Electronic Supplementary Material (ESI) for RSC Advances.

Electrochemical Proton Reduction Catalysed by Selenolato-Manganese Carbonyl Complexes

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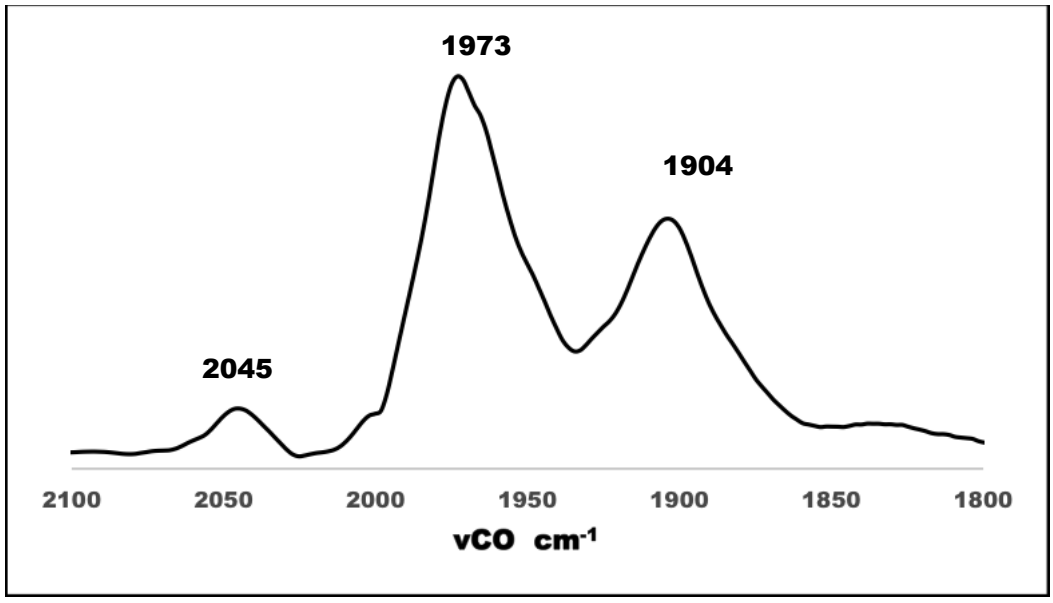
Infrared spectrum resulting from the reaction of 1 with Na in thf



νCO peaks of Complex 1 in THF after Na is added.

General Single crystal X-ray structural study details. Crystals were grown from solvents in dichloromethane/hexane . The X-ray data were collected with a Bruker AXS D8 Venture Kappa four cycles X-ray diffractometer system equipped with a Photon 100 detector, using a Mo sealed microfocusing Source, with the Bruker Apex 2 suite program[1] .

Data were integrated with the Bruker SAINT program[2] using a narrow-frame algorithm. Sadabs (Sheldrick G.M. 2012)[3] was used for absorption correction. Structural solution and refinement were carried out with the SHELXTL[4] suite of programs. The structures were solved by direct methods, followed by difference maps and refined with full-matrix least-squares on F2. All non-hydrogen atoms were generally given anisotropic displacement parameters in the final model. All hydrogen atoms were put at calculated positions. The thermal ellipsoid plots were created using the XP component of SHELXTL.

For complex 2, two terminal C atoms of one of the n-butyl groups were disordered into two positions with occupancy ratio=84:16. Restraints in bond lengths and thermal parameters were applied to the disordered atoms. The minor parts were kept isotropic. The high residue peaks could be due to the crystal was a thin plate.

For complex 4, a twin refinement was performed and found the twin component refinement has a BASF value of 0.01265.

Reference:

1. Apex2 v2013,9.0 , Bruker AXS Inc.
2. SAINT V8.32B, 2013, Bruker AXS Inc.
3. G.M . Sheldrick, Sadabs, v2012/1, Bruker AXS Inc.
4. G.M . Sheldrick, SHELXTL, Bruker AXS Inc

1. Crystal structure information of complex 2.

(1) Data collection and structure refinement for complex 2.

Theta range for data collection	2.08 to 27.50°
Index ranges	-14<=h<=14, -26<=k<=26, -26<=l<=26
Reflections collected	75699
Independent reflections	10274 [R(int) = 0.0857]
Max. and min. transmission	0.5633 and 0.4485
Structure solution technique	direct methods

Structure solution program	SHELXS-97 (Sheldrick 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2013 (Sheldrick, 2013)	
Function minimized	$\Sigma\ w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	10274 / 6 / 484	
Goodness-of-fit on F^2	1.007	
Δ/σ_{max}	0.002	
Final R indices	7501 data; I>2σ(I)	R1 = 0.0387, wR2 = 0.0731
	all data	R1 = 0.0706, wR2 = 0.0805
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0340P)^2+3.3988P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	1.228 and -0.446 eÅ^{-3}	
R.M.S. deviation from mean	0.098 eÅ^{-3}	

(2) Bond lengths (Å) for complex 2.

