Electronic Supporting Information

Study on the Coordination and Solution Structures for the Interaction Systems between Diperoxovanadate Complexes and the 4-(Pyridin-2-yl)pyrimidine-like Ligands

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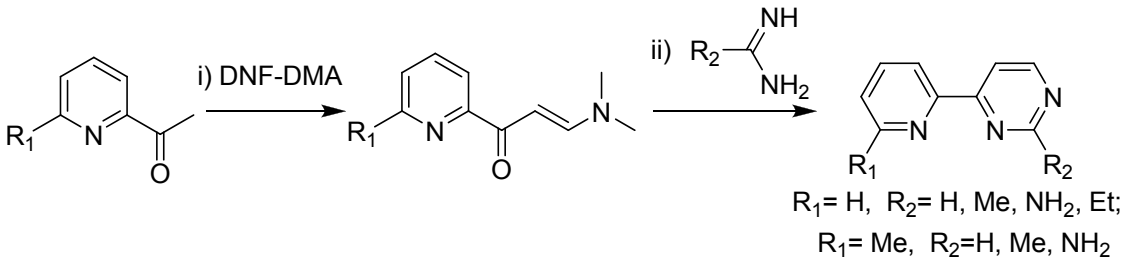
1. The syntheses rout of the organic ligands:



Scheme 1. The syntheses rout of 4-(2'-pyridyl)pyrimidine-like ligands. i) DMF-DMA, 110 °C; ii) $R_2C(NH)NH_2$, NaOEt, 65~85 °C

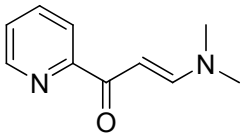
2. The synthesis of the organic ligands (1 ~ 7):

2.1 Synthesis of the organic ligands (1 ~ 4)

2.1.1 Synthesis of 3-dimethylamino-1-pyridin-2-yl-propan-1-one:

A mixture of 2-acetyl-pyridine (1 mol) and *N*,*N*-dimethylformide dimethyl acetal (1.8 mol)

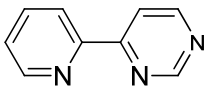
was heated at 110 °C for 1h, shown in **Scheme 1**. The mixture was cooled to room temperature and refrigerated overnight. The yellow solid was filtered, washed with petroleum ether and dried. Yield: 2.82 g (60%).



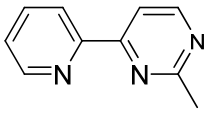
2.1.2 General method for syntheses of 1 ~ 4:

Amidine(3 mol) and a ethanol solution of sodium ethylate (3 mol) was added to a solution of 3-dimethylamino-1-pyridin-2-yl-propan-1-one (1 mol) in ethanol. The mixture was reacted under high pressure and heated at 65 °C for 4 h, shown in **Scheme 1.** Progress of the reaction was monitored by TLC. The solvent was evaporated in vacuum. The residue was purified by column chromatography on silica gel using petroleum ether and ethyl acetate as eluent to afford the cooresponding 4-(2'-pyridyl)pyrimidine-like ligands.

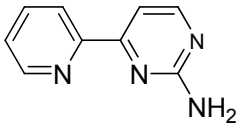
4-pyridin-2-yl-pyrimidine (1, abbr. pprd): white solid, 29% yield, m.p. 75-76 °C; ^{1}H NMR ($CDCl_3$, 500 MHz) δ: 7.41-7.45(m, 1H, Py-**H**), 7.88(t, *J*=7.9 Hz, 1H, Py-**H**), 8.38(d, *J*=5.2 Hz, 1H, Pym-**H**), 8.51(d, *J*=7.9 Hz, 1H, Py-**H**), 8.74(d, *J*=4.7 Hz, Py-**H**), 8.88(d, *J*=5.2 Hz, 1H, Pym-**H**), 9.30(s, 1H, Pym-**H**); ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 162.7, 158.7, 158.0, 153.8, 149.6, 137.2, 125.5, 121.7, 117.8; FT-IR (KBr, cm^{-1}): ν 1576, 1541, 1456, 1392, 861, 801, 748, 641; MS (ESI) 158 (M^++H); HRMS calcd. *m/e* 180.0538 $(M+Na)^+$; found *m/e* 180.0531.



