

$R_3\text{Au}_9Pn$ ($R = \text{Y, Gd-Tm}$; $Pn = \text{Sb, Bi}$): A Link between $\text{Cu}_{10}\text{Sn}_3$ and $\text{Gd}_{14}\text{Ag}_{51}$

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Supporting Information

Table S1. Summary of the thermal synthesis techniques used for each sample including: high temperature reactions in tube furnaces, annealing in tube furnaces, Differential Thermal Analysis (DTA), and arc melting.

| $R_3\text{Au}_9\text{Pn}$ | Thermal Treatment |
|---|---|
| Gd ₃ Au ₉ Sb | 1000°C for 3 hrs, annealed at 850°C for 12 hrs |
| Tb ₃ Au ₉ Sb | DTA, annealed at 960°C for 5 days |
| Dy ₃ Au ₉ Sb | 1050°C for 5 hrs, annealed at 850 for 72 hrs |
| Ho ₃ Au ₉ Sb | 900°C for 10 days |
| Er ₃ Au ₉ Sb | 900°C for 7 days |
| Tm ₃ Au ₉ Sb | Arc melted |
| Y ₃ Au ₉ Sb | DTA, annealed at 900°C for 10 days |
| Gd ₃ Au ₉ Bi | Arc melted, annealed at 850°C for 2 days and 700°C for 5 days |

Table S2. Anisotropic displacement parameters U_{ij} [\AA^2] for Gd₃Au₉Sb.

| Atom | U_{11} | U_{22} | U_{33} | U_{12} | U_{13} | U_{23} |
|-------------|----------------------------|----------------------------|----------------------------|----------------------------|----------------------------|----------------------------|
| Au1 | 0.00202(17) | 0.00202(17) | 0.0064(3) | 0.000 | 0.000 | 0.00101(9) |
| Au2 | 0.00436(18) | 0.00506(18) | 0.00296(18) | -0.00150(12) | -0.00125(13) | 0.00292(14) |
| Au3 | 0.0028(2) | 0.0028(2) | 0.0107(5) | 0.000 | 0.000 | 0.00138(12) |
| Gd | 0.0025(3) | 0.0018(3) | 0.0013(3) | 0.000 | 0.000 | 0.0017(2) |
| Sb | 0.0007(4) | 0.0007(4) | 0.0015(7) | 0.000 | 0.000 | 0.00037(18) |

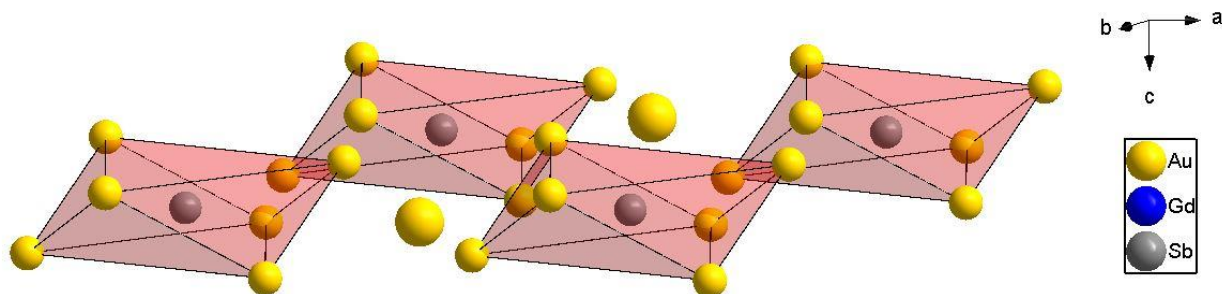


Figure S1. View of the isolated Sb@Au₆ trigonal prisms in Gd₃Au₉Sb. The unbound (slightly larger for differentiation) Au atoms represent the caps of the Au@Au₈ clusters in neighboring layers.

