

Crystal structure of bis(2-nitrobenzoato-*O*)bis(1,10-phenanthroline-*N,N'*)manganese(II) tetrahydrate, $[\text{Mn}(\text{C}_7\text{H}_4\text{NO}_4)_2(\text{C}_{12}\text{H}_8\text{N}_2)_2] \cdot 4\text{H}_2\text{O}$

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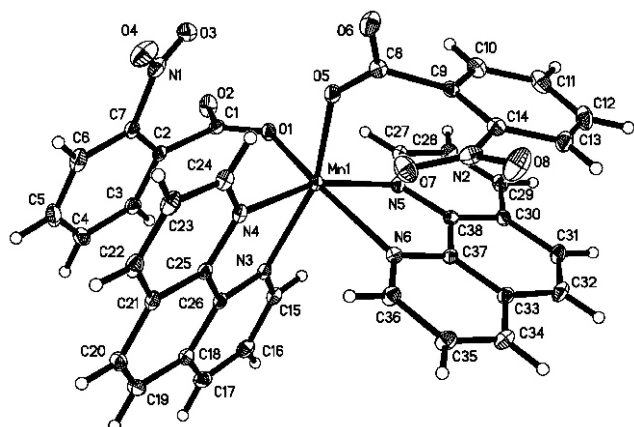


Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
C(1)	4e	0.6389(1)	0.6884(2)	0.0836(1)	0.017(1)	0.019(1)	0.022(1)	0.0029(9)	0.0076(9)	0.0005(9)
C(2)	4e	0.6719(1)	0.7626(2)	0.1518(1)	0.014(1)	0.023(1)	0.021(1)	−0.0014(9)	0.0109(9)	−0.0023(9)
C(3)	4e	0.7216(2)	0.7268(2)	0.2291(1)	0.022(1)	0.030(1)	0.022(1)	0.004(1)	0.013(1)	0.004(1)
C(4)	4e	0.7593(2)	0.7916(2)	0.2935(2)	0.024(1)	0.057(2)	0.019(1)	0.001(1)	0.010(1)	−0.003(1)
C(5)	4e	0.7479(2)	0.8941(2)	0.2818(2)	0.029(1)	0.047(2)	0.032(2)	−0.011(1)	0.018(1)	−0.021(1)
C(6)	4e	0.6981(2)	0.9320(2)	0.2063(2)	0.028(1)	0.028(1)	0.040(2)	−0.006(1)	0.022(1)	−0.011(1)
C(7)	4e	0.6604(1)	0.8658(2)	0.1430(1)	0.020(1)	0.024(1)	0.021(1)	0.0018(9)	0.013(1)	0.0001(9)
C(8)	4e	0.7119(2)	0.8837(2)	−0.1313(1)	0.022(1)	0.020(1)	0.021(1)	−0.0007(9)	0.010(1)	0.0001(9)
C(9)	4e	0.7532(1)	0.8196(2)	−0.1749(1)	0.021(1)	0.018(1)	0.015(1)	0.0037(9)	0.0077(9)	0.0042(9)
C(10)	4e	0.7089(2)	0.7324(2)	−0.2129(1)	0.029(1)	0.021(1)	0.023(1)	−0.003(1)	0.011(1)	0.002(1)
C(11)	4e	0.7420(2)	0.6747(2)	−0.2570(1)	0.046(2)	0.019(1)	0.023(1)	−0.002(1)	0.012(1)	−0.002(1)
C(12)	4e	0.8204(2)	0.7026(2)	−0.2640(2)	0.049(2)	0.025(1)	0.026(1)	0.011(1)	0.021(1)	0.003(1)
C(13)	4e	0.8654(2)	0.7887(2)	−0.2278(1)	0.029(1)	0.025(1)	0.026(1)	0.009(1)	0.017(1)	0.006(1)
C(14)	4e	0.8313(1)	0.8453(2)	−0.1840(1)	0.023(1)	0.015(1)	0.019(1)	0.0019(9)	0.007(1)	0.0015(9)
C(15)	4e	0.8924(1)	0.6090(2)	0.1799(1)	0.021(1)	0.020(1)	0.026(1)	0.0011(9)	0.014(1)	0.0006(9)
C(16)	4e	0.9489(2)	0.5833(2)	0.2587(1)	0.024(1)	0.023(1)	0.031(1)	0.004(1)	0.015(1)	0.006(1)
C(17)	4e	0.9878(2)	0.6577(2)	0.3136(1)	0.021(1)	0.036(1)	0.023(1)	0.003(1)	0.011(1)	0.006(1)
