

Room temperature, one atmosphere

Shashank Dixit, ERP.AI · 6 October 2026 · Draft 4

No material is known to superconduct at room temperature and ambient pressure, so a model to find one has no examples. The target needs pairing and phase-stiffness scales above 300 K in a phase persisting at one atmosphere; no reproduced superconductor is within a factor of two on all three. For phonon pairing the known large-coupling limit is $k_B T_c \rightarrow 0.1827 \hbar \sqrt{S}$, with the Hopfield sum S fixed by a sum rule at fixed structure and linear coupling. Four published spectra of ambient-pressure hydride candidates reach 0.35 to 0.52 of it. A single mode needs a hydrogen Hopfield parameter of 8.7 to 12 eV/Å² for 300 K; the largest found at ambient pressure is 5.2. This parameter is hydrogen density times a scattering strength per proton, known for an electron gas (2.3 to 2.5 e^2 at metallic densities) and 23 eV Å within a factor of about 1.5 across 75 published calculations. At the densest hydrogen known near one atmosphere typical values give about 70 to 150 K, and the largest computed scattering strength and efficiency about 200 K; no factor is bounded. In 8,323 near-hull compounds calculated T_c has an exponential tail, scale 4.0 K, that fails at the sample's top. No hydride predicted above 60 K at ambient pressure has been made at, or recovered to, one atmosphere. We specify a model, roomtsc, with supervised label S , and fix baselines and tests before training.

A search without examples

The highest transition temperature of any equilibrium phase at ambient pressure has belonged to the mercury cuprates since 1993, at 133 to 135 K in HgBa₂Ca₂Cu₃O_{8+δ} [1, 2] and 138 K with partial thallium substitution [3]. For a phonon-mediated superconductor at ambient pressure it is 39 K, in MgB₂, found in 2001 and still the record in a 2025 survey [4, 5]. Under pressure the accepted record is about 250 K, in LaH₁₀ near 170 GPa, with zero resistance, an isotope effect and reproduction by a second group [6, 7].

Later reports exceed these values, and we found no independent reproduction of any. A 2025 preprint reports resistive onsets up to 298 K in LaSc₂H₂₄ at 260 GPa, without a measurement of magnetic screening or an isotope substitution [8]. A second group saw no transition between 245 and 300 K in the four cells that gave transport data, and identified the claimed phase by diffraction in none [9]. A 2026 paper reports a pressure-quenched state of HgBa₂Ca₂Cu₃O_{8+δ} with a resistive onset of up to 151 K at ambient pressure. Zero resistance is not reported [10]. Another 2026 paper claims phonon-mediated transitions at 112 to 187 K at ambient pressure in boron-doped quenched carbon [11]. Figure 1 shows both records against time.

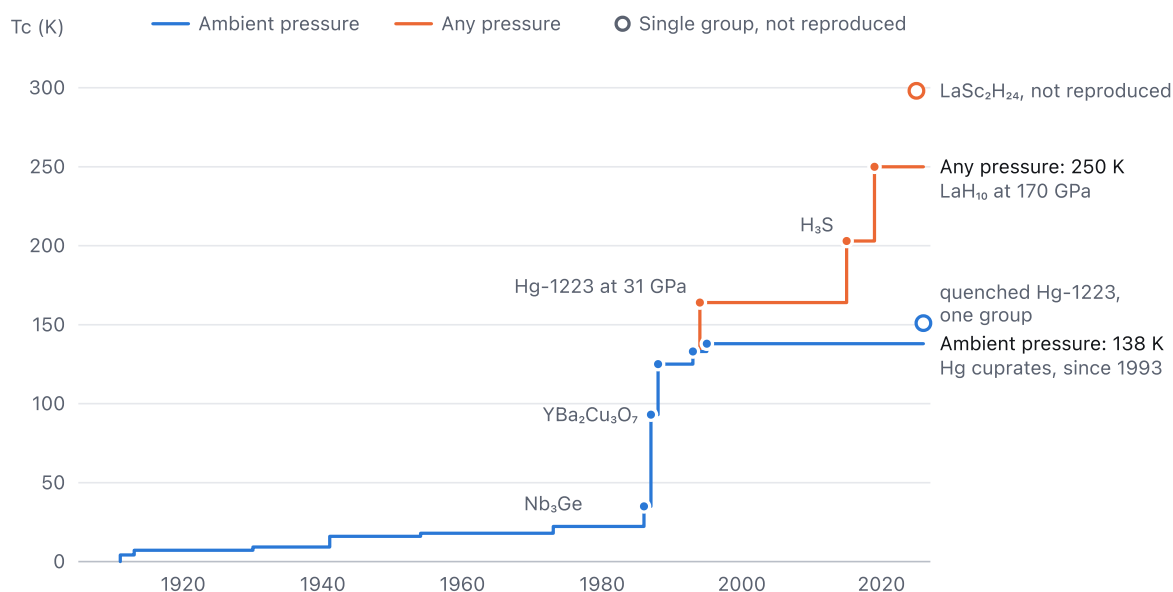


Figure 1. Highest accepted superconducting transition temperature by year, at ambient pressure and at any pressure. Open markers are two single-group results that have not been independently reproduced: the pressure-quenched state of Hg-1223 (onset 151 K, ambient pressure, metastable) and $\text{LaSc}_2\text{H}_{24}$ (onset 298 K at 260 GPa). Retracted claims and the quenched-carbon claim are not plotted. Values and sources are in the data file that accompanies the paper.

A model built to find a superconductor at 300 K and one atmosphere therefore has no example to learn from, and the nearest verified material is a factor of 2.2 to 2.3 below the target.

A random-forest model of T_c from chemical composition reaches R^2 of 0.88 for $\ln T_c$ on a random train-test split of the SuperCon entries above 10 K, but one trained on low- T_c compounds alone underestimates cuprates and iron-based materials [12]. Random splits overstate what such a model can do in discovery [13]. SuperCon holds many doping series [12], and near-duplicate compositions account for part of the high score of a nearest-neighbour model on such a split [14].

Five superconductors first suggested by a learned model have been made with an identified phase in three peer-reviewed reports, at 0.8 to 5.4 K [15, 16, 17], and a fourth adds Pd_2NiTe_2 at 1.1 K [18, 19]. Nine alloys from a generative model superconduct at 4.8 to 9.7 K without forming the predicted structure [20], and a signal near 9 K has no isolated phase [21]. All were found at ambient pressure and are below 10 K. Mg_2RhH_6 , from a machine-learning-accelerated search [22], reaches 29 K at 53 GPa [23]. The target is ten times that.

Two of the five came from a model of the electron-phonon spectral function. Its authors state that it is unlikely to predict hydride-like high- T_c materials, because its training spectra are at ambient pressure and truncated at 100 meV [16].

This paper asks what limits superconductivity at 300 K and one atmosphere and what a model aimed at that target should estimate, and it makes five claims.

A transition at 300 K and one atmosphere needs a pairing scale and a phase-stiffness scale above 300 K [24] in a phase that persists at one atmosphere. LaH₁₀ at 170 GPa pairs to 250 K, has a stiffness scale far above that, and does not exist at one atmosphere. The mercury cuprate exists there with a stiffness scale of 130 to 190 K and a spectroscopic gap scale above 300 K that may not be a pairing gap [25, 26]. MgB₂ exists there with a stiffness scale of 1400 K and pairs at 39 K. No material with a reproduced transition is within a factor of two of the target on all three at once.

For phonon-mediated pairing we use a known limit, $k_B T_c \rightarrow 0.1827 \hbar \sqrt{S}$ at large coupling, where the Hopfield sum S is the sum over atoms of the Hopfield parameter divided by the mass [27, 28, 29]. S is an upper scale for T_c , and the published hydride spectra for which we solved the Eliashberg equations reach about half of it or less. By a sum-rule identity S is fixed at fixed structure and linear coupling, so renormalising the phonons cannot change it. It is not protected against Fermi-surface sampling at a density-of-states peak, a change of structure under nuclear quantum motion, or a non-linear or averaged vertex.

The Hopfield parameter of hydrogen, η_H , is its number density times a scattering strength per proton, h . For a proton in an electron gas h is the free-electron limit of the Gaspari-Gyorffy formula [30], with self-consistent calculations since 1974 [31, 32, 33, 34], and our evaluation gives about 2.3 to 2.5 e^2 at metallic densities. Our addition is the normalisation, with a census of 75 published calculations of 68 hydrides in which S scales with hydrogen density and h is 23 eV Å to within a factor of about 1.5. Megabar hydrides have 5.7 times the hydrogen density of ambient-pressure ones and an h about 40% higher, so density carries most of the difference in η_H . Within each of the five megabar hydrides computed by Quan and coauthors, further pressure lowers T_c [28]. At a hydrogen density of 0.10 Å⁻³, about the highest known near one atmosphere, typical values of h and of the efficiency give about 70 to 150 K, and the largest h and best efficiency computed so far give about 200 K. None of the factors is bounded.

In the 8,323 compounds within 50 meV per atom of the convex hull that we recovered from the figures of the largest ambient-pressure survey [5], the fraction above a given calculated T_c falls exponentially between 2 and about 30 K, with a scale of 4.0 K. The sample is not a random draw, and the exponential form fails at its top, where it gives 34 K for the largest value and the sample has 54 K. These data cannot say whether a calculated 300 K lies in the tail; our conclusion that it does not rests on the Hopfield sum. If true values have an exponential tail and calculations a log-normal error whose size we have not estimated, selection on the calculated value overstates the leaders by factors we tabulate.

No hydride predicted to superconduct above 60 K at ambient pressure has been made at, or recovered to, one atmosphere. Of eleven named predictions, Mg₂IrH₆ and Mg₂PtH₆ did not form when their metals were heated in hydrogen [35, 36], Li₂AuH₆ and Li₂AgH₆ are unstable in one path-integral simulation [37], Li₂CuH₆ stayed intact in a short simulation with classical nuclei [38], and for six we found no test. Mg₂RhH₆, predicted at 45 to 59 K, is the one member of its family that has been made, and it reverted below about 30 GPa on decompression [23].

We then specify a model, roomtsc, whose supervised label is S , with its baselines and its tests. None of it has been trained.

Three conditions

Superconductivity at a temperature T requires that electrons are paired at T and that the pairs are phase coherent at T . Emery and Kivelson wrote this as two temperature scales, each of which limits T_c [24, 25]:

$$T_c \lesssim \min(T_{\text{pair}}, T_\theta). \quad (1)$$

T_{pair} is the temperature at which pairs form, estimated from the zero-temperature gap as $k_B T_{\text{pair}} = \Delta_0/2$. T_θ is the temperature at which phase order would be lost if the pairs survived. It is set by the superfluid stiffness at zero temperature, which is obtained from the magnetic penetration depth λ_L :

$$k_B T_\theta = A \frac{\hbar^2 a}{4\mu_0 e^2 \lambda_L^2}, \quad (2)$$

with $A \approx 0.9$ and a the layer spacing d for a layered material, and $A \approx 2.2$ and $a = \sqrt{\pi} \xi$ for an isotropic one with coherence length ξ . Carlson and coauthors present the numerical factors as estimates that depend on microscopic details [25]. Neither inequality is a theorem. Weak-coupling BCS theory has $k_B T_c = \Delta_0/1.76$, which is above $\Delta_0/2$, and explicit models exist in which T_c exceeds any fixed multiple of the zero-temperature stiffness [39]. A rigorous bound exists in two dimensions, $k_B T_c \leq \pi \tilde{D}/2$ with $\tilde{D}$ fixed by the optical sum rule, which becomes $k_B T_c \leq E_F/8$ for a single parabolic band [40]. We use equation (1) as an organising estimate.

The third condition is that the phase carrying the condensate exists at one atmosphere and at the operating temperature for as long as it is used, either as the thermodynamic ground state or behind a kinetic barrier. We call this persistence.

A transition at 300 K and one atmosphere therefore needs T_{pair} and T_θ above 300 K in a phase that persists there. Table 1 sets three well-characterised superconductors against each condition.

Table 1. Pairing scale, stiffness scale and existence at one atmosphere for three superconductors. For LaH₁₀ and MgB₂ the pairing scale is T_c . The transition temperatures, and the pressure for LaH₁₀, are those of the introduction [1, 2, 4, 6, 7]. The cuprate gap scale $\Delta_0/2$ and the cuprate and MgB₂ stiffness scales are from the tabulation of Carlson and coauthors, which gives 130 K for the mercury compound with the stiffness in three CuO₂ planes and 190 K with it in the outer two [25]. The pairing onset is the one measured in Bi-2201 and Bi-2212 [26]. The LaH₁₀ stiffness scale is our evaluation of equation (2) with the penetration depth of 14 to 35 nm inferred from magnetisation at 130 GPa, where T_c is 231 K, and a coherence length of 1.5 nm [41].

Material	Measured at	T_c (K)	Pairing scale (K)	Stiffness scale T_θ (K)	Exists at 1 atm	Factor short of 300 K
LaH ₁₀	170 GPa	250	250	3×10^4 to 2×10^5 (inferred)	no	pairing 1.2
HgBa ₂ Ca ₂ Cu ₃ O _{8+δ}	1 atm	133 to 135	435 (gap scale); 120 to 150 (onset in Bi cuprates)	130 to 190	yes	stiffness 1.6 to 2.3; pairing 2.0 to 2.5 on the onset
MgB ₂	1 atm	39	39	1400	yes	pairing 7.7

No material with a reproduced transition is within a factor of two of 300 K on all three conditions at once. The highest established T_c at one atmosphere, 133 to 135 K in the mercury cuprate and 138 K with thallium substitution [3], is a factor of 2.2 to 2.3 below. The pressure-quenched state of the unsubstituted compound has a resistive onset up to 151 K in one group's measurements, with no zero resistance reported, and one sample's onset fell from 147 to 143 K after cycling to room temperature [10].

LaH₁₀ pairs at 250 K, a factor of 1.2 below the target. Its cubic phase distorts below 135 GPa [42], and we found no report of LaH₁₀ at one atmosphere. Its stiffness scale, on the penetration depth inferred from magnetisation, is about a hundred times the target or more. MgB₂ exists at one atmosphere with a stiffness scale of 1400 K and pairs at 39 K, a factor of 7.7 below the target. The mercury cuprate exists at one atmosphere, and its stiffness scale of 130 to 190 K is a factor of 1.6 to 2.3 below the target. Its gap scale of 435 K, or $2\Delta_0/k_B T_c \approx 13$, is above the target. Carlson and coauthors tabulate it as the pairing scale [25], which it is only if the gap seen by spectroscopy is a pairing gap, and that reading is contested. Kondo and coauthors find in Bi-2201 and Bi-2212 that pairing sets in at 120 to 150 K and attribute the pseudogap above that temperature to a state without pair formation [26]. If the same holds in the mercury compound, its pairing scale is a factor of 2.0 to 2.5 below the target.

The stiffness scale of the hydrides is inferred through models, and we found no direct measurement of the penetration depth in a hydride superconductor above 150 K. For H₃S the values derived from one laboratory's magnetisation data run from 22 to 189 nm [41, 43, 44], over which equation (2) gives T_θ/T_c from 475 down to 7.5. An October 2026 addendum to the first of these re-derives 24 nm for H₃S, which lowers the upper ratio to about 400, and 36 nm for LaH₁₀, just outside the range used in Table 1 [45]. Critical-current analyses by a second group give 211 nm for YH₆ and 500 nm for ThH₁₀ [46, 47], for which we obtain T_θ/T_c of 4.8 and 1.8. Each of these estimates, and the one for LaH₁₀, puts the stiffness scale above T_c , by a factor between 1.8 and about 800.

The three conditions involve different physics and are constrained by different data, so we treat them as separate estimation problems. A single regression on T_c mixes them. The next three sections concern the pairing scale when phonons provide it, where a forward theory exists. The two after them concern persistence at one atmosphere, and the pairing and stiffness scales when phonons do not provide the pairing, where no controlled, validated forward theory exists.

Usability

A superconductor carries loss-free current only below its irreversibility field, which falls to zero as the temperature approaches T_c and is smaller the stronger the thermal fluctuations. Gurevich gives the scale as [48]

$$H^*(T) \sim 0.005 H_{c2}(0) \frac{(T_c/T - 1)^2}{Gi}, \quad (3)$$

where the Ginzburg number $Gi = \frac{1}{2} [2\pi\mu_0 k_B T_c \gamma \lambda_L^2 / (\Phi_0^2 \xi)]^2$ measures the strength of thermal fluctuations, with γ the anisotropy and Φ_0 the flux quantum [49]. A material with T_c of 300 K therefore carries no useful current at 300 K. Pickett puts the T_c needed for room-temperature use at 375 to 400 K, and more for high current density [50].

The margin needed depends on Gi , which is 2×10^{-9} in niobium, 8×10^{-7} in Nb-Ti and about 10^{-2} in YBa₂Cu₃O₇ [49]. Holding the coherence length, penetration depth and anisotropy of YBa₂Cu₃O₇ fixed and raising T_c to 400 K gives $Gi \approx 0.2$. The lower limit on the vortex creep rate proposed by Eley and coauthors, $Gi^{1/2} T/T_c$, is then above 0.3 at 300 K, about four times its value for YBa₂Cu₃O₇ at 77 K [49]. That limit was tested at $T_c/4$ and we extrapolate it to $0.75 T_c$. On this estimate a layered, low-carrier-density superconductor of that kind with T_c of 400 K would not hold a useful current at room temperature.

Gi varies as λ_L^4 , so for the hydrides it is less certain than the penetration depth. Over the 22 to 189 nm published for H₃S it runs from about 10^{-6} to 3×10^{-3} , which is four orders of magnitude below YBa₂Cu₃O₇ at one end and a third of it at the other. The critical-current analyses of YH₆ and ThH₁₀ give 3×10^{-3} to 7×10^{-3} and 0.039 to 0.085 [46, 47]. A free-electron estimate from the carrier density of H₃S, without mass enhancement, gives 18 nm [41], at the low end. Carrier density therefore predicts a small Gi for dense three-dimensional metals of this kind, and measurement has not yet established it.

We keep usability out of the search objective and report an uncalibrated estimate of Gi for every phonon-mediated candidate, from its penetration depth, coherence length and anisotropy.

What 300 K costs when phonons do the pairing

Phonon-mediated superconductivity has a forward model, the Migdal-Eliashberg equations, which return T_c from the Eliashberg spectral function $\alpha^2 F(\omega)$ and a Coulomb pseudopotential μ^* . Fully first-principles calculations, benchmarked with density functional theory for supercon-

ductors, come within about 20% of the measured T_c for most elemental superconductors [51, 52]. We use three moments of the spectral function:

$$\lambda = 2 \int_0^\infty \frac{\alpha^2 F(\omega)}{\omega} d\omega, \quad \omega_{\log} = \exp \left[\frac{2}{\lambda} \int_0^\infty \ln \omega \frac{\alpha^2 F(\omega)}{\omega} d\omega \right], \quad \langle \omega^2 \rangle = \frac{2}{\lambda} \int_0^\infty \omega \alpha^2 F(\omega) d\omega$$

To find what a 300 K transition requires we solved the linearised isotropic Eliashberg equations on the Matsubara axis for a single Einstein mode of frequency ω_E (methods and checks are in the appendix). For this spectrum $k_B T_c = \hbar \omega_E f(\lambda, \mu^*)$, and Table 2 gives f and the frequency that 300 K requires at each coupling.

Table 2. Phonon frequency and hydrogen Hopfield parameter required for $T_c = 300$ K, from the Eliashberg equations for an Einstein mode. $\mu^* = 0.13$ at a Matsubara cutoff of $10 \omega_E$, which corresponds to $\mu^* = 0.10$ at the mode frequency. The last column is $\eta_H = \lambda M_H \omega_E^2$, the Hopfield parameter of equation (5).

λ	$k_B T_c / \hbar \omega_E$	ω_E for 300 K (meV)	ω_E for 300 K (K)	η_H (eV/Å ²)
1.0	0.072	357	4146	30.8
1.5	0.124	209	2421	15.7
2.0	0.164	158	1833	12.0
2.5	0.196	132	1529	10.5
3.0	0.225	115	1336	9.6
4.0	0.273	95	1099	8.7
5.0	0.314	82	956	8.2

At $\lambda = 1$ the required frequency is 357 meV. Trachenko and coauthors estimate from fundamental constants that phonon frequencies in a non-molecular solid stay below 317 meV (3680 K), which a single mode would meet at $\lambda = 1.1$; some calculated spectra under pressure exceed the estimate [53]. At the second-moment frequencies of hydrogen in the megabar hydrides of Table 3, 113 to 163 meV [28], a single mode needs λ between 1.9 and 3.1. The table assumes an isotropic gap, a constant density of states and Migdal's approximation, whose expansion parameter $\lambda \hbar \omega / E_F$ [29] is below 0.1 in these rows only where the Fermi energy exceeds 3 to 4 eV.

Figure 2 places published calculations against the same solution. Among the 12,053 compounds in the coupling figure of the largest ambient-pressure survey, which reports more than 20,000, none combines λ above 2 with $\omega_{\log}$ above 600 K, and the largest $\omega_{\log}$ is 1275 K, at $\lambda = 0.23$ [5]. The abstract of that paper quotes 1800 K; the appendix explains why we use the figures.

