

Thermodynamic properties of group-III nitrides and related species

I. N. Przhevskii¹, S. Yu. Karpov² and Yu. N. Makarov³

¹Russian Research Center "Applied Chemistry",

²Soft-Impact Ltd (St.Petersburg, Russia),

³Lehrstuhl für Strömungsmechanik, University of Erlangen-Nürnberg,

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A database for thermodynamic properties of group-III nitrides and relevant species involved into growth of these materials is developed in this paper. Standard formation enthalpies of materials and coefficients of polynomial approximations of the reduced Gibbs free energies are collected in the tables. They allow one to determine the Gibbs free energy, enthalpy, entropy and specific heat of a species as a function of temperature. The database covers solid and gaseous group-III nitrides, elemental species, gaseous metal-organic compounds, chlorides and hydrides of group-III elements, nitrogen containing precursors and organic byproducts of various chemical reactions proceeding during growth processes. Thermodynamic properties of adducts which can be formed in the vapor phase while mixing ammonia and metal-organic compounds are presented in the database as well. Much of the data given in this paper is presented for the first time. All the data are checked for self-consistency and therefore can be used for thermodynamic calculations.

1 Introduction

Group-III nitrides are semiconductor materials that are expected to play a revolutionary role in modern optoelectronics and high-power, high-temperature electronics. Development of the technological base for growth and processing of these materials demands detailed knowledge of their physical properties. Much effort has been made in the recent years to examine various characteristics and parameters of GaN, AlN, InN and their ternary compounds. Some carefully selected results are summarized in reference [1]. However, the scientific field related to group-III nitrides has broadened so quickly that the appearance of such books does not keep pace with the needs of the nitride community. More ongoing development of the reference database is desirable both for fundamental and applied studies covering growth, processing and characterization of these promising materials.

In this paper we make an attempt to develop a self-consistent database of thermodynamic properties of group-III nitrides and the species related to growth of these materials. Part of the data is taken from the reliable sources. The rest of the data are either refined using new information on the properties of the nitrides and rel-

evant species available from the literature or presented here for the first time.

The organization of the paper is as follows. In Section 2 we explain the notation used throughout the paper and give the main expressions for calculation of thermodynamic functions of the materials. Section 3 gives a short guide to the database. In Section 4 we discuss the origin of the thermodynamic properties of the species refined or obtained in this paper.

2 Notation and general relationships

The Gibbs free energy $G(P, T)$ of a certain species as a function of pressure P and temperature T is defined by the expression

$$G(P, T) = G^{\circ}(P_0, T) + \int_{P_0}^P \left(\frac{\partial G}{\partial P} \right)_T dP \quad (1)$$

where $G^{\circ}(P_0, T)$ is the Gibbs thermodynamic potential taken at the standard pressure $P_0 = 1$ atm. For $G^{\circ}(P_0, T)$ we use the standard approximation accepted

in the reference books [2] [3] [4]. According to these works the temperature dependence of $G^0(P_0, T)$ can be approximated by a polynomial

$$G^0(P_0, T) = H(298 \text{ K}) - T \cdot \Phi(x)$$

$$\Phi(x) = \varphi \ln x + \sum_{k=-2}^3 \varphi_k x^k, \quad x = T/10^4$$

(2)

Here $H(298 \text{ K})$ is the standard formation enthalpy of the species (for elemental species this value is defined to be equal to zero) corresponding to the standard temperature $T_0 = 298.15 \text{ K}$, $\Phi(x)$ is the so called reduced Gibbs free energy. The polynomial approximation (2) differs from those used in JANNAF tables or in well-known database "Chemkin". By special comparison we have found that our polynomial form provides more accurate approximation of the thermodynamic properties of various species in a wide temperature range.

Using the array of coefficients $\varphi, \varphi_1, \dots, \varphi_3$ one can calculate the enthalpy $H(T)$, entropy $S(T)$ and specific heat $C_p(T)$ of the species corresponding to the standard pressure $P_0 = 1 \text{ atm}$ and arbitrary temperature

$$H(T) = H(298 \text{ K}) + T \cdot \left(\varphi + \sum_{k=-2}^3 k \varphi_k x^k \right)$$

$$S(T) = \varphi (1 + \ln x) + \sum_{k=-2}^3 (k+1) \varphi_k x^k$$

$$C_p(T) = \varphi + \sum_{k=-2}^3 k(k+1) \varphi_k x^k$$

(3)

In this paper thermodynamic functions of materials are calculated by commonly accepted methods discussed in detail in [2]. For gaseous species the molecular constants (bond lengths, angles between the bond directions, oscillation frequencies etc.), either taken from literature or estimated (in the case of lack of experimental information), are used in the calculations. Therewith the "rigid rotator – harmonic oscillator" approximation is applied to account for internal rotational degrees of freedom of molecules.

3 Organization of the database

For convenience the thermodynamic database of the materials involved into growth of group-III nitrides is split into seven tables [1]. In Table 1 the data on elemental materials are collected. Table 2 and Table 3 contain the data on group-III hydrides and chlorides respectively. Table 4 presents the data on gaseous group-III metal-organic compounds. In Table 5 the data on various (first of all, gaseous) species which are either nitrogen carrying precursors or byproducts of chemical reactions are given. Table 6 contains thermodynamic properties of the adducts forming during MOVPE or HVPE growth of group-III nitrides. And, finally, in Table 7 properties of solid and gaseous binary nitrides are presented. Every table contains in separate columns

- The chemical notation for the species
- The phase state of the species: solid (s), liquid (l) or gaseous (g)
- The temperature range where the polynomial approximation (2) is proven to be valid
- The formation enthalpy $H(298 \text{ K})$ of the species corresponding to the standard temperature $T_0 = 298.15 \text{ K}$, and seven coefficients $\varphi, \varphi_1, \dots, \varphi_3$ measured in $\text{J/mol}\cdot\text{K}$ to provide the Gibbs free energy measured in J/mol
- A reference to the work where the corresponding thermodynamic data have been reported (there is no reference in this column if the thermodynamic properties are refined or estimated in this paper)

Thermodynamic properties of 44 species – Al(s), Al(l), Al(g), Al₂(g), AlH(g), AlH₂(g), AlH₃(g), AlN(g), CH(g), CH₂(g), CH₃(g), CH₄(g), s-C₂H₂(g), C₂H₄(g), C₂H₅(g), C₂H₆(g), Cl(g), Cl₂(g), H(g), H₂(g), HCl(g), HN₃(g), In(s), In(l), In(g), InH(g), Ga(s), Ga(l), Ga(g), GaH(g), GaCl(g), GaCl₂(g), GaCl₃(s), GaCl₃(l), GaCl₃(g), Ga₂Cl₆(g), N(g), N₂(g), NH(g), NH₂(g), NH₃(g), N₂H₂(g), N₂H₄(g), NH₄Cl(s) – are taken from references [2] [3] [4] [5]. For these components no special comments will be made. The properties of 31 other species (including adducts forming during MOVPE and HVPE process) – AlN(s), AlCH₃(g), Al(CH₃)₃(g), Al₂(CH₃)₆(g), a-C₂H₂(g), GaH₂(g), GaH₃(g), GaN(s), GaN(g), GaCH₃(g), Ga(CH₃)₃(g), InH₂(g), InH₃(g), InN(s), InCH₃(g), In(CH₃)₃(g), Al·NH₃(g), AlCH₃·NH(g), (AlCH₃·NH)₃(g), Al(CH₃)₃·NH₃(g), (Al(CH₃)₂·NH₂)₃(g), (Al·N)₃, (Al(CH₃)₂·NH₂)₂(Ga(CH₃)₂·NH₂)(g), (Al(CH₃)₂·NH₂)(Al(CH₃)₂·NH₂)₂(g), Ga·NH₃(g), GaCH₃·NH(g), Ga(CH₃)₃·NH₃(g), (GaCH₃·NH)₃(g), (Ga(CH₃)₂·NH₂)₃(g), (Ga·N)₃, GaCl₃·NH₃(g) – are

either refined or derived in this paper. For these species the thermodynamic data are attended by necessary comments given in Section 4.

All the data are verified for self-consistency and therefore can be used for thermodynamic calculations.

4 Comments

In this section we make short comments on the thermodynamic properties of various species and the way in which these properties are estimated. The main species are arranged in alphabetical order, the adducts are considered at the end of section.