2-Methyl-4-pyridin-2-yl-pyrimidine (2, abbr. 2-Me-pprd): white solid, 46% yield, m.p. 60-61 °C; ^{1}H NMR ($CDCl_3$, 500 MHz) δ: 2.82(s, 3H, C**H**$_3$), 7.37-7.42(m, 1H, Py-**H**), 7.85(t, *J*=7.8 Hz, 1H, Py-**H**), 8.13(d, *J*=5.2 Hz, 1H, Pym-**H**), 8.48(d, *J*=7.9 Hz, 1H, Py-**H**), 8.71(d, *J*=4.7 Hz, 1H, Py-**H**), 8.76(d, *J*=5.2 Hz, 1H, Pym-**H**); ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 168.0, 162.8, 158.0, 154.1, 149.5, 137.0, 125.2, 121.6, 114.2, 26.2; FT-IR (KBr, cm^{-1}): ν 1574, 1547, 1431, 1396, 799, 759; MS (ESI) 172 (M^++H); HRMS calcd. *m/e* 194.0694 $(M+Na)^+$; found *m/e* 194.0682.

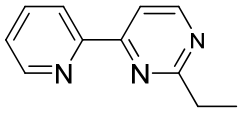


4-pyridin-2-yl-pyrimidine-2-ylamine (3, abbr. 2-NH$_2$-pprd): white solid, 51% yield, m.p. 137-138 °C; ^{1}H NMR ($CDCl_3$, 500 MHz) δ: 5.41(s, 2H, N**H**$_2$), 7.35-7.40(m, 1H, Py-**H**), 7.64(d, *J*=5.1 Hz, 1H, Pym-**H**), 7.82(t, *J*=7.5 Hz, 1H, Py-**H**), 8.33(d, *J*=7.8 Hz, 1H, Py-**H**), 8.45(d, *J*=5.1 Hz, 1H, Pym-**H**), 8.71(d, *J*=4.1 Hz, 1H, Py-**H**); ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 164.1, 163.3, 159.4, 154.4, 149.5, 136.9, 125.1, 121.5, 108.1; FT-IR (KBr, cm^{-1}): ν 3330, 3188, 1655, 1565, 1551, 1486, 1469, 1437, 792, 781; MS (ESI) 173 (M^++H); HRMS calcd. *m/e* 195.0647 $(M+Na)^+$; found *m/e* 195.0640.



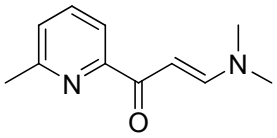
2-Et-4-pyridin-2-yl-pyrimidine (4, abbr. 2-Et-pprd): yellow liquid, 53% yield; ^{1}H NMR ($CDCl_3$, 500 MHz) δ: 1.45(t, *J*=7.6 Hz, 3H, C**H**$_3$), 3.08(q, *J*=7.6 Hz, 2H, C**H**$_2$),7.37-7.42(m, 1H, Py-**H**), 7.86(t, *J*=7.7 Hz, 1H, Py-**H**), 8.15(d, *J*=5.2 Hz, 1H, Pym-**H**), 8.53(d, *J*=7.9 Hz, 1H,

Py-**H**), 8.72(d, *J*=4.2 Hz, 1H, Py-**H**), 8.79(d, *J*=5.2 Hz, 1H, Pym-**H**); ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 172.0, 162.8, 158.0, 154.3, 149.5, 137.1, 125.2, 121.7, 114.4, 32.7, 12.7; FT-IR (KBr, cm^{-1}): ν 2974, 1574, 1548, 1431, 1396, 861, 746, 795; MS (ESI) 186 (M^++H); HRMS calcd. *m/e* 208.0851 $(M+Na)^+$; found *m/e* 208.0844.



