Low-Potential Cyclometalated Osmium(II) Mediators of Glucose Oxidase

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Table 1S. X-ray experimental data for complex **2**.

Formula	: $C_{17}H_{14}ClNOs$
Molecular weight	: 457.96
Crystal system	: triclinic
Space group	: P-1
a(Å)	: 10.2556(2)
b(Å)	: 12.0349(2)
c(Å)	: 12.5450(2)
α(deg)	: 70.647(5)
β(deg)	: 77.229(5)
γ(deg)	: 74.994(5)
V(Å^3)	: 1395.44(6)
Z	: 4
Color	: orange
Crystal dim(mm)	: 0.12×0.10×0.08
Dcalc(g cm^{-3})	: 2.18
F000	: 864
μ(mm^{-1})	: 9.317
Trans. min and max	: 0.339/0.475
Temperature(K)	: 173
Wavelength(Å)	: 0.71073
Radiation	: MoKα graphitemonochromated
Diffractometer	: KappaCCD
Scan mode	: 'phi scans'
hkl limits	: -14,14/-16,16/-17,17
Theta limits(deg)	: 2.5/30.04
Number of data meas.	: 17211
Number of data with I > 3 σ(I)	: 6899
Number of variables	: 361
R	: 0.025
Rw	: 0.052
GOF	: 1.002
Largest peak in final difference (e^{-3})	: 0.860

Table 2S. Positional Parameters and Their E.S.D.

Atom	x	y	z	Ueqv
OS1	0.48742(1)	0.60497(1)	-0.27234(1)	0.01978(6)
CL1	0.5955(1)	0.65090(9)	-0.47059(8)	0.0242(4)
N1	0.4893(3)	0.7837(3)	-0.2974(3)	0.020(1)
C1	0.3852(5)	0.8770(4)	-0.3409(4)	0.028(2)
C2	0.3965(7)	0.9953(4)	-0.3700(4)	0.034(2)
C3	0.5114(6)	1.0227(4)	-0.3553(5)	0.034(2)
C4	0.6144(5)	0.9316(4)	-0.3102(4)	0.029(2)
C5	0.6019(4)	0.8125(4)	-0.2810(3)	0.021(2)
C6	0.7040(4)	0.7058(3)	-0.2357(3)	0.020(2)
C7	0.8208(4)	0.7123(4)	-0.1996(4)	0.027(2)
C8	0.9145(5)	0.6068(4)	-0.1605(4)	0.034(2)
C9	0.8897(5)	0.4982(5)	-0.1588(5)	0.034(2)
C10	0.7734(5)	0.4927(4)	-0.1917(4)	0.028(2)
C11	0.6743(4)	0.5947(4)	-0.2280(3)	0.020(2)
C12	0.3475(5)	0.5150(4)	-0.3162(4)	0.038(2)
C13	0.4464(6)	0.4295(4)	-0.2548(5)	0.041(2)
C14	0.4653(5)	0.4286(5)	-0.1483(5)	0.042(2)
C15	0.3857(5)	0.5231(6)	-0.1027(4)	0.038(2)
C16	0.2900(5)	0.6137(5)	-0.1669(5)	0.036(2)
C17	0.2652(4)	0.6050(5)	-0.2724(4)	0.032(2)
OS2	0.06385(1)	0.81672(1)	0.33593(1)	0.01546(6)
CL2	-0.0221(1)	1.03231(8)	0.28131(8)	0.0213(4)
N2	-0.0516(3)	0.8109(3)	0.2209(3)	0.018(1)
C18	-0.1808(4)	0.7882(4)	0.2522(3)	0.022(2)
C19	-0.2539(4)	0.7859(4)	0.1744(4)	0.028(2)
C20	-0.1982(4)	0.8089(4)	0.0594(4)	0.028(2)
C21	-0.0684(4)	0.8328(4)	0.0271(3)	0.024(2)
C22	0.0044(4)	0.8325(3)	0.1081(3)	0.015(1)
C23	0.1449(4)	0.8519(3)	0.0854(3)	0.016(1)
C24	0.2217(4)	0.8743(4)	-0.0229(4)	0.023(2)
C25	0.3561(5)	0.8892(4)	-0.0350(4)	0.024(2)
C26	0.4069(4)	0.8852(4)	0.0582(4)	0.023(2)
C27	0.3268(4)	0.8670(4)	0.1650(3)	0.022(2)
C28	0.1951(4)	0.8474(3)	0.1829(3)	0.016(1)
C29	0.1261(5)	0.8202(4)	0.4911(4)	0.034(2)
C30	-0.0110(6)	0.8055(5)	0.5230(4)	0.028(2)
C31	-0.0510(5)	0.7148(6)	0.5001(4)	0.037(2)
C32	0.0499(6)	0.6367(4)	0.4413(4)	0.030(2)
C33	0.1852(6)	0.6470(4)	0.4190(4)	0.032(2)
C34	0.2251(5)	0.7399(5)	0.4434(4)	0.031(2)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as one third of the trace of the orthogonalized Uij tensor.