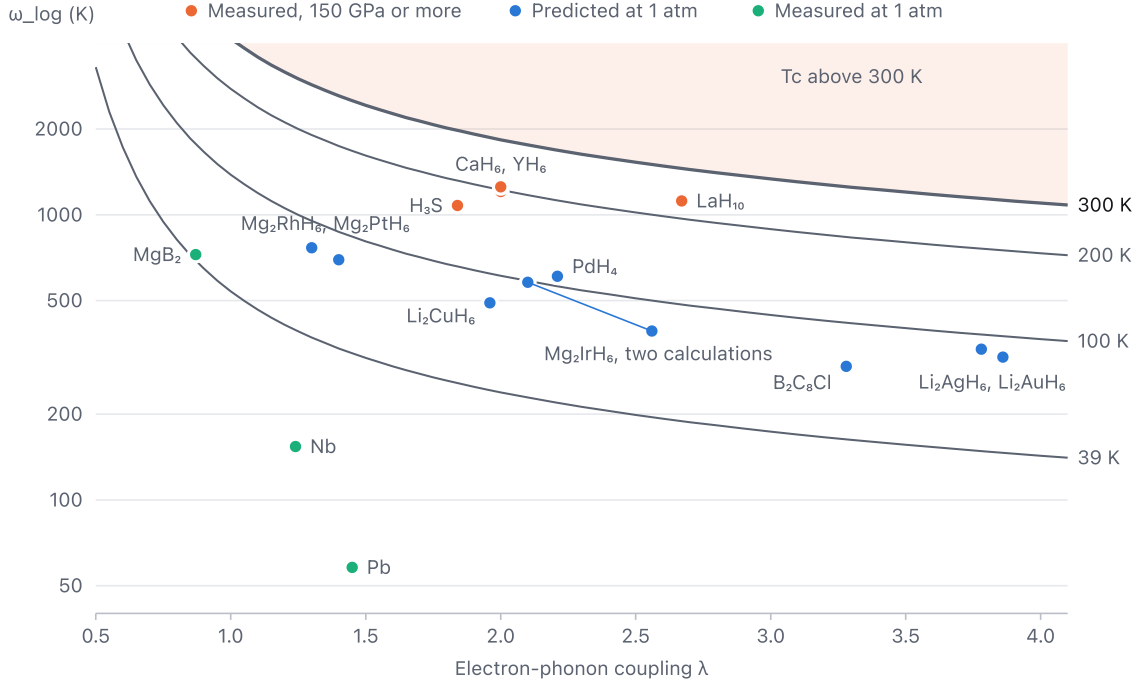


Figure 2. Coupling strength and logarithmic phonon frequency from published calculations, against isotherms of T_c from our solution of the Eliashberg equations for a single mode at $\omega_E = \omega_{\log}$ (μ^* as in Table 2). A broad spectrum has a second moment above its $\omega_{\log}$, and for the four ambient-pressure spectra we solved T_c is 3 to 22% above the isotherm through the point. The four superhydrides exist only at megabar pressure. The ambient-pressure predictions with λ of 2 or more have $\omega_{\log}$ of 290 to 610 K, against 1080 to 1250 K for the superhydrides. Sources are in the data file that accompanies the paper.

Which phonons count

T_c depends on the frequencies at which the coupling sits, and the total λ does not record them. We recomputed the functional derivative $\delta T_c / \delta \alpha^2 F(\Omega)$ of Bergmann and Rainer, the response of T_c to a small spectral weight added at frequency Ω [54], for an Einstein spectrum with $\lambda = 2$. It peaks near $\hbar\Omega = 7 k_B T_c$. Per unit of spectral area, the most valuable phonons for a 300 K superconductor are therefore near 180 meV, in the range of hydrogen stretching vibrations.

Per unit of $S = \lambda \langle \omega^2 \rangle$, which the next subsection calls the Hopfield sum, the ranking reverses. A weight ϵ added at Ω adds $2\Omega\epsilon$ to S , so the response per unit of S is the same derivative divided by 2Ω . It decreases monotonically with frequency: relative to its low-frequency value it is 0.92 at $2 k_B T_c$, 0.56 at $6 k_B T_c$ and 0.22 at $13 k_B T_c$. At fixed S a softer spectrum gives a higher T_c . The gain is limited, because the efficiency Φ of equation (6) is below one in every solution we computed and is already 0.63 for a single mode at $\lambda = 2$, and because a mode can soften only until the lattice becomes unstable. This section treats S as the scarce quantity, so the second ranking applies.

Split $\lambda = 2$ between a 15 meV mode, typical of a heavy host lattice, and a 150 meV mode, typical of hydrogen. With all of the coupling on the soft mode T_c is 30 K, with an even split 134 K, and with all of it on the stiff mode 285 K. This comparison is at fixed λ . The Hopfield sums of the two extremes differ by a factor of 100 and their T_c by about ten, its square root.

The Hopfield sum

One moment of the spectral function does not depend on the phonon frequencies. McMillan showed for a metal with one kind of atom that $\lambda\langle\omega^2\rangle = N(0)\langle I^2\rangle/M$, and Hopfield identified the numerator as a local electronic quantity [55, 56]. With one term for each atom type, as it is written for hydrides [28, 57], the relation is

$$S \equiv \lambda\langle\omega^2\rangle = 2 \int_0^\infty \omega \alpha^2 F(\omega) d\omega = \sum_j \frac{\eta_j}{M_j}, \quad \eta_j = N(0) \langle I_j^2 \rangle, \quad (5)$$

where the sum runs over atom types, M_j is the mass, $N(0)$ the density of states per spin at the Fermi level and $\langle I_j^2 \rangle$ the Fermi-surface average of the squared electron-ion matrix element, summed over the atoms of type j in the cell. η_j has the units of a force constant. The phonon frequencies and eigenvectors cancel out of S because the eigenvectors form a complete set. We call S the Hopfield sum and quote it in the units of η_H (eV/Å²) by multiplying by the hydrogen mass. For the megabar hydrides of Table 3 it equals η_H to within 3%. Where lithium, beryllium or boron couple, or hydrogen is a small part of the cell, it exceeds η_H by an amount we have not measured (appendix).

Allen and Dynes found that at large coupling the Eliashberg equations give $k_B T_c \rightarrow 0.18 \hbar \sqrt{\lambda\langle\omega^2\rangle}$, with a constant of 0.1827 at $\mu^* = 0$, and concluded that the phonon frequencies do not limit T_c [27, 29]. By equation (5) the limit is $0.18 \hbar \sqrt{\eta/M}$ for one atom type, as Quan, Ghosh and Pickett and Sadovskii write it [28, 29]. We use this known limit as a scale and write, at any coupling,

$$k_B T_c = 0.1827 \Phi \hbar \sqrt{S}, \quad (6)$$

where the efficiency Φ depends on λ , on μ^* and on the shape of the spectrum. For hydrogen the prefactor is $136.5 \text{ K} \times \sqrt{\eta_H/(\text{eV} \text{ Å}^{-2})}$. Φ is below one in every isotropic solution we have computed, and the bound of this form proved for a general spectrum has a constant 2.03 times larger [58]. S is therefore an upper scale for T_c . Our additions are Φ for single modes and for published spectra, S and η_H for ambient-pressure hydrides from published tables, and an account of which errors S is protected against.

For a single mode with the μ^* of Table 2, Φ is 0.40, 0.55, 0.63, 0.71, 0.75 and 0.81 at $\lambda = 1, 1.5, 2, 3, 4$ and 10. Our solutions for four published spectra of hydrides predicted at ambient pressure give 0.35 to 0.52, against 0.50 to 0.68 for a single mode with the same λ and S , and 0.03 for the anharmonic spectrum of PdH, where $\lambda = 0.40$. With the first-principles Coulomb interaction of the authors of three of those spectra, the published T_c is 0.21 to 0.41 of the asymptote [22]. For the five superhydrides of Table 3 the hydrogen-mode T_c of Quan and coauthors, an Allen-Dynes value that we reproduce with $\mu^* = 0.13$, a stronger Coulomb term than that of Table 2, is 0.51 to 0.58 of the asymptote [28]. Leaving PdH aside, Φ runs from about 0.2 to 0.6.

Once the structure and the linear electron-ion matrix elements are fixed, equation (5) fixes S whatever the frequencies and eigenvectors are, so renormalising the phonons at a fixed structure cannot change it. The published anharmonic calculations change only the phonons, and their tables obey the rule to rounding. For Li_2AuH_6 with harmonic phonons and two anharmonic treatments, λ is 3.86, 2.10 and 2.67, and the S we compute from the tabulated λ and second moment is 3.62, 3.63 and 3.62 $\text{eV}/\text{\AA}^2$ [5]. For PdH λ falls from 1.55 to 0.40, and our reading of the published cumulative coupling curves gives 0.42 $\text{eV}/\text{\AA}^2$ for both, within a reading error of about 15% and with the harmonic calculation done at the volume of PdT [59]. This agreement is an identity. It checks the tables and is no evidence about the accuracy of S .

The sum rule does not protect S against errors in the electronic factor or in the structure, and three kinds are documented in hydrides. Three published calculations of one structure of Mg_2IrH_6 , whose Fermi level sits on a peak in the density of states, give 2.3, 3.7 and 5.2 $\text{eV}/\text{\AA}^2$ (Table 3). Path-integral dynamics pairs part of the hydrogen in Li_2AuH_6 into molecules, and S in that state is 0.86 $\text{eV}/\text{\AA}^2$ against 3.6 for the crystal, a factor of 4.2 between two different methods [5, 37]. In PdH, on the same anharmonic phonons, λ is 0.42 with the bare linear vertex, 0.27 when that vertex is averaged over the quantum distribution of the nuclei, and 0.64 when averaged second-order terms are added [60].

At fixed S an error in the phonons moves T_c less than the same fractional error in η . With $a = d \ln T_c / d \ln \lambda$ at fixed S , errors in η and in the force constants k give $\delta T_c / T_c = (\frac{1}{2} + a) \delta \eta / \eta - a \delta k / k$. For a single mode a is 0.61, 0.39, 0.22 and 0.15 at $\lambda = 1.5, 2, 3$ and 4. Real spectra are more sensitive than a single mode with the same λ , because their soft modes add to λ and little to S or T_c . Scaling every force constant in the four ambient-pressure spectra by 1.3 or 1/1.3 at fixed S moves T_c by 12 to 25%, and the same factor in η at fixed frequencies moves it by 24 to 41%, about twice as much. A non-uniform change in the phonons can exceed the single-mode rule. In H_3S at 200 GPa anharmonicity lowers λ from 2.64 to 1.84 and the Eliashberg T_c from 250 to 194 K, where the rule gives 222 K [61]. At small λ a fixed S constrains T_c little, and in PdH it falls from 47 to 5 K [59].

In these terms the requirement for 300 K is the last column of Table 2: η_H of 12.0 $\text{eV}/\text{\AA}^2$ at $\lambda = 2$ and 8.7 at $\lambda = 4$ for a single mode, with a floor of 4.83 at infinite coupling and $\mu^* = 0$. At the efficiencies of the megabar hydrides (0.51 to 0.58) it is 14 to 19 $\text{eV}/\text{\AA}^2$, and at those of the four ambient-pressure spectra (0.35 to 0.52) it is 18 to 39. The floor scales with mass, so boron needs at least 52 $\text{eV}/\text{\AA}^2$ and carbon 58, about four times the largest value in Table 3. Semenok, Altshuler and Yuzbashyan conclude from a different argument that phonon-mediated room-temperature superconductivity is feasible only in hydrogen compounds [62].

Table 3 compares the requirement with published calculations. We found no paper that prints η_H for the hydrides predicted at ambient pressure, but λ and the second moment are tabulated for more than sixty of them and four published spectra cover three, so the values follow from equation (5).

Table 3. Hopfield parameter of hydrogen from linear-response calculations. Megabar rows are from [28] at the lowest pressure tabulated for each compound, with the Allen-Dynes T_c of the hydrogen modes alone. Ambient rows are our evaluation of equation (5) from published λ and second moments [5, 63] or, where marked $^+$, from our reading of published cumulative coupling curves, with a reading error of 15 to 20% [22, 59, 64]; their T_c is the published range. The lithium values are upper bounds because lithium modes contribute. The asymptote is $136.5 \text{ K} \times \sqrt{\eta_H}$.

Compound	Pressure	η_H (eV/ $\text{\AA}^2$)	Asymptote (K)	Calculated T_c (K)	Status at that pressure
MgH ₆	300 GPa	13.5	502	280	no synthesis reported
YH ₁₀	300 GPa	13.4	500	270	did not form up to 410 GPa and 2250 K [65]
H ₃ S	220 GPa	10.1	434	222	made; 203 K measured at 155 GPa [66]
LaH ₁₀	250 GPa	8.9	407	217	made; 250 K measured at 170 GPa [6]
CaH ₆	150 GPa	6.7	353	204	made; 215 K measured at 172 GPa [67]
Mg ₂ IrH ₆ [64]	1 atm	5.2 $^+$	311	160 to 175	attempted; Mg ₂ IrH ₆ forms [35]
Mg ₂ IrH ₆ [22]	1 atm	3.7 $^+$	263	66 to 77	as above
Mg ₂ IrH ₆ [63]	1 atm	2.3	207	59	as above
Li ₂ AuH ₆	1 atm	at most 3.6	260	88 to 140 [5, 68]	unstable in one path-integral simulation [37]
Li ₂ AgH ₆	1 atm	at most 2.9	233	83 to 132	unstable in the same simulation
Mg ₂ RhH ₆	1 atm	2.2 to 2.7 $^+$	203 to 224	45 to 59	made at 30 to 74 GPa only; onsets 18 to 29 K [23]
Mg ₂ PtH ₆	1 atm	1.9 to 2.0 $^+$	188 to 193	64 to 80	did not form when Mg ₃ Pt and 2:1 Mg-Pt mixtures were heated in hydrogen at 160 bar (no ternary hydride) and at 9 to 24 GPa (Mg ₄ Pt ₃ H ₆); the study did not name Mg ₂ PtH ₆ as its target [36]
Mg ₂ PdH ₆	1 atm	1.6	173	51 to 67	untested
PdH	1 atm	0.42 $^+$	88	5	exists; 8 to 9 K measured, as tabulated in [59]

The five megabar hydrides of the table, each with a calculated T_c above 200 K, have 6.7 to 13.5 eV/ $\text{\AA}^2$, at 150 to 300 GPa. The hypothetical ambient-pressure compounds have 1.6 to 5.2, a factor of 1.7 to 7.5 short of the single-mode requirement. PdH, the one ambient-pressure hydride in the table that exists, is short by a factor of more than twenty.

The three rows for Mg₂IrH₆ are calculations of one structure, and their published T_c comes from different methods: the Allen-Dynes formula with $\mu^* = 0.10$ (59 K), the Eliashberg equations and density functional theory for superconductors with a first-principles Coulomb interac-

tion (77 K and 66 to 71 K), and anisotropic Eliashberg equations with μ^* of 0.10 to 0.16 (160 to 175 K). At a common μ^* of 0.10 our solutions of the two published spectra give 134 and 174 K.

Within one phase, compression raises η_H and lowers T_c , because the force constants stiffen faster. In the calculations of Quan and coauthors, between 150 and 300 GPa η_H of CaH₆ rises from 6.7 to 8.8 eV/Å², $M_H\langle\omega^2\rangle$ rises by a factor of 2.1, and the T_c of the full spectrum falls from 200 to 175 K. Their other four compounds behave in the same way [28].

The ambient-pressure candidates have low efficiency for the reason given under "Which phonons count". In our reading of the published spectra of Mg₂IrH₆ and Mg₂RhH₆, modes above 150 meV hold about 60% of S and contribute λ of 0.2 to 0.4 [22, 64]. In Li₂AuH₆ about 70% of λ comes from modes below 30 meV [68].

Proposed ceilings

None of the proposed bounds on T_c for phonon pairing reviewed below excludes 300 K, and they disagree about the range of coupling in which a room-temperature material would have to lie.

Esterlis, Kivelson and Scalapino proposed $k_B T_c \lesssim 0.1 \hbar \bar{\omega}$ from measured ratios of T_c to the Debye temperature and from quantum Monte Carlo for the two-dimensional Holstein model, from which they infer a maximum near 0.08 of the bare phonon frequency and 0.12 of the renormalised one [69]. In that model the simulations agree with Migdal-Eliashberg theory up to a bare coupling of about 0.4 and depart from it beyond [70]. In the same calculations bare couplings of 0.4 and 0.5 correspond to renormalised λ of 1.7 and 4.6, a range that contains the four superhydrides of Figure 2 [69, 71]. H₃S sits at 0.08 if $\bar{\omega}$ is the top of its calculated phonon spectrum, 0.23 eV [69]. Kivelson and other coauthors later built models in which the ratio is unbounded, and concluded that the bound is no theorem and is hard to exceed in real materials [39].

Semenok, Altshuler and Yuzbashyan argue that an instability of the electron-phonon system limits λ to 3.7 for Einstein and 4.7 for Debye spectra [62]. Zhang, Berg and Chubukov dispute the instability and the proponents have replied [72, 73]. Sadovskii's review agrees with Zhang and coauthors on the equilibrium specific heat and leaves the kinetic argument of the reply open [29]. He argues that the renormalised λ is unbounded inside the stable metallic phase, takes equation (6) with $\Phi = 1$ as the upper limit on T_c , and estimates it for an electron gas as $(0.2/r_s)\sqrt{m/M}$ Ry, about 650 K for hydrogen at $r_s = 1$ [29]. Trachenko and coauthors bound the phonon frequency by fundamental constants and obtain a maximum T_c between 370 and 740 K [53].

Leavens showed that $k_B T_c \leq 0.2309 A$ at $\mu^* = 0$, with A the area under $\alpha^2 F$ [29, 74]. Our solver reproduces the constant for a single mode at $\lambda = 1.14$ and gives 0.166 with the μ^* of Table 2, so a single mode needs A of at least 156 meV for 300 K. Moussa and Cohen derived two further bounds within Eliashberg theory [75].

A cap on λ at 3.7 lowers the single-mode Φ from 0.81, its value at $\lambda = 10$, to 0.74. A cap on $k_B T_c / \hbar \bar{\omega}$ of 0.10 to 0.12, with $\bar{\omega}$ the top of the spectrum, removes every row of Table 2 from $\lambda = 1.5$ up, because for a single mode the top of the spectrum is ω_E . A single mode then needs ω_E of 2500 to 3000 K at λ of 1.25 to 1.46, which is η_H of 16 to 20 eV/Å² against 8.7 to 12.0 without the cap, above every value in Table 3. At 0.08, where H₃S sits, 300 K needs a top frequency of 3750 K, above the 3680 K estimate of Trachenko and coauthors. The cap does not hold on a mean frequency, since LaH₁₀ superconducts at 250 K with a calculated $\omega_{\log}$ of 1119 K, a ratio of 0.22 [6, 76]. Whether it holds on the top frequency of a three-dimensional multi-band hydride is not settled. Under either cap the requirement falls on S , and the section "What hydrogen density buys at one atmosphere" asks what sets it.

How wrong a computed T_c can be

Any model trained on computed electron-phonon data inherits the errors of the calculations. For strongly coupled hydrides the documented cases run from 7% to a factor of three between published values for one structure, and to a factor of four or more where quantum nuclear motion changes the structure (Table 4).

Table 4. Sources of error in first-principles T_c for strongly coupled hydrides, with documented cases.

Source	Documented size	Case
Closed-form formula in place of the Eliashberg solution	McMillan form 32 to 36% low; Allen-Dynes 19% RMS error	H ₃ S: 173 K against 256 K, and 125 K against 194 K, for the same inputs [61, 77, 78]
Harmonic phonons	λ 43% high (2.64 against 1.84); T_c 250 K against 194 K	H ₃ S at 200 GPa [61]
Classical nuclei, structure	spurious instability below 230 GPa	LaH ₁₀ [76]
Quantum nuclei, structure	S lower by a factor of 4.2; T_c 22 K against 88 to 140 K	Li ₂ AuH ₆ in path-integral dynamics at 80 K [5, 37, 68]
Eliashberg equations against density functional theory for superconductors, same phonons, first-principles Coulomb interaction in both	7 to 24%	LaH ₁₀ 243 against 225 K; Li ₂ AgH ₆ 109 against 83 K [5, 76]
High-throughput against converged settings	λ differs by a factor of 1.8 to 2.2	Mg ₂ IrH ₆ 1.16 against 2.13; Li ₂ AuH ₆ 1.75 against 3.86 [5, 63]
Settings and methods combined, Fermi level on a peak in the density of states	T_c differs by a factor of 3.0; η_H by 2.3	Mg ₂ IrH ₆ : 59 to 175 K and 2.3 to 5.2 eV/Å ² for one structure [22, 35, 63, 64]

Anharmonic calculations come within about 10% of the measured T_c of H₃S and LaH₁₀ [61, 76]. The high-throughput calculations, which make up most of the published data, are harmonic, use $\mu^* = 0.10$ and run on coarse grids [5, 63]. H₃S was predicted at 191 to 204 K at 200 GPa and measured at 203 K at 155 GPa [66, 79]. YH₆ was measured at 224 K against a prediction above 270 K and YH₉ about 30 K under its predictions, and the predicted YH₁₀ did not form

[65, 80]. Mg₂RhH₆ has onsets of 18 to 29 K at 30 to 74 GPa against about 60 K calculated at 30 to 50 GPa [23]. Ranking on a calculated value adds a further overestimate of the leaders, which the subsection "Selection on the calculated value" calculates under stated assumptions.

What hydrogen density buys at one atmosphere

We define the scattering strength per proton, h , by dividing the Hopfield parameter of hydrogen by the hydrogen number density,

$$\eta_H = \rho_H h, \quad \rho_H = \frac{n_H}{V}, \quad h = \nu_F s^2, \quad (7)$$

where n_H is the number of hydrogen atoms in a cell of volume V , ν_F is the density of states per spin per unit volume, and $s^2 = V^2 \langle I_H^2 \rangle / n_H$ is the squared matrix element of the force on one proton for states normalised to unit volume. h has the units of energy times length and does not depend on the choice of cell. Equation (7) is a definition and assumes nothing. It is useful to the extent that h varies less between compounds than η_H does, which the rest of this section measures.