2.2.1 Synthesis of 3-dimethylamino-1-(6-Methylpyridin-2-yl)-propan-1-one:

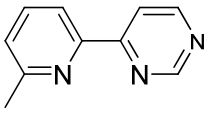
.A mixture of 2-acetyl-6-Methylpyridine (1 mol) and *N*,*N*-dimethylformide dimethyl acetal (1.587 g) was heated at 110 °C for 7h, shown in **Scheme 1**. The mixture was cooled to room temperature and refrigerated overnight. The yellow solid was filtered, washed with petroleum ether and dried. Yield: 1.25 g (89%).



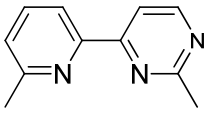
2.2.2 General method for syntheses of 5 ~ 7:

Amidine(3 mol) and a ethanol solution of sodium ethylate(3 mol) was added to a solution of 3-dimethylamino-1-(6-Methylpyridin-2-yl)-propan-1-one (1 mol) in ethanol. The mixture was reacted under high pressure and heated at 85 °C for 5 h, shown in **Scheme 1.** Progress of the reaction was monitored by TLC. The solvent was evaporated in vacuum. The residue was purified by column chromatography on silica gel using petroleum ether and ethyl acetate as eluent to afford the cooresponding 4-(2'-pyridyl)pyrimidine-like ligands.

4-(6-Methyl-pyridin-2-yl)-pyrimidine (5, abbr. 6'-Me-pprd): white solid, 23% yield, m.p. 69-70 °C; ^{1}H NMR ($CDCl_3$, 500 MHz) δ: 2.65(s, 3H, C**H**$_3$), 7.26-7.27(m, 1H, Py-**H**), 7.75(t, *J*=7.8 Hz, 1H, Py-**H**), 8.28(d, *J*=7.8 Hz, 1H, Py-**H**), 8.39(d, *J*=5.2 Hz, 1H, Pym-**H**), 8.85(d, *J*=5.2 Hz, 1H, Pym-**H**), 9.28(s, 1H, Pym-**H**); ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 163.0, 158.7, 158.6, 157.9, 153.1, 137.3, 125.2, 118.8, 117.6, 24.6; FT-IR (KBr, cm^{-1}): ν 2923, 1579, 1542, 1456, 1392, 805, 766, 635; MS (ESI) 172 (M^++H); HRMS calcd. *m/e* 172.0875 $(M+H)^+$; found *m/e* 172.0870.

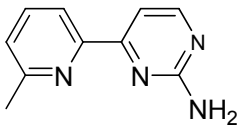


2-Methyl-4-(6-Methyl-pyridin-2-yl)-pyrimidine (6, abbr. 2-Me-6'-Me-pprd): white solid, 79% yield, m.p. 93-94 °C; ^{1}H NMR ($CDCl_3$, 500 MHz) δ: 2.64(s, 3H, C**H**$_3$), 2.81(s, 3H, C**H**$_3$), 7.25(d, *J*=7.7 Hz, 1H, Py-**H**), 7.73(t, *J*=7.7 Hz, 1H, Py-**H**), 8.17(d, *J*=5.2 Hz, 1H, Pym-**H**), 8.28(d, *J*=7.8 Hz, 1H, Py-**H**), 8.74(d, *J*=5.2 Hz, 1H, Pym-**H**); ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 167.9, 163.2, 158.4, 157.9, 153.5, 137.2, 124.9, 118.7, 114.4, 26.2, 24.6; FT-IR (KBr, cm^{-1}): ν 1573, 1549, 1449, 1425, 801, 765, 642; MS (ESI) 186 (M^++H); HRMS calcd. *m/e* 208.0851 $(M+Na)^+$; found *m/e* 208.0845.