4.1 $\text{AlCH}_3(\text{g})$ monomethylaluminum (MMA)

Molecules AlCH_3 (MMA) have been observed experimentally in the gas phase [6]. Thermodynamic functions of MMA are obtained using molecular constants calculated theoretically in references [7] [8] [9]. According to these works the molecule MMA in the ground X^1A_1 state has the structure of C_{3V} symmetry. Formation enthalpy of MMA is calculated using the value of $\text{Al}-\text{CH}_3$ bond energy estimated by comparison of the bond energies in such pairs of molecules as AlCH_3 and GaCH_3 , $\text{Al}(\text{CH}_3)_3$ and $\text{Ga}(\text{CH}_3)_3$. This procedure is applied because theoretical estimation of the formation enthalpy of MMA carried out in reference [7] results in an evidently underestimated value (this was mentioned by authors of reference [7] themselves). Our data are in a reasonable agreement with those obtained in reference [10].

4.2 $\text{Al}(\text{CH}_3)_3(\text{g})$ trimethylaluminum (TMA)

Thermodynamic functions of $\text{Al}(\text{CH}_3)_3$ are calculated using the molecular constants taken from experimental [11] [12] [13] [14] [15] [16] [17] and theoretical [11] studies. According to these works, the TMA molecule in the ground X^1A_1 state has the structure of D_{3h} symmetry. The formation enthalpy of TMA is taken after reference [18]. Earlier thermodynamic functions of TMA were calculated in reference [19] using approximate values of molecular constants and in reference [10]. Our data are in a reasonable agreement with the results of both these works.

4.3 $\text{Al}_2(\text{CH}_3)_6(\text{g})$

Thermodynamic properties of gaseous $\text{Al}_2(\text{CH}_3)_6$ are calculated using the molecular constants obtained experimentally in references [13] [15] [16] [17] [20] [21]. According to these works the $\text{Al}_2(\text{CH}_3)_6$ molecule in the ground X^1A_1 state has the structure of D_{2h} symmetry. The formation enthalpy of $\text{Al}_2(\text{CH}_3)_6$ is taken from reference [18].

Earlier thermodynamic functions of $\text{Al}_2(\text{CH}_3)_6$ were calculated in reference [19] using approximate values of molecular constants and in reference [10]. The value of entropy at 298.15 K given in [10] is lower than that accepted in the current work. The cause of the discrepancy could not be revealed since the authors of reference [10] did not refer to their source of data on molecular constants. The formation enthalpy of $\text{Al}_2(\text{CH}_3)_6$ reported in reference [10] is somewhat lower than that recommended in reference [18], although it remains within the experimental error bars.

4.4 $\text{AlN}(\text{s})$

The specific heat $C_p(T)$ of solid AlN has been measured by different groups in the temperature range of 50-300 K. The results are summarized in reference [1] and plotted in Figure 1 (numerical values are given also in the Data file 1). These data were used in references [4] [5] for calculation of thermodynamic functions of solid AlN. We refine the thermodynamic properties of AlN accounting for the results of AlN specific heat measurements carried out in the temperature range of 2.6-300 K [22] (the data on specific heat are shown in Figure 1 and also given in the Data file 2). The formation enthalpy of AlN is taken according to references [4] [5].

Free evaporation of AlN in vacuum has been investigated in reference [23]. The evaporation of AlN is found to be congruent. The total pressure of evaporating species (Al and N_2) measured at different temperatures is shown in Figure 2 and numerical data given in Data file 3. Comparison to thermodynamic calculations (the solid line in Figure 2) shows that the evaporation of AlN is kinetically limited. Due to this kinetic effect the experimental data on AlN evaporation can not be used for estimation of thermodynamic properties of this compound.

4.5 $\text{a-C}_2\text{H}_2(\text{g})$ vinylidene

Thermodynamic properties of vinylidene are calculated using the molecular constants found in theoretical and experimental studies [24] [25]. According to the results of these studies the vinylidene molecule has a configuration of C_{2V} symmetry in the ground state. The formation enthalpy of vinylidene is determined using the formation enthalpy of $s\text{-C}_2\text{H}_2(\text{g})$ [4] and the isomerization energy of acetylene- vinylidene – 43 kcal/mol obtained in references [24] [25]

4.6 GaCH_3 monomethylgallium (MMG)

Thermodynamic functions for gaseous GaCH_3 (MMG) are calculated using molecular constants determined in experimental [26] and theoretical [27] [28] [29] studies of the molecules MMG and CH_3GaH [30] [31]. According to these works the molecule GaCH_3 in the

ground X^1A_1 state has the configuration of C_{3v} symmetry. The formation enthalpy of MMG is calculated using the value of the Ga–CH₃ bond energy determined while studying the pyrolysis of trimethylgallium (Ga(CH₃)₃) [32] [33]. Theoretical calculation of this energy [27] gave a remarkably underestimated value. Earlier thermodynamic functions of MMG were reported in reference [10]. Our data are in a reasonable agreement with the results of this work.

4.7 Ga(CH₃)₃(g) trimethylgallium (TMG)

Thermodynamic functions of gaseous Ga(CH₃)₃ (TMG) are calculated using the molecular constants determined both experimentally [13] [34] [35] [36] [37] and theoretically [27] [28]. According to these studies the TMG molecule in the ground X^1A_1 state has the configuration of D_{3h} symmetry. Formation enthalpy of TMG is taken from reference [18]. Earlier thermodynamic properties of TMG have been estimated in [38] and [10] using the approximate values of the molecular constants. Our data agree with the results obtained in reference [10].

4.8 GaH₂(g)

Molecular constants of gaseous GaH₂ are determined using the experimental data of references [30] [39] [40] [41] and results of theoretical calculations carried out for molecules GaH₂ [30] [39] [40] [31] [42] [43] [44] and Ga₂H₄ [45]. According to the experimental and theoretical results the molecule GaH₂ in the ground state X^2A_1 has a non-linear configuration of C_{2v} symmetry. We calculate the formation enthalpy of GaH₂ using the value of Ga–H bond energy in the molecule GaH₂ obtained theoretically in [44] [46]. Recently thermodynamic functions of GaH₂ have been estimated in Reference [10]. The authors of [10] reported the value of entropy of GaH₂ at 298.15 K as well as the polynomial approximation of the specific heat which agree well with our estimates. However, the formation enthalpy of GaH₂ – $H(298\text{ K}) = 164\text{ kJ/mol}$ accepted in [10] exceeds significantly the value obtained in this work. This is related to overestimation in reference [10] the Ga–H bond energy in the molecule GaH₂ – 273.6 kJ/mol instead 171.5 kJ/mol as follows from the theoretical calculations of references [44] [46].

4.9 GaH₃(g)

Molecular constants of gaseous GaH₃ are taken from experimental [39] [47] and theoretical [39] [43] [44] [47] [48] [49] [50] [51] [52] [53] studies of molecules GaH₃ and Ga₂H₆ [48] [49]. According to the results obtained in these works the molecule GaH₃ in the

ground state X^1A_1 has a flat configuration of D_{3h} symmetry. We calculate the formation enthalpy of GaH₂ using the value of Ga–H bond energy in the molecule GaH₃ obtained theoretically in reference [44] [46]. Thermodynamic functions of gaseous GaH₃ have been reported also in reference [10]. The value of entropy of GaH₃ at 298.15 K and the polynomial approximation for specific heat agree well with our data. The formation enthalpy of GaH₃ – $H(298\text{ K}) = 108\text{ kJ/mol}$ accepted in reference [10] is significantly less than the value obtained in this work. This is related to the underestimation in reference [10] of the Ga–H bond energy in the molecule GaH₃ – 273.6 kJ/mol instead 338.7 kJ/mol predicted based on theoretical calculations [44] [46].

4.10 GaN(s)

The specific heat $C_p(T)$ of solid GaN has been measured by calorimetry in the temperature interval of 5–60 K [54] and in the temperature interval of 55–300 K [55]. The experimental data obtained in these works are shown in Figure 3 and given numerically in Data file 4. For comparison in Figure 3 is shown the approximation of the specific heat versus temperature recommended in reference [1].