Mn1-C14	1.790(3)	Mn1-C15	1.795(3)
Mn1-C13	2.032(3)	Mn1-P1	2.3021(8)
Mn1-Se2	2.4601(5)	Mn1-Se1	2.4672(5)
Mn1-Mn2	2.6528(6)	Mn2-C16	1.786(3)
Mn2-C17	1.794(3)	Mn2-C13	2.017(3)
Mn2-P2	2.3014(9)	Mn2-Se1	2.4640(5)
Mn2-Se2	2.4647(5)	Se1-C1	1.932(3)
Se2-C7	1.935(3)	P1-C22	1.833(3)
P1-C26	1.835(3)	P1-C18	1.836(3)
P2-C30	1.836(3)	P2-C38	1.840(3)
P2-C34	1.841(3)	O1-C13	1.170(3)
O2-C14	1.152(3)	O3-C15	1.156(3)
O4-C16	1.161(3)	O5-C17	1.157(3)
C1-C6	1.384(4)	C1-C2	1.392(4)
C2-C3	1.385(4)	C2-H2	0.95

C3-C4	1.382(4)	C3-H3	0.95
C4-C5	1.389(4)	C4-H4	0.95
C5-C6	1.386(4)	C5-H5	0.95
C6-H6	0.95	C7-C12	1.381(4)
C7-C8	1.397(4)	C8-C9	1.383(4)
C8-H8	0.95	C9-C10	1.374(5)
C9-H9	0.95	C10-C11	1.380(4)
C10-H10	0.95	C11-C12	1.400(4)
C11-H11	0.95	C12-H12	0.95
C18-C19	1.532(4)	C18-H18A	0.99
C18-H18B	0.99	C19-C20	1.524(4)
C19-H19A	0.99	C19-H19B	0.99
C20-C21	1.521(4)	C20-H20A	0.99
C20-H20B	0.99	C21-H21A	0.98
C21-H21B	0.98	C21-H21C	0.98
C22-C23	1.534(4)	C22-H22A	0.99
C22-H22B	0.99	C23-C24	1.534(4)
C23-H23A	0.99	C23-H23B	0.99
C24-C25	1.507(5)	C24-H24A	0.99
C24-H24B	0.99	C25-H25A	0.98
C25-H25B	0.98	C25-H25C	0.98
C26-C27	1.537(4)	C26-H26A	0.99
C26-H26B	0.99	C27-C28	1.519(4)
C27-H27A	0.99	C27-H27B	0.99
C28-C29	1.520(4)	C28-H28A	0.99
C28-H28B	0.99	C29-H29A	0.98
C29-H29B	0.98	C29-H29C	0.98
C30-C31	1.530(4)	C30-H30A	0.99
C30-H30B	0.99	C31-C32	1.528(4)
C31-H31A	0.99	C31-H31B	0.99
C32-C33	1.516(4)	C32-H32A	0.99
C32-H32B	0.99	C33-H33A	0.98
C33-H33B	0.98	C33-H33C	0.98
C34-C35	1.538(4)	C34-H34A	0.99
C34-H34B	0.99	C35-C36	1.528(4)
C35-H35A	0.99	C35-H35B	0.99
C36-C37	1.520(4)	C36-H36A	0.99
C36-H36B	0.99	C37-H37A	0.98
C37-H37B	0.98	C37-H37C	0.98
C38-C39	1.543(4)	C38-H38A	0.99

C38-H38B	0.99	C39-C40A	1.515(15)
C39-C40	1.538(5)	C40-C41	1.510(6)
C40-H40A	0.99	C40-H40B	0.99
C41-H41A	0.98	C41-H41B	0.98
C41-H41C	0.98	C40A-C41A	1.509(16)
C40A-H40C	0.99	C40A-H40D	0.99
C41A-H41D	0.98	C41A-H41E	0.98
C41A-H41F	0.98		

(3)Bond angles (°) for complex 2.

