

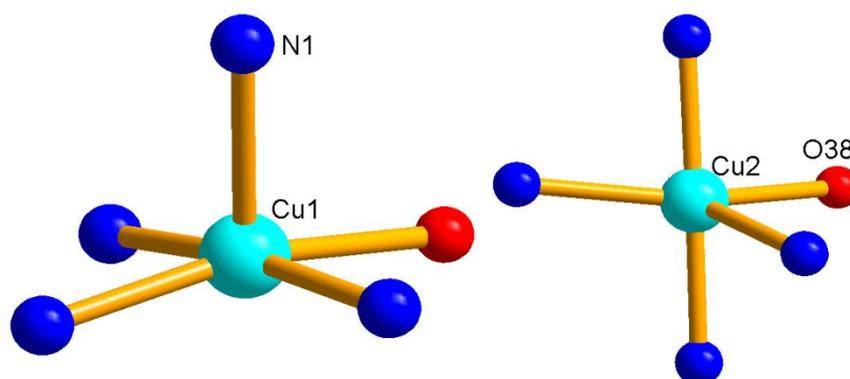
## Supporting information

# Synthesis and antibacterial activity of polyoxometalates with different structures

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Table S1 W-O bond lengths (Å)

| Bond   | Length    | Bond    | Length    | Bond    | Length    | Bond    | Length    |
|--------|-----------|---------|-----------|---------|-----------|---------|-----------|
| W1 O34 | 1.722(8)  | W2 O32  | 1.698(9)  | W3 O17  | 1.710(9)  | W4 O30  | 1.712(9)  |
| W1 O13 | 1.847(9)  | W2 O1   | 1.865(10) | W3 O23  | 1.896(8)  | W4 O19  | 1.911(8)  |
| W1 O14 | 1.917(9)  | W2 O10  | 1.893(8)  | W3 O12  | 1.921(10) | W4 O21  | 1.915(8)  |
| W1 O11 | 1.936(10) | W2 O2   | 1.942(10) | W3 O6   | 1.945(9)  | W4 O11  | 1.920(9)  |
| W1 O38 | 2.010(8)  | W2 O27  | 2.007(8)  | W3 O38  | 1.949(8)  | W4 O12  | 1.933(9)  |
| W1 O35 | 2.210(8)  | W2 O24  | 2.284(8)  | W3 O35  | 2.271(8)  | W4 O35  | 2.392(9)  |
| W5 O7  | 1.740(10) | W6 O33  | 1.704(10) | W7 O37  | 1.683(8)  | W8 O8   | 1.709(9)  |
| W5 O25 | 1.883(8)  | W6 O19  | 1.892(8)  | W7 O6   | 1.869(8)  | W8 O3   | 1.883(9)  |
| W5 O2  | 1.896(8)  | W6 O15  | 1.898(9)  | W7 O18  | 1.880(10) | W8 O16  | 1.901(9)  |
| W5 O21 | 1.906(8)  | W6 O26  | 1.906(8)  | W7 O15  | 1.939(10) | W8 O1   | 1.938(10) |
| W5 O22 | 1.956(9)  | W6 O25  | 1.942(8)  | W7 O29  | 2.077(8)  | W8 O39  | 1.959(9)  |
| W5 O24 | 2.221(9)  | W6 O40  | 2.396(9)  | W7 O40  | 2.226(8)  | W8 O20  | 2.299(8)  |
| W9 O4  | 1.698(10) | W10 O31 | 1.710(9)  | W11 O36 | 1.709(9)  | W12 O5  | 1.709(8)  |
| W9 O9  | 1.915(8)  | W10 O39 | 1.891(8)  | W11 O22 | 1.888(11) | W12 O27 | 1.807(9)  |
| W9 O18 | 1.934(9)  | W10 O28 | 1.907(10) | W11 O14 | 1.893(8)  | W12 O16 | 1.902(9)  |
| W9 O23 | 1.934(8)  | W10 O9  | 1.932(9)  | W11 O28 | 1.913(10) | W12 O26 | 1.933(9)  |
| W9 O3  | 1.951(8)  | W10 O13 | 1.966(8)  | W11 O10 | 1.950(8)  | W12 O29 | 2.112(8)  |
| W9 O20 | 2.207(9)  | W10 O20 | 2.338(8)  | W11 O24 | 2.311(8)  | W12 O40 | 2.174(7)  |