Thermodynamic properties of solid GaN are determined using the experimental data on specific heat [22] [54] [55] and the enthalpy increment of GaN [56]. We take the formation enthalpy of GaN averaged over two values – one of them based on the calorimetric measurements of GaN heat of burning [57], the other obtained using the 3rd law and the experimental data of reference [58]. The value accepted in reference [18] is an underestimate. This was pointed out by authors of reference [59], where results of reference [57] were discussed in regard to the determination of the formation enthalpy of solid InN. The thermodynamic functions of GaN reported in references [60] [61] were obtained using rough estimates of the GaN specific heat, entropy and formation enthalpy; therefore they are not quite accurate.

Langmuir (free) evaporation of GaN in vacuum has been studied in reference [62]. The evaporation was found to be congruent. The total pressure of the evaporating species (Ga and N₂) was measured versus temperature by a torsion-effusion method. The results of the measurements are plotted in Figure 4 and given numerically in Data file 5. Comparison to thermodynamic calculations (the solid line in Figure 4) shows that the evaporation of GaN is kinetically limited. Due to this limitation the experimental data on GaN evaporation can not be used for estimation of the thermodynamic properties of this compound.

4.11 GaN(g)

There is no information on the molecular constants of gaseous GaN. To calculate the thermodynamic functions of GaN(g) we use the oscillation frequencies and interatomic distance estimated in references [63] [64] assuming by analogy with AlN(g) that the ground state of GaN molecule is $X^2\Pi$. The formation enthalpy of gaseous GaN is calculated by using the dissociation energy of the molecule equal to 523 kJ/mol as determined in reference [65]. Thermodynamic functions of gaseous GaN reported in reference [63] have been calculated using the molecular constants obtained in references [63] [64]. The formation enthalpy of GaN(g) was not determined in reference [63].

4.12 InCH₃ monomethylindium (MMI)

We could not find in the literature any information on the molecular constants of gaseous InCH₃ (MMI). That is why we estimate these constants assuming in analogy with MMA and MMG that the MMI molecule in the ground state X^1A_1 state has the configuration of C_{3V} symmetry. The formation enthalpy of MMI is found using the value of In-CH₃ bond energy extracted in reference [66] from the experimental data on pyrolysis of In(CH₃)₃.

4.13 In(CH₃)₃(g) trimethylindium (TMI)

Thermodynamic functions of gaseous In(CH₃)₃ (TMI) are calculated using the molecular constants obtained in experimental studies [34] [67] [68] [69] [70] [71] [72]. According to these works the TMI molecule in the ground X^1A_1 state has the configuration of D_{3h} symmetry. To determine the value of formation enthalpy of TMI we use the experimental data on the formation enthalpy of solid In(CH₃)₃ as well as the heat of In(CH₃)₃(s) sublimation [73] [74]. Earlier rough estimations of thermodynamic properties of TMI have been made in reference [75].

4.14 InH₂(g)

Thermodynamic functions of gaseous InH₂ are calculated on the base of molecular constants measured in references [39] [40] and theoretically calculated in reference [40]. According to these works the molecule InH₂ in the ground X^2A_1 state has non-linear configuration of C_{2V} symmetry. The formation enthalpy of InH₂ is estimated using the value of In-H bond energy in the InH₂ molecule calculated in reference [76].

4.15 InH₃(g)

The thermodynamic functions of gaseous InH₃ are calculated using the molecular constants determined in

experimental [39] [47] and theoretical studies [40]. According to these works the molecule InH₃ in the ground X^1A_1 state has a flat configuration of D_{3h} symmetry. The formation enthalpy of InH₃ is estimated using the value of the In-H bond energy in the InH₃ molecule calculated in reference [76].

4.16 InN(s)

There is no experimental information on thermodynamic properties of solid InN. The published data on InN evaporation [77] [78] [59] [79] cannot be used to determine the enthalpy of InN formation since equilibrium conditions were not met in these experiments. Evaporation of InN occurs with decomposition into the liquid and gas phases starting at least from 450°C [22]. No experimental data on Langmuir evaporation of InN in vacuum are available at the present time.

The value of $H(298\text{ K})$ estimated using the heat of InN burning [57] and accepted in [58] is apparently underestimated (this was mentioned by the authors of reference [59] who especially analyzed the work [57]) and cannot serve as the basis for estimation of properties of InN. That is why we take the available data on the properties of other III-V compounds and use the analogy method [80] to extrapolate the respective thermodynamic functions of InN.

4.17 Adducts formed while mixing gaseous group-III compounds and ammonia

Spectral investigations of the chemical reactions between Al atoms in a ground electron state and NH₃ molecules [81], theoretical studies of Al-NH₃ adducts [82] [83] and numerous experimental data [84] [85] [86] [87] [88] [89] [90] [91] [92] [93] [94] [95] [96] [97] [97] [98] [99] [100] provide evidence of the formation in the gaseous mixture of metal-organic group-III compounds and ammonia of such adducts as TMA·NH₃ and TMG·NH₃. With gradual liberation of methane these adducts transform into the radicals DMA·NH₂ and DMG·NH₂ which, in turn, can combine into the complexes (DMA·NH₂)₃, (DMG·NH₂)₃, (DMA·NH₂)₂(DMG·NH₂) and (DMA·NH₂)(DMG·NH₂)₂. Further liberation of CH₄ molecules is assumed from these complexes with their transition into (MMA·NH)₃, (MMG·NH)₃, (MMA·NH)₂(MMG·NH), (MMA·NH)(MMG·NH)₂, and then into gaseous polymers of (Al·N)₃, (Ga·N)₃, (Al·N)₂(Ga·N), (Al·N)(Ga·N)₂ type. Below the thermodynamic properties of some of these adducts are estimated. In addition the properties of GaCl₃·NH₃, which can be formed during hydride vapor phase epitaxy of GaN, are discussed.

4.17.1 $\text{AlNH}_3(\text{g})$

The molecular constants of gaseous $\text{Al}\cdot\text{NH}_3$ necessary for estimation of thermodynamic functions are taken from theoretical studies [82] [83]. According to these works the molecule $\text{Al}\cdot\text{NH}_3$ in the ground X^1A_1 state has configuration of C_{3V} symmetry. The formation enthalpy of $\text{Al}\cdot\text{NH}_3$ is found using the value of $\text{Al}\text{--}\text{NH}_3$ bond energy calculated theoretically in [82] [83].

4.17.2 $\text{GaNH}_3(\text{g})$

There is no information on molecular constants of the gaseous $\text{Ga}\cdot\text{NH}_3$ adduct. In analogue with $\text{Al}\cdot\text{NH}_3$ we assume that molecule $\text{Ga}\cdot\text{NH}_3$ is stable in the ground X^1A_1 state and has the structure of C_{3V} symmetry. Molecular constants of $\text{Ga}\cdot\text{NH}_3$ are found by extrapolation of the corresponding constants for the pairs TMA and TMG, $\text{TMA}\cdot\text{NH}_3$ and $\text{TMG}\cdot\text{NH}_3$, $\text{Al}\cdot\text{NH}_3$ and $\text{Ga}\cdot\text{NH}_3$. The formation enthalpy of $\text{Ga}\cdot\text{NH}_3$ is calculated using the estimated value of the $\text{Ga}\text{--}\text{NH}_3$ bond energy. The estimation procedure is based on a comparison of the values of bond energies in the pairs of molecules $\text{Al}\cdot\text{NH}_3$ and $\text{Ga}\cdot\text{NH}_3$, $\text{TMA}\cdot\text{NH}_3$ and $\text{TMG}\cdot\text{NH}_3$.

4.17.3 $\text{Al}(\text{CH}_3)_3\cdot\text{NH}_3(\text{g})$

Thermodynamic functions of gaseous $\text{Al}(\text{CH}_3)_3\cdot\text{NH}_3$ (or $\text{TMA}\cdot\text{NH}_3$) are calculated using the molecular constants found both experimentally [84] [85] [86] [87] and theoretically [86] [101] [102]. According to these studies the molecule $\text{Al}(\text{CH}_3)_3\cdot\text{NH}_3$ in the ground X^1A_1 state has the configuration of C_{3V} symmetry. The formation enthalpy of $\text{Al}(\text{CH}_3)_3\cdot\text{NH}_3$ is determined using the value of $\text{TMA}\text{--}\text{NH}_3$ bond energy obtained in references [86] [87] [102] [103] [104] [105].