A proton in an electron gas

For one proton in a uniform electron gas h is a known quantity,

$$h = \frac{4\hbar^2 k_F}{m} \sum_{l \geq 0} (l+1) \sin^2(\delta_l - \delta_{l+1}), \quad (8)$$

where the δ_l are the phase shifts at the Fermi momentum k_F and the sum is the transport cross-section of the proton in units of $4\pi/k_F^2$. This is the free-electron limit of the formula of Gaspari and Gyorffy [30], which Papaconstantopoulos and Klein applied to metallic hydrogen in 1977 [81]. The same cross-section gives the residual resistivity of a dissolved proton and the friction coefficient of a slow proton, $Q = mk_F h / 3\pi\hbar$. The friction was calculated from self-consistent phase shifts in 1981 [82], and such values agree with the measured stopping of slow ions better than linear theory does [83, 84]. Self-consistent density-functional calculations of a proton in an electron gas date from 1974 [31, 32, 33], and Fermi-level phase shifts and transport cross-sections of embedded atoms were tabulated in 1983 [34].

Table 5 gives our own evaluation, a self-consistent Kohn-Sham calculation in the local-density approximation (appendix). At $r_s = 2.5$ it returns $\delta_0 = 1.217$ and $\delta_1 = 0.091$, against 1.221 and 0.089 published by Nagy and Zawadowski [84].

Table 5. Scattering strength of a proton in an electron gas of density parameter r_s , from equation (8) with self-consistent phase shifts. The last column is h for the Yukawa potential $-e^2 e^{-\kappa r}/r$ with κ fixed by the Friedel sum rule.

r_s	k_F ($\text{\AA}^{-1}$)	δ_0	δ_1	h (eV $\text{\AA}$)	h/e^2	Yukawa model, h (eV $\text{\AA}$)
1.0	3.63	0.63	0.16	25.8	1.80	21.3
1.5	2.42	0.85	0.15	32.8	2.28	26.0
2.0	1.81	1.05	0.12	36.3	2.52	28.6
2.5	1.45	1.22	0.09	36.6	2.54	29.4
3.0	1.21	1.36	0.05	34.5	2.40	28.8
4.0	0.91	1.59	-0.01	27.6	1.92	25.4
6.0	0.60	1.85	-0.11	16.3	1.13	18.2

For r_s between 1.5 and 3, h is 2.3 to 2.5 e^2 (33 to 37 eV $\text{\AA}$), which we use as the single-proton reference. The Yukawa model of the last column, which has been used for ion stopping and for a proton in an electron gas [85, 86], satisfies the same Friedel sum rule and is 17 to 21% lower for r_s up to 3.

With equation (6), equation (7) gives

$$k_B T_c = 0.1827 \Phi \hbar \sqrt{\frac{\rho_H h}{M_H}} = 0.0515 \Phi \sqrt{\frac{h}{e^2}} \hbar \Omega_p, \quad \Omega_p = \sqrt{\frac{4\pi \rho_H e^2}{M_H}}, \quad (9)$$

where Ω_p is the plasma frequency of the protons. In practical units the asymptote, at $\Phi = 1$, is $136.5 \text{ K} \times \sqrt{\rho_H h}$ with ρ_H in $\text{\AA}^{-3}$ and h in eV $\text{\AA}$. For $h = 2.4e^2$ the asymptote is $0.080 \hbar \Omega_p$, an estimate for hydrogen in a free-electron-like metal. It does not bound T_c , since h in H₃S is about 3 e^2 (Table 6). Sadovskii gives a dimensional estimate of the same asymptote for one electron per atom, $(0.2/r_s) \sqrt{m/M} \text{ Ry}$ with factors of order unity dropped, and quotes about 650 K at $r_s = 1$ [29]. Equation (9) with the h of Table 5 and one proton per electron gives 880, 369 and 114 K at $r_s = 1, 2$ and 4. His estimate scales with density as r_s^{-1} and ours as $r_s^{-3/2} \sqrt{h}$.

Equation (9) is McMillan's expression for $\lambda \langle \omega^2 \rangle$ in simple metals, with the phase-shift sum in place of his average of the pseudopotential form factor [55], joined to the asymptote of Allen and Dynes [27]. In simple metals the Hopfield parameter is known empirically to scale as the inverse volume under pressure [87], which makes h constant within a metal. Quan and coauthors normalised the hydrogen coupling by the density of states and found that the squared matrix element differs by a factor of five among the five superhydrides [28]. We add to these known results the division of η_H by the hydrogen density of a compound, taken separately from its electron density, and the comparison of h across pressures and compounds that follows. We have not found either in the literature.

The single-site assumption

Equation (8) is exact, within the Kohn-Sham description, for one proton in a uniform gas. Applying it to each proton of a crystal assumes that the protons scatter free-electron states independently. That is not controlled in the superhydrides, where the mean proton spacing is 0.5 to 0.7 Fermi wavelengths. In a compound the formula of Gaspari and Gyorffy weights each term of the sum by the site-projected densities of states of the two channels relative to those of a single scatterer [30], and these band factors can lie on either side of one. Published rigid-muffin-tin values of η_H for H₃S, LaH₁₀ and YH₁₀ [57, 88] are 1.2 to 1.9 times smaller than the linear-response values at the same or a nearby pressure [28]. The comparison is ours and assumes that Hutcheon and coauthors sum η_H over the ten hydrogen atoms; Papaconstantopoulos and coauthors report a λ consistent with linear response. We therefore take every value of h for a compound from linear-response calculations, and use the single-proton value as a reference scale.

Computed hydrides

Table 6 lists h for the hydrides of Table 3. The paper that reports the megabar η_H prints no cell volumes [28], so each megabar density uses a volume from another calculation of the same structure [61, 89, 90, 91, 92, 93]. Five of the eleven volumes behind the megabar rows are printed at the pressure used, and the others are interpolated, extrapolated or read from a figure. Where two calculations print a volume at the same pressure they differ by about 2%.

Table 6. Hydrogen number density and scattering strength per proton, $h = \eta_H / \rho_H$. Megabar η_H is from [28] over the pressure range given. Mg₂IrH₆ has a row for each of the three published calculations from which η_H can be extracted [22, 63, 64]; others print no second moment or spectrum that we could use [35, 94]. The 3.7 and 5.2 eV/Å² are read from published curves, with the reading error given in Table 3. For the lithium compounds the numerator includes lithium modes, so the entry is an upper bound. The PdH row is the stoichiometric compound. Cell volumes and their sources are in the data file that accompanies the paper.

Compound	Pressure	ρ_H (Å ⁻³)	η_H (eV/Å ²)	h (eV Å)	h/e^2
CaH ₆	150 to 300 GPa	0.280 to 0.348	6.7 to 8.8	24.0 to 25.3	1.7 to 1.8
LaH ₁₀	250 to 300 GPa	0.353 to 0.374	8.9 to 9.2	24.6 to 25.2	1.7 to 1.8
YH ₁₀	300 GPa	0.411	13.4	32.6	2.3
MgH ₆	300 GPa	0.399	13.5	33.9	2.4
H ₃ S	220 to 280 GPa	0.231 to 0.248	10.1 to 10.7	43.1 to 44.6	3.0 to 3.1
Mg ₂ IrH ₆ , high-throughput	1 atm	0.083	2.3	28	1.9
Mg ₂ IrH ₆ , Sanna and coauthors	1 atm	0.083	3.7	45	3.1
Mg ₂ IrH ₆ , Dolui and coauthors	1 atm	0.081	5.2	64	4.4
Li ₂ AuH ₆	1 atm	0.084	at most 3.6	at most 43	at most 3.0
Li ₂ AgH ₆	1 atm	0.086	at most 2.9	at most 34	at most 2.3
Mg ₂ RhH ₆	1 atm	0.085	2.2 to 2.7	26 to 32	1.8 to 2.2
Mg ₂ PtH ₆	1 atm	0.083	1.9 to 2.0	23 to 24	1.6 to 1.7
Mg ₂ PdH ₆	1 atm	0.084	1.6	19	1.3

Compound	Pressure	ρ_H ($\text{\AA}^{-3}$)	η_H (eV/ $\text{\AA}^2$)	h (eV $\text{\AA}$)	h/e^2
PdH	1 atm	0.058	0.42	7.2	0.50

Within each superhydride h is constant to about 3% under pressure, so η_H follows the hydrogen density. Over the pressure ranges tabulated by Quan and coauthors, which reach 400 GPa for MgH₆ and YH₁₀, η_H rises by 3 to 31% and the T_c they calculate from the hydrogen modes falls by 4 to 16%, for the reason given in the previous section [28].

The five superhydrides span 24 to 45 eV $\text{\AA}$, a factor of 1.9 that is about as wide as the spread of their η_H , so density does not order them. The six candidates at one atmosphere span 19 to 45 eV $\text{\AA}$, apart from one calculation of Mg₂IrH₆ at 64, at hydrogen densities three to five times lower. Against the single-proton value the superhydrides lie at 0.7 to 1.3, with a geometric mean of 31 eV $\text{\AA}$, about 0.9. The three calculations of Mg₂IrH₆ lie at 0.8, 1.2 and 1.8, and PdH at 0.2. In PdH a tenth of the density of states at the Fermi level is on hydrogen, against nearly half in H₃S [95].

A census of published calculations

We computed h for every hydride in the published tables we know of that give both λ and the second-moment frequency ω_2 , where we could find the cell. That gives 62 ambient-pressure hydrides, PdH, and 12 pressure points of the five superhydrides, one of them (YH₁₀ at 400 GPa) with an estimated volume. Of the 62, 57 are from the tables of Cerqueira and coauthors, which list compounds with a harmonic Allen-Dynes T_c above 20 K after a machine-learning pre-screen [63], and five are from Gao and coauthors [5]. For these rows the numerator is the Hopfield sum, $S = M_H \lambda \omega_2^2$, which also contains the coupling of the other atoms. The cells are the PBE cells of the Alexandria database [96], matched by formula and structure. The coupling was computed in PBEsol cells [5, 63], which are smaller by a median of 3% in the 24 database records we compared, so the ambient values of h are high by about 3%. Table 7 gives the statistics and Figure 3 shows the rows.

Table 7. Scattering strength per proton in the census, S/ρ_H for ambient-pressure rows and η_H/ρ_H for megabar rows. The spread factor is the exponential of the standard deviation of $\ln h$.

Group	Rows	Geometric mean (eV $\text{\AA}$)	Spread factor	Quartiles (eV $\text{\AA}$)	Range (eV $\text{\AA}$)
Ambient pressure	62	22.0	1.44	19.1, 25.4	7.4 to 83
Ambient pressure, no atom lighter than sodium besides hydrogen	47	21.3	1.39	18.9, 25.4	7.4 to 37
Megabar	12	30.7	1.28	25.2, 36.2	24 to 45
All rows, with PdH	75	22.9	1.47	19.3, 26.0	7.2 to 83

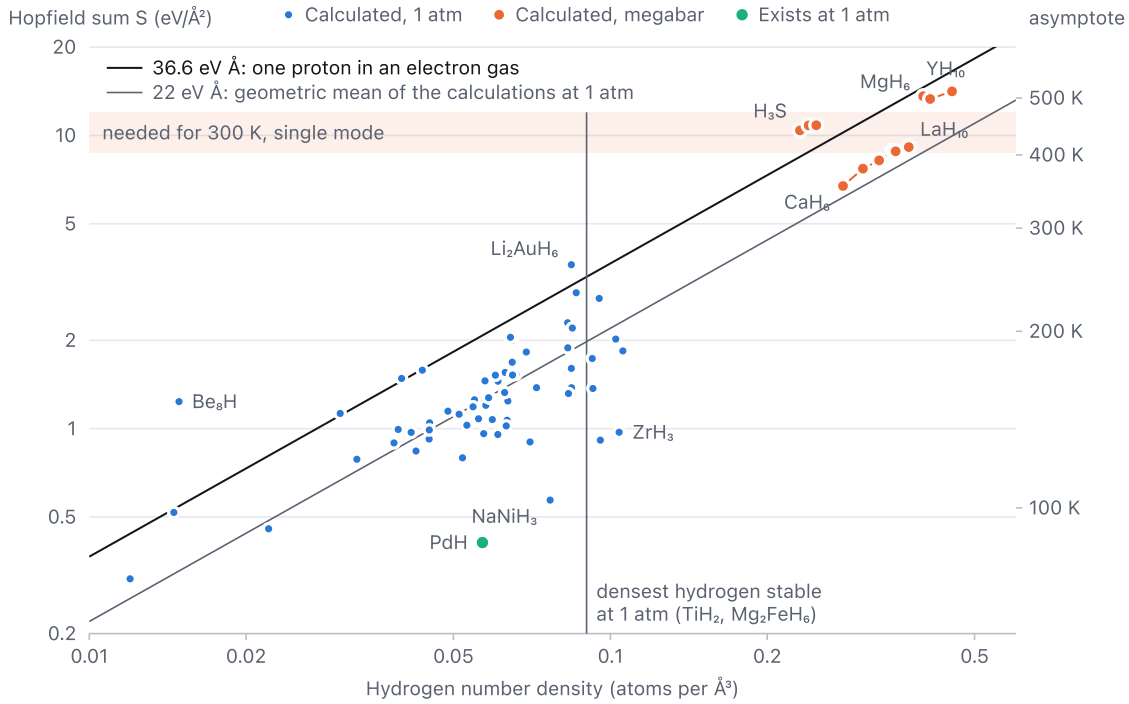


Figure 3. Hopfield sum against hydrogen number density, on logarithmic scales, for the 75 rows of the census: 62 ambient-pressure hydrides, PdH, and 12 pressure points of the 5 megabar superhydrides, for which the ordinate is η_H . The lines are constant scattering strength per proton, 22 eV Å (the geometric mean of the ambient rows) and 36.6 eV Å (one proton in an electron gas at $r_s = 2.5$). The shaded band, 8.7 to 12 eV/Å², is what a 300 K transition needs with a single mode. The vertical line marks 0.090 Å⁻³, the densest hydrogen we find in a compound stable at one atmosphere and room temperature. The right-hand scale is the asymptote of equation (6), $136.5 \text{ K} \times \sqrt{S}$, which T_c reaches only at $\Phi = 1$.

The largest ambient value, 83 eV Å, is Be₈H, whose coupling is mainly on beryllium modes [63], so its S is not η_H . Between the ambient and megabar groups the geometric mean of S rises from 1.24 to 9.9 eV/Å², a factor of 8.0. Hydrogen density accounts for a factor of 5.7 (0.057 to 0.32 Å⁻³) and h for 1.4 (22 to 31 eV Å).

All but two of the ambient rows were selected for high calculated T_c , and h rises with it. Its geometric mean is 18 eV Å below 30 K, 23 from 30 to 50 K and 30 above 50 K. Small values are therefore under-represented, and 22 eV Å is the mean of a selected sample. The smallest values in the census are 7.2 (PdH), 7.4 (NaNiH₃) and 9.4 (ZrH₃).

Hydrogen density at one atmosphere

Among compounds stable at one atmosphere and room temperature, the densest hydrogen we find from crystallographic cell volumes is 0.090 atoms per Å³, or 150 kg per cubic metre, in the metal TiH₂ [97] and the insulator Mg₂FeH₆ [97, 98]. Liquid hydrogen has 0.042 [98]. VH₂, a metal in equilibrium with about two atmospheres of hydrogen at 25 °C [99, 100], reaches 0.103 at full stoichiometry [97], and we found no compound above it. The candidates of Table 6 have 0.081 to 0.086 and the superhydrides 0.23 to 0.41.

The first effect of pressure is to make metallic phases with hydrogen states at the Fermi level exist at all, and Table 6 does not show it. Quan and coauthors call the stabilisation of structures of atomic hydrogen the essential role of pressure [28]. The six candidates are hypothetical at

one atmosphere. In the chemical systems of the five superhydrides, the hydrogen-richest phases that exist at one atmosphere (H_2S , LaH_3 and YH_3 [101], CaH_2 and MgH_2) are insulators or semiconductors, for which η_H is zero. In the two existing metallic hydrides for which we have a computed hydrogen coupling, it is small. PdH has $h = 7.2 \text{ eV } \text{\AA}$, and for TiH_2 a calculation finds the hydrogen contribution to the coupling much smaller than in PdH or H_3S [102].

An estimate at the densest packing

We take a round density of $0.10 \text{ \AA}^{-3}$, between TiH_2 and VH_2 . The asymptote of equation (9) is then 203 K for the census mean of $22 \text{ eV } \text{\AA}$, 261 K for the single-proton value of 36.6, 286 K for the 44 of H_3S , and 345 K for the 64 of one calculation of Mg_2IrH_6 , the largest value we have extracted from a published calculation whose coupling is on hydrogen. The hydride spectra of the previous section reach 0.35 to 0.52 of their asymptote at one atmosphere and 0.51 to 0.58 at megabar pressure, the second range with a stronger Coulomb term, and a single mode at $\lambda = 4$ reaches 0.75. With typical values, T_c at this density is about 70 to 120 K for the census mean and 90 to 150 K for the single-proton value. With the largest scattering strength and the best efficiency computed so far it is about 200 K, which restates the 175 K calculation of Mg_2IrH_6 [64] at a 23% higher hydrogen density. A single mode at $\lambda = 4$ with the same h would give about 260 K. If $k_B T_c$ cannot exceed 0.10 to 0.12 of the top phonon frequency, the cap discussed under "Proposed ceilings", a single mode reaches at most 0.49 to 0.54 of the asymptote, which is 170 to 190 K. These are conditional estimates. The efficiency is below one in every solution we computed and is otherwise unconstrained, and we know of no bound on h or on the hydrogen density of a metastable phase. The estimates may also be high, since among the ambient rows of the census h falls as hydrogen density rises, and the seven rows above $0.090 \text{ \AA}^{-3}$ have h between 9 and $29 \text{ eV } \text{\AA}$.

A 300 K transition needs $\rho_H h$ of 8.7 to $12 \text{ eV}/\text{\AA}^2$ with a single mode (Table 2). At $0.10 \text{ \AA}^{-3}$ that is a scattering strength of 87 to $120 \text{ eV } \text{\AA}$, which is 2.4 to 3.3 times the single-proton value, 2.0 to 2.7 times the largest megabar value and 1.4 to 1.9 times the largest in Table 6. Under the cap on the top frequency the single-mode requirement is 16 to $20 \text{ eV}/\text{\AA}^2$, or 160 to $200 \text{ eV } \text{\AA}$ at this density. At megabar scattering strengths, 24 to $45 \text{ eV } \text{\AA}$, it is a hydrogen density of $0.19 \text{ \AA}^{-3}$ or more, twice that of the densest compound we found stable at one atmosphere.

The estimates would be too low if band structure concentrates the states at the Fermi level on hydrogen, if the coupling is not linear in the hydrogen displacement, or if hydrogen packs more densely in a metastable structure than in any stable one.

In Mg_2IrH_6 the Fermi level sits on a peak in the density of states, and three calculations give h from 28 to $64 \text{ eV } \text{\AA}$ depending on how the peak is sampled [35]. RbPH_3 may lie above the range of Table 6. Its T_c of 126 K from the isotropic Eliashberg equations at $\mu^* = 0.14$, at 0.040 hydrogen atoms per $\text{\AA}^3$ [103], implies S/ρ_H of at least $64 \text{ eV } \text{\AA}$ unless its efficiency exceeds 0.58, and the 90 K the same paper gives with a first-principles Coulomb interaction implies at least 33. Its Hopfield sum has not been published.

In PdH , Bianco and Errea average the vertices over the nuclear distribution, and adding the second-order vertex then raises λ from 0.27 to 0.64. Of their four treatments only this one gives the inverse isotope effect and a T_c near the measured one, 11 K against 8 to 9 K, and the sec-

ond-order term with bare vertices gives 50 K [60]. If effects of that size are general, linear-response values of S are low by an unknown amount.

The cubic PdH₄ predicted by Li and coauthors [104] has 0.118 hydrogen atoms per Å³ in its cell in the Alexandria database, where it lies 319 meV per atom above the hull [96].

MgB₂ has a scattering strength per atom several times the single-proton value, and this implies nothing for hydrogen. From $\lambda = 0.87$ and $\omega_{\log} = 725$ K [105] its Hopfield sum in boron units is at least 8.8 eV/Å², which at a boron density of 0.069 Å⁻³ is 128 eV Å per boron atom. The electron-gas calculation of Table 5, repeated for a boron nucleus at the valence density of MgB₂ ($r_s = 1.80$), gives 121 eV Å, so MgB₂ sits at its electron-gas value.

What the census supports

Across published calculations the Hopfield sum scales with hydrogen number density. The slope of $\ln S$ on $\ln \rho_H$ over the 75 rows is 1.03 ± 0.06 , with a scattering strength per proton of 23 eV Å to within a factor of about 1.5, which is 0.6 to 0.7 of the single-proton value. One common h describes the step from one atmosphere to megabar pressure.

The census does not support a constant h among ambient-pressure compounds. Within the 62 ambient rows the slope is 0.62 ± 0.09 , the correlation of $\ln h$ with $\ln \rho_H$ is -0.47 , and h is only slightly narrower than S itself, with a standard deviation of the logarithm of 0.36 against 0.42. The three calculations of Mg₂IrH₆ alone have a standard deviation of the logarithm of 0.42, so part of the spread between compounds comes from the settings of the calculations. The census does not support the same h at megabar pressure as at one atmosphere either, since megabar values are about 40% higher.

Gao and coauthors deposited their electron-phonon data in the Alexandria database [5, 96], and the dynamically stable records we inspected store λ and ω_2 with the spectrum resolved by mode. We have not checked that compounds below the T_c cut are among them and have not computed h from them, so its distribution among unselected hydrides and the hydrogen share of S in each row remain to be measured.

What screening at ambient pressure has found

The largest set of calculated T_c at ambient pressure that we found is that of Gao and coauthors, who report more than 20,000 metals [5]. From the vector figures of their paper we recovered the Allen-Dynes T_c (harmonic phonons, $\mu^* = 0.1$) and the energy above the convex hull of 12,079 of them. The calculation is isotropic, and its authors note that it underestimates MgB₂, measured at 39 K, by almost a factor of two [4, 5].

