*Electronic Supplementary Information*

# $SrPt_3In_2$ – An orthorhombically distorted coloring variant of $SrIn_5$

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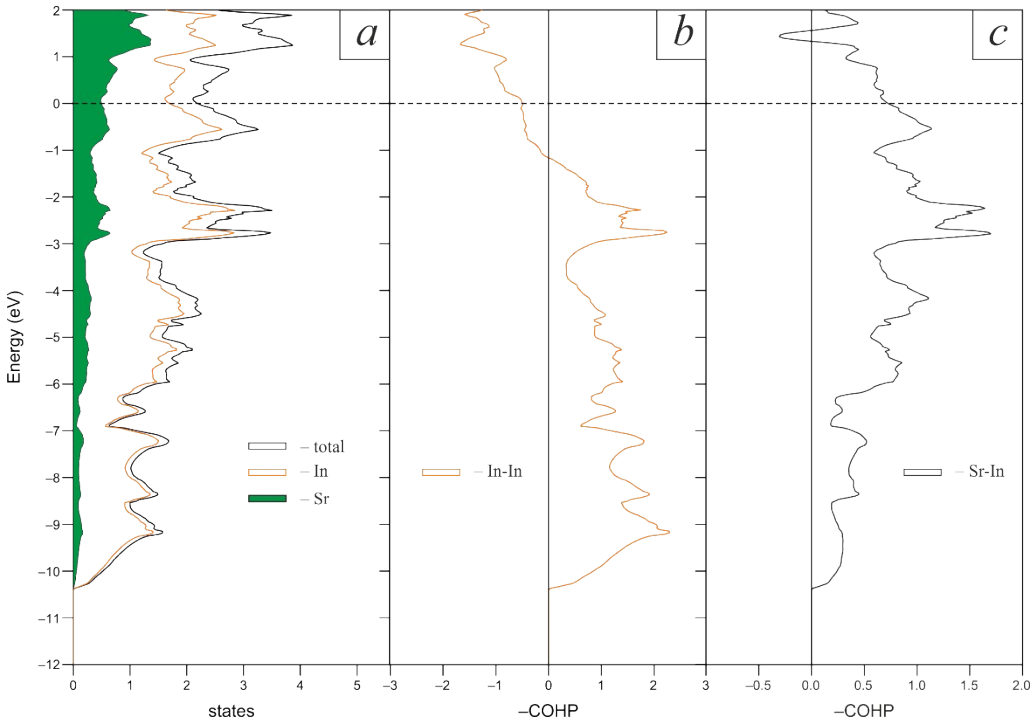


**Figure 1S.** Total and projected DOS for $SrIn_5$ (*a*); cumulative COHP curves for different interactions: In–In interactions (*b*); Sr–In interactions (*c*).

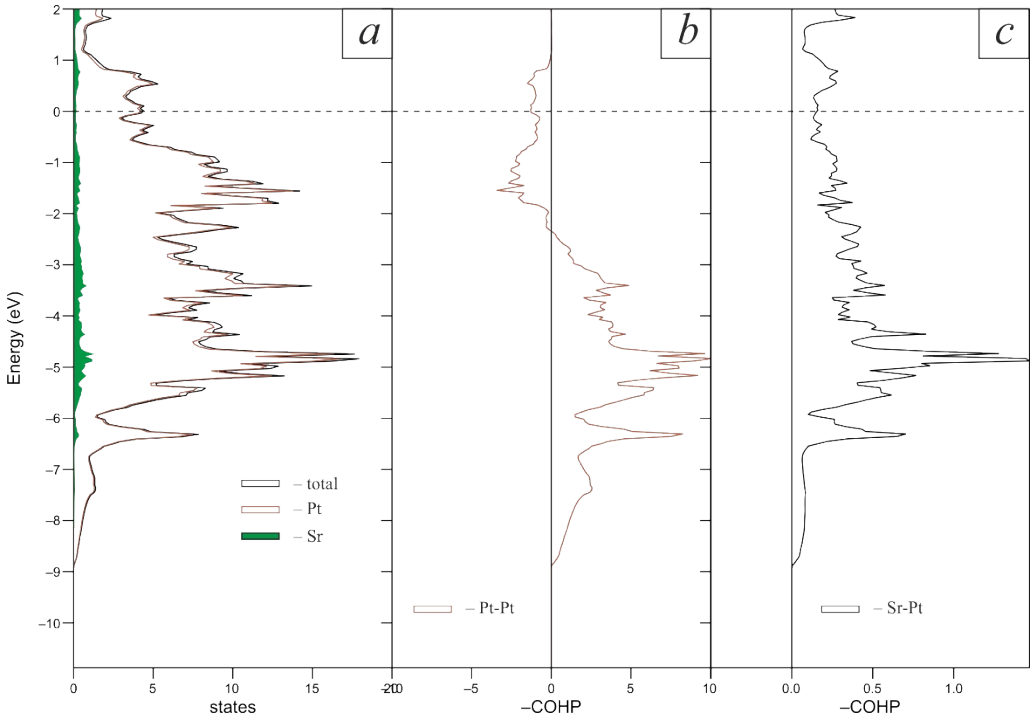


**Figure 2S.** Total and projected DOS for $SrPt_5$ (*a*); cumulative COHP curves for different interactions: Pt–Pt interactions (*b*); Sr–Pt interactions (*c*).

