

**Supplementary data B for**  
**[Cu<sub>2</sub>(dpyam)<sub>2</sub>(μ-C<sub>2</sub>O<sub>4</sub>)(CF<sub>3</sub>SO<sub>3</sub>)<sub>2</sub>]<sub>n</sub> (II)**

**Table B1** Atomic Coordinates [ $\times 10^4$ ] and equivalent isotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for complex **II**. U(eq) is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor

|       | <b>x</b>   | <b>y</b>  | <b>z</b>    | <b>U(eq)</b> |
|-------|------------|-----------|-------------|--------------|
| Cu(1) | 6855.1(3)  | 2664(4)   | 1103.53(13) | 24.37(13)    |
| S(1)  | 7579.3(7)  | 5076.4(8) | 1034.6(3)   | 29.81(17)    |
| F(1)  | 8082.(3)   | 3910(3)   | -73.1(10)   | 72.3(6)      |
| F(2)  | 6472(3)    | 5953(4)   | -168.2(9)   | 78.5(7)      |
| F(3)  | 8625(2)    | 6684(3)   | 138.6(11)   | 73.8(7)      |
| O(1)  | 6824.8(19) | 147(2)    | 154.4(9)    | 28(4)        |
| O(2)  | 4759.3(19) | 23(2)     | 795.6(9)    | 29.4(4)      |
| O(3)  | 6630(2)    | 3562(3)   | 1011.4(11)  | 45.9(5)      |
| O(4)  | 7019(2)    | 6763(3)   | 1213.5(10)  | 48.6(5)      |
| O(5)  | 9019(3)    | 4686(4)   | 1348.8(13)  | 61.5(7)      |
| N(1)  | 8943(2)    | 162(3)    | 1360.2(11)  | 24(4)        |
| N(2)  | 6684(2)    | 472(3)    | 2020.1(10)  | 23.8(4)      |
| N(3)  | 8970(2)    | -681(3)   | 2454.9(10)  | 33(5)        |
| C(1)  | 9702(3)    | 491(4)    | 892.7(13)   | 32.6(5)      |
| C(2)  | 11133(3)   | 208(4)    | 990(15)     | 36.9(6)      |
| C(3)  | 11843(3)   | -442(4)   | 1590.1(15)  | 37.9(6)      |
| C(4)  | 11111(3)   | -728(4)   | 2074.5(13)  | 35.6(6)      |
| C(5)  | 9658(3)    | -402(3)   | 1944.7(12)  | 26.6(5)      |
| C(6)  | 7668(3)    | -120(3)   | 2532.8(12)  | 25.8(5)      |
| C(7)  | 7397(3)    | -173(4)   | 164.6(13)   | 33.7(6)      |
| C(8)  | 6132(3)    | 459(4)    | 3268.2(13)  | 38.8(6)      |
| C(9)  | 5142(3)    | 1150(4)   | 2743.4(12)  | 34.3(6)      |
| C(10) | 5455(2)    | 1140(3)   | 2140.1(11)  | 29.9(5)      |
| C(11) | 5614(3)    | 38(3)     | -184.1(12)  | 22.8(5)      |
| C(12) | 7688(4)    | 5414(4)   | 187.7(15)   | 43.3(7)      |

**Table B2** Bond lengths [Å] for [Cu<sub>2</sub>(dpyam)<sub>2</sub>(μ-C<sub>2</sub>O<sub>4</sub>)(CF<sub>3</sub>SO<sub>3</sub>)<sub>2</sub>]<sub>n</sub> **II**

