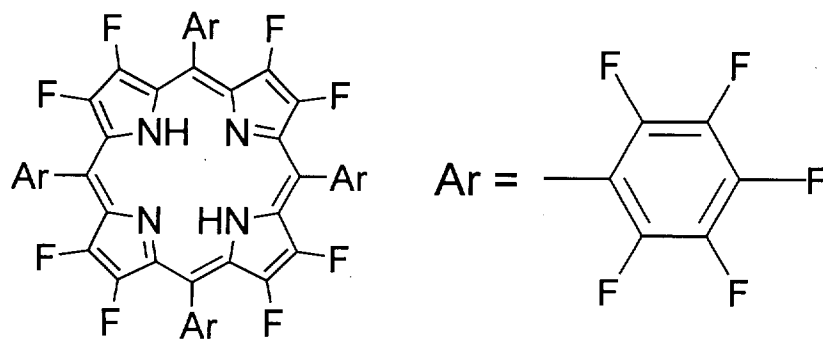
Emission spectrum of **Zn(TPP)** in benzonitrile. Excitation frequency was set to 560 nm.



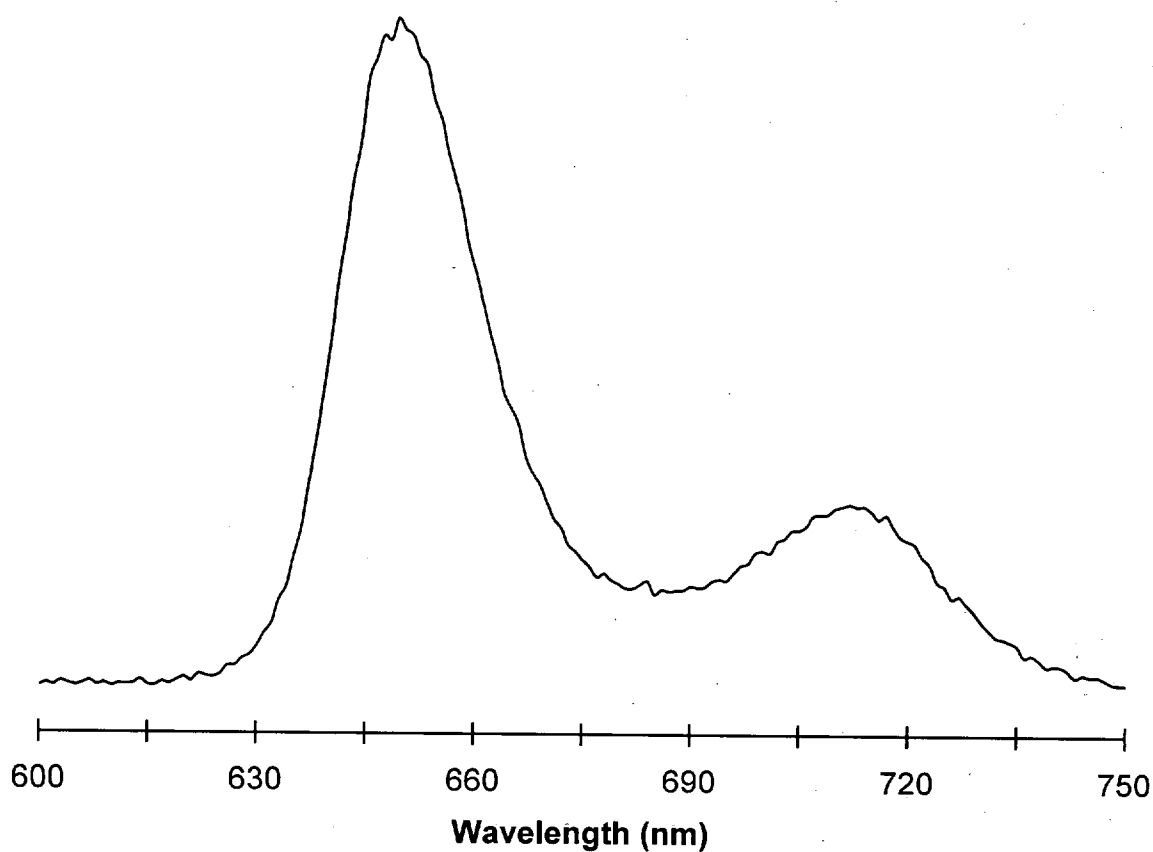
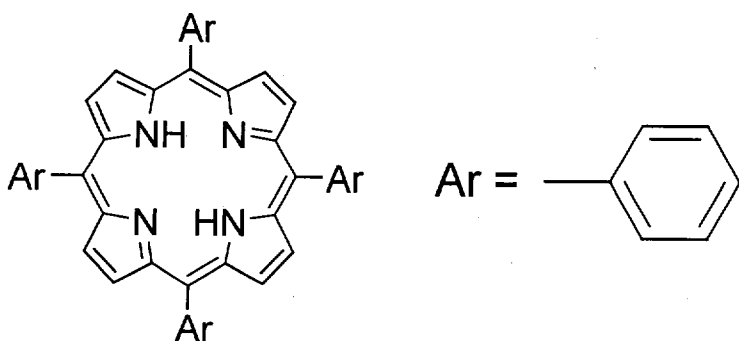
Emission spectrum of $\text{H}_2(\text{F}_8\text{TPP})$ in CH_2Cl_2 . Excitation frequency was set to 407 nm.