**Table.** Selected bond distances and corresponding -ICOHP (eV/bond) as integrated up to $E_F$ for $SrIn_5$ and $SrPt_5$ together with a contribution of each type of interactions to the total bonding population per cell.

| #1 | #2 | Dist (Å) | eV/bond | mult | eV/cell | % |
|---|---|---|---|---|---|---|
| *$SrIn_5$* | | | | | | |
| In1– | In2 (4x) | 2.960 | 1.03 | 3 | 12.36 | 35.6 |
| | In1 (4x) | 2.968 | 1.10 | 3 | 13.2 | 38.0 |
| In2– | In2 (3x) | 3.428 | 0.39 | 2 | 2.34 | 6.7 |
| | | | | | Σ= | 80.4 |
| Sr– | In2 (6x) | 3.428 | 0.47 | 1 | 2.82 | 8.1 |
| | In1 (12x) | 3.826 | 0.33 | 1 | 3.96 | 11.4 |
| | | | | | Σ= | 19.6 |
| *$SrPt_5$* | | | | | | |
| Pt1– | Pt2 (4x) | 2.681 | 1.76 | 3 | 21.12 | 40.4 |
| | Pt1 (4x) | 2.698 | 1.76 | 3 | 21.12 | 40.4 |
| Pt2– | Pt2 (3x) | 3.116 | 0.58 | 2 | 3.48 | 6.7 |
| | | | | | Σ= | 87.6 |
| Sr– | Pt2 (6x) | 3.116 | 0.46 | 1 | 2.76 | 5.2 |
| | Pt1 (12x) | 3.470 | 0.31 | 1 | 3.72 | 7.1 |
| | | | | | Σ= | 12.4 |

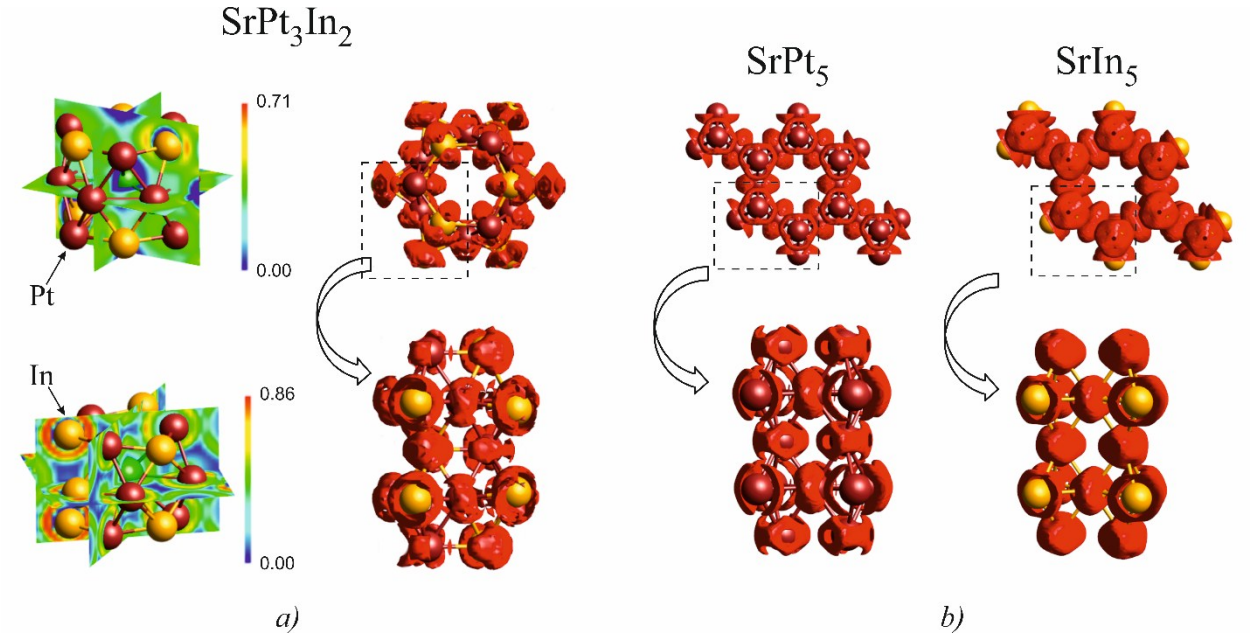


**Figure 3S.** (*a*) ELF plane sections representing the first coordination sphere of Sr2 and Sr1, respectively together with ELF isosurfaces (η = 0.8) within the $[Pt_3In_2]$ framework. For a comparative goal, the analogous ELF isosurfaces for $SrPt_5$ and $SrIn_5$ are shown in *b)*. A partial fragment shown by dotted line includes all crystallographically independent sites of Pt and In for chosen compounds (for more details see main text).