# Supporting Information for:

## Cyano-Bridged Terbium(III)–Chromium(III) Bimetallic Quasi-One-Dimensional Assembly Exhibiting Long-Range Magnetic Ordering

Yang Guo, Gong-Feng Xu, Chao Wang, Ting-Ting Cao, Jinkui Tang,* Zhan-Quan Liu, Yue Ma,* Shi-Ping Yan, Peng Cheng, Dai-Zheng Liao
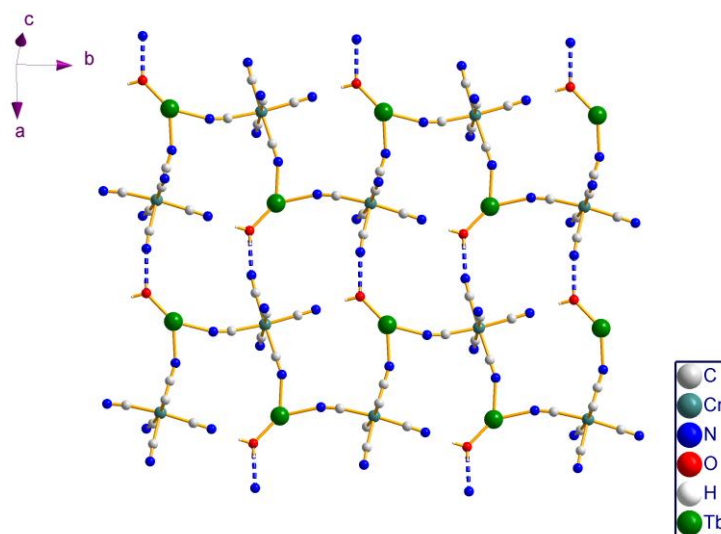


Figure S1. Weak interactions (O–H⋯N) between the 1D chains of **1** leading to 2D hydrogen-bonded network along *ab* plane.
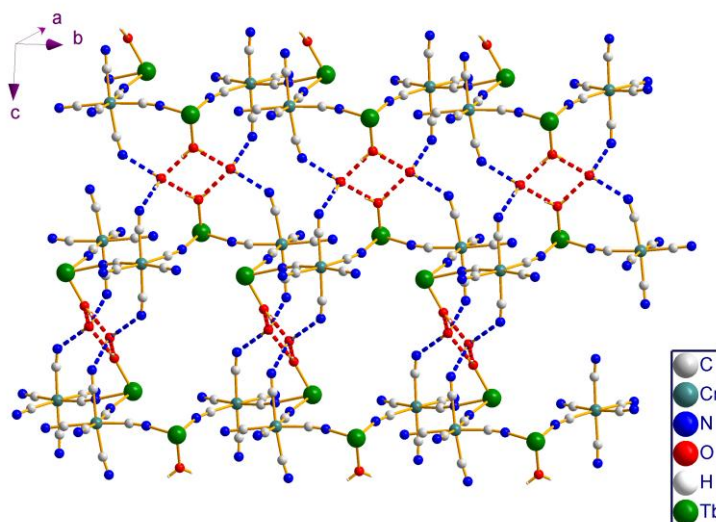


Figure S2. Weak interactions (O–H⋯N and O–H⋯O) between the 1D chains of **1** leading to 2D hydrogen-bonded network along *bc* plane.
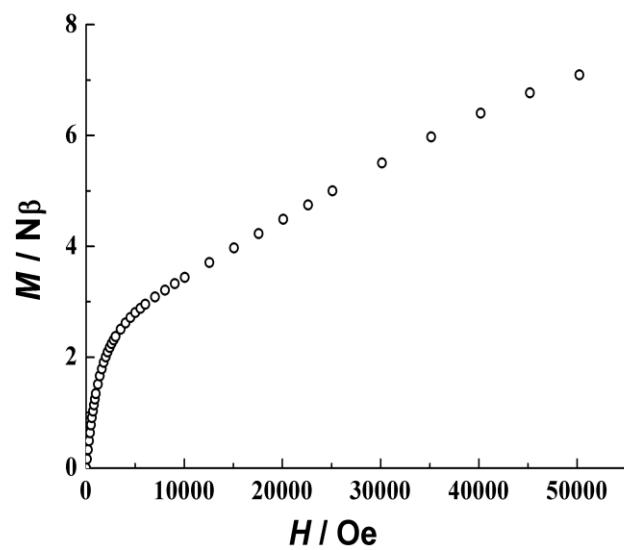
Figure S3. Magnetization versus magnetic field at 2 K for **1**.

