SUPPORTING INFORMATION

Ternary Gold Hydrides: Routes to Stable and Potentially Superconducting Compounds

Martin Rahm, Roald Hoffmann and N. W. Ashcroft

1 Table of Contents

2 Comparison with Experiment (Li_2PdH_2 and Na_2PdH_2)

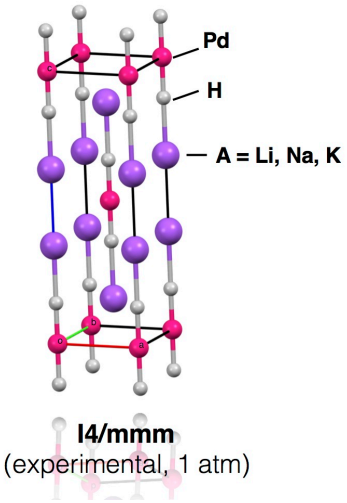

Figure S1. *The experimental I4/mmm 1atm structures of $[A]_2PdH_2$ (A = Li, Na) were correctly identified as the ground states by CALYPSO. We did not search for K_2PdH_2. The structural agreement with experiment was excellent, and their close relation to proposed ternaries of AuH_2 validates our approach.*

Table S1. *Comparisons of unit cell volumes (in Ångström) with experimental references and at different levels of theory. Calculations used a kinetic energy cutoff of 800 eV, unless otherwise stated. Experimental structures are from the ICSD database.*

Compound	Space group	V(exp)	V(PBE)	V(PBE+D3)	V(HSE06)
Na_2PdH_2	*I4mmm*	146.22	145.9	134.9	-
Li_2PdH_2	*I4mmm*	99.97	99.7	91.4	-
$Ba(AuH_2)_2$	*I4*	n/a	125.5	117.9 (116.7[a])	(123.71) [a]

[a] *Volume was calculated using a 400 eV kinetic energy cutoff.*

3 3D Convex Hulls for Selected Ternaries

3.1 K-Au-H

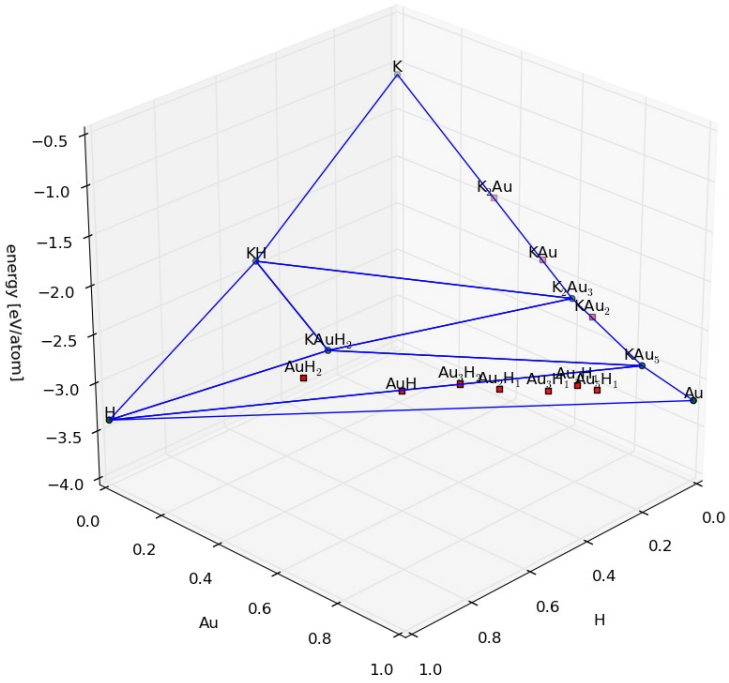

Figure S2. A calculated segment of the three-component phase diagram of K, Au and H in the ground state (left). Blue lines between green circles connect stable phases. $K(AuH_2)_2$ is stable.

3.2 Ba-Au-H

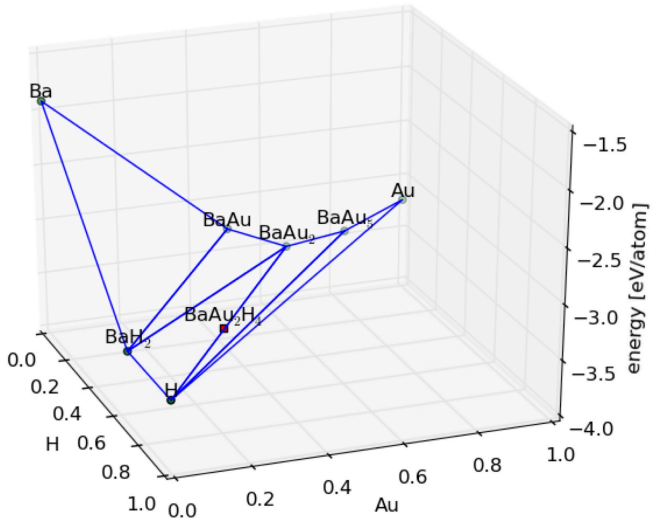

Figure S3. *A calculated segment of the three-component phase diagram of Ba, Au and H in the ground state (left). Blue lines between green circles connect stable phases. Unstable Au_xH_y binaries have been omitted. $Ba(AuH_2)_2$ is metastable (but just barely) with respect to decomposition into $BaAu_2$ and H_2. Its synthesis nevertheless appears possible from $CsAuH_2$.*

3.3 Sr-Au-H

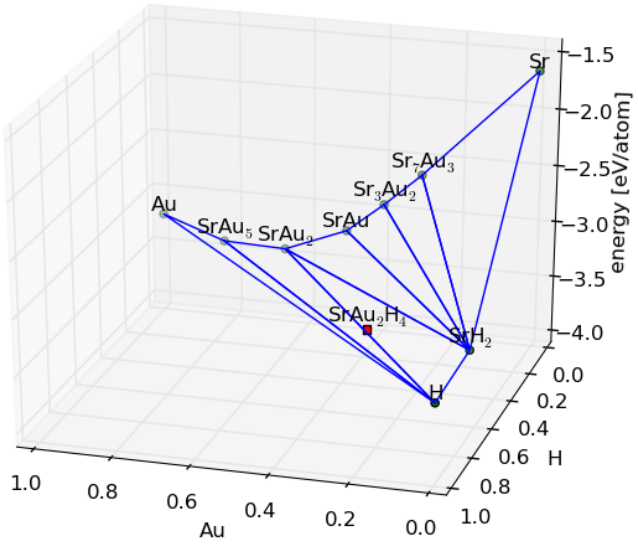

Figure S4. *A calculated segment of the three-component phase diagram of Sr, Au and H in the ground state (left). Blue lines between green circles connect stable phases. Unstable Au_xH_y binaries have been omitted. $Sr(AuH_2)_2$ is metastable (but just barely) with respect to decomposition into $SrAu_2$ and H_2. Its synthesis nevertheless appears possible from $CsAuH_2$.*

4 Electronic Structure Data for Select Materials

4.1 Molecular Orbitals for AuH_2^-

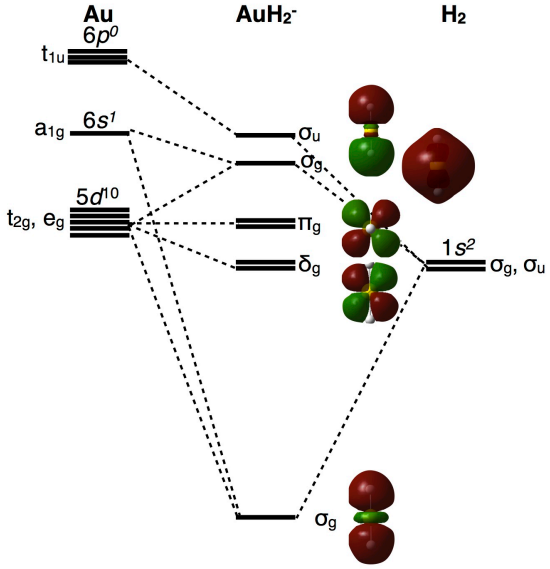

Figure S5. *Approximate MO diagram for AuH_2^- formation from Au and H_2. The composite molecule has 14 valence electrons, so all orbitals shown for AuH_2^- are occupied, and their relative ordering is taken from a PBE/Def2-TZVPD calculation. Note the distinct Au-6p character of the frontier orbital, and the lowering of the delta δ_g relative π_g.*

