



## Ab initio study of phase transition and bulk modulus of NaH

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### ABSTRACT

The phase transition of NaH from NaCl- to CsCl-type structure is investigated by an *ab initio* plane-wave pseudopotential density functional theory method with the norm-conserving pseudopotential scheme in the frame of the generalized gradient approximation correction; the isothermal bulk modulus and its first and second pressure derivatives of the NaCl- and CsCl-type structures under high pressure and temperature are obtained through the quasi-harmonic Debye model. The phase transition obtained from the usual condition of equal enthalpies occurs at the pressure of 32 GPa, which is consistent with the experimental and other calculated values. Through the quasi-harmonic Debye model, in which the phononic effects are considered, the dependences of cell volume  $V$  and lattice constant  $a$  on temperature  $T$  at zero pressure, the isothermal bulk modulus  $B_0$  and its pressure derivatives  $B'_0$  and  $B''_0$  on pressure  $P$  along isotherms 0, 300, and 600 K, are also successfully obtained.

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### 1. Introduction

Hydrogen forms stable stoichiometric hydrides by reaction with all of the alkali metals: Li, Na, K, Rb, and Cs. The alkali hydrides XH ( $X = \text{Li, Na, K, Rb, and Cs}$ ) are interesting, because of the possibility to use them for fusion to obtain high energy fuels. In these materials, experimental evidence seems consistent with hydrogen being present in the form of anions or modified anions: electron distribution investigations [1] estimated the ionic charge in an LiH to fall in range 0.4–1.0 electron charges, indicating that the alkali hydrides are probably very similar to the alkali halides, with respect to the electronic structure, and that XH ( $X = \text{Li, Na, K, Rb, and Cs}$ ) might even be regarded as the lightest alkali halides, not far from alkaline fluoride compounds: XF ( $X = \text{Li, Na, K, Rb, and Cs}$ ). Like other alkali hydrides, an NaH adopts an NaCl-type structure in which each  $\text{Na}^+$  ion is surrounded by six  $\text{H}^-$  ions in an octahedral configuration under normal conditions. At elevated temperatures of 698 K, an NaH undergoes thermal decomposition in which molecular hydrogen is released [2]. It has been received wide attention partly, due to the fact that it is of interest as the model compound with the simplest anion and cations in the periodic

table, but as potential hydrogen storage materials. So, it is extensively investigated both experimentally [3,4] and theoretically [5–9].

Duclos et al. [3] have performed high-pressure measurements with the diamond anvil cell on an NaH in 1987. Their high-pressure data shows a structural phase transition from the low-pressure NaCl-type structure to the high-pressure CsCl-type structure at  $29.3 \pm 0.9$  GPa. Hochheimer et al. [4] have reported the transition pressures for CsH, RbH, and KH, as well as the equation of state (EOS) of an NaH to 28 GPa. On the theoretical side, Martins [5] had calculated equations of the LiH, NaH, and KH as a function of pressure for the NaCl- and CsCl-type structures using the pseudopotential method. Their calculated transition pressures in NaH and KH are in agreement with experiments. Ahuja et al. [6] have calculated the transition pressure for an NaH used the full-potential linear muffin-tin-orbital (FP-LMTO) method based on the local-density approximation, and given the value 37 GPa, which is high than the experimental result [3]. Besides the crystal structure, the thermodynamic properties are the most fundamental parameter obtained from high-pressure experiments. Using plane wave pseudopotential density functional theory and density functional perturbation theory within the framework of the quasiharmonic approximation, Yu et al. [7] have calculated the phonon dispersions and thermodynamic properties for the lighter alkali-metal hydrides LiH and NaH. The high-pressure studies for an NaH have completed the data for the series and have enabled a systematic comparison of transition pressures as well as EOSs, bulk moduli, and effective charges with those of alkali halides. Such comparisons will lead to an improved understanding of bonding in ionic and partly ionic materials at equilibrium conditions and at high pressures. On the other hand, despite the publication of numerous

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experimental and theoretical studies to understand more about an NaH, the variation of the isothermal bulk modulus and its first and second pressure derivatives which play a central role in the formulation of approximate EOSs at high pressure and temperature is still scarce.

