Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Superconducting Be_2SH_3 with hydrogen kagome lattice at high pressure

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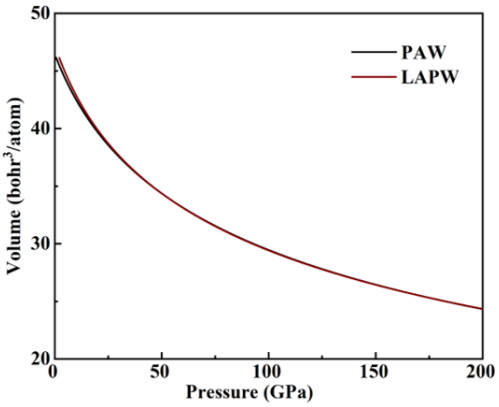

Fig. S00 Comparison of the fitted Birch-Murnaghan equation of states for *P*6/*mmm* Be_2SH_3 using calculated results with the PAW pseudopotentials and full-potential LAPW methods.

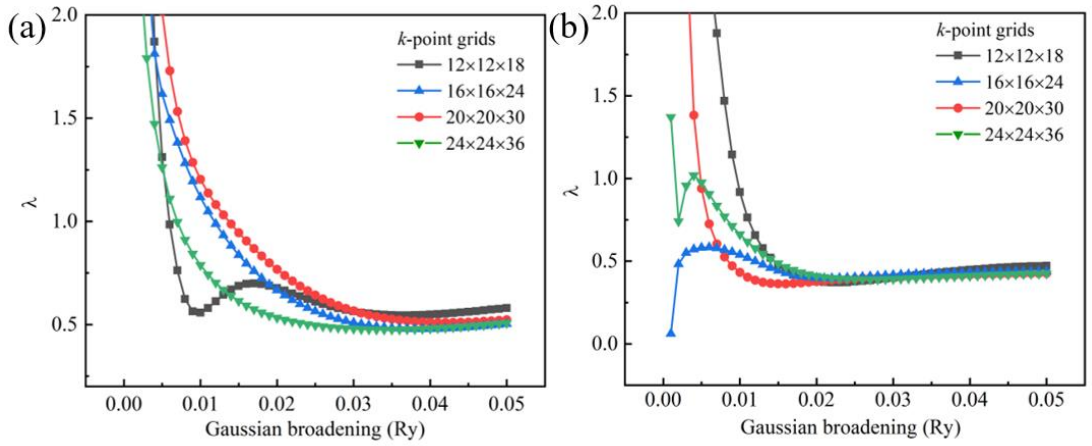

Fig. S01 Electron-phonon coupling constant, λ, versus Gaussian broadening, σ, for *P*6/*mmm* Be_2SH_3 at 200 GPa at q = (0, 0, 0) (a) and q = (0, 0, 0.554628) (b) using various k-grids. In (a) and (b) the k-meshes 16 × 16 × 24 are considered to be converged for acquiring an accurate λ .

Table. S1. Superconducting parameters for *P6/mmm* Be_2SH_3 at 200 GPa: electron-phonon coupling parameter (λ), logarithmic average of phonon frequencies (ω_{log}) and estimated superconducting critical temperature (T_c) for values of the Coulomb pseudopotential, using the listed q-grids.

q-meshes	λ	ω_{log} (K)	T_c (K)
4 × 4 × 6	0.53	1161.28	18
6 × 6 × 9	0.58	1029.08	22

