

## Electronic Supplementary Information (ESI)

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# Novel intercluster compound between heptakis{triphenylphosphinegold(I)}dioxonium cation and $\alpha$ -Keggin polyoxometalate anion

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**Table S1** Bond lengths (Å) of the Keggin polyoxoanion in **1**

**Table S1** Bond lengths (Å) around the Keggin polyoxoanion in **1**

| W–O <sub>t</sub> (O <sub>t</sub> : terminal oxygen)       |          |             |          |
|---|----------|-------------|----------|
| W(1)–O(3)   | 1.682(8) | W(7)–O(9)   | 1.714(8) |
| W(2)–O(4)   | 1.689(7) | W(8)–O(10)  | 1.702(8) |
| W(3)–O(5)   | 1.698(7) | W(9)–O(11)  | 1.699(7) |
| W(4)–O(6)   | 1.708(7) | W(10)–O(12) | 1.711(7) |
| W(5)–O(7)   | 1.704(8) | W(11)–O(13) | 1.724(7) |
| W(6)–O(8)   | 1.701(8) | W(12)–O(14) | 1.688(7) |
|   |          | average     | 1.702    |
| W–O <sub>c</sub> (O <sub>c</sub> : corner-sharing oxygen) |          |             |          |
| W(1)–O(15)  | 1.906(7) | W(7)–O(27)  | 1.925(7) |
| W(1)–O(16)  | 1.934(7) | W(7)–O(33)  | 1.915(7) |
| W(2)–O(16)  | 1.864(7) | W(8)–O(27)  | 1.885(7) |
| W(2)–O(17)  | 1.908(7) | W(8)–O(34)  | 1.879(7) |
| W(3)–O(15)  | 1.895(7) | W(9)–O(29)  | 1.886(7) |
| W(3)–O(17)  | 1.896(7) | W(9)–O(35)  | 1.922(7) |
| W(4)–O(29)  | 1.905(7) | W(10)–O(30) | 1.893(7) |
| W(4)–O(30)  | 1.907(7) | W(10)–O(35) | 1.884(7) |
| W(5)–O(25)  | 1.906(7) | W(11)–O(31) | 1.907(7) |
| W(5)–O(31)  | 1.895(7) | W(11)–O(32) | 1.900(7) |
| W(6)–O(25)  | 1.895(7) | W(12)–O(33) | 1.885(7) |
| W(6)–O(32)  | 1.902(7) | W(12)–O(34) | 1.928(7) |
|   |          | average     | 1.901    |
| W–O <sub>e</sub> (O <sub>e</sub> : edge-sharing oxygen)   |          |             |          |
| W(1)–O(18)  | 1.907(7) | W(3)–O(23)  | 1.929(7) |
| W(1)–O(19)  | 1.914(7) | W(4)–O(18)  | 1.919(7) |
| W(2)–O(20)  | 1.910(7) | W(4)–O(24)  | 1.907(7) |
| W(2)–O(21)  | 1.943(7) | W(5)–O(19)  | 1.917(7) |
| W(3)–O(22)  | 1.917(7) | W(5)–O(24)  | 1.914(7) |

|            |          |             |          |
|------------|----------|-------------|----------|
| W(6)–O(20) | 1.911(7) | W(9)–O(28)  | 1.914(8) |
| W(6)–O(26) | 1.926(7) | W(10)–O(36) | 1.918(8) |
| W(7)–O(21) | 1.908(7) | W(10)–O(38) | 1.911(7) |
| W(7)–O(26) | 1.915(8) | W(11)–O(36) | 1.913(7) |
| W(8)–O(22) | 1.917(7) | W(11)–O(37) | 1.914(7) |
| W(8)–O(28) | 1.907(8) | W(12)–O(37) | 1.910(7) |
| W(9)–O(23) | 1.896(7) | W(12)–O(38) | 1.908(7) |
|            |          | average     | 1.914    |

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| W–O <sub>a</sub> (O <sub>a</sub> : oxygen coordinating to heteroatom) |          |             |          |
|---|----------|-------------|----------|
| W(1)–O(39)  | 2.453(7) | W(7)–O(40)  | 2.405(6) |
| W(2)–O(40)  | 2.473(6) | W(8)–O(41)  | 2.462(7) |
| W(3)–O(41)  | 2.422(7) | W(9)–O(41)  | 2.445(7) |
| W(4)–O(39)  | 2.427(7) | W(10)–O(42) | 2.417(7) |
| W(5)–O(39)  | 2.428(7) | W(11)–O(42) | 2.444(7) |
| W(6)–O(40)  | 2.426(7) | W(12)–O(42) | 2.450(7) |
|   |          | average     | 2.438    |

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