In the present work, we focus on investigating the phase transition of an NaH from the NaCl- to the CsCl-type structure and the bulk modulus of an NaH by the plane-wave pseudopotential density functional theory method through the Cambridge Sequential Total Energy Package (CASTEP) program [10] and by the quasi-harmonic Debye model [11], which allows us to obtain all thermodynamic quantities from the calculated energy-volume points. Major advantages of this *ab initio* approach are: the ease of computing forces and stresses; good convergence control with respect to all computational parameters employed; favorable scaling with the number of atoms in the system and the ability to make cheaper calculations by neglecting core electrons. The isothermal bulk modulus and its pressure derivatives, especially their pressure, and temperature dependencies have been studied by many scientific research workers, because of its basic role for the EOS and the description of the behavior of solids in the area of high-pressure and high-temperature sciences [12–14]. Here, we can calculate the isothermal bulk modulus and its pressure derivatives of an NaH not only at the normal state, but also at an extended temperature and pressure ranges. The properties of an NaH summarized in the pressure 0–65 GPa ranges and the temperature up to 600 K.

## 2. Theoretical methods

In the electronic structure calculations, we employ a non-local norm-conserving pseudopotential together with Perdew–Burke–Ernzerhof (PBE) [15] generalized gradient approximation (GGA) for the interactions of the electrons with the ion cores. Density functional calculations were conducted with the plane-wave pseudopotential method [16]. Pseudo-atomic calculations are performed for an Na  $2s^2 2p^6 3s^1$  and H  $1s^1$ . The energy cutoff of the plane-wave basis was chosen as 770 eV. For the Brillouin-zone sampling, we adopted the  $9 \times 9 \times 9$  Monkhorst–Pack mesh [17], where the self-consistent convergence of the total energy is at  $5.0 \times 10^{-7}$  eV/atom. The chosen plane-wave cutoff and the number of  $k$  points were carefully checked to ensure the total energy converged. For a given external hydrostatic pressure, both parameters of the unit cell and the internal coordinates of the atoms are fully relaxed until forces had converged to  $< 0.01$  eV/Å and all the stress components are  $< 0.02$  GPa. The relative stability of different structural phases was examined by comparing their enthalpy values, which were computed from  $H = E + PV$ .

All the calculations for the equilibrium structure are performed at  $T = 0$ , because of the lack of an extension of density-functional theory to high temperature. To investigate the thermodynamic properties of an NaH with NaCl- and CsCl-type structures, we here applied the quasi-harmonic Debye model [11], in which the phononic effect is considered. In the quasi-harmonic Debye model, the non-equilibrium Gibbs function  $G^*(V; P, T)$  can be written as  $G^*(V; P, T) = E(V) + PV + A_{vib}(\Theta; T)$ , (1) where  $E(V)$  is the total energy per unit cell, which can be determined by electronic structure calculations,  $PV$  corresponds to the constant hydrostatic pressure condition,  $\Theta(V)$  is the Debye temperature, and  $A_{vib}$  is the vibrational Helmholtz free energy, including both the vibrational contribution to the internal energy and the  $TS$  constant temperature condition term, which can be written as [18]

$$A_{vib}(\Theta; T) = nkT \left[ \frac{9}{8} \frac{\Theta}{T} + 3 \ln(1 - e^{-\Theta/T}) - D(\Theta/T) \right], \quad (2)$$

where  $D(\Theta/T)$  represents the Debye integral,  $n$  is the number of atoms per formula unit. By solving the following equation with respect to  $V$

$$\left[ \frac{\partial G^*(V; P, T)}{\partial V} \right]_{P,T} = 0, \quad (3)$$

one could obtain the isothermal bulk modulus  $B_T$

$$B_T(P, T) = V \left[ \frac{\partial^2 G^*(V; P, T)}{\partial V^2} \right]_{P,T}, \quad (4)$$

and the adiabatic bulk modulus  $B_S$

$$B_S = B_T(1 + \alpha\gamma T), \quad (5)$$

where  $\alpha$  is the thermal expansion coefficient, and  $\gamma$  is the Grüneisen parameter.