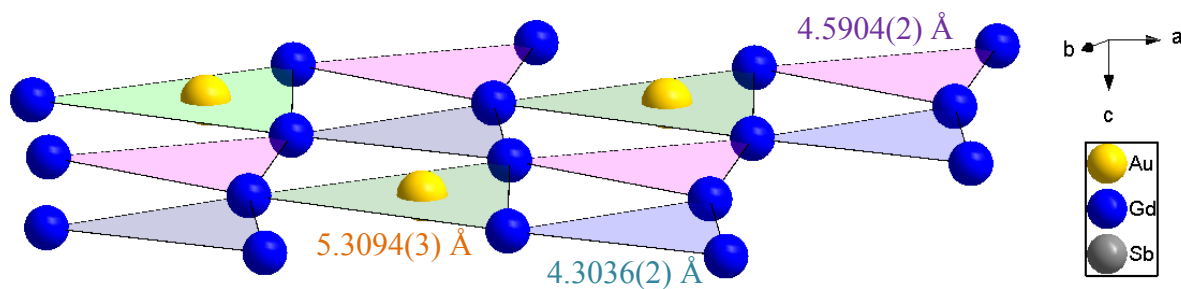


Figure S2. A view of the Gd trigonal planes in Gd₃Au₉Sb and interatomic atomic distances within each triangle. The green planes are centered by the central atom of the Au@Au₈ clusters.