4.17.4 $\text{Ga}(\text{CH}_3)_3\cdot\text{NH}_3(\text{g})$

Molecular constants of gaseous $\text{Ga}(\text{CH}_3)_3\cdot\text{NH}_3$ (or $\text{TMG}\cdot\text{NH}_3$) needed for estimation of the thermodynamic functions are taken from experimental studies [88] [89] [90] [91] [92] [93] [94] [95]. According to the results of these works the molecule $\text{Ga}(\text{CH}_3)_3\cdot\text{NH}_3$ in the ground X^1A_1 state has the structure of C_{3V} symmetry. The formation enthalpy of $\text{Ga}(\text{CH}_3)_3\cdot\text{NH}_3$ is obtained through the $\text{TMG}\text{--}\text{NH}_3$ bond energy determined in references [104] [96].

4.17.5 $(\text{Al}(\text{CH}_3)_2\cdot\text{NH}_2)_3(\text{g})$

Thermodynamic properties of $(\text{Al}(\text{CH}_3)_2\cdot\text{NH}_2)_3$ or $(\text{DMA}\cdot\text{NH}_2)_3$ are calculated using the molecular constants taken from experimental studies of $(\text{DMA}\cdot\text{NH}_2)_3$ [100], $(\text{DMG}\cdot\text{NH}_2)_3$ [97] [98], $(\text{DMA}\cdot\text{NH}_2)_2$ [97], $\text{TMA}\cdot\text{NH}_3$, $\text{TMG}\cdot\text{NH}_3$ and theoretical investigations of

$\text{DMA}\cdot\text{NH}_2$ [86] and $(\text{HAl}\cdot\text{NH}_3)$ [106]. In accordance with these works it is accepted that in the ground state X^1A the complex $(\text{DMA}\cdot\text{NH}_2)_3$ has non-flat ring configuration of C_1 symmetry. The formation enthalpy of $(\text{DMA}\cdot\text{NH}_2)_3$ is found using the experimental data of reference [103].

4.17.6 $(\text{Ga}(\text{CH}_3)_2\cdot\text{NH}_2)_3(\text{g})$

Thermodynamic properties of $(\text{Ga}(\text{CH}_3)_2\cdot\text{NH}_2)_3$ or $(\text{DMG}\cdot\text{NH}_2)_3$ are calculated using the molecular constants taken from experimental studies of $(\text{DMG}\cdot\text{NH}_2)_3$ [97] [98], $(\text{DMG}\cdot\text{NH}_2)_2$ [97], and $\text{TMG}\cdot\text{NH}_3$. According to these works the complex $(\text{DMG}\cdot\text{NH}_2)_3$ in the ground state X^1A has non-flat ring configuration of C_1 symmetry. There is no information on the formation enthalpy of $(\text{DMG}\cdot\text{NH}_2)_3$. We estimate this value by comparison the formation energies of the pairs $(\text{DMA}\cdot\text{NH}_2)_3$ and $(\text{DMG}\cdot\text{NH}_2)_3$, $\text{TMA}\cdot\text{NH}_3$ and $\text{TMG}\cdot\text{NH}_3$.

4.17.7 $(\text{Al}(\text{CH}_3)_2\cdot\text{NH}_2)_2(\text{Ga}(\text{CH}_3)_2\cdot\text{NH}_2)(\text{g})$ and $(\text{Al}(\text{CH}_3)_2\cdot\text{NH}_2)(\text{Ga}(\text{CH}_3)_2\cdot\text{NH}_2)_2(\text{g})$

The complexes $(\text{Al}(\text{CH}_3)_2\cdot\text{NH}_2)_2(\text{Ga}(\text{CH}_3)_2\cdot\text{NH}_2)$ and $(\text{Al}(\text{CH}_3)_2\cdot\text{NH}_2)(\text{Ga}(\text{CH}_3)_2\cdot\text{NH}_2)_2$ have not been studied. The molecular constants of these species as well as their formation enthalpies are calculated using extrapolation of corresponding data on the properties of $(\text{Al}(\text{CH}_3)_2\cdot\text{NH}_2)_3$ and $(\text{Ga}(\text{CH}_3)_2\cdot\text{NH}_2)_3$ adducts.

4.17.8 $\text{AlCH}_3\text{NH}(\text{g})$ and $\text{GaCH}_3\text{NH}(\text{g})$

Decomposition of $\text{TMA}\cdot\text{NH}_3$ and $\text{TMG}\cdot\text{NH}_3$ can lead to appearance of gaseous radicals $\text{AlCH}_3\cdot\text{NH}$ and $\text{GaCH}_3\cdot\text{NH}$ which, in turn, can combine into the ring complexes $(\text{AlCH}_3\cdot\text{NH})_3$ and $(\text{GaCH}_3\cdot\text{NH})_3$. There is no information on molecular constants of these species in literature. We estimate them using corresponding data obtained for molecules $\text{TMA}\cdot\text{NH}_3$, $\text{TMG}\cdot\text{NH}_3$, $\text{DMA}\cdot\text{NH}_2$, $\text{DMG}\cdot\text{NH}_2$, MMA , MMG , $\text{Al}\cdot\text{NH}_3$, $\text{Ga}\cdot\text{NH}_3$, HGaCH_3 and HAlCH_3 . Therewith we assume that molecules $\text{AlCH}_3\cdot\text{NH}(\text{g})$ and $\text{GaCH}_3\cdot\text{NH}(\text{g})$ in the ground X^1A state have an asymmetric configuration of C_1 symmetry. The formation enthalpies of $\text{AlCH}_3\cdot\text{NH}(\text{g})$ and $\text{GaCH}_3\cdot\text{NH}(\text{g})$ are estimated based on experimental data for $\text{TMA}\cdot\text{NH}_3$ and $\text{TMG}\cdot\text{NH}_3$ decomposition obtained in references [86] [103] [99].

4.17.9 $(\text{AlCH}_3\cdot\text{NH})_3(\text{g})$ and $(\text{GaCH}_3\cdot\text{NH})_3(\text{g})$

Thermodynamic functions of gaseous $(\text{AlCH}_3\cdot\text{NH})_3$ and $(\text{GaCH}_3\cdot\text{NH})_3$ are calculated based on molecular constants estimated using results of experimental and theoretical studies of $(\text{AlH}\cdot\text{NH}_3)$, $(\text{DMA}\cdot\text{NH}_2)_3$,

(DMG·NH₂)₃ , (DMG·NH₂)₂(DMA·NH₂) , TMA·NH₃ and TMG·NH₃ . Therewith is assumed that molecules considered in their ground states have asymmetric configuration of C₁ symmetry. The formation enthalpies are estimated using the results of study of TMA·NH₃ and TMG·NH₃ decomposition accompanied by release of methane [86] [103] [99].

4.17.10 (AlN)₃ and (GaN)₃

Ring molecular complexes (Al·N)₃ and (Ga·N)₃ are assumed to be the final products in the chain of consequent adduct formation when mixing group-III metal-organic compounds and ammonia. The thermodynamic functions of these molecules are calculated using the estimated values of molecular constants. For this we use the results of experimental and theoretical studies of AlH·NH₃ [106], (BH·NH₃)₃ [4] and (B·N)₃ [107] [108]. We also assume that in their ground states the molecules (Al·N)₃ and (Ga·N)₃ have a flat structure of D_{3h} symmetry. Formation enthalpies of (Al·N)₃ and (Ga·N)₃ are estimated on the base of studies of TMA·NH₃ and TMG·NH₃ decomposition with simultaneous release of methane [86] [103] [99].

4.17.11 GaCl₃·NH₃

Thermodynamic properties of GaCl₃·NH₃ are calculated using the molecular constants experimentally found in [109] [110]. According to these works the GaCl₃·NH₃ molecule has in the ground state X¹A₁ a configuration of C_{3v} symmetry. The formation enthalpy of GaCl₃·NH₃ is determined using the value of formation enthalpy of solid GaCl₃·NH₃ as well as the evaporation enthalpy of liquid GaCl₃·NH₃ recommended in [18]. The enthalpy of GaCl₃·NH₃(s) melting necessary for the calculations is estimated by a method proposed in reference [111].

