Supplemental Information

Pressure-induced Superconductivity and Structure Phase Transition in Pt_2HgSe_3

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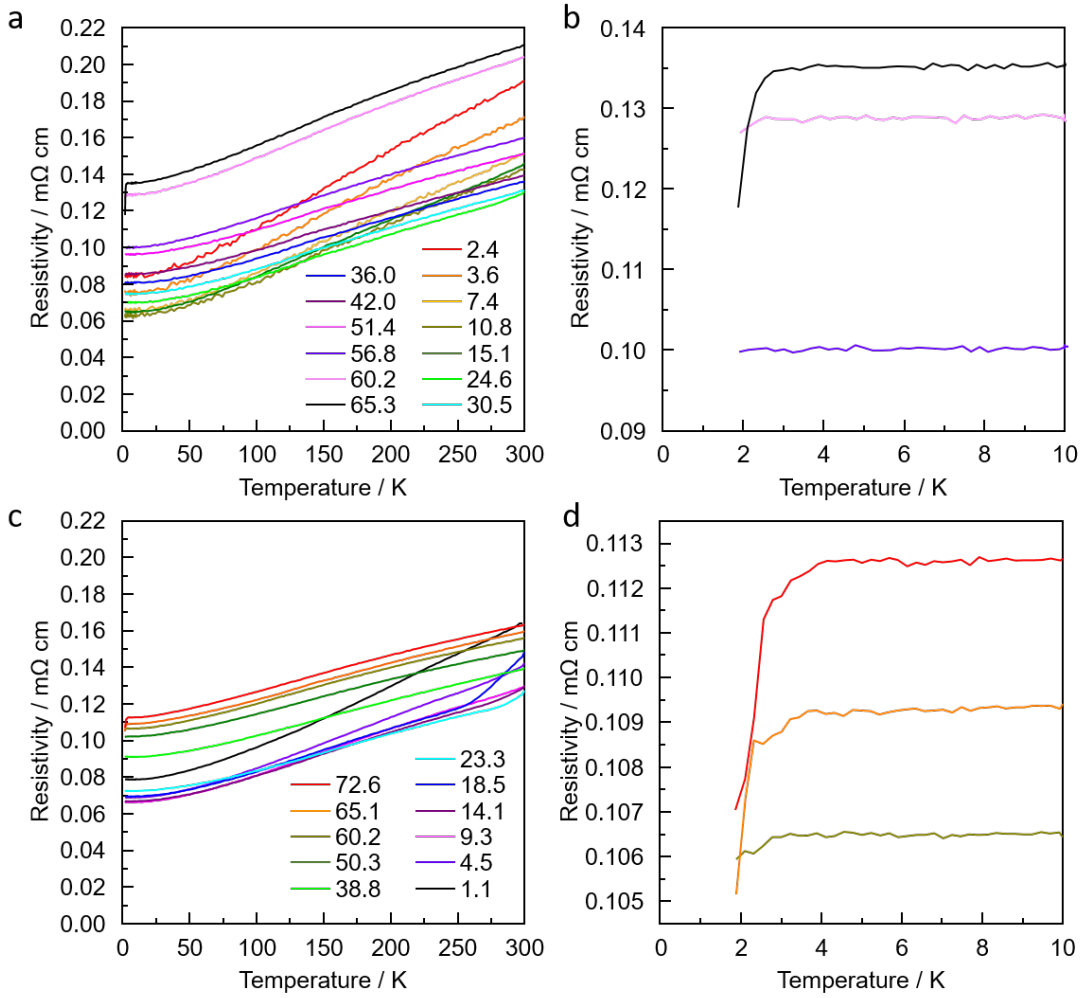
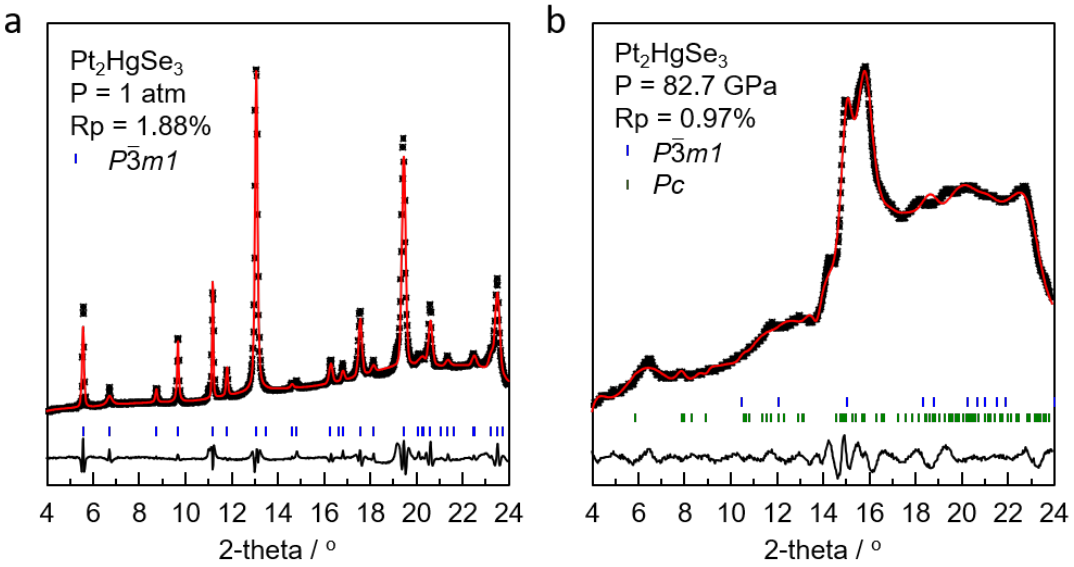
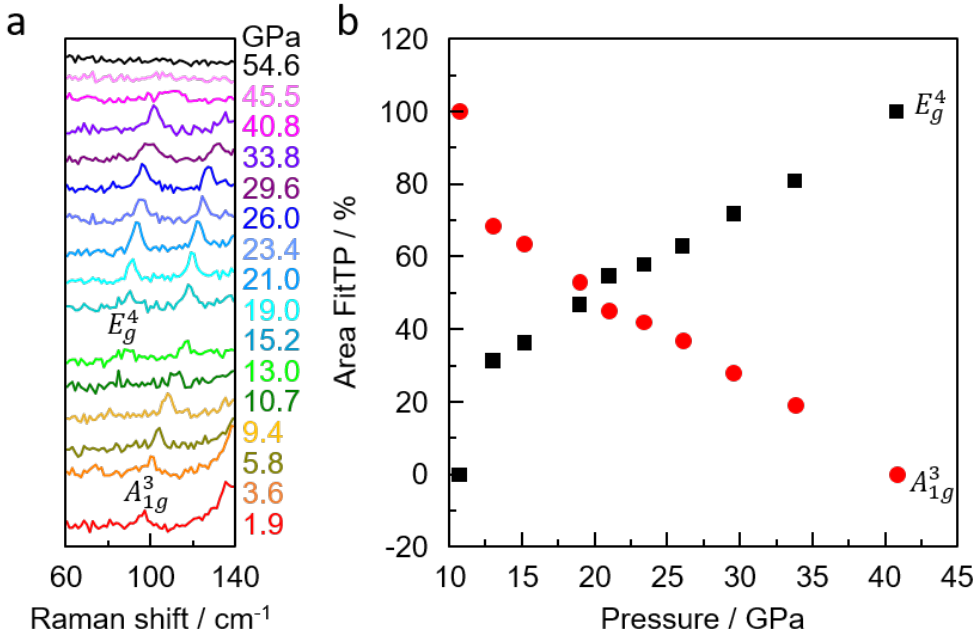