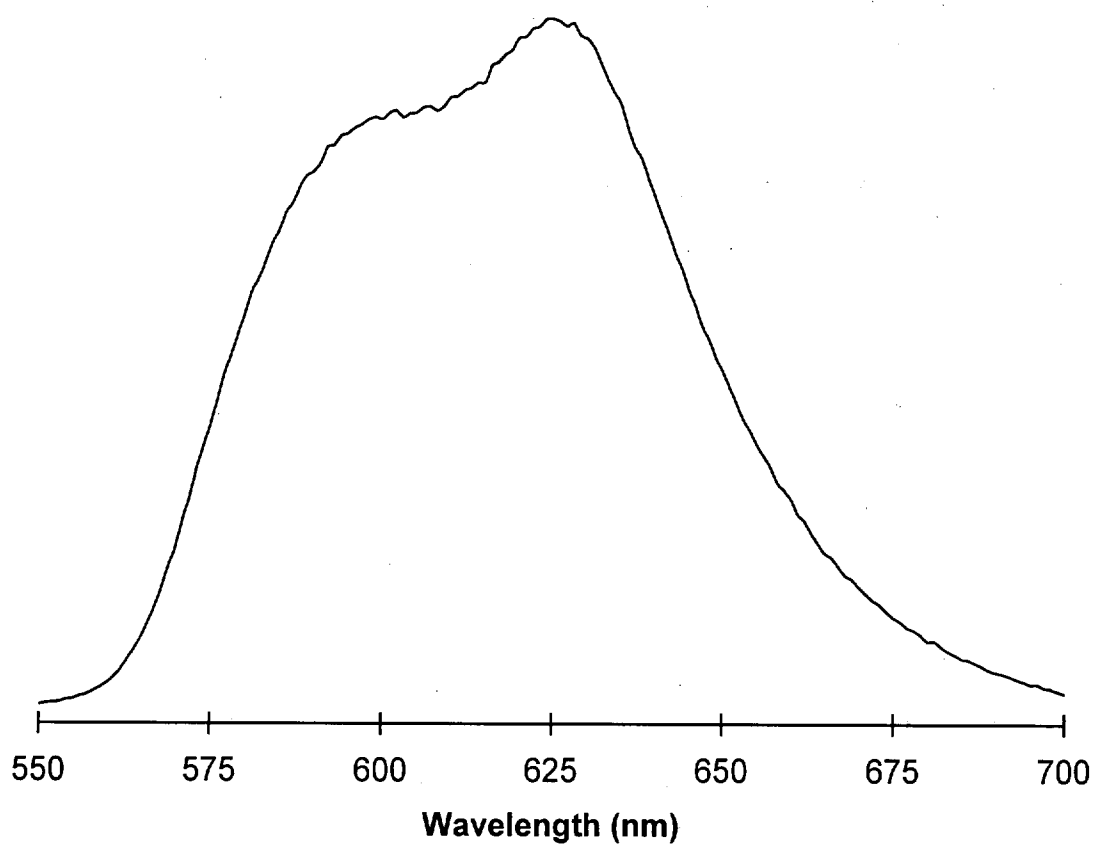
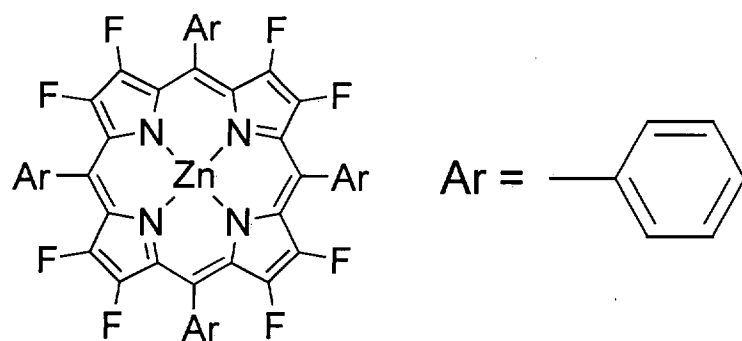
Emission spectrum of $\text{H}_2(\text{F}_{28}\text{TPP})$ in CH_2Cl_2 . Excitation frequency was set to 395 nm.