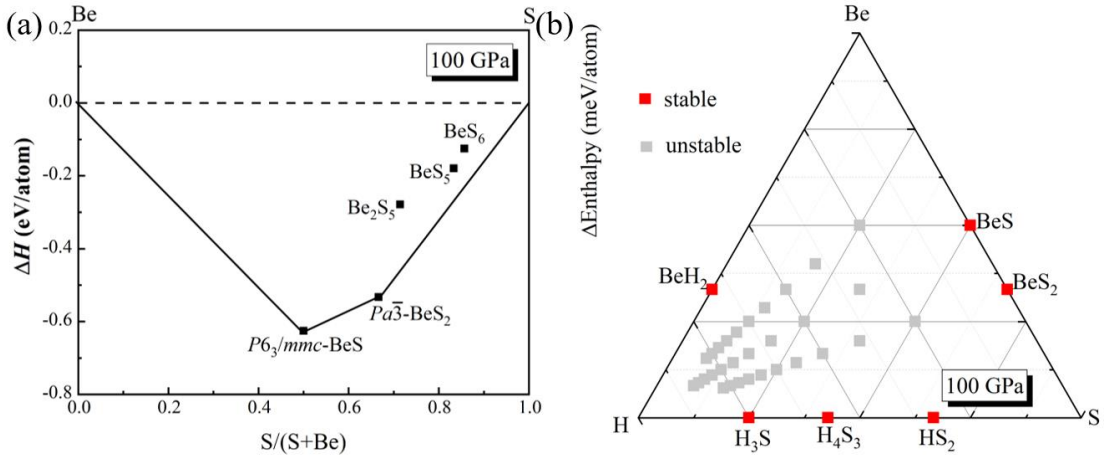

Fig. S1 (a) Convex hull of Be-S system and (b) Phase diagram of Be-S-H system at 100 GPa.

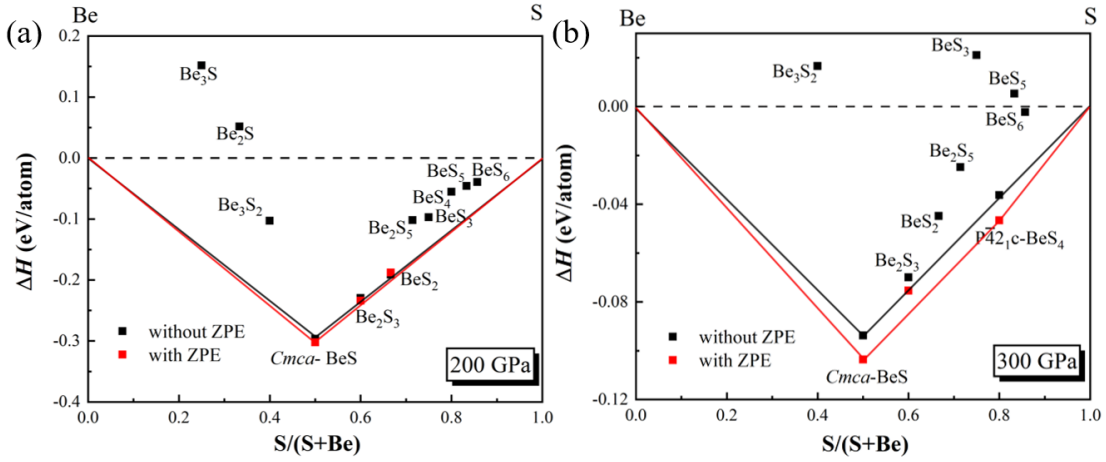

Fig. S2 Phase diagram of Be-S system at (a) 200 GPa, (b) 300 GPa. Convex hulls are shown as continuous lines, with (red) and without (black) the inclusion of zero-point vibrational enthalpy (ZPE).

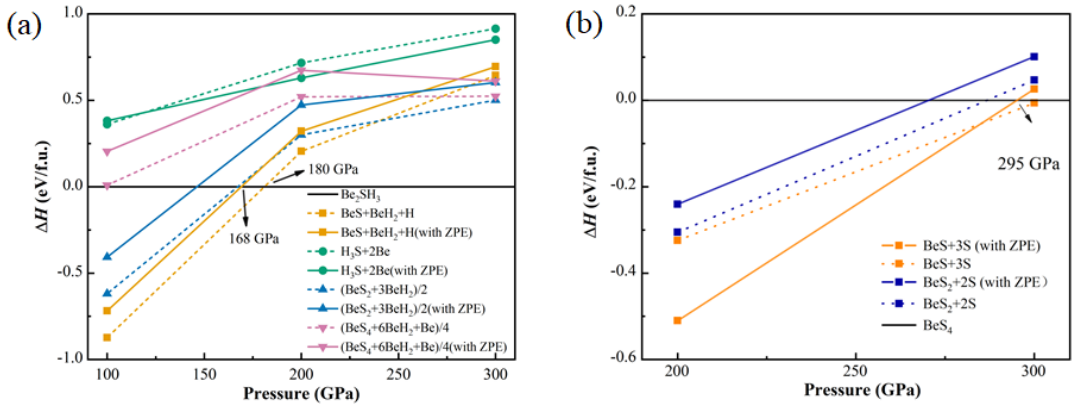

Fig. S3 The calculated formation enthalpy of (a) *P6/mmm* Be_2SH_3 and (b) $P\bar{4}2_1c$ BeS_4 and crystal as a function of pressure relative to the competing element and binary compounds.