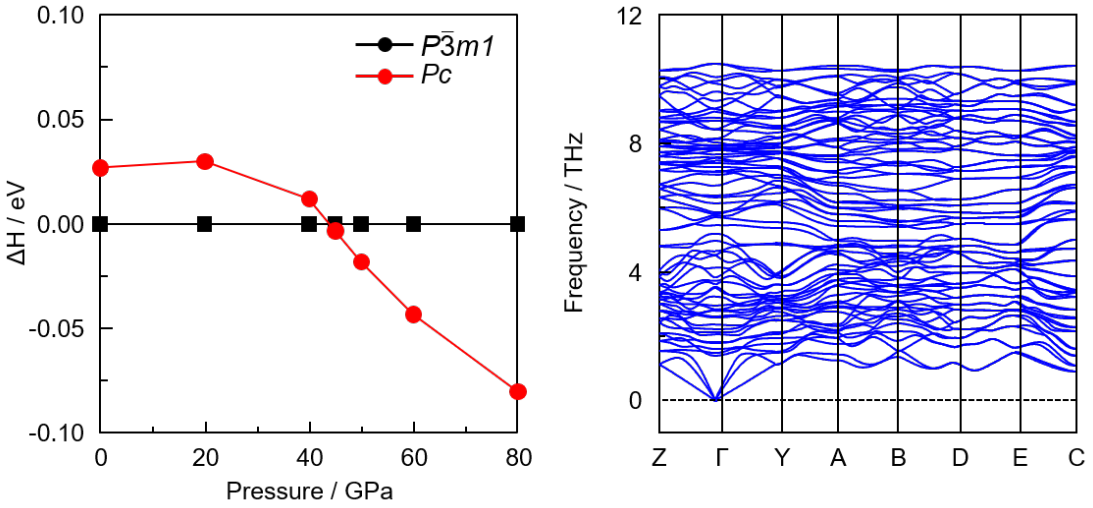
Supplementary Figure 1. (a-b) Electrical resistivity of Pt_2HgSe_3 as a function of temperature for pressures in run I; (c-d) Electrical resistivity of Pt_2HgSe_3 as a function of temperature for pressures in run III; The electrical resistivity drops were shown at low temperatures, indicating the superconducting transition. Since the max pressure is around 70 GPa in run I and run III, we did not observe zero-resistance behavior.