5 Summary

In conclusion, a database of thermodynamic properties of group-III nitrides and substances related to growth of these materials is developed in this paper. A polynomial approximation of the reduced Gibbs free energy as a function of temperature corresponding to the standard pressure of 1 atm is given for 75 species. Among them data for 31 species (including adducts frequently formed during vapor phase epitaxy) are either refined or obtained here for the first time. Using the polynomial one can calculate temperature dependencies of enthalpy, entropy and specific heat of a certain species. The database is checked for self-consistency and therefore can be used for thermodynamic calculations.

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FIGURES

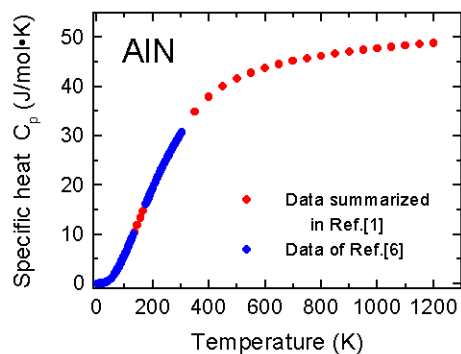


Figure 1. Specific heat of solid AlN as a function of temperature (after reference [1] and reference [22]).

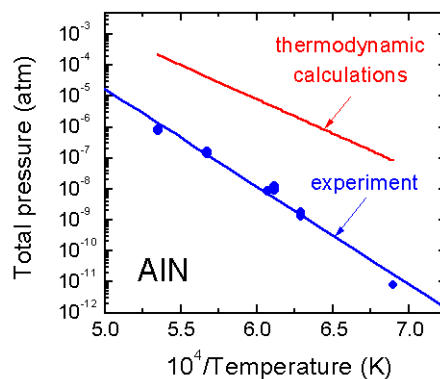


Figure 2. Total pressure (sum of Al and N₂ partial pressures) measured during free evaporation of AlN in vacuum by torsion method [23]. For comparison the result of thermodynamic calculation of the total pressure is plotted in the figure.

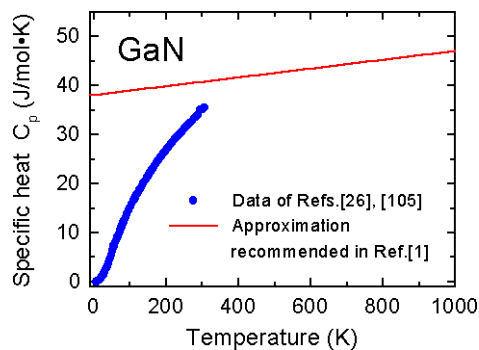


Figure 3. Specific heat of solid GaN versus temperature [54] [55].

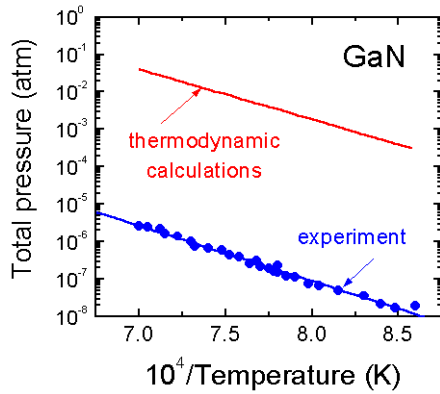


Figure 4. Total pressure (sum of Ga and N₂ partial pressures) measured during free evaporation of GaN in vacuum by torsion-effusion method [62]. For comparison the result of thermodynamic calculation of the total pressure is plotted in the figure.

TABLES

Table 1. Thermodynamic properties of elemental materials related to growth of group-III nitrides.

Component	Phase	Temperature range (K)	H(298K) J/mol	φ_0	φ	φ_2	φ_{-1}	φ_1	φ_2	φ_3	reference
Al	s	298.15–933.61	0	172.8289	50.51806	-0.00411847	1.476107	-458.1279	2105.75	-4168.337	[4]
Al	l	933.61–3000	0	103.0714	26.00912	0.008181946	-0.4129445	32.24031	-43.76215	30.68377	[4]
Al	g	298.15–3000	329700	217.0413	20.81346	0.000249045	0.60354813	-0.2495735	0.5140443	-0.5629165	[4]
Al ₂	g	298.15–3000	490380	353.35	48.47124	-0.00369942	1.6604767	-42.89068	106.9097	-115.6532	[4]
Ga	s	100–302.91	0	241.3354	66.94004	-0.00324457	1.676481	-602.4515	0	0	[4]
Ga	l	302.91–3000	0	126.5938	26.24945	0.001124295	0.1477694	-3.306797	7.960486	-4.117994	[4]
Ga	g	298.15–3000	271979	268.3674	38.19512	-0.00269398	1.226597	-118.8071	194.3493	-161.9061	[4]
In	s	100–429.78	0	28.56306	0.173385	0.001116428	0.3581493	621.9059	-2378.554	0	[4]
In	l	429.78–3000	0	136.5535	27.6628	0.002004388	0.3864998	-7.11553	11.33041	-2.563969	[4]
In	g	298.15–3000	240389	179.4259	5.544982	0.002369352	0.1624565	199.5227	-392.3531	350.0412	[4]
Cl	g	298.15–3000	121302	230.4749	26.0518	-0.001404393	0.8484566	-26.44172	33.95742	-23.09449	[2]
Cl ₂	g	298.15–3000	0	315.6297	37.6554	-0.001818968	1.2427151	-0.7480257	-3.237695	19.2696	[2]
H	g	298.15–3000	217998	166.7375	20.75064	0.000011002	0.61825525	0.3951741	-0.9575932	1.072888	[2]
H ₂	g	298.15–3000	0	205.5368	29.50487	0.000168424	0.86065612	-14.95312	78.18955	-82.78981	[2]
N	g	298.15–3000	472680	205.2031	20.71029	0.000020737	0.61679049	0.9006424	-2.39269	3.047489	[2]
N ₂	g	298.15–3000	0	242.8156	21.47467	0.001748786	0.5910039	81.08497	-103.6265	71.30775	[2]

Table 2. Thermodynamic properties of group-III hydrides.

Component	Phase	Temperature range (K)	H(298K) J/mol	φ_0	φ	φ_2	φ_1	φ_1	φ_2	φ_3	reference
AlH	g	298.15–3000	248949	241.7735	23.45061	0.000267033	0.7561976	94.52152	-149.8564	133.8216	[4]
AlH ₂	g	298.15–3000	247058	263.5826	24.47025	0.000052127	0.887457	201.8884	-305.6576	247.8367	[4]
AlH ₃	g	298.15–3000	208143	247.6922	25.23092	-0.00247941	1.1974457	351.8847	-534.7299	424.2375	[4]
GaH	g	298.15–3000	214301	256.9793	24.75093	-0.00017796	0.81698595	85.2476	-130.322	112.485	[4]
GaH ₂	g	298.15–3000	261000	283.1801	27.73824	-0.00098536	1.04260905	189.6211	-292.8738	234.49034	
GaH ₃	g	298.15–3000	140000	262.5014	25.64802	0.000707271	1.05328668	360.1502	-557.6752	447.1876	
InH	g	298.15–3000	214704	268.5535	26.25779	-0.00068009	0.88853891	77.20851	-119.0338	104.2369	[4]
InH ₂	g	298.15–3000	301000	300.4066	30.93877	-0.00176795	1.1772364	174.5085	-275.3281	224.5262	
InH ₃	g	298.15–3000	226000	298.3732	36.02385	-0.00383638	1.5631789	294.7202	-457.1725	368.1224	

Table 3. Thermodynamic properties of group-III chlorides.

Component	Phase	Temperature range (K)	H(298K) J/mol	φ_0	φ	φ_2	φ_1	φ_1	φ_2	φ_3	reference
GaCl	g	298.15–3000	-70553	332.2718	37.11052	-0.000746187	1.1606512	4.891346	-4.467591	5.506236	[4]
GaCl ₂	g	298.15–3000	-241238	443.2976	57.74584	-0.002265112	1.8755545	3.66186	-9.356338	15.88245	[4]
GaCl ₃	s	298.15–351	-525000	117.602	22.661	0	1.768938	1229.9	0	0	[4]
GaCl ₃	l	351.–1000	-525000	426.622	105.0455	0.000857935	2.0378948	55.82225	-187.023	316.5247	[4]
GaCl ₃	g	298.15–3000	-431573	526.8113	82.03355	-0.003486473	2.6855923	8.278878	-14.5678	12.8899	[4]
Ga ₂ Cl ₆	g	298.15–3000	-957552	945.776	180.9567	-0.007721776	5.923436	14.74793	-26.29971	23.6243	[4]

Table 4. Thermodynamic properties of group-III metal-organic compounds.

