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A BINARY DATABASE FOR III-V COMPOUND SEMICONDUCTOR SYSTEMS

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Abstract

A thermodynamic database for binary III-V semiconductor systems has been compiled. It is based upon individual assessments which have been or will be published separately, but each assessment is based on the SGTE recommendation for the pure elements and uses the same solution model expression. The 15 possible binary systems between the group III elements Al, Ga and In on one hand, and the group V elements As, Sb and P are included.

Introduction

The group III-V compound semiconductors and their solid solutions are important materials used in optoelectronic and high speed electronic device applications. The fabrication of these devices can involve processes that require contact between the solid and a fluid phase at near equilibrium conditions. Examples of processes that involve contact between the solid and liquid phases include bulk crystal growth and liquid phase epitaxy, and between the solid and vapour phases include chemical vapour deposition, molecular beam expitaxy and rapid thermal annealing. Therefore, knowledge of the phase diagrams and thermochemistry for these semiconductor systems is important for providing boundary conditions in the analysis of a variety of processing steps.

The collection, assessment and recommendation of thermodynamic properties for a material system of this size is a significant task. Though databases have been previously published by several investigators for group III–V systems [1, 2, 3], additional experimental measurements have been reported for many systems that modify the conclusions of the previous databases. In addition to these databases, there have been several excellent assessments of selected systems reported in the literature. Given the important objective of predicting the equilibrium behaviour of higher order systems, combining the results of these independent assessments

[1] A. Leonhardt, and G. Kühn, J. Less-Common Metals, 39, 247-264 (1975)
[2] L. Kaufman, J. Nell, K. Taylor, and F. Hayes, Calphad, 5, 3, 185-215 (1981)
[3] K. Ishida, H. Tokunaga, H. Ohtani, and T. Nishizawa, J. Cryst. Growth, 98, 140-147 (1989)

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is difficult since different solution models and reference state properties have often been used.

For these reasons, an international collaboration was initiated to develop a consistent thermodynamic database for the binary III-V semiconductor systems. Though the database consists of the contributions from individual assessments, each of them used the same model description for the solution phases, the same expression for the temperature dependence of the Gibbs energies of the compounds, and the SGTE recommendation for the thermodynamic properties of the elements [4]. The database includes all nine binary systems between Al, Ga and In on one hand, and P, As and Sb on the other hand, as well as the six related III-III and V-V systems. Values of the parameters for the solution models and the Gibbs energy expressions are represented together with the assessed phase diagram. In addition, the partial pressures of the species in equilibrium with the liquid and compound phases are presented for the nine III-V systems.

Thermodynamic Description

Elements

The Gibbs energy of the pure element i, ${}^{\circ}G_i^{\phi}(T)$, referred to the enthalpy for its stable state ϕ at 298.15K, ${}^{\circ}H_i^{\phi}(298.15K)$, is denoted by $GHSER_i$. This quantity is described as a function of temperature by the following equation:

$$\begin{aligned} GHSER_i &= {}^{\circ}G_i^{\phi}(T) - {}^{\circ}H_i^{\phi}(298.15K) \\ &= a + b\,T + c\,T ln T + d\,T^2 + e\,T^3 + f\,T^{-1} + g\,T^7 + h\,T^{-9} \end{aligned} \quad (1)$$

The coefficients of the above expression (a through h) for each element are taken from the SGTE database[4].

The same functional form is also used to represent the same element that is in a solution with a structure φ^* different from the structure of the pure stable element. The expression ${}^{\circ}G_i^{\varphi^*}(T) - {}^{\circ}H_i^{\phi}(298.15K)$ is equivalent to ${}^{\circ}G_i^{\varphi^*}(T) - {}^{\circ}G_i^{\phi}(T) + GHSER_i$. The term ${}^{\circ}G_i^{\varphi^*}(T) - {}^{\circ}G_i^{\phi}(T)$ is often called the lattice stability of element *i*.

The coefficients for the expressions of the Gibbs energies of the six pure elements are given in Appendix I. It should be noted that for phosphorous, the P(white) phase at 298.15K, has been chosen as the reference state.

Binary Compounds

The only solid phase compounds that form in these 15 binary systems are the III-V compounds (e.g., GaAs, InSb) with the zinc blende structure. The Gibbs energy of formation of the compound $A_{0.5}B_{0.5}$ is expressed as:

[4] A. T. Dinsdale, Calphad, 15, 4, 317-425 (1991)

$$G_{A_{0.5}B_{0.5}} - 0.5\ {}^{\circ}H_A^{\phi}(298.15K) - 0.5\ {}^{\circ}H_B^{\phi}(298.15K) = f(T) \qquad (2)$$

The expression for $f(T)$ is identical to that given by equation 1.

Equation 2 can be transformed by applying equation 1 for each component

$$\begin{aligned} f(T) &= G^T_{A_{0.5}B_{0.5}} - 0.5\ {}^{\circ}G_A^{\phi,T} - 0.5\ {}^{\circ}G_B^{\phi,T} + 0.5\,GHSER_A + 0.5\,GHSER_B \\ &= \Delta_f G^T_{A_{0.5}B_{0.5}} + 0.5\,GHSER_A + 0.5\,GHSER_B \end{aligned} \qquad (3)$$

The term $\Delta_f G^T_{A_{0.5}B_{0.5}}$ is the Gibbs energy of formation of the compound referred to the stable elements at T. The Gibbs energy of formation for each compound is listed, after the table of invariant reactions for each III-V system, in units of joule per mole of atoms.

Gaseous species

An expression identical to equation 2 is used to describe the Gibbs energy of formation of the gaseous species with the additional $RT\ \ln P$ term, where P is the total pressure. The gas phase is assumed to form an ideal solution. The reference state for each vapor species is taken to be the pure component at 0.1 MPa pressure. The thermodynamic properties of the vapour species used in this calculation are summarized in Appendix II.

Liquid and Solid Solutions

The excess Gibbs energy of a binary solution phase ϕ, ${}^{E}G_m^{\phi}$, is described by the Redlich-Kister equation [5] which is expressed as follows:

$${}^{E}G_m^{\phi} = x_i x_j \sum_{\nu=0}^{n} {}^{\nu}L_{ij}^{\phi}\,(x_i - x_j)^{\nu} \qquad (4)$$

where x_i and x_j are the mole fractions of components i and j, and the model parameter ${}^{\nu}L_{ij}$ can be temperature dependent. The assessed values of these parameters are listed below each phase diagram.