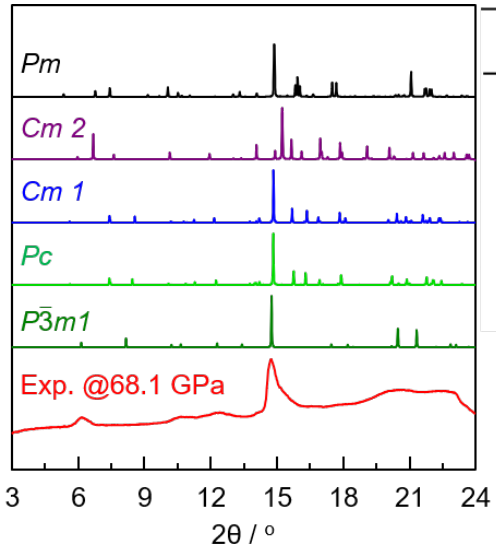
Supplementary Figure 2. Typical Rietveld refinement of Pt_2HgSe_3 at 1atm (a) and 82.7 GPa (b), respectively. The experimental and simulated data are indicated by black stars and red lines, respectively. The solid lines shown at the bottom of the figures are the residual intensities. The vertical bars indicate peak positions of the Bragg reflections for Pt_2HgSe_3 in $P\bar{3}m1$ (blue) and *Pc* (olive) space groups.



Supplementary Figure 3. (a) Raman spectra of Pt_2HgSe_3 under high pressure amplified in the range of 60 to 140 cm^{-1}; (b) fitted peak area of E_g^4 and A_{1g}^3 contained in fitting range from 60 to 150 cm^{-1}.