Component	Phase	Temperature range (K)	H(298K) J/mol	φ_0	φ	φ_2	φ_1	φ_1	φ_2	φ_3	reference
AlCH ₃	g	298.15–3000	70000	305.5526	35.03927	-0.00174578	1.4497961	350.8434	-441.7573	302.0432	
Al(CH ₃) ₃	g	298.15–3000	-87864	439.3127	67.03525	-0.00997983	3.579156	1117.969	-1438.63	1005.325	
Al ₂ (CH ₃) ₆	g	298.15–3000	-268000	732.0682	153.8187	-0.02210495	7.934453	2291.222	-2980.321	2100.53	
GaCH ₃	g	298.15–3000	79000	310.9298	33.36529	-0.00299805	1.4928029	363.5709	-463.8545	321.0485	
Ga(CH ₃) ₂	g	298.15–3000	78000	420.9466	58.61963	-0.00830238	2.828981	634.9377	-719.8074	425.8506	
Ga(CH ₃) ₃	g	298.15–3000	-45100	419.6335	56.51964	-0.00623311	3.1207383	1253.185	-1835.496	1583.225	
InCH ₃	g	298.15–3000	215000	327.9518	37.02704	-0.00234819	1.5345267	331.9569	-408.1081	273.5027	
In(CH ₃) ₃	g	298.15–3000	207000	486.1998	75.34946	-0.00966392	3.760722	1060.398	-1344.147	926.5466	

Table 5. Thermodynamic properties of compound species related to growth of group-III nitrides. (*) Indexes s- and a- denotes the molecules C_2H_2 having different bond configurations: $HC=CH$ and $H_2C=C$ respectively.

Component	Phase	Temperature range (K)	H(298K) J/mol	φ_0	φ	φ_2	φ_1	φ_1	φ_2	φ_3	reference
CH	g	298.15–3000	597370	242.7524	24.00883	0.001670102	0.6407824	37.86651	15.51023	-45.27447	[3]
CH ₂	g	298.15–3000	390421	240.600	20.52894	0.002739503	0.5603418	152.657	-143.930	66.92434	[3]
CH ₃	g	298.15–3000	146300	235.311	21.73794	0.001495276	0.7668275	260.1063	-286.5025	170.8566	[3]
CH ₄	g	298.15–3000	-74600	160.1245	0.1376158	0.003060968	0.2359966	530.4743	-641.3777	443.8204	[3]
s-C ₂ H ₂ *	g	298.15–3000	227400	290.1858	41.22485	-0.00318242	1.5993697	185.8367	-182.5197	98.56432	[3]
a-C ₂ H ₂ *	g	298.15–3000	406000	295.9776	34.44796	-0.000729682	1.2620663	225.396	-274.2221	181.7939	
C ₂ H ₄	g	298.15–3000	52400	235.4331	20.90119	-0.004640969	1.384579	557.1087	-729.554	519.1573	[3]
C ₂ H ₅	g	298.15–3000	107000	232.3991	10.06969	-0.00231435	1.0455083	730.0119	-972.2628	700.7000	[3]
C ₂ H ₆	g	298.15–3000	-84000	210.8502	12.79009	-0.00332157	1.28072185	834.093	-1099.041	784.2161	[3]
HCl	g	298.15–3000	-92310	243.9878	23.15984	0.001819985	0.6147384	51.16604	-36.89502	9.174252	[2]
HN ₃	g	298.15–3000	294000	318.1457	37.99594	-0.003275438	1.5385397	231.3021	-308.8172	225.2746	[2]
NH ₄ Cl	s	298.15–1500	-314553	1655.076	514.7979	-0.05652215	14.5633	-6619.275	24457.48	-41827.86	[5]
NH ₃	g	298.15–3000	-45940	231.1183	20.52222	0.000716251	0.7677236	244.6296	-251.69	146.6947	[2]
NH ₂	g	298.15–3000	190000	242.1951	21.06781	0.002580563	0.5819481	147.4422	-141.0088	79.39323	[2]
NH	g	298.15–3000	338885	241.3573	24.14921	0.001711517	0.6418191	38.52613	-13.20793	-8.079821	[2]
N ₂ H ₂	g	298.15–3000	211860	259.887	22.8261	-0.000935	0.966786	245.36	-151.638	0	[2]
N ₂ H ₄	g	298.15–3000	95180	301.5557	37.05947	-0.006113206	1.8485832	412.1844	-493.5967	319.4443	[2]

Table 6. Thermodynamic properties of adducts related to growth of group-III nitrides.

Component	Phase	Temperature range (K)	H(298K) J/mol	φ_0	φ	φ_2	φ_1	φ_1	φ_2	φ_3	reference
Al-NH ₃	g	298.15–3000	250000	348.4526	41.86005	0.000211864	1.4472277	255.1086	-257.7037	141.7346	
(Al-N) ₃	g	298.15–3000	-525000	543.3702	108.7302	-0.01831327	4.594580	171.8226	-290.5235	248.8242	
MMA-NH	g	298.15–3000	-190000	414.2169	61.61885	-0.00253783	2.3779207	423.3068	-509.5931	332.8755	
(MMA-NH) ₃	g	298.15–3000	-750000	892.3664	202.2196	-0.03836758	9.739639	1407.448	-1800.317	1257.067	
TMA-NH ₃	g	298.15–3000	-246000	588.4401	112.231	-0.01885472	5.621111	1273.086	-1552.79	1055.969	
(DMA-NH ₂) ₃	g	298.15–3000	-760000	1195.758	324.3533	-0.06284943	15.81051	2406.101	-2903.563	1950.622	
Ga-NH ₃	g	298.15–3000	200000	353.3958	40.79851	0.000266934	1.4191327	264.0403	-272.4233	153.5392	
(Ga-N) ₃	g	298.15–3000	-360000	609.4856	122.2825	-0.01653284	4.809612	77.69752	-1333.739	1154.612	
MMG-NH	g	298.15–3000	-130000	418.7216	60.2648	-0.00183430	2.3002024	434.3678	-528.0146	347.8084	
(MMG-NH) ₃	g	298.15–3000	-520000	946.5981	213.6344	-0.03663681	9.919197	1347.501	-1711.188	1184.161	
TMG-NH ₃	g	298.15–3000	-170000	530.7141	87.98152	-0.00725578	4.304382	1467.071	-1874.727	1297.835	
(DMG-NH ₂) ₃	g	298.15–3000	-525000	1021.0	264.9086	-0.04829547	13.504477	2918.077	-3839.803	2751.129	
(DMA-NH ₂) ₂ (DMG-NH ₂)	g	298.15–3000	-680000	1129.111	302.3056	-0.05821187	15.004891	2596.184	-3249.624	2246.259	
(DMA-NH ₂) (DMG-NH ₂) ₂	g	298.15–3000	-600000	1084.095	285.9634	-0.05281923	14.281768	2738.584	-3512.749	2471.468	
GaCl ₃ -NH ₃	g	298.15–3000	-619000	602.7288	99.90594	-0.003368528	3.512104	365.2924	-445.3745	295.2586	

Table 7. Thermodynamic properties of group-III nitrides.

Component	Phase	Temperature range (K)	H(298K) J/mol	φ_0	φ	φ_2	φ_1	φ_1	φ_2	φ_3	reference
AlN	s	298.15–2000	-319000	124.0509	45.23707	-0.00732285	1.861658	25.72751	-26.7394	39.61092	
AlN	g	298.15–3000	438530	307.9826	32.62139	-0.00060462	1.0388258	25.05068	29.55234	-64.15543	[4]
GaN	s	298.15–2000	-114000	160.2647	52.86351	-0.00799055	2.113389	1.313428	-2.441129	1.945731	
GaN	g	298.15–3000	221659	313.033	33.77197	-0.00212262	1.1675484	25.48238	-42.78832	36.53425	
InN	s	298.15–1400	-71000	182.0219	58.73762	-0.00885117	2.347111	2.118085	-2.740333	-1.525678	

Table 1s. Thermodynamic properties of elemental materials related to growth of group-III nitrides (ChemKin format).