4.2 Orbital-projected DOS for Pure Gold

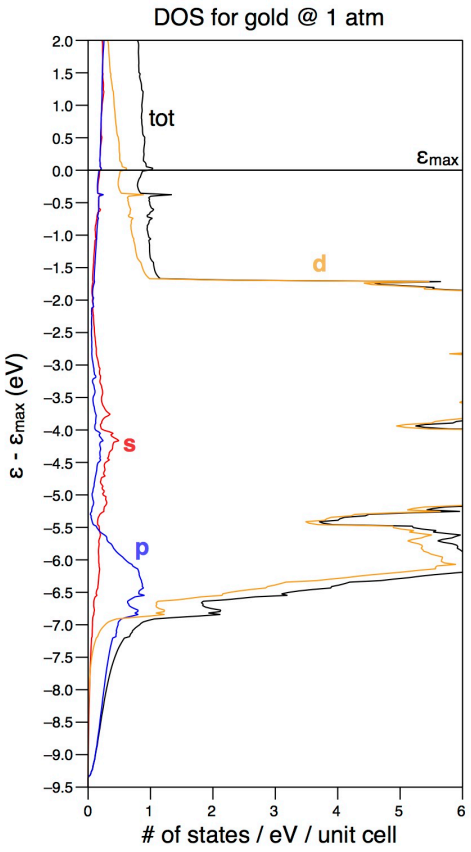

Figure S6. *Density of States (DOS) for gold at 1atm. The DOS at the Fermi level is dominated by d-levels, with an admixture of s and p in equal amounts.*

4.3 Effect of Spin-Orbit Coupling

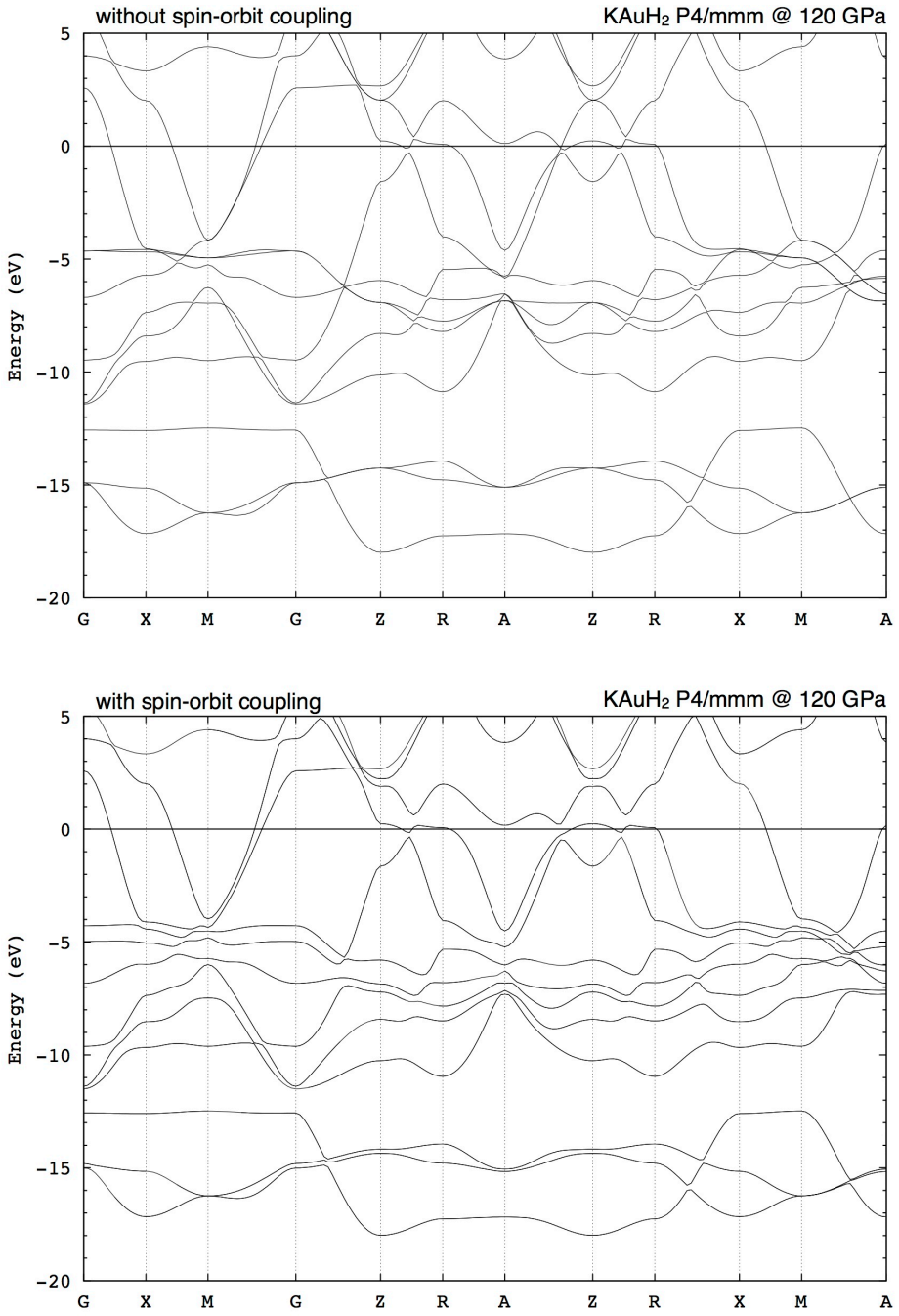

Figure S7. *Stability of the band structure of P4/mmm $KAuH_2$ at 1atm, with and without spin-orbit coupling.*

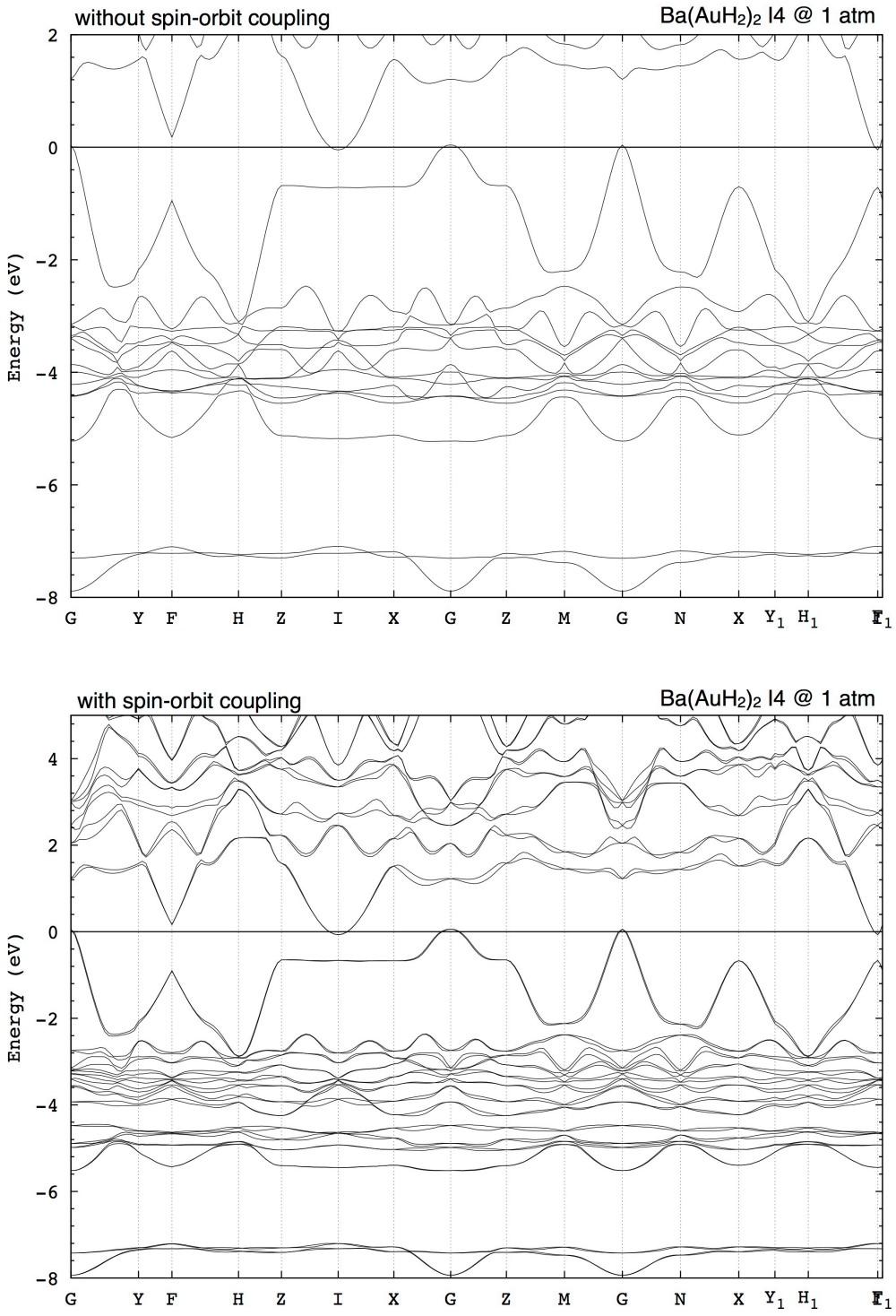

Figure S8. *Stability of the band structure of I4 $Ba(AuH_2)_2$ at 1atm with and without spin-orbit coupling. This figure does not follow the Brillouin zone path shown in the main article, but a longer one, with incorrect labeling. This does not matter - it captures all the important points, and demonstrates the insensitivity of the Fermi surface with respect to spin-orbit coupling.*