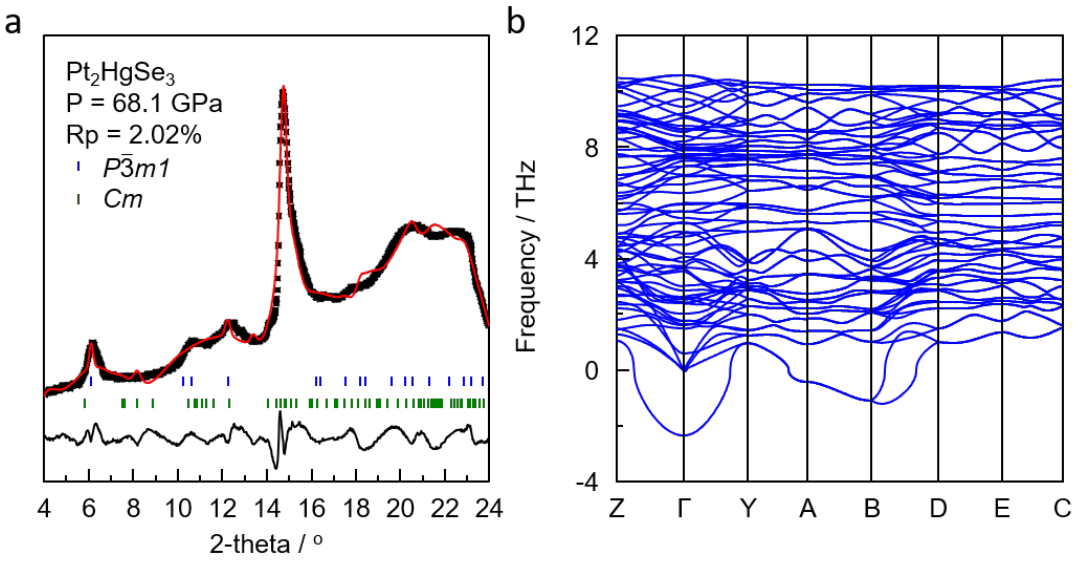


Supplementary Figure 4. (a) Enthalpy curves (relative to *Pc* phase) of Pt_2HgSe_3 as a function of pressure; (b) Calculated phonon dispersion of the *Pc* structure Pt_2HgSe_3 at 68 GPa.

