Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic Supporting Information

Tuning the Visible Colour of Octahedral Manganese(III) Phthalocyanines via Axial Ligand Exchange

Declan McKearney, Kyle MacDonald, Min Suk Kim, Vance E. Williams and Daniel B. Leznoff*

Department of Chemistry, Simon Fraser University, 8888 University Drive, Burnaby, British Columbia, V5A 1S6, Canada. Email: dleznoff@sfu.ca

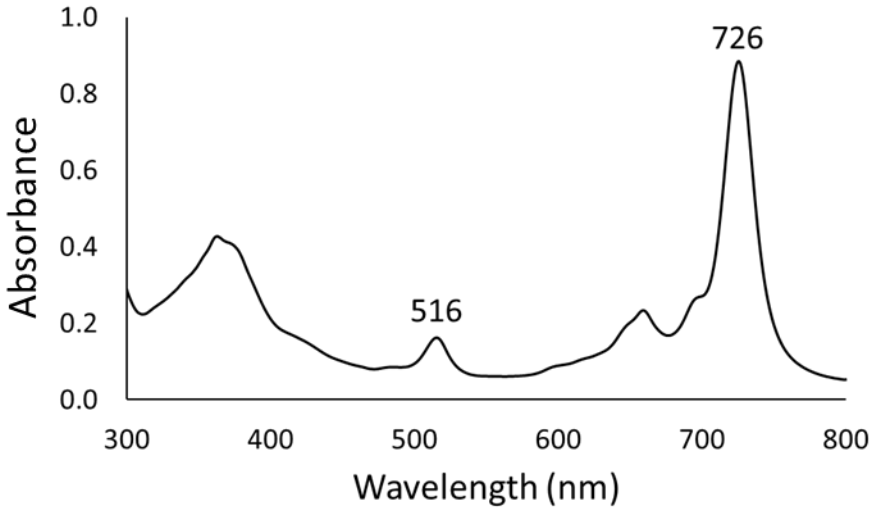

Figure S1. Electronic absorption spectrum of **$[PcMnMeIm_2]^+$** in DCB.

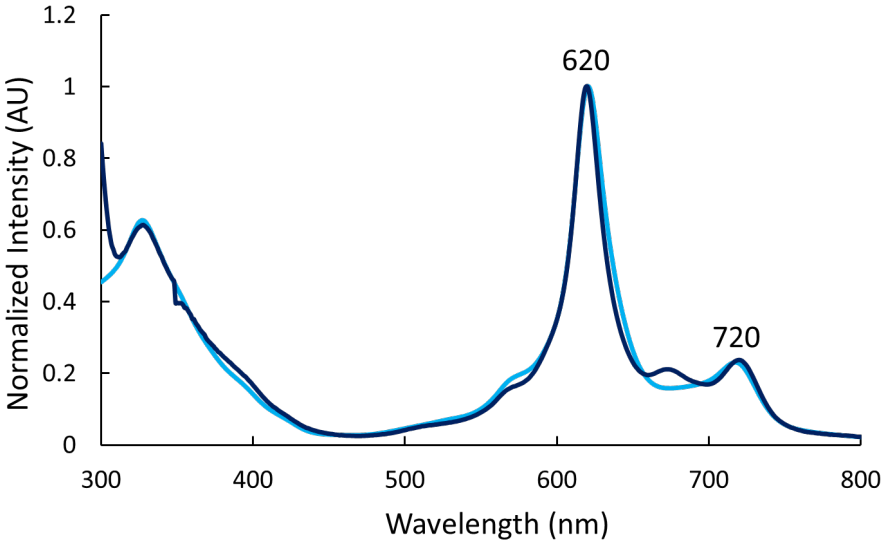

Figure S2. Electronic absorption spectra of **[PcMn]$^+$** in DCB with an excess of water and Py (light blue) or DMAP (dark blue) after 24 hours.

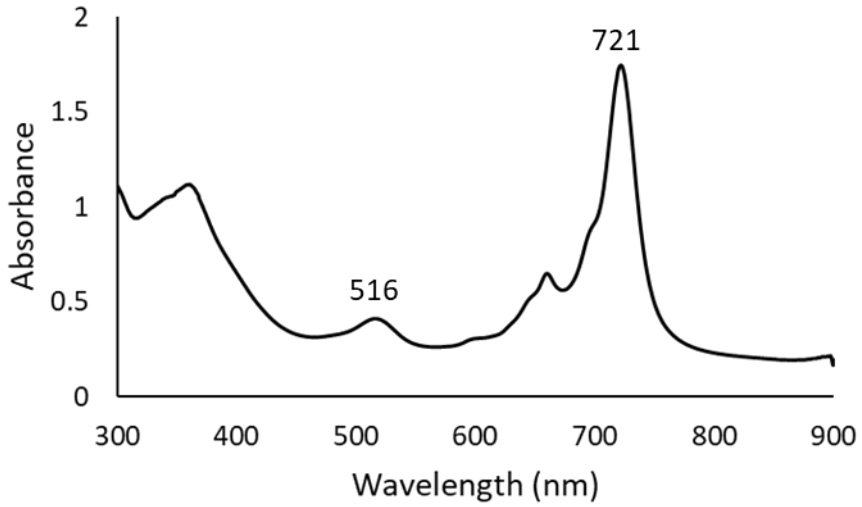

Figure S3. Electronic absorption spectrum of **[PcMn(MeCN)$_2$]$^+$** in the presence of an excess of water for 24 hours to produce **[PcMn(H$_2$O)$_2$]$^+$** in DCB.