The chemical potential of component i, derived from equation 4, is then equal to

$$\mu_i - {}^{\circ}\mu_i^{ref} = RT ln a_i = RT ln x_i + {}^{E}G_m^{\phi} + (1 - x_i)\partial {}^{E}G_m^{\phi}/\partial x_i \qquad (5)$$

where a_i is the activity of component i referred to the pure component at the temperature and phase of the solution.

[5] O. Redlich and A. Kister, Ind. Eng. Chem., 40, 345-348 (1948)

The partial pressures $p_{A_iB_j}$ of the various species A_iB_j existing in the gaseous phase are related to the activity of the components of the binary phase by the following equation:

$$p_{A_iB_j} = a_A^i \cdot a_B^j \cdot K_p \tag{6}$$

where K_p represents the equilibrium constant corresponding to the formation of the gaseous species from the elements.

The same reference state for the condensed and gaseous phases is used. For the binary systems for which the values of plots $lnp_{A_iB_j}$ are represented versus $1/T$, the reference state pressure is taken as 0.1 MPa.

Results

Standard CALPHAD procedures were used to assess the 15 binary systems amongst the elements Al, Ga, In, P, As and Sb. The importance of the III-V systems to electronic and optoelectronic industries has resulted in considerable experimental investigations of the phase diagram and thermodynamic properties for most of these systems. Similarly, the group III-III systems are well studied, primarily motivated by metallurgical applications. The group V-V systems, however, are experimentally difficult systems and the database is small.

Each system was fully assessed with a detailed description of the database and conclusions givent in a separate report, as cited below. The figures and properties given in this report include:

- the calculated solid - liquid equilibrium phase diagram
- the thermodynamic properties of the compound and solution phases
- for the III-V systems, a figure presenting values of $lnpA_iB_j = f(1/T)$ for the various gaseous species A_iB_j
- for the III-V systems, a calculated temperature - composition phase diagram at a constant pressure, P = 0.1 MPa, including the gas phase

Acknowledgements

The assessments were performed by the different contributors either with the optimization program developed by Lukas *et al.* [6, 7], or with Parrot developed by Jansson [8]. All the diagrams have been calculated with Thermo-Calc [9].

[6] H.L. Lukas, B. Zimmerman, and E.-Th. Henig, Calphad, 1, 225-236 (1977) 6, and 229-251 (1982)

[7] H.L.Lukas, and S. Fries, J. Phase Equil., 13, 5, 532-541 (1992).

[8] B. Jansson, Ph.D. Thesis, KTH, Stockholm, Sweden (1983).

[9] B. Sundman, B. Jansson and J. O. Andersson, Calphad 9, 153-190 (1985).

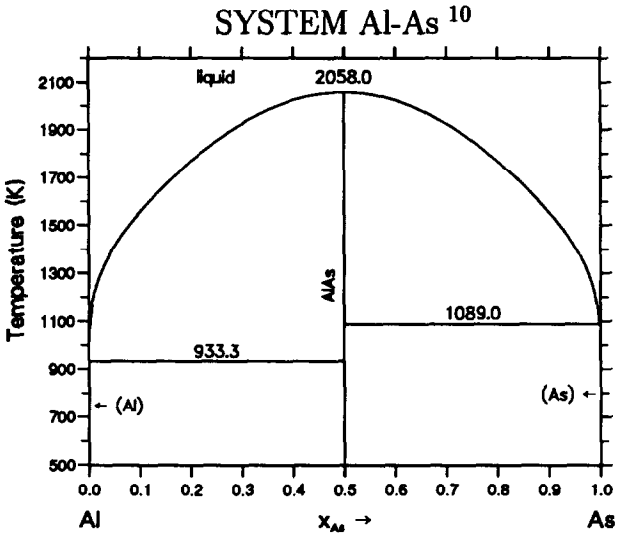

Figure 1: Calculated phase diagram of the Al–As system.

Invariant Reactions.

Reaction	*Type*	*Compositions* x_{As}			$T(K)$
liquid ⇌ *(Al)* + *AlAs*	*Degenerate*	0.000	0.000	0.500	933.3
liquid ⇌ *AlAs* + *(As)*	*Degenerate*	0.998	0.500	1.000	1089.0
liquid ⇌ *AlAs*	*Congruent*	0.500	.....	.....	2058.0

Thermodynamic properties of the compound and solution phases in the Al–As system ($J.mol^{-1}$)

Phase AlAs

$${}^{\circ}G^{Zincblende}_{Al_{0.5}As_{0.5}}(T) - 0.5\ {}^{\circ}H^{fcc-A1}_{Al}(298.15K) - 0.5\ {}^{\circ}H^{rhombo-A7}_{As}(298.15K) = - 58565 + 3.89\ T + 0.5\ GHSER_{Al} + 0.5\ GHSER_{As}$$

Phase Liquid

$${}^{0}L^{liq}_{Al,As} = - 15693.0 - 34.163\ T$$

[10] I. Ansara, and D. Dutartre, Calphad, 8, 4, 323-342 (1984)

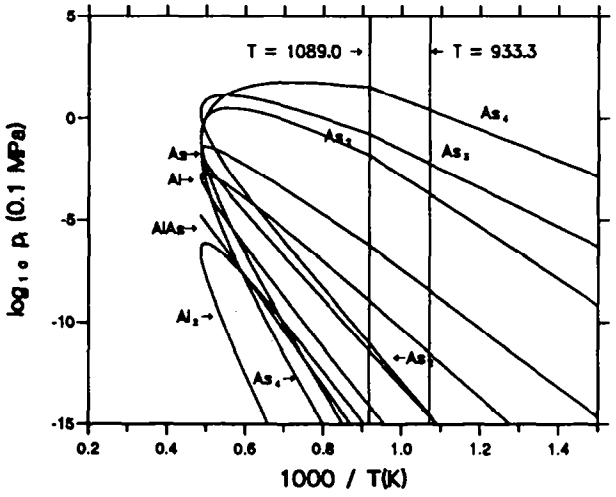

Figure 2: Calculated partial pressures of the various species in the gaseous phase along the equilibrium lines.