4.4 Band Structure and COHP Analysis of KAuH2, $P2_12_12_1$

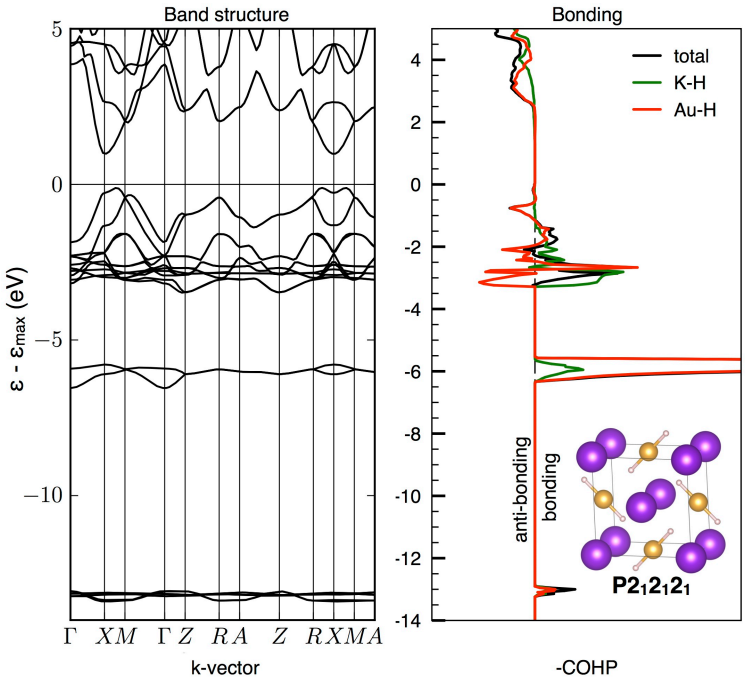

Figure S9. *PBE Band structure and crystal orbital Hamilton population (COHP) analysis of the predicted metastable* $P2_12_12_1$ *phase of* $KAuH_2$ *at 1atm.*

4.5 Band Structure of *I*4 $Ba(AuH_2)_2$ with PBE and HSE06

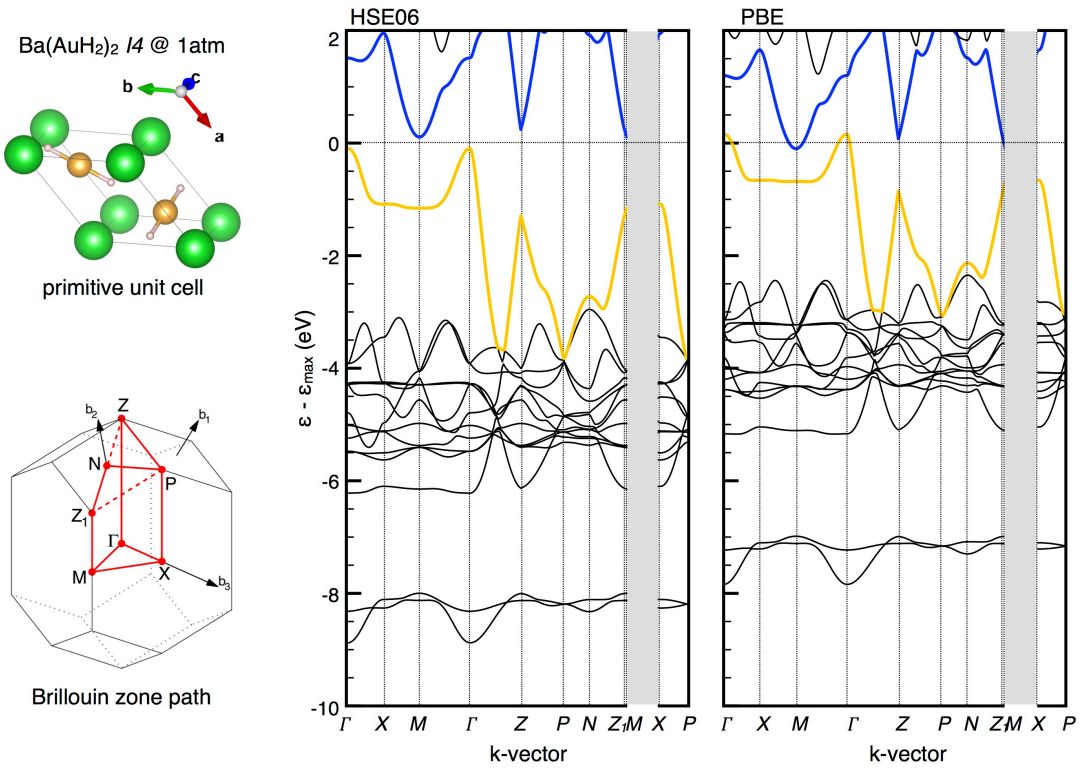

Figure S10. *The band structure of I4 $Ba(AuH_2)_2$ calculated with PBE and HSE06, a 80meV gap opens up at the latter level of theory. The gap is small and thermal excitation under ambient conditions is likely to close it.*

4.6 Band Structure of *I*4 $Sr(AuH_2)_2$ with PBE and HSE06, and Fermi surface.

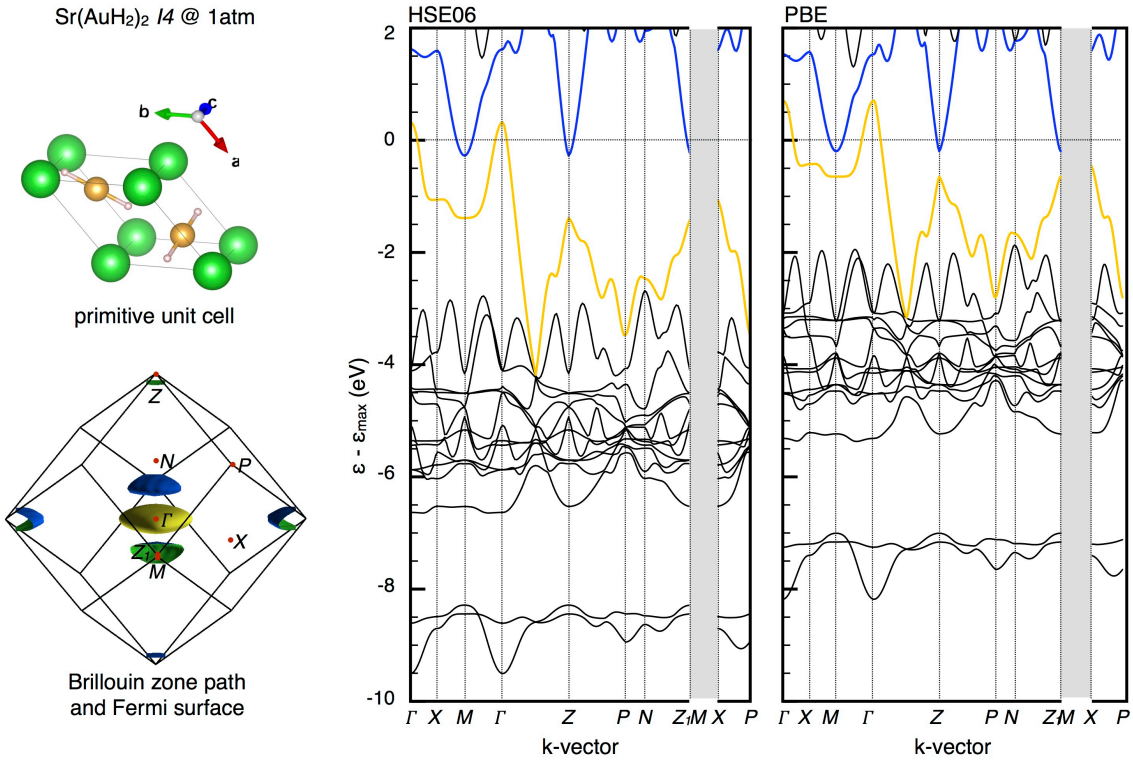

Figure S11. *Stability of the band structure of I4 $Sr(AuH_2)_2$ with respect to the level of theory. The Fermi surface is slightly more complex than the $Ba(AuH_2)_2$-analog (shown in Figure S10) due to one additional band crossing the Fermi surface close to the Z-point.*

5 Calculated Radii of Some Atoms, Anions and Cations and their Correlation with Energies of Formation.

A selection of radii for atoms and ions are shown in Table S2 for comparison. One reasonable assumption is that the packing of similarly sized ions makes for higher lattice energy. This argument is corroborated by the trend in formation energies calculated for alkali metal ternaries of AuH_2^- , which vary linearly with cation size (Figure S3).

