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Yue Zhao(赵玥), Sihan Liu(刘思涵), Jiao Liu(刘骄), Tingting Gu(顾婷婷), Jian Hao(郝健), Jingming Shi(石景明), Wenwen Cui(崔文文), and Yinwei Li(李印威)

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SPECIAL TOPIC — Structures and properties of materials under high pressure

Design of superconducting compounds at lower pressure via intercalating $X\mathrm{H_4}$ molecules (X = B, C, and N) into fcc lattices

Yue Zhao(赵玥)[†], Sihan Liu(刘思涵)[†], Jiao Liu(刘骄)[†], Tingting Gu(顾婷婷), Jian Hao(郝健), Jingming Shi(石景明), Wenwen Cui(崔文文)[‡], and Yinwei Li(李印威)[§]

Laboratory of Quantum Functional Materials Design and Application, School of Physics and Electronic Engineering, Jiangsu Normal University, Xuzhou 221116, *China*

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Recently, many encouraging experimental advances have been achieved in ternary hydrides superconductors under high pressure. However, the extreme pressure required is indeed a challenge for practical application, which promotes a further exploration for high temperature (T_c) superconductors at relatively low pressure. Herein, we performed a systematic theoretical investigation on a series of ternary hydrides with stoichiometry AX_2H_8, which is constructed by interacting molecular $X\mathrm{H_4}$ (X = B, C, and N) into the fcc metal A lattice under low pressure of 0–150 GPa. We uncovered five compounds which are dynamically stable below 100 GPa, e.g., AcB_2H_8 (25 GPa), LaB_2H_8 (40 GPa), RbC_2H_8 (40 GPa), CsC_2H_8 (60 GPa), and SrC_2H_8 (65 GPa). Among them, AcB_2H_8, which is energetically stable above 2.5 GPa, exhibits the highest T_c of 32 K at 25 GPa. The superconductivity originates mainly from the coupling between the electron of Ac atoms and the associated low-frequency phonons, distinct from the previous typical hydrides with H-derived superconductivity. Our results shed light on the future exploration of superconductivity among ternary compounds at low pressure.

Keywords: ternary superconductors, low pressure, $X\mathrm{H_4}$ molecules, fcc lattice

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1. Introduction

It has been a long-term pursuit to search for high temperature and even room temperature superconductivity since the first discovery of superconductivity in 1911.[1] Hydrogen is considered as a promising candidate for high-T_c superconductors because the H atom has a smaller mass and a higher phonon vibration frequency.[2,3] However, the metallization of hydrogen is not unambiguously achieved and may require pressures over 400 GPa.[4] Alternately, compressed hydrides can be metalized at much lower pressures due to the "chemical pre-compression".[5] Indeed, increasing amounts of binary hydrides have been measured to exhibit high-T_c superconductivity, e.g., H_3S with T_c of 203 K at 155 GPa,[6–9] LaH_{10} with T_c of 250–260 K at 170 GPa,[10–13] YH_9 with T_c of 243–262 K at 182–201 GPa,[14,15] YH_6 with T_c of 220 K at 166 GPa or 237 GPa,[15–17] and the recent CaH_6 with T_c of 220 K at 160 GPa or 172 K.[18–20] All these discoveries are in good agreement with the theoretical predictions,[7,9,12,13,21] however, the pressures required to stabilize these hydrides are higher than 150 GPa,[22,23] which significantly limits the further application. Thus it is a primary challenge to search for high-T_c superconductors at lower pressure or even ambient pressure.