C14-Mn1-C15	90.53(13)	C14-Mn1-C13	84.71(11)
C15-Mn1-C13	82.14(12)	C14-Mn1-P1	86.21(9)
C15-Mn1-P1	88.18(9)	C13-Mn1-P1	166.64(9)
C14-Mn1-Se2	171.69(9)	C15-Mn1-Se2	97.67(9)
C13-Mn1-Se2	95.08(8)	P1-Mn1-Se2	95.32(2)
C14-Mn1-Se1	96.80(9)	C15-Mn1-Se1	171.73(10)
C13-Mn1-Se1	94.68(8)	P1-Mn1-Se1	96.11(2)
Se2-Mn1-Se1	74.931(15)	C14-Mn1-Mn2	117.54(9)
C15-Mn1-Mn2	115.62(9)	C13-Mn1-Mn2	48.84(8)
P1-Mn1-Mn2	144.52(3)	Se2-Mn1-Mn2	57.492(14)
Se1-Mn1-Mn2	57.397(14)	C16-Mn2-C17	91.12(12)
C16-Mn2-C13	84.80(12)	C17-Mn2-C13	81.10(12)
C16-Mn2-P2	87.84(9)	C17-Mn2-P2	87.47(9)
C13-Mn2-P2	166.25(8)	C16-Mn2-Se1	169.83(9)
C17-Mn2-Se1	98.93(9)	C13-Mn2-Se1	95.14(8)
P2-Mn2-Se1	94.14(2)	C16-Mn2-Se2	94.96(9)
C17-Mn2-Se2	172.64(9)	C13-Mn2-Se2	95.31(8)
P2-Mn2-Se2	96.88(2)	Se1-Mn2-Se2	74.906(15)
C16-Mn2-Mn1	116.41(9)	C17-Mn2-Mn1	116.08(9)
C13-Mn2-Mn1	49.30(8)	P2-Mn2-Mn1	144.19(3)
Se1-Mn2-Mn1	57.513(14)	Se2-Mn2-Mn1	57.324(14)
C1-Se1-Mn2	112.42(8)	C1-Se1-Mn1	113.29(8)
Mn2-Se1-Mn1	65.090(15)	C7-Se2-Mn1	112.86(9)
C7-Se2-Mn2	113.67(8)	Mn1-Se2-Mn2	65.185(15)
C22-P1-C26	102.74(14)	C22-P1-C18	103.06(14)
C26-P1-C18	103.38(13)	C22-P1-Mn1	112.61(10)
C26-P1-Mn1	117.02(10)	C18-P1-Mn1	116.22(10)
C30-P2-C38	101.31(13)	C30-P2-C34	103.01(13)
C38-P2-C34	103.24(14)	C30-P2-Mn2	116.61(10)

C38-P2-Mn2	117.42(10)	C34-P2-Mn2	113.25(10)
C6-C1-C2	119.6(3)	C6-C1-Se1	124.5(2)
C2-C1-Se1	115.9(2)	C3-C2-C1	120.2(3)
C3-C2-H2	119.9	C1-C2-H2	119.9
C4-C3-C2	120.1(3)	C4-C3-H3	120.0
C2-C3-H3	120.0	C3-C4-C5	119.8(3)
C3-C4-H4	120.1	C5-C4-H4	120.1
C6-C5-C4	120.2(3)	C6-C5-H5	119.9
C4-C5-H5	119.9	C1-C6-C5	120.0(3)
C1-C6-H6	120.0	C5-C6-H6	120.0
C12-C7-C8	119.4(3)	C12-C7-Se2	125.7(2)
C8-C7-Se2	114.9(2)	C9-C8-C7	120.6(3)
C9-C8-H8	119.7	C7-C8-H8	119.7
C10-C9-C8	120.1(3)	C10-C9-H9	119.9
C8-C9-H9	119.9	C9-C10-C11	119.9(3)
C9-C10-H10	120.1	C11-C10-H10	120.1
C10-C11-C12	120.6(3)	C10-C11-H11	119.7
C12-C11-H11	119.7	C7-C12-C11	119.5(3)
C7-C12-H12	120.3	C11-C12-H12	120.3
O1-C13-Mn2	139.3(2)	O1-C13-Mn1	138.8(2)
Mn2-C13-Mn1	81.86(11)	O2-C14-Mn1	175.7(2)
O3-C15-Mn1	175.3(3)	O4-C16-Mn2	177.1(2)
O5-C17-Mn2	175.1(2)	C19-C18-P1	112.75(19)
C19-C18-H18A	109.0	P1-C18-H18A	109.0
C19-C18-H18B	109.0	P1-C18-H18B	109.0
H18A-C18-H18B	107.8	C20-C19-C18	114.3(2)
C20-C19-H19A	108.7	C18-C19-H19A	108.7
C20-C19-H19B	108.7	C18-C19-H19B	108.7
H19A-C19-H19B	107.6	C21-C20-C19	111.0(2)
C21-C20-H20A	109.4	C19-C20-H20A	109.4
C21-C20-H20B	109.4	C19-C20-H20B	109.4
H20A-C20-H20B	108.0	C20-C21-H21A	109.5
C20-C21-H21B	109.5	H21A-C21-H21B	109.5
C20-C21-H21C	109.5	H21A-C21-H21C	109.5
H21B-C21-H21C	109.5	C23-C22-P1	117.3(2)
C23-C22-H22A	108.0	P1-C22-H22A	108.0
C23-C22-H22B	108.0	P1-C22-H22B	108.0
H22A-C22-H22B	107.2	C24-C23-C22	112.5(3)
C24-C23-H23A	109.1	C22-C23-H23A	109.1
C24-C23-H23B	109.1	C22-C23-H23B	109.1