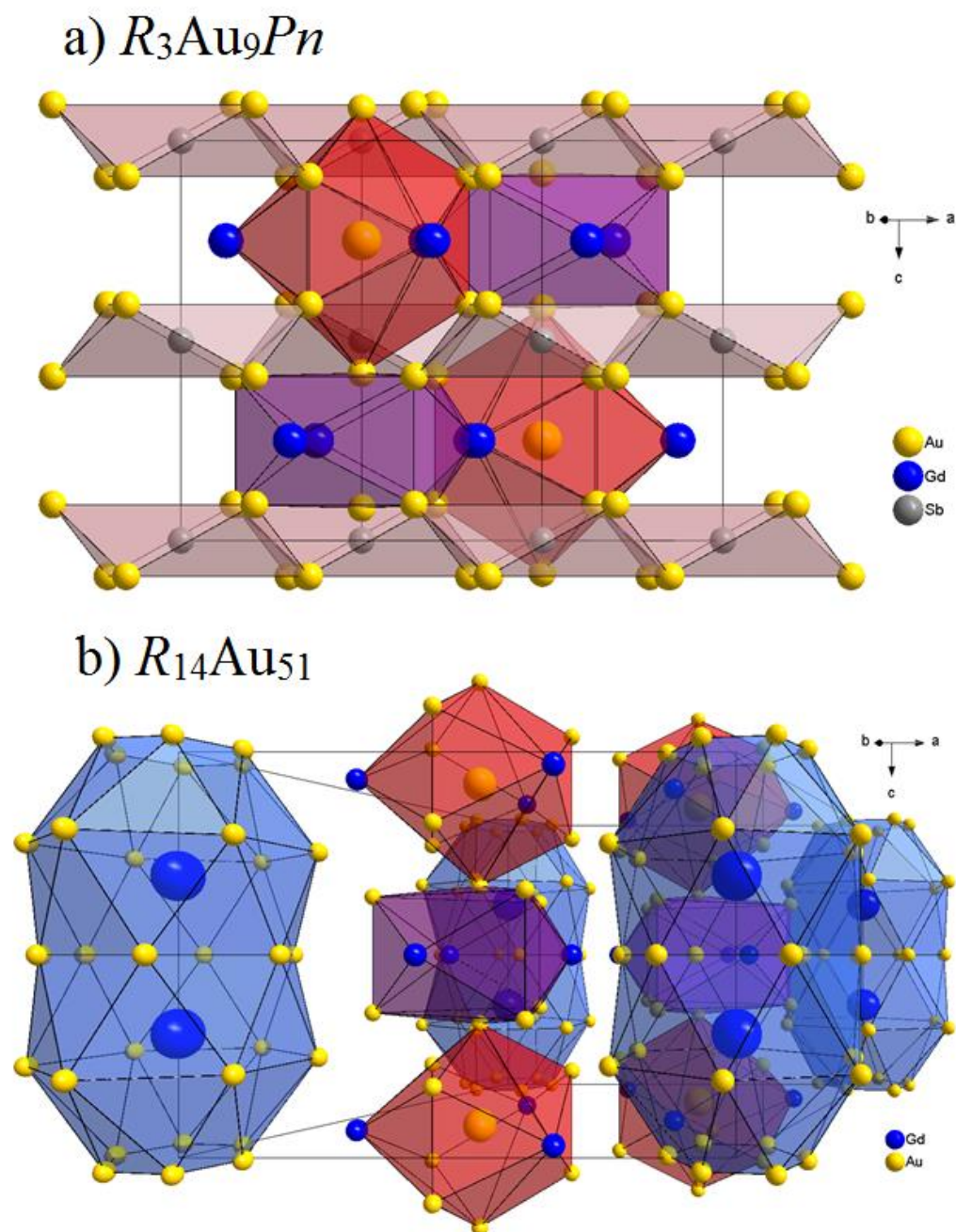


Figure S3. Comparison of coordination polyhedral observed in $R_3\text{Au}_9\text{Pn}$ (a) and $R_{14}\text{Au}_{51}$ (b). The red and purple polyhedra appear isostructural and are not present in the $R_3\text{Au}_7\text{Sn}_3$ structure, demonstrating a previously unrecognized relationship between $R_{14}\text{Au}_{51}$ and $\text{Cu}_{10}\text{Sn}_3$ type structures.

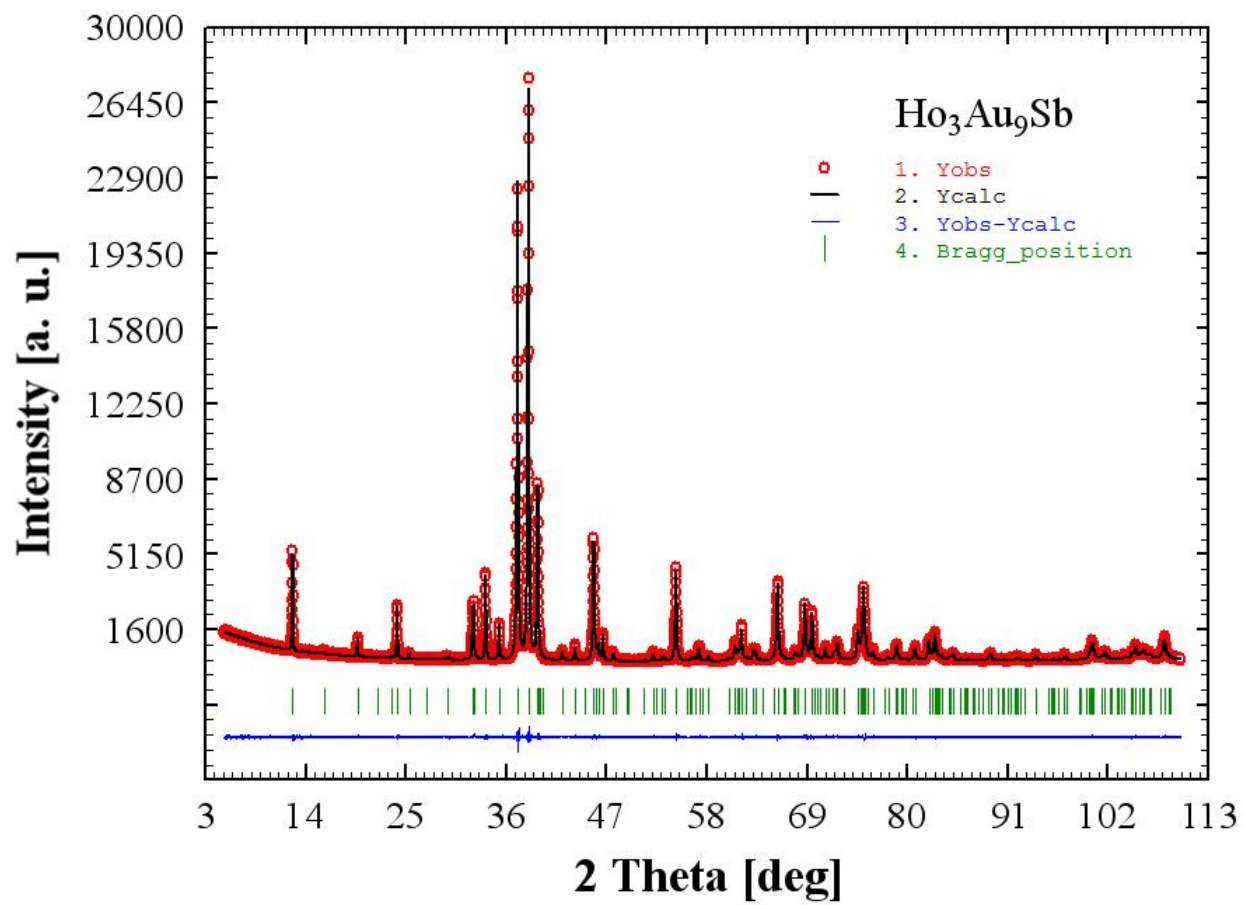


Figure S4. PXRD pattern of single phase $\text{Ho}_3\text{Au}_9\text{Sb}$ used for magnetic testing.