The focus in the field of superconductivity has been shifted to ternary hydrides,[29,30] because adding a light element X could bind with the atoms to form $X\mathrm{H}_x$ units, which can produce increased chemical pre-compression on the parent binary lattice and further reduce the metallization pressure.[31] For example, CH_4 molecular in CSH_7 (181 K at 100 GPa),[32,33] BeH_8 units in La/Ac/Lu/BeH_8,[34–37] BH_6 units in $AcBH_7$,[38] and BH_8 units in $LaBH_8$[39–41] make the compounds dynamically stable down to relatively low pressures compared with those of binary hydrides. Encouragingly, $LaBeH_8$[34] and LaB_2H_8[42] have been successfully synthesized with measured T_c of 100 K at 80 GPa and 106 K at 90 GPa, respectively. Moreover, ternary alkaline (Am) boron hydrides AmB_2H_8 (Am = K/Rb/Cs) constructed by intercalating BH_4 into fcc lattice of alkaline metals are predicted to possess T_c above 100 K at 15 GPa.[24,25] Similarly, CH_4 and NH_4 can also be inserted into metal fcc lattice to obtain high-T_c superconductors below megabar pressure, e.g., AlN_2H_8 (118 K at 40 GPa), MgN_2H_8 (105 K at 30 GPa), MgC_2H_8 (55 K at 40 GPa), ScC_2H_8 (49 K at 50 GPa),[26] and AlC_2H_8 (67 K at 80 GPa).[43,44] Note that LaC_2H_8 has the highest T_c in XC_2H_8 group with T_c of 140 K but at ultrahigh pressure (250 GPa),[27] while YC_2H_8 could be stabilized at 50 GPa with the estimated T_c of 24 K.[28]

Thus in this work, we systematically investigated the superconductivity and stability of AX_2H_8 structures constructed by inserting $X\mathrm{H_4}$ (X = B, C, and N) molecules into metal

[†]These authors contributed equally to this work.
[‡]Corresponding author. E-mail: wenwencui@jsnu.edu.cn
[§]Corresponding author. E-mail: yinwei_li@jsnu.edu.cn

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atoms A (A are alkali metals, alkaline earth metal, and real earth metals). In addition to known compounds, we identified five new dynamically stable compounds below 100 GPa: AcB_2H_8 with T_c of 32 K at 25 GPa, LaB_2H_8 with T_c of 18.09 K at 40 GPa, RbC_2H_8 with T_c of 3.29 K at 40 GPa, SrC_2H_8 with T_c of 5.05 K at 65 GPa, and CsC_2H_8 with T_c of 4.29 K at 60 GPa. Our results indicate that ternary hydrides with AX_2H_8 stoichiometry are an ideal class of superconducting materials stabilized at submegabar pressures due to the pre-compression of the XH_4 molecules by the metal fcc lattice.

2. Computational details

We constructed the compounds with AX_2H_8 structure under pressures below 150 GPa (A = Li, Na, K, Rb, Cs, Be, Mg, Ca, Sr, Ba, Sc, Y, La, Ac, Ce; X = C, B, N). Optimization and self-consistent energy calculations of the structures were performed using Vienna *Ab initio* Simulation Package (VASP)[45,46] with the exchange–correlation functional of the generalized gradient approximation (GGA) from the Perdew–Burke–Ernzerhof (PBE)[47] and the projector-augmented wave pseudopotential.[48] We set the corresponding plane wave cutoff energy to 600 eV. During the optimization process, the crystal structure of AX_2H_8 achieved energy and force convergence smaller than 10^{-5} eV/Å and 10^{-4} eV/Å, respectively. The dynamic stability of the AX_2H_8 ternary crystal structure was studied using phonopy code based on density-functional theory.[49] To consider the chemical bonding states of the structure, the covalent bonding was explored by the electron localization function (ELF)[50] and charge transfer using Bader.[51] The electron–phonon coupling (EPC) and the superconducting critical temperature T_c were calculated using the quantum espresso package[52,53] based on the broadening parameter of 0.04 Ry. To get the EPC parameter λ, the Brillouin zone was sampled with a k-point $24\times24\times24$ grid and a $6\times6\times6$ q-point grid. T_c was further estimated using the Allen-Dynes-modified McMillan (ADM) equation[54]

$$T_c = \frac{\omega_{\log}}{1.2}\exp\left[-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right]. \quad (1)$$