Table S2. *A selection of relevant ionic and atomic VdW radii (Å).*[a]

AuH_2^-	2.63[b]	Au	2.26	Li^+	0.98	Ba^{2+}	1.97
H^-	2.10	Au^+	1.99	Na^+	1.33	Ca^{2+}	1.58
H	1.54	Au^-	2.55	K^+	1.75		
				Rb^+	1.91		
				Cs^+	2.12		

[a] *Data is from ref.* [59]*, supplemented with the radius of Ca^{2+} and Ba^{2+}.*
[b] *Calculated from the volume of the molecular anion, averaged to a sphere.*

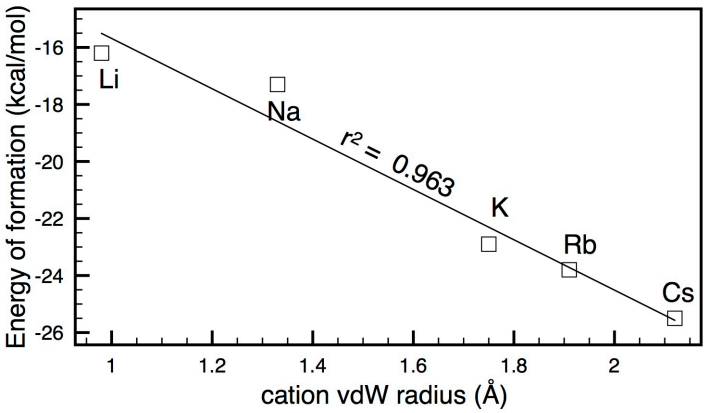

Figure S12. *The formation energy of gold hydride ternaries is related to the counterion radius.*

6 Vibrational Analyses

6.1 Convergence with Respect to Size of Supercell

We typically used 3x3x3 supercells when calculating phonon dispersion and thermal corrections in VASP. The two exceptions are electron-phonon calculations on $Ba(AuH_2)_2$ and $Sr(AuH_2)_2$ using the all-electron ELK code. The latter are very computationally intensive and we were limited to 2x2x2 supercells. Using VASP we verified that the phonon density of states and the total Gibbs energy at 300K did not change with further expansion of the supercell (Table S3). The fortunate circumstance of a small supercell (or small q-mesh) likely arises due to the molecular character of these solids.

Table S3. *Stability of thermal corrections with respect to supercell size for the I4 phase of $Sr(AuH_2)_2$ at 1 atm. Energies are given in kcal/mol formula unit.*

Supercell size	ZPE	G^0_{300K}
2x2x2	18.21	10.60
3x3x3	18.22	10.59
4x4x4	18.23	10.60

6.2 $KAuH_2$ phases

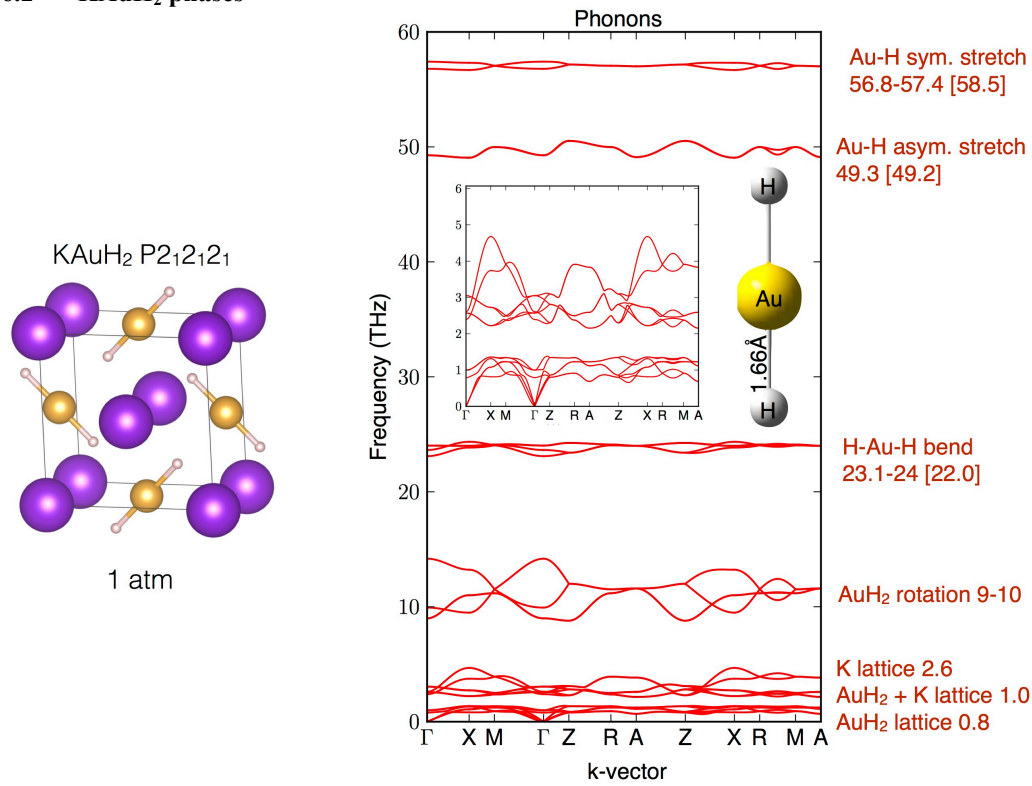

Figure S13. *Phonon spectrum of $KAuH_2$ in the metastable phase $P2_12_12_1$ at 1 atm. Inset shows the low energy part of the phonon spectrum. Assignments and comparison with of gas-phase AuH_2^- is shown at right. Molecular vibrational frequencies are within brackets. Model shows geometry of AuH_2^-, which is near identical in the gas phase and in the $KAuH_2$ crystal at 1atm.*

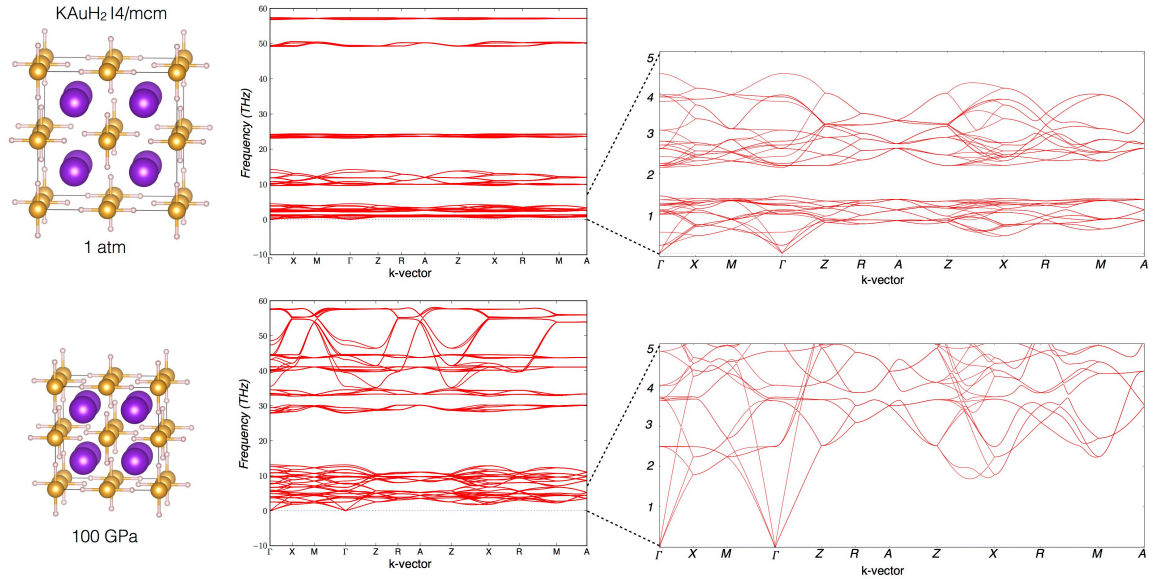

Figure S14. *The phonon spectra of the I4/mcm phase of $KAuH_2$ at 1 atm (metastable) and at 100 GPa (ground state). Insets at right show the low energy part of the phonon spectra.*

6.3 $Ba(AuH_2)_2$

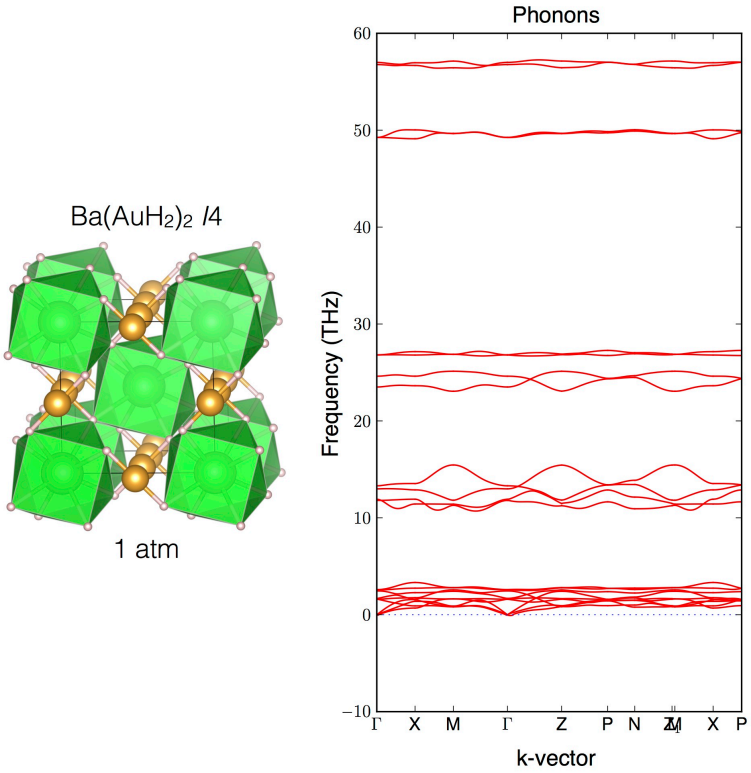

Figure S15. *Phonon spectrum of $Ba(AuH_2)_2$ I4 phase at 1 atm. Note the similarity with $KAuH_2$ shown above.*