H23A-C23-H23B	107.8	C25-C24-C23	113.5(3)
C25-C24-H24A	108.9	C23-C24-H24A	108.9
C25-C24-H24B	108.9	C23-C24-H24B	108.9
H24A-C24-H24B	107.7	C24-C25-H25A	109.5
C24-C25-H25B	109.5	H25A-C25-H25B	109.5
C24-C25-H25C	109.5	H25A-C25-H25C	109.5
H25B-C25-H25C	109.5	C27-C26-P1	113.7(2)
C27-C26-H26A	108.8	P1-C26-H26A	108.8
C27-C26-H26B	108.8	P1-C26-H26B	108.8
H26A-C26-H26B	107.7	C28-C27-C26	113.1(3)
C28-C27-H27A	109.0	C26-C27-H27A	109.0
C28-C27-H27B	109.0	C26-C27-H27B	109.0
H27A-C27-H27B	107.8	C27-C28-C29	112.6(3)
C27-C28-H28A	109.1	C29-C28-H28A	109.1
C27-C28-H28B	109.1	C29-C28-H28B	109.1
H28A-C28-H28B	107.8	C28-C29-H29A	109.5
C28-C29-H29B	109.5	H29A-C29-H29B	109.5
C28-C29-H29C	109.5	H29A-C29-H29C	109.5
H29B-C29-H29C	109.5	C31-C30-P2	114.6(2)
C31-C30-H30A	108.6	P2-C30-H30A	108.6
C31-C30-H30B	108.6	P2-C30-H30B	108.6
H30A-C30-H30B	107.6	C32-C31-C30	111.9(2)
C32-C31-H31A	109.2	C30-C31-H31A	109.2
C32-C31-H31B	109.2	C30-C31-H31B	109.2
H31A-C31-H31B	107.9	C33-C32-C31	112.2(3)
C33-C32-H32A	109.2	C31-C32-H32A	109.2
C33-C32-H32B	109.2	C31-C32-H32B	109.2
H32A-C32-H32B	107.9	C32-C33-H33A	109.5
C32-C33-H33B	109.5	H33A-C33-H33B	109.5
C32-C33-H33C	109.5	H33A-C33-H33C	109.5
H33B-C33-H33C	109.5	C35-C34-P2	116.2(2)
C35-C34-H34A	108.2	P2-C34-H34A	108.2
C35-C34-H34B	108.2	P2-C34-H34B	108.2
H34A-C34-H34B	107.4	C36-C35-C34	111.9(2)
C36-C35-H35A	109.2	C34-C35-H35A	109.2
C36-C35-H35B	109.2	C34-C35-H35B	109.2
H35A-C35-H35B	107.9	C37-C36-C35	111.8(3)
C37-C36-H36A	109.3	C35-C36-H36A	109.3
C37-C36-H36B	109.3	C35-C36-H36B	109.3
H36A-C36-H36B	107.9	C36-C37-H37A	109.5

C36-C37-H37B	109.5	H37A-C37-H37B	109.5
C36-C37-H37C	109.5	H37A-C37-H37C	109.5
H37B-C37-H37C	109.5	C39-C38-P2	114.6(2)
C39-C38-H38A	108.6	P2-C38-H38A	108.6
C39-C38-H38B	108.6	P2-C38-H38B	108.6
H38A-C38-H38B	107.6	C40A-C39-C38	112.2(11)
C40-C39-C38	112.3(3)	C41-C40-C39	114.1(3)
C41-C40-H40A	108.7	C39-C40-H40A	108.7
C41-C40-H40B	108.7	C39-C40-H40B	108.7
H40A-C40-H40B	107.6	C40-C41-H41A	109.5
C40-C41-H41B	109.5	H41A-C41-H41B	109.5
C40-C41-H41C	109.5	H41A-C41-H41C	109.5
H41B-C41-H41C	109.5	C41A-C40A-C39	111.1(19)
C41A-C40A-H40C	109.4	C39-C40A-H40C	109.4
C41A-C40A-H40D	109.4	C39-C40A-H40D	109.4
H40C-C40A-H40D	108.0	C40A-C41A-H41D	109.5
C40A-C41A-H41E	109.5	H41D-C41A-H41E	109.5
C40A-C41A-H41F	109.5	H41D-C41A-H41F	109.5
H41E-C41A-H41F	109.5		

2. Crystal structure information of complex 3.

(1) Data collection and structure refinement for complex 3.