3. Results and discussion

The dynamical stability of AX_2H_8 compounds is first examined by calculating the phonons by using the supercell approach as implemented in the phonopy code[55,56] at 150 GPa. For the dynamically stable compounds, we then perform further calculations at lower pressures to determine their threshold of dynamic stability. As shown in Fig. 1(a), in addition to previously reported compounds, we screen five new compounds that are dynamically stabilized below 150 GPa, which are divided into two groups according to molecule XH_4: (i) LaB_2H_8 (40 GPa) and AcB_2H_8 (25 GPa); (ii) RbC_2H_8 (40 GPa), CsC_2H_8 (60 GPa), and SrC_2H_8 (65 GPa). The pressures here are remarked as the minimum dynamically stable pressures at which all the following calculations and discussions are focused. We investigate the thermodynamic stability of these compounds by calculating their enthalpy as a function of pressure relative to binary compounds and elemental forms, as shown in Fig. S1. Our results indicate that AcB_2H_8 and LaB_2H_8 are energetically stable around 2.5 GPa, making them the primary focus of our study due to their relatively high T_c (Table 1) and the lower pressure required compared to other compounds. For the three low-T_c compounds, RbC_2H_8 becomes stable below 17 GPa and above 39 GPa, while ScC_2H_8 stabilizes above 26 GPa. In contrast, CsC_2H_8 is calculated to be energetically unstable across the entire pressure range. All these structures adopt the space group of $Fm\bar{3}m$ characterized by the XH_4 molecules into metal fcc lattice [Fig. 1(b)]. The metal atom A, the light element X, and H atoms occupy the $4a$ (0.000, 0.000, 0.000), $8c$ (0.250, 0.250, 0.250), and $32f$ (0.357, 0.357, 0.357) Wyckoff positions, respectively. The angle between H–C(B)–H in C(B)H_4 tetrahedra has the same values of 109.47°. The lengths of C–H bonds have the same value of 1.110 Å in RbC_2H_8 (at 40 GPa) and CsC_2H_8 (at 60 GPa), which are a litter smaller than those of SrC_2H_8 (at 65 GPa), MgC_2H_8 (at 40 GPa), and AlC_2H_8 (at 80 GPa)[43] with the values of 1.136 Å, 1.128 Å, 1.124 Å, and 1.115 Å, respectively. These values are comparable with those of typical CH_4 (at ambient pressure) molecules with 1.11 Å bond length and 109.5° bond angle. B–H bonds have longer distances with values of 1.216 Å, 1.196 Å, and 1.227 Å in AcB_2H_8 (at 25 GPa), LaB_2H_8 (at 40 GPa), and KB_2H_8 (12 GPa),[25] respectively. The chemical boning characters of C–H and B–H are examined by the electron localization functions (ELF). The strong covalent nature is demonstrated by the clear electron localization between B/C [Fig. 1(c) and S2]. The Bader charges reveal that the charges from metal A transferred to CH_4 are $0.37e$ and $0.36e$ per C atom in RbC_2H_8 and CsC_2H_8, respectively. In fact, the electrons are accepted by C atoms, and almost no electrons ($<0.02e$) are transferred to H atoms, which is consist

Table 1. The calculated electron–phonon coupling parameter (λ), logarithmic average of phonon frequencies ($\omega_{\log}$) and estimated T_c ($\mu^* = 0.10$) for fcc AcB_2H_8, LaB_2H_8, RbC_2H_8, CsC_2H_8, and SrC_2H_8 at their lowest dynamical stability pressure.

				T_c (K)	
Phases	Pressure (GPa)	λ	$\omega_{\log}$ (K)	ADM	Eliashberg
AcB_2H_8	25	1.68	152.88	19.22	32
LaB_2H_8	40	1.23	196.94	18.09	
RbC_2H_8	40	0.45	448.53	3.29	
CsC_2H_8	60	0.47	456.44	4.29	
SrC_2H_8	65	0.63	194.23	5.05	

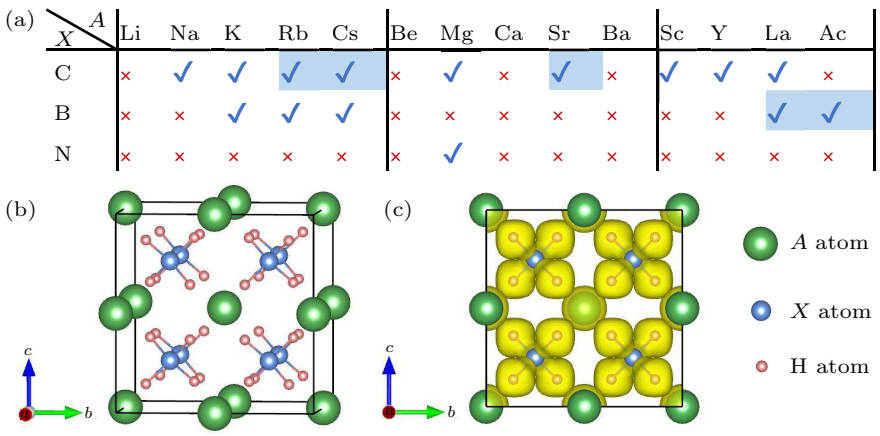


Fig. 1. (a) Dynamical stability of the AX_2H_8 structures below 150 GPa for various combinations of A and X elements. Dynamically stable and unstable compounds are indicated by red crosses and blue ticks, receptively. The unfilled and filled areas represent the known[24–28] and our proposed structures, respectively. (b) The crystal structure of $Fm\bar{3}m$ AX_2H_8. (c) The ELF of AcB_2H_8, with isosurfaces value of 0.75.