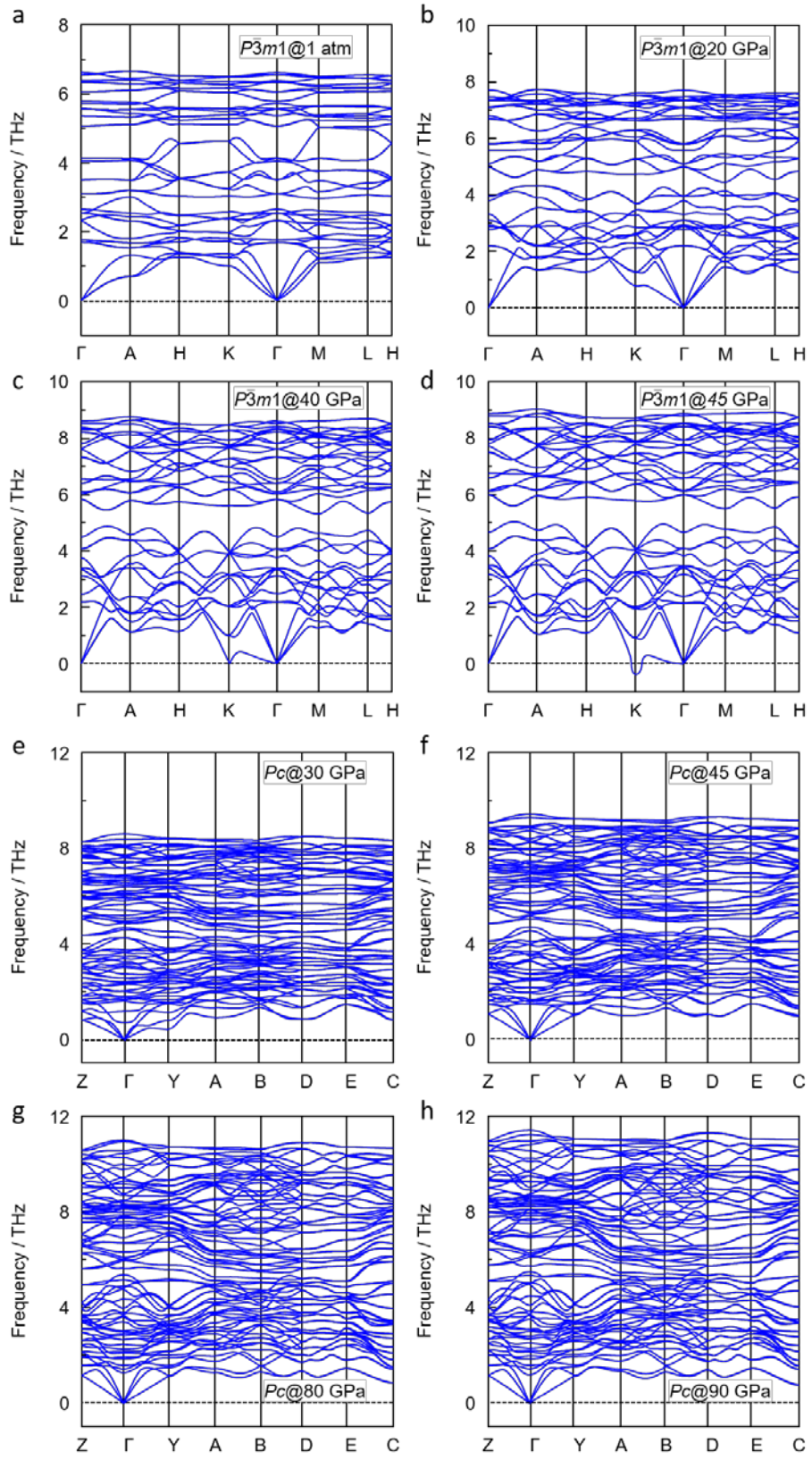


Space group	a / Å	b / Å	c / Å	β / °	Enthalpy eV/atom
Pm	6.9073	4.7926	5.4466	105.2791	3.129
Cm 2	11.0974	2.6055	6.2090	73.6806	3.122
Cm 1	12.6726	6.6089	7.5445	146.5574	3.108
Pc	7.5345	6.5546	12.6281	146.0107	3.103

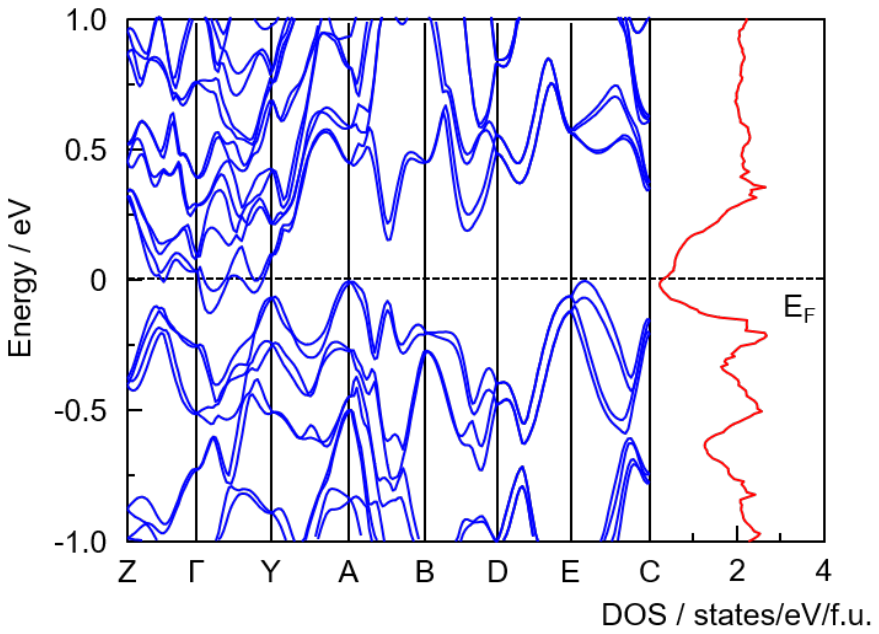
Supplementary Figure 5. Typical simulated XRD patterns of Pt_2HgSe_3 with different structures in comparison with the experimental spectrum at 68.1 GPa (red line). $P\bar{3}m1$ is the structure of phase I. *Pc*, *Cm* (1), *Cm* (2) and *Pm* are the candidates of phase II.