Theta range for data collection	2.37 to 27.50°
Index ranges	-21<=h<=21, -16<=k<=15, -14<=l<=14
Reflections collected	16556
Independent reflections	2955 [R(int) = 0.0526]
Max. and min. transmission	0.7700 and 0.6900
Structure solution technique	direct methods
Structure solution program	SHELXS-97 (Sheldrick 2008)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2013 (Sheldrick, 2013)
Function minimized	$\Sigma\ w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	2955 / 0 / 178
Goodness-of-fit on F^2	1.057

Δ/σ_{max}	0.001	
Final R indices	2346 data; I>2σ(I)	R1 = 0.0288, wR2 = 0.0510
	all data	R1 = 0.0474, wR2 = 0.0560
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0231P)^2+0.7096P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.569 and -0.438 eÅ^{-3}	
R.M.S. deviation from mean	0.106 eÅ^{-3}	

(2)Bond lengths (Å) for complex 3.

Se1-C1	1.936(2)	Se1-Mn2	2.5104(4)
Se1-Mn1	2.5301(4)	Mn1-C7	1.793(3)
Mn1-C7	1.794(3)	Mn1-C8	1.804(4)
Mn1-N1	2.103(3)	Mn1-Se1	2.5301(4)
Mn2-C10	1.804(3)	Mn2-C10	1.804(3)
Mn2-C9	1.865(4)	Mn2-C11	1.864(4)
Mn2-Se1	2.5104(4)	O1-C7	1.158(3)
O2-C8	1.146(4)	O3-C9	1.140(4)
O4-C10	1.150(3)	O5-C11	1.137(4)
N1-C12	1.346(3)	N1-C12	1.346(3)
C1-C2	1.386(3)	C1-C6	1.388(3)
C2-C3	1.383(3)	C3-C4	1.377(4)
C4-C5	1.384(4)	C5-C6	1.389(4)
C12-C13	1.378(4)	C13-C14	1.383(3)
C14-C13	1.383(3)		

(3) Bond angles (°) for complex 3.

C1-Se1-Mn2	109.97(7)	C1-Se1-Mn1	108.44(7)
Mn2-Se1-Mn1	95.730(13)	C7-Mn1-C7	86.71(15)
C7-Mn1-C8	90.76(11)	C7-Mn1-C8	90.76(11)
C7-Mn1-N1	91.82(10)	C7-Mn1-N1	91.83(10)
C8-Mn1-N1	176.44(14)	C7-Mn1-Se1	94.97(7)
C7-Mn1-Se1	178.16(8)	C8-Mn1-Se1	89.96(8)
N1-Mn1-Se1	87.38(6)	C7-Mn1-Se1	178.16(8)
C7-Mn1-Se1	94.97(7)	C8-Mn1-Se1	89.96(8)
N1-Mn1-Se1	87.38(6)	Se1-Mn1-Se1	83.329(18)
C10-Mn2-C10	87.81(15)	C10-Mn2-C9	92.75(11)
C10-Mn2-C9	92.75(11)	C10-Mn2-C11	94.86(11)
C10-Mn2-C11	94.86(11)	C9-Mn2-C11	169.43(15)

C10-Mn2-Se1	176.03(8)	C10-Mn2-Se1	93.92(7)
C9-Mn2-Se1	83.61(8)	C11-Mn2-Se1	88.55(8)
C10-Mn2-Se1	93.92(7)	C10-Mn2-Se1	176.03(8)
C9-Mn2-Se1	83.61(8)	C11-Mn2-Se1	88.55(8)
Se1-Mn2-Se1	84.132(19)	C12-N1-C12	116.7(3)
C12-N1-Mn1	121.38(15)	C12-N1-Mn1	121.38(15)
C2-C1-C6	119.2(2)	C2-C1-Se1	122.07(18)
C6-C1-Se1	118.70(19)	C3-C2-C1	120.3(2)
C4-C3-C2	120.7(3)	C3-C4-C5	119.3(3)
C4-C5-C6	120.4(3)	C1-C6-C5	120.1(3)
O1-C7-Mn1	175.5(2)	O2-C8-Mn1	179.4(3)
O3-C9-Mn2	176.2(3)	O4-C10-Mn2	176.2(2)
O5-C11-Mn2	178.8(3)	N1-C12-C13	123.2(2)
C12-C13-C14	119.6(3)	C13-C14-C13	117.7(4)

3. Crystal structure information of complex 4.

(1)Data collection and structure refinement for complex 4.

Theta range for data collection	1.74 to 27.50°	
Index ranges	-22<=h<=22, -10<=k<=21, -15<=l<=15	
Reflections collected	10940	
Independent reflections	6913 [R(int) = 0.0305]	
Max. and min. transmission	0.7457 and 0.6002	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2013 (Sheldrick, 2013)	
Function minimized	$\Sigma\ w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	6913 / 2 / 388	
Goodness-of-fit on F^2	0.914	
Δ/σ_{max}	0.001	
Final R indices	6160 data; I>2σ(I)	R1 = 0.0397, wR2 = 0.0775
	all data	R1 = 0.0460, wR2 = 0.0803
Weighting scheme	$w=1/[\sigma^2(F_o^2)]$ where $P=(F_o^2+2F_c^2)/3$	
Absolute structure parameter	0.0(0)	
Largest diff. peak and hole	0.706 and -0.291 $eÅ^{-3}$	

R.M.S. deviation from mean	0.061 eÅ^{-3}

(2). Bond lengths (Å) for complex 4.