6.4 $Sr(AuH_2)_2$

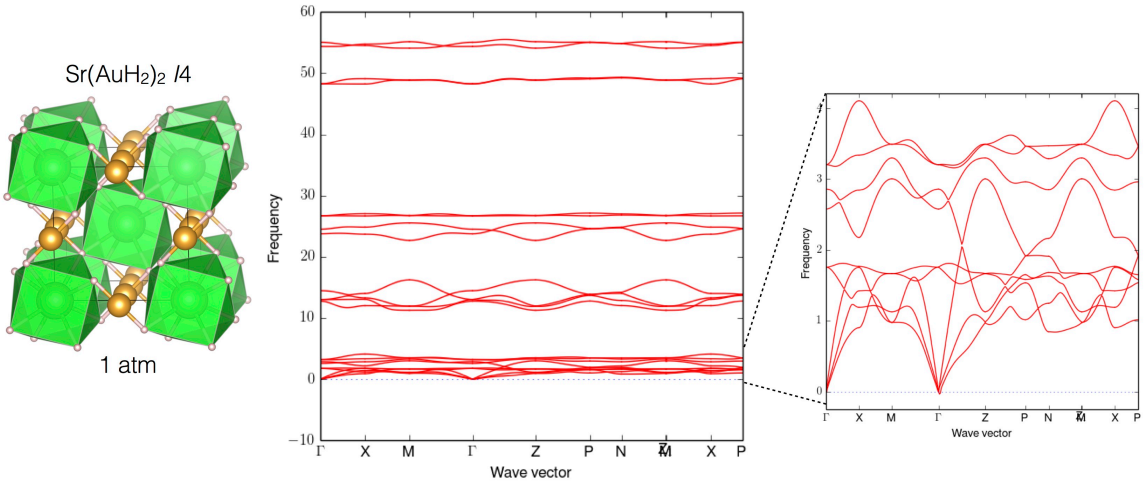

Figure S16. *Phonon spectrum of $Sr(AuH_2)_2$ I4 phase at 1 atm. Note the similarity with $KAuH_2$ shown above. Inset at right show the low energy part of the phonon spectra.*

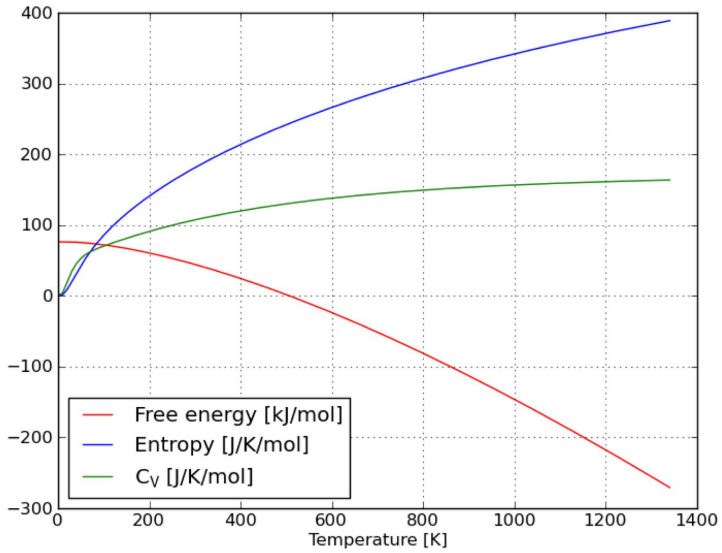

Figure S17. *Thermal corrections to the free energy and enthalpy, and the molar heat capacity of I4 $Sr(AuH_2)_2$ as a function of temperature.*

7 Optimized geometries in .cif format

Copy data (omitting caption in bold) into a text file, change the file ending to .cif and then you can view the structure in, for example, VESTA.

7.1 Selection of Gold Hydride Binary (AuH_n) Structures at 200 GPa

Gold hydride binaries are all unstable with respect to decomposition into H_2 and Au. We have *not* investigated the dynamic stability of anyone of these compositions. The structure data shown below represent a selection of geometry-optimized lower-energy minima identified by our structure searches. The AuH_n structures were all identified at either 100 or 200 GPa, and were subsequently scanned between 0-300 GPa. We reproduce the structures optimized at 200 GPa below.

7.1.1 AuH_2 *Cc* @ 200GPa

```
data_image0
_cell_length_a       3.58055
_cell_length_b       3.57998
_cell_length_c       3.59749
_cell_angle_alpha    90
_cell_angle_beta     90
_cell_angle_gamma    89.968

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
  _symmetry_equiv_pos_as_xyz
  'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
```

```
 _atom_site_thermal_displace_type
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
 Au1      1.0000 0.50000  0.00000  0.89588  Biso   1.000  Au
 Au2      1.0000 0.00000  0.00000  0.39671  Biso   1.000  Au
 Au3      1.0000 0.50000  0.50000  0.39671  Biso   1.000  Au
 H1       1.0000 0.00000  0.00000  0.89959  Biso   1.000  H
 H2       1.0000 0.91639  0.41631  0.75444  Biso   1.000  H
 H3       1.0000 0.00000  0.50000  0.99654  Biso   1.000  H
 H4       1.0000 0.08361  0.58369  0.75444  Biso   1.000  H
 H5       1.0000 0.00000  0.50000  0.23780  Biso   1.000  H
 H6       1.0000 0.50000  0.50000  0.89956  Biso   1.000  H
```

7.1.2 AuH *P*1 @ 200GPa

```
data_image0
_cell_length_a       3.59441
_cell_length_b       3.59533
_cell_length_c       7.74733
_cell_angle_alpha    103.443
_cell_angle_beta     103.408
_cell_angle_gamma    90.0492

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'

loop_
 _atom_site_label
 _atom_site_occupancy
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_thermal_displace_type
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
 Au1      1.0000 0.11251  0.60576  0.54365  Biso   1.000  Au
 Au2      1.0000 0.61244  0.10567  0.54373  Biso   1.000  Au
 Au3      1.0000 0.24240  0.23445  0.80243  Biso   1.000  Au
 Au4      1.0000 0.86677  0.35993  0.05221  Biso   1.000  Au
 Au5      1.0000 0.36659  0.85974  0.05219  Biso   1.000  Au
 Au6      1.0000 0.48827  0.48399  0.29789  Biso   1.000  Au
 Au7      1.0000 0.73793  0.72997  0.79346  Biso   1.000  Au
 H1       1.0000 0.09755  0.09060  0.51340  Biso   1.000  H
 H2       1.0000 0.12357  0.85959  0.30841  Biso   1.000  H
 H3       1.0000 0.87257  0.90626  0.29281  Biso   1.000  H
 H4       1.0000 0.98329  0.37741  0.29826  Biso   1.000  H
 H5       1.0000 0.59643  0.98934  0.29833  Biso   1.000  H
 H6       1.0000 0.06188  0.09412  0.29247  Biso   1.000  H
 H7       1.0000 0.88550  0.86993  0.08128  Biso   1.000  H
```

7.1.3 Au_3H_2 *P*1 @ 200GPa

```
data_image0
_cell_length_a       2.56326
_cell_length_b       8.67412
_cell_length_c       8.05348
_cell_angle_alpha    126.816
_cell_angle_beta     72.6978
_cell_angle_gamma    125.656

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'

loop_
 _atom_site_label
 _atom_site_occupancy
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_thermal_displace_type
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
 Au1      1.0000 0.27372  0.45418  0.16388  Biso   1.000  Au
 Au2      1.0000 0.01667  0.81809  0.15096  Biso   1.000  Au
 Au3      1.0000 0.56982  0.17846  0.82383  Biso   1.000  Au
 Au4      1.0000 0.36221  0.18086  0.52220  Biso   1.000  Au
 Au5      1.0000 0.25728  0.53118  0.81850  Biso   1.000  Au
 Au6      1.0000 0.41325  0.81582  0.75364  Biso   1.000  Au
 Au7      1.0000 0.49763  0.46684  0.46572  Biso   1.000  Au
 Au8      1.0000 0.21476  0.81358  0.44673  Biso   1.000  Au
 Au9      1.0000 0.12325  0.10207  0.10422  Biso   1.000  Au
 H1       1.0000 0.42820  0.41187  0.90576  Biso   1.000  H
 H2       1.0000 0.80018  0.04476  0.32082  Biso   1.000  H
 H3       1.0000 0.87451  0.98036  0.63323  Biso   1.000  H
 H4       1.0000 0.13414  0.62239  0.14190  Biso   1.000  H
 H5       1.0000 0.73003  0.26229  0.31613  Biso   1.000  H
 H6       1.0000 0.80436  0.81726  0.93248  Biso   1.000  H
```