Table. S2. Charge transfer of Be, S and H atoms in one unit cell. The negative and positive signs indicate electron gain and loss, respectively.

Phases	Pressure (GPa)	Atoms	Charge (e)
$P\bar{4}2_1c$ BeS_4	180	Be (2*a*)	-1.63
		S (8*e*)	0.41
$P\bar{4}2_1c$ BeS_4	300	Be (2*a*)	-1.62
		S (8*e*)	0.41
P6/mmm Be_2SH_3	100	Be (2*d*)	-1.65
		S (1*b*)	0.97
		H (3*f*)	0.78
P6/mmm Be_2SH_3	200	Be (2*d*)	-1.65
		S (1*b*)	1.11
		H (3*f*)	0.73
P6/mmm Be_2SH_3	300	Be (2*d*)	-1.64
		S (1*b*)	1.17
		H (3*f*)	0.70

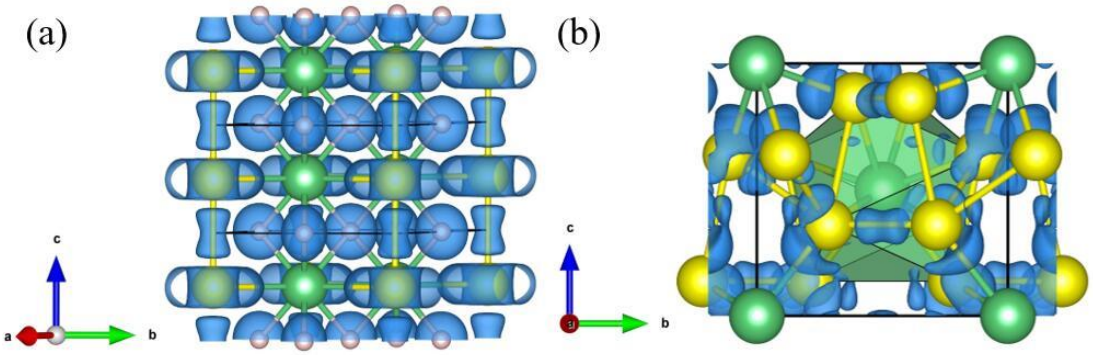

Fig. S4 The ELF of (a) *P6/mmm* Be_2SH_3 at 200 GPa and (b) $P\bar{4}2_1c$ BeS_4 at 300 GPa, the ELF isosurfaces with a value of 0.75.

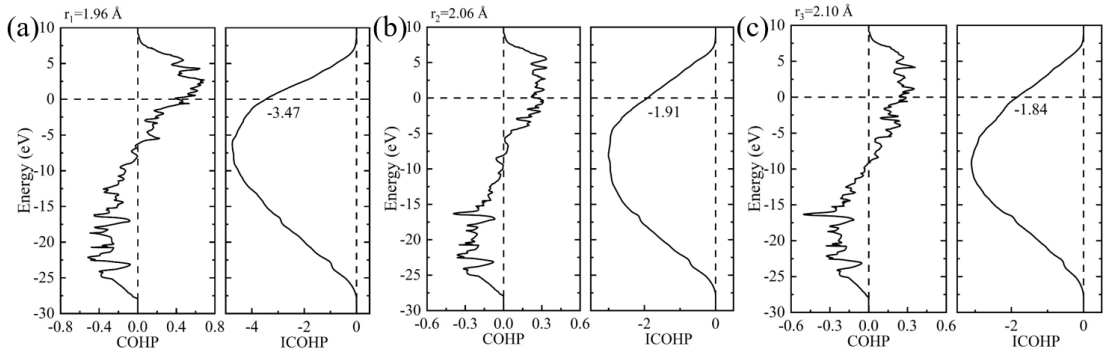

Fig. S5 The calculated Crystalline Orbital Hamiltonian Population (COHP) and Integrated Crystalline Orbital Hamiltonian Population (ICOHP) of BeS_4 with S-S distances of (a) 1.96, (b) 2.06 and (c) 2.10 Å at 300 GPa. The horizontal lines present the Fermi levels. The negative COHP indicates bonding and positive COHP indicates antibonding and the negative ICOHP values represent the bonding interactions between the S atoms.