4-(6-Methyl-pyridin-2-yl)-pyrimidine-2-ylamine (7, abbr. 2-NH$_2$-6'-Me-pprd): white solid, 33% yield, m.p. 159-161 °C; ^{1}H NMR ($CDCl_3$, 500 MHz) δ: 2.63(s, 3H, C**H**$_3$), 5.37(s, 2H, N**H**$_2$), 7.23(d, *J*=7.7 Hz, 1H, Py-**H**), 7.66(d, *J*=5.2 Hz, 1H, Pym-**H**), 7.69(t, *J*=7.7 Hz, 1H,

Py-**H**), 8.11(d, *J*=7.8 Hz, 1H, Py-**H**), 8.43(d, *J*=5.2 Hz, 1H, Pym-**H**); ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 164.5, 163.2, 159.2, 158.3, 153.8, 137.1, 124.7, 118.6, 108.2, 24.6; FT-IR (KBr, cm^{-1}): ν 3486, 1625, 1580, 1557, 1453, 790; MS (ESI) 187 (M^++H); HRMS calcd. *m/e* 187.0984 $(M+H)^+$; found *m/e* 187.0979.



3. The detailed spectroscopic characterization of 8 and 9:

$NH_4[OV(O_2)_2(pprd)]\cdot 2H_2O$ (8): ^{1}H NMR (D_2O, 500 MHz): **Isomer A:** 7.84(t, *J*= 6.0 Hz, 1H), 8.08(d, *J*= 4.5 Hz, 1H), 8.26(t, *J*= 7.1 Hz, 1H), 8.43(d, *J*= 7.4 Hz, 1H), 8.60(s, 1H), 8.76(d, *J*= 4.5 Hz, 1H), 9.51(d, *J*= 4.0 Hz, 1H); **Isomer B:** 7.38(s, 1H), 7.89(s, 1H), 8.07(s, 1H), 8.18(s, 1H), 8.38(s, 1H), 9.12(s, 1H), 10.0(s, 1H); ^{13}C NMR (D_2O, 125 MHz): **Isomer A:** 159.3, 156.5, 155.0, 154.6, 150.9, 142.5, 128.8, 124.8, 117.3; **Isomer B:** 161.7, 161.4, 161.0, 146.6, 146.5, 139.4, 128.1, 123.1, 119.0; IR (KBr): *v* = 1637 w, 1603 w, 1589 vs, 1470 m, 1393 s, 1318 m, 1027 w, 940 s (V=O), 877 m $(O-O)_{peroxo}$, 855 vs $(O-O)_{peroxo}$, 756 s, 652 m, 623 m $(V-O)_{peroxo}$, 594 s $(V-O)_{peroxo}$ cm^{-1}.

$NH_4[OV(O_2)_2(2\text{-}NH_2\text{-}pprd)]\cdot 3H_2O$ (9): ^{1}H NMR (D_2O, 500 MHz): 7.31 (d, *J*=5.2 Hz, 1H), 7.87 (t, *J*=6.0 Hz, 1H), 8.23-8.31 (m, 2H), 8.31-8.39 (m, 1H), 9.58 (d, *J*=4.6 Hz, 1H); ^{13}C NMR (D_2O, 125 MHz): 160.4, 160.2, 157.7, 154.7, 152.1, 141.8, 128.0, 124.7, 106.5. IR (KBr): *v* = 1615 vs, 1568 vs, 1470 s, 947 s (V=O), 876 m $(O-O)_{peroxo}$, 857 vs $(O-O)_{peroxo}$, 828 w, 796 w, 782 s, 655 s, 623 s $(V-O)_{peroxo}$, 595 s $(V-O)_{peroxo}$ cm^{-1}.

