

## Supplementary Material 1

**Table 3**

Occupation and Temperature B factors for the atoms composing the trinuclear copper cluster moiety for both molecules A and B

<i>Atom</i>	<i>Occupancy</i>	<i>B Factors (Å<sup>2</sup>)</i>
<b>Molecule A</b>		
Cu1A	0.75	19.18
Cu2A	0.5	19.78
Cu3(a)A	0.75	22.30
Cu3(b)A	0.75	21.25
OH O1	0.75	21.79
Oxo O2	0.5	26.72
<b>Molecule B</b>		
Cu1B	0.75	24.22
Cu2B	0.5	23.87
Cu3(a)B	0.75	26.90
Cu3(b)B	0.75	24.14
Per O1	0.75	33.73
Per O2	0.75	23.57