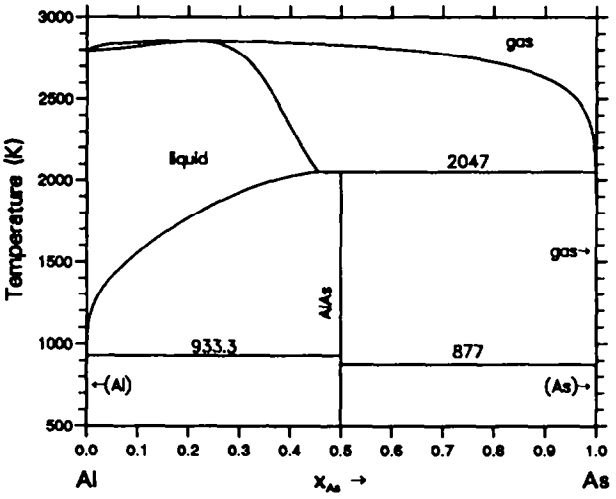

Figure 3: Calculated phase diagram at 0.1 MPa.

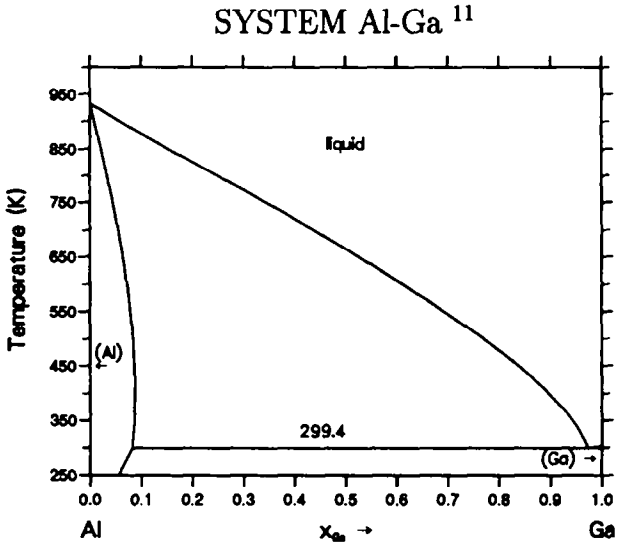

Figure 4: Calculated phase diagram of the Al–Ga system.

Table I - Invariant Reactions.

Reaction	*Type*	*Compositions* x_{Ga}			$T(K)$
liquid $\rightleftharpoons$ *(Al) + (Ga)*	*Eutectic*	0.974	0.082	1.000	299.4

Thermodynamic properties of the solution phases in the Al–Ga system ($J.mol^{-1}$)

Phase Al (fcc-A1)

$${}^{0}L^{fcc-Al}_{Al,Ga} = 9195.8 + 8.18764\ T$$
$${}^{1}L^{fcc-Al}_{Al,Ga} = -\ 7678.5$$

Phase Liquid

$${}^{0}L^{liq}_{Al,Ga} = 2613.3 - 2.94533\ T$$
$${}^{1}L^{liq}_{Al,Ga} = 692.4 - 0.09271\ T$$
$${}^{2}L^{liq}_{Al,Ga} = 319.5$$

[11] A. Watson, Calphad, 16, 2, 207-217 (1992)

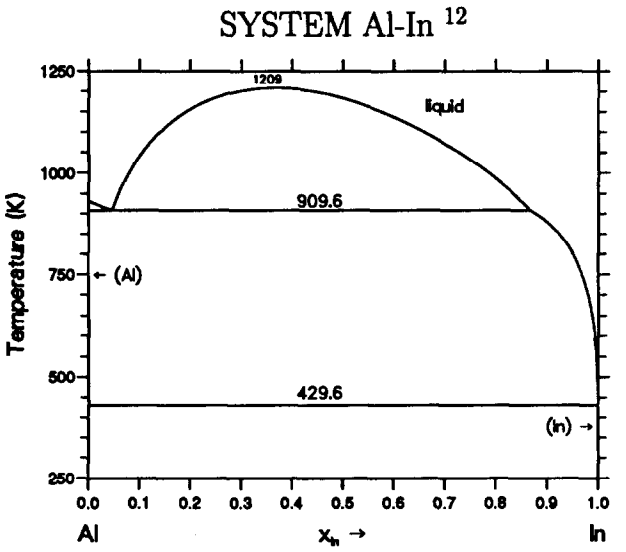

Figure 5: Calculated phase diagram of the Al–In system.

Invariant Reactions.

Reaction	*Type*	*Compositions* x_{In}			$T(K)$
$liquid(1) \rightleftharpoons (Al) + liquid(2)$	*Monotectic*	0.046	0.000	0.866	909.6
$liquid \rightleftharpoons (Al) + (In)$	*Degenerate*	1.000	0.000	1.000	429.6
	Critical point	0.361	.....	.....	1209.0

Thermodynamic properties of the liquid phase in the Al–In system ($J.mol^{-1}$)

Phase Liquid

$$^{0}L^{liq}_{Al,In} = 21259.6 - 0.48737\ T$$
$$^{1}L^{liq}_{Al,In} = 3850.3 - 1.20564\ T$$
$$^{2}L^{liq}_{Al,In} = 5479.2 - 3.16805\ T$$

[12]C.A.Coughanowr, Ph.D Thesis, University of Florida U.S.A., 1989)

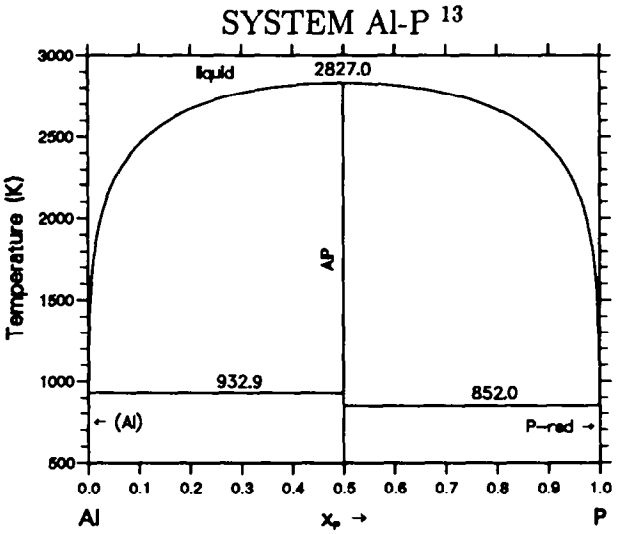

Figure 6: Calculated phase diagram of the Al–P system.