|                           |            |             |          |
|---------------------------|------------|-------------|----------|
| Cu(1)-N(2)                | 1.970(2)   | N(1)-C(5)   | 1.338(3) |
| Cu(1)-N(1)                | 1.977(2)   | N(1)-C(1)   | 1.366(3) |
| Cu(1)-O(1)                | 1.9859(18) | N(2)-C(6)   | 1.347(3) |
| Cu(1)-O(2)                | 1.9987(18) | N(2)-C(10)  | 1.359(3) |
| S(1)-O(5)                 | 1.436(3)   | N(3)-C(6)   | 1.368(3) |
| S(1)-O(4)                 | 1.438(2)   | N(3)-C(5)   | 1.390(3) |
| S(1)-O(3)                 | 1.440(2)   | C(1)-C(2)   | 1.371(4) |
| S(1)-C(12)                | 1.818(3)   | C(2)-C(3)   | 1.384(4) |
| F(1)-C(12)                | 1.328(3)   | C(3)-C(4)   | 1.373(4) |
| F(2)-C(12)                | 1.312(4)   | C(4)-C(5)   | 1.394(3) |
| F(3)-C(12)                | 1.322(4)   | N(3)-H(5)   | 0.6930   |
| O(1)-C(11)                | 1.235(3)   | C(1)-H(1)   | 0.9300   |
| O(2)-C(11) <sup>i</sup>   | 1.256(3)   | C(2)-H(2)   | 0.9300   |
| C(6)-C(7)                 | 1.405(4)   | C(4)-H(4)   | 0.9300   |
| C(7)-C(8)                 | 1.369(4)   | C(3)-H(3)   | 0.9300   |
| C(8)-C(9)                 | 1.391(4)   | C(8)-H(8)   | 0.9300   |
| C(9)-C(10)                | 1.362(3)   | C(7)-H(7)   | 0.9300   |
| C(11) <sup>i</sup> -O(2)  | 1.256(3)   | C(9)-H(9)   | 0.9300   |
| C(11) <sup>i</sup> -C(11) | 1.549(5)   | C(10)-H(10) | 0.9300   |
| Cu(1)-Cu(1) <sup>i</sup>  | 5.228(3)   |             |          |

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<sup>i</sup> [1-x,-y,-z]

**Table B3** Bond angle [°] for [Cu<sub>2</sub>(dpyam)<sub>2</sub>(μ-C<sub>2</sub>O<sub>4</sub>)(CF<sub>3</sub>SO<sub>3</sub>)<sub>2</sub>]<sub>n</sub> **II**