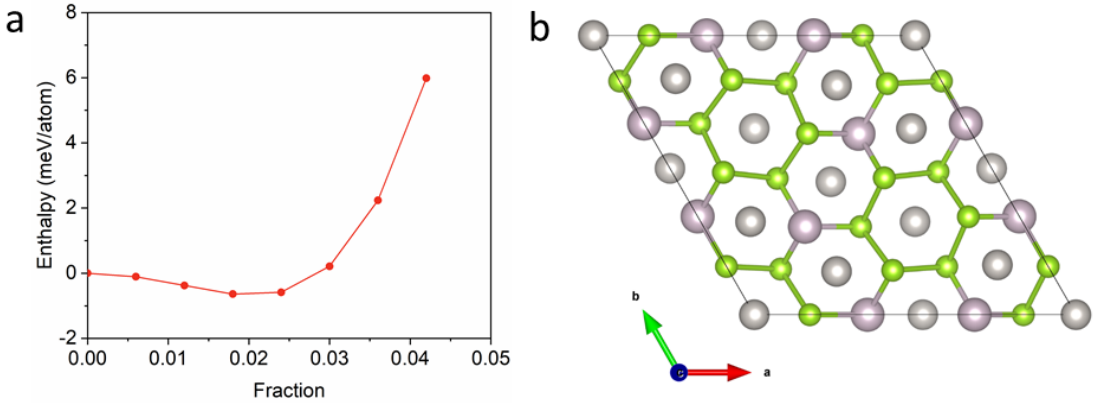
Supplementary Figure 6. (a) Typical Rietveld refinement of Pt_2HgSe_3 at 68.1 GPa. The experimental and simulated data are indicated by black stars and red lines, respectively. The solid lines shown at the bottom of the figures are the residual intensities. The vertical bars indicate peak positions of the Bragg reflections for Pt_2HgSe_3 in $P\bar{3}m1$ (blue) and *Cm* (olive) space groups; (b) Phonon dispersion of Pt_2HgSe_3 in *Cm* space group at 68 GPa.



Supplementary Figure 7. Calculated phonon dispersion of the $P\bar{3}m1$ structure Pt_2HgSe_3 at 1 atm (a), 20 GPa (b), 40 GPa (c) and 45 GPa (d); *Pc* structure Pt_2HgSe_3 at 30 GPa (e), 45 GPa (f), 80 GPa (g) and 90 GPa (h).