Invariant Reactions.

Reaction	*Type*	*Compositions* x_P			$T(K)$
$liquid \rightleftharpoons (Al) + AlP$	*Degenerate*	0.000	0.000	0.500	932.9
$liquid \rightleftharpoons AlP + P - red$	*Degenerate*	0.999	0.500	1.000	852.0
$liquid \rightleftharpoons AlP$	*Congruent*	0.500	.....	.....	2827.0

Thermodynamic properties of the solution and compound phases in the Al–P system ($J.mol^{-1}$)

Phase AlP

$${}^{\circ}G^{Zincblende}_{Al_{0.5}P_{0.5}}(T) - 0.5\ {}^{\circ}H^{fcc-Al}_{Al}(298.15K) - 0.5\ {}^{\circ}H^{white}_{P}(298.15K) =$$
$$- 68243.51 - 240.02438\ T + 23.054000\ T\ \ln T - 1.433000E\text{-}3\ T^2 + 105650\ T^{-1}$$

Phase Liquid

$${}^{0}L^{liq}_{Al,P} = - 209476.90 + 64.70238\ T$$

[13] H.L. Lukas, private communication

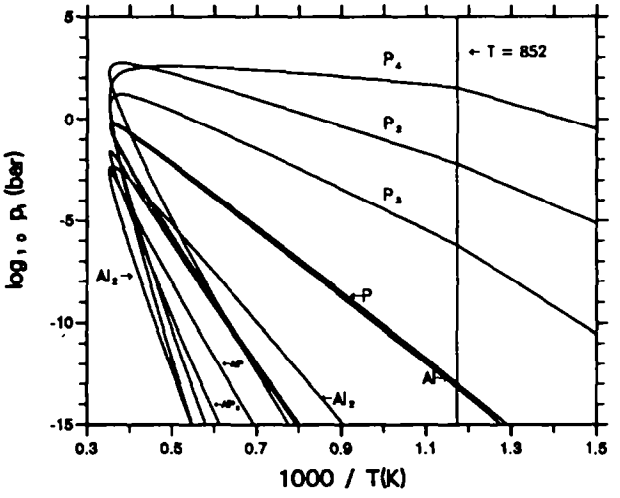

Figure 7: Calculated partial pressures of the various species in the gaseous phase along the equilibrium lines.

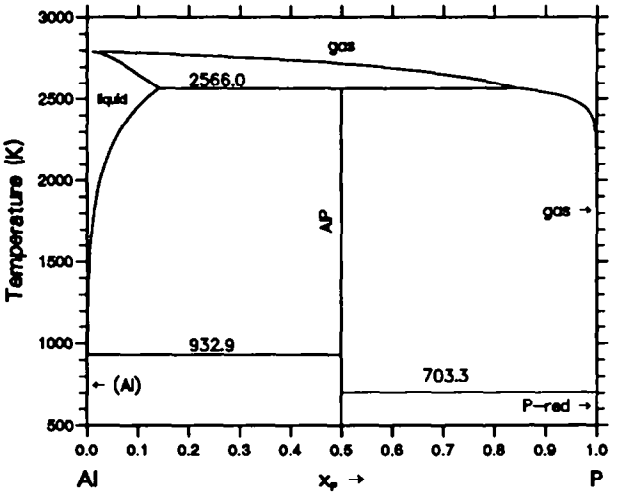

Figure 8: Calculated phase diagram at 0.1 MPa.

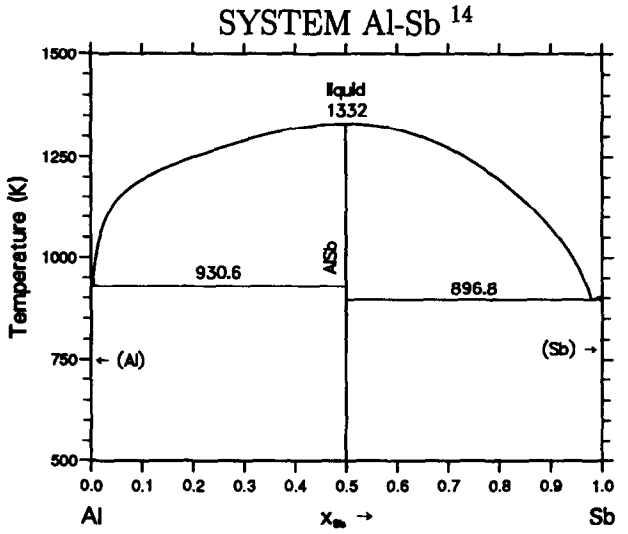

Figure 9: Calculated phase diagram of the Al–Sb system.

Invariant Reactions.

Reaction	*Type*	*Compositions* x_{Sb}			*T(K)*
liquid ⇌ *(Al) + AlSb*	*Eutectic*	0.004	0.000	0.500	930.6
liquid ⇌ *AlSb + (Sb)*	*Eutectic*	0.979	0.500	1.000	896.8
liquid ⇌ *AlSb*	*Congruent*	0.500	.....	.....	1332.0

Thermodynamic properties of the solution and compound phases in the Al–Sb system ($J.mol^{-1}$)

Phase AlSb

$$^{\circ}G^{Zincblende}_{Al_{0.5}Sb_{0.5}}(T) - 0.5\ ^{\circ}H^{fcc-A1}_{Al}(298.15K) - 0.5\ ^{\circ}H^{rhombo-A7}_{Sb}(298.15K) = 0.5\ GHSER_{Al} + 0.5\ GHSER_{Sb} - 24486.0 + 7.528437\ T - 0.827827\ T\ lnT + 2.6797E{-}03\ T^2$$

Phase Liquid

$$^{0}L^{liq}_{Al,Sb} = -41894.5 + 185.6213\ T - 22.67728\ T\ lnT$$
$$^{1}L^{liq}_{Al,Sb} = 5685.8 + 1.93333\ T \qquad ^{2}L^{liq}_{Al,Sb} = 17158.5 - 9.54781\ T$$