with the previous work.[43] While in AcB_2H_8 and LaB_2H_8, H accepts 0.59e and 0.57e, respectively, which are from both metal Ac/La and B atoms. The variation in the replacement atoms exerts a significant influence on their electron–phonon properties, subsequently impacting their superconductivity. The relevant properties will be analyzed next according to the classification of the molecule XH_4.

Ac/LaB$_2$H$_8$ We further investigate the electronic density of states (DOS) and band structures of AcB_2H_8 (at 25 GPa) and LaB_2H_8 (40 GPa) as shown in Figs. 2(a) and 2(b), respectively. They have similar band spectra due to the same crystal structures and in the same main group as well. Both of them are metallic with the presence of two flat energy bands crossing the Fermi energy (E_f), suggesting their potential as the high-temperature superconductors. The band structures at high-energy level, especially around E_f, are mainly contributed by the metal atoms Ac and La, where the electrons can easily flee from the atoms and thus turn into free electrons, which strongly strengthen the electrical conductivity. The low-energy level band is primarily contributed by B and H with a strong overlap in DOS, suggesting the existence of stable covalent B–H bonds. Note that superconductivity is closely associated with the occupation of electrons at the E_f. Here, the DOS at E_f in AcB_2H_8 is primarily contributed by the metal atom Ac, accounting for more than half (60%), while the light atoms B and H contribute 28% and 12%, respectively [Fig. 2(a)]. For LaB_2H_8, the contribution of metal atoms La reaches an astonishing 73%, followed by B atoms with a share of 19%, while H atoms contribute only a minimal percentage of 8% [Fig. 2(b)]. However, it fails to satisfy the basic criteria of a high contribution of H-derived DOS at E_f, indicating a relatively weak superconductivity as compared with those of the typical hydrides.

The dynamical stability of AcB_2H_8 (25 GPa) and LaB_2H_8 (40 GPa) is demonstrated by the absence of imaginary frequencies in phonon dispersions [Figs. 2(c) and 2(d)]. The stabilization of AcB_2H_8 occurs at a lower pressure mainly due to the larger atomic mass of Ac atoms, resulting in a greater chemical pre-compression compared to LaB_2H_8. Their phonons display very similar features with a large gap in 1250–2250 cm^{-1} region, which divides the phonons into three distinctive parts of high, middle and low frequencies. For both hydrides, the low-frequency phonon is mainly dominated by the metal atoms due to the large atomic mass. The middle frequency modes are generally contributed by B and H atoms, and the high-frequency one is exclusively due to H atoms. The superconductivity is estimated by the modified Allen–Dynes McMillan equation.[54] We use the typical value of the Coulomb pseudopotential $\mu^* = 0.10$. A summary of the results can be found in Table 1. AcB_2H_8 shows the strongest EPC parameter $\lambda = 1.68$, contributed by low frequencies about 67.7%, middle frequencies 21.8%, and high frequencies 10.5%. There is an obvious soft mode at high symmetry point W. With a phonon frequency logarithmic average ω_{log} of 152.88 K, the T_c is estimated to be 19.22 K. For the strongly coupled superconductors with $\lambda > 1.5$, Eliashberg theory[57] gives a better estimation, and the T_c is increased to 32 K by numerically solving the Eliashberg equations. For LaB_2H_8, the λ is calculated to 1.23 at 40 GPa, with 67.0% contribution from low-frequencies. Middle and high frequencies contribute 28.3% and 4.7%, respectively. The T_c is about 18 K, slightly lower than that of AcB_2H_8 due to its lower EPC. In summary, the electron–phonon coupling primarily involves the metal atoms La and Ac, which contributes significantly to the participation of electrons and phonons interactions.