The compounds were not drawn at random. The core of the set is the training set of an earlier screen by the same group, 6,912 non-magnetic metals within 50 meV per atom of the hull with small high-symmetry cells and an estimated Debye temperature above 300 K [106]. To these were added the compounds that a model predicted above 5 K, hydrides predicted above 20 K,

and in the later survey compounds predicted above 10 K [5, 63, 106]. We analyse the 8,323 compounds within 50 meV per atom of the hull. All passed the harmonic stability filter of the source calculations [5, 106], and the statistics below describe that sample.

An exponential tail between 2 and 30 K

The mean amount by which the calculated T_c exceeds a threshold is constant within its standard error from 2 to 15 K. It is 4.10 ± 0.08 K above 2 K (2,482 compounds), 4.08 ± 0.12 above 5 K, 4.01 ± 0.16 above 7.5 K, 4.03 ± 0.23 above 10 K (355), 3.92 ± 0.34 above 12.5 K and 4.02 ± 0.53 above 15 K (100). Above 20 K, where 25 compounds remain, it is 5.05 ± 1.58 K. A constant mean excess is the property of an exponential tail, the zero-shape generalised Pareto case of the peaks-over-threshold method [107, 108],

$$P(T_c \geq T) = p_u e^{-(T-u)/\tau}, \quad u = 10 \text{ K}, \quad p_u = 0.043, \quad \tau = 4.0 \text{ K}, \quad (10)$$

with a bootstrap 95% interval of 3.6 to 4.5 K for τ that treats the compounds as independent. An Anderson-Darling test does not reject the exponential form above 10 K ($p = 0.59$). The source of the training set reported 214 of its 6,912 compounds above 10 K, and chances of about 0.4% above 20 K and 0.03% above 30 K [106], which correspond to scales of 4.9 and 3.9 K. The mean-excess analysis and the fitted form are ours. Between 2 and about 30 K a threshold 9.3 K higher is exceeded by one tenth as many compounds (Figure 4). The fraction p_u is the composition of this sample and carries over to no other pool.

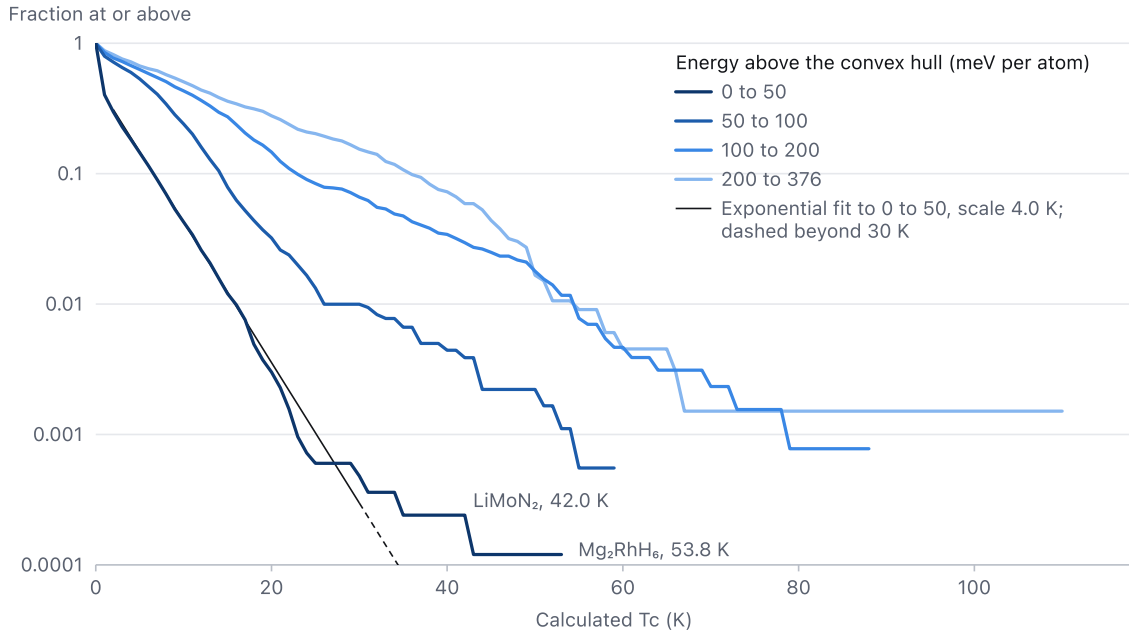


Figure 4. Fraction of compounds with calculated T_c at or above a given value, in four ranges of energy above the convex hull (key inside the frame), for the 12,079 compounds recovered from the figures of [5]. The straight line is equation (10), fitted to the range from 0 to 50 meV per atom, solid from 2 to 30 K and dashed beyond. The two highest compounds of that range, LiMoN_2 and Mg_2RhH_6 , are labelled. The three upper curves are samples chosen for high predicted T_c , and neither their height nor their slope describes a population.

The top of the sample

If equation (10) held at all temperatures, the level exceeded once among N compounds chosen the same way would be

$$T_{\max}(N) = u + \tau \ln(Np_u), \quad (11)$$

and the largest of the N would scatter about it with a standard deviation of 1.28τ , which is 5 K. For the 355 compounds above 10 K the level is 34 K. The sample has Mg_2RhH_6 at 54 K, 49.7 meV per atom above the hull, and LiMoN_2 at 42 K. Under equation (10) a largest value of 54 K or more has a probability of 0.007. The equation expects 2.5, 0.27 and 0.017 compounds at or above 30, 39 and 50 K, and the sample has 4, 2 and 1. The exponential form fails at the top of the sample it was fitted to. The failure rests on those two compounds. With the hull cut at 49 meV per atom, which removes Mg_2RhH_6 , the largest value is 42 K and its probability is 0.09.

With the shape left free the data do not determine the tail. A generalised Pareto fit has a shape of 0.05 above 10 K, with a bootstrap 95% interval of -0.13 to 0.15 , and 0.16 (-0.14 to 0.35) above 15 K. Return levels are therefore illustrations, conditional on the shape and on p_u . For a million compounds equation (11) gives 53 K if 4.3% exceed 10 K, as here, and 42 K if 0.27% do. That is the fraction confirmed among the roughly 200,000 compounds of the earlier screen, a lower bound because most were calculated only if its model flagged them [106]. With p_u as in the sample, the two generalised Pareto fits give 63 K (34 to 104 K) and 89 K (35 to 230 K).

For a calculated 300 K the three fits give probabilities per compound of 2×10^{-33} , 4×10^{-16} and 8×10^{-10} , so these data make no statement about 300 K either way. The argument that ranking this population will not produce a 300 K compound is the one from the Hopfield sum. A single mode with λ between 4 and 2 needs a hydrogen Hopfield parameter of 8.7 to 12 eV/Å² for 300 K (Table 2), and the largest we have found in a published ambient-pressure calculation is 5.2 (Table 3).

One later screen gives a weak check of the scale. Among the stable cubic hydrides of the GNoME database, 25 have an Allen-Dynes T_c of 4.2 K or more, and the largest is 23.5 K [109]. For 25 exceedances equation (11) gives 17 K, and a largest value of 23.5 K or more has a probability of 0.19. The candidates were chosen by a model whose training data include the 2024 screens behind the sample fitted here [63, 106], and the count of 25 is an input, so p_u is not tested.

Best calculated T_c against hull distance

Beyond 50 meV per atom the compounds are in the set because a model predicted a high T_c for them or an earlier paper proposed them [5, 63, 106]. The share above 10 K is 24%, 43% and 51% in the ranges 50 to 100, 100 to 200 and 200 to 376 meV per atom, against 4.3% inside 50. We assign no tail scale to those ranges.

The best calculated T_c at or below a given hull distance, the front drawn in the source figure [5], is a record of what has been found. It is 22.9 K on the hull, 42.0 K within 25 meV per atom, 53.8 K within 50, 59.4 K within 100, 88.4 K within 200 and 110.6 K at 319, a rise of about 0.3

K per meV per atom. Past LiMoN₂ the front runs through hydrides only, Mg₂RhH₆, Mg₂IrH₆, KInH₃, Li₂AuH₆ and Li₂AgH₆.

Selection on the calculated value

Ranking on a noisy number overstates the compounds at the top, an effect known in decision analysis as the optimizer's curse [110]. We calculate its size on two assumptions. The true T_c , t , has an exponential density of scale τ_t . The calculated value is $y = t e^\epsilon$, with ϵ normally distributed with zero mean and standard deviation σ . The posterior density of t given y is then proportional to $\exp[-t/\tau_t - \ln^2(y/t)/2\sigma^2]$, and at its mode the ratio $R = y/t$ satisfies

$$R \ln R = \frac{\sigma^2 y}{\tau_t}. \quad (12)$$

This is a special case of the correction for Eddington bias in survey astronomy [111], whose prior-free form is Tweedie's formula [112], and we apply it to calculated T_c . The ratio grows with y/τ_t and requires no bias in the calculation.

We have not estimated σ , the spread of the high-throughput value about the true one across the screened population, and we found no published estimate. The calculated and measured values tabulated for known superconductors could supply one, and with it a test that we have not made [113]. The only number we have is the spread of six published values of T_c for one compound, Mg₂IrH₆ (two are midpoints of quoted ranges) [22, 35, 63, 64, 94]. It is 0.39 in $\ln T_c$, with a 95% interval of 0.25 to 0.97, and 0.22 without the largest value. The compound is atypical, with its Fermi level on a peak in the density of states [35] and an Alexandria hull distance of 86 meV per atom [96]. The zero mean is an assumption as well, since the errors of Table 4 have signs and their net is unknown.

Whatever the distribution of true values, calculated values with log-normal error of width σ cannot have an exponential tail of scale τ , as in equation (10), above $y = \tau/\sigma^2$, where Tweedie's formula would make the posterior variance negative. The limit is 45 K at $\sigma = 0.3$ and 25 K at $\sigma = 0.4$. The simulation behind Table 8 keeps the two assumptions, and its calculated values have a heavier tail than equation (10).

Table 8. Median ratio of calculated to true T_c in bins of the calculated value, from a simulation with exponentially distributed true T_c and log-normal calculation error of width σ . The true scale τ_t is set so that the calculated values have the observed mean excess of 4.03 K above 10 K. The second column is the number of compounds of the near-hull sample in each bin.

Calculated T_c (K)	Compounds in sample	$\sigma = 0.15$	$\sigma = 0.2$	$\sigma = 0.3$	$\sigma = 0.4$
10 to 15	255	1.05	1.09	1.23	1.47
15 to 20	75	1.07	1.14	1.34	1.68
20 to 30	21	1.11	1.20	1.47	1.92
30 to 45	3	1.16	1.29	1.69	2.31
45 to 70	1	1.25	1.42	1.96	2.88
True scale τ_t (K)		3.77	3.57	3.05	2.45
Limit τ/σ^2 (K)		179	101	45	25

On these assumptions a compound calculated at 53 K has a median true T_c of 41, 36, 26 and 18 K at $\sigma = 0.15, 0.2, 0.3$ and 0.4 . In a pool of a million compounds of which 4.3% are calculated above 10 K, the most probable highest true T_c is 50, 48, 42 and 34 K. The last two rows of ratios depend on the exponential form assumed for the true values, which the four compounds above 30 K cannot check.

For compounds predicted before they were made, the record cannot yet test the calculation. We have one such comparison at matched pressure for a compound calculated above 10 K. The highest onsets of Mg_2RhH_6 , 24 K near 30 GPa and 29 K at 53 GPa, are a factor of 2.1 to 2.5 below the roughly 60 K its makers calculated for 30 to 50 GPa, in samples whose hydrogen content was inferred (the section on one atmosphere) [23]. Four intermetallics with an identified phase, whose calculations after screening gave 1.9 to 9.3 K, were measured lower by factors of 1.2 to 3.4 [16, 17]. The introduction of the second source prints values that would give 4.2. For σ from 0.15 to 0.4 equation (12) gives ratios of 1.01 to 1.50 there, so selection as modelled does not account for the larger of the measured factors.

Correcting for selection means ranking on the posterior of the true value given the calculated one [110], which needs σ and the distribution of true values in the candidate's own population. Neither is known beyond 50 meV per atom, and we give no corrected value for the compounds there.

One atmosphere

The third condition is persistence at one atmosphere. No hydride predicted to superconduct above 60 K at ambient pressure has been made at, or recovered to, one atmosphere. Table 9 lists eleven such predictions. Two did not form when their metals were heated in hydrogen at the right ratio, two are unstable in the one path-integral simulation run on them, one stayed intact in a short simulation with classical nuclei, and for six we found no test.

Outcomes for the predicted candidates

Figure 5 places the candidates against the scale of known metastability. Half of the known inorganic crystalline phases are metastable, with a median energy above the ground state of 15 meV per atom and a 90th percentile of 67 meV per atom [114].

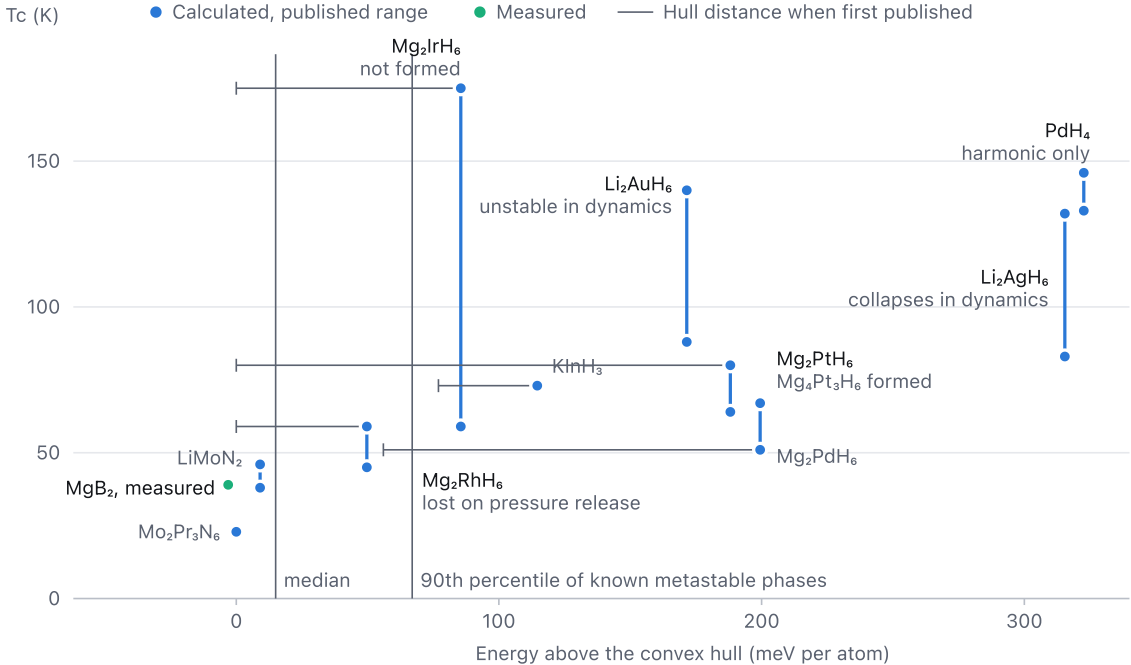


Figure 5. Calculated transition temperature against calculated energy above the convex hull for ambient-pressure candidates. Vertical bars span the published range of T_c for each compound. Horizontal whiskers run from the hull distance first published to the value in the Alexandria database in October 2026. The vertical lines mark the median and 90th percentile of energy above the ground state among known metastable inorganic phases [114]. MgB_2 is the measured value. Sources are in the data file that accompanies the paper.

Table 9. Ambient-pressure hydride predictions whose published range of calculated T_c reaches 60 K, and the test each has had. Hull distances are calculated energies above the convex hull in meV per atom; an arrow runs from the first published value to the value in the Alexandria database in October 2026 [96]. The last two rows lie below 60 K. The list is not complete.

Compound	Calculated T_c (K)	Hull distance	Test and outcome	Sources
Mg_2IrH_6	59 to 175	0 → 85.5	Laboratory: did not form; Mg_2IrH_6 formed	[22, 35, 63, 64]
Mg_2PtH_6	64 to 80	0 → 191.8	Laboratory: did not form; $\text{Mg}_4\text{Pt}_3\text{H}_6$ formed. Not the study's named target	[22, 36, 63]
Li_2AuH_6	88 to 140	171.5	Path-integral simulation: hydrogen pairs into H_2 and diffuses at 80 K	[5, 37, 68]
Li_2AgH_6	83 to 132	319.1	Path-integral simulation: collapses at 80 K	[5, 37]
Li_2CuH_6	80 to 152	80 → 203.9	Simulation with classical nuclei: intact after 10 ps at 300 K. No path-integral simulation or synthesis found	[38, 63, 94]
Mg_2PdH_6	51 to 67	56 → 195.7	Untested	[22, 63]
KInH_3	73	77 → 114.6	Untested	[5, 63]

Compound	Calculated T_c (K)	Hull distance	Test and outcome	Sources
RbPH ₃	90 to 126	none published at 1 atm	Untested; dynamically stable only with quantum anharmonic phonons	[103]
PdH ₄	133 to 146	318.9	Untested; harmonic phonons only	[104]
AcRhH ₈	78	6 (authors' own hull)	Untested; harmonic phonons only	[115]
RbH ₆	180	not known to us	No test found; we read the abstract only	[116]
Mg ₂ RhH ₆	45 to 59	0 → 49.7 (30 in the same group's second survey)	Laboratory: made at 30 to 74 GPa, onsets 18 to 29 K; reverted below about 30 GPa at room temperature	[22, 23, 63, 94]
BaRhH ₈	52	0 (authors' own hull)	Untested; harmonic phonons only	[115]

Mg₂IrH₆. Of the two papers that predicted this compound, one placed it on the hull and the other described it as metastable [22, 64]. Syntheses up to 28 GPa and 2500 K, and a low-pressure autoclave route, produced Mg₂IrH₅ each time. Mg₂IrH₅ has the same metal sublattice with five sixths of the hydrogen sites filled and is a charge-balanced insulator [35]. The hydrogen-rich neighbour Mg₂IrH₇ forms above about 40 GPa, is also an insulator, and on decompression at room temperature reverts to Mg₂IrH₅ near 20 GPa without passing through the metallic composition between them [117]. Mg₂IrH₆ has not been observed, so whether it would last if made by another route is untested.

Li₂AuH₆ and Li₂AgH₆. They have the two highest calculated T_c in the hull figure of the largest ambient-pressure survey, 88 and 111 K [5], and Li₂AuH₆ had passed harmonic and anharmonic phonon checks. In path-integral molecular dynamics at 80 K about a quarter of its hydrogen pairs into H₂ molecules and the rest diffuses. Superconductivity recalculated in that state gives 22 K, and the Hopfield sum we form from it is a factor of 4.2 below the linear-response value for the crystal [5, 37]. Li₂AgH₆ collapses in the same simulation [37]. The evidence is one study with density-functional forces, on 72 atoms for 1 ps and 243 atoms for 6 ps. We found no synthesis attempt for either compound.

The other predictions. Mg₂PtH₆ did not form in a study that explored the Mg-Pt-H system and did not name it as a target. Mg₃Pt and 2:1 Mg-Pt mixtures were heated in hydrogen at 160 bar and at 9 to 24 GPa, and all six high-pressure runs gave Mg₄Pt₃H₆ [36]. Li₂CuH₆ stayed intact in one molecular-dynamics run with classical nuclei [38], a weak test, since Li₂AuH₆ also stayed solid with classical nuclei at 80 K [37]. For the other six rows above 60 K we found no synthesis aimed at the compound and no simulation with moving nuclei. By our count from its figures, which carry no compositions, the largest survey holds 42 compounds of all chemistries calculated at or above 60 K [5].

Mg₂RhH₆. The calculations cited by its synthesis paper put this compound at 45 to 59 K, below the 60 K line. It is the one member of the family that has been made, by one group [23]. Nine cells gave resistive onsets between 18 and 29 K, with no magnetic measurement. The paper quotes 24 K near 30 GPa and 29 K at 53 GPa, against about 60 K that the same authors calculate for 30 to 50 GPa, a ratio of 2.1 to 2.5. The hydrogen content was inferred from the cell volume and one Raman mode, and the authors attribute part of the shortfall to hydrogen deficiency.

cy. On decompression at room temperature the resistance turned insulating at 28 GPa, and diffraction at 0.7 GPa showed Mg_2RhH_5 . Release at low temperature has not been reported. Mg_2RhH_6 is the only compound in Table 9 that was made and then lost.

A low-pressure case: BaSiH_8 . BaSiH_8 was never predicted at one atmosphere. Calculations place it on the hull above 130 GPa and find it dynamically stable down to 3 GPa in an anharmonic estimate, 5 GPa harmonically and 20 GPa with quantum nuclei, with a T_c near 71 K at 5 GPa, and protected against loss of H_2 only above about 30 GPa [118, 119]. In 2026 a cubic Ba-Si-H phase was made by laser heating at 18 and at 31 GPa, and its diffraction pattern persists to ambient pressure [120]. Samples in that study are semiconducting or poorly metallic below about 40 to 50 GPa, and the only superconducting transition reported is 9 K at 142 GPa, where the authors' harmonic estimate is 52 K. The authors assign the phase as BaSiH_8 , propose that its hydrogen has converted to molecular or Si-H covalent units, and note that BaSiH_6 and BaSiH_8 have nearly the same cell volume, so diffraction does not fix the hydrogen content. If the phase is BaSiH_8 , its lattice outlasted the calculated limit of retention by 30 GPa. If it is not, the prediction is untested.