[14] C.A. Coughanowr, U.R. Kattner, and T.J. Anderson, Calphad, 14, 2, 193-303 (1990)

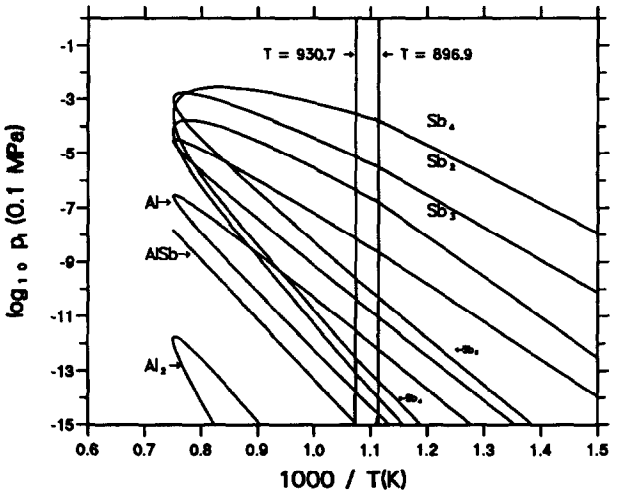

Figure 10: Calculated partial pressures of the various species in the gaseous phase along the equilibrium lines.

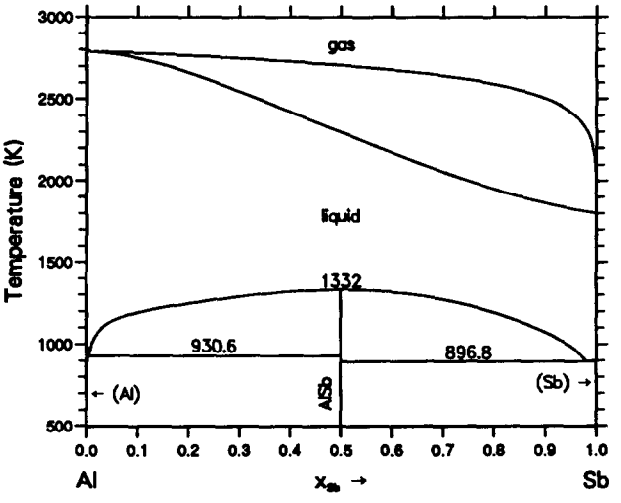

Figure 11: Calculated phase diagram at 0.1 MPa.

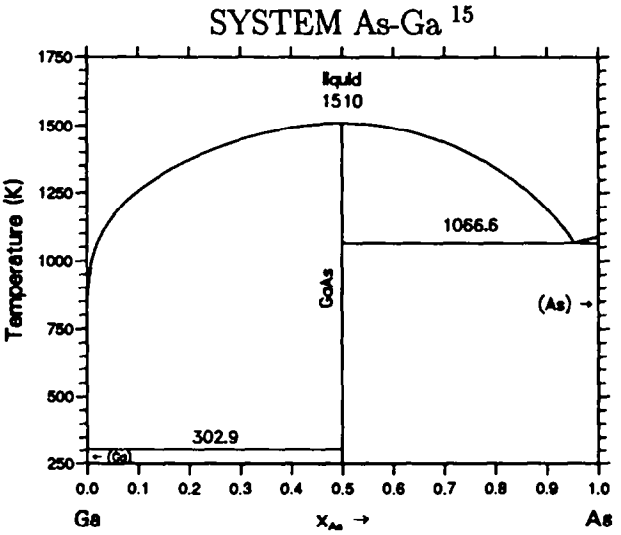

Figure 12: Calculated phase diagram of the As–Ga system.

Invariant Reactions.

Reaction	*Type*	*Compositions* x_{As}			*T(K)*
liquid ⇌ *(Ga)* + *GaAs*	*Degenerate*	0.000	0.000	0.500	302.9
liquid ⇌ *GaAs* + *(As)*	*Eutectic*	0.953	0.500	1.000	1066.6
liquid ⇌ *GaAs*	*Congruent*	0.500	.....	.....	1510.0

Thermodynamic properties of the solution and compound phases in the As–Ga system ($J.mol^{-1}$)

Phase GaAs

$${}^{\circ}G^{Zincblende}_{As_{0.5}Ga_{0.5}}(T) - 0.5\ {}^{\circ}H^{orthorhombic}_{Ga}(298.15K) - 0.5\ {}^{\circ}H^{rhombo-A7}_{As}(298.15K) =$$
$$- 52176 + 132.71628\ T - 24.340629\ T\ lnT - 0.0005579\ T^2 + 63835.0\ T^{-1}$$
$$- 3.5689E\text{-}7\ T^3$$

Phase Liquid

$${}^{0}L^{liq}_{As,Ga} = - 25503.6 - 4.3109\ T \qquad {}^{1}L^{liq}_{As,Ga} = - 5174.7$$

[15] C. Chatillon, I. Ansara, A. Watson, and B.B.Argent, Calphad, 14,2, 203-214(1990)

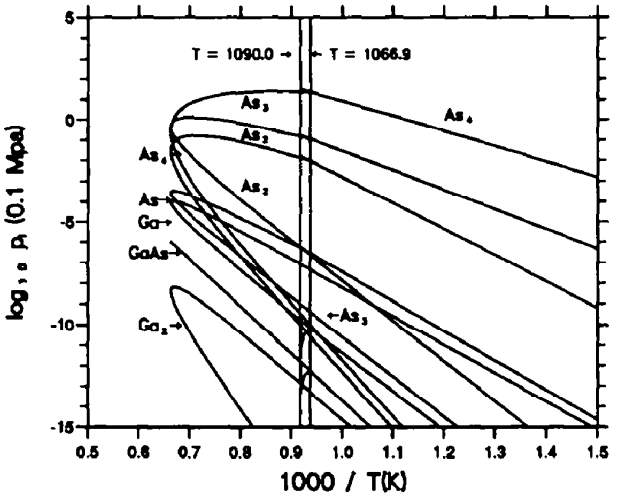

Figure 13: Calculated partial pressures of the various species in the gaseous phase along the equilibrium lines.