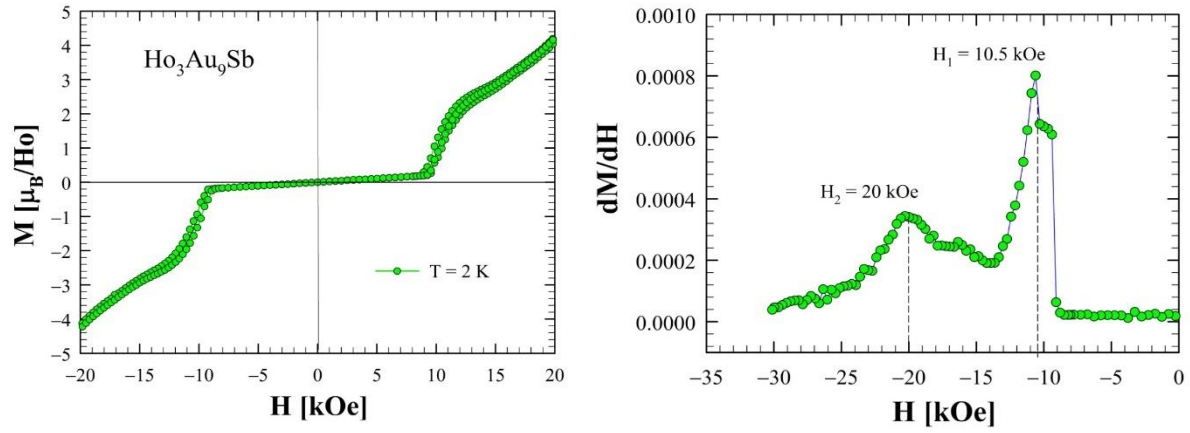


Figure S5. (left) A magnification of the isothermal magnetization in between ± 20 kOe showing magnetic hysteresis after the AFM region. (right) The derivative of the same isothermal magnetization curve showing peak positions used for determination of critical field values.