C(18)	4e	0.9704(2)	0.7588(2)	0.2896(1)	0.018(1)	0.029(1)	0.021(1)	−0.0003(9)	0.010(1)	−0.002(1)
C(19)	4e	1.0067(2)	0.8412(2)	0.3434(1)	0.020(1)	0.041(2)	0.019(1)	−0.000(1)	0.006(1)	−0.003(1)
C(20)	4e	0.9861(2)	0.9370(2)	0.3173(1)	0.021(1)	0.035(1)	0.026(1)	−0.006(1)	0.009(1)	−0.013(1)
C(21)	4e	0.9285(1)	0.9588(2)	0.2353(1)	0.019(1)	0.022(1)	0.026(1)	−0.0029(9)	0.013(1)	−0.0072(9)
C(22)	4e	0.9034(2)	1.0565(2)	0.2059(2)	0.025(1)	0.021(1)	0.036(2)	−0.005(1)	0.018(1)	−0.010(1)
C(23)	4e	0.8467(2)	1.0713(2)	0.1268(2)	0.029(1)	0.016(1)	0.040(2)	0.000(1)	0.021(1)	−0.002(1)
C(24)	4e	0.8163(2)	0.9878(2)	0.0765(1)	0.024(1)	0.020(1)	0.027(1)	0.0005(9)	0.014(1)	−0.000(1)
C(25)	4e	0.8932(1)	0.8793(2)	0.1807(1)	0.015(1)	0.021(1)	0.021(1)	−0.0011(9)	0.0099(9)	−0.0029(9)
C(26)	4e	0.9140(1)	0.7776(2)	0.2083(1)	0.016(1)	0.021(1)	0.020(1)	−0.0001(9)	0.0105(9)	−0.0027(9)
C(27)	4e	0.7300(1)	0.5375(2)	−0.0608(1)	0.020(1)	0.022(1)	0.021(1)	0.0007(9)	0.010(1)	−0.0010(9)
C(28)	4e	0.7302(2)	0.4536(2)	−0.1062(1)	0.025(1)	0.019(1)	0.025(1)	−0.0042(9)	0.009(1)	−0.0044(9)
C(29)	4e	0.8007(2)	0.4420(2)	−0.1276(1)	0.030(1)	0.019(1)	0.021(1)	0.002(1)	0.010(1)	−0.0044(9)
C(30)	4e	0.8705(1)	0.5140(2)	−0.1035(1)	0.023(1)	0.020(1)	0.016(1)	0.0040(9)	0.0082(9)	0.0008(9)
C(31)	4e	0.9464(2)	0.5063(2)	−0.1235(1)	0.029(1)	0.023(1)	0.027(1)	0.007(1)	0.016(1)	−0.004(1)
C(32)	4e	1.0133(2)	0.5756(2)	−0.0970(1)	0.026(1)	0.026(1)	0.033(1)	0.007(1)	0.018(1)	0.001(1)
C(33)	4e	1.0102(1)	0.6588(2)	−0.0496(1)	0.020(1)	0.021(1)	0.021(1)	0.0059(9)	0.010(1)	0.0041(9)
C(34)	4e	1.0801(2)	0.7308(2)	−0.0195(1)	0.021(1)	0.024(1)	0.034(1)	0.003(1)	0.015(1)	0.005(1)
C(35)	4e	1.0717(2)	0.8088(2)	0.0249(1)	0.021(1)	0.023(1)	0.034(1)	−0.003(1)	0.012(1)	−0.002(1)
C(36)	4e	0.9935(2)	0.8159(2)	0.0385(1)	0.023(1)	0.019(1)	0.028(1)	0.0004(9)	0.012(1)	−0.002(1)
C(37)	4e	0.9352(1)	0.6702(2)	−0.0316(1)	0.019(1)	0.015(1)	0.017(1)	0.0059(8)	0.0077(9)	0.0045(8)