## 3. Results and discussion

The estimation of the zero-temperature transition pressure between NaCl- and CsCl-type structures of an NaH can be obtained from the usual condition of equal enthalpies; in other words, the pressure  $P$ , at which enthalpy  $H = E + PV$  of both two phases is the same. We calculate the enthalpy of the two-ion primitive cell of an NaH in both the NaCl- and CsCl-type structures as a function of pressure from 0 to 65 GPa, as shown in Fig. 1. In the inset, the relative enthalpy versus pressure is presented. From this figure, we can see that the NaCl-type structure has the lower enthalpy under low pressure and the CsCl-type structure has the lower enthalpy under pressure higher than the transition pressure. The thermodynamic requirement, for the equality of free energies, at a phase boundary, suggests that the transition pressure of an NaH should occur at 32 GPa. The transition involves the coordination number increasing from 6 for the NaCl-type structure to 8 for the CsCl-type structure, resulting in denser packing. Compared with an FP-LMTO calculated value 37 GPa based on the local-density approximation [6], our result 32 GPa is in very good agreement with the diamond-anvil-cell high-pressure experimental value of  $29.3 \pm 0.9$  GPa [3]. The differences among all theoretical data result from the different methods used. Each calculation method also has its own limitations related to the basic material parameters, basis sets, and the precisions used, in addition to the approximations of the method itself, leading to variations in the calculated parameters. For the

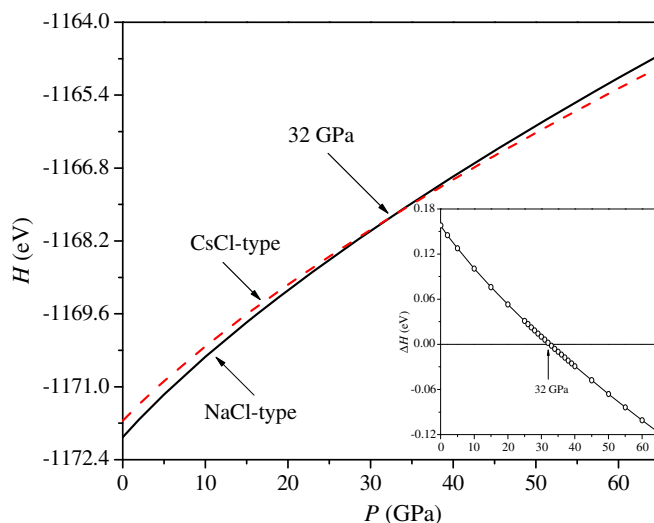


Fig. 1. Enthalpy as a function of pressure for an NaH. In the inset, the relative enthalpy versus pressure is presented.

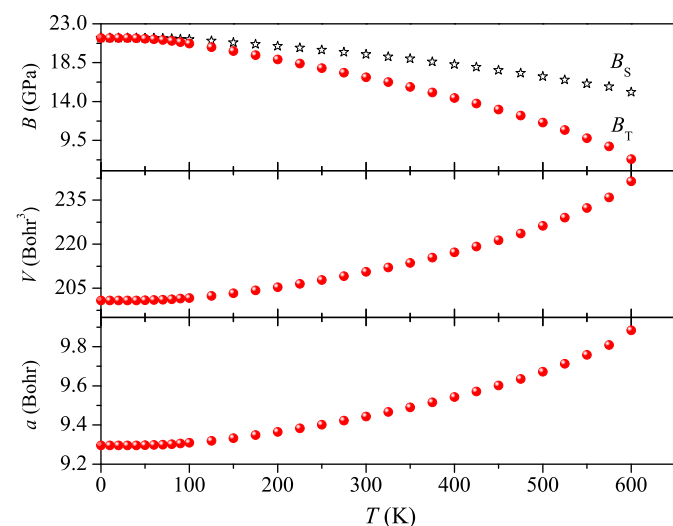
NaCl-type structure, the charge transfer increase from 0.47 to 0.55, when the pressure is increased from 0 to 32 GPa, the bond length is compressed from 4.594 to 3.861 Bohr, and the bond population is reduced from 0.64 to 0.50. When the CsCl-type structure is compressed from 32 to 65 GPa, the charge transfer is also increased, while the bond length and the bond population are reduced. A high value of the bond population indicates a covalent bond, while a low value indicates an ionic interaction. It can be found that the ionicity interaction becomes more and more stronger as the pressure applied from 0 to 65 GPa. In the following, considering the phase transition pressure, we investigate the bulk modulus and its pressure derivatives of the NaCl-type structure of an NaH over a range of pressures from 0 to 32 GPa, and those of the CsCl-type structure over a range of pressures from 33 to 65 GPa through the quasi-harmonic Debye model.