7.1.4 Au_2H *Cm* @ 200GPa

```
data_image0
_cell_length_a       8.26647
_cell_length_b       3.69924
_cell_length_c       3.68411
_cell_angle_alpha    90
_cell_angle_beta     116.707
_cell_angle_gamma    90

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
```

```
loop_
 _atom_site_label
 _atom_site_occupancy
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_thermal_displace_type
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
 Au1     1.0000 0.52334  0.00000  0.69078  Biso   1.000  Au
 Au2     1.0000 0.77332  0.00000  0.44070  Biso   1.000  Au
 Au3     1.0000 0.54049  0.50000  0.20766  Biso   1.000  Au
 Au4     1.0000 0.79049  0.50000  0.95762  Biso   1.000  Au
 Au5     1.0000 0.02334  0.50000  0.69078  Biso   1.000  Au
 Au6     1.0000 0.27332  0.50000  0.44070  Biso   1.000  Au
 Au7     1.0000 0.04049  1.00000  0.20766  Biso   1.000  Au
 Au8     1.0000 0.29049  1.00000  0.95762  Biso   1.000  Au
 H1      1.0000 0.78196  0.00000  0.94947  Biso   1.000  H
 H2      1.0000 0.53182  0.50000  0.69878  Biso   1.000  H
 H3      1.0000 0.28196  0.50000  0.94947  Biso   1.000  H
 H4      1.0000 0.03182  1.00000  0.69878  Biso   1.000  H
```

7.1.5 Au_3H *P*1 @ 200GPa

```
data_image0
_cell_length_a       2.5921
_cell_length_b       4.97381
_cell_length_c       6.1635
_cell_angle_alpha    105.19
_cell_angle_beta     90.0395
_cell_angle_gamma    105.097

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'

loop_
 _atom_site_label
 _atom_site_occupancy
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_thermal_displace_type
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
 Au1     1.0000 0.47462  0.45037  0.19690  Biso   1.000  Au
 Au2     1.0000 0.19075  0.88059  0.14119  Biso   1.000  Au
 Au3     1.0000 0.13799  0.77730  0.52428  Biso   1.000  Au
 Au4     1.0000 0.52538  0.54963  0.80310  Biso   1.000  Au
 Au5     1.0000 0.86201  0.22270  0.47572  Biso   1.000  Au
 Au6     1.0000 0.80925  0.11941  0.85881  Biso   1.000  Au
 H1      1.0000 0.83413  0.16870  0.17325  Biso   1.000  H
 H2      1.0000 0.16587  0.83130  0.82675  Biso   1.000  H
```

7.1.6 Au_4H *P4mm* @ 200GPa

```
data_image0
_cell_length_a       2.60278
_cell_length_b       2.60278
_cell_length_c       7.18758
_cell_angle_alpha    90
_cell_angle_beta     90
_cell_angle_gamma    90

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'

loop_
 _atom_site_label
 _atom_site_occupancy
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_thermal_displace_type
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
 Au1      1.0000 0.00000  0.00000  0.01615  Biso   1.000  Au
 Au2      1.0000 0.50000  0.50000  0.77278  Biso   1.000  Au
 Au3      1.0000 0.00000  0.00000  0.51622  Biso   1.000  Au
 Au4      1.0000 0.50000  0.50000  0.25958  Biso   1.000  Au
 H1       1.0000 0.50000  0.50000  0.51612  Biso   1.000  H
```

7.1.7 Au_5H *Pm* @ 200GPa

```
data_image0
_cell_length_a       8.55032
_cell_length_b       2.5815
_cell_length_c       7.69445
_cell_angle_alpha    90
_cell_angle_beta     134.637
_cell_angle_gamma    90

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'

loop_
 _atom_site_label
 _atom_site_occupancy
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_thermal_displace_type
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
```

```
 Au1     1.0000 0.20121  0.50000  0.88689  Biso   1.000  Au
 Au2     1.0000 0.11539  0.00000  0.09604  Biso   1.000  Au
 Au3     1.0000 0.40834  0.50000  0.49145  Biso   1.000  Au
 Au4     1.0000 0.01039  0.50000  0.29527  Biso   1.000  Au
 Au5     1.0000 0.80619  0.50000  0.68753  Biso   1.000  Au
 Au6     1.0000 0.70121  0.00000  0.88689  Biso   1.000  Au
 Au7     1.0000 0.61539  0.50000  0.09604  Biso   1.000  Au
 Au8     1.0000 0.90834  0.00000  0.49145  Biso   1.000  Au
 Au9     1.0000 0.51039  0.00000  0.29527  Biso   1.000  Au
 Au10    1.0000 0.30619  0.00000  0.68753  Biso   1.000  Au
 H1      1.0000 0.90810  0.50000  0.99100  Biso   1.000  H
 H2      1.0000 0.40810  0.00000  0.99100  Biso   1.000  H
```

7.2 $Au[A]_n$ Binaries (A=Alkali/Alkaline earth metal) not Available in ICSD

Structures of alkali and alkaline earth-gold binaries used can be found in the Inorganic Crystal Structure Database (ICSD). Exceptions mentioned in Table 1 of the main article are reproduced below.

7.2.1 K_2Au *I*4/*mcm* @ 1atm

```
data_image0
_cell_length_a       8.16346
_cell_length_b       8.16346
_cell_length_c       7.54984
_cell_angle_alpha    90
_cell_angle_beta     90
_cell_angle_gamma    90

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
  _symmetry_equiv_pos_as_xyz
  'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_thermal_displace_type
  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
 K1      1.0000 0.80598  0.30598  0.50000  Biso   1.000  K
 K2      1.0000 0.30598  0.19402  0.50000  Biso   1.000  K
 K3      1.0000 0.69402  0.19402  0.00000  Biso   1.000  K
 K4      1.0000 0.19402  0.30598  0.00000  Biso   1.000  K
 K5      1.0000 0.30598  0.80598  0.00000  Biso   1.000  K
 K6      1.0000 0.80598  0.69402  0.00000  Biso   1.000  K
 K7      1.0000 0.19402  0.69402  0.50000  Biso   1.000  K
 K8      1.0000 0.69402  0.80598  0.50000  Biso   1.000  K
 Au1     1.0000 0.00000  0.00000  0.75000  Biso   1.000  Au
 Au2     1.0000 0.00000  0.00000  0.25000  Biso   1.000  Au
 Au3     1.0000 0.50000  0.50000  0.25000  Biso   1.000  Au
 Au4     1.0000 0.50000  0.50000  0.75000  Biso   1.000  Au
```

7.2.2 Cs_2Au_3 *Immm* @ 1atm

```
data_image0
_cell_length_a       5.2461
_cell_length_b       5.57867
_cell_length_c       6.84555
_cell_angle_alpha    114.046
_cell_angle_beta     112.531
_cell_angle_gamma    90

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
  _symmetry_equiv_pos_as_xyz
  'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_thermal_displace_type
  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
  Cs1      1.0000 0.80756  0.30756  0.61512  Biso   1.000  Cs
  Cs2      1.0000 0.19244  0.69244  0.38488  Biso   1.000  Cs
  Au1      1.0000 0.50000  0.24932  0.00000  Biso   1.000  Au
  Au2      1.0000 0.50000  0.75068  1.00000  Biso   1.000  Au
  Au3      1.0000 0.00000  0.00000  0.00000  Biso   1.000  Au
```

7.3 Ternary compounds

7.3.1 $Li_2(PdH_2)_2$ *I4/mmm* @ 1 atm

```
data_image0
_cell_length_a       3.11332
_cell_length_b       3.11332
_cell_length_c       10.2893
_cell_angle_alpha    90
_cell_angle_beta     90
_cell_angle_gamma    90

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
  _symmetry_equiv_pos_as_xyz
  'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_thermal_displace_type
```

```
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
 Li1     1.0000 0.50000  0.50000  0.14623  Biso   1.000  Li
 Li2     1.0000 0.50000  0.50000  0.85377  Biso   1.000  Li
 Li3     1.0000 0.00000  0.00000  0.64623  Biso   1.000  Li
 Li4     1.0000 0.00000  0.00000  0.35377  Biso   1.000  Li
 H1      1.0000 0.00000  0.00000  0.83648  Biso   1.000  H
 H2      1.0000 0.00000  0.00000  0.16352  Biso   1.000  H
 H3      1.0000 0.50000  0.50000  0.33648  Biso   1.000  H
 H4      1.0000 0.50000  0.50000  0.66352  Biso   1.000  H
 Pd1     1.0000 0.00000  0.00000  0.00000  Biso   1.000  Pd
 Pd2     1.0000 0.50000  0.50000  0.50000  Biso   1.000  Pd
```

