Supplementary Materials: The Exploration and Analysis of the Magnetic Relaxation Behavior in Three Isostructural Cyano-Bridged 3d−4f Linear Heterotrinuclear Compounds

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

|  |  |  |  |
| --- | --- | --- | --- |
| **1** | | | |
| Y(1)−N(1)#1 | 2.353(11) | Fe(1)−C(3) | 1.963(10) |
| Y(1)−N(1) | 2.353(11) | Fe(1)−C(3)#3 | 1.963(10) |
| Y(1)−O(1) | 2.208(11) | Fe(1)−C(3)#6 | 1.963(10) |
| Fe(1)−C(1) | 1.915(13) | Fe(1)−C(3)#7 | 1.963(10) |
| Fe(1)−C(2) | 1.922(13) |  |  |
|  |  |  |  |
| N(1)−Y(1)−N(1)#1 | 180 | O1#3−Y1−O1#7 | 89.92(45) |
| O1−Y(1)−O1#6 | 89.92(45) | O(1)−Y(1)−N(1) | 88.0(8) |
| O1#6−Y1−O1#7 | 89.92(45) | O(1)−Y(1)−N(1)#1 | 92.0(8) |
| O1−Y1−O1#3 | 89.92(45) |  |  |
|  |  |  |  |
| C(1)−Fe(1)−C(2) | 180 | C(3)#7−Fe(1)−C(3) | 178.3(5) |
| C(1)−Fe(1)−C(3) | 89.1(2) | C(3)#3−Fe(1)−C(3)#6 | 178.3(5) |
| C(1)−Fe(1)−C(3)#3 | 89.1(2) | C(3)#3−Fe(1)−C(3) | 89.987(8) |
| C(1)−Fe(1)−C(3)#6 | 89.1(2) | C(3)#6−Fe(1)−C(3) | 89.987(8) |
| C(1)−Fe(1)−C(3)#7 | 89.1(2) | C(3)#7−Fe(1)−C(3)#3 | 89.987(8) |
| C(2)−Fe(1)−C(3) | 90.9(2) | C(3)#7−Fe(1)−C(3)#6 | 89.987(8) |
| C(2)−Fe(1)−C(3)#3 | 90.9(2) |  |  |
| C(2)−Fe(1)−C(3)#6 | 90.9(2) |  |  |
| C(2)−Fe(1)−C(3)#7 | 90.9(2) |  |  |

Symmetry codes: #1 −x, −y, −z; #3 −y, x, z; #6 y, −x, z; #7 −x, −y, z.

**Table S2.** Hydrogen bonding geometry for **1**: lengths (Å) and angles (°).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| D−H···A | d(D−H) | d(H···A) | d(D···A) | <(DHA) |
| N(2)−H(2)···N(2)#13 | 0.85 | 1.72 | 2.57(2) | 180 |
| O(2)−H(2A)···N(3) | 0.85 | 1.85 | 2.70(3) | 179.6 |
| O(2)−H(2A)···N(3)#2 | 0.85 | 2.10 | 2.91(3) | 159.0 |
| O(2)−H(2B)···N(3)#9 | 0.85 | 2.12 | 2.92(3) | 158.3 |
| O(2)−H(2B)···N(3)#10 | 0.85 | 1.84 | 2.68(32) | 179.3 |

Symmetry codes: #2 −x, y, z; #9 −y+1/2, x+1/2, −z+1/2; #10 −y+1/2, −x+1/2, −z+1/2; #13 −x, −y, −z+1.