Table 3S. Positional Parameters.

Atom	x	y	z	Ueqv
H1	0.3046	0.8589	-0.3508	0.0367
H2	0.3246	1.0579	-0.4003	0.0553
H3	0.5200	1.1042	-0.3760	0.0481
H4	0.6941	0.9501	-0.2991	0.0399
H5	0.8361	0.7876	-0.2018	0.0355
H6	0.9944	0.6092	-0.1354	0.0425
H7	0.9546	0.4263	-0.1343	0.0487
H8	0.7600	0.4168	-0.1897	0.0365
H9	0.3371	0.5111	-0.3882	0.0474
H10	0.5030	0.3693	-0.2874	0.0555
H11	0.5297	0.3666	-0.1069	0.0563
H12	0.3965	0.5254	-0.0302	0.0563
H13	0.2420	0.6806	-0.1402	0.0469
H14	0.1937	0.6600	-0.3109	0.0457
H15	-0.2208	0.7736	0.3302	0.0286
H16	-0.3429	0.7686	0.1988	0.0368
H17	-0.2483	0.8081	0.0045	0.0341
H18	-0.0286	0.8496	-0.0510	0.0306
H19	0.1841	0.8793	-0.0875	0.0313
H20	0.4115	0.9020	-0.1078	0.0356
H21	0.4979	0.8951	0.0500	0.0364
H22	0.3634	0.8679	0.2279	0.0274
H23	0.1508	0.8858	0.5025	0.0456
H24	-0.0761	0.8579	0.5603	0.0503
H25	-0.1427	0.7041	0.5226	0.0589
H26	0.0231	0.5791	0.4186	0.0474
H27	0.2524	0.5914	0.3868	0.0501
H28	0.3181	0.7468	0.4273	0.0466

Table 4S. General Displacement Parameter Expressions - U's.