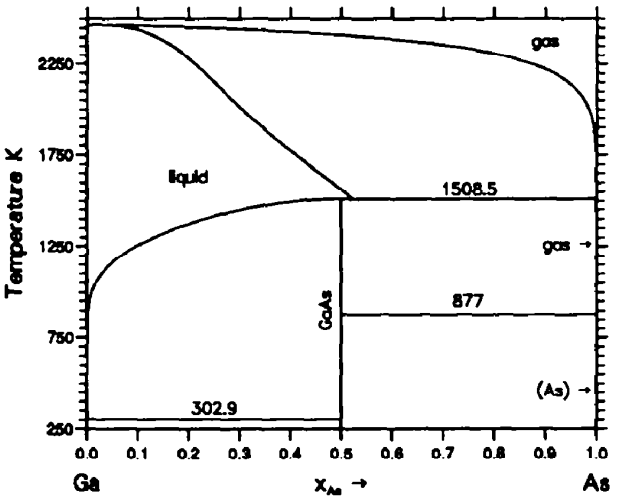

Figure 14: Calculated phase diagram at 0.1 MPa.

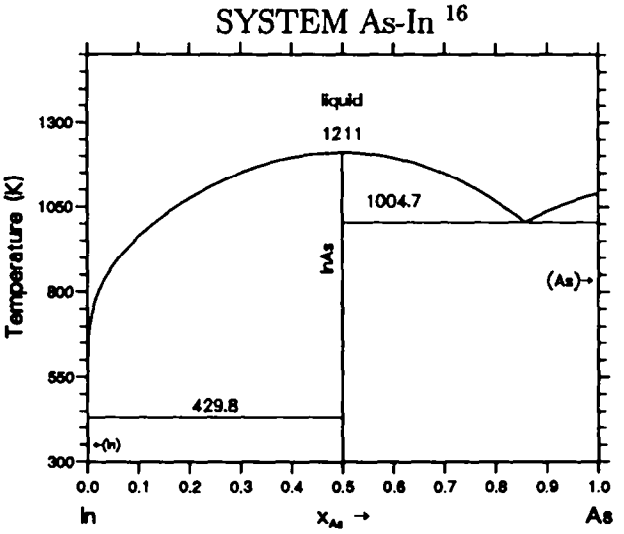

Figure 15: Calculated phase diagram of the As–In system.

Invariant Reactions.

Reaction	*Type*	*Compositions* x_{As}			*T(K)*
liquid ⇌ *(In) + InAs*	*Degenerate*	0.000	0.000	0.500	429.8
liquid ⇌ *InAs + (As)*	*Eutectic*	0.857	0.500	1.000	1004.7
liquid ⇌ *InAs*	*Congruent*	0.500	.....	.....	1211.0

Thermodynamic properties of the solution and compound phases in the As–In system ($J.mol^{-1}$)

Phase InAs

$${}^{\circ}G^{Zincblende}_{As_{0.5}In_{0.5}}(T) - 0.5\ {}^{\circ}H^{bct-A6}_{In}(298.15K) - 0.5\ {}^{\circ}H^{rhombo-A7}_{As}(298.15K) =$$
$$- 36528.6 + 115.45948\ T - 22.593971\ T\ lnT - 0.003865\ T^2 + 34719.0\ T^{-1}$$
$$+ 7.09E\text{-}8\ T^3$$

Phase Liquid

$${}^{0}L^{liq}_{As,In} = - 15851.0 - 11.27053\ T \qquad {}^{1}L^{liq}_{As,In} = - 1219.5$$

[16] C. Chatillon, I. Ansara, A. Watson, and B.B.Argent, Calphad, 14,2, 203-214(1990)

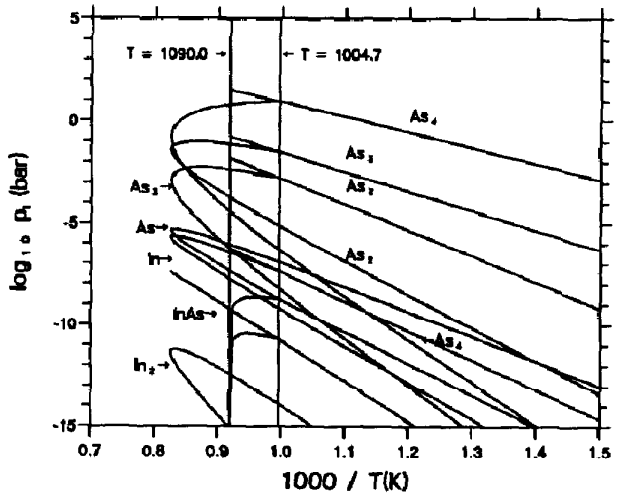

Figure 16: Calculated partial pressures of the various species in the gaseous phase along the equilibrium lines.

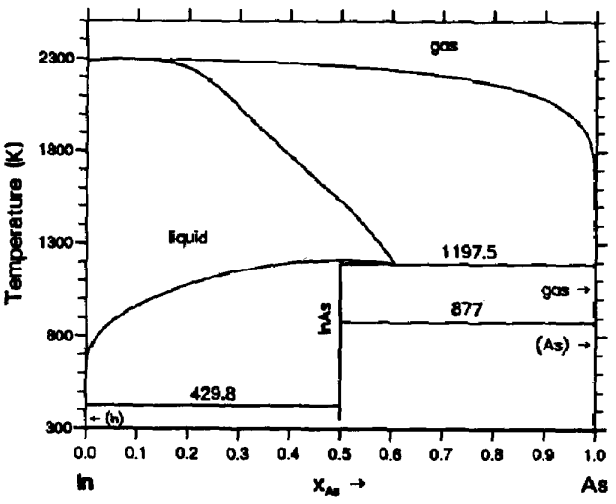

Figure 17: Calculated phase diagram at 0.1 MPa.