Table S1. Crystallographic information table for **$(PcMnDMAP)_2O$**, **$(PcMnMeIm)_2O$**, and **$[PcMn(H_2O)_2]^+$:**

Compound Reference	**$(PcMnDMAP)_2O$**	**$(PcMnMeIm)_2O$**	**$[PcMn(H_2O)_2]^+$**
Chemical Formula	$C_{97.5}H_{58}N_{22}O_1Mn_2Cl_4SbF_6$	$C_{84}H_{52}N_{20}OMn_2Cl_4$	$C_{40}H_{32}N_{12}O_2MnSbF_6$
Formula Mass	2041.08	1609.14	1003.46
a/Å	13.9153(5)	10.2034(3)	6.7827(1)
b/Å	14.9330(4)	13.0541(4)	11.8143(2)
c/Å	25.6822(8)	13.5633(4)	13.0385(2)
α/°	89.600(2)	91.015(2)	87.0700(10)
β/°	80.169(2)	109.836(2)	80.0800(10)
γ/°	88.144(2)	91.205(2)	83.3940(10)
Unit cell volume/$Å^3$	5255.6(3)	1698.42(9)	1021.84(3)
Temperature/K	150(2)	150(2)	150(2)
Space group	P-1	P-1	P-1
Number of formula unit per cell/Z	2	1	1
Radiation type	Cu Kα	Cu Kα	Cu Kα
Absorption coefficient, μ/mm^{-1}	5.425	5.035	8.454
No. of reflections collected	76360	15081	14604
No. unique reflections	18219	5844	3536
R_{int}	0.0664	0.0212	0.0444
Final R_1 values (I>2σ(I))	0.0986	0.0333	0.0252
Final wR(F^2) values (I>2σ(I))	0.2809	0.0933	0.0685
Final R_1 values (all data)	0.1180	0.0350	0.0272
Final wR(F^2) (all data)	0.2989	0.0947	0.0698
Goodness of fit	1.065	1.089	1.060

Table S2. Crystallographic information table for **$[PcMn(MeIm)_2]^+$** and **$[PcMn(Py)_2]^+$:**

Compound Reference	**$[PcMn(MeIm)_2]^+$**	**$[PcMn(Py)_2]^+$**
Chemical Formula	$C_{48}H_{40}N_{16}MnSbF_6$	$C_{125}H_{76}N_{20}Mn_2Sb_2F_{12}Cl_{14}$
Formula Mass	1131.65	2935.74
a/Å	8.7345(2)	23.6576(4)
b/Å	9.3932(2)	23.6576 (4)
c/Å	15.3182(2)	42.1881(9)
α/˚	85.4520(10)	90
β/˚	89.3170(10)	90
γ/˚	70.5600(10)	90
Unit cell volume/$Å^3$	1181.26(4)	23611.9(9)
Temperature/K	150(2)	150(2)
Space group	P-1	I 41/a
Number of formula unit per cell/Z	1	8
Radiation type	Cu Kα	Cu Kα
Absorption coefficient, μ/mm^{-1}	7.382	8.886
No. of reflections collected	18116	62105
No. unique reflections	4089	10438
R_{int}	0.0356	0.0343
Final R_1 values ($I>2\sigma(I)$)	0.0267	0.0768
Final $wR(F^2)$ values ($I>2\sigma(I)$)	0.0706	0.2240
Final R_1 values (all data)	0.0275	0.0912
Final $wR(F^2)$ (all data)	0.0713	0.2249
Goodness of fit	1.056	1.017

Table S3. Crystallographic information table for **$[PcMn(THF)_2]^+$** and **$[PcMn(OPPh_3)_2]^+$:**

Compound Reference	**$[PcMn(OPPh_3)_2]^+$**	**$[PcMn(THF)_2]^+$**
Chemical Formula	$C_{74}H_{46}N_8O_2P_2Cl_2MnSbF_6$	$C_{44}H_{39}N_8MnO_3SbF_6$
Formula Mass	1502.72	1018.52
a/Å	9.3814(4)	8.5811(1)
b/Å	11.7093(5)	10.4045(1)
c/Å	15.1727(7)	23.5751(2)
α/°	77.135(4)	87.2870(10)
β/°	81.131(4)	81.7290(10)
γ/°	89.347(4)	80.1210(10)
Unit cell volume/Å^3	1604.99(13)	2051.50(4)
Temperature/K	150(2)	150(2)
Space group	P1	P-1
Number of formula unit per cell/Z	1	2
Radiation type	Cu Kα	Cu Kα
Absorption coefficient, μ/mm^{-1}	6.791	8.420
No. of reflections collected	16858	32711
No. unique reflections	8272	7379
R_{int}	0.0548	0.0516
Final R_1 values (I>2σ(I))	0.0766	0.0633
Final wR(F^2) values (I>2σ(I))	0.1962	0.1491
Final R_1 values (all data)	0.0805	0.0702
Final wR(F^2) (all data)	0.1998	0.1538
Goodness of fit	1.066	1.050