Mn1-C10	1.798(6)	Mn1-C12	1.807(5)
Mn1-C11	1.812(5)	Mn1-P2	2.3446(14)
Mn1-P1	2.3536(14)	Mn1-Se1	2.5417(8)
Se1-C1	1.933(5)	P1-C7	1.828(5)
P1-C1B	1.841(5)	P1-C1A	1.843(5)
P2-C1D	1.826(5)	P2-C9	1.833(5)
P2-C1C	1.846(5)	O1-C10	1.137(6)
O2-C11	1.137(6)	O3-C12	1.138(6)
C1-C6	1.374(8)	C1-C2	1.378(8)
C2-C3	1.374(8)	C3-C4	1.367(11)
C4-C5	1.366(11)	C5-C6	1.382(9)
C7-C8	1.516(8)	C8-C9	1.533(8)
C1A-C2A	1.375(8)	C1A-C6A	1.384(7)
C2A-C3A	1.388(8)	C3A-C4A	1.361(9)
C4A-C5A	1.371(9)	C5A-C6A	1.381(8)
C1B-C6B	1.379(7)	C1B-C2B	1.392(7)
C2B-C3B	1.375(8)	C3B-C4B	1.370(9)
C4B-C5B	1.372(9)	C5B-C6B	1.382(7)
C1C-C2C	1.381(8)	C1C-C6C	1.387(8)
C2C-C3C	1.369(7)	C3C-C4C	1.381(10)
C4C-C5C	1.349(10)	C5C-C6C	1.376(8)
C1D-C6D	1.387(7)	C1D-C2D	1.389(7)
C2D-C3D	1.374(8)	C3D-C4D	1.373(9)
C4D-C5D	1.382(9)	C5D-C6D	1.384(8)

(3). Bond angles (°) for complex 4.

C10-Mn1-C12	90.4(2)	C10-Mn1-C11	90.3(2)
C12-Mn1-C11	88.8(2)	C10-Mn1-P2	92.72(16)
C12-Mn1-P2	92.01(15)	C11-Mn1-P2	176.84(15)
C10-Mn1-P1	99.79(16)	C12-Mn1-P1	169.41(17)
C11-Mn1-P1	88.24(15)	P2-Mn1-P1	90.37(5)
C10-Mn1-Se1	172.31(16)	C12-Mn1-Se1	82.46(16)
C11-Mn1-Se1	92.40(14)	P2-Mn1-Se1	84.70(4)
P1-Mn1-Se1	87.49(4)	C1-Se1-Mn1	105.25(15)
C7-P1-C1B	103.9(2)	C7-P1-C1A	103.1(2)
C1B-P1-C1A	101.5(2)	C7-P1-Mn1	113.50(18)
C1B-P1-Mn1	119.21(17)	C1A-P1-Mn1	113.69(15)
C1D-P2-C9	104.1(2)	C1D-P2-C1C	99.9(2)
C9-P2-C1C	101.9(2)	C1D-P2-Mn1	115.23(16)
C9-P2-Mn1	115.47(17)	C1C-P2-Mn1	118.02(17)

C6-C1-C2	118.7(6)	C6-C1-Se1	119.3(5)
C2-C1-Se1	122.0(4)	C3-C2-C1	120.9(7)
C4-C3-C2	119.7(8)	C5-C4-C3	120.3(7)
C4-C5-C6	119.9(7)	C1-C6-C5	120.5(7)
C8-C7-P1	115.2(3)	C7-C8-C9	115.0(4)
C8-C9-P2	114.4(3)	O1-C10-Mn1	173.4(5)
O2-C11-Mn1	176.8(4)	O3-C12-Mn1	176.1(4)
C2A-C1A-C6A	118.5(5)	C2A-C1A-P1	121.2(4)
C6A-C1A-P1	120.1(4)	C1A-C2A-C3A	120.5(5)
C4A-C3A-C2A	120.8(6)	C3A-C4A-C5A	119.1(6)
C4A-C5A-C6A	120.8(6)	C5A-C6A-C1A	120.3(6)
C6B-C1B-C2B	118.7(5)	C6B-C1B-P1	119.1(4)
C2B-C1B-P1	122.2(4)	C3B-C2B-C1B	120.0(5)
C4B-C3B-C2B	120.8(6)	C3B-C4B-C5B	119.7(5)
C4B-C5B-C6B	119.9(6)	C1B-C6B-C5B	120.8(5)
C2C-C1C-C6C	117.8(5)	C2C-C1C-P2	120.5(4)
C6C-C1C-P2	121.6(4)	C3C-C2C-C1C	121.2(6)
C2C-C3C-C4C	119.7(7)	C5C-C4C-C3C	119.9(5)
C4C-C5C-C6C	120.7(6)	C5C-C6C-C1C	120.6(6)
C6D-C1D-C2D	118.9(5)	C6D-C1D-P2	117.8(4)
C2D-C1D-P2	123.2(4)	C3D-C2D-C1D	120.3(6)
C4D-C3D-C2D	120.4(6)	C3D-C4D-C5D	120.3(6)
C4D-C5D-C6D	119.4(6)	C5D-C6D-C1D	120.7(5)

4. Crystal structure information of complex 5.

(1). Data collection and structure refinement for complex 5.

