10.1071/CH12077_AC
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Australian Journal of Chemistry 2012, 65(6), 672-679

# Supplementary Material (ESI)

# A new quinoxalinyl-substituted nitronyl nitroxide radical and its five-spin Cu(II) and four-spin Mn(II) complexes: syntheses, crystal structures and magnetic properties

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Table 1. Selected bond lengths (Å) and angles (deg) for QNXL-2NIT (**1**)

| | | | |
|---|---|---|---|
| C(1)-N(2) | 1.332(6) | N(1)-O(1) | 1.286(17) |
| C(1)-N(1) | 1.334(6) | N(2)-O(2) | 1.263(5) |
| C(1)-C(8) | 1.466(6) | N(5)-O(3) | 1.274(4) |
| C(2)-N(1) | 1.476(6) | N(6)-O(4) | 1.269(4) |
| C(2)-C(3) | 1.499(8) | C(9)-N(3) | 1.291(5) |
| C(2)-C(5) | 1.516(8) | C(10)-N(3) | 1.369(6) |
| C(2)-C(4) | 1.558(8) | C(5)-N(2) | 1.500(7) |
| N(2)-C(1)-N(1) | 110.2(4) | N(2)-C(1)-C(8) | 126.3(4) |
| N(1)-C(1)-C(8) | 123.4(4) | N(1)-C(2)-C(3) | 112.8(4) |
| O(1)-N(1)-C(1) | 124.1(11) | O(1)-N(1)-C(2) | 122.3(10) |
| O(2)-N(2)-C(1) | 126.6(4) | O(2)-N(2)-C(5) | 123.8(4) |
| O(3)-N(5)-C(16) | 124.9(3) | O(3)-N(5)-C(20) | 123.3(3) |
| O(4)-N(6)-C(16) | 125.6(3) | O(4)-N(6)-C(17) | 122.2(3) |

Table 2. Selected bond lengths (Å) and angles (deg) for complex **2**

| | | | |
|---|---|---|---|
| Cu(1)-O(8) | 1.950(3) | Cu(1)-O(3) | 1.955(3) |
| Cu(1)-O(2) | 1.960(3) | Cu(1)-O(4) | 1.961(3) |
| Cu(1)-O(1) | 2.257(3) | Cu(1)-N(1) | 2.476(3) |
| Cu(2)-O(5) | 1.950(3) | Cu(2)-O(6) | 1.966(3) |
| Cu(2)-N(2) | 2.394(3) | N(3)-O(7) | 1.268(4) |
| N(4)-O(8) | 1.308(4) | | |
| O(8)-Cu(1)-O(3) | 92.32(12) | O(8)-Cu(1)-O(2) | 88.47(12) |
| O(3)-Cu(1)-O(2) | 173.65(12) | O(8)-Cu(1)-O(4) | 174.03(12) |
| O(3)-Cu(1)-O(4) | 91.29(13) | O(2)-Cu(1)-O(4) | 88.46(12) |
| O(8)-Cu(1)-O(1) | 94.82(12) | O(3)-Cu(1)-O(1) | 86.09(12) |
| O(2)-Cu(1)-O(1) | 87.56(12) | O(4)-Cu(1)-O(1) | 90.17(12) |
| O(8)-Cu(1)-N(1) | 78.07(12) | O(3)-Cu(1)-N(1) | 97.77(12) |
| O(2)-Cu(1)-N(1) | 88.56(12) | O(4)-Cu(1)-N(1) | 96.72(12) |
| O(1)-Cu(1)-N(1) | 171.99(12) | O(5)-Cu(2)-O(6) | 87.84(12) |
| O(5)-Cu(2)-N(2) | 87.59(12) | O(6)-Cu(2)-N(2) | 89.00(12) |

Table 3. Selected bond lengths (Å) and angles (deg) for complex **3**

| | | | |
|---|---|---|---|
| Mn(1)-O(4) | 2.124(3) | Mn(1)-O(1) | 2.133(3) |
| Mn(1)-O(5) | 2.143(3) | Mn(1)-O(3) | 2.177(3) |
| Mn(1)-O(6) | 2.204(3) | Mn(1)-N(1) | 2.309(3) |
| N(3)-O(1) | 1.306(4) | N(4)-O(2) | 1.269(4) |
| O(4)-Mn(1)-O(1) | 92.90(11) | O(4)-Mn(1)-O(5) | 160.31(11) |
| O(1)-Mn(1)-O(5) | 105.03(11) | O(4)-Mn(1)-O(3) | 81.07(11) |
| O(1)-Mn(1)-O(3) | 173.94(11) | O(5)-Mn(1)-O(3) | 80.86(11) |
| O(4)-Mn(1)-O(6) | 92.76(12) | O(1)-Mn(1)-O(6) | 86.39(11) |
| O(5)-Mn(1)-O(6) | 80.55(11) | O(3)-Mn(1)-O(6) | 93.32(12) |
| O(4)-Mn(1)-N(1) | 103.65(11) | O(1)-Mn(1)-N(1) | 85.42(11) |
| O(5)-Mn(1)-N(1) | 86.12(11) | O(3)-Mn(1)-N(1) | 96.50(11) |
| O(6)-Mn(1)-N(1) | 161.98(12) | N(3)-O(1)-Mn(1) | 124.9(2) |