The isothermal bulk modulus is defined as the volume derivative of pressure. For many purposes, it is desirable to investigate the temperature dependence of the bulk modulus of solids. An adequate knowledge of the temperature dependence of the bulk modulus is necessary for understanding the thermoelastic and anharmonic properties of crystals [19–21]. In Fig. 2, we illustrate the relationship between bulk modulus  $B$  of an NaH with NaCl-type structure and temperature at zero pressure. Meanwhile, the volume  $V$  and lattice constant  $a$  dependent on the temperature at zero pressure are presented too. X-ray diffraction experiments lead to the determination of the isothermal bulk modulus [3]. Besides the experimental investigations, many theoretical calculations have also been employed to determine the structural and mechanical properties of an NaH [22–25]. For NaCl- and CsCl-type structures of an NaH, a series of different values of lattice constant  $a$  is set to calculate the total energy  $E$  and the corresponding primitive cell volumes  $V$ . Here, we fit the calculated  $E$ - $V$  points to Birch–Murnaghan EOS [26], in which the pressure–volume relationship expanded to the fourth-order in strain is

$$P = 3B_0 f_E (1 + f_E)^{5/2} \left\{ 1 + \frac{3}{2} (B' - 4) f_E + \frac{3}{2} \left[ B_0 B'' + (B' - 4)(B' - 3) + \frac{35}{9} f_E^2 \right] f_E^2 \right\}, \quad (6)$$

where  $f_E$  is written as

$$f_E = [(V_0/V)^{2/3} - 1]/2. \quad (7)$$



**Fig. 2.** The isothermal bulk modulus  $B_T$ , adiabatic bulk modulus  $B_S$ , primitive cell volume  $V$ , and lattice constant  $a$  of an NaH with an NaCl-type structure as a function temperature  $T$  at zero pressure.

The lattice constant, primitive cell volumes, isothermal bulk modulus, and its pressure derivatives are obtained as shown in Table 1. The NaCl- and CsCl-type NaH have theoretical bulk modulus of 22.90 and 23.21 GPa, with pressure derivatives  $B'_0$  and  $B''_0$  of 3.78, 3.75 and  $-0.162$ ,  $-0.159$ , respectively. Compared with experimental values [3], our GGA results are slightly scattered. High-pressure X-ray diffraction data on an NaH to 54 GPa at room temperature show the isothermal bulk modulus  $B_0$  with an NaCl-type structure is  $19.40 \pm 2.00$  GPa, with a pressure derivative  $B'_0$  of  $4.40 \pm 0.50$  [3]. We note that our calculations are in very good agreement with the theoretical value 22.80 GPa by Gupta and Kumar [22] and other theoretical calculations [23–25], and provide further support for the bulk modulus of an NaH determined by Duclos et al. [3] in comparison to that reported by Hochheimer et al. [4]. The results, together with earlier measurements on KH, RbH, and CsH, indicate that the alkali hydrides show the same strong dependence of phase transition pressure on cation as do the alkali halides. The systematically lower bulk moduli of the alkali hydrides as compared to the alkali halides can be attributed to an incomplete charge transfer in this series of partly ionic compounds.

From Fig. 2, one can obviously see that when  $T < 100$  K,  $B$  nearly keeps constant; when  $T > 100$  K,  $B$  decreases dramatically as  $T$  increases. Correspondingly, when  $T < 100$  K, the primitive cell volume and lattice constant of an NaH with an NaCl-type structure have a little change; when  $T > 100$  K, the primitive cell volume or lattice constant change rapidly as  $T$  increases. It is the rapid volume or lattice constant variation that makes the bulk modulus  $B$  rapidly decrease. The primitive cell volume and lattice constant calculated are 200.79 Bohr<sup>3</sup> and 9.194 Bohr for an NaH with an NaCl-type structure, respectively. The lattice constant is in very good agreement with the theoretical prediction from 9.140 to 9.362 Bohr [2,7,24], as shown in Table 1.