Theta range for data collection	1.75 to 27.50°
Index ranges	-11<=h<=12, -15<=k<=14, -17<=l<=17
Reflections collected	10408
Independent reflections	6675 [R(int) = 0.0315]
Max. and min. transmission	0.7456 and 0.6071
Structure solution technique	direct methods
Structure solution program	Bruker SHELXTL
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2013 (Sheldrick, 2013)
Function minimized	$\Sigma\ w(F_o^2 - F_c^2)^2$

Data / restraints / parameters	6675 / 0 / 388	
Goodness-of-fit on F^2	1.033	
Final R indices	5615 data; I>2σ(I)	R1 = 0.0483, wR2 = 0.1149
	all data	R1 = 0.0579, wR2 = 0.1206
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0629P)^2+0.2204P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.716 and -0.325 eÅ^{-3}	
R.M.S. deviation from mean	0.086 eÅ^{-3}	

(2). Bond lengths (Å) for complex 5.

Mn1-C4	1.782(3)	Mn1-C3	1.834(3)
Mn1-C5	1.835(3)	Mn1-O5	2.055(2)
Mn1-P1	2.3449(12)	Mn1-P2	2.3661(13)
P1-C1B	1.827(3)	P1-C1A	1.833(2)
P1-C6	1.837(2)	P2-C1C	1.818(2)
P2-C8	1.832(2)	P2-C1D	1.839(3)
F1-C2	1.346(3)	F2-C2	1.321(3)
F3-C2	1.309(3)	O1-C4	1.157(3)
O2-C3	1.147(3)	O3-C5	1.138(3)
O4-C1	1.215(3)	O5-C1	1.269(3)
C1-C2	1.541(3)	C6-C7	1.531(3)
C6-H6A	0.99	C6-H6B	0.99
C7-C8	1.532(3)	C7-H7A	0.99
C7-H7B	0.99	C8-H8A	0.99
C8-H8B	0.99	C1A-C2A	1.389(3)
C1A-C6A	1.391(3)	C2A-C3A	1.390(4)
C2A-H2A	0.95	C3A-C4A	1.389(4)
C3A-H3A	0.95	C4A-C5A	1.376(4)
C4A-H4A	0.95	C5A-C6A	1.387(4)
C5A-H5A	0.95	C6A-H6A1	0.95
C1B-C6B	1.391(3)	C1B-C2B	1.403(3)
C2B-C3B	1.395(4)	C2B-H2B	0.95
C3B-C4B	1.376(4)	C3B-H3B	0.95
C4B-C5B	1.388(4)	C4B-H4B	0.95
C5B-C6B	1.387(3)	C5B-H5B	0.95
C6B-H6B1	0.95	C1C-C2C	1.386(3)
C1C-C6C	1.398(3)	C2C-C3C	1.379(3)
C2C-H2C	0.95	C3C-C4C	1.392(4)

C3C-H3C	0.95	C4C-C5C	1.383(4)
C4C-H4C	0.95	C5C-C6C	1.377(3)
C5C-H5C	0.95	C6C-H6C	0.95
C1D-C6D	1.392(3)	C1D-C2D	1.397(3)
C2D-C3D	1.392(4)	C2D-H2D	0.95
C3D-C4D	1.373(4)	C3D-H3D	0.95
C4D-C5D	1.387(4)	C4D-H4D	0.95
C5D-C6D	1.393(3)	C5D-H5D	0.95
C6D-H6D	0.95		

(3). Bond angles (°) for complex 5.