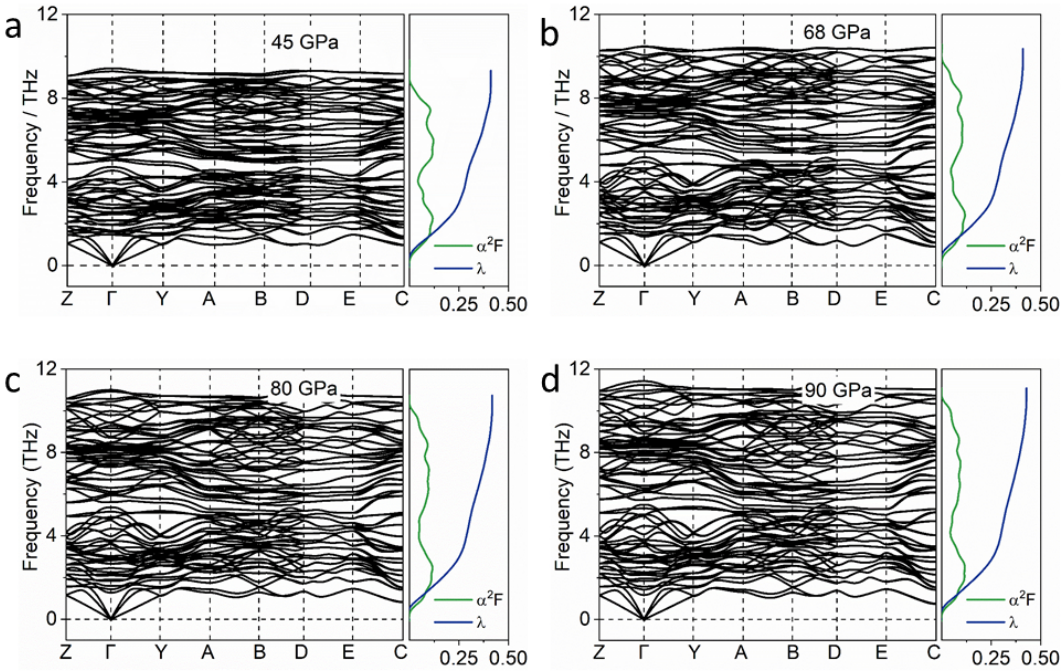


Supplementary Figure 8. Electronic band structure and density of states of Pt_2HgSe_3 at 68 GPa with SOC. red line stands for the DOS of whole.



Supplementary Figure 9. (a) Enthalpy with respect the $P\bar{3}m1$ phase when the atoms are displaced along the eigenvector of the transverse mode at K point; (b) Crystal structure of the $P\bar{3}m1$ phase.

The total energy as a function of the atomic displacements along the eigenvector of the transverse phonon mode at K point for phase I have been calculated. For such a calculation, a 3×3×1 supercell was constructed. A new structure with space group of $P\bar{3}m1$ is found after optimization. The enthalpy is 1 meV/atom lower than the $P\bar{3}m1$ phase (phase I), but 2 meV/atom lower than the Pc phase (phase II) at 45 GPa. These results imply that the softening at K in phase I shown in Figure S7 is not directly associated with an instability towards phase II.



Supplementary Figure 10. (a-d) The phonon dispersion, electron-phonon coupling parameter and Eliashberg spectral function of phase II at 45, 68, 80 and 90 GPa.

Supplementary Table 1. The T_c convergence data with respect to q-mesh.

k-mesh	q-mesh	T_c (K)
3 3 3	1 1 1	1.78
4 4 4	2 2 2	0.76
3 3 3	3 3 3	0.87

Supplementary Table 2. The summary of electron-phonon coupling parameter (λ) and estimated T_c from the Allen-Dynes formula of the Pc phase under high pressures.

P / GPa	45	55	68	80	90
λ	0.41	0.41	0.41	0.42	0.43
T_c / K	0.68	0.69	0.72	0.80	0.87

Appendix (optimized structural parameters in POSCAR format)

P-3m1 (ambient)

```
   1.00000000000000
     7.4948896428286300    0.0000000000000000    0.0000000000000000
    -3.7474448214143150    6.4907648293097955    0.0000000000000000
     0.0000000000000000    0.0000000000000000    5.4542251166764295
   Pt   Hg   Se
     4    2    6
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000
  0.5000000000000000  0.0000000000000000  0.0000000000000000
  0.0000000000000000  0.5000000000000000  0.0000000000000000
  0.5000000000000000  0.5000000000000000  0.0000000000000000
  0.3333333429999996  0.6666666870000029  0.3493550214678152
  0.6666666269999979  0.3333333129999971  0.6506449485321824
  0.8277778371501867  0.1722221478498227  0.2334687530243258
  0.1722221628498133  0.8277778371501796  0.7665312619756719
  0.8277778371501796  0.6555556743003663  0.2334687530243258
  0.1722221478498227  0.3444443256996337  0.7665312619756719
  0.3444443256996337  0.1722221628498204  0.2334687530243258
  0.6555556743003663  0.8277778371501796  0.7665312619756719
```