4. Detailed structural data (bond distances and angles) of 8 and 9:

Table S1 Bond lengths [Å] and angles [°] around the vanadium center in $NH_4[OV(O_2)_2(pprd)]\cdot 2H_2O$ (**8**) or $NH_4[OV(O_2)_2(2\text{-}NH_2\text{-}pprd)]\cdot 3H_2O$ (**9**)

$NH_4[OV(O_2)_2(pprd)]\cdot 2H_2O$ (**8**)				$NH_4[OV(O_2)_2(2\text{-}NH_2\text{-}pprd)]\cdot 3H_2O$ (**9**)			
V(1)-O(3)	1.611(3)	O(1)#1-V(1)-O(1)	155.74(13)	V(1)-O(3)	1.606(3)	O(3)-V(1)-N(3)	92.85(17)
V(1)-O(2)	1.887(2)	O(3)-V(1)-N(3)	93.73(15)	V(1)-O(4)	1.878(4)	O(4)-V(1)-N(3)	131.93(18)
V(1)-O(2)#1	1.887(2)	O(2)-V(1)-N(3)	130.00(7)	V(1)-O(2)	1.882(4)	O(2)-V(1)-N(3)	130.90(16)
V(1)-O(1)#1	1.895(2)	O(2)#1-V(1)-N(3)	130.00(7)	V(1)-O(1)	1.901(3)	O(1)-V(1)-N(3)	86.29(15)
V(1)-O(1)	1.895(2)	O(1)#1-V(1)-N(3)	85.27(7)	V(1)-O(5)	1.912(4)	O(5)-V(1)-N(3)	86.85(17)
V(1)-N(3)	2.142(3)	O(1)-V(1)-N(3)	85.27(7)	V(1)-N(3)	2.128(4)	O(3)-V(1)-N(2)	164.44(17)
V(1)-N(2)	2.332(3)	O(3)-V(1)-N(2)	166.13(15)	V(1)-N(2)	2.400(4)	O(4)-V(1)-N(2)	89.57(16)
O(2)-O(1)	1.472(3)	O(2)-V(1)-N(2)	85.63(9)	O(1)-O(2)	1.465(5)	O(2)-V(1)-N(2)	87.36(15)
		O(2)#1-V(1)-N(2)	85.63(9)	O(5)-O(4)	1.473(6)	O(1)-V(1)-N(2)	78.94(14)
O(3)-V(1)-O(2)	103.97(10)	O(1)#1-V(1)-N(2)	77.93(7)			O(5)-V(1)-N(2)	79.86(15)
O(3)-V(1)-O(2)#1	103.97(10)	O(1)-V(1)-N(2)	77.93(7)	O(3)-V(1)-O(4)	102.02(18)	N(3)-V(1)-N(2)	71.62(14)
O(2)-V(1)-O(2)#1	90.70(13)	N(3)-V(1)-N(2)	72.40(12)	O(3)-V(1)-O(2)	102.78(18)	O(2)-O(1)-V(1)	66.55(19)
O(3)-V(1)-O(1)#1	101.43(7)	O(1)-O(2)-V(1)	67.41(11)	O(4)-V(1)-O(2)	90.11(18)	O(4)-O(5)-V(1)	65.9(2)
O(2)-V(1)-O(1)#1	133.91(10)	C(8)-N(3)-V(1)	120.7(3)	O(3)-V(1)-O(1)	99.62(18)	O(1)-O(2)-V(1)	67.88(19)
O(2)#1-V(1)-O(1)#1	45.78(9)	C(4)-N(3)-V(1)	121.2(3)	O(4)-V(1)-O(1)	134.12(18)	C(8)-N(3)-V(1)	119.6(3)
O(3)-V(1)-O(1)	101.43(7)	O(2)-O(1)-V(1)	66.81(11)	O(2)-V(1)-O(1)	45.57(15)	C(4)-N(3)-V(1)	122.0(3)
O(2)-V(1)-O(1)	45.78(9)	C(9)-N(2)-V(1)	126.9(3)	O(3)-V(1)-O(5)	100.73(19)	O(5)-O(4)-V(1)	68.4(2)
O(2)#1-V(1)-O(1)	133.92(10)	C(3)-N(2)-V(1)	115.1(3)	O(4)-V(1)-O(5)	45.71(19)	C(3)-N(2)-C(9)	117.5(4)
				O(2)-V(1)-O(5)	133.47(18)	C(3)-N(2)-V(1)	113.7(3)
				O(1)-V(1)-O(5)	158.81(17)	C(9)-N(2)-V(1)	128.7(3)

