# Supporting Information:Synthesis and Characterization of Barium Hexafluoridoosmates

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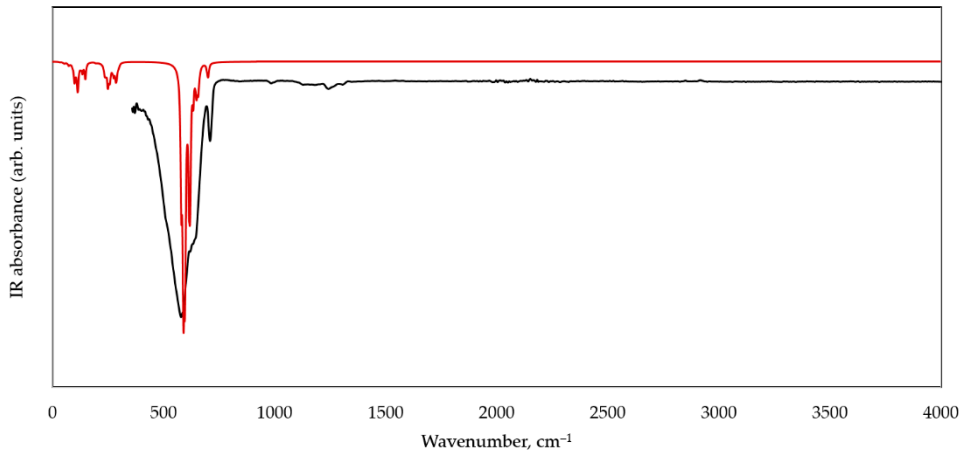


**Figure S1.** IR spectra of $BaOs_2F_{12}$: experimentally observed (black) and calculated with DFT-PBE0 (red).

**Table S1.** Region assignment for the theoretical IR spectrum of $Ba(OsF_6)_2$. .

| **IR peak ($cm^{-1}$)** | **Assignment** |
|---|---|
| 702, 698, 696, 695, 667, 660, 657, 655, 648, 644, 634, 633, 619, 618, 614, 606, 598, 596, 594, 593, 589, 587, 580 | Os–F stretching |
| 301, 296, 289, 284, 282, 281, 275, 269, 268, 264, 263, 259, 256, 254, 253, 249, 248, 241, 239, 235, 232, 231, 230, 222, 221, 214, 210, 204, 201, 199, 196, 194 | $OsF_6^-$ deformations |

| | |
|---|---|
| 148, 134, 130, 126, 116, 115, 112, 111, 107, 105, 99, 94, 90, 88, 81, 76, 73, 66, 59, 55, 54, 51 45, 33, 27 | Lattice vibrations |

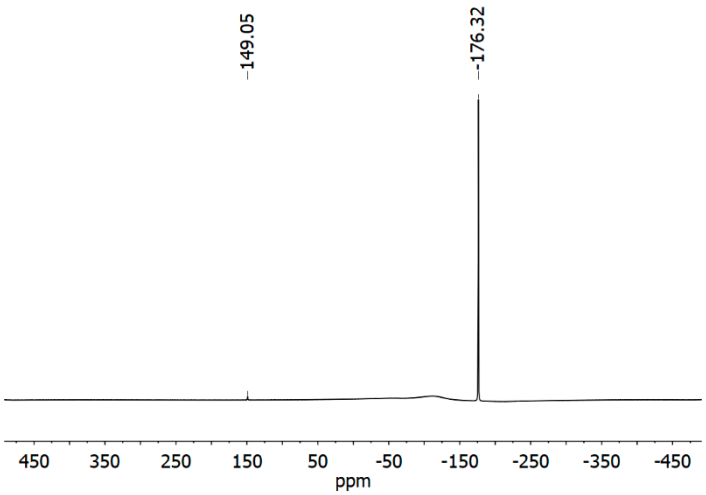


**Figure S2.** $^{19}F$ NMR spectrum of $Ba(OsF_6)_2$ in anhydrous HF.

## Additional basis set details

The following split-valence + polarization (SVP) basis sets were applied for Ba, Os, and F:

```
Full basis set listing for Ba in CRYSTAL14 input format
256 6
INPUT
10. 0 2 2 2 1 0
9.526986 427.845816 0
4.487510 204.417530 0
8.315930 293.605864 0
4.292217 294.193316 0
5.916108 112.550402 0
2.874842 181.782621 0
3.589465 -33.473174 0
0 0 3 2.0 1.0
  2.3961900000     -5.9554766710
  2.2433050000      6.6805648241
  0.71740200000    -0.57055347037
0 0 1 2.0 1.0
  0.27420073547     1.0000000000
0 1 1 0.0 1.0
 0.13               1.0 1.0
0 2 4 6.0 1.0
  2.9267420000      0.79815276764
  2.5207180000     -1.0707548832
  0.67578180854     0.34940781448
  0.31985844531     0.65041110673
0 3 2 0.0 1.0
  0.966315         -0.908938
  0.893828          0.947240
0 3 1 0.0 1.0
```

```
  0.273195          0.322057
```

**Full basis set listing for Os in CRYSTAL14 input format**

```
276 8
INPUT
16. 0 2 2 2 1 1
13.875754 885.405719 0
6.937877 25.967040 0
10.193793 320.083902 0
5.096896 26.148765 0
7.099238 115.044843 0
3.549619 13.622575 0
2.767075 18.909457 0
4.349905 -19.027595 0
0 0 2 2.0 1.0
  15.286736000     -1.0647114485
  12.700638000      1.8433193269
0 0 1 2.0 1.0
  5.7094832504      1.0000000000
0 0 1 0.0 1.0
  1.0689228744      1.0000000000
0 0 1 0.0 1.0
 0.46783543749      1.0000000000
0 1 1 0.0 1.0
  0.13              1.0 1.0
0 2 4 6.0 1.0
  7.9362790000      .33899369659
  6.3036410000     -.56379438345
  1.4351579676      .52360040577
 0.68442749722      .52445339821
0 3 4 6.0 1.0
  3.5808150000     -.42773932262
  3.1961650000      .44501403992
  1.0550226354      .43689459722
 0.41588406618      .48220605798770
0 3 1 0.0 1.0
 0.20794203309      1.0
```

**Full basis set listing for F in CRYSTAL14 input format**

```
9 5
0 0 5 2.0 1.0
  2894.8325990     -0.53408255515E-02
  435.41939120     -0.39904258866E-01
  98.843328866     -0.17912768038
  27.485198001     -0.46758090825
  8.5405498171     -0.44653131020
0 0 1 2.0 1.0
  1.0884995861      1.00000000000
0 1 1 0.0 1.0
 0.35000000000      1.0 1.0
0 2 3 5.0 1.0
  22.736269492     -0.45212874436E-01
  4.9973682193     -0.23754317067
  1.3537773703     -0.51287353587
0 3 1 0.0 1.0
  1.4000000000      1.00000000000
```