P-3m1 (20 GPa)

```
   1.00000000000000
     7.0950748245798341    0.0000000000000000    0.0000000000000000
    -3.5475374122899170    6.1445150400466071   -0.0000000000000000
     0.0000000000000000    0.0000000000000000    4.9735498264961349
   Pt   Hg   Se
     4    2    6
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000
  0.5000000000000000  0.0000000000000000  0.0000000000000000
  0.0000000000000000  0.5000000000000000  0.0000000000000000
  0.5000000000000000  0.5000000000000000  0.0000000000000000
  0.3333333429999996  0.6666666870000029  0.3519128351466755
  0.6666666269999979  0.3333333129999971  0.6480871348533221
  0.8303178385765493  0.1696821464234247  0.2697453146980688
  0.1696821614234507  0.8303178385765776  0.7302547003019358
  0.8303178385765776  0.6606356771531482  0.2697453146980688
  0.1696821464234247  0.3393643228468518  0.7302547003019358
  0.3393643228468730  0.1696821614234224  0.2697453146980688
  0.6606356771531269  0.8303178385765776  0.7302547003019358
```

P-3m1 (45 GPa)

1.00000000000000

6.7703754221268468 0.0000000000000000 0.0000000000000000

-3.3851877110634234 5.8633171163211912 -0.0000000000000000

0.0000000000000000 0.0000000000000000 4.8549508312246488

Pt Hg Se

4 2 6

Direct

-0.0000000000000000 -0.0000000000000000 -0.0000000000000000

0.5000000000000000 -0.0000000000000000 -0.0000000000000000

-0.0000000000000000 0.5000000000000000 -0.0000000000000000

0.5000000000000000 0.5000000000000000 -0.0000000000000000

0.3333333429999996 0.6666666870000029 0.3522883129092710

0.6666666269999979 0.3333333129999971 0.6477116570907265

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0.1680223389588950 0.8319776610410766 0.7131627280855453

0.8319776610410766 0.6639553220821461 0.2868372869144525

0.1680223239589257 0.3360446779178539 0.7131627280855453

0.3360446779178254 0.1680223389589234 0.2868372869144596

0.6639553220821746 0.8319776610410766 0.7131627280855453

Pc (45GPa)

1.00000000000000

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0.0000000000000000 6.7693886291358831 0.0000000000000000

-4.7217811915522399 0.0000000000000000 7.2260615667631862

Pt Hg Se

8 4 12

Direct

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0.5670782847853310 0.2418857736669688 0.6908018735106919

0.4436513932727016 0.7300611092165232 0.7170646918524707

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0.0980914311767791 0.7709392211119515 0.6937295308974952

0.7472545660029760 0.7361016570473066 0.6665163305349515

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0.9015209203157590 0.2500118014941084 0.7102536178054771
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0.3998993993147575 0.4771458051336402 0.4430355220608600
0.2330960096326874 0.7504034883614837 0.1719678987712452
0.9015209203157590 0.7499881985058916 0.2102536178054771

Pc (68GPa)
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0.0000000000000000 6.5546147531536301 0.0000000000000000
-4.6014738027300295 0.0000000000000000 7.0576844564793149
Pt Hg Se
8 4 12
Direct
0.0517311736889317 0.0062478138416418 0.4349838829910236
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0.5687047298179446 0.2448284036716459 0.6904085441953213
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0.3859492298687266 0.0221248449940166 0.9715494769614385
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0.4022049822734138 0.4834002957995219 0.4421112507362756
0.2371148094777433 0.7517938927728244 0.1763145317485728
0.9005246741738617 0.7489141707373068 0.2051339472644707

Pc (80 GPa)

1.00000000000000

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0.0000000000000000 6.4436304308872128 0.0000000000000000

-4.5571148129415304 0.0000000000000000 7.0136870045807269

Pt Hg Se

8 4 12

Direct

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