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
OS1	.01991(6)	.01983(6)	.01959(6)	-.00408(5)	-.00500(5)	-.00392(5)
CL1	.0282(4)	.0248(4)	.0204(4)	-.0060(3)	-.0005(3)	-.0068(3)
N1	.020(1)	.020(1)	.021(1)	.000(1)	-.005(1)	-.006(1)
C1	.031(2)	.023(2)	.031(2)	.005(2)	-.012(2)	-.010(1)
C2	.070(3)	.018(2)	.032(2)	.007(2)	-.013(2)	-.006(2)
C3	.048(3)	.021(2)	.038(2)	-.006(2)	-.000(2)	-.008(2)
C4	.039(2)	.029(2)	.022(2)	-.010(2)	.005(2)	-.009(1)
C5	.023(2)	.025(2)	.017(1)	-.003(1)	.002(1)	-.013(1)
C6	.021(2)	.019(1)	.020(2)	-.002(1)	.003(1)	-.009(1)
C7	.023(2)	.036(2)	.025(2)	-.010(1)	.001(1)	-.011(1)
C8	.028(2)	.043(2)	.032(2)	-.009(2)	-.009(2)	-.014(2)
C9	.022(2)	.040(2)	.045(2)	.008(2)	-.011(2)	-.012(2)
C10	.028(2)	.027(2)	.030(2)	-.001(2)	-.011(1)	-.008(1)
C11	.020(2)	.023(2)	.017(1)	-.005(1)	-.004(1)	-.005(1)
C12	.047(2)	.047(2)	.025(2)	-.033(1)	-.003(2)	-.008(1)
C13	.048(2)	.023(2)	.061(3)	-.020(2)	-.001(2)	-.014(2)
C14	.042(2)	.036(2)	.048(3)	-.021(2)	-.026(2)	.016(2)
C15	.043(2)	.075(3)	.017(2)	-.033(2)	-.006(2)	-.003(2)
C16	.027(2)	.046(2)	.037(2)	-.016(2)	.006(2)	-.014(2)
C17	.022(2)	.047(3)	.031(2)	-.012(2)	-.011(2)	.005(2)
OS2	.01862(6)	.01649(6)	.01202(5)	-.00371(5)	-.00214(5)	-.00208(4)
CL2	.0293(4)	.0172(4)	.0192(4)	-.0023(3)	-.0053(3)	-.0046(3)
N2	.023(1)	.017(1)	.016(1)	-.008(1)	-.001(1)	-.002(1)
C18	.021(2)	.022(2)	.023(2)	-.006(1)	-.002(1)	-.006(1)
C19	.023(2)	.027(2)	.038(2)	-.010(1)	-.009(1)	-.006(1)
C20	.023(2)	.033(2)	.028(2)	-.005(1)	-.011(1)	-.011(1)
C21	.028(2)	.029(2)	.017(1)	-.003(1)	-.009(1)	-.008(1)
C22	.020(1)	.011(1)	.015(1)	-.004(1)	-.003(1)	-.002(1)
C23	.023(2)	.014(1)	.014(1)	-.004(1)	-.004(1)	.000(1)
C24	.027(2)	.024(2)	.019(2)	-.005(1)	-.000(1)	-.005(1)
C25	.028(2)	.029(2)	.018(2)	-.010(2)	.005(2)	.000(2)
C26	.023(2)	.017(2)	.033(2)	-.002(2)	.000(2)	.002(2)
C27	.020(2)	.021(2)	.024(2)	-.006(1)	-.007(1)	-.005(1)
C28	.018(1)	.017(1)	.013(1)	-.006(1)	.002(1)	-.002(1)
C29	.054(2)	.036(2)	.019(2)	-.012(2)	-.016(2)	-.006(1)
C30	.044(3)	.049(3)	.010(2)	.005(2)	-.003(2)	-.004(2)
C31	.036(2)	.064(3)	.022(2)	-.023(2)	-.004(2)	.016(2)
C32	.063(3)	.022(2)	.019(2)	-.017(2)	-.011(2)	.009(2)
C33	.059(3)	.022(2)	.026(2)	.003(2)	-.021(2)	.005(2)
C34	.029(2)	.047(3)	.021(2)	.001(2)	-.011(2)	.003(2)

Table 5S. Bond Distances in Angstroms.