C(38)	4e	0.8645(1)	0.5957(2)	−0.0586(1)	0.018(1)	0.017(1)	0.016(1)	0.0049(9)	0.0064(9)	0.0033(9)
Mn(1)	4e	0.79168(2)	0.75264(2)	0.02540(2)	0.0180(2)	0.0164(2)	0.0175(2)	0.0003(1)	0.0091(1)	−0.0019(1)
N(1)	4e	0.6039(1)	0.9080(2)	0.0637(1)	0.030(1)	0.025(1)	0.035(1)	0.0115(9)	0.021(1)	0.0066(9)
N(2)	4e	0.8811(1)	0.9360(1)	−0.1446(1)	0.021(1)	0.022(1)	0.032(1)	0.0020(8)	0.0092(9)	0.0025(9)
N(3)	4e	0.8758(1)	0.7030(1)	0.1542(1)	0.0168(9)	0.0178(9)	0.021(1)	0.0001(7)	0.0107(8)	−0.0018(8)
N(4)	4e	0.8378(1)	0.8939(1)	0.1016(1)	0.0204(9)	0.0173(9)	0.022(1)	−0.0003(8)	0.0128(8)	−0.0027(8)
N(5)	4e	0.7945(1)	0.6072(1)	−0.0371(1)	0.0201(9)	0.0174(9)	0.018(1)	0.0009(7)	0.0093(8)	−0.0011(7)
N(6)	4e	0.9265(1)	0.7492(1)	0.0115(1)	0.0190(9)	0.0171(9)	0.018(1)	−0.0004(7)	0.0080(8)	−0.0001(7)
O(1)	4e	0.67552(9)	0.6899(1)	0.03584(9)	0.0202(8)	0.0242(8)	0.0204(9)	−0.0033(6)	0.0114(7)	−0.0040(7)
O(2)	4e	0.5803(1)	0.6263(1)	0.0820(1)	0.0319(9)	0.0266(9)	0.039(1)	−0.0136(7)	0.0217(8)	−0.0098(8)
O(3)	4e	0.5483(1)	0.8533(1)	0.0134(1)	0.035(1)	0.037(1)	0.025(1)	0.0129(8)	0.0072(8)	−0.0003(8)
O(4)	4e	0.6146(1)	0.9972(1)	0.0524(1)	0.044(1)	0.027(1)	0.059(1)	0.0106(8)	0.030(1)	0.0179(9)
O(5)	4e	0.7091(1)	0.8461(1)	−0.06958(9)	0.0232(8)	0.0241(8)	0.0201(9)	0.0028(7)	0.0119(7)	0.0018(7)
O(6)	4e	0.6792(1)	0.9652(1)	−0.1622(1)	0.045(1)	0.0250(9)	0.038(1)	0.0147(8)	0.0273(9)	0.0123(8)
O(7)	4e	0.8777(1)	0.9634(1)	−0.0828(1)	0.046(1)	0.028(1)	0.029(1)	−0.0052(8)	0.0134(9)	−0.0063(8)
O(8)	4e	0.9239(1)	0.9803(1)	−0.1759(1)	0.041(1)	0.034(1)	0.072(1)	−0.0104(9)	0.040(1)	−0.003(1)
O(9)	4e	0.3985(1)	0.5653(1)	0.9809(1)	0.0264(9)	0.036(1)	0.043(1)	0.0013(8)	0.0151(8)	−0.0046(8)
O(10)	4e	0.7860(1)	0.7653(2)	0.4824(1)	0.029(1)	0.059(1)	0.035(1)	−0.0081(9)	0.0128(8)	−0.0017(9)
O(11)	4e	0.4661(1)	0.7173(1)	0.1518(1)	0.054(1)	0.032(1)	0.059(1)	0.0058(9)	0.043(1)	0.0053(9)
O(12)	4e	0.5932(1)	0.0878(1)	0.9025(1)	0.082(2)	0.035(1)	0.054(1)	0.030(1)	0.049(1)	0.018(1)

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