C4-Mn1-C3	87.58(10)	C4-Mn1-C5	90.54(11)
C3-Mn1-C5	90.52(11)	C4-Mn1-O5	176.75(9)
C3-Mn1-O5	92.59(9)	C5-Mn1-O5	92.70(9)
C4-Mn1-P1	94.53(9)	C3-Mn1-P1	91.30(8)
C5-Mn1-P1	174.68(7)	O5-Mn1-P1	82.22(6)
C4-Mn1-P2	95.72(8)	C3-Mn1-P2	176.55(8)
C5-Mn1-P2	88.45(8)	O5-Mn1-P2	84.17(5)
P1-Mn1-P2	89.44(5)	C1B-P1-C1A	100.23(12)
C1B-P1-C6	103.70(11)	C1A-P1-C6	100.86(11)
C1B-P1-Mn1	114.23(9)	C1A-P1-Mn1	122.74(9)
C6-P1-Mn1	112.59(9)	C1C-P2-C8	105.58(12)
C1C-P2-C1D	102.43(11)	C8-P2-C1D	99.77(10)
C1C-P2-Mn1	116.32(8)	C8-P2-Mn1	115.10(8)
C1D-P2-Mn1	115.56(8)	C1-O5-Mn1	122.67(15)
O4-C1-O5	130.6(2)	O4-C1-C2	118.7(2)
O5-C1-C2	110.6(2)	F3-C2-F2	108.2(2)
F3-C2-F1	105.9(2)	F2-C2-F1	106.0(2)
F3-C2-C1	113.3(2)	F2-C2-C1	112.6(2)
F1-C2-C1	110.3(2)	O2-C3-Mn1	176.0(2)
O1-C4-Mn1	176.1(2)	O3-C5-Mn1	176.8(2)
C7-C6-P1	112.18(16)	C7-C6-H6A	109.2
P1-C6-H6A	109.2	C7-C6-H6B	109.2
P1-C6-H6B	109.2	H6A-C6-H6B	107.9
C6-C7-C8	113.81(19)	C6-C7-H7A	108.8
C8-C7-H7A	108.8	C6-C7-H7B	108.8
C8-C7-H7B	108.8	H7A-C7-H7B	107.7
C7-C8-P2	116.21(15)	C7-C8-H8A	108.2
P2-C8-H8A	108.2	C7-C8-H8B	108.2
P2-C8-H8B	108.2	H8A-C8-H8B	107.4
C2A-C1A-C6A	118.9(2)	C2A-C1A-P1	122.07(19)

C6A-C1A-P1	118.95(19)	C1A-C2A-C3A	119.9(2)
C1A-C2A-H2A	120.1	C3A-C2A-H2A	120.1
C4A-C3A-C2A	120.5(3)	C4A-C3A-H3A	119.8
C2A-C3A-H3A	119.8	C5A-C4A-C3A	119.8(2)
C5A-C4A-H4A	120.1	C3A-C4A-H4A	120.1
C4A-C5A-C6A	119.8(3)	C4A-C5A-H5A	120.1
C6A-C5A-H5A	120.1	C5A-C6A-C1A	121.0(3)
C5A-C6A-H6A1	119.5	C1A-C6A-H6A1	119.5
C6B-C1B-C2B	118.9(2)	C6B-C1B-P1	121.95(18)
C2B-C1B-P1	119.18(19)	C3B-C2B-C1B	120.1(3)
C3B-C2B-H2B	119.9	C1B-C2B-H2B	119.9
C4B-C3B-C2B	120.2(3)	C4B-C3B-H3B	119.9
C2B-C3B-H3B	119.9	C3B-C4B-C5B	120.0(3)
C3B-C4B-H4B	120.0	C5B-C4B-H4B	120.0
C6B-C5B-C4B	120.2(3)	C6B-C5B-H5B	119.9
C4B-C5B-H5B	119.9	C5B-C6B-C1B	120.5(2)
C5B-C6B-H6B1	119.7	C1B-C6B-H6B1	119.7
C2C-C1C-C6C	119.0(2)	C2C-C1C-P2	123.32(18)
C6C-C1C-P2	117.64(18)	C3C-C2C-C1C	120.3(2)
C3C-C2C-H2C	119.9	C1C-C2C-H2C	119.9
C2C-C3C-C4C	120.5(2)	C2C-C3C-H3C	119.8
C4C-C3C-H3C	119.8	C5C-C4C-C3C	119.4(2)
C5C-C4C-H4C	120.3	C3C-C4C-H4C	120.3
C6C-C5C-C4C	120.2(2)	C6C-C5C-H5C	119.9
C4C-C5C-H5C	119.9	C5C-C6C-C1C	120.6(2)
C5C-C6C-H6C	119.7	C1C-C6C-H6C	119.7
C6D-C1D-C2D	118.4(2)	C6D-C1D-P2	118.77(18)
C2D-C1D-P2	122.83(18)	C3D-C2D-C1D	120.1(2)
C3D-C2D-H2D	119.9	C1D-C2D-H2D	119.9
C4D-C3D-C2D	121.2(2)	C4D-C3D-H3D	119.4
C2D-C3D-H3D	119.4	C3D-C4D-C5D	119.3(2)
C3D-C4D-H4D	120.3	C5D-C4D-H4D	120.3
C4D-C5D-C6D	120.1(2)	C4D-C5D-H5D	119.9
C6D-C5D-H5D	119.9	C1D-C6D-C5D	120.9(2)
C1D-C6D-H6D	119.5	C5D-C6D-H6D	119.5