7.3.2 $Na_2(PdH_2)_2$ *I*4/*mmm* @ 1 atm

```
data_image0
_cell_length_a       3.59658
_cell_length_b       3.59658
_cell_length_c       11.343
_cell_angle_alpha    90
_cell_angle_beta     90
_cell_angle_gamma    90

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'

loop_
 _atom_site_label
 _atom_site_occupancy
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_thermal_displace_type
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
 Na1     1.0000 0.50000  0.50000  0.14031  Biso   1.000  Na
 Na2     1.0000 0.50000  0.50000  0.85969  Biso   1.000  Na
 Na3     1.0000 0.00000  0.00000  0.64031  Biso   1.000  Na
 Na4     1.0000 0.00000  0.00000  0.35969  Biso   1.000  Na
 Pd1     1.0000 0.00000  0.00000  0.00000  Biso   1.000  Pd
 Pd2     1.0000 0.50000  0.50000  0.50000  Biso   1.000  Pd
 H1      1.0000 0.00000  0.00000  0.85072  Biso   1.000  H
 H2      1.0000 0.00000  0.00000  0.14928  Biso   1.000  H
 H3      1.0000 0.50000  0.50000  0.35072  Biso   1.000  H
 H4      1.0000 0.50000  0.50000  0.64928  Biso   1.000  H
```

7.3.3 $LiAuH_2$ *C*2 @ 1 atm

```
data_image0
_cell_length_a       5.00778
_cell_length_b       5.00777
_cell_length_c       6.03552
_cell_angle_alpha    90.0009
```

```
_cell_angle_beta     89.9991
_cell_angle_gamma    120

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'

loop_
 _atom_site_label
 _atom_site_occupancy
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_thermal_displace_type
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
 Li1      1.0000 0.35485  1.00000  0.66668  Biso   1.000  Li
 Li2      1.0000 1.00000  0.35485  0.33332  Biso   1.000  Li
 Li3      1.0000 0.64515  0.64515  0.00000  Biso   1.000  Li
 Au1      1.0000 0.25946  0.99999  0.16666  Biso   1.000  Au
 Au2      1.0000 0.99999  0.25946  0.83334  Biso   1.000  Au
 Au3      1.0000 0.74053  0.74053  0.50000  Biso   1.000  Au
 H1       1.0000 0.35933  0.44012  0.72052  Biso   1.000  H
 H2       1.0000 0.55988  0.91920  0.38719  Biso   1.000  H
 H3       1.0000 0.08079  0.64067  0.05386  Biso   1.000  H
 H4       1.0000 0.44012  0.35933  0.27948  Biso   1.000  H
 H5       1.0000 0.91920  0.55988  0.61281  Biso   1.000  H
 H6       1.0000 0.64068  0.08079  0.94614  Biso   1.000  H
```

7.3.4 $NaAuH_2$ *C*2 @ 1 atm

```
data_image0
_cell_length_a       5.46402
_cell_length_b       5.46402
_cell_length_c       6.42376
_cell_angle_alpha    89.9989
_cell_angle_beta     90.0011
_cell_angle_gamma    120

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'

loop_
 _atom_site_label
 _atom_site_occupancy
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_thermal_displace_type
```

```
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
 Na1     1.0000 0.64594  0.64594  0.50000  Biso   1.000  Na
 Na2     1.0000 0.35406  0.00000  0.16667  Biso   1.000  Na
 Na3     1.0000 0.00000  0.35406  0.83333  Biso   1.000  Na
 Au1     1.0000 1.00000  0.26735  0.33333  Biso   1.000  Au
 Au2     1.0000 0.73264  0.73264  0.00000  Biso   1.000  Au
 Au3     1.0000 0.26735  1.00000  0.66667  Biso   1.000  Au
 H1      1.0000 0.31168  0.42631  0.20986  Biso   1.000  H
 H2      1.0000 0.57368  0.88537  0.87653  Biso   1.000  H
 H3      1.0000 0.11464  0.68833  0.54320  Biso   1.000  H
 H4      1.0000 0.42631  0.31168  0.79014  Biso   1.000  H
 H5      1.0000 0.68833  0.11464  0.45680  Biso   1.000  H
 H6      1.0000 0.88537  0.57368  0.12347  Biso   1.000  H
```

7.3.5 $KAuH_2$ *C*2 @ 1atm

```
data_image0
_cell_length_a       5.96331
_cell_length_b       5.96331
_cell_length_c       7.14353
_cell_angle_alpha    90.0013
_cell_angle_beta     89.9987
_cell_angle_gamma    120.002

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'

loop_
 _atom_site_label
 _atom_site_occupancy
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_thermal_displace_type
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
 K1      1.0000 0.34455  0.00000  0.66667  Biso   1.000  K
 K2      1.0000 0.00000  0.34455  0.33333  Biso   1.000  K
 K3      1.0000 0.65543  0.65543  0.00000  Biso   1.000  K
 Au1     1.0000 0.30409  1.00000  0.16668  Biso   1.000  Au
 Au2     1.0000 1.00000  0.30409  0.83332  Biso   1.000  Au
 Au3     1.0000 0.69591  0.69591  0.50000  Biso   1.000  Au
 H1      1.0000 0.26897  0.43639  0.70451  Biso   1.000  H
 H2      1.0000 0.56361  0.83257  0.37118  Biso   1.000  H
 H3      1.0000 0.16743  0.73104  0.03785  Biso   1.000  H
 H4      1.0000 0.43639  0.26897  0.29549  Biso   1.000  H
 H5      1.0000 0.83257  0.56361  0.62882  Biso   1.000  H
 H6      1.0000 0.73104  0.16743  0.96215  Biso   1.000  H
```

7.3.6 $KAuH_2$ $P2_12_12_1$ @ 1atm

```
data_image0
_cell_length_a       6.23982
_cell_length_b       3.76758
_cell_length_c       6.23975
_cell_angle_alpha    90
_cell_angle_beta     90
_cell_angle_gamma    90

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
  _symmetry_equiv_pos_as_xyz
  'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_thermal_displace_type
  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
  K1       1.0000 0.00000  0.99997  0.00000  Biso   1.000  K
  K2       1.0000 0.50000  0.00003  0.50000  Biso   1.000  K
  Au1      1.0000 0.00000  0.50012  0.50000  Biso   1.000  Au
  Au2      1.0000 0.50000  0.49988  0.00000  Biso   1.000  Au
  H1       1.0000 0.68848  0.49988  0.18853  Biso   1.000  H
  H2       1.0000 0.81152  0.50012  0.68853  Biso   1.000  H
  H3       1.0000 0.18848  0.50012  0.31147  Biso   1.000  H
  H4       1.0000 0.31152  0.49988  0.81147  Biso   1.000  H
```

7.3.7 $KAuH_2$ $I4/mcm$ @ 1atm

```
data_image0
_cell_length_a       8.85414
_cell_length_b       8.85414
_cell_length_c       7.4481
_cell_angle_alpha    90
_cell_angle_beta     90
_cell_angle_gamma    90

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
  _symmetry_equiv_pos_as_xyz
  'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
```

```
 _atom_site_fract_z
 _atom_site_thermal_displace_type
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
 Au1     1.0000 0.00000  0.00000  0.00000  Biso   1.000  Au
 Au2     1.0000 0.00000  0.00000  0.50000  Biso   1.000  Au
 Au3     1.0000 0.00000  0.50000  0.00000  Biso   1.000  Au
 Au4     1.0000 0.00000  0.50000  0.50000  Biso   1.000  Au
 Au5     1.0000 0.50000  0.00000  0.00000  Biso   1.000  Au
 Au6     1.0000 0.50000  0.00000  0.50000  Biso   1.000  Au
 Au7     1.0000 0.50000  0.50000  0.00000  Biso   1.000  Au
 Au8     1.0000 0.50000  0.50000  0.50000  Biso   1.000  Au
 H1      1.0000 0.00000  0.18786  0.00000  Biso   1.000  H
 H2      1.0000 0.31214  0.00000  0.00000  Biso   1.000  H
 H3      1.0000 0.00000  0.31214  0.50000  Biso   1.000  H
 H4      1.0000 0.18786  0.00000  0.50000  Biso   1.000  H
 H5      1.0000 0.00000  0.81214  0.00000  Biso   1.000  H
 H6      1.0000 0.18786  0.50000  0.00000  Biso   1.000  H
 H7      1.0000 0.00000  0.68786  0.50000  Biso   1.000  H
 H8      1.0000 0.31214  0.50000  0.50000  Biso   1.000  H
 H9      1.0000 0.50000  0.31214  0.00000  Biso   1.000  H
 H10     1.0000 0.68786  0.00000  0.00000  Biso   1.000  H
 H11     1.0000 0.50000  0.18786  0.50000  Biso   1.000  H
 H12     1.0000 0.81214  0.00000  0.50000  Biso   1.000  H
 H13     1.0000 0.50000  0.68786  0.00000  Biso   1.000  H
 H14     1.0000 0.81214  0.50000  0.00000  Biso   1.000  H
 H15     1.0000 0.50000  0.81214  0.50000  Biso   1.000  H
 H16     1.0000 0.68786  0.50000  0.50000  Biso   1.000  H
 K1      1.0000 0.25000  0.25000  0.25000  Biso   1.000  K
 K2      1.0000 0.25000  0.25000  0.75000  Biso   1.000  K
 K3      1.0000 0.25000  0.75000  0.25000  Biso   1.000  K
 K4      1.0000 0.25000  0.75000  0.75000  Biso   1.000  K
 K5      1.0000 0.75000  0.25000  0.25000  Biso   1.000  K
 K6      1.0000 0.75000  0.25000  0.75000  Biso   1.000  K
 K7      1.0000 0.75000  0.75000  0.25000  Biso   1.000  K
 K8      1.0000 0.75000  0.75000  0.75000  Biso   1.000  K
```