|                                |            |                                             |          |
|--------------------------------|------------|---------------------------------------------|----------|
| N(2)-Cu(1)-N(1)                | 91.80(9)   | N(1)-C(1)-C(2)                              | 123.1(3) |
| N(2)-Cu(1)-O(1)                | 174.16(8)  | C(1)-C(2)-C(3)                              | 118.5(3) |
| N(1)-Cu(1)-O(1)                | 93.80(8)   | C(4)-C(3)-C(2)                              | 119.5(2) |
| N(2)-Cu(1)-O(2)                | 91.79(8)   | C(3)-C(4)-C(5)                              | 119.1(2) |
| N(1)-Cu(1)-O(2)                | 172.02(8)  | N(1)-C(5)-N(3)                              | 120.8(2) |
| O(1)-Cu(1)-O(2)                | 82.86(7)   | N(1)-C(5)-C(4)                              | 122.3(2) |
| O(5)-S(1)-O(4)                 | 115.84(15) | C(6)-N(3)-H(5)                              | 112.7    |
| O(5)-S(1)-O(3)                 | 114.07(14) | C(5)-N(3)-H(5)                              | 113.7    |
| O(4)-S(1)-O(3)                 | 114.03(13) | N(1)-C(1)-H(1)                              | 118.4    |
| O(5)-S(1)-C(12)                | 102.86(17) | C(2)-C(1)-H(1)                              | 118.4    |
| O(4)-S(1)-C(12)                | 103.87(13) | C(1)-C(2)-H(2)                              | 120.8    |
| O(3)-S(1)-C(12)                | 104.07(14) | C(3)-C(2)-H(2)                              | 120.8    |
| C(11)-O(1)-Cu(1)               | 112.80(16) | C(4)-C(3)-H(3)                              | 120.3    |
| C(11) <sup>i</sup> -O(2)-Cu(1) | 112.50(16) | C(2)-C(3)-H(3)                              | 120.3    |
| C(5)-N(1)-C(1)                 | 117.5(2)   | C(3)-C(4)-H(4)                              | 120.4    |
| C(5)-N(1)-Cu(1)                | 123.96(17) | C(5)-C(4)-H(4)                              | 120.4    |
| C(1)-N(1)-Cu(1)                | 118.15(17) | N(3)-C(5)-C(4)                              | 116.9(2) |
| C(6)-N(2)-C(10)                | 117.8(2)   | N(2)-C(6)-N(3)                              | 120.9(2) |
| C(6)-N(2)-Cu(1)                | 124.16(17) | N(2)-C(6)-C(7)                              | 121.3(2) |
| C(10)-N(2)-Cu(1)               | 117.90(16) | N(3)-C(6)-C(7)                              | 117.8(2) |
| C(6)-N(3)-C(5)                 | 130.6(2)   | C(8)-C(7)-C(6)                              | 119.6(3) |
| C(8)-C(7)-H(7)                 | 120.2      | N(2)-C(10)-H(10)                            | 118.3    |
| C(6)-C(7)-H(7)                 | 120.2      | O(1)-C(11)-O(2) <sup>i</sup>                | 128.2(2) |
| C(7)-C(8)-C(9)                 | 119.1(2)   | O(1)-C(11)-C(11) <sup>i</sup>               | 116.7(3) |
| C(7)-C(8)-H(8)                 | 120.5      | O(2) <sup>i</sup> -C(11)-C(11) <sup>i</sup> | 115.1(3) |
| C(9)-C(8)-H(8)                 | 120.5      | F(2)-C(12)-F(3)                             | 106.7(3) |
| C(10)-C(9)-C(8)                | 118.7(2)   | F(2)-C(12)-F(1)                             | 108.6(3) |
| C(10)-C(9)-H(9)                | 120.6      | F(3)-C(12)-F(1)                             | 107.4(3) |
| C(8)-C(9)-H(9)                 | 120.6      | F(2)-C(12)-S(1)                             | 111.4(2) |
| C(9)-C(10)-N(2)                | 123.4(2)   | F(3)-C(12)-S(1)                             | 110.9(2) |
| C(9)-C(10)-H(10)               | 118.3      | F(1)-C(12)-S(1)                             | 111.7(2) |

<sup>i</sup> [1-x,-y,-z]

**Table B4** Anisotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for complex **II**.  
The anisotropic displacement factor exponent takes the form:  
 $-2\pi^2[(ha^*)^2 U_{11} + \dots + 2hka^*b^*U_{12}]$