Component	Phase	a1	a2	a3	a4	a5	a6	a7	reference
Al	s	0.19463122E+01	0.57014083E-02	-0.11246948E-04	0.11906191E-07	-0.40549592E-11	-0.75595051E+03	-0.89767193E+01	[4]
Al	l	0.38186714E+01	0.35092866E-13	-0.29243825E-16	0.10296049E-19	-0.13010214E-23	0.31529158E+03	-0.17522257E+02	[4]
Al	g	0.26386461E+01	-0.33361981E-03	0.29072954E-06	-0.10687702E-09	0.14019385E-13	0.39560925E+05	0.48317142E+01	[4]
Al ₂	g	0.40327689E+01	0.31080371E-02	-0.26555275E-05	0.10139488E-08	-0.14265000E-12	0.57660543E+05	0.42808346E+01	[4]
Ga	s	0.31516549E+01	0.47487811E-03	-0.13114719E-05	0.66957280E-09	-0.10309042E-12	0.31761301E+05	0.22722336E+01	[4]
Ga	l	0.37332207E+01	-0.14576218E-02	0.12593146E-05	-0.45013529E-09	0.58809512E-13	-0.78157088E+03	-0.13777782E+02	[4]
Ga	g	0.31516549E+01	0.47487811E-03	-0.13114719E-05	0.66957280E-09	-0.10309042E-12	0.31761301E+05	0.22722336E+01	[4]
In	s	0.28708331E+01	0.50895697E-03	0.23897104E-05	0	0	-0.89967232E+3	-0.96810646E+01	[4]
In	l	0.40047221E+01	-0.16093120E-02	0.12357138E-05	-0.40475261E-09	0.50565275E-13	-0.11326205E+04	-0.14615689E+02	[4]
In	g	0.17106240E+01	0.27284880E-02	-0.15237756E-05	0.24935117E-09	-0.13543811E-14	0.28294009E+05	0.10393415E+02	[4]
Cl	g	0.24863802E+01	0.85400259E-03	-0.10102948E-05	0.41513823E-090	-0.57351897E-13	0.13818230E+05	0.54745422E+01	[2]
Cl ₂	g	0.36723063E+01	0.19959920E-02	-0.17664869E-05	0.67118808E-09	-0.85427189E-13	-0.11692930E+04	0.53710238E+01	[2]
H	g	0.24999969E+01	0.40554262E-16	-0.69589660E-19	0.36480813E-22	-0.59810677E-26	0.25473925E+05	-0.46019397E+00	[2]
H ₂	g	0.35835513E+01	-0.50820648E-03	0.80582475E-06	-0.26671703E-09	0.28964961E-13	-0.10611936E+04	-0.45955646E+01	[2]
N	g	0.25022205E+01	-0.10929503E-04	0.17136711E-07	-0.10629382E-10	0.22781404E-14	0.56105014E+05	0.41705817E+01	[2]
N ₂	g	0.33489922E+01	0.22852471E-03	0.66433042E-06	-0.38603865E-09	0.60257282E-13	-0.10137940E+03	0.38564836E+01	[2]

Table 2s. Thermodynamic properties of group-III hydrides (ChemKin format).

Component	Phase	a1	a2	a3	a4	a5	a6	a7	reference
AlH	g	0.29920505E+01	0.19313058E-02	-0.89008762E-06	0.17659140E-09	-0.66198110E-14	0.28971460E+05	0.49959763E+01	[4]
AlH ₂	g	0.29899556E+01	0.49326258E-02	-0.25346247E-05	0.60656427E-09	-0.53207711E-13	0.28624960E+05	0.72437680E+01	[4]
AlH ₃	g	0.19873363E+01	0.11164632E-01	-0.65786378E-05	0.18095101E-08	-0.19009482E-12	0.23999886E+05	0.10457201E+02	[4]
GaH	g	0.29623752E+01	0.21304955E-02	-0.11056997E-05	0.27502882E-09	-0.23505502E-13	0.24805959E+01	0.65474670E+01	[4]
GaH ₂	g	0.29812282E+01	0.55323277E-02	-0.31765828E-05	0.84445499E-09	-0.85359368E-13	0.30282972E+05	0.85657017E+01	
GaH ₃	g	0.24500013E+01	0.10867555E-01	-0.66409192E-05	0.18952949E-08	-0.20627448E-12	0.15680233E+05	0.93830393E+01	
InH	g	0.29152219E+01	0.24766074E-02	-0.14984347E-05	0.44210391E-09	-0.47914809E-13	0.24856256E+05	0.76777967E+01	[4]
InH ₂	g	0.30615829E+01	0.60170750E-02	-0.38185434E-05	0.11155913E-08	-0.12315586E-12	0.35053547E+05	0.91236129E+01	
InH ₃	g	0.29241131E+01	0.10796226E-01	-0.69214730E-05	0.20533707E-08	-0.23055240E-12	0.25887243E+05	0.79935951E+01	

Table 3s. Thermodynamic properties of group-III chlorides (ChemKin format).

Component	Phase	a1	a2	a3	a4	a5	a6	a7	reference
GaCl	g	0.40828200E+01	0.10275066E-02	-0.82584758E-06	0.30159693E-09	-0.38982556E-13	-0.18930553E+05	0.53481325E+01	[4]
GaCl ₂	g	0.58256772E+01	0.27618590E-02	-0.24086603E-05	0.89405236E-09	-0.11624406E-12	-0.30854559E+05	0.22752045E+01	[4]
GaCl ₃	s	0.27254950E+01	0.29584829E-01	0	0	0	-0.65270941E+05	-0.82328905E+01	[4]
GaCl ₃	l	0.13109770E+02	0	0	0	0	-0.67257972E+05	-0.54894857E+02	[4]
GaCl ₃	g	0.81264039E+01	0.43397075E-02	-0.37045176E-05	0.13443762E-08	-0.17473299E-12	-0.54492248E+05	-0.83485211E+01	[4]
Ga ₂ Cl ₆	g	0.17907141E+02	0.95219173E-02	-0.81418255E-05	0.29569337E-08	-0.38442017E-12	-0.12086372E+06	-0.44330387E+02	[4]

Table 4s. Thermodynamic properties of group-III metal-organic compounds (ChemKin format).

Component	Phase	a1	a2	a3	a4	a5	a6	a7	reference
AlCH ₃	g	0.33152363E+01	0.10730808E-01	-0.53649153E-05	0.13219641E-08	-0.12963324E-12	0.69985773E+04	0.69088112E+01	
Al(CH ₃) ₃	g	0.32762275E+01	0.38648068E-01	-0.21169742E-04	0.57086106E-08	-0.60677829E-12	-0.13086231E+05	0.12164379E+02	
Al ₂ (CH ₃) ₆	g	0.77694495E+01	0.81503404E-01	-0.45707472E-04	0.12565890E-07	-0.13556605E-11	-0.37792596E+05	-0.66613696E+01	
GaCH ₃	g	0.25578342E+01	0.12336949E-01	-0.66536191E-05	0.17697148E-08	-0.18602651E-12	0.82459942E+04	0.11507155E+02	
Ga(CH ₃) ₂	g	0.31015884E+01	0.24665912E-01	-0.13279303E-04	0.35247826E-08	-0.36978377E-12	0.74707731E+04	0.13886280E+02	
Ga(CH ₃) ₃	g	0.19674198E+01	0.47163954E-01	-0.37019398E-04	0.17197050E-07	-0.34877739E-11	-0.78124671E+04	0.18869043E+02	
InCH ₃	g	0.32606827E+01	0.10945619E-01	-0.56676425E-05	0.14649582E-08	-0.15127365E-12	0.24447299E+05	0.92182406E+01	
In(CH ₃) ₃	g	0.43958263E+01	0.36932913E-01	-0.20120601E-04	0.54175515E-08	-0.57640580E-12	0.22113910E+05	0.89579139E+01	

Table 5s. Thermodynamic properties of compound species related to growth of group-III nitrides (ChemKin format). (*) Indexes s- and a- denotes the molecules C₂H₂ having different bond configurations: HC=CH and H₂C=C respectively.