5. Detailed NMR results for the interaction systems of bpV and the pprd-like ligand:

Table S2 NMR results for the interaction systems of bpV and the pprd-like ligands

Systems	Species	Chemical shifts		
		^{1}H (ppm)	^{13}C (ppm)	^{51}V (ppm)
bpV + **1** [a]	$[OV(O)_2(pprd)]^-$ (**Isomer A**)	7.74-7.80(m, 1H, Py-**H**), 8.02-8.04(d, *J*=4.5 Hz, 1H, Pym-**H**), 8.18(t, *J*=7.0 Hz, 1H, Py-**H**), 8.35(d, *J*=7.4 Hz, 1H, Py-**H**), 8.60(s, 1H, Pym-**H**), 8.72(d, *J*=4.5 Hz, 1H, Pym-**H**), 9.47(d, *J*=4.2 Hz, 1H, Py-**H**)	159.2, 156.5, 155.0, 154.6, 150.8, 142.0, 128.7, 124.8, 117.2	−741
	$[OV(O)_2(pprd)]^-$ (**Isomer B**)	7.37(s, 1H, Py-**H**), 7.85(s, 1H, Pym-**H**), 8.05(s, 1H, Py-**H**), 8.11(s, 1H, Pym-**H**), 8.31(s, 1H, Py-**H**), 9.06(s, 1H, Py-**H**), 9.98(s, 1H, Pym-**H**)	161.6, 161.4, 161.0, 146.6, 146.5, 139.3, 128.1, 123.0, 119.0	−745
	pprd (**1**)	7.40(dd, *J*= 6.8, 5.2 Hz, 1H, Py-**H**), 7.76-7.82(m, 1H, Py-**H**), 7.84(d, *J*= 5.3 Hz, 1H, Pym-**H**), 7.92(d, *J*=7.8 Hz, 1H, Py-**H**), 8.43(d, *J*=4.0 Hz, 1H, Py-**H**), 8.66(d, *J*=5.3 Hz, 1H, Pym-**H**), 8.95(s, 1H, Pym-**H**)	161.9, 158.1, 157.6, 151.7, 149.2, 138.9, 126.5, 122.8, 118.4	
bpV + **2** [b]	$[OV(O)_2(2\text{-Me-pprd})]^-$	2.61(s, 3H, C**H**$_3$), 7.74(t, *J*=6.3 Hz, 1H, Py-**H**), 7.83(d, *J*=5.4 Hz, 1H, Pym-**H**), 8.16(t, *J*=7.5 Hz, 1H, Py-**H**), 8.31(d, *J*=8.0 Hz, 1H, Py-**H**), 8.52(d, *J*=5.4 Hz, 1H, Pym-**H**), 9.46(d, *J*=4.8 Hz, 1H, Py-**H**)	167.2, 158.3, 157.5, 155.0, 151.6, 141.9, 128.3, 125.1, 115.0, 23.6	−732
	2-Me-pprd (**2**)	2.52(s, 3H, C**H**$_3$), 7.39(t, *J*=5.9 Hz, 1H, Py-**H**), 7.60(d, *J*=5.2 Hz, 1H, Pym-**H**), 7.78-7.82(m, 1H, Py-**H**), 7.84-7.88(m, 1H, Py-**H**), 8.43(d, *J*=4.3 Hz, 1H, Py-**H**), 8.49-8.51(m, 1H, Pym-**H**)	167.5, 162.4, 157.9, 152.0, 149.1, 138.8, 126.3, 122.9, 115.5, 24.3	
bpV + **3** [a]	$[OV(O)_2(2\text{-}NH_2\text{-pprd})]^-$	7.26(d, *J*=5.2 Hz, 1H, Py-**H**), 7.85(t, *J*=6.0 Hz, 1H, Py-**H**), 8.22-8.27(m, 1H, Py-**H**), 8.27-8.32(m, 1H, Pym-**H**), 8.29-8.32(m, 1H, Pym-**H**), 9.58(d, *J*=4.6 Hz, 1H, Py-**H**)	160.3, 160.1, 157.7, 154.6, 152.0, 141.7, 128.0, 124.6, 106.4	−739