**Table S3.** Selected bond lengths (Å) and angles (°) for **2**.

|  |  |  |  |
| --- | --- | --- | --- |
| **2** | | | |
| Dy(1)−N(1)#1 | 2.372(13) | Fe(1)−C(3) | 1.946(10) |
| Dy(1)−N(1) | 2.372(13) | Fe(1)−C(3)#3 | 1.946(10) |
| Dy(1)−O(1) | 2.244(11) | Fe(1)−C(3)#4 | 1.946(10) |
| Fe(1)−C(1) | 1.904(15) | Fe(1)−C(3)#5 | 1.946(10) |
| Fe(1)−C(2) | 1.906(14) |  |  |
|  |  |  |  |
| N(1)−Dy(1)−N(1)#1 | 180 | O1#4−Dy1−O1#5 | 89.98(44) |
| O1−Dy(1)−O1#3 | 89.98(44) | O(1)−Dy(1)−N(1) | 89.20(70) |
| O1#3−Dy1−O1#5 | 89.98(44) | O(1)−Dy(1)−N(1)#1 | 90.80(70) |
| O1−Dy1−O1#4 | 89.98(44) |  |  |
|  |  |  |  |
| C(1)−Fe(1)−C(2) | 180 | C(3)#5−Fe(1)−C(3) | 178.3(5) |
| C(1)−Fe(1)−C(3) | 89.20(30) | C(3)#4−Fe(1)−C(3)#3 | 178.3(5) |
| C(1)−Fe(1)−C(3)#3 | 89.20(30) | C(3)#3−Fe(1)−C(3) | 89.987(8) |
| C(1)−Fe(1)−C(3)#4 | 89.20(30) | C(3)#4−Fe(1)−C(3) | 89.989(8) |
| C(1)−Fe(1)−C(3)#5 | 89.20(30) | C(3)#5−Fe(1)−C(3)#4 | 89.988(8) |
| C(2)−Fe(1)−C(3) | 90.80(30) | C(3)#5−Fe(1)−C(3)#3 | 89.988(8) |
| C(2)−Fe(1)−C(3)#3 | 90.80(30) |  |  |
| C(2)−Fe(1)−C(3)#4 | 90.80(30) |  |  |
| C(2)−Fe(1)−C(3)#5 | 90.80(30) |  |  |

Symmetry codes: #1 −x, −y, −z; #3 y, −x, z; #4 −y, x, z; #5 −x, −y, z.

**Table S4.** Hydrogen bonding geometry for **2**: lengths (Å) and angles (°).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| D−H···A | d(D−H) | d(H···A) | d(D···A) | <(DHA) |
| N(2)−H(2)···N(2)#13 | 0.86 | 1.69 | 2.54(3) | 180 |
| O(2)−H(2A)···N(3) | 0.85 | 1.86 | 2.70(2) | 179.3 |
| O(2)−H(2A)···N(3)#2 | 0.85 | 2.10 | 2.91(3) | 159.0 |
| O(2)−H(2B)···N(3)#11 | 0.85 | 2.10 | 2.91(3) | 158.4 |
| O(2)−H(2B)···N(3)#10 | 0.85 | 1.83 | 2.68(3) | 178.7 |

Symmetry codes: #2 −x, y, z; #10 −y+1/2, −x+1/2, −z+1/2; #11 −y+1/2, x+1/2, −z+1/2; #13 −x, −y, −z+1.

**Table S5.** Selected bond lengths (Å) and angles (°) for **3**.

|  |  |  |  |
| --- | --- | --- | --- |
| **3** | | | |
| Dy(1)−N(1) | 2.380(12) | Co(1)−C(3) | 1.904(10) |
| Dy(1)−N(1)#1 | 2.380(12) | Co(1)−C(3)#2 | 1.904(10) |
| Dy(1)−O(1) | 2.235(11) | Co(1)−C(3)#3 | 1.904(10) |
| Co(1)−C(1) | 1.860(13) | Co(1)−C(3)#4 | 1.904(10) |
| Co(1)−C(2) | 1.869(13) |  |  |
|  |  |  |  |
| N(1)#1−Dy(1)−N(1) | 180 | O1#3−Dy1−O1#4 | 89.969(1) |
| O1−Dy(1)−O1#2 | 89.969(1) | O(1)−Dy(1)−N(1)#1 | 90.7(7) |
| O1#2−Dy1−O1#4 | 89.969(1) | O(1)−Dy(1)−N(1) | 89.3(7) |
| O1−Dy1−O1#3 | 89.969(1) |  |  |
|  |  |  |  |
| C(1)−Co(1)−C(2) | 180 | C(3)−Co(1)−C(3)#4 | 178.2(5) |
| C(1)−Co(1)−C(3) | 89.1(3) | C(3)#3−Co(1)−C(3)#2 | 178.2(5) |
| C(1)−Co(1)−C(3)#2 | 89.1(3) | C(3)−Co(1)−C(3)#2 | 89.986(9) |
| C(1)−Co(1)−C(3)#3 | 89.1(3) | C(3)−Co(1)−C(3)#3 | 89.985(8) |
| C(1)−Co(1)−C(3)#4 | 89.1(3) | C(3)#4−Co(1)−C(3)#2 | 89.986(8) |
| C(2)−Co(1)−C(3) | 90.9(3) | C(3)#4−Co(1)−C(3)#3 | 89.986(9) |
| C(2)−Co(1)−C(3)#2 | 90.9(3) |  |  |
| C(2)−Co(1)−C(3)#3 | 90.9(3) |  |  |
| C(2)−Co(1)−C(3)#4 | 90.9(3) |  |  |