FigS1 Coordination geometries of Cu ions

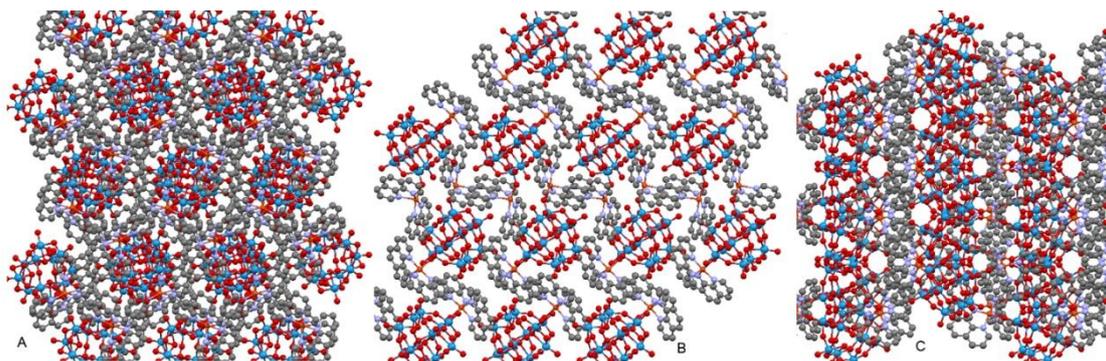


Fig S2 Stacking representation of **1** from three directions of (A) *a*-axis, (B) *b*-axis and (C) *c*-axis

Table S2 CH...O hydrogen bonds in **1**

| D-H      | <i>d</i> (D-H) | <i>d</i> (H...A) | <DHA   | <i>d</i> (D...A) | A  |
|----------|----------------|------------------|--------|------------------|--|
| C10-H10A | 0.930          | 2.335            | 154.31 | 3.199            | O39 [ <i>x</i> , - <i>y</i> +3/2, <i>z</i> -1/2 ]  |
| C22-H22A | 0.930          | 2.325            | 145.04 | 3.132            | O4 [ - <i>x</i> +1, - <i>y</i> +2, - <i>z</i> +1 ] |
| C22-H22A | 0.930          | 2.512            | 130.61 | 3.196            | O9 [ - <i>x</i> +1, - <i>y</i> +2, - <i>z</i> +1 ] |
| C23-H23A | 0.930          | 2.571            | 110.75 | 3.028            | O7   |

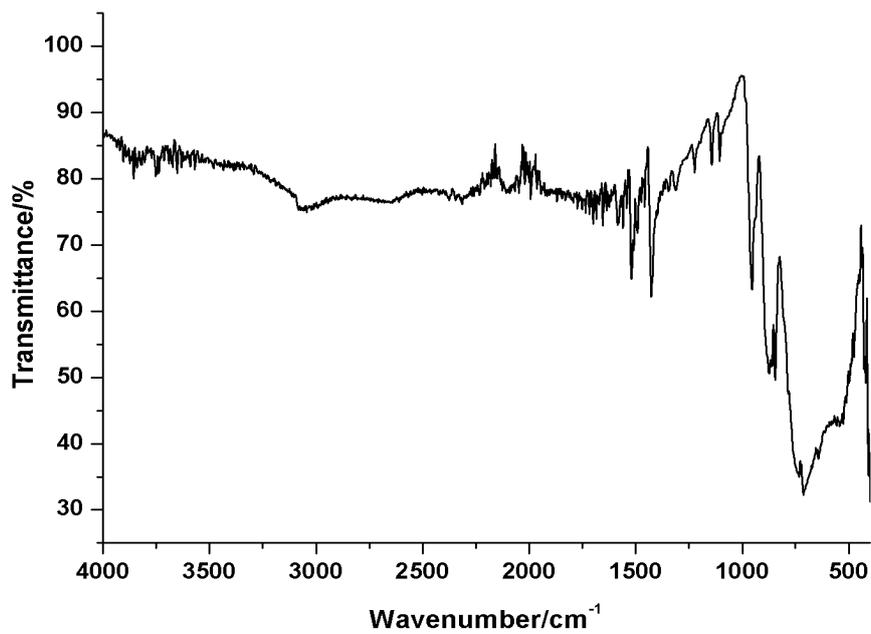


Fig S3 IR spectrum of **1**

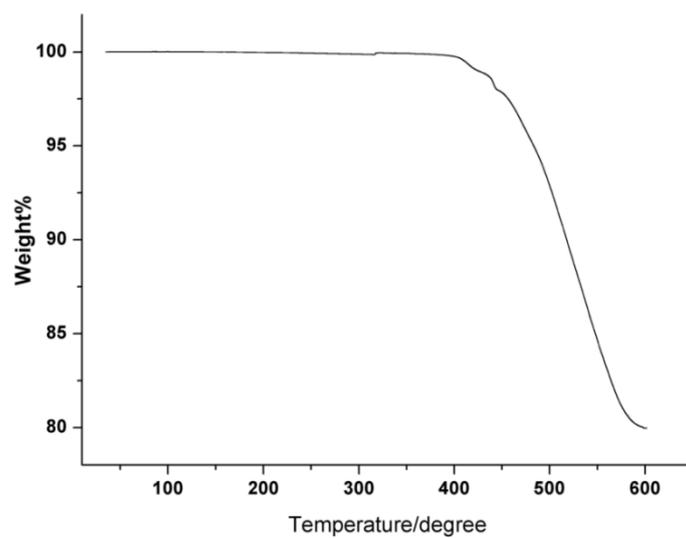


Fig S4 TG plot of **1** in 0-600 °C