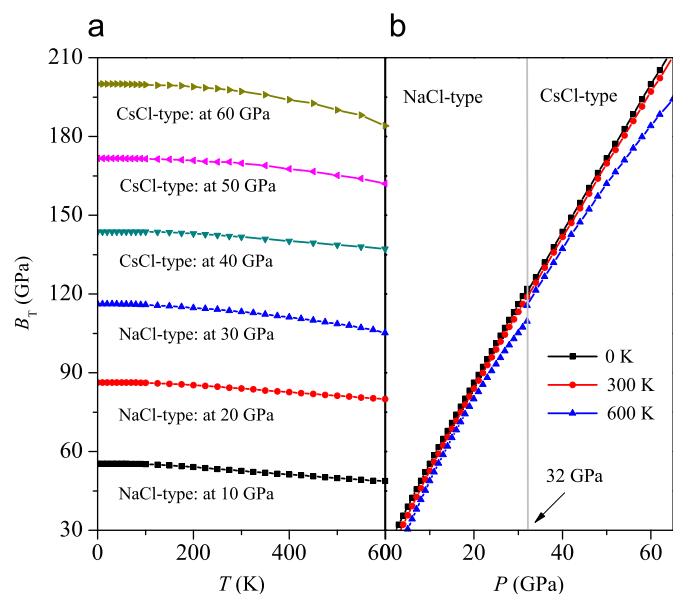
In the context of bulk modulus, it is also of interest to investigate an isothermal bulk modulus  $B_T$  under various pressures and temperatures. Fig. 3 shows the predicted values of the isothermal bulk modulus of an NaH dependence of the temperature  $T$  at 10, 20, and 30 GPa for an NaCl-type structure and at 40, 50, and 60 GPa for the CsCl-type structure, and dependence of the pressure  $P$  at 0, 300, and 600 K, respectively. It is easily seen that the isothermal bulk modulus of an NaH with NaCl- and CsCl-type structures increases with the increase of pressure, and decreases with an increasing temperature.

The pressure derivative of the isothermal bulk modulus at a given temperature and pressure,  $B'_{T,P}$  and  $B''_{T,P}$ , where the subscripts  $T$  and  $P$  denote the iso- $T$  and iso- $P$ , respectively, are very important in high-pressure studies. From a geophysical viewpoint,  $B'_{T,P}$  and  $B''_{T,P}$  are parameters that are necessary for the accurate inversion of seismic data into composition, structure, and texture,

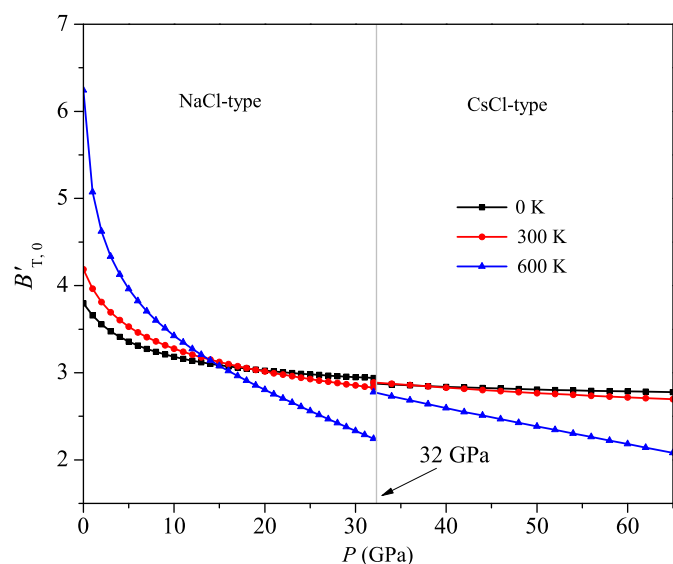
**Table 1**

The lattice constant  $a$ , primitive cell volumes  $V$ , isothermal bulk modulus  $B_T$ , and its pressure derivatives  $B'_0$  and  $B''_0$  of an NaH with NaCl- and CsCl-type structures at zero pressure and temperature.

	NaCl-type	Present Calc.	Other Theor. Calc.	Expt.
$a$ /Bohr		9.194	9.140 [2] 9.362 [7] 9.150 [24]	9.222 [3]
$V$ /Bohr <sup>3</sup>		200.79	176.30 [23] 191.515 [24]	196.072 [3]
$B_0$ /GPa		22.90	22.80 [22] 24.08 [24] 23.50 [25]	$19.40 \pm 2.00$ [3]
$B'_0$		3.78	3.16 [25]	$4.40 \pm 0.50$ [3]
$B''_0$		$-0.162$		
CsCl-type				
$a$ /Bohr		5.637		
$V$ /Bohr <sup>3</sup>		89.56		
$B_0$ /GPa		23.21		$28.30 \pm 3.00$ [3]
$B'_0$		3.75		$4.30 \pm 0.40$ [3]
$B''_0$		$-0.159$		