We tabulated the decompression outcomes of about twenty hydrides made under pressure, from papers published between 2020 and 2026; the list is ours and is not a census. Those recovered to ambient conditions include $\text{Y}_3\text{Fe}_4\text{H}_{20}$, U_4H_{15} , $\text{PdH}_{1.3}$, seven lanthanide trihydrides, $\text{Mg}_4\text{Pt}_3\text{H}_6$ and the cubic Ba-Si-H lattice [36, 120, 121, 122, 123, 124]. Those lost on release include Mg_2IrH_7 , Mg_2RhH_6 , UH_7 and PdH_3 [23, 117, 122, 123], and we found no report of a clathrate superhydride recovered to one atmosphere. Within the list the highest measured T_c is 2.9 K, in $\text{Mg}_4\text{Pt}_3\text{H}_6$, among compounds recovered at room temperature and 11.6 K, in ZrH_3 , among those kept only cold [125]. Hydrides loaded by ion implantation or electrochemistry are outside the list. Among them PdH superconducts at 8 to 9 K (Table 3), and a palladium-copper alloy, implanted with hydrogen at liquid-helium temperature, at 16.6 K [126]. The hydride Th_4H_{15} superconducts at about 8 K [127].

Stability and T_c trade against each other

In the largest survey the best calculated T_c at a given distance from the hull rises from 23 K on the hull to 111 K at 319 meV per atom, about 0.3 K for each meV per atom, and that front is a record of the best found (the section on screening) [5]. Among the stable cubic hydrides of the GNoME database the highest calculated T_c is 23.5 K by the Allen-Dynes formula and 17 K after refinement with a first-principles Coulomb interaction, and the authors write that values of order 100 K appear systematically linked to thermodynamic instability [109]. A 2026 survey of about two million hydride structures finds more than 600 above 20 K, at roughly 100 meV per atom or more from the hull [128].

A 2025 calculation places fluorite-type BaRhH_8 on the ambient-pressure hull with a calculated T_c of 52 K, and AcRhH_8 6 meV per atom above it with 78 K [115]. Its hull uses a different set of competing phases from the surveys above, and neither compound has been tested beyond harmonic phonons. If the calculation stands, the two are exceptions to the trade.

For the six rows of Table 9 that give a first published value, the hull distance rose by about 40 to 190 meV per atom by October 2026. The papers do not say which competing phases moved them, but the database lists the decomposition products [96]. For Mg_2IrH_6 and Mg_2RhH_6 they

are the compositions with five and seven hydrogen atoms. For Mg_2PdH_6 , KInH_3 and Li_2CuH_6 they include MgH_6 , KH_7 and CuH_4 , which we do not know to have been made at one atmosphere, so part of the rise for those three may not correspond to compounds that exist. In the Matbench Discovery benchmark about 33,000 structures lie below the Materials Project hull, and about 20,000 of them remain on the hull once the benchmark's own structures are added [129].

That strong coupling at the Fermi level drives phonons toward instability is known [75], and two hydride surveys report that high calculated T_c goes with distance from the hull [63, 109]. We put the link in the terms of this paper, as a hypothesis. A large η_H means that the energies of electrons at the Fermi level change steeply when hydrogen moves. A lattice can use the same sensitivity to lower its energy, by rearranging its hydrogen at fixed composition or by taking up or releasing hydrogen until the electron count closes a shell. The Mg_2IrH_6 family shows the second route. Its metallic composition sits between two insulators one hydrogen atom away on either side, Mg_2IrH_5 with a calculated gap of 0.65 eV and Mg_2IrH_7 with 2.46 eV [35, 117]. Li_2AuH_6 shows the first in simulation, where pairing a quarter of its hydrogen into molecules removes three quarters of its Hopfield sum. In the Fröhlich model with a structureless coupling, the conduction electrons lower the force constant of a mode by twice its Hopfield parameter [29, 75]. The bare force constant is not observable in a real metal, so we take from the relation only that the most strongly coupled modes are the ones at risk. Li_2AuH_6 , which has about 70% of its λ below 30 meV [68] and fails once its nuclei move, fits this account. One case does not test it.

Pressure opposes these instabilities through the PV term in the enthalpy. A phase that is denser by one cubic ångström per atom is favoured by 624 meV per atom at 100 GPa, nine times the 90th-percentile metastability of known compounds, and it loses all of that on release. In the superhydrides pressure therefore stabilises a hydrogen-rich metal against the insulating phases that compete with it, and it raises the hydrogen density and with it η_H .

Hull distance and phonon stability do not predict survival

The standard computational filters are energy above the hull and the absence of imaginary phonon frequencies. That neither is a criterion for lifetime is known. The authors of the metastability scale present it as a description of observed phases and leave kinetics to later work [114], and the prediction of BaSiH_8 added a kinetic threshold for this reason [118].

Mg_2RhH_6 passed both filters and was lost on decompression. Li_2AuH_6 passed the phonon test, with and without anharmonic corrections, and is unstable in path-integral dynamics. The cubic Ba-Si-H lattice is recovered below both limits calculated for BaSiH_8 . The high-pressure phases of $\text{Bi}_{0.5}\text{Sb}_{1.5}\text{Te}_3$ fail the phonon test at zero pressure, and superconductivity was retained there after a quench [130]. Aluminium hydride lies 120 meV per atom above aluminium and hydrogen gas in Gibbs energy at room temperature and is stable only above about 7 kbar of hydrogen, yet it keeps at ambient conditions because its hydrogen release is limited by kinetics [131].

The barrier needed for a lifetime of one year at 300 K depends on which step limits the loss. If each hydrogen site empties independently by one activated event with an attempt frequency of 10^{13} per second, the barrier must be 1.22 eV, or 1.0 eV at 10^{10} per second; a week at 200 K needs 0.75 eV. If one such event anywhere among N sites starts a transformation that then runs

quickly, the requirement rises by $k_B T \ln N$, to 1.9 eV for $N = 10^{12}$, the number of hydrogen atoms in a grain about 2 μm across. If loss is limited by diffusion to a free surface, a plate of thickness L empties in a time $L^2/\pi^2 D$, and with a diffusion prefactor of 10^{-3} cm^2 per second the migration barrier must be 0.68 eV at 10 μm , 0.45 eV at 1 mm and 0.33 eV at 1 cm.

The calculated activation energy for hydrogen migration is 0.23 eV in palladium and 0.46 eV for hydride ions in the polyhydride CaH_4 under pressure, the second from molecular dynamics at 1000 K and above [132, 133]. With the same prefactor a 10 μm grain empties in about a second at 0.23 eV and in an hour and a half at 0.46 eV, so bulk diffusion does not hold hydrogen in grains of the size made in diamond anvil cells. At 0.46 eV a plate 1 mm thick has a relaxation time of 1.7 years, so slow diffusion could contribute to retention in a bulk sample. In a grain the hydrogen has to be held by a barrier to nucleating the hydrogen-poor phase, by a barrier to recombination at the surface, or by strong binding in a closed-shell unit. The complex hydrides Mg_2IrH_5 and $\text{Mg}_4\text{Pt}_3\text{H}_6$ have the last of these, and neither superconducts above 3 K [35, 36].

A decomposition temperature can be read as a barrier through the per-site formula, $E = k_B T \ln(\nu t)$ for loss in a time t . The result is a scale that assumes one rate-limiting step and moves by 0.04 to 0.08 eV for each factor of ten in the assumed prefactor ν . With $\nu = 10^{13}$ per second, ZrH_3 , which decomposes to ZrH_2 between 200 and 270 K when heated at 10 K per minute in vacuum, reads 0.6 to 0.85 eV [125]. $\text{Y}_3\text{Fe}_4\text{H}_{20}$, unchanged after 30 hours in air at room temperature and 7 to 8% smaller in volume after one to three months, reads 1.1 to 1.2 eV [121]. AlH_3 is the one hydride here with measured kinetics. It decomposes between 60 and 140 $^\circ\text{C}$ by nucleation and growth, with an activated complex of about nine formula units and an activation energy of about 1.06 eV [131, 134], where the per-site reading of the same decomposition times is about 1.2 eV. Isothermal decomposition curves from the same laboratory [135], as we read them, correspond to an effective prefactor near 10^{10} per second and extrapolate to about a third of the hydrogen lost in roughly a year at 300 K. That report describes fresh material as pyrophoric and surface-treated material as stored at ambient conditions for more than twenty years. In the one case with known kinetics the lifetime depends on nucleation and on the surface as well as on a barrier.

For the compounds of Table 9 we found no published rate, single-event barrier or lifetime for hydrogen loss. The only path calculations we found are nudged-elastic-band results for Mg_2IrH_6 , which give no barrier along one path for inserting hydrogen into Mg_2IrH_5 and 32 meV per atom between two Mg_2IrH_6 polymorphs [35].

States retained at ambient pressure

Cooling under pressure and releasing cold is an established way to recover binary transition-metal hydrides made at several GPa, and it is how ZrH_3 is kept [125, 136]. Deng, Chu and coworkers applied cold release to pressure-enhanced superconductors in diamond anvil cells. In FeSe a quench from 4 GPa at 4.2 K retains an onset of 37 K against 9 K for the ambient phase. That state is gone after warming to about 200 K, and heating to 300 K leaves a strained crystal with a T_c near 20 K [137]. On the per-site scale a state lost near 200 K within minutes to a week reads 0.6 to 0.75 eV at 10^{13} per second. For prefactors from 10^6 to 10^{13} per second the reading stays between 0.4 and 0.6 of the requirement for a year at 300 K.

In $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_{8+\delta}$ quenched from 10 to 30 GPa, five samples retained resistive onsets of 139 to 151 K, against 133 to 135 K for the equilibrium phase. Zero resistance after the quench is not reported. Cycling to 170 K lowered the onset slightly, cycling to room temperature lowered one sample from 147 to 143 K, and a sample retrieved from the cell through room temperature showed about 140 K with a shielding fraction of about 78% in magnetisation. Part of the enhancement therefore outlasts room temperature for the time of handling, and a loss this gradual is not described by one barrier. Diffraction finds the same tetragonal structure with broader peaks, and the authors attribute the retention to strain or defects [10]. The quench results on superconductors come from one group, and we found no independent replication.

Epitaxial strain substitutes for pressure in films a few unit cells thick. Bulk $\text{La}_3\text{Ni}_2\text{O}_7$ shows signatures of superconductivity near 80 K only above about 14 GPa [138]. Compressively strained $\text{La}_3\text{Ni}_2\text{O}_7$ films superconduct at ambient pressure [139], and $(\text{La},\text{Pr})_3\text{Ni}_2\text{O}_7$ films reach an onset of 63 K and zero resistance at 37 K [140].

The boron-carbon clathrate SrB_3C_3 was recovered from about 50 GPa to one atmosphere, where it persists in an inert atmosphere and degrades in moist air within hours [141]. Its superconducting onset is about 20 K at 40 GPa, and we found no measurement of its transition at one atmosphere [142]. Across chemistries the accessible range of metastability scales with cohesive energy [114].

Data on persistence

Electron-phonon calculations have been published for more than ten thousand metals at ambient pressure [5]. The record of persistence has not been assembled. Beyond the twenty or so outcomes we tabulated, older records exist that we have not collected. Binary hydrides of the 3d and 4d metals of groups VI to VIII have been made at several GPa, cooled under pressure and studied at one atmosphere [136]. RhH_2 , made at 8 GPa and released cold, keeps its hydrogen indefinitely at 77 K and for minutes at 150 K [143]. Room-temperature equilibrium pressures have been compiled for about five thousand storage-hydride compositions; they describe stable phases and do not record whether a metastable hydride survives [144]. We found no compilation of recovery outcomes with their protocols, and no test of a descriptor against one.

We found calculated barriers along a transformation path for two hydrides, BaSiH_8 and Mg_2IrH_6 , and one path-integral simulation that tests whether an ambient-pressure candidate survives [35, 37, 118]. A model that ranks candidates by a predicted T_c and filters on hull distance and harmonic phonons ranks on the quantity for which data are plentiful and filters with two tests that have each failed in the cases above. For the four candidates above 60 K that did not form or were unstable in simulation, the outcome was decided by which phase forms or by the motion of hydrogen, and we found no labelled set for either.

When phonons do not provide the pairing

The ambient-pressure record belongs to the cuprates, which are classed as unconventional superconductors and whose pairing mechanism is not settled [138, 145]. The iron-based superconductors reach 55 to 56 K in bulk [146, 147]. A review of single-layer FeSe on SrTiO_3 quotes a T_c

of 65 K, and 109 K from a single in situ transport measurement, against 9 K for bulk FeSe, and weighs phonon pairing, magnetic or orbital pairing, and the two acting together [148, 149]. This paper treats the two kinds of pairing separately and does not cover a mixed case.

The cuprate stiffness scale is close to T_c

From equation (2) Carlson and coauthors tabulate a T_θ of 130 to 190 K for the mercury compound, whose T_c is 133 to 135 K, 140 K against a T_c of 85.5 K for optimally doped $\text{Y}_{0.8}\text{Ca}_{0.2}\text{Ba}_2\text{Cu}_3\text{O}_{7-\delta}$, and 54 K against 38 K for optimally doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. The ratios are 1.0 to 1.6, where MgB_2 has 36 [25]. The authors caution that the prefactor depends on microscopic details, so these ratios suggest that stiffness limits T_c in the cuprates and do not establish it. In underdoped cuprates T_c rises linearly with superfluid density over part of the doping range [150].

Putting T_θ at 300 K in equation (2) requires an in-plane penetration depth of 106 nm or less at a layer spacing of 6 Å. The optimally doped cuprates in the same tabulation have 150 to 270 nm. For the mercury cuprate the requirement is 1.6 to 2.3 times its tabulated stiffness.

Uemura's empirical upper limit on T_c/T_F , about 0.05 with T_F derived from the superfluid density, describes the cuprates and the other strongly correlated superconductors in his compilation [151]. Gate-doped Li_xZrNCl , a two-dimensional superconductor, reaches $T_{\text{BKT}}/T_F = 0.12$ at low carrier density [152], close to the bound of 1/8 for a single parabolic band in two dimensions [40]. At a ratio of 0.05 a 300 K transition needs a Fermi temperature of 6000 K, which is 1.3 carriers per CuO_2 cell if the effective mass is four electron masses, the value we assume for a cuprate-like band. At 0.12 it needs 2500 K and about half a carrier per cell.

Calculated T_c is a few percent of the electronic energy scales

Qin and Yang find T_c/J peaking between 0.04 and 0.07 across several effective pairing models, with the best cuprates at 0.06 to 0.067, and conclude that 300 K at ambient pressure would need a superexchange J of 400 to 700 meV [153]. The cuprates in their table have 105 to 176 meV. The dynamical cluster result $T_c = 0.023t$ for the Hubbard model at $U = 4t$ and 10% doping [154] would need a hopping t near 1.1 eV, against the 0.4 eV we take for the bare one-band hopping of a cuprate. Both are numerical results on simplified models, and Qin and Yang say that theirs carries no proof. On these two results a cuprate-like route to 300 K needs J at 2.3 to 4.0 times the largest value in that table, or t at 2.8 times the value we take.

No validated forward model

We know of no controlled, validated theory that returns T_c from a crystal structure in this class. A dynamical vertex calculation on a one-band model of NdNiO_2 gave the doping range of the infinite-layer nickelates three weeks before the measured dome was posted, with a maximum T_c of 36 K against the 15 K then measured at 20% strontium; changing one interaction parameter from $8t$ to $9t$ nearly removes the difference [155, 156]. A density-matrix embedding calculation from the crystal structure returns d -wave order and a pairing gap for CaCuO_2 at three pressures and for two mercury cuprates. Its T_c is a weak-coupling conversion of the gap, about 180 K for CaCuO_2 at ambient pressure against about 110 K measured in the strontium-substi-

tuted compound [157]. We found no blind test of either method on a second family. A 2022 review of the numerical methods calls the mapping from a material to model parameters neither systematic nor controlled [158].

Ground-state studies of the Hubbard and t - t' - J models find stripes with no superconducting order in the pure Hubbard model at 1/8 doping [159] and disagree on whether next-nearest-neighbour hopping gives pairing on the hole-doped side [160, 161]. None of the three reports a T_c .

Four material-specific descriptors have been correlated with the maximum T_c within the cuprates: the charge-transfer energy, the hopping range that grows with the apical oxygen distance, the superexchange and the hole content on planar oxygen [162, 163, 164, 165]. They are not independent, since the superexchange depends on the charge-transfer energy E as $J \approx 4t^4/E^3$ [166]. The published correlations are in-sample trends across eight to sixteen compounds or families [162, 164, 165], and we found no test of any descriptor on compounds held out of the fit. $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ has 1.5 times the J of $\text{YBa}_2\text{Cu}_3\text{O}_8$ and half its T_c [153].

A nickel analogue of the cuprates was proposed in 1999 and found in 2019, at 9 to 15 K [167, 168]. $\text{La}_3\text{Ni}_2\text{O}_7$ was named in 2017 as a possible realisation of a bilayer model that might exceed cuprate T_c , with the note that it did not superconduct. Signatures of superconductivity near 80 K were reported in 2023 between 14 and 43.5 GPa, and the proposal did not mention pressure [138, 169]. Norman wrote in 2016 that the heavy-fermion, cuprate and iron-based superconductors each took the community by surprise [145].

What a model can do in this class

From a band structure a model can compute an upper bound on the superfluid stiffness of a hypothetical layered compound, because the stiffness cannot exceed the optical sum-rule weight of the bands [40]. Inside a known family it can rank compounds on the descriptors above, which have been tested only in sample. The record gives no basis for proposing a new family, and we do not ask roomtsc to try.

The pressure-quenched mercury cuprate, with an onset up to 151 K, and compressively strained nickelate films, with an onset of 63 K, each show at ambient pressure a T_c that the bulk equilibrium material reaches only under pressure [10, 140]. Both are treated under "States retained at ambient pressure". The strain in the films is held by their substrate.

What roomtsc estimates

roomtsc is a staged estimator, and none of it has been trained. For a candidate crystal structure at one atmosphere it returns an estimate of each condition with an uncertainty, and a decision layer uses those estimates to choose which calculation or experiment to run next. Table 10 lists the components.

Table 10. Specification of roomtsc by component. Label counts are as of October 2026.

Component	Input	Output	Labels	Uncertainty
Hopfield sum	relaxed structure at 1 atm	tensor h_j on each atom; S	S in the dynamically stable Alexandria records, hydrides not yet counted; S and a cell for 62 ambient-pressure hydrides and PdH; η_H for 5 megabar compounds	ensemble spread, rescaled on held-out prototypes
Phonons	the same structure	force constants, frequencies, eigenvectors	none; a universal potential checked against stored linear-response dynamical matrices	errors of $\langle \omega^2 \rangle$ and of the lowest optical branch in that check
Spectrum and T_c	the two rows above	$\alpha^2 F$, λ , Φ , T_c	none; equation (13) and the Eliashberg equations	propagated samples; $\mu^* = 0.10, 0.13, 0.16$
Hull distance	composition, enumerated competitors	energy above the hull with zero-point energy	density-functional energies	none for competitors not enumerated
Survival	structure, fine-tuned potential	survives or decomposes in path-integral dynamics at 77 and 300 K	one density-functional simulation of two compounds	a run without an event bounds the barrier from below
Barrier and lifetime	structure, decomposition paths	barrier per event; lifetime at the operating temperature	outcomes of Table 12; two published barriers	range over the limiting step and prefactors of 10^{10} to 10^{13} s^{-1}
Stiffness and G_i	structure, λ , plasma frequency, Fermi velocity	penetration depth, coherence length, G_i	none	not calibrated

Pairing by phonons

No part of roomtsc is trained on T_c . The supervised label is the Hopfield sum S . For a dynamically stable compound, a record of the Alexandria electron-phonon release of 11 August 2025 holds the relaxed cell, the dynamical matrices, the spectral function at ten smearing widths with its split by phonon branch, and λ , $\omega_{\log}$ and the second moment, from which S follows [5, 96]. We read this layout from the files we opened and the survey's workflow script, and neither paper describes it. S depends on the smearing. In the one record we read in full, λ is 0.78 at a width of 0.005 Ry and 0.61 at 0.020 Ry. Each label carries its width, and the model is trained at one width.

The hydrogen part of S is a label only where the hydrogen vibrations separate from the rest. A split by branch gives $\sum_j \eta_j/M_j$, and the term of one atom type needs the coupling in the basis of atomic displacements, which the records do not hold. Where each of the $3n_H$ highest branches has at least 90% of its eigenvector weight on hydrogen at every stored wavevector, their first moment is η_H/M_H to that accuracy and $h = \eta_H/\rho_H$ is a label. Quan and coauthors formed the megabar values from the high-frequency part of spectra in which the hydrogen and metal

modes are disjoint [28]. Where the criterion fails, as we expect in Li_2AgH_6 , whose lowest optical branches mix hydrogen and lithium [5], S alone is supervised and its division between atoms is latent.

Labels for h are few. The census of Table 7 has 62 ambient-pressure hydrides and PdH , with S from published tables standing in for η_H , and five megabar compounds. The public sets under pressure add none so far. About 1,900 literature pairs of λ and $\omega_{\log}$ carry no second moment and no cell [170]. About 900 uniform calculations up to 500 GPa use a $2 \times 2 \times 2$ grid of phonon wavevectors, and we have not opened their archive to see whether it holds the spectral functions [171]. We have not counted how many Alexandria records contain hydrogen or pass the branch criterion.