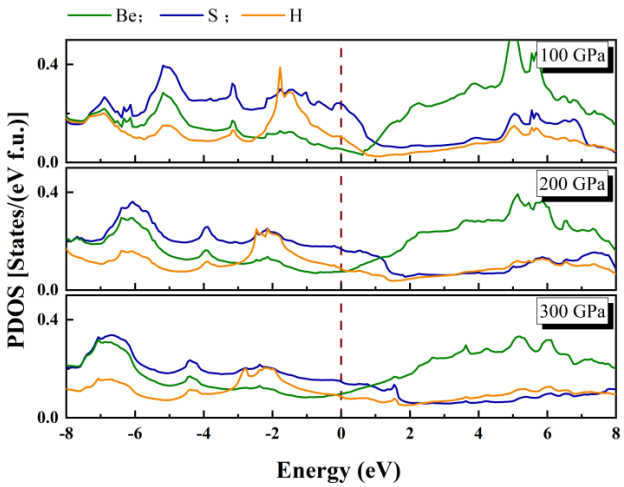

Fig. S6 Atom-projected density of states near the Fermi level for *P6/mmm* Be_2SH_3 at 100 GPa, 200 GPa and 300 GPa.

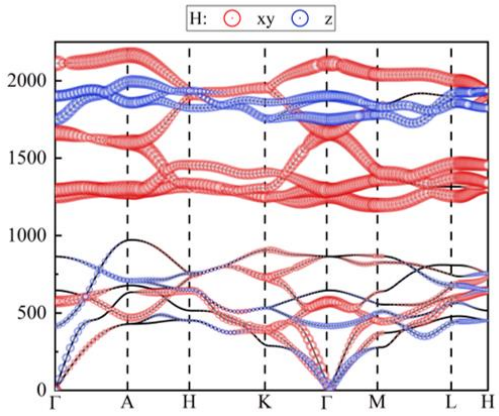

Fig. S7. Calculated phonon spectra for *P*6/*mmm* Be_2SH_3 at 200 GPa highlighting the primary nature of the different modes. *xy* shown as red are in-plane vibrations and *z* shown as blue are out-of-plane vibrations.

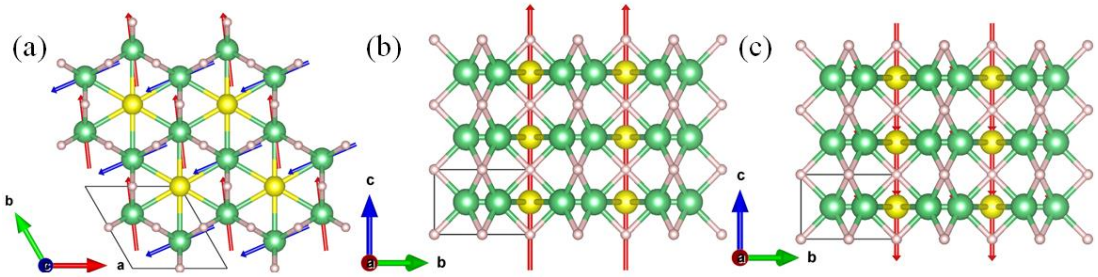

Fig. S8 The vibrational modes at (a) Γ-A (b) H-K and (c) M-L of *P*6/*mmm* Be_2SH_3 at 100 GPa. The arrows represent the direction of atomic vibration.