|       | <b>U11</b> | <b>U22</b> | <b>U33</b> | <b>U23</b> | <b>U13</b> | <b>U12</b> |
|-------|------------|------------|------------|------------|------------|------------|
| Cu(1) | 15.47(19)  | 40.7(2)    | 15.95(19)  | -0.22(10)  | 1.1(12)    | 0.34(10)   |
| S(1)  | 30.5(4)    | 35.4(3)    | 22.7(3)    | 0.8(2)     | 3.8(3)     | -1.4(2)    |
| F(1)  | 122.2(19)  | 56.4(12)   | 46.5(11)   | -4.8(10)   | 36.4(12)   | 18.7(12)   |
| F(2)  | 91.3(16)   | 92.2(17)   | 37.8(11)   | 6.2(11)    | -18.2(10)  | 21.5(14)   |
| F(3)  | 95.7(16)   | 61.6(13)   | 79.1(16)   | 16.2(11)   | 52.4(13)   | -7.6(11)   |
| O(1)  | 15.8(8)    | 48.7(10)   | 19.1(9)    | -2.4(7)    | 2.6(7)     | -1(6)      |
| O(2)  | 20.5(9)    | 49.9(11)   | 17.1(8)    | -1.6(7)    | 2.7(7)     | -0.9(7)    |
| O(3)  | 46.8(11)   | 36.0(11)   | 58.2(13)   | 6.5(9)     | 18.5(10)   | -2.5(9)    |
| O(4)  | 66.8(14)   | 37.4(11)   | 49.5(13)   | -7.6(9)    | 30(11)     | -6.7(9)    |
| O(5)  | 38.5(14)   | 97(2)      | 41.7(14)   | 5.6(12)    | -6.9(11)   | 5.8(11)    |
| N(1)  | 16.1(10)   | 30.3(10)   | 24.2(11)   | 0.8(7)     | 1.1(8)     | -0.7(7)    |
| N(2)  | 21.2(9)    | 31.4(10)   | 17.7(9)    | -0.3(7)    | 1.9(7)     | -0.6(7)    |
| N(3)  | 24.8(10)   | 51.3(13)   | 19.8(10)   | 8.2(9)     | -2.0(8)    | 7.4(9)     |
| C(1)  | 23 (12)    | 45.5(14)   | 29.3(13)   | 4.6(11)    | 5.3(10)    | -2.6(10)   |
| C(2)  | 24.2(13)   | 50.5(16)   | 37.3(15)   | -1.0(11)   | 97.(11)    | -3.9(10)   |
| C(3)  | 18.8(12)   | 49.5(16)   | 44.5(16)   | -4.5(12)   | 4.9(11)    | 2.8(10)    |
| C(4)  | 23.5(12)   | 46.8(15)   | 32.2(13)   | 0.8(11)    | -4.0(10)   | 3.7(11)    |
| C(5)  | 22 (12)    | 29.4(12)   | 27.3(12)   | -1.5(9)    | 3.1(9)     | -0.2(8)    |
| C(6)  | 25(12)     | 31(12)     | 19.6(12)   | 0.8(8)     | 1.4(9)     | -2.1(8)    |
| C(7)  | 34(15)     | 52.3(16)   | 22.1(13)   | 6.6(10)    | 0.2(11)    | -1.1(11)   |
| C(8)  | 40(16)     | 56.2(17)   | 22.2(12)   | 0.5(11)    | 11.1(11)   | -1.8(12)   |
| C(9)  | 30.2(12)   | 46.8(15)   | 28.3(12)   | -4.4(11)   | 11.4(10)   | 2.7(11)    |
| C(10) | 27.8(12)   | 38.5(13)   | 22.9(11)   | -1.4(10)   | 4.1(9)     | 4.7(10)    |
| C(11) | 19.3(11)   | 27.5(10)   | 21.5(12)   | 0.9(8)     | 4.3(9)     | 1.1(8)     |
| C(12) | 60(2)      | 41.9(16)   | 29(15)     | 1.6(11)    | 12.4(14)   | 2.9(13)    |

**Table B5** Hydrogen coordinates [ $\times 10^4$ ] and isotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for  $[\text{Cu}_2(\text{dpyam})_2(\mu\text{-C}_2\text{O}_4)(\text{CF}_3\text{SO}_3)_2]_n$  **II**

|      | <b>x</b> | <b>y</b>  | <b>z</b>   | <b>U(eq)</b> |
|------|----------|-----------|------------|--------------|
| H(1) | 0.917(3) | 0.099(4)  | 0.0479(15) | 0.038(8)     |
| H(2) | 1.158(4) | 0.049(5)  | 0.0663(17) | 0.044(9)     |
| H(3) | 1.280(4) | -0.064(4) | 0.1661(16) | 0.042(9)     |
| H(4) | 1.152(3) | -0.122(4) | 0.2477(16) | 0.042(8)     |
| H(5) | 0.942(3) | -0.090(4) | 0.2745(15) | 0.028(8)     |
| H(6) | 0.811(4) | -0.064(5) | 0.3487(19) | 0.055(10)    |
| H(7) | 0.601(4) | 0.044(4)  | 0.3640(18) | 0.038(9)     |
| H(8) | 0.434(3) | 0.160(4)  | 0.2806(13) | 0.029(7)     |
| H(9) | 0.485(3) | 0.159(4)  | 0.1777(16) | 0.040(8)     |