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
OS1	CL1	2.431(1)	OS1	C15	2.180(5)
OS1	N1	2.073(4)	OS1	C16	2.158(5)
OS1	C11	2.074(4)	N1	C1	1.390(6)
OS1	C12	2.254(5)	N1	C5	1.362(6)
OS1	C13	2.191(5)	C1	C2	1.377(8)
OS1	C14	2.210(6)	C2	C3	1.37(1)
OS1	C15	2.180(5)	C3	C4	1.376(8)
OS1	C16	2.158(5)	C4	C5	1.389(7)
OS1	C17	2.279(5)	C5	C6	1.466(6)
OS2	CL2	2.426(1)	C6	C7	1.399(7)
OS2	N2	2.086(4)	C6	C11	1.415(6)
OS2	C28	2.069(4)	C7	C8	1.393(8)
OS2	C29	2.195(5)	C8	C9	1.387(8)
OS2	C30	2.272(5)	C9	C10	1.369(7)
OS2	C31	2.266(5)	C10	C11	1.391(6)
OS2	C32	2.155(5)	C12	C13	1.401(9)
OS2	C33	2.157(5)	C12	C17	1.379(9)
OS2	C34	2.185(5)	C13	C14	1.39(1)
OS1	N1	2.073(4)	C14	C15	1.43(1)
OS1	C11	2.074(4)	C15	C16	1.419(9)
OS1	C13	2.191(5)	C16	C17	1.444(8)
OS2	N2	2.086(4)	C23	C24	1.391(6)
OS2	C28	2.069(4)	C23	C28	1.409(6)
OS2	C29	2.195(5)	C24	C25	1.405(7)
OS2	C32	2.155(5)	C25	C26	1.363(7)
OS2	C33	2.157(5)	C26	C27	1.389(6)
OS2	C34	2.185(5)	C27	C28	1.387(6)
N2	C18	1.368(6)	C29	C30	1.414(9)
N2	C22	1.369(5)	C29	C34	1.389(8)
C18	C19	1.367(7)	C30	C31	1.39(1)
C19	C20	1.392(7)	C31	C32	1.46(1)
C20	C21	1.379(7)	C32	C33	1.384(9)
C21	C22	1.386(6)	C33	C34	1.424(9)
C22	C23	1.470(6)			

Table 6S. Bond Angles in Degrees.

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
CL1	OS1	N1	82.1(1)	C12	OS1	C13	36.7(2)
CL1	OS1	C11	87.7(1)	C12	OS1	C14	66.6(2)
CL1	OS1	C12	88.9(1)	C12	OS1	C15	79.2(2)
CL1	OS1	C13	98.5(2)	C12	OS1	C16	66.7(2)
CL1	OS1	C14	129.2(2)	C12	OS1	C17	35.4(2)
CL1	OS1	C15	165.6(2)	C13	OS1	C14	36.8(3)
CL1	OS1	C16	142.2(2)	C13	OS1	C15	67.1(3)
CL1	OS1	C17	106.8(1)	C13	OS1	C16	79.3(2)
N1	OS1	C11	77.3(2)	C13	OS1	C17	65.2(2)
N1	OS1	C12	132.7(2)	C14	OS1	C15	37.9(3)
N1	OS1	C13	169.1(2)	C14	OS1	C16	68.3(2)
N1	OS1	C14	147.1(2)	C14	OS1	C17	78.7(2)
N1	OS1	C15	112.0(2)	C15	OS1	C16	38.2(2)
N1	OS1	C16	93.6(2)	C15	OS1	C17	67.7(2)
N1	OS1	C17	104.2(2)	C16	OS1	C17	37.9(2)
C11	OS1	C12	148.8(2)	CL2	OS2	N2	86.5(1)
C11	OS1	C13	113.5(2)	CL2	OS2	C28	86.1(1)
C11	OS1	C14	92.2(2)	CL2	OS2	C29	92.0(1)
C11	OS1	C15	98.2(2)	CL2	OS2	C30	90.6(2)
C11	OS1	C16	128.1(2)	CL2	OS2	C31	114.0(2)
C11	OS1	C17	165.5(2)	CL2	OS2	C32	151.9(2)
CL2	OS2	C33	157.7(2)	C30	OS2	C32	67.2(2)
CL2	OS2	C34	119.4(2)	C30	OS2	C33	78.7(2)
N2	OS2	C28	77.2(2)	C30	OS2	C34	66.3(2)
N2	OS2	C29	162.6(2)	C31	OS2	C32	38.3(3)
N2	OS2	C30	125.8(2)	C31	OS2	C33	67.2(2)
N2	OS2	C31	98.8(2)	C31	OS2	C34	79.0(2)
N2	OS2	C32	92.7(2)	C32	OS2	C33	37.4(2)
N2	OS2	C33	115.6(2)	C32	OS2	C34	68.5(2)
N2	OS2	C34	152.8(2)	C33	OS2	C34	38.3(2)
C28	OS2	C29	120.0(2)	N1	OS1	C11	77.3(2)
C28	OS2	C30	156.5(2)	N1	OS1	C13	169.1(2)
C28	OS2	C31	159.4(2)	N1	OS1	C15	112.0(2)
C28	OS2	C32	121.2(2)	N1	OS1	C16	93.6(2)
C28	OS2	C33	96.0(2)	C11	OS1	C13	113.5(2)
C28	OS2	C34	95.3(2)	C11	OS1	C15	98.2(2)
C29	OS2	C30	36.9(2)	C11	OS1	C16	128.1(2)
C29	OS2	C31	66.1(2)	C13	OS1	C15	67.1(3)
C29	OS2	C32	80.5(2)	C13	OS1	C16	79.3(2)
C29	OS2	C33	67.8(2)	C15	OS1	C16	38.2(2)
C29	OS2	C34	37.0(2)	OS1	N1	C1	122.4(3)
C30	OS2	C31	35.7(3)	OS1	N1	C5	119.3(3)
C1	N1	C5	118.0(4)	C12	C13	C14	122.9(6)
N1	C1	C2	121.3(5)	C13	C14	C15	118.3(5)
C1	C2	C3	119.9(5)	OS1	C15	C14	72.2(3)
C2	C3	C4	119.6(5)	OS1	C15	C16	70.1(3)
C3	C4	C5	120.0(5)	C14	C15	C16	119.1(5)
N1	C5	C4	121.1(4)	OS1	C16	C15	71.7(3)
N1	C5	C6	112.4(4)	OS1	C16	C17	75.6(3)
C4	C5	C6	126.5(5)	C15	C16	C17	120.5(6)
C5	C6	C7	122.8(4)	C12	C17	C16	118.6(5)
C5	C6	C11	115.2(4)	N2	OS2	C28	77.2(2)
C7	C6	C11	122.0(4)	N2	OS2	C29	162.6(2)
C6	C7	C8	119.1(5)	N2	OS2	C32	92.7(2)
C7	C8	C9	119.1(5)	N2	OS2	C33	115.6(2)
C8	C9	C10	121.3(5)	N2	OS2	C34	152.8(2)
C9	C10	C11	122.0(5)	C28	OS2	C29	120.0(2)
OS1	C11	C6	115.5(3)	C28	OS2	C32	121.2(2)

