Electronic Supplementary Information

# A novel octacyanido dicobalt(III) building block for the construction of heterometallic compounds†

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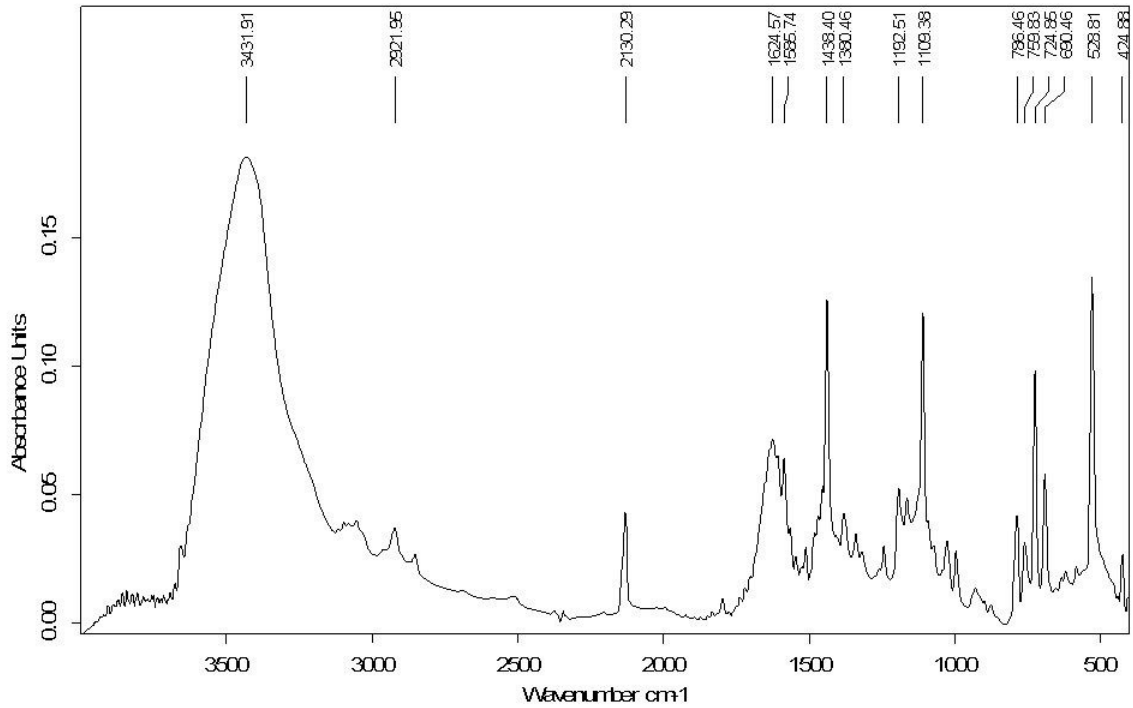