Across the census h is 23 eV Å to within a factor of about 1.5. The 62 ambient-pressure values have a geometric mean of 22 eV Å and a spread of a factor of 1.44, the five megabar compounds lie between 24 and 45 eV Å, and a proton in an electron gas has 33 to 37 eV Å at metallic densities (Table 7, Table 5). The estimator is therefore scored against two baselines in every test. The first is the electron-gas value, 36.6 eV Å, for every hydrogen atom, which is high at one atmosphere, where the census mean is 0.6 of it. The second is a constant, fitted on the training split, times the hydrogen-projected density of states at the Fermi level per unit volume. A model can improve on them only where h departs from the typical value, in compounds with little hydrogen weight at the Fermi level, such as PdH at 7.2 eV Å, and in the rare compounds well above it. The present labels cannot show whether it does, because the three calculations of Mg_2IrH_6 in Table 6 differ by more than the spread between compounds. Calibration is measured on a reference set of a few hundred calculations with dense Fermi-surface sampling, drawn at random within strata of predicted h before any acquisition guided by the model. Calculations acquired later on the model's own output are reported separately, because they carry the selection effect of the section on screening.

Learning h leaves an extrapolation of a stated size. A 300 K transition at a hydrogen density of 0.10 Å^{-3} needs 87 to 120 eV Å for a single mode, which is 2.0 to 2.7 times the largest megabar value and 1.4 to 1.9 times the largest in any calculation, the 64 eV Å of one calculation of Mg_2IrH_6 . Megabar calculations add chemistry and add nothing to the range of the target. Whether a model trained on them transfers to one atmosphere is untested. The next section specifies the test, which five compounds are too few to run, and until it is passed megabar labels stay out of the training of the estimator used at one atmosphere.

S and the phonons do not give λ . Each mode contributes its share of S divided by the square of its frequency, so λ depends on how S is divided among displacement directions and wavevectors. The learned output is therefore a symmetric 3×3 tensor h_j on each atom j , whose trace averaged over the hydrogen atoms is h . The spectrum is built from it in a local approximation, which drops the coupling between displacements of different atoms and its dependence on wavevector:

$$\lambda = \frac{1}{N_{\mathbf{q}}} \sum_{\mathbf{q}\nu} \frac{s_{\mathbf{q}\nu}}{\omega_{\mathbf{q}\nu}^2}, \quad s_{\mathbf{q}\nu} = \sum_j \frac{1}{M_j V} \mathbf{e}_j^\dagger(\mathbf{q}\nu) h_j \mathbf{e}_j(\mathbf{q}\nu), \quad (13)$$

where $\mathbf{e}_j(\mathbf{q}\nu)$ is the part of the normalised eigenvector of branch ν on atom j and V is the cell volume. The shares $s_{\mathbf{q}\nu}$ sum to S at every wavevector. A scalar spread equally over directions is inadequate. In the spectra of Mg_2IrH_6 and Mg_2RhH_6 we binned from published figures [22, 64], the bins above 150 meV, which we read as the six metal-hydrogen stretching branches, are one third of the hydrogen modes and hold 58 to 63% of the hydrogen Hopfield sum. Giving them one third at the same S and the same frequencies raises T_c by 21 to 39% at $\mu^* = 0.13$. We have not measured the error of the local tensor against the full coupling. The tests include that measurement against the branch-resolved Alexandria spectra, made before training, and an end-to-end requirement on held-out prototypes: Φ within 15% and T_c within 25% of the values from the linear-response spectrum.

The force constants come from an interatomic potential. For non-magnetic semiconductors at ambient pressure the best of seven universal potentials reproduces the maximum phonon frequency with a mean absolute error of 17 K, and two of the seven are off by 291 and 780 K [172]. No benchmark of that size covers metals or hydrides, and the maximum frequency says little about the modes below 100 meV, which carry more than 80% of λ in the four ambient-pressure spectra we solved. We check the potential against the linear-response dynamical matrices of the Alexandria release before it is used. T_c is computed from the Eliashberg equations at μ^* of 0.10, 0.13 and 0.16, because the closed forms are 19 to 36% off for strongly coupled hydrides (Table 4). roomtsc does not estimate the Coulomb term.

The alternative design learns the matrix elements. Networks that predict the Kohn-Sham Hamiltonian, with its gradient predicted or taken by finite differences, have given electron-phonon interactions for individual systems [173, 174]. We know of none with the reach that universal potentials have for phonons, and we learn h because public labels exist for it. The rigid-muffin-tin approximation gives η from a band-structure calculation alone [30]. For H_3S , LaH_{10} and YH_{10} , where we compared published values, its η_H is 1.2 to 1.9 times smaller than the linear-response value [28, 57, 88]. If that deficit proves predictable, the approximation becomes the first stage.

The reference set leaves two defects of the labels in place. The harmonic frequencies do not enter S , but the classical structure and the linear vertex that a harmonic calculation assumes do. In Li_2AuH_6 the structure reached in path-integral dynamics has S of 0.86 eV/Å², which we form from that study's λ and second-moment frequency, against 3.6 for the crystal in linear response, a factor of 4.2 between two different methods [5, 37]. The treatment of the vertex moves λ of PdH between 0.27 and 0.64 [60]. The persistence component tests for the first, and nothing in roomtsc estimates the second. The harmonic filter also decides which compounds have labels. Records with imaginary harmonic modes carry no spectral function, and the peer-review file of the survey reports that about 85% of nearly 40,000 hydrides sent to linear response were dropped for that reason [5]. Strong coupling at the Fermi level drives phonons toward instability [75], so the unlabelled compounds may include those with the largest h . S is defined whether or not a mode is unstable, and we will compute it for a random sample of the unstable hydride records to measure the bias.

Persistence

This component replaces the usual pair of filters with three estimates of increasing cost.

The first is energy above the convex hull against a competitor set that is enumerated for the candidate as well as read from a database. For Mg_2IrH_6 the phase that formed in its place, Mg_2IrH_5 , was its neighbour in hydrogen content [35]. For a hydride the set includes the same metal sublattice at each nearby hydrogen count, the closed-shell variants allowed by electron counting, molecular and covalently bound forms of the hydrogen, and decomposition into those plus H_2 gas at its room-temperature chemical potential. Zero-point energy is included; in RbPH_3 at 25 GPa it lowers the hull distance from 33 to 6 meV per atom [103].

The second is survival in path-integral molecular dynamics at 77 K and 300 K, at one atmosphere. In the retrodiction test of the next section the dynamics run at the temperature of each recorded protocol. The one such simulation of ambient-pressure candidates used density-functional forces with 16 beads on at most 243 atoms for 6 ps [37], which is too expensive for a filter. A potential fitted to BaSiH_8 was about 20,000 times faster than the reference method in a self-consistent harmonic calculation [119]. The precedent is for cost alone. That potential was fitted around one structure and would not describe hydrogen pairing or decomposition products, and the calculation put the limit of dynamical stability near 20 GPa. A cubic Ba-Si-H lattice assigned to that compound was later recovered at ambient pressure [120]. We have not measured the cost per candidate of fine-tuning a potential that describes those products and running path-integral dynamics with it.

A molecular-dynamics run in which nothing decomposes gives a lower bound on the barrier. Half a nanosecond at 700 K on 750 hydrogen atoms with no event excludes per-site barriers below about 0.9 eV at an attempt frequency of 10^{13} per second, which guarantees no more than minutes of per-site lifetime at 300 K. The third estimate is therefore a barrier per event along the lowest decomposition path found, converted to a lifetime at the operating temperature. The paths to search are hydrogen pairing into molecules, hydrogen loss at a surface, nucleation of the hydrogen-poor neighbour, and reversion to the nearest closed-shell competitor. The conversion depends on which step limits the loss and on the prefactor, so the lifetime is reported as a range over the three limiting steps of the section on one atmosphere and over prefactors from 10^{10} to 10^{13} per second.

The first universal potentials, trained on structures near equilibrium, soften the energy surface, which lowers migration barriers [175], and the energy errors of the eight universal potentials tested grow by a factor of 7 to 28 between 0 and 150 GPa [176]. Fine-tuning corrects much of the softening [175]. Fine-tuning on high-pressure structures lowered the error of the two potentials it was applied to at 150 GPa and raised it at ambient pressure by factors of 6.0 and 6.6 [176]. The estimator uses potentials fine-tuned on hydrogen-rich structures along decomposition paths, and every barrier used to accept or reject a candidate is recomputed with density functional theory.

The labels for this component are those counted under "Data on persistence": our tabulation of about twenty decompression outcomes, which is not a census, calculated barriers for two hydrides, and one path-integral simulation. The main data cost of the project is a few thousand simulated survive-or-decompose outcomes with barriers, for hydrides near the hull at one atmosphere. Those outcomes are a surrogate for the simulator and carry no information about experiment, for which the anchor is the retrodiction set of Table 12.

Stiffness and fluctuations

Over the 22 to 189 nm inferred for the penetration depth of H_3S , the stiffness scale is 7.5 to 475 times T_c and Gi runs from about 10^{-6} to 3×10^{-3} [41, 43, 44]. An October 2026 addendum to the first paper re-derives 24 nm from unsmoothed data, for which the ratio is about 400 [45]. For dense three-dimensional metals roomtsc does not filter on stiffness. It estimates the penetration depth from the plasma frequency and the mass renormalisation $1 + \lambda$, and the coherence length from the Fermi velocity and the gap, and reports Gi from them without calibration. For layered and low-density candidates the same estimate is used as a filter.

Unconventional candidates

For compounds in the known unconventional families roomtsc reports what the section on pairing without phonons supports, an upper bound on the stiffness from the band structure and the family descriptors. It reports no T_c and no Gi for them.

The dossier

Every shortlisted candidate leaves roomtsc with a dossier. It names the composition to load and the route. It lists the phases to expect beside the target, from a convex-hull calculation at the loaded composition that includes the elements of the precursors, the hydrogen source, the electrodes and the gasket, repeated over the range of pressure in the sample. That calculation misses metastable phases selected by the heating, so the dossier also lists every known phase of each chemical subsystem with its superconducting, structural and magnetic transitions. It states the signatures a true positive would show: the upper critical field implied by the coherence length, the isotope shift implied by the share of the Hopfield sum on hydrogen, and the gap. It states the predicted T_c at the pressure of measurement, for $\mu^* = 0.13$, and the persistence prediction under a named protocol, which the prospective test of the next section scores.

The decision layer

The stages run in order of cost: relaxation and phonons with an interatomic potential, at minutes per structure [177]; the pairing estimate; the hull against enumerated competitors; path-integral dynamics and barriers; a converged electron-phonon calculation; synthesis. A computed T_c is reported with a value corrected for selection only where the distribution of calculated values in the candidate's own population has been measured on members chosen without regard to predicted T_c , and then at each σ of Table 8, since we have not estimated σ . Beyond 50 meV per atom of the hull we give no corrected value. Where a component fails its test, the decision layer falls back as the next section fixes. It uses the better baseline in place of the estimator of h , reports no T_c without a linear-response spectrum, and filters on the hull stage alone.

Thresholds between the computational stages are set jointly, because a fixed top fraction at each stage cannot be chosen well in advance. In a four-stage synthetic benchmark with 100 true positives and neighbouring stage scores correlated at 0.8, passing the top tenth found 26. Passing the top three quarters found all of them at 49% of the cost of running the last stage on every candidate, and jointly optimised thresholds did so at 20% [178]. Our stages share a density functional and a structure, so their errors are correlated, and the joint distribution of the computational stage scores has to be estimated from a random sample of candidates carried

through all of them. No candidate has been carried through to synthesis, so nothing connects those scores to laboratory outcomes. roomtsc therefore returns a ranked shortlist with the estimates behind each entry and does not multiply them into a probability that all conditions hold.

The tests, fixed before training

roomtsc has no example of its target and cannot be scored on finding one. It can be scored on scattering strengths computed for compounds it has not seen, on spectra from linear response, and on the recorded outcomes of hydrides at one atmosphere. This section fixes those tests before any component is trained. Each has a baseline, a mark and an action that follows from failing it. Where no measurement dictates a threshold the choice is ours, and it is made here.

Base rates and likelihood ratios

Take a pool of 10^6 candidate structures that contains one compound meeting all three conditions. A perfect ranking that keeps the top hundred yields one success in a hundred syntheses, so the probability per shortlisted candidate averages one percent, and no ranking gives more. That figure is conditional on the pool containing such a compound. Unconditionally it is one percent times our credence that one exists, which the section on the odds puts at about one in a hundred or lower, so at most about 10^{-4} per candidate.

Even odds for one named candidate would need a cumulative likelihood ratio of 10^6 . The entry ranked first on the Matbench Discovery leaderboard on 6 October 2026 and the superconductor classifier of Stanev and coauthors reach about 70 and 80, which we compute from their reported precision, 0.927 and 0.74, at prevalences of 15% and 3% [12, 129, 179]. Each figure belongs to the operating point its authors chose and to held-out data of the same origin as the training set, and we found no classifier in this field measured at a selected fraction near 10^{-4} . The stages of roomtsc share inputs, and a second screening step adds less the more it is correlated with the first [180], so their likelihood ratios would not multiply.

roomtsc is therefore judged on the shortlist it returns and on what that shortlist costs to test. LK-99, made by solid-state synthesis at ambient pressure, was claimed as a superconductor on 22 July 2023. Insulating single crystals were reported 20 days after the claim, and the question was reported settled after 25 [181, 182]. A refutation of the lutetium hydride claim at 1 GPa was posted after 7 days and published after 64 [183]. The first outside attempt we found on $\text{LaSc}_2\text{H}_{24}$ at 260 GPa was posted eight months after the claim and was not decisive [8, 9]. On that record a claim testable below a few GPa is settled in weeks, and one that needs megabar synthesis takes months.

Rules for every split

Records are de-duplicated before any split, and every record of one compound goes to the same side, whatever its source, settings or pressure. The literature compilation cites the survey of Shipley and coauthors for some of its rows [170, 184], and the public high-pressure set computes each of its materials at 0, 100, 200, 300 and 500 GPa [171], so a cut in pressure alone would leave the zero-pressure record of a megabar test compound in training.

Splits assign whole structural prototypes, because members of one prototype fall on both sides of a cut in value. Of the sixteen cubic A₂MH₆ hydrides in the tables of one survey, fourteen lie above the 90th percentile of $M_H \lambda \omega_{\log}^2$ that we compute for the 12,053 compounds plotted in the largest survey, 0.23 eV/Å², and two below [5, 63]. Each result is also reported without the prototype rule, and the grouped result is the one that counts.

A reference value is the label of the held-out record where one exists. Where none exists it is a new calculation at the settings of the training labels, made by someone who does not see the predictions. References are deposited before training, with the predictions of the baselines and the database identifiers on each side of each split.

Each test of h is scored by the mean absolute error in $\ln h$ over the held-out compounds that pass the branch criterion, for the estimator and for the two baselines of the previous section, the constant 36.6 eV Å and a constant fitted on the training side times the hydrogen-projected density of states at the Fermi level per unit volume. The estimator passes if its error is at most half that of the better baseline and the 95% interval of the ratio of the two, from resampling held-out prototypes, lies below one. We set the margin at one half. The baselines need no electron-phonon labels, the constant is off by a factor of 1.26 on the megabar compounds below, and a factor of 1.3 in η moves T_c of the four ambient-pressure spectra by 24 to 41% (the section on what 300 K costs). Where the estimator fails a test, roomtsc uses the better baseline for that quantity and the failure is reported with every shortlist.

We had seen some of the targets when we wrote the tests. The megabar values of the first test and the Mg₂XH₆ values of the fourth are rows of Table 3 and Table 6, so a pass on those rows shows that the estimator reproduces numbers that shaped the design. The targets we have not seen are the second moments of the Alexandria records outside the census, the new megabar references, the references for the cubic A₂MH₆ compounds without a converged calculation, and every laboratory outcome published after the tests are deposited.

Pairing: the scattering strength held out

Published tests on measured T_c show that models trained on T_c do not extrapolate upward. With the lowest 90% of a SuperCon-derived table for training and the top 10% for testing, the best of ten methods have errors near 37 K against about 10 K on random splits, and none places more than about 5% of the held-out entries above the training ceiling [185]. In forward cross-validation a random forest cannot predict above its training maximum, and a neural network did so in 3% of cases [14]. Trained on data from before 2008, one deep-learning model gives a finite predicted T_c to 3 to 6% of the iron-based superconductors, or 9% with two iron-based compounds left in training, and a random-forest classifier finds none [186]. Two cases have gone better. A model trained on part of the lowest 99% of six calculated properties recovered about three quarters of the top 1% [187], and a formula in λ , $\omega_{\log}$ and μ^* , fitted to superconductors below 10 K, gave a reasonable value for H₃S [188]. A hold-out of calculated h therefore shows skill only against baselines.

The first test holds out pressure. The estimator is trained on calculations at or below 50 GPa, with the prototypes of the test compounds removed at every pressure, and asked for h in hydrides at 100 GPa or above. We found no paper that prints h for the five megabar compounds

of Table 3, and the paper that gives their η_H prints no cell volumes [28]. The references in Table 11 divide that η_H by the hydrogen density from other calculations of the same structures, as in Table 6.

Table 11. Reference values for the pressure test. η_H is from [28]. The volumes, those behind Table 6, are printed at that pressure for YH₁₀ [91], taken from lattice constants quoted at second hand for CaH₆ and MgH₆ [93], and interpolated for H₃S and LaH₁₀ [61, 89] (appendix). The last column is the error of the constant 36.6 eV Å against the reference.

Compound	Pressure (GPa)	Volume per formula unit (Å ³)	ρ_H (Å ⁻³)	η_H (eV/Å ²)	h (eV Å)	Baseline error
H ₃ S	220	13.0	0.231	10.1	43.7	−16%
LaH ₁₀	250	28.3	0.353	8.9	25.2	+45%
CaH ₆	150	21.5	0.280	6.7	24.0	+53%
MgH ₆	300	15.1	0.399	13.5	33.9	+8%
YH ₁₀	300	24.3	0.411	13.4	32.6	+12%

The constant 36.6 eV Å is within 30% of three of the five, with a mean absolute error of 0.23 in $\ln h$, and the constant 31 eV Å is within 30% of all five. A tolerance on each value would therefore be met without a model. Five compounds cannot carry a comparison with the baselines either, since a paired sign test on five needs all five in the estimator's favour to reach $p = 0.03$. The mark applies to a held-out set of at least twenty hydrides at 100 GPa or above, for which fifteen in the estimator's favour give $p = 0.02$. Their references are new calculations at the training settings. The five compounds of Table 11 are reported as a named subset, against those references and against the tabulated ones, which were computed with other settings.

The second test runs the other way, from megabar pressure to one atmosphere, which is the direction in which megabar data would be used. The estimator is trained only on calculations at or above 100 GPa and scored on the ambient-pressure hydrides of the reference set, with the same baselines and the same mark. It cannot be run yet, because megabar labels with a cell exist for five compounds. We will run it when the megabar training set is as large as the smallest ambient-pressure training set with which the estimator passes the third test. Until it is passed, no megabar label enters the training of the estimator used at one atmosphere.

The third test holds out the top. Hydrogen-bearing prototypes are ranked by the largest h among their members, the prototypes that hold the top tenth of compounds are removed with all their members, and the estimator is trained on the rest. Besides the common mark we require that at least half of the held-out compounds whose h exceeds every training value are predicted above every training value, the quantity on which the models cited above score 0 to 5%, and that at most a tenth of the other held-out compounds are. The same split in S over all compounds is reported without a mark, because $S = \sum_j \rho_j h_j / M_j$ and the composition and cell volume, which the estimator is given, fix part of its ordering.

The fourth test holds out a structure type. Every compound with the cubic A₂MH₆ structure of Mg₂IrH₆ (space group $Fm\bar{3}m$) is removed from every training source at every pressure. The tables of our census hold eighteen such compounds. Sixteen are in one survey, five of them with magnesium, and the other two are Li₂AgH₆ and Li₂AuH₆ [5, 63]. The interval is resampled over

compounds, since the test holds out one prototype. The mark is set at the training settings and says nothing about how far those settings are from a converged calculation. For Mg_2IrH_6 the high-throughput label, $2.3 \text{ eV}/\text{\AA}^2$, lies below the 3.7 and 5.2 of the two calculations with denser sampling (Table 3). The reference set of the previous section measures that gap.

Before training, the tensor of equation (13) is fitted to the branch-resolved linear-response spectrum of each compound, which gives the error of the local approximation for a perfect estimator. After training, the whole chain is run on held-out prototypes from the structure alone and compared with the linear-response spectrum of the same record at the same μ^* . In both we require a median absolute error of at most 15% in Φ and 25% in T_c over records with λ of at least 1, below which a fixed S constrains T_c little. The baseline is the scalar closure, which shares each atom's part of S equally among its modes and raises T_c by 21 to 39% in the spectra examined in the previous section, and the chain must have the smaller median error. The end-to-end result is given with linear-response phonons and with those of the interatomic potential, which separates the two sources of error. The training set of the potential may contain the held-out structures, and we report whether it does. If the fitted tensor misses the marks, the closure is abandoned before any model is trained. If the trained chain misses them, roomtsc reports S and its asymptote for a candidate and gives no T_c until a linear-response calculation has been made.

Calibration is measured on the reference set of the previous section, which is drawn before any acquisition guided by the model. The 90% intervals must contain between 85% and 95% of the reference values, and their median width must be smaller than the central 90% range of the residuals of the better baseline on the same compounds. Intervals that fail are refitted and tested on a fresh draw before any shortlist is issued.

The last test is prospective. Before a shortlisted compound is attempted, its dossier states the predicted T_c at the pressure of measurement, for $\mu^* = 0.13$, and the persistence prediction under a stated protocol. Every attempt enters a ledger as not formed, formed and lost under the protocol, or formed and measured, and a measured compound is scored by the ratio of measured to predicted T_c for the phase made in the predicted structure. For compounds predicted before they were made and calculated above 10 K, the record holds one comparison at matched pressure, Mg_2RhH_6 , with highest onsets a factor of 2.1 to 2.5 below the value its makers calculated, in samples whose hydrogen content was not measured [23]. It predates the deposit and does not count.