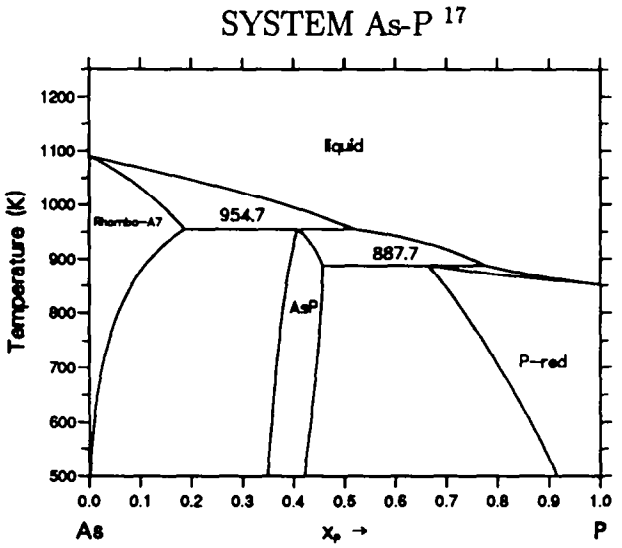

Figure 18: Calculated phase diagram of the As–P system.

Invariant Reactions.

Reaction	*Type*	*Compositions* x_P			$T(K)$
Liquid + *Rhombo* − *A7* ⇌	*Peritectic*	0.521	0.187	0.408	954.7
Liquid + *AsP* ⇌ *P* − *red*	*Peritectic*	0.775	0.457	0.663	887.7

Thermodynamic properties of the solution phases in the As–P system ($J.mol^{-1}$)

Phase Rhombo-A7 : ${}^0L^{rhombo-A7}_{As,P}$ = 106922

Phase Liquid : ${}^0L^{liq}_{As,P}$ = 4014.47

: ${}^1L^{liq}_{As,P}$ = 1780.77

Phase P-red : ${}^0L^{P-red}_{As,P}$ = 3453.04

Phase AsP : ${}^0L^{AsP}_{As,P}$ = − 66342.56 + 21.986 T

[17] I. Ansara, and C. Chatillon

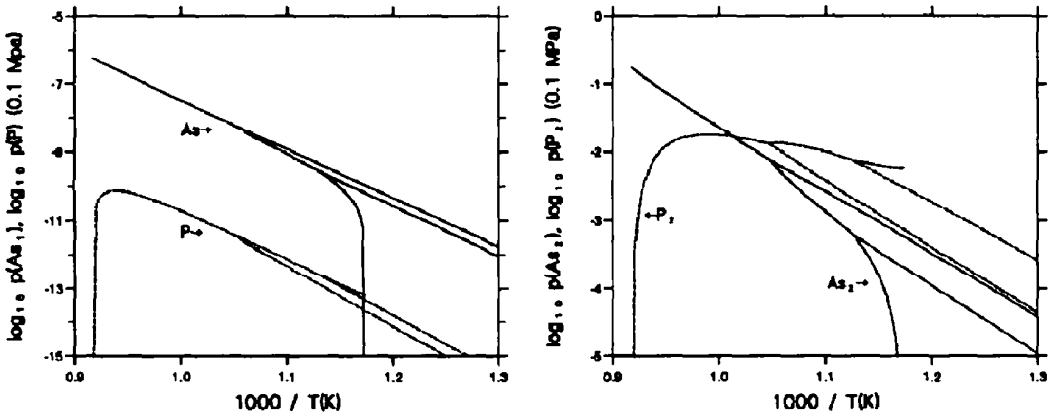

Figure 19: Partial pressures: a) As and P, b) As_2 and P_2.

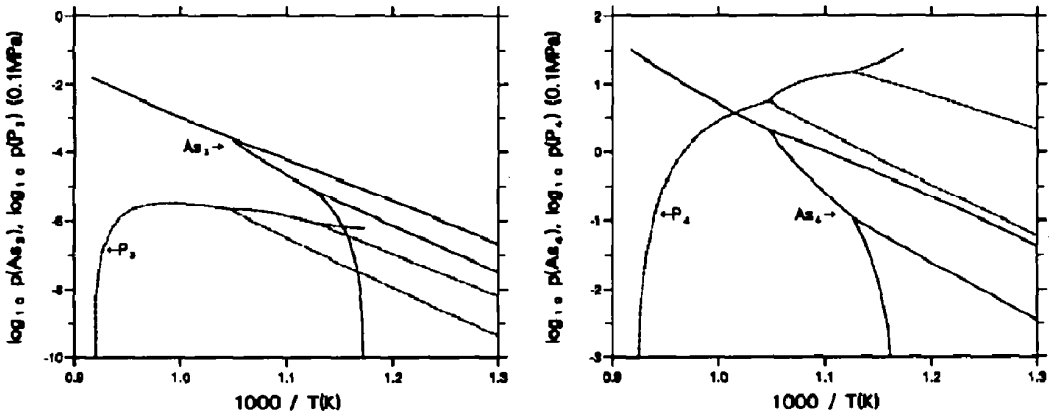

Figure 20: Partial pressures: c) As_3 and P_3 d) As_4 and P_4.

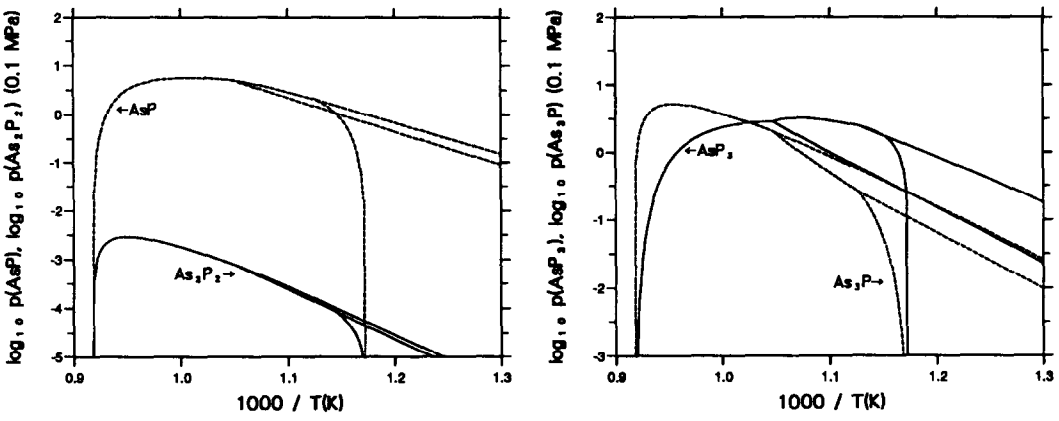

Figure 21: Partial pressures: e) AsP and As_2P_2 , f) As_3P and AsP_3.