Fig. S1. FTIR spectrum of **1**

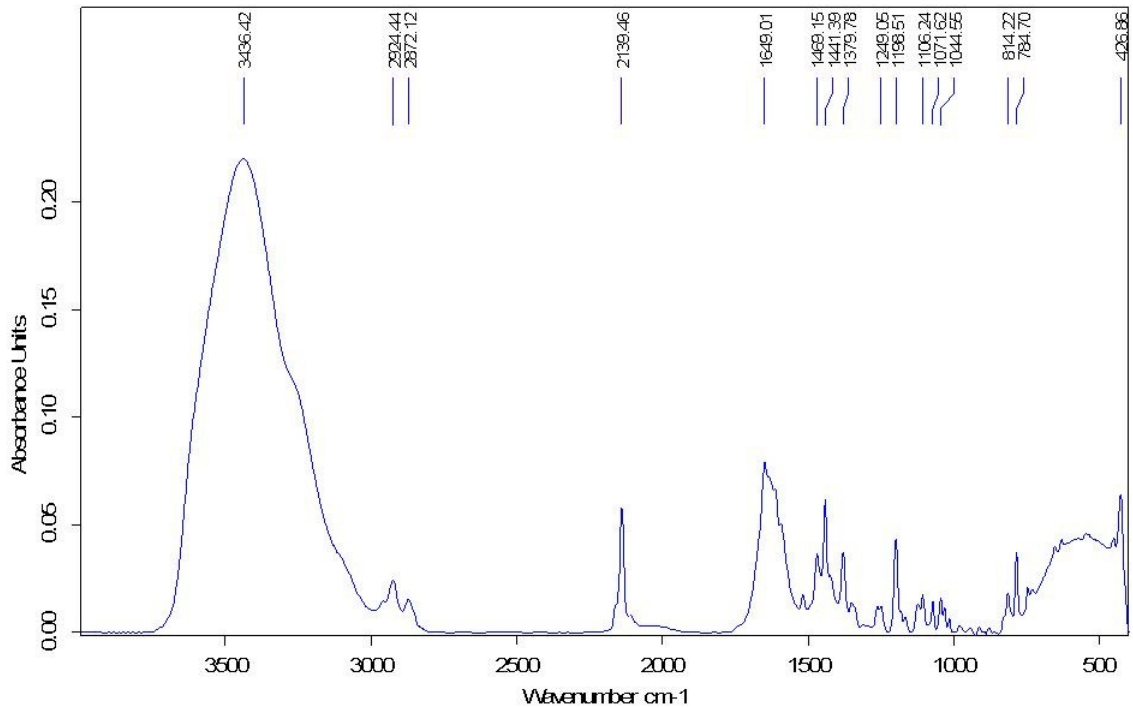


Fig. S2. FTIR spectrum of **2**.

**Table S1.** Selected bond lengths (Å) and angles (°) for **1**

| | | | |
|---|---|---|---|
| Co(1)-N(1) | 1.9659(14) | Co(1)-C(9) | 1.8657(18) |
| Co(1)-N(2) | 1.9603(13) | Co(1)-C(10) | 1.8683(19) |
| Co(1)-C(8) | 1.908(2) | Co(1)-C(11) | 1.908(2) |
| | | | |
| C(9)-Co(1)-C(10) | 87.64(8) | C(9)-Co(1)-N(1) | 95.71(7) |
| C(9)-Co(1)-C(11) | 88.26(8) | C(10)-Co(1)-N(1) | 176.63(6) |
| C(10)-Co(1)-C(11) | 89.37(8) | C(11)-Co(1)-N(1) | 90.36(7) |
| C(9)-Co(1)-C(8) | 91.93(8) | C(8)-Co(1)-N(1) | 89.83(7) |
| C(10)-Co(1)-C(8) | 90.43(9) | N(2)-Co(1)-N(1) | 82.12(6) |
| C(11)-Co(1)-C(8) | 179.72(8) | N(3)-C(8)-Co(1) | 175.6(2) |
| C(9)-Co(1)-N(2) | 176.02(7) | N(4)-C(9)-Co(1) | 178.4(2) |
| C(10)-Co(1)-N(2) | 94.51(6) | N(5)-C(10)-Co(1) | 178.71(17) |
| C(11)-Co(1)-N(2) | 88.42(7) | N(6)-C(11)-Co(1) | 177.3(2) |
| C(8)-Co(1)-N(2) | 91.40(7) | | |