Persistence: retrodiction of recorded outcomes

The persistence estimator is one decision rule, and it is fixed here. A phase on the hull of the enumerated competitors at the temperature and pressure of a protocol is predicted to persist. A phase off that hull is predicted to persist if it shows no decomposition event in path-integral dynamics at the protocol temperature and its computed lifetime exceeds the hold time at every prefactor from 10^{10} to 10^{13} per second. It is predicted to be lost if an event occurs or the lifetime falls short of the hold time at every prefactor in that range. Between the two the rule returns no prediction, which is scored as an error. For a heating ramp the rate is integrated along the ramp, and the predicted temperature of loss is the one at which half the hydrogen is gone at 3×10^{11} per second. For a decompression the rule is applied at one atmosphere and 300 K, and

the pressure of reversion is not scored. The run lengths and cell sizes of the dynamics, the competitor and path lists, the limiting step assumed for each path, the hold time coded for each row (one hour where the source gives none) and the coded outcome of each row are deposited in a dated manifest before any score is computed for a case in Table 12. No case in the table is used to set them.

Table 12. Retrodiction set for the persistence estimator, with the protocol under which each outcome was observed. The fourth column is the result of the standard filters at one atmosphere, energy above the hull under 100 meV per atom and no imaginary harmonic phonon, where published values decide it. Hull distances are those of Table 9. Only the first group counts toward the mark. Rows marked [†] were read from an abstract or a data record, and their protocols are checked against the full text before the manifest is deposited.

Case	Protocol	Observed	Standard filters	Source
Counted: experiment, outcome identified				
Mg ₂ IrH ₇ , made above 40 GPa	pressure released at 300 K	reverts to Mg ₂ IrH ₅ near 20 GPa	not found	[117]
Mg ₂ RhH ₆ , made at 30 to 74 GPa	pressure released at 300 K	insulating at 28 GPa; Mg ₂ RhH ₅ at 0.7 GPa	pass at 0 to 50 meV per atom, harmonically stable; wrong	[23]
UH ₇ , made at 41 GPa [†]	pressure released, temperature not stated	UH ₅ below 27 GPa, U ₄ H ₁₅ below 12 GPa	not found	[122]
U ₄ H ₁₅ from that release [†]	ambient pressure and temperature	recovered; a metal; oxidises over hours	not found	[122]
Y ₃ Fe ₄ H ₂₀ , made at 60 to 83 GPa	air, 300 K	unchanged for 30 h; 7 to 8% smaller in volume after one to three months; metallic by calculation	phonons pass; off the hull by an amount not given	[121]
Mg ₄ Pt ₃ H ₆ , made at 9 to 24 GPa	ambient conditions	recovered; superconducts at 2.9 K	not found	[36]
Seven fcc lanthanide trihydrides, made in a large-volume press [†]	ambient conditions	recovered; semiconductors	at most 70 meV per atom above the ground state, which passes the first filter; harmonic phonons not found	[124]
SrB ₃ C ₃ , released from about 50 GPa	1 atm, inert atmosphere	recovered; degrades in moist air within hours	not found	[141]
Th ₄ H ₁₅ [†]	ambient conditions	structure determined in 1953; superconducts at 8.05 to 8.35 K	not found	[127, 189]
α-AlH ₃	ambient conditions	kept; metastable	not found; one answer for both rows	[131]
α-AlH ₃ [†]	held at 60 to 140 °C	hydrogen evolves by nucleation and growth	as above	[134]
hcp ZrH ₃ , made at 9 GPa, released at 100 K [†]	1 atm, 100 K and below	kept; superconducts at 11.6 K	not found; one answer for both rows	[125]

Case	Protocol	Observed	Standard filters	Source
hcp ZrH ₃ †	heated in vacuum at 10 K per minute	hydrogen lost between 200 and 270 K, leaving ZrH ₂	as above	[125]
RhH ₂ , made at 8 GPa, released cold †	1 bar, 77 K	hydrogen kept indefinitely	not found; one answer for both rows	[143]
RhH ₂ †	1 bar, 150 K	hydrogen kept for minutes only	as above	[143]
Listed: two outcomes of synthesis and three simulations				
Mg ₂ IrH ₆	synthesis up to 28 GPa and 2500 K, and in an autoclave	not formed; Mg ₂ IrH ₅ forms	pass at 0 to 86 meV per atom, harmonically stable; wrong	[35]
Mg ₂ PtH ₆	Mg ₃ Pt and 2:1 Mg-Pt mixtures heated in hydrogen at 9 to 24 GPa	not formed; Mg ₄ Pt ₃ H ₆ forms	pass at the first published 0 meV per atom, fail at the current 192; harmonically stable	[36]
Li ₂ AuH ₆	path-integral dynamics at 80 K and 1 atm	hydrogen pairs into H ₂ and diffuses	fail on hull distance, 172 meV per atom	[37]
Li ₂ AgH ₆	the same simulation	collapses	fail on hull distance, 319 meV per atom	[37]
Li ₂ CuH ₆	molecular dynamics with classical nuclei, 10 ps at 300 K	intact	pass at the first published 80 meV per atom, fail at the current 204	[38]
Listed: quenched non-hydrides, and a hydride of undetermined hydrogen content				
Cubic Ba-Si-H phase assigned as BaSiH ₆ , made at 18 and 31 GPa	pressure released to 1 atm	lattice kept; semiconducting or poorly metallic	fail: imaginary harmonic modes below 5 GPa	[119, 120]
FeSe, 37 K state	quenched from 4 GPa at 4.2 K, then warmed	gone after warming to about 200 K	not found	[137]
FeSe, hexagonal phase	quenched from 11 GPa	survives to 300 K	not found	[137]
Hg-1223, enhanced state	quenched from 10 to 30 GPa	at least three days at 77 K; zero resistance not reported	nothing to test: the structure is that of the ambient phase	[10]
Bi _{0.5} Sb _{1.5} Te ₃ , 10 K state	quenched from 33 GPa at 77 K	degrades above about 77 K	fail for the high-pressure phases: imaginary harmonic modes at 0 GPa	[130]

The first group holds the experimental outcomes in our tabulation for which the text we read states the protocol and identifies the outcome, by diffraction of the phase or, for α -AlH₃, by the hydrogen evolved, with one row for each protocol. Th₄H₁₅ is included as a control, though the texts we read state no protocol for it. The other outcomes in the tabulation are left out because the text we read does not state both. The second group holds two outcomes of synthesis, Mg₂IrH₆, from which the competitor list was written, and Mg₂PtH₆, and three simulated outcomes, which test a fitted potential against the density-functional dynamics that produced them. In the third group the estimator has no identified end state to predict. Diffraction of quenched Hg-1223 shows the ambient structure, we found no diffraction reported for the quenched states of FeSe and Bi_{0.5}Sb_{1.5}Te₃, and the hydrogen content of the Ba-Si-H phase is undetermined. The rows of the last two groups are scored and reported separately.

The mark is twelve of the fifteen counted rows. Two kinds of error fail the check whatever the count. One is a persisting metal predicted to be lost, of which the group has five rows (Mg₄Pt₃H₆, U₄H₁₅, Th₄H₁₅, ZrH₃ kept cold, and Y₃Fe₄H₂₀, metallic by calculation). The other is hydrogen that was lost predicted to stay, of which it has six. For ZrH₃ the predicted temperature of loss must fall within 25% of the midpoint of the measured interval, 200 to 270 K, and for RhH₂ within 25% of 150 K. α -AlH₃ was measured in isothermal runs between 333 and 413 K and has no single temperature of loss, so there the rule must predict loss within the run at both ends of that range. Predicted for one ramp, the three temperatures of loss must come in the order RhH₂, ZrH₃, AlH₃. The tolerance is set by what a computed barrier can deliver. For ZrH₃ on its ramp an error of 0.1 eV in the barrier moves the predicted temperature by 14% and a factor of thirty in the prefactor by about 10%.

Passing is a necessary check and carries no statistical weight on its own. The fifteen rows come from ten compounds or families, with Mg₂IrH₇ and Mg₂RhH₆ as one family and the two uranium rows as one. An estimator that is right on 80% of independent cases reaches twelve of fifteen 65% of the time, and one that is right on 60%, the share of rows that persist, reaches it 9% of the time. Twelve of fifteen bounds the accuracy only to between 0.52 and 0.96 (exact 95% interval). A pass is also in-sample. The competitor and path lists were written with the Mg₂IrH₆ family, Li₂AuH₆ and the Ba-Si-H phase in view, and the section on one atmosphere has already read barriers from the outcomes of ZrH₃, Y₃Fe₄H₂₀ and AlH₃.

The baseline is the standard pair of filters. The pair returns one answer for a structure whatever the temperature, so it is wrong on one row for each of ZrH₃, RhH₂ and AlH₃, and it passes Mg₂RhH₆, which was lost. That is at least four errors in fifteen, below the mark. Where the table says not found we have no hull distance or phonon calculation at one atmosphere, and we will compute both before the estimator is scored. The estimator is compared with the filters by a paired sign test on the rows where the two disagree, with one vote for each compound or family. Five votes, all for the estimator, are needed to reach $p = 0.03$, and the filters are known to err in four families.

Separating an accuracy of 0.85 from 0.60 at the 5% level with 80% power takes 21 independent outcomes. Recoveries and failed recoveries published after the manifest is deposited are scored with the same rule on a separate list, and that list is the only out-of-sample result we will report for persistence.

Results that would refute the approach

The census of h is repeated on the Alexandria records, for the hydrides that pass the branch criterion, listed before the calculation. If the standard deviation of $\ln h$ among them is not smaller than that of $\ln S$, dividing by hydrogen density removes none of the variation between ambient-pressure compounds. That is the case when the slope of $\ln S$ on $\ln \rho_H$ is one half or less. In the published tables, which were selected on T_c , the two standard deviations are 0.36 and 0.42 and the slope is 0.62 ± 0.09 . If the criterion is met the estimator learns S directly, and we withdraw the estimates of the section on hydrogen density for ambient-pressure compounds.

If linear response with converged Fermi-surface sampling finds η_H of $8.7 \text{ eV/\AA}^2$ or more in a compound that exists at one atmosphere, those estimates are too low by enough to admit 300 K with a single mode at $\lambda = 4$ (Table 2). We withdraw them, and the structure family of that compound becomes the first target.

The tail of calculated T_c is refitted by structural prototype on the full public dataset, with the list of prototypes fixed beforehand. The criterion is a generalised Pareto shape, fitted by maximum likelihood above the prototype's 90th percentile on at least 300 exceedances, whose 95% lower bound is above zero after a Bonferroni correction for the number of prototypes and stays above zero when the two largest values are removed. The pooled near-hull sample does not meet it, with a shape of 0.05 (-0.13 to 0.15) above 10 K and 0.16 (-0.14 to 0.35) above 15 K. If a prototype meets it, sampling that prototype more densely could reach high calculated T_c , and the decision layer ranks on calculated T_c within it.

If the frozen rule scores below twelve on the counted rows of Table 12, makes either kind of excluded error, or misses a temperature of loss by more than 25%, roomtsc does not filter on persistence. Its shortlists then carry the hull stage alone and say so, and a revised rule is scored only on outcomes published after its own deposit.

If a screen of the hydride records of the Alexandria database [96] finds no structure that passes the persistence rule at one atmosphere and has η_H above $4.8 \text{ eV/\AA}^2$, the floor of equation (6) at infinite coupling, we publish the null and stop proposing phonon-mediated candidates for 300 K from that pool. The null counts only if the estimator can return large values, so it is conditional on the estimator placing at least four of the five compounds of Table 11 above $4.8 \text{ eV/\AA}^2$ when they are held out.

If the median ratio of measured to predicted T_c over the first five compounds made in the predicted structure is below 0.7, or three of the first five attempted compounds do not form or do not persist under the protocol in their dossier, no further synthesis is proposed until the estimator at fault has been revised and has passed its held-out tests again. An unbiased prediction with a scatter of 0.3 to 0.4 in $\ln T_c$ crosses the first line by chance in 1 to 5% of cases.

What counts as finding one

Since 1986 eight claims of a record T_c have survived, five in cuprates at ambient pressure [1, 190, 191, 192, 193] and one each in the mercury cuprate under pressure [194], H_3S [66] and LaH_{10} [6]. From Wikipedia's article "Room-temperature superconductor", read on 6 October

2026, and one further report [195], we count eleven prominent claims above the record of their day that were refuted, retracted or never corroborated, nine of them at or above 273 K, where no claim of an equilibrium transition has been corroborated. Two of the nine were retracted from Nature, and a university investigation found research misconduct by the senior author of both [196, 197, 198]. The article omits older reports of superconductivity that were never established [2], so eleven undercounts the claims that did not survive. The data file that accompanies the paper lists the eight and the eleven.

In LK-99 a first-order structural transition of a copper sulfide impurity, which shows thermal hysteresis, produced a tenfold drop in resistivity that did not reach zero. Ferromagnetic fragments produced the partial levitation, and sulfur-free single crystals are transparent insulators [181, 182, 199]. Magnetic imaging of CeH₉ shows superconducting regions of 10 micrometres or less in a sample whose resistance falls to near zero [200], so zero resistance in a four-probe measurement can come from a connected minority phase. The LaSc₂H₂₄ preprint, whose authors checked that all four electrodes conducted, shows negative resistance between 230 and 277 K in one cell [8]. A diamagnetic signal after zero-field cooling measures shielding, which a surface or a network also gives, and in a diamond-anvil cell it is obtained by subtracting the cell's signal [41, 201].

We found no formally adopted checklist for superconductivity claims. The nearest is a comment by fifteen authors on the hydrides, which relies on reproduction by different groups and on magnetisation that is diamagnetic before background subtraction, and asks that data be public [201]. With the cases above it gives a working standard, which at megabar pressure has seven items:

- zero resistance in a four-probe measurement, with a stated noise floor, the contact pairs permuted and current-voltage curves shown;
- a shift of the transition in applied field;
- a magnetic signature visible before background subtraction;
- warming and cooling sweeps, to expose hysteresis from a structural transition;
- identification of the phase that carries the superconductivity;
- release of the raw data;
- reproduction by a second group.

A percolating minority phase can pass the first four. roomtsc candidates are compounds at one atmosphere, where more can be measured, and they will be held to four further items:

- a bulk signature (a specific-heat anomaly, a muon-spin-rotation volume fraction or field-cooled flux expulsion), set against the measured fraction of the identified phase;
- for a hydride, the hydrogen content of the measured sample, from neutron diffraction, thermal desorption or nuclear magnetic resonance, because X-ray diffraction locates the metal atoms and Mg₂IrH₆ shares its metal sublattice with the Mg₂IrH₅ that formed in its place [35];
- for a hydride, the transition in the deuteride, against the isotope shift stated in the dossier;
- the transition and the phase fraction measured again after a stated time at the claimed temperature and pressure.

H₃S has most of the first seven, and they took about eight years to accumulate. A second group reported the transition in alternating-current susceptibility 22 months after the first preprint [202]. Flux trapped at zero applied field, which needs no background subtraction, followed after seven and a half years [43]. Hirsch disputes the magnetisation data and reports that the raw data behind the 2015 measurement are not available [203]. The highest transitions of lanthanum hydride with magnetic evidence in a static field are 231 K at 130 GPa, by magnetisation [41], and about 240 K at 155 GPa, where an independent group imaged screening and the Meissner effect [204]. We found no static-field magnetic evidence above about 240 K in any hydride, the 250 K transition of LaH₁₀ at 170 GPa included. Two alternating-field reports on lanthanum hydride, with two authors in common, lie higher. Modulated susceptibility gave an onset near 250 K, and 278 K three weeks later, in results the authors call initial [205]. Radio-frequency and nuclear magnetic resonance screening has onsets of 260 to 279 K at 165 GPa, with no resistance measured on those cells [206]. We found no specific-heat measurement on a megabar hydride.

The phases listed in the dossier cannot be read from a convex hull computed for the target, because the phases in a real sample are set by the loaded composition, the route and the kinetics. LK-99 contains no sulfur, so no hull of the target contains a copper sulfide. The reaction as written yields 17 parts of copper and 5 of sulfur for each part of product [182]. The H₃S cell used for flux trapping has a second transition near 15 K from elemental sulfur on the anvil bevels, where the pressure falls from about 140 to 95 GPa [43]. One of the two LaSc₂H₂₄ cells with zero resistance has unindexed diffraction peaks that its authors leave to undetermined hydrides [8], and a later calculation by the same group assigns the secondary phase to a metastable La₂ScH₃₆ from a new structure search [207]. The list therefore starts from a hull at the loaded composition, over the range of pressure in the sample, and adds the known phases of each chemical subsystem, on the hull or off it. A phase that has not been reported when the list is made is still missed, which may be the case of La₂ScH₃₆.

Of the sixteen model-suggested superconductors cited in the first section, eight contain niobium. Six of the eight are arc-melted alloys with transitions at 4.8 to 9.7 K that did not form the predicted structure and lie in alloy families already known to superconduct [20]. The other two have specific-heat measurements [16], which the bulk item asks for. They show one jump in Be₂Hf₂Nb and two in Be₂HfNb₂, which the authors read as a second superconducting phase.

The dossier is deposited before the synthesis is attempted.

The odds, and what is worth finding

None of the bounds reviewed under "Proposed ceilings" excludes a phonon-mediated superconductor at 300 K [39, 53, 62]. A single mode needs a hydrogen Hopfield parameter of 8.7 to 12.0 eV/Å² for 300 K, and the largest we found in a published ambient-pressure calculation is 5.2, in one of three calculations of a compound that did not form (Table 2, Table 3). At a hydrogen density of 0.10 Å⁻³, about the highest we found near one atmosphere, the requirement is a scattering strength per proton of 87 to 120 eV Å, 1.4 to 1.9 times the largest in any calculation whose coupling is on hydrogen.

The largest ambient-pressure survey has its best cases near 110 K, 170 to 320 meV per atom above the hull, and its authors conclude that room temperature is extremely unlikely [5]. Its tail of calculated T_c makes no statement about 300 K either way. No hydride predicted to superconduct above 60 K at ambient pressure has been made at, or recovered to, one atmosphere. Of the eleven predictions above 60 K in Table 9, two did not form when their metals were heated in hydrogen, two are unstable in one path-integral simulation, one stayed intact in a short simulation with classical nuclei, and for six we found no test.

These results are not independent. The survey's dataset was computed by one group with one workflow, starting from its two earlier screens [5, 63, 106]. All 62 ambient-pressure rows of our census of h come from that group's tables, and seven of the eleven predictions appear in them. An error common to that harmonic workflow would move the census, the tail and the survey's conclusion together. The megabar values of η_H [28], the electron-gas reference, the crystallographic hydrogen densities and the laboratory outcomes for Mg_2IrH_6 and Mg_2RhH_6 [23, 35] do not depend on it.

Our credence that a phonon-mediated superconductor with T_c above 300 K exists and can be kept at one atmosphere is about one in a hundred, and one in a thousand is as defensible. It is a judgement, derived from no measured frequency. It is low because one compound must combine persistence, which no hydride predicted above 60 K has shown, with a Hopfield sum 1.7 times the largest computed at ambient pressure or more. That factor assumes the efficiency of a single mode at $\lambda = 4$, which is 0.75, and the hydride spectra evaluated here reach 0.2 to 0.6. It is above zero because no factor is bounded and the calculations have known gaps. The survey's authors state in its published peer-review file that about 85% of the hydrides sent to linear response had imaginary harmonic modes and were left out [5], the treatment of the vertex moves λ of PdH between 0.27 and 0.64 [60], and for six of the eleven predictions we found no test. Two measurements would move it, h in unselected and in harmonically unstable hydride records and a screen of persistent structures for η_H above the floor of $4.8 \text{ eV}/\text{\AA}^2$. The section on the tests bounds the chance per candidate on a shortlist of a hundred from a million at one percent if the pool contains a positive, so the unconditional figure is at most 10^{-4} .

For unconventional pairing we give no credence, because we know of no controlled, validated theory that returns T_c from a crystal structure in that class. The equilibrium record at ambient pressure has belonged to the mercury cuprates since 1993 [1]. A cuprate-like route to 300 K needs a stiffness 1.6 to 2.3 times that tabulated for the mercury cuprate [25] and, on the model calculations reviewed in the section on pairing without phonons, a superexchange 2.3 to 4.0 times the largest tabulated cuprate value [153]. On the creep estimate under "Usability", a layered material with the parameters of $\text{YBa}_2\text{Cu}_3\text{O}_7$ and a T_c of 400 K would not hold a useful current at room temperature.

A large Hopfield parameter and thermodynamic stability can coexist on atoms heavier than hydrogen. From $\lambda = 0.87$ and $\omega_{\log} = 725 \text{ K}$ [105] boron in MgB_2 , which is stable at one atmosphere, has at least $8.8 \text{ eV}/\text{\AA}^2$, since $\omega_{\log}$ stands in for the second moment, and rigid-muffin-tin calculations give niobium 9.1 and vanadium 8.0, against 7.6 and 6.9 in the earlier calculations that paper quotes [208]. Hydrogen in the megabar hydrides has 6.7 to 13.5 (Table 3). The

floor for 300 K scales with mass and is $52 \text{ eV}/\text{\AA}^2$ for boron (the section on what 300 K costs). MgB_2 carries no further inference for hydrogen, because boron there sits at its electron-gas value (the section on hydrogen density).

Persistence is better supported for covalent frameworks than for the hydrides of Table 9. The accessible range of metastability rises with cohesive energy across chemistries [114], and the boron-carbon clathrate SrB_3C_3 was recovered from about 50 GPa to one atmosphere, where it keeps under an inert atmosphere and degrades in moist air [141]. In two predictions that put hydrogen in such frameworks, hole-doped graphane and boron-carbon clathrates with ammonium units in their cages, the states at the Fermi level belong to the framework and the high-frequency hydrogen modes contribute little or nothing to the coupling [209, 210]. In one of two computed structures of $\text{SrNH}_4\text{B}_6\text{C}_6$, rotations of the ammonium units supply 21% of λ [210]. roomtsc will search hydrogen-bearing covalent frameworks first, on the evidence for persistence alone. Whether hydrogen can carry the coupling in one is open.