Rb/Cs/SrC$_2$H$_8$ Figure 3 shows the electronic band structures and DOS of RbC_2H_8 at 40 GPa, CsC_2H_8 at 60 GPa and SrC_2H_8 at 65 GPa. Rb/CsC_2H_8 have very similar band structures with one band crossing the E_f. The Van Hove singularity in the DOS indicates that they are the potential superconductors. Interestingly, C atoms dominate more than half of the total DOS at E_f with the similar contribution (63%), followed

by H (25%) and meta atoms (12%). Rb/CsC_2H_8 compounds have similar features with distinct gaps divided by low, middle and high frequencies. The low frequencies dominated by Rb and Cs contribute 41.7% and 44.0% to the total λ. The middle-frequencies from the C–H bonds have 41.7% and 37.0% contributions in RbC_2H_8 and CsC_2H_8, respectively. Due to the similar contribution in DOS and phonon dispersions, they exhibit similar superconductivity with T_c of 3.29 K and 4.29 K for RbC_2H_8 and CsC_2H_8, respectively. For SrC_2H_8 [Fig. 3(c)], it exhibits weak metallic nature, where the Fermi energy level locates in the pseudo gap with only one band crossing the Fermi energy. The DOS occupation of SrC_2H_8 at E_f is mainly contributed by Sr (50%). Similar to that of La/AcB_2H_8, low frequencies derived from heavy metal atoms contribute mostly to the total λ, e.g., 73.7% to 0.63 for Sr. The corresponding T_c is estimated to be 5.05 K.

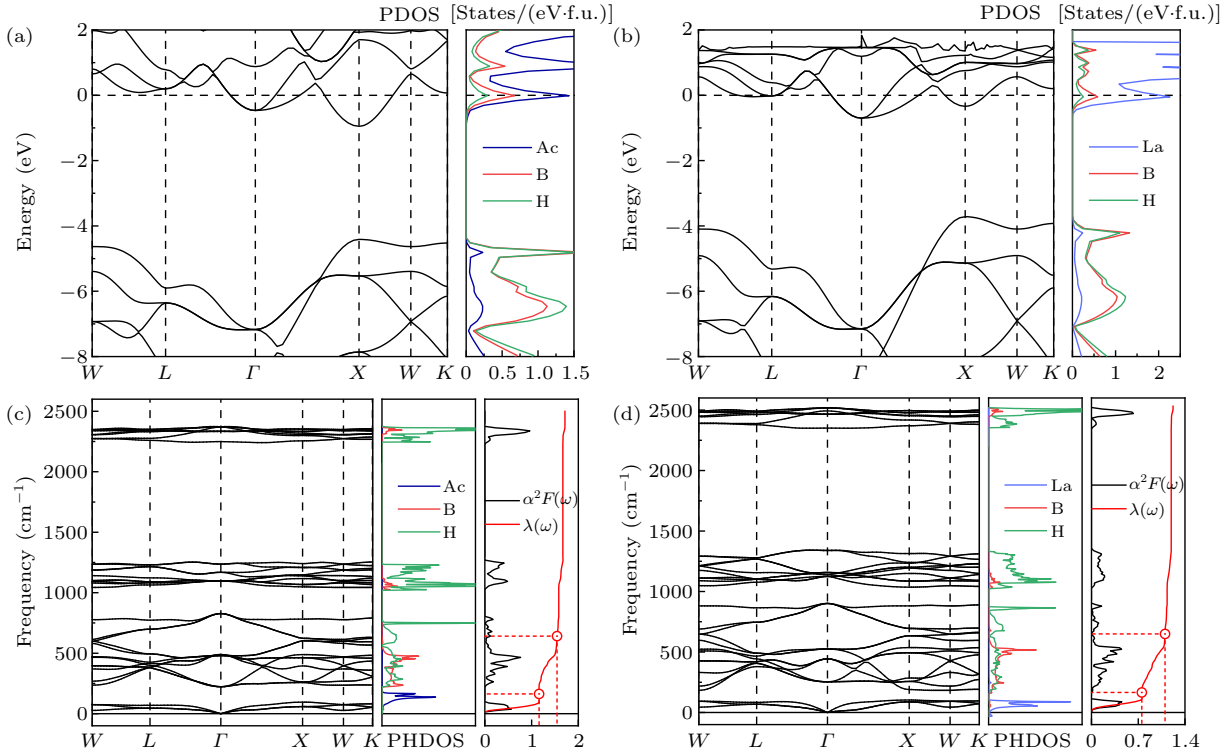


Fig. 2. Electronic band structure, and atom projected density of states near the Fermi level of (a) AcB_2H_8 at 25 GPa, and (b) LaB_2H_8 at 40 GPa. Panels (c) and (d) show the phonon-dispersion curves, PHDOS, projected on each atom, Eliashberg spectral function, $\alpha^2F(\omega)$ and λ for AcB_2H_8 at 25 GPa and LaB_2H_8 at 40 GPa, respectively.

