# Supplementary information

# Pressure-induced structures and properties in indium hydrides

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**Table S1** Structural parameters of $InH_3$-*R*-3, $InH_5$-$P2_1/m$ and $InH_5$-*P*-1 structures at selected pressure.

| Space group pressure | Lattice parameters (Å, °) | Atomic coordinates (fractional) | Sites |
|---|---|---|---|
| *R*-3 | a=4.384 | H1 0.401 0.129 0.009 | 18f |
| 100 GPa | b=4.384 | H7 -0.167 0.167 -0.333 | 9e |
| | c=9.510 | In1 0.000 0.000 -0.139 | 6c |
| | α=β=90 | In3 -0.333 0.333 -0.167 | 3b |
| | γ=120 | | |
| $P2_1/m$ | a=4.108 | H1 0.571 0.750 0.430 | 2e |
| 200 GPa | b=2.759 | H2 0.272 0.750 0.294 | 2e |
| | c=7.547 | H3 0.058 0.250 1.142 | 2e |
| | α=γ=90 | H4 0.344 0.250 0.396 | 2e |
| | β=94.697 | H6 0.411 0.250 0.304 | 2e |
| | | H8 0.386 0.750 0.448 | 2e |
| | | H9 0.133 0.750 1.222 | 2e |
| | | H11 0.020 0.750 1.071 | 2e |
| | | H12 0.244 0.250 1.132 | 2e |
| | | H13 0.152 0.750 1.003 | 2e |
| | | In1 -0.106 0.250 0.372 | 2e |
| | | In2 0.600 0.750 1.133 | 2e |
| *P*-1 | a=5.174 | H1 0.098 0.361 0.180 | 2i |
| 300 GPa | b=4.198 | H2 0.358 0.141 0.439 | 2i |
| | c=3.587 | H4 0.106 0.591 0.192 | 2i |
| | α=90.65 | H5 0.143 0.976 0.064 | 2i |
| | β=109.09 | H7 0.614 0.271 0.639 | 2i |
| | γ=90.70 | H8 -0.132 0.228 -0.107 | 2i |
| | | H9 0.351 0.912 0.433 | 2i |
| | | H10 0.605 0.475 0.682 | 2i |
| | | H12 0.618 0.693 0.674 | 2i |
| | | H19 -0.143 0.806 -0.085 | 2i |
| | | In1 0.749 0.499 0.249 | 2i |
| | | In2 0.500 1.000 0.000 | 1d |
| | | In3 0.000 1.000 0.500 | 1b |

**Table S2** Bader analysis for $InH_3$-*R*-3, $InH_5$-*P*$2_1$/*m* and $InH_5$-*P*-1 at 100, 200 and 300 GPa, respectively.

| $InH_3$-*R*-3-100 GPa | | | | | |
|---|---|---|---|---|---|
| Atom | Charge value(e) | δ(e) | Atom | Charge value(e) | δ(e) |
| H | 1.27 | -0.27 | H | 0.99 | 0.01 |
| H | 1.27 | -0.27 | H | 0.99 | 0.01 |
| H | 1.27 | -0.27 | H | 0.99 | 0.01 |
| H | 1.27 | -0.27 | In | 2.50 | 0.50 |
| H | 1.27 | -0.27 | In | 2.50 | 0.50 |
| H | 1.27 | -0.27 | In | 2.41 | 0.59 |

| $InH_5$-*P*$2_1$/*m*-200 GPa | | | $InH_5$-*P*-1-300 GPa | | |
|---|---|---|---|---|---|
| Atom | Charge value(e) | δ(e) | Atom | Charge value(e) | δ(e) |
| H | 1.22 | -0.22 | H | 1.13 | -0.13 |
| H | 1.06 | -0.06 | H | 1.12 | -0.12 |
| H | 1.11 | -0.11 | H | 1.12 | -0.12 |
| H | 1.04 | -0.04 | H | 1.14 | -0.14 |
| H | 1.10 | -0.10 | H | 1.09 | -0.09 |
| H | 1.13 | -0.13 | H | 1.09 | -0.09 |
| H | 1.22 | -0.22 | H | 1.14 | -0.14 |
| H | 1.06 | -0.06 | H | 1.14 | -0.14 |
| H | 1.11 | -0.11 | H | 1.11 | -0.11 |
| H | 1.04 | -0.04 | H | 1.11 | -0.11 |
| H | 1.10 | -0.10 | H | 1.13 | -0.13 |
| H | 1.13 | -0.13 | H | 1.12 | -0.12 |
| H | 1.09 | -0.09 | H | 1.13 | -0.13 |
| H | 1.07 | -0.07 | H | 1.14 | -0.14 |
| H | 1.11 | -0.11 | H | 1.09 | -0.09 |
| H | 1.14 | -0.14 | H | 1.09 | -0.09 |
| H | 1.09 | -0.09 | H | 1.14 | -0.14 |
| H | 1.07 | -0.07 | H | 1.14 | -0.14 |
| H | 1.11 | -0.11 | H | 1.11 | -0.11 |
| H | 1.14 | -0.14 | H | 1.11 | -0.11 |
| In | 2.50 | 0.50 | In | 2.40 | 0.60 |
| In | 2.50 | 0.50 | In | 2.40 | 0.60 |
| In | 2.53 | 0.47 | In | 2.40 | 0.60 |
| In | 2.53 | 0.47 | In | 2.40 | 0.60 |

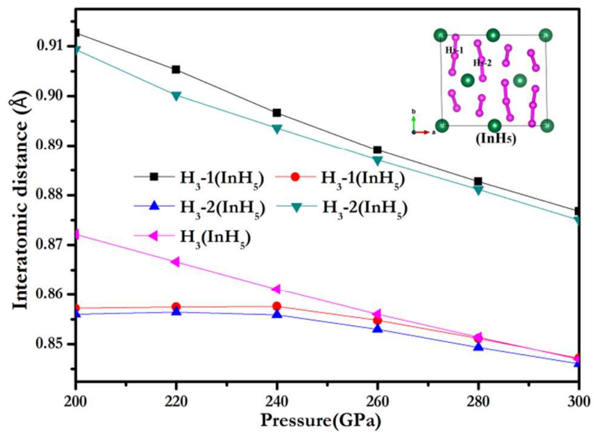


**Figure S1** The pressure dependence of the H-H distance in $H_3$ units in $InH_3$-*R*-3 and $InH_5$-*P*-1 structures. And $H_3$-1 and $H_3$-2 represent the two different types of $H_3$ in $InH_5$-*P*-1 phase.

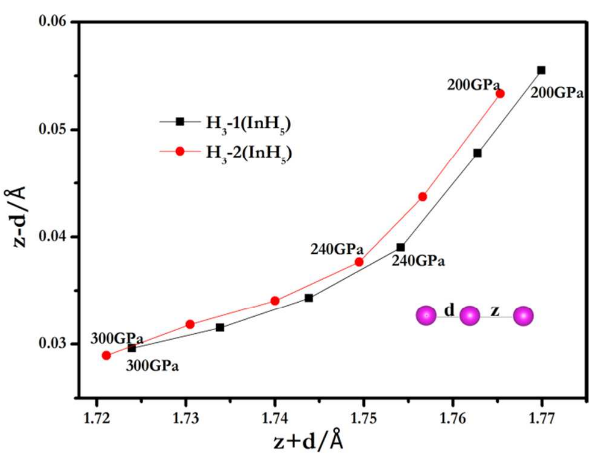


**Figure S2** The difference between the z and d distances in an $H^{-}\cdots H_2$ fragment is plotted vs their sum for $H_3$ units in $InH_5$ at different pressures.