**Table S2.** Selected bond lengths (Å) and angles (°) for **2**[a]

| | | | | | |
|---|---|---|---|---|---|
| Co(1)-N(1) | 1.973(3) | Co(2)-N(3) | 1.967(3) | Mn(1)-N(9) | 2.277(4) |
| Co(1)-N(2) | 1.966(3) | Co(2)-N(4) | 1.975(3) | Mn(1)-N(13) | 2.210(2) |
| Co(1)-C(15) | 1.899(4) | Co(2)-C(19) | 1.905(4) | Mn(1)-N(14) | 2.297(4) |
| Co(1)-C(16) | 1.865(3) | Co(2)-C(20) | 1.871(4) | Mn(1)-N(15) | 2.306(4) |
| Co(1)-C(17) | 1.875(4) | Co(2)-C(21) | 1.873(4) | Mn(1)-N(16) | 2.292(4) |
| Co(1)-C(18) | 1.900(4) | Co(2)-C(22) | 1.900(5) | Mn(1)-N(17) | 2.308(4) |
| | | | | Mn(1)-N(5a) | 2.273(4) |
| | | | | | |
| C(16)-Co(1)-C(17) | 89.02(15) | C(20)-Co(2)-C(21) | 88.22(16) | N(13)-Mn(1)-N(5a) | 90.81(12) |
| C(16)-Co(1)-C(15) | 87.91(16) | C(20)-Co(2)-C(22) | 89.50(18) | N(13)-Mn(1)-N(9) | 92.80(12) |
| C(17)-Co(1)-C(15) | 90.70(16) | C(21)-Co(2)-C(22) | 89.85(19) | N(5a)-Mn(1)-N(9) | 176.33(12) |
| C(16)-Co(1)-C(18) | 88.40(16) | C(20)-Co(2)-C(19) | 86.09(16) | N(13)-Mn(1)-N(16) | 142.97(16) |
| C(17)-Co(1)-C(18) | 90.1725(16) | C(21)-Co(2)-C(19) | 89.62(16) | N(5a)-Mn(1)-N(16) | 93.16(14) |
| C(15)-Co(1)-C(18) | 176.18(15) | C(22)-Co(2)-C(19) | 175.57(16) | N(9)-Mn(1)-N(16) | 84.34(13) |
| C(16)-Co(1)-N(2) | 176.84(14) | C(20)-Co(2)-N(3) | 177.35(15) | N(13)-Mn(1)-N(14) | 69.82(17) |
| C(17)-Co(1)-N(2) | 94.13(13) | C(21)-Co(2)-N(3) | 93.26(13) | N(5a)-Mn(1)-N(14) | 88.07(14) |
| C(15)-Co(1)-N(2) | 91.99(13) | C(22)-Co(2)-N(3) | 92.70(15) | N(9)-Mn(1)-N(14) | 93.78(14) |
| C(18)-Co(1)-N(2) | 91.64(13) | C(19)-Co(2)-N(3) | 91.72(13) | N(16)-Mn(1)-N(14) | 73.5(2) |
| C(16)-Co(1)-N(1) | 94.71(14) | C(20)-Co(2)-N(4) | 96.61(14) | N(13)-Mn(1)-N(15) | 69.54(15) |
| C(17)-Co(1)-N(1) | 176.05(13) | C(21)-Co(2)-N(4) | 174.90(13) | N(5a)-Mn(1)-N(15) | 92.31(14) |
| C(15)-Co(1)-N(1) | 88.14(14) | C(22)-Co(2)-N(4) | 88.57(17) | N(9)-Mn(1)-N(15) | 88.34(14) |
| C(18)-Co(1)-N(1) | 91.15(14) | C(19)-Co(2)-N(4) | 92.33(13) | N(16)-Mn(1)-N(15) | 146.83(19) |
| N(2)-Co(1)-N(1) | 82.14(11) | N(3)-Co(2)-N(4) | 81.98(11) | N(14)-Mn(1)-N(15) | 139.35(19) |
| N(5)-C(15)-Co(1) | 174.9(3) | N(9)-C(19)-Co(2) | 176.4(3) | N(13)-Mn(1)-N(17) | 141.32(16) |
| N(6)-C(16)-Co(1) | 178.2(4) | N(10)-C(20)-Co(2) | 177.6(4) | N(5a)-Mn(1)-N(17) | 84.87(14) |
| N(7)-C(17)-Co(1) | 176.7(3) | N(11)-C(21)-Co(2) | 175.7(3) | N(9)-Mn(1)-N(17) | 91.90(13) |
| N(8)-C(18)-Co(1) | 178.9(4) | N(12)-C(22)-Co(2) | 178.0(5) | N(16)-Mn(1)-N(17) | 75.70(18) |
| C(15)-N(5)-Mn(1b) | 161.1(3) | C(19)-N(9)-Mn(1) | 159.0(3) | N(14)-Mn(1)-N(17) | 148.0(2) |
| | | | | N(15)-Mn(1)-N(17) | 72.26(17) |

[a]Symmetry codes: (a) = *x*, *y*-1, *z*; (b) *x*, *y*+1, *z*.