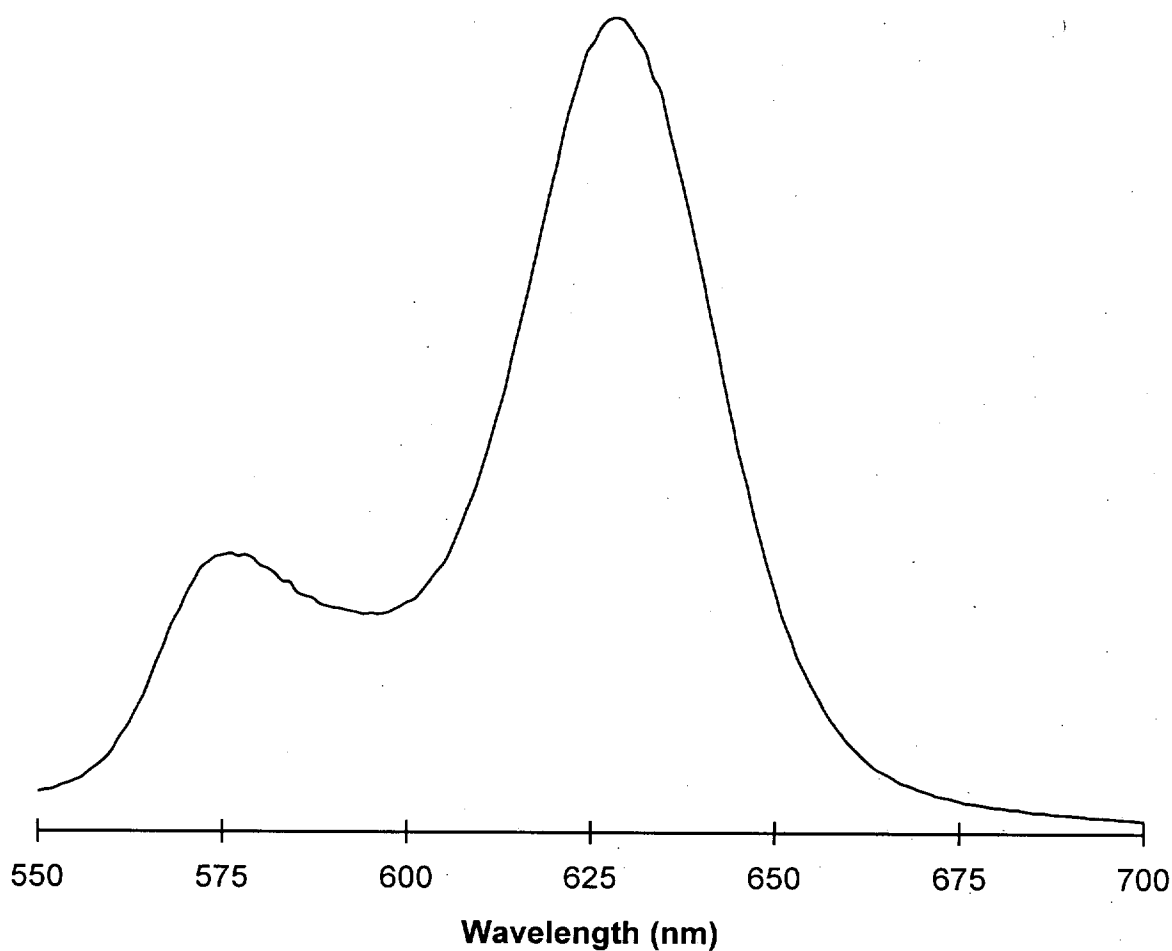
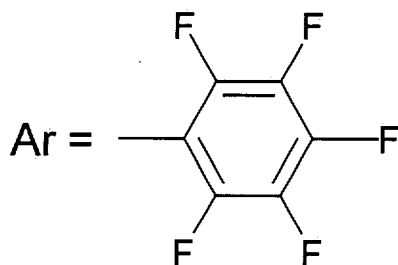
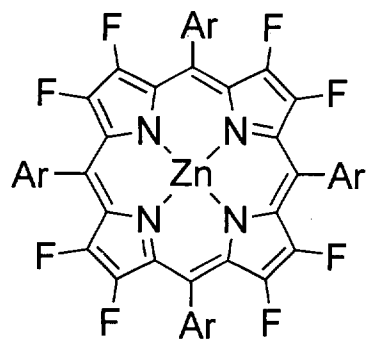
Emission spectrum of $\text{H}_2(\text{TPP})$ in CH_2Cl_2 . Excitation frequency was set to 425 nm.



Emission spectrum of **Zn(F₈TPP)** in CH₂Cl₂. Excitation frequency was set to 400 nm.



Emission spectrum of **Zn(F₂₈TPP)** in CH₂Cl₂. Excitation frequency was set to 400 nm.



Emission spectrum of **Zn(TPP)** in CH_2Cl_2 . Excitation frequency was set to 400 nm.