7.3.8 $KAuH_2$ *I*4/*mcm* @ 50 GPa

```
data_image0
_cell_length_a       7.43053
_cell_length_b       7.43053
_cell_length_c       5.48959
_cell_angle_alpha    90
_cell_angle_beta     90
_cell_angle_gamma    90

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'

loop_
 _atom_site_label
```

```
 _atom_site_occupancy
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_thermal_displace_type
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
 Au1      1.0000 0.00000  0.00000  0.00000  Biso   1.000  Au
 Au2      1.0000 0.00000  0.00000  0.50000  Biso   1.000  Au
 Au3      1.0000 0.00000  0.50000  0.00000  Biso   1.000  Au
 Au4      1.0000 0.00000  0.50000  0.50000  Biso   1.000  Au
 Au5      1.0000 0.50000  0.00000  0.00000  Biso   1.000  Au
 Au6      1.0000 0.50000  0.00000  0.50000  Biso   1.000  Au
 Au7      1.0000 0.50000  0.50000  0.00000  Biso   1.000  Au
 Au8      1.0000 0.50000  0.50000  0.50000  Biso   1.000  Au
 H1       1.0000 0.00000  0.22466  0.00000  Biso   1.000  H
 H2       1.0000 0.27534  0.00000  0.00000  Biso   1.000  H
 H3       1.0000 0.00000  0.27534  0.50000  Biso   1.000  H
 H4       1.0000 0.22466  0.00000  0.50000  Biso   1.000  H
 H5       1.0000 0.00000  0.77534  0.00000  Biso   1.000  H
 H6       1.0000 0.22466  0.50000  0.00000  Biso   1.000  H
 H7       1.0000 0.00000  0.72466  0.50000  Biso   1.000  H
 H8       1.0000 0.27534  0.50000  0.50000  Biso   1.000  H
 H9       1.0000 0.50000  0.27534  0.00000  Biso   1.000  H
 H10      1.0000 0.72466  0.00000  0.00000  Biso   1.000  H
 H11      1.0000 0.50000  0.22466  0.50000  Biso   1.000  H
 H12      1.0000 0.77534  0.00000  0.50000  Biso   1.000  H
 H13      1.0000 0.50000  0.72466  0.00000  Biso   1.000  H
 H14      1.0000 0.77534  0.50000  0.00000  Biso   1.000  H
 H15      1.0000 0.50000  0.77534  0.50000  Biso   1.000  H
 H16      1.0000 0.72466  0.50000  0.50000  Biso   1.000  H
 K1       1.0000 0.25000  0.25000  0.25000  Biso   1.000  K
 K2       1.0000 0.25000  0.25000  0.75000  Biso   1.000  K
 K3       1.0000 0.25000  0.75000  0.25000  Biso   1.000  K
 K4       1.0000 0.25000  0.75000  0.75000  Biso   1.000  K
 K5       1.0000 0.75000  0.25000  0.25000  Biso   1.000  K
 K6       1.0000 0.75000  0.25000  0.75000  Biso   1.000  K
 K7       1.0000 0.75000  0.75000  0.25000  Biso   1.000  K
 K8       1.0000 0.75000  0.75000  0.75000  Biso   1.000  K
```

7.3.9 $KAuH_2$ *P4/mmm* @ 120 GPa

```
data_image0
_cell_length_a       3.46155
_cell_length_b       3.46155
_cell_length_c       2.54059
_cell_angle_alpha    90
_cell_angle_beta     90
_cell_angle_gamma    90

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
```

```
loop_
 _atom_site_label
 _atom_site_occupancy
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_thermal_displace_type
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
 Au1     1.0000 0.00000  0.00000  0.00000  Biso   1.000  Au
 H1      1.0000 0.00000  0.50000  0.00000  Biso   1.000  H
 H2      1.0000 0.50000  0.00000  0.00000  Biso   1.000  H
 K1      1.0000 0.50000  0.50000  0.50000  Biso   1.000  K
```

7.3.10 $RbAuH_2$ *C*2 @ 1 atm

```
data_image0
_cell_length_a       6.20477
_cell_length_b       6.20477
_cell_length_c       7.48732
_cell_angle_alpha    90.0002
_cell_angle_beta     89.9998
_cell_angle_gamma    120

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'

loop_
 _atom_site_label
 _atom_site_occupancy
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_thermal_displace_type
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
 Rb1     1.0000 0.34416  0.00001  0.66666  Biso   1.000  Rb
 Rb2     1.0000 0.00001  0.34416  0.33334  Biso   1.000  Rb
 Rb3     1.0000 0.65585  0.65585  0.00000  Biso   1.000  Rb
 Au1     1.0000 0.30969  0.99996  0.16664  Biso   1.000  Au
 Au2     1.0000 0.99996  0.30969  0.83336  Biso   1.000  Au
 Au3     1.0000 0.69032  0.69032  0.50000  Biso   1.000  Au
 H1      1.0000 0.25492  0.43544  0.70762  Biso   1.000  H
 H2      1.0000 0.56457  0.81950  0.37427  Biso   1.000  H
 H3      1.0000 0.18052  0.74505  0.04093  Biso   1.000  H
 H4      1.0000 0.43544  0.25492  0.29238  Biso   1.000  H
 H5      1.0000 0.81950  0.56457  0.62573  Biso   1.000  H
 H6      1.0000 0.74505  0.18052  0.95907  Biso   1.000  H
```

7.3.11 $CsAuH_2$ *C*2 @ 1 atm

```
data_image0
_cell_length_a       6.48446
_cell_length_b       6.48446
_cell_length_c       7.90403
_cell_angle_alpha    90.0006
_cell_angle_beta     89.9994
_cell_angle_gamma    120

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'

loop_
 _atom_site_label
 _atom_site_occupancy
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_thermal_displace_type
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
 Cs1      1.0000 0.34403  0.99999  0.66667  Biso   1.000  Cs
 Cs2      1.0000 0.99999  0.34403  0.33333  Biso   1.000  Cs
 Cs3      1.0000 0.65601  0.65601  0.00000  Biso   1.000  Cs
 Au1      1.0000 0.31562  0.99999  0.16666  Biso   1.000  Au
 Au2      1.0000 0.99999  0.31562  0.83334  Biso   1.000  Au
 Au3      1.0000 0.68437  0.68437  0.50000  Biso   1.000  Au
 H1       1.0000 0.24078  0.43502  0.71171  Biso   1.000  H
 H2       1.0000 0.56498  0.80575  0.37837  Biso   1.000  H
 H3       1.0000 0.19424  0.75922  0.04503  Biso   1.000  H
 H4       1.0000 0.43502  0.24078  0.28829  Biso   1.000  H
 H5       1.0000 0.80575  0.56498  0.62163  Biso   1.000  H
 H6       1.0000 0.75922  0.19424  0.95497  Biso   1.000  H
```

7.3.12 $Sr(AuH_2)_2$ *I*4 @ 1atm

```
data_image0
_cell_length_a       5.22014
_cell_length_b       5.22014
_cell_length_c       5.22014
_cell_angle_alpha    109.292
_cell_angle_beta     109.292
_cell_angle_gamma    109.831

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'

loop_
 _atom_site_label
```

```
 _atom_site_occupancy
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_thermal_displace_type
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
 Sr1     1.0000 0.59756  0.59756  0.00000  Biso   1.000  Sr
 Au1     1.0000 0.84742  0.34742  0.50000  Biso   1.000  Au
 Au2     1.0000 0.34742  0.84742  0.50000  Biso   1.000  Au
 H1      1.0000 0.65170  0.54282  0.49975  Biso   1.000  H
 H2      1.0000 0.04307  0.15195  0.50025  Biso   1.000  H
 H3      1.0000 0.15195  0.65170  0.10888  Biso   1.000  H
 H4      1.0000 0.54282  0.04307  0.89112  Biso   1.000  H
```

7.3.13 $Ba(AuH_2)_2$ *I*4 @ 1atm

```
data_image0
_cell_length_a       5.46616
_cell_length_b       5.46616
_cell_length_c       5.46616
_cell_angle_alpha    108.177
_cell_angle_beta     108.177
_cell_angle_gamma    112.092

_symmetry_space_group_name_H-M    "P 1"
_symmetry_int_tables_number       1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'

loop_
 _atom_site_label
 _atom_site_occupancy
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_thermal_displace_type
 _atom_site_B_iso_or_equiv
 _atom_site_type_symbol
 Ba1     1.0000 0.59748  0.59748  0.00000  Biso   1.000  Ba
 Au1     1.0000 0.84741  0.34741  0.50000  Biso   1.000  Au
 Au2     1.0000 0.34741  0.84741  0.50000  Biso   1.000  Au
 H1      1.0000 0.66395  0.53076  0.49990  Biso   1.000  H
 H2      1.0000 0.03086  0.16404  0.50010  Biso   1.000  H
 H3      1.0000 0.16404  0.66395  0.13318  Biso   1.000  H
 H4      1.0000 0.53076  0.03086  0.86682  Biso   1.000  H
```