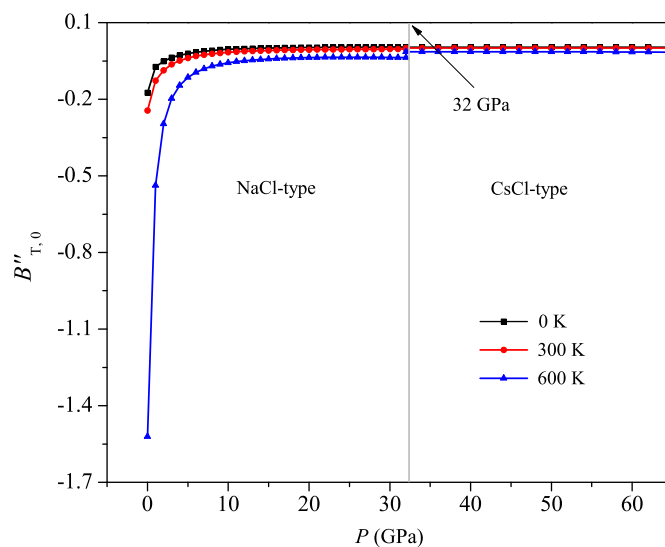
**Fig. 3.** The predicted isothermal bulk modulus of an NaH versus temperatures and pressures.



**Fig. 4.** The predicted first pressure derivative of isothermal bulk modulus of an NaH versus pressure at different temperatures.

as well as for determining the thermal profile of the deep Earth [27] and also for determining the isothermal empirical equation of the state of materials in the deep Earth [28]. Since the variation in many of the macroproperties of solids with temperature and pressure are closely related to  $B_{T,p}$  and  $B''_{T,p}$ , then  $B_{T,p}$  and  $B''_{T,p}$  are crucial for thermodynamic calculations of the properties at high temperatures and high pressures [29]. In point defect thermodynamics,  $B_{T,p}$  and  $B''_{T,p}$  are also the key parameters constraining the behavior of point defects, such as their formation, clustering, and migration [30]. Thus, precise determination of the temperature dependence of  $B_{T,p}$  and  $B''_{T,p}$  are significant in many fields, including geophysics, condensed matter physics, and materials science.

Figs. 4 and 5 show the predicted first and second pressure derivatives of the isothermal bulk modulus  $B_{T,p}$  and  $B''_{T,p}$  of an NaH with NaCl- and CsCl-type structures versus pressure along isotherms 0, 300, and 600 K. It can be seen that the  $B''_{T,p}$  increases with the increase of temperature in the whole pressure 0–65 GPa ranges,



**Fig. 5.** The predicted second pressure derivative of isothermal bulk modulus of an NaH versus pressure at different temperatures.

and  $B''_{T,p}$  decreases with the increase of temperature when  $P > 15$  GPa. Note that the effect of decreasing pressure on the first pressure derivative  $B_{T,p}$  of the isothermal bulk modulus for an NaH is the same as an increasing temperature of an NaH. The second pressure derivative,  $B''_{T,p}$ , of the isothermal bulk modulus for an NaH rather steep when  $P < 5$  GPa, rapidly flattens with an increasing pressure, and it keeps a constant on the whole when  $P > 10$  GPa. Thus, the  $B''_{T,p}$  of an NaH at high pressures is a weak function of temperature.

#### 4. Conclusions

In summary, we use the *ab initio* plane-wave pseudopotential density functional theory together with the GGA-PBE to investigate the high-pressure phase transition and the bulk modulus in an NaH. The transition pressure from NaCl- to CsCl-type structure occurs at 32 GPa, which is in good agreement with the experimental value. The primitive cell volume, lattice constants, bulk modulus, and its pressure derivatives for an NaH are obtained. All the results are well consistent with the experimental data and other theoretical results. At an extended pressure and temperature ranges, the isothermal bulk modulus and its pressure derivatives of an NaH with NaCl- and CsCl-type structures are predicted by using the quasi-harmonic Debye model which the phononic effects are considered. It can be found that the isothermal bulk modulus decreases with increasing temperatures and increases with an increasing pressure. The first pressure derivative of the isothermal bulk modulus  $B_{T,p}$  of an NaH decreases with the increase of temperature when  $P > 15$  GPa, and the effect of decreasing pressure is the same as an increasing temperature. The second pressure derivative of the isothermal bulk modulus  $B''_{T,p}$  of an NaH at high pressures is a weak function of temperature.

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