Milestones below room temperature

The first target is a phonon-mediated superconductor above 39 K that persists at one atmosphere, where MgB_2 , found in 2001, was still the record in a 2025 survey [4, 5]. In the near-hull sample of the survey two of 8,323 compounds are calculated above 39 K, LiMoN_2 at 42 K and Mg_2RhH_6 at 54 K. The survey's authors report that intrinsic defects destroy superconductivity in LiMoN_2 [5], and Mg_2RhH_6 was measured at 18 to 29 K under pressure and reverted on release [23]. For a million compounds chosen as that sample was, the exponential fit, which fails at the top of its own sample, puts the largest calculated value near 53 K. On the selection calculation of the section on screening, a compound calculated at 53 K has a median true T_c of 18 to 41 K, and the most probable highest true T_c in the pool is 34 to 50 K, for σ from 0.4 down to 0.15. We have not estimated σ and found no published estimate, and the same group's isotropic Eliashberg calculation gives MgB_2 18.9 K at $\mu^* = 0.10$ [106].

The second is 77 K, the boiling point of nitrogen. The survey's coupling figure has 13 points calculated at or above 77 K. Its hull figure shows three of them, 172 to 319 meV per atom above the hull, and the best within 100 meV per atom is 59 K [5]. With the shape of the tail left free, the level exceeded once among a million compounds chosen like the near-hull sample is 63 K (34 to 104 K) or 89 K (35 to 230 K), so those data do not say whether such a pool holds one calculated at 77 K.

The ideal work to carry one watt of heat to 300 K is 70 W from 4.2 K, 2.9 W from 77 K and 1.5 W from 120 K, so most of the saving is made by 77 K. A 2006 U.S. Department of Energy report argued that an isotropic superconductor with T_c near 120 K would have a large current margin at 77 K and would cover nearly all new applications there [211]. For the dense three-dimensional metallic hydrides considered here, carrier density predicts a small Ginzburg number, which measurement has not established (under "Usability"). A T_c of 120 K lies in the upper half of the 70 to 150 K that typical values give at the highest hydrogen density we found near one atmosphere.

The third is a retained state. It is made under pressure and held at one atmosphere without a substrate, has zero resistance and a bulk magnetic transition at least 10 K above the T_c of the equilibrium phase, is unchanged after a month at 300 K, and is reproduced by a second group.

The quench results cited in the section on one atmosphere come from one group and do not reach it. One sample of the quenched mercury cuprate lost 4 K of onset in a cycle to room temperature, and a sample retrieved from the cell showed about 140 K by magnetisation, against 133 to 135 K, with no zero resistance reported [10]. The 37 K state of FeSe did not survive warming to 300 K [137].

Of these targets we judge the 120 K phonon superconductor the most valuable. The pairing estimates leave it inside the computed range, its persistence is untested, and the search for it uses the estimators and tests specified for 300 K.

Appendix: methods and data

The calculations described here are scripts in the repository that accompanies the paper, each with its output file beside it. `eliashberg.py`, `requirements.py` and `spectra.py` give the Eliashberg results, `jellium.py` the electron gas, `h_census.py` the census, and `tails.py`, `tails_checks.py` and `selection_checks.py` the tail and selection results. Numbers derived from these results or from closed formulas are stored in the directory `derived`, one script per group with its printed output beside it. Its five `pairing` scripts hold the response of T_c per unit of S , the single-mode requirement under a cap on the top frequency, the Leavens constant and the scaling of force constants and of η , `closure.py` the comparison of closures, `kinetics.py` the kinetic estimates and `test_statistics.py` the test statistics. Some numbers are direct arithmetic on published values and have no stored output, among them the stiffness scales, the Ginzburg numbers, the spread of the six published values of T_c for Mg₂IrH₆, the mean proton spacing in Fermi wavelengths and the refrigeration work.

Eliashberg equations

We solve the linearised isotropic Eliashberg equations on the Matsubara axis. For a spectral function made of Einstein modes with couplings λ_i and frequencies ω_i ,

$$\lambda(i\nu_l) = \sum_i \frac{\lambda_i \omega_i^2}{\omega_i^2 + \nu_l^2}, \quad \nu_l = 2\pi l k_B T, \quad (14)$$

and T_c is the temperature at which the largest eigenvalue of the symmetric kernel of Allen and Dynes [27] crosses zero:

$$K_{nm} = \lambda(i\nu_{n-m}) + \lambda(i\nu_{n+m+1}) - 2\mu^* - \delta_{nm} \left[2n + 1 + \lambda(0) + 2 \sum_{l=1}^n \lambda(i\nu_l) \right], \quad n, m \geq 0. \quad (15)$$

Matsubara frequencies are kept up to a cutoff of ten times the highest mode frequency, and never fewer than four. μ^* is defined at that cutoff. A value of 0.13 at a cutoff of $10\omega_E$ corresponds to 0.10 at ω_E under the usual logarithmic rescaling, $1/\mu^*(\omega_1) = 1/\mu^*(\omega_2) + \ln(\omega_2/\omega_1)$.

Five checks were made. With $\mu^* = 0$ the Allen-Dynes formula, including its strong-coupling and shape factors, is 6% below the solution at $\lambda = 0.3$ and within 1% of it from $\lambda = 1.5$ to 10; the formula was fitted to solutions of this kind [27], so this checks the code against the literature. At large coupling the ratio $k_B T_c / \hbar \omega_E \sqrt{\lambda}$ approaches the asymptotic value 0.1827 of the same paper from below, reaching 0.176 at $\lambda = 10$. Doubling the cutoff changes T_c by less than 0.2% at $\mu^* = 0$. A second implementation, written from the equations alone without access to the first, agrees with it to two parts in a million or better at 32 of 35 combinations of λ from 0.3 to 10 and μ^* of 0, 0.10 and 0.16. The other three are at λ of 7 and 10, where three Matsubara frequencies lie below the cutoff and the first implementation keeps four, and there the two differ by 0.3% at $\mu^* = 0$ and by 0.008% at $\mu^* = 0.10$. For a real spectrum, the published spectral function of Mg₂IrH₆ from Dolui and coauthors, coarse-grained into five modes, the solver returns 174, 165 and 157 K at $\mu^* = 0.10, 0.13$ and 0.16, against a T_c between 160 and 175 K given in that paper for μ^* of 0.10, 0.125 and 0.16 [64]. The published values are from the anisotropic equations and the five modes are our reading of a published curve, so this check tests the reading and the solver together.

Table 13 gives $f(\lambda, \mu^*) = k_B T_c / \hbar \omega_E$. The efficiency of equation (6) for a single mode is $\Phi = f / (0.1827 \sqrt{\lambda})$.

Table 13. $k_B T_c / \hbar \omega_E$ for an Einstein spectrum. μ^* is defined at a Matsubara cutoff of $10 \omega_E$.

λ	$\mu^* = 0$	$\mu^* = 0.10$	$\mu^* = 0.13$	$\mu^* = 0.16$
1.0	0.1146	0.0799	0.0724	0.0657
1.5	0.1691	0.1321	0.1239	0.1167
2.0	0.2117	0.1723	0.1637	0.1557
2.5	0.2474	0.2057	0.1963	0.1877
3.0	0.2789	0.2346	0.2246	0.2155
4.0	0.3330	0.2840	0.2729	0.2629
5.0	0.3793	0.3261	0.3139	0.3028
7.0	0.4587	0.3975	0.3833	0.3704
10.0	0.5570	0.4853	0.4688	0.4539

At fixed λ and fixed Hopfield sum a single mode has the largest Matsubara couplings. Each $\lambda(i\nu_l)$ with $l \geq 1$ is λ times a weighted average of $\omega_i^2 / (\omega_i^2 + \nu_l^2)$, a concave function of ω_i^2 , so by Jensen's inequality it is largest when the weight sits at one frequency. Equation (15) contains the spectrum only through these couplings, because $\lambda(0)$ cancels from it. We have not proved that T_c rises with each of them. In the four spectra of hypothetical hydrides that we solved, the single mode with the same λ and S has the higher T_c , by 14 to 41%, and on that evidence we read each η_H of Table 2 as the least that a spectrum of that λ needs. The comparison used a cutoff of ten times the highest frequency of each spectrum, which for the published spectra is 2.0 to 2.3 times the cutoff of the single mode. By the rescaling above and Table 13, the single-mode T_c at a common cutoff is about 2% higher still.

The published spectra are solved as the five to seven Einstein modes that we read from their cumulative coupling curves. The functional derivative was obtained by adding a mode of spectral area $2 \times 10^{-3} \omega_E$ at frequency Ω to an Einstein spectrum with $\lambda = 2$ and re-solving for T_c at a fixed absolute cutoff. The two-mode calculation uses modes at 15 and 150 meV with a common cutoff of 1500 meV.

Hopfield sums from published tables and spectra

Where a paper tabulates λ and the second-moment frequency ω_2 , the Hopfield sum in hydrogen units is $S = M_H \lambda \omega_2^2$, with $M_H \omega^2 = 1.790 \text{ eV}/\text{\AA}^2$ at $\hbar\omega = k_B \times 1000 \text{ K}$. It equals η_H plus the terms of the other atoms weighted by M_H/M_j . For the megabar hydrides of Quan and coauthors, who print both, the two agree to within 3% [28]. The difference is larger where lithium, beryllium or boron couple or where hydrogen is a small part of the cell, and we have not measured it there. The efficiency quoted for the megabar hydrides is the Allen-Dynes T_c that Quan and coauthors give for the hydrogen modes alone, which the formula returns with $\mu^* = 0.13$, divided by the asymptote of the same η_H .

Where only a figure of the cumulative coupling is published, we read the increments of λ in five to seven frequency bins, and η_H is the sum over the bins above the metal modes, which is 1 to 2% below S [22, 59, 64]. The reading reproduces the λ of the source and, where it is printed, the $\omega_{\log}$ to within 9%. That check constrains the low-frequency increments. The second moment weights the high-frequency ones, which are constrained only by the reading error of 15 to 20%, and an error of 0.03 in λ near 190 meV moves η_H by $0.3 \text{ eV}/\text{\AA}^2$.

For the comparison of closures in the section on the model, the bins of each read spectrum above 40 meV are taken as hydrogen modes and those at or above 150 meV as the metal-hydrogen stretching branches. The scalar closure gives the stretching bins one third of the hydrogen part of S and the other hydrogen bins two thirds, each bin in proportion to its original share and at its original frequency, and T_c is solved again at $\mu^* = 0.13$. In the two spectra of Mg_2IrH_6 and that of Mg_2RhH_6 the stretching bins hold 58 to 63% of the hydrogen part and T_c rises by 21 to 39%. In Mg_2PtH_6 , where our reading puts 3% of S above 150 meV, the same construction lowers T_c by 25%. In the four spectra 83 to 86% of λ lies below 100 meV.

Scattering by a proton

The self-consistent values of Table 5 are from a Kohn-Sham calculation for a point charge in a uniform electron gas with a rigid neutralising background, the problem solved by Almladh and coauthors and by Zaremba and coauthors in 1976 and 1977 [32, 33]. The calculation is spin-unpolarised and uses the local-density approximation with the Perdew-Zunger parametrisation of the correlation energy [212]. The induced density is built from radial scattering states for l up to 12 on a grid of momenta up to k_F and from a doubly occupied bound s state, which is present at $r_s = 2.0$ and above and absent at 1.8. The potential is iterated to self-consistency inside a sphere of at least 40 Bohr radii, and the phase shifts at k_F enter equation (8).

Neutrality is not imposed, and the Friedel sum of the converged phase shifts equals the nuclear charge to within 7×10^{-5} . Doubling the sphere radius, the momentum grid or the number of partial waves, or halving the radial step, changes h by at most 1.2 parts in 10^5 . For a charge of

10^{-3} the induced density reproduces the analytic linear response with the same local exchange-correlation kernel to a few parts in a million. Four parametrisations of the local-density correlation energy give h within 0.7% of each other. At $r_s = 2.5$ the phase shifts are $\delta_0 = 1.2172$ and $\delta_1 = 0.0906$, against 1.2213 and 0.0894 published by Nagy and Zawadowski [84]; with the Gunnarsson-Lundqvist parametrisation [213] the same code gives 1.2217 and 0.0897. An independent calculation supplied in review of an earlier draft gives the same h to within 0.1 eV Å at ten densities. The friction coefficient $Q = mk_F h / 3\pi\hbar$ agrees with the values published by Gerrits and coauthors for nuclear charges of 1 to 6 at r_s from 1.5 to 5 to within 1.3%, and to within 0.7% for the proton and 0.5% for boron [214]. We have not compared with the tables of Puska and Nieminen [34], which we could not obtain.

For a boron nucleus with all five electrons the same code gives 149, 121 and 101 eV Å at $r_s = 1.5, 1.8$ and 2.07 . The middle value is the one compared with MgB₂.

The last column of Table 5 is the potential $-e^2 e^{-\kappa r} / r$ with κ fixed by the Friedel sum rule [85, 86]. Its phase shifts for l up to 8 come from the variable-phase equation

$$\frac{d\delta_l}{dr} = -\frac{2m}{\hbar^2 k} V(r) [\cos \delta_l \hat{j}_l(kr) - \sin \delta_l \hat{n}_l(kr)]^2, \quad (16)$$

with Riccati-Bessel functions, integrated outward from the origin. The equation returns the absolute phase, so the Friedel sum counts the s state that this potential binds at low density. The model is 17 to 21% below the self-consistent h for r_s up to 3 and 12% above it at $r_s = 6$. It lies within 6% of a self-consistent calculation that keeps the Hartree potential alone, so most of the difference is the exchange-correlation potential.

Census of the scattering strength

The census takes every hydride in three sources that tabulate both λ and ω_2 . Tables I and II of Cerqueira and coauthors hold 59 hydrides with a harmonic Allen-Dynes T_c above 20 K after a machine-learning pre-screen [63]. Of these, 57 are ambient rows, PdH is counted on its own, and Al₂TcH₆ is left out because we found no matching cell. The supplement of Gao and coauthors adds four hydrides from its data cards and Li₂AuH₆ from a table [5]. The megabar rows are the 13 pressure points of Quan and coauthors less MgH₆ at 400 GPa, for which we found no volume [28]. The other papers we opened on megabar hydrides and atomic hydrogen print no second moment [61, 90, 92, 215, 216, 217]. Each ambient compound is counted once. For Mg₂IrH₆ the counted value is the high-throughput 28 eV Å, and the 45 and 64 eV Å from digitised spectra are outside the statistics. As a guard on transcription, the Allen-Dynes formula applied to the λ , $\omega_{\log}$ and ω_2 we entered returns the printed T_c of all 66 ambient-pressure rows to within 0.4 K with $\mu^* = 0.10$, and of the 13 megabar rows to within 0.5% with $\mu^* = 0.13$.

The tables print no cell volumes. For the ambient rows we took the primitive cell of the matching entry in the Alexandria database [96], read on 6 October 2026. The four data cards print the database identifier. For 47 rows the formula and the structure described in the source select one entry. For five perovskites two entries share the space group, and we took the one nearer the hull. For six rows the source does not fix the structure, and we took the metallic entry

whose hull distance is nearest the printed one. The alternatives change h by up to 20% for InH_3 and by 3 to 12% for the others, and without the six rows the ambient geometric mean is 22.6 eV Å.

The database cells were relaxed with the PBE functional [96] and the coupling was computed in cells relaxed with PBEsol [5, 63]. In 24 hydride records for which we could compare the two, none of them a census compound, the median ratio of PBEsol to PBE volume is 0.967, and 22 of the 24 lie between 0.930 and 0.984. The ambient hydrogen densities are therefore low, and the ambient values of h high, by about 3%.

Each megabar density uses the volume of the same structure at the same nominal pressure from another calculation [61, 89, 91, 92, 93], and the census data file names the source of each. Three of the twelve volumes are printed at that pressure, two are quoted at second hand, six are interpolated, extrapolated or read from a figure, and one, for YH_{10} at 400 GPa, is an estimate. Independent calculations of one phase differ by up to 2% in volume (LaH_{10} at 300 GPa), and the extrapolated values are uncertain by a further 1 to 2.5%.

The ambient rows are not a sample of hydrides. The rows from Cerqueira and coauthors passed a cut on calculated T_c , and three of the five from Gao and coauthors were singled out there for a high T_c or a large λ . The statistics of Table 7 are the geometric mean and the exponential of the sample standard deviation of $\ln h$. The slopes are least-squares fits of $\ln S$ on $\ln \rho_H$, and their standard errors treat the rows as independent. The twelve megabar rows are five compounds, so the error on the slope over all 75 rows is understated.

Figure data from the ambient-pressure survey

The energy above the hull and the calculated T_c were read from the 12,079 marker positions of a vector figure in the arXiv source of [5] (arXiv:2502.18281), and λ and $\omega_{\log}$ from a second figure with 12,059 markers. Six of those repeat a labelled compound, which leaves 12,053 distinct compounds, and compounds with a T_c of zero are not drawn there. The reading reproduces the supplementary values of $\omega_{\log}$ and λ for five labelled compounds to 0.5 K and 0.001. Markers above 376 meV per atom were not written to the hull figure and are absent. The paper reports more than 20,000 compounds and its histograms hold about 13,160, so the figures are a subset, and we do not know how the remainder is distributed. The data carry no compositions or identifiers. The article is published under a CC BY 4.0 licence.

No part of the set is a random sample. The section on screening describes how the compounds within 50 meV per atom of the hull were chosen, and those further away were added because a model or an earlier paper had predicted a high T_c for them.

The abstract of [5] states that $\omega_{\log}$ rarely exceeds 1800 K. No compound in the coupling figure or on the six data cards exceeds 1275 K, and the histogram of $\omega_{\log}$ in the same paper has no entry above 1360 K. Two other frequencies in the text of that paper, 425 K and "almost 300 K", are 1.44 to 1.45 times the 294 and 204 K on the data cards of the same compounds, and one inverse centimetre is 1.44 K. On each card λ and $\omega_{\log}$ return the card's own McMillan T_c . We use the values in the figures and on the cards. We have not confirmed this reading with the au-

thors. The figures hold about 12,000 of the more than 20,000 compounds, so a compound above 1275 K outside them is not excluded, and the maximum of $\omega_{\log}$ over the public data files, which we have not taken, would settle it.

Tail statistics

The statistics are for the 8,323 compounds within 50 meV per atom of the hull. The scale τ is the mean excess above 10 K, with a 95% interval from 2,000 bootstrap resamples of the 355 exceedances, and the errors quoted for the mean excess at other thresholds are standard errors of the mean. Both treat the compounds as independent. They come in structural families, and without identifiers we could not resample by family, so the stated intervals are too narrow by an amount we cannot give.

The Anderson-Darling statistic for an exponential with its scale estimated from the data is 0.43, and 59% of 4,000 simulated exponential samples of 355 give a larger value. Under equation (10) the largest of n exceedances lies below $u + x$ with probability $(1 - e^{-x/\tau})^n$, which gives the probability of 0.007 for the observed maximum, and for large n its standard deviation is $\pi\tau/\sqrt{6}$. Moving the cut to 49 meV per atom leaves 8,191 compounds with $\tau = 3.9$ K. The generalised Pareto fits are by maximum likelihood on the excesses above 10 K and above 15 K, with intervals from 1,000 bootstrap resamples. Return levels for a million compounds use a fraction above 10 K of 4.27% for a pool composed like the sample and 0.27% for the pool of the earlier screen [106].

Selection calculation

The calculation behind Table 8 draws 8×10^7 true values from an exponential distribution that starts at zero and multiplies each by log-normal noise of width σ . The true scale τ_t is found by root-finding so that the calculated values have a mean excess of 4.03 K above 10 K. That is the only threshold at which the simulated values are matched to the data. Their mean excess rises with the threshold, where that of the data is flat from 2 to 15 K, so the simulation is not a fit to the sample. The table gives the median ratio of calculated to true value in bins of the calculated value. The true T_c quoted for a compound calculated at 53 K is the median true value among calculated values from 49 to 57 K. The most probable highest true T_c in a pool is $\tau_t \ln n$, where n is the number of draws that gives as many calculated values above 10 K as 4.27% of a million.

Kinetic estimates and test statistics

The barriers in the section on one atmosphere use three limiting cases. For loss by independent events at each site with attempt frequency ν , a lifetime t at temperature T needs a barrier $E = k_B T \ln(\nu t)$. If one event among N sites starts a fast transformation, the barrier needed is larger by $k_B T \ln N$. For loss limited by diffusion to the faces of a plate of thickness L , the slowest mode decays in a time $L^2/\pi^2 D$ with $D = D_0 e^{-E/k_B T}$, and we take $D_0 = 10^{-3}$ cm² per second. A barrier read from a decomposition temperature is the first formula with t the observed time of loss. A molecular-dynamics run of length t on N sites without an event excludes barriers below $k_B T \ln(\nu t N)$.

In the section on the tests, the chance of reaching twelve of fifteen at a given accuracy is the binomial tail, the interval for twelve of fifteen is the exact (Clopper-Pearson) 95% interval, and the sign-test values are one-sided binomial tails at probability one half. The sensitivity of the temperature of loss of ZrH₃ is for first-order loss integrated along the measured ramp of 10 K per minute [125], with the barrier set so that half the hydrogen is gone at 235 K, the midpoint of the measured 200 to 270 K, for a prefactor of 10¹³ per second.

Conversions

1 meV corresponds to 11.6045 K; 1 GPa Å³ = 6.2415 meV; $e^2 = 14.40$ eV Å; 1 kg of hydrogen per cubic metre is 5.975×10^{-4} hydrogen atoms per Å³.

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