Component	Phase	a1	a2	a3	a4	a5	a6	a7	reference
CH	g	0.36138827E+01	-0.82828147E-03	0.16896253E-05	-0.68730072E-09	0.89176108E-13	0.70792073E+05	0.15886242E+01	[3]
CH ₂	g	0.36456497E+01	0.95155874E-03	0.13138435E-05	-0.78153507E-09	0.11901737E-12	0.45817667E+05	0.23139800E+01	[3]
CH ₃	g	0.32140185E+01	0.49932545E-02	-0.10666071E-05	-0.94179151E-10	0.41825069E-13	0.16425353E+05	-0.32620959E+00	[3]
CH ₄	g	0.15216894E+01	0.94206100E-02	-0.20358736E-05	-0.16954382E-09	0.84231104E-13	-0.98265001E+04	0.11015042E+02	[3]
s-C ₂ H ₂ *	g	0.32873503E+01	0.84711075E-02	-0.47845151E-05	0.14062688E-08	-0.16380579E-12	0.26033038E+05	0.30977851E+01	[3]
a-C ₂ H ₂ *	g	0.37432140E+01	0.64649821E-02	-0.29878974E-05	0.67863179E-09	-0.61508807E-13	0.47452584E+05	0.36880757E+01	
C ₂ H ₄	g	0.51347290E+00	0.18255281E-01	-0.97529218E-05	0.25543735E-08	-0.26359173E-12	0.54190726E+04	0.18407655E+02	[3]
C ₂ H ₅	g	0.41356879E+00	0.19656915E-01	-0.92762870E-05	0.20790714E-08	-0.17976542E-12	0.11950162E+05	0.22444201E+02	[3]
C ₂ H ₆	g	0.14469981E+00	0.23658897E-01	-0.11545008E-04	0.27146353E-08	-0.24972355E-12	-0.11100895E+05	0.20160466E+02	[3]
HCl	g	0.35477617E+01	-0.52495759E-03	0.12539209E-05	-0.55704126E-09	0.77853020E-13	-0.12146858E+05	0.23571698E+01	[2]
HN ₃	g	0.30696955E+01	0.91823215E-02	-0.55000486E-05	0.16008807E-08	-0.18008554E-12	0.34082455E+05	0.87750511E+01	[2]
NH ₄ Cl	s	0.15779218E+02	-0.32826760E-01	0.68126014E-04	-0.42994252E-07	0.91512370E-11	-0.41599526E+05	-0.71376421E+02	[5]
NH ₃	g	0.28571756E+01	0.49698173E-02	-0.10459846E-05	-0.59616310E-10	0.33876824E-13	-0.65887633E+04	0.54578631E+01	[2]
NH ₂	g	0.36485140E+01	0.99709004E-03	0.11450996E-05	-0.67166863E-09	0.10319335E-12	0.21710932E+05	0.23089927E+01	[2]
NH	g	0.36081623E+01	-0.70482845E-03	0.13400834E-05	-0.56265529E-09	0.77335350E-13	0.39703545E+05	0.13808122E+01	[2]
N ₂ H ₂	g	0.22848311E+01	0.65332679E-02	-0.10485018E-05	-0.26377069E-09	0.67449391E-13	0.24519210E+05	0.11328618E+02	[2]
N ₂ H ₄	g	0.18125618E+01	0.16115998E-01	-0.90347623E-05	0.25420769E-08	-0.28283711E-12	0.10250740E+05	0.13915855E+02	[2]

Table 6s. Thermodynamic properties of adducts related to growth of group-III nitrides (ChemKin format).

Component	Phase	a1	a2	a	a4	a5	a6	a7	reference
Al-NH ₃	g	0.51515143E+01	0.58573417E-02	-0.16170505E-05	0.11451009E-09	0.12133096E-13	0.28286069E+05	-0.48274682E-01	
(Al-N) ₃	g	0.45513774E+01	0.24224744E-01	-0.19583472E-04	0.68617042E-08	-0.87066457E-12	-0.65417224E+05	0.37152416E+01	
MMA-NH	g	0.53000416E+01	0.15817580E-01	-0.89597704E-05	0.25398503E-08	-0.28426358E-12	-0.19047211E+05	-0.38015130E-01	
(MMA-NH) ₃	g	0.58446617E+01	0.78028253E-01	-0.51959593E-04	0.16480119E-07	-0.19828760E-11	-0.94988106E+05	0.64522837E+01	
TMA-NH ₃	g	0.63159729E+01	0.46337132E-01	-0.24201379E-04	0.62752490E-08	-0.64727423E-12	-0.33328111E+05	-0.89507418E+00	
(DMA-NH ₂) ₃	g	0.11133625E+02	0.12201319E+00	-0.75594693E-04	0.22848140E-07	-0.26665328E-11	-0.99526181E+05	-0.26267281E+02	
Ga-NH ₃	g	0.50415777E+01	0.60423017E-02	-0.17099375E-05	0.13220508E-09	0.11191167E-13	0.22297756E+05	0.14946460E+01	
(Ga-N) ₃	g	0.67417325E+01	0.20698420E-01	-0.17293197E-04	0.61883733E-08	-0.79656592E-12	-0.79656592E-12	-0.47959352E+01	
MMG-NH	g	0.54128110E+01	0.15466515E-01	-0.85993868E-05	0.23946771E-08	-0.26421186E-12	-0.14257212E+05	0.34268502E+00	
(MMG-NH) ₃	g	0.78421436E+01	0.75178598E-01	-0.50082986E-04	0.15895148E-07	-0.19139941E-11	-0.67809637E+05	-0.17042245E+01	
TMG-NH ₃	g	0.72199138E+01	0.43905101E-01	-0.21992163E-04	0.54490488E-08	-0.53816240E-12	-0.24366705E+05	-0.51898207E+01	
(DMG-NH ₂) ₃	g	0.87149890E+01	0.12611576E+00	-0.78186312E-04	0.23569819E-07	-0.27410200E-11	-0.70701723E+05	-0.15101017E+02	
(DMA-NH ₂) ₂ (DMG-NH ₂)	g	0.73936341E+01	0.13562588E+00	-0.92917003E-04	0.31735301E-07	-0.42292280E-11	-0.89258078E+05	-0.90006738E+01	
(DMA-NH ₂) (DMG-NH ₂) ₂	g	0.97937059E+01	0.12425531E+00	-0.76968702E-04	0.23215922E-07	-0.27027562E-11	-0.79971211E+05	-0.20135984E+02	
GaCl ₃ -NH ₃	g	0.99445135E+01	0.14131038E-01	-0.81793973E-05	0.23593607E-08	-0.26734087E-12	-0.77974368E+05	-0.15271713E+02	

Table 7s. Thermodynamic properties of group-III nitrides (ChemKin format).

Component	Phase	a1	a2	a3	a4	a5	a6	a7	reference
AlN	s	0.16484984E+00	0.16906333E-01	-0.19156391E-04	0.95997888E-08	-0.17389262E-11	-0.39016612E+05	-0.27932794E+01	
AlN	g	0.35951625E+01	0.12581327E-02	-0.17178569E-06	-0.42709248E-10	0.83346116E-14	0.51617150E+05	0.66104571E+01	[4]
GaN	s	0.51341560E+00	0.18306308E-01	-0.21633569E-04	0.11081026E-07	-0.20603428E-11	-0.14507663E+05	-0.31255765E+01	
GaN	g	0.31180378E+01	0.28153203E-02	-0.22191154E-05	0.76417778E-09	-0.95775476E-13	0.25622984E+05	0.93780951E+01	
InN	s	-0.17387340E+01	0.34314485E-01	-0.52155647E-04	0.35199074E-07	-0.87726745E-11	-0.91507858E+04	0.70544505E+01	

SUPPLEMENTARY MATERIALS

Datafile #1 (available at <http://data1.txt>): Specific heat of solid AlN as a function of temperature

Datafile #2 (available at <http://data2.txt>): Specific heat of solid AlN as a function of temperature [22].

Datafile #3 (available at <http://data3.txt>): Total pressure of gaseous species measured by torsion method

Datafile #4 (available at <http://data4.txt>): Specific heat of solid GaN as a function of temperature

Datafile #5 (available at <http://data5.txt>): Total pressure of gaseous species measured by torsion method