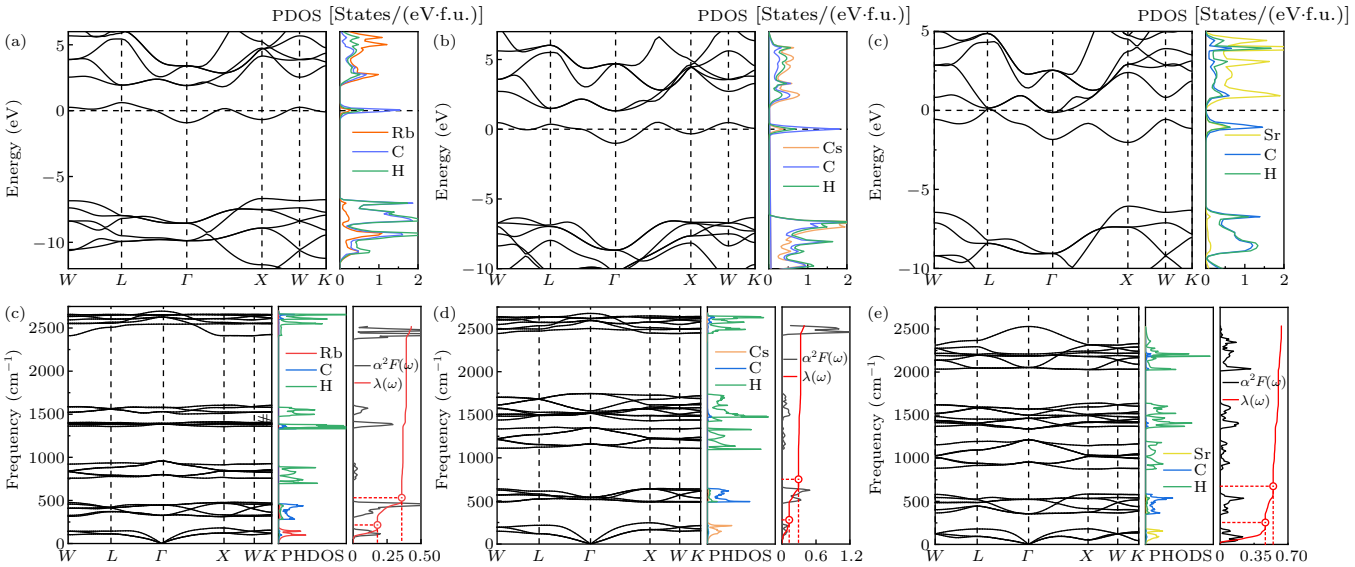


Fig. 3. Electronic band structure, atom projected density of states near the Fermi level of (a) RbC_2H_8 at 40 GPa, (b) CsC_2H_8 at 60 GPa, and (c) SrC_2H_8 at 65 GPa. Panels (d)–(f) show phonon-dispersion curves, PHDOS, projected on the *A*, *B*, and H atoms, Eliashberg spectral function, $\alpha^2F(\omega)$ and λ for RbC_2H_8 at 40 GPa, CsC_2H_8 at 60 GPa, and SrC_2H_8 at 65 GPa, respectively.

4. Conclusions

We systematically investigated the stability and superconductivity with $Fm\bar{3}m$ AX_2H_8 structures in the pressure range of 0–150 GPa. We identified five new dynamically stable structures and all of them are superconductors. Among these, AcB_2H_8 could be dynamically stable down to 25 GPa, and has the highest T_c of 32 K. Analysis demonstrates that their superconductivity is attributed to the coupling between electron from metals and its associated low-frequency phonons, which is distinct from other typical hydrides superconductors, where the H atoms play a key role in the superconductivity. This may also explain why these compounds exhibit relatively weak superconductivity. Our results are expected to bring certain light for future design of high-T_c superconductors stabilized at low pressure.

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