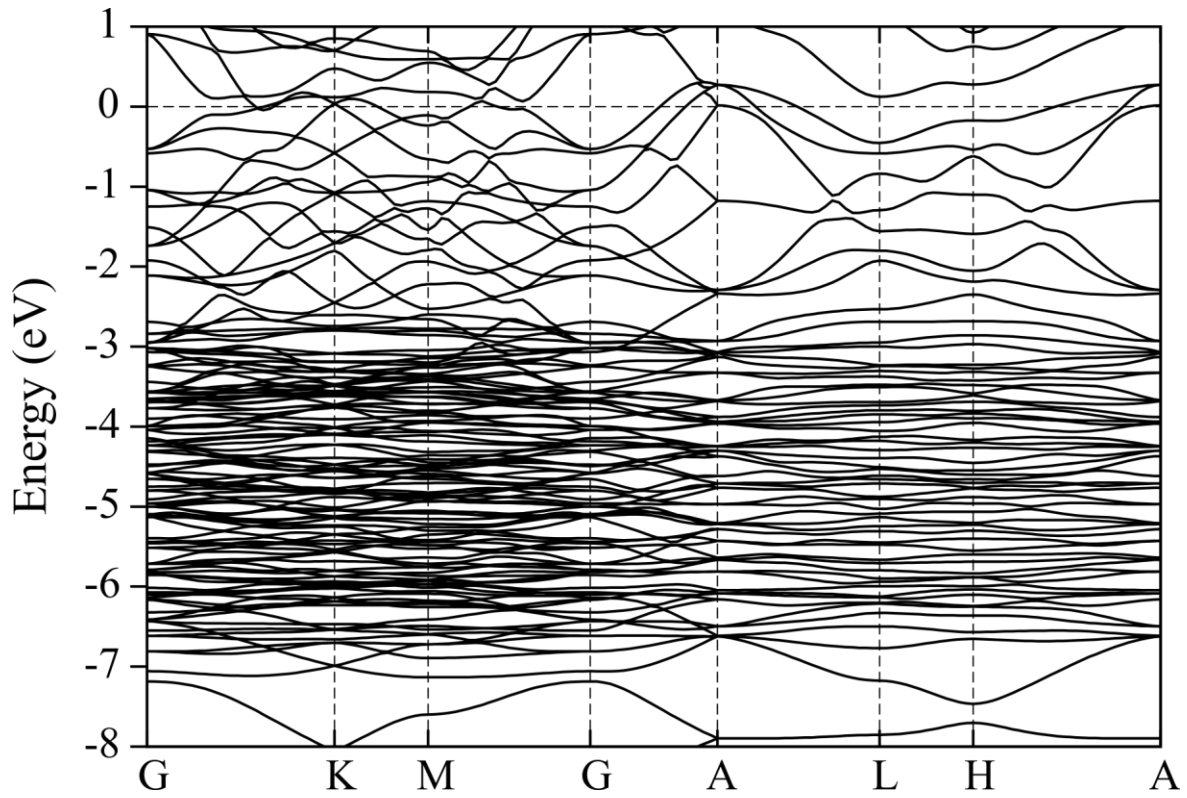


Figure S6. Band structure plot for $\text{Y}_3\text{Au}_9\text{Sb}$.

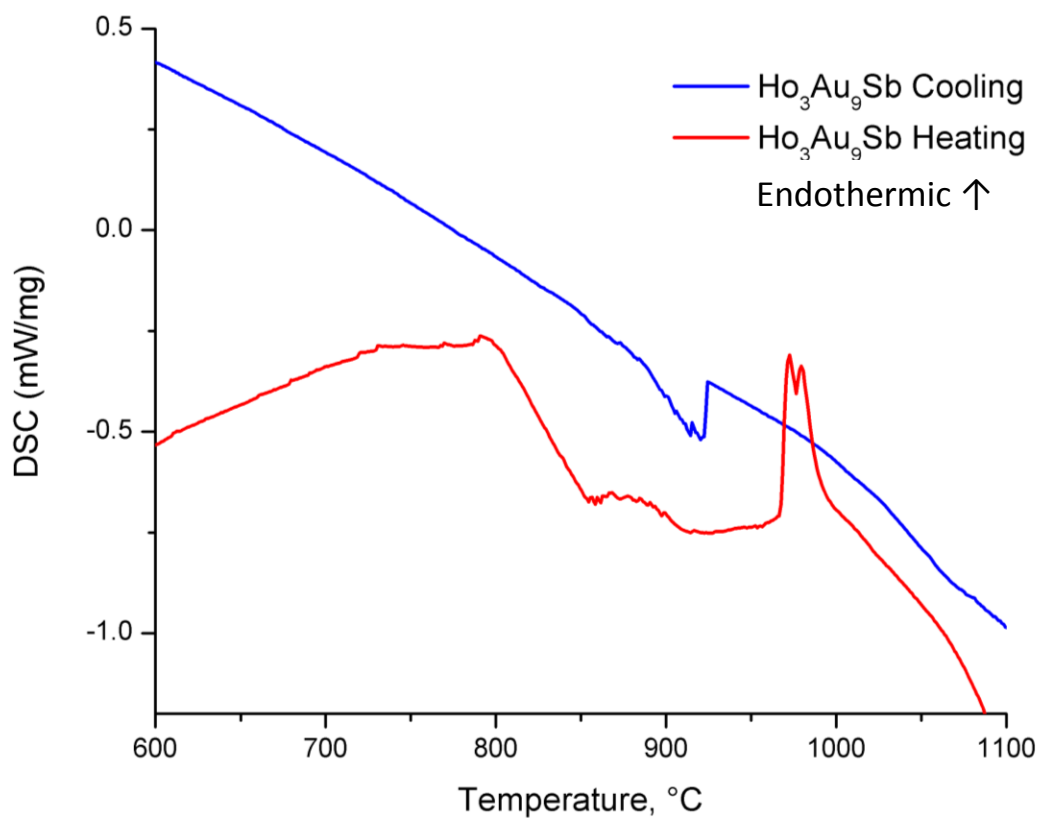


Figure S7. DSC plot for the $\text{Ho}_3\text{Au}_9\text{Sb}$ sample recorded on heating and cooling at 20 °C/min for both measurements.