Symmetry codes: #1 −x, −y, −z; #2 y, −x, z; #3 −y, x, z; #4 −x, −y, z.

**Table S6.** Hydrogen bonding geometry for **3**: lengths (Å) and angles (°).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| D−H···A | d(D−H) | d(H···A) | d(D···A) | <(DHA) |
| N(2)−H(2)···N(2)#13 | 0.85 | 1.71 | 2.56(2) | 180 |
| O(2)−H(2A)···N(3) | 0.85 | 1.83 | 2.68(4) | 179.2 |
| O(2)−H(2A)···N(3)#7 | 0.85 | 2.09 | 2.90(4) | 158.6 |
| O(2)−H(2B)···N(3)#9 | 0.85 | 2.15 | 2.95(4) | 157.8 |
| O(2)−H(2B)···N(3)#10 | 0.85 | 1.86 | 2.71(4) | 178.3 |

Symmetry codes: #7 −x, y, z ; #9 −y+1/2, x+1/2, −z+1/2 ; #10 −y+1/2, −x+1/2, −z+1/2 ; #13 −x, −y, −z+1.

**Table S7.** Continuous shaped measures (CShM) for **1**−**3** using SHAPE 2.1.

|  |  |  |  |
| --- | --- | --- | --- |
|  | **1** | **2** | **3** |
| HP-6 | 33.391 | 33.363 | 33.374 |
| PPY-6 | 30.016 | 30.116 | 30.072 |
| OC-6 | 0.131 | 0.079 | 0.105 |
| TPR-6 | 16.841 | 16.800 | 16.822 |
| JPPY-5 | 33.446 | 33.556 | 33.490 |

|  |  |
| --- | --- |
| HP-6 = (D6h) Hexagon | TPR-6 = (D3h) Trigonal prism |
| PPY-6 = (C5v) Pentagonal pyramid | JPPY-5 = (C5v) Johnson pentagonal pyramid (J2) |
| OC-6 = (Oh) Octahedron |  |



**Figure S1.** The disorder in the molecular structure of compound **2**.



**Figure S2.** Powder X-ray diffraction patterns of compound **1** for the as-synthesized samples and the simulated one.



**Figure S3.** Powder X-ray diffraction patterns of compound **2** for the as-synthesized samples and the simulated one.



**Figure S4.** Powder X-ray diffraction patterns of compound **3** for the as-synthesized samples and the simulated one.



**Figure S5.** Field dependence of the magnetization at the temperatures of 2 K, 3 K, 5 K, 10 K and 15 K for a polycrystalline sample of **1**.



**Figure S6.** Plots of the reduced magnetization *M*vs *H*/*T*at the temperatures of 2 K, 3 K, 5 K, 10 K and 15 K for a polycrystalline sample of **1**.



**Figure S7.** Field dependence of the magnetization at the temperatures of 2 K, 3 K, 5 K, 10 K and 15 K for a polycrystalline sample of **3**.



**Figure S8.** Plots of the reduced magnetization *M*vs *H*/*T*at the temperatures of 2 K, 3 K, 5 K, 10 K and 15 K for a polycrystalline sample of **3**.



**Figure S9.** Field dependence of the in-phase (*χ*', inset) and out-of-phase (*χ''*) ac susceptibilities for **2** with *f* = 10, 100 and 999 Hz.



**Figure S10.** Field dependence of the in-phase (*χ*', inset) and out-of-phase (*χ''*) ac susceptibilities for **3** with *f* = 10, 100 and 999 Hz.



**Figure S11.** Temperature dependence of the in-phase (*χ*') and out-of-phase (*χ''*) ac susceptibilities for **3** under a 3 kOe dc field.