Table S1. Selected Bond Lengths (Å) and Angles (deg) for **1**[a].

| | | | |
|---|---|---|---|
| O(1)-Tb(1) | 2.363(3) | O(2)-Tb(1) | 2.376(4) |
| O(3)-Tb(1) | 2.353(4) | O(4)-Tb(1) | 2.340(3) |
| O(5)-Tb(1) | 2.343(3) | O(6)-Tb(1) | 2.400(4) |
| N(6)-Tb(1)#1 | 2.515(4) | Tb(1)-N(6)#2 | 2.515(4) |
| N(1)-Tb(1) | 2.498(4) | | |
| C(1)-Cr(1) | 2.084(4) | C(2)-Cr(1) | 2.082(5) |
| C(3)-Cr(1) | 2.072(4) | C(4)-Cr(1) | 2.064(5) |
| C(5)-Cr(1) | 2.071(5) | C(6)-Cr(1) | 2.098(4) |
| O(1)-Tb(1)-N(1) | 144.64(12) | O(2)-Tb(1)-N(1) | 115.43(14) |
| O(3)-Tb(1)-N(1) | 72.72(14) | O(4)-Tb(1)-N(1) | 74.40(12) |
| O(5)-Tb(1)-N(1) | 138.85(11) | O(6)-Tb(1)-N(1) | 81.72(14) |
| O(1)-Tb(1)-N(6)#2 | 78.35(12) | O(2)-Tb(1)-N(6)#2 | 71.62(13) |
| O(3)-Tb(1)-N(6)#2 | 111.98(15) | O(4)-Tb(1)-N(6)#2 | 141.53(12) |
| O(5)-Tb(1)-N(6)#2 | 144.73(12) | O(6)-Tb(1)-N(6)#2 | 82.33(13) |
| O(1)-Tb(1)-O(2) | 76.69(13) | O(1)-Tb(1)-O(6) | 71.94(13) |
| O(2)-Tb(1)-O(6) | 142.55(13) | O(3)-Tb(1)-O(6) | 145.48(13) |
| O(3)-Tb(1)-O(1) | 140.10(13) | O(3)-Tb(1)-O(2) | 71.14(14) |
| O(4)-Tb(1)-O(1) | 116.39(12) | O(4)-Tb(1)-O(2) | 144.02(13) |
| O(4)-Tb(1)-O(5) | 71.74(12) | O(4)-Tb(1)-O(6) | 70.64(13) |
| O(4)-Tb(1)-O(3) | 80.25(14) | O(5)-Tb(1)-O(3) | 79.09(15) |
| O(5)-Tb(1)-O(1) | 73.36(12) | O(5)-Tb(1)-O(2) | 81.62(15) |
| O(5)-Tb(1)-O(6) | 107.79(16) | N(1)-Tb(1)-N(6)#2 | 75.05(12) |
| C(1)-N(1)-Tb(1) | 159.5(3) | C(6)-N(6)-Tb(1)#1 | 163.4(3) |
| N(1)-C(1)-Cr(1) | 174.7(4) | N(2)-C(2)-Cr(1) | 174.6(5) |
| N(3)-C(3)-Cr(1) | 176.5(4) | N(4)-C(4)-Cr(1) | 178.6(5) |
| N(5)-C(5)-Cr(1) | 171.8(5) | N(6)-C(6)-Cr(1) | 170.9(4) |
| C(1)-Cr(1)-C(6) | 94.29(16) | C(5)-Cr(1)-C(3) | 91.57(19) |
| C(2)-Cr(1)-C(1) | 84.98(19) | C(2)-Cr(1)-C(6) | 92.60(18) |
| C(3)-Cr(1)-C(2) | 90.71(19) | C(3)-Cr(1)-C(6) | 88.99(16) |
| C(4)-Cr(1)-C(1) | 89.29(17) | C(4)-Cr(1)-C(2) | 91.9(2) |
| C(4)-Cr(1)-C(3) | 87.77(18) | C(4)-Cr(1)-C(5) | 92.83(19) |
| C(5)-Cr(1)-C(1) | 92.99(19) | C(5)-Cr(1)-C(6) | 82.75(18) |

a. Symmetry transformations used to generate equivalent atoms: #1 -x+2, y-1/2, -z+3/2; #2 -x+2, y+1/2, -z+3/2.

Table S2. Interatomic Distances and Angles for the Hydrogen Bonds in **1** (Å and deg)[b].

| D–H···A | d(D–H) | d(H···A) | d(D···A) | <(DHA) |
|---|---|---|---|---|
| O5–H5A···N3#3 | 0.848 | 1.926 | 2.772 | 174.93 |
| O5–H5B···N4#1 | 0.849 | 1.916 | 2.763 | 175.28 |
| O6–H6A···O7#5 | 0.848 | 2.047 | 2.885 | 169.79 |
| O6–H6B···O7#4 | 0.851 | 1.973 | 2.811 | 167.86 |
| O7–H7A···N5#3 | 0.851 | 2.055 | 2.907 | 179.25 |
| O7–H7B···N2#6 | 0.846 | 2.036 | 2.875 | 171.38 |

b. Symmetry transformations used to generate equivalent atoms: #1 -x+2, y-1/2, -z+3/2; #2 -x+2, y+1/2, -z+3/2; #3 x-1, y, z; #4 -x+1, y+1/2, -z+3/2; #5 x+1, -y+3/2, z+1/2; #6 x-1, -y+3/2, z-1/2.