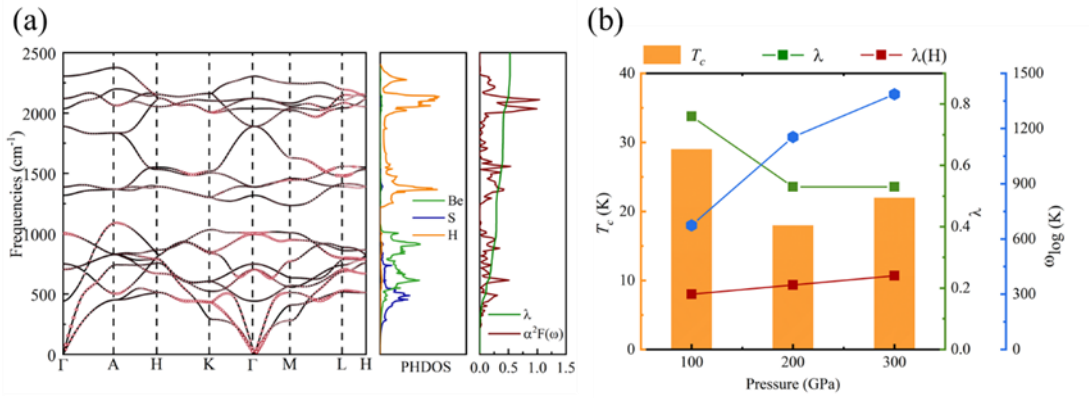

Fig. S9 (a) Phonon-dispersion curves, PHDOS, projected on the Be, S, and H atoms, Eliashberg spectral function, $\alpha^2F(\omega)$ and λ for *P*6/*mmm* Be_2SH_3 at 300 GPa. (b) Pressure dependence of T_C, the logarithmic average phonon frequency ω_{log}, the total EPC parameter λ and the contribution of H atoms to the total λ, namely λ(H), for *P*6/*mmm* Be_2SH_3.

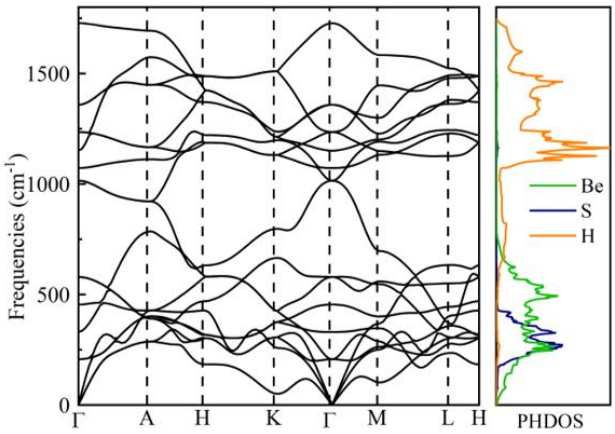

Fig. S10 Phonon dispersion curves of *P6/mmm* Be_2SH_3 at the pressure of 60 GPa, PHDOS, projected on the Be, S, and H atoms.

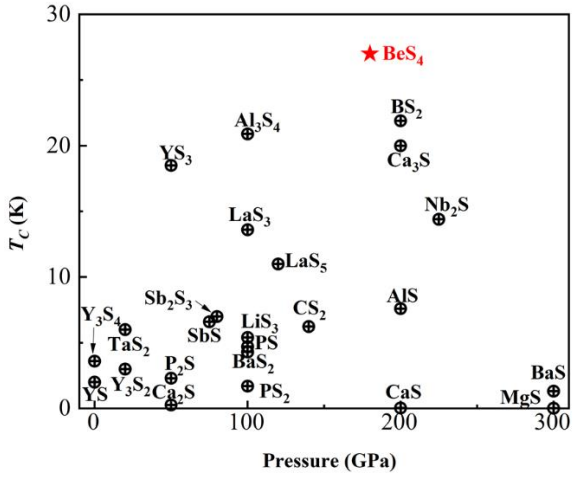

Fig. S11 T_c values of the reported binary chalcogenides at high pressure.

Table S3. The structure information of *P6/mmm* Be_2SH_3 at 200 GPa and $P\bar{4}2_1c$ BeS_4 at 300 GPa.

Space group Pressure	Lattice parameters (Å)	Atomic coordinates				Sites
P6/mmm Be_2SH_3	a=3.48	Be	0.33333	0.66667	0.50000	2*d*
200 GPa	c=2.06	S	0.00000	-0.00000	0.50000	1*b*
		H	0.50000	-0.00000	0.00000	3*f*
$P\bar{4}2_1c$ BeS_4	a=4.21	Be	0.00000	0.00000	0.00000	2*a*
300 GPa	c=4.37	S	0.88184	0.70802	0.37436	8*e*