# Supplementary material

The table below gives the periodic box and atom positions (all in Angstroms) for the geometry shown in Fig. 2a of the manuscript. This is provided for additional information concerning the geometries not only of this particular structure, but also for similar structures also shown in Fig. 2.

|  |  |  |  |
| --- | --- | --- | --- |
| **Vector Number** | **x** | **y** | **z** |
| 1 | 5.42565 | 0.00000 | 0.00000 |
| 2 | 2.71283 | 4.69875 | 0.00000 |
| 3 | 0.00000 | 0.00000 | 10.90124 |
|  |  |  |  |
| **Atom Number** | **x** | **y** | **z** |
| 1 | 0.00000 | 0.00000 | 2.12810 |
| 2 | 1.35161 | -2.35212 | 4.25627 |
| 3 | -1.35161 | -2.35212 | 4.25627 |
| 4 | -2.71281 | 0.00554 | 4.25627 |
| 5 | -2.71281 | -1.56624 | 2.14307 |
| 6 | -2.71281 | 1.56624 | 2.11312 |
| 7 | -1.36120 | -2.34659 | -0.00007 |
| 8 | -2.71281 | -0.00554 | -0.00007 |
| 9 | 1.36120 | -2.34659 | -0.00007 |
| 10 | -1.33745 | -0.77217 | -2.18946 |
| 11 | 0.00000 | 1.54435 | -2.18946 |
| 12 | -2.71281 | 1.56624 | -2.21430 |
| 13 | 1.33745 | -0.77217 | -2.18946 |
| 14 | -1.33745 | 0.77218 | -4.45551 |
| 15 | -2.71281 | -1.56624 | -4.43067 |
| 16 | 0.00000 | -1.54435 | -4.45551 |
| 17 | 1.33745 | 0.77218 | -4.45551 |

Table S1 – (Caption) Translation vectors in angstroms and atom positions for the ThIr16 unit cell. The first atom in the Table is the thorium atom. The remaining atoms are all iridium. Units of coordinates are Angstroms.