OS1	C11	C10	128.2(4)	C28	OS2	C33	96.0(2)
C6	C11	C10	116.3(4)	C28	OS2	C34	95.3(2)
C13	C12	C17	120.1(5)	C29	OS2	C32	80.5(2)
OS1	C13	C12	74.1(3)	C29	OS2	C33	67.8(2)
OS1	C13	C14	72.4(3)	C29	OS2	C34	37.0(2)
C32	OS2	C33	37.4(2)	C26	C27	C28	122.1(4)
C32	OS2	C34	68.5(2)	OS2	C28	C23	116.8(3)
C33	OS2	C34	38.3(2)	OS2	C28	C27	127.0(3)
OS2	N2	C18	123.4(3)	C23	C28	C27	116.1(4)
OS2	N2	C22	118.2(3)	OS2	C29	C30	74.5(3)
C18	N2	C22	118.3(4)	OS2	C29	C34	71.1(3)
N2	C18	C19	121.9(4)	C30	C29	C34	120.8(5)
C18	C19	C20	120.1(4)	C29	C30	C31	120.5(5)
C19	C20	C21	118.4(4)	C30	C31	C32	118.9(5)
C20	C21	C22	120.3(4)	OS2	C32	C31	75.0(3)
N2	C22	C21	121.0(4)	OS2	C32	C33	71.4(3)
N2	C22	C23	113.4(4)	C31	C32	C33	119.4(6)
C21	C22	C23	125.6(4)	OS2	C33	C32	71.2(3)
C22	C23	C24	123.2(4)	OS2	C33	C34	71.9(3)
C22	C23	C28	114.2(4)	C32	C33	C34	120.9(5)
C24	C23	C28	122.6(4)	OS2	C34	C29	71.9(3)
C23	C24	C25	118.7(4)	OS2	C34	C33	69.8(3)
C24	C25	C26	119.7(4)	C29	C34	C33	119.1(5)
C25	C26	C27	120.7(4)				