	2-NH_2-pprd (**3**)	7.16(d, *J*=5.2 Hz, 1H, Pym-**H**), 7.51(t, *J*=5.5 Hz, 1H, Py-**H**), 7.83-7.90(m, 1H, Py-**H**), 7.92(t, *J*=7.6 Hz, 1H, Py-**H**), 8.27-8.32(m, 1H, Pym-**H**), 8.54(d, *J*=4.4 Hz, 1H, Py-**H**)	163.5, 162.3, 159.2, 152.2, 148.9, 138.6, 126.1, 122.6, 107.9	
bpV + **4** [b]	$[OV(O)_2$(2-Et-pprd)$]^-$	1.19(t, *J*=7.5 Hz, 3H, C**H**$_3$), 3.10(q, *J*=7.5 Hz, 2H, C**H**$_2$), 7.87-7.94(m, 1H, Py-**H**), 8.00(d, *J*=5.3 Hz, 1H, Pym-**H**), 8.35(t, *J*=7.7 Hz, 1H, Py-**H**), 8.50(d, *J*=8.0 Hz, 1H, Py-**H**), 8.74(d, *J*=5.3 Hz, 1H, Pym-**H**), 9.62(d, *J*=5.0 Hz, 1H, Py-**H**)	171.7, 158.6, 157.6, 155.0, 151.9, 141.9, 128.3, 125.2, 115.0, 30.2, 12.8	−729
	2-Et-pprd (**4**)	1.28(t, *J*=7.5 Hz, 3H, C**H**$_3$), 2.88(q, *J*=7.5 Hz, 2H, C**H**$_2$), 7.52(d, *J*=6.0 Hz, 1H, Py-**H**), 7.67(d, *J*=5.3 Hz, 1H, Pym-**H**), 7.91(t, *J*=7.5 Hz, 1H, Py-**H**), 7.98(d, *J*=8.0 Hz, 1H, Py-**H**), 8.54(d, *J*=4.2 Hz, 1H, Py-**H**), 8.63(d, *J*=5.3 Hz, 1H, Pym-**H**)	171.7, 162.7, 158.0, 152.3 , 149.3, 138.5, 126.2, 122.8, 115.6, 31.6, 12.4	
bpV + **5** [b]	$[OV(O)_2$(6-Me-pprd)$]^-$	2.55(s, 1H, C**H**$_3$), 7.35-7.42(m, 1H, Py-**H**), 7.85(t, *J*=7.9 Hz, 1H, Py-**H**), 8.15(d, *J*=7.7 Hz, 1H, Py-**H**), 8.45(d, *J*=4.0 Hz, 1H, Pym-**H**), 9.18(d, *J*=4.0 Hz, 1H, Pym-**H**), 10.13(s, 1H, Pym-**H**)	162.0, 161.8, 161.4, 159.7, 146.8, 138.4, 126.3, 121.2, 119.2, 22.5	−736
	6-Me-pprd (**5**)	2.66(s, 1H, C**H**$_3$), 7.35-7.42(m, 1H, Py-**H**), 7.74-7.84(m, 2H, Py-**H,** Pym-**H**), 7.94(s, 1H, Py-**H**), 8.80(s, 1H, Pym-**H**), 9.09(s, 1H, Pym-**H**)	161.0, 159.1, 157.8, 157.6, 151.2, 138.8, 129.4, 120.1, 118.6, 22.9	

[a] The molar ratio between bpV and the pprd-like ligands is 1:1.5;

[b] The molar ratio between bpV and the pprd-like ligands is 1:1.