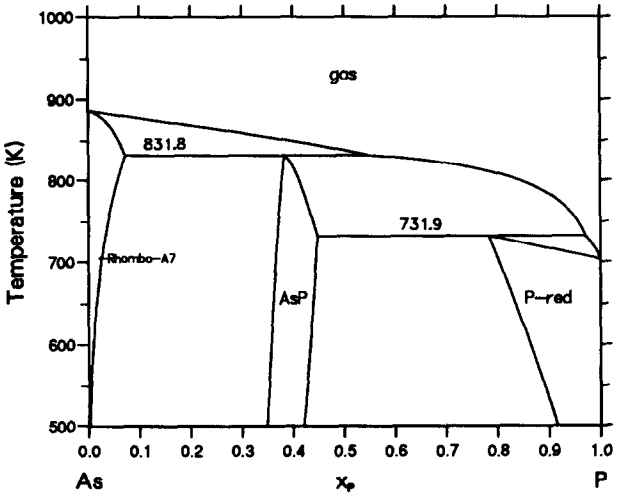

Figure 22: Calculated phase diagram at 0.1 MPa.

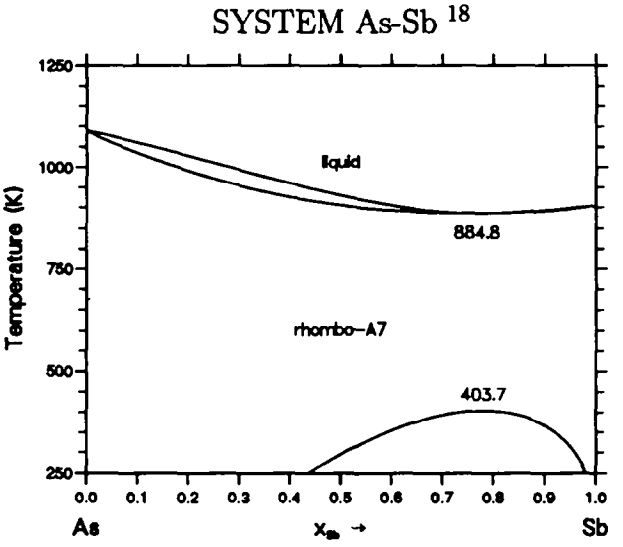

Figure 23: Calculated phase diagram of the As–Sb system.

Invariant Reactions.

Reaction	*Type*	*Compositions* x_{Sb}	$T(K)$
liquid $\rightleftharpoons$ *rhombo* – *A7*	*Congruent*	0.773	884.8
	Critical point	0.775	403.7

Thermodynamic properties of the solution phases in the As–Sb system ($J.mol^{-1}$)

Phase Rhombo-A7

$${}^{0}L^{rhombo-A7}_{As,Sb} = 2176.3 - 3.2164\ T$$
$${}^{1}L^{rhombo-A7}_{As,Sb} = -5300.0$$

Phase Liquid

$${}^{0}L^{liq}_{As,Sb} = -16197.1 + 8.9167\ T$$
$${}^{1}L^{liq}_{As,Sb} = -5018.$$

[18] H. Ohtani, private commuication

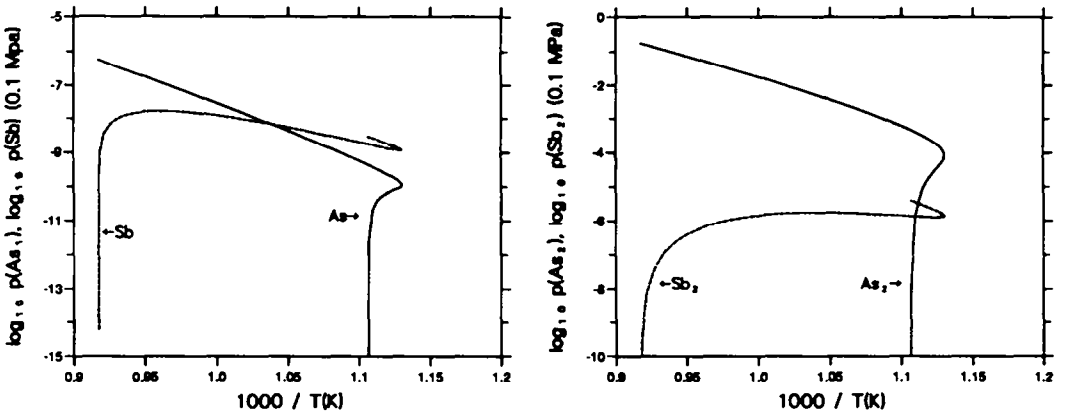

Figure 24: Partial pressures: a) As and Sb, b) As_2 and Sb_2.

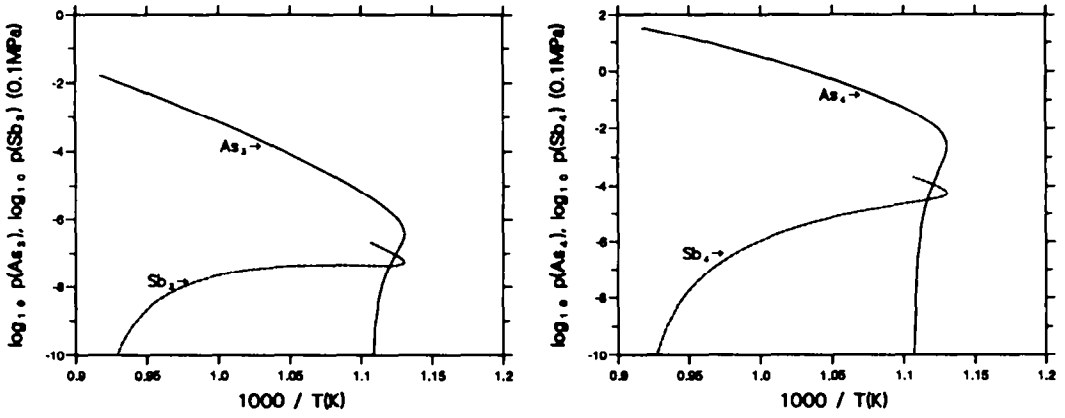

Figure 25: Partial pressures: c) As_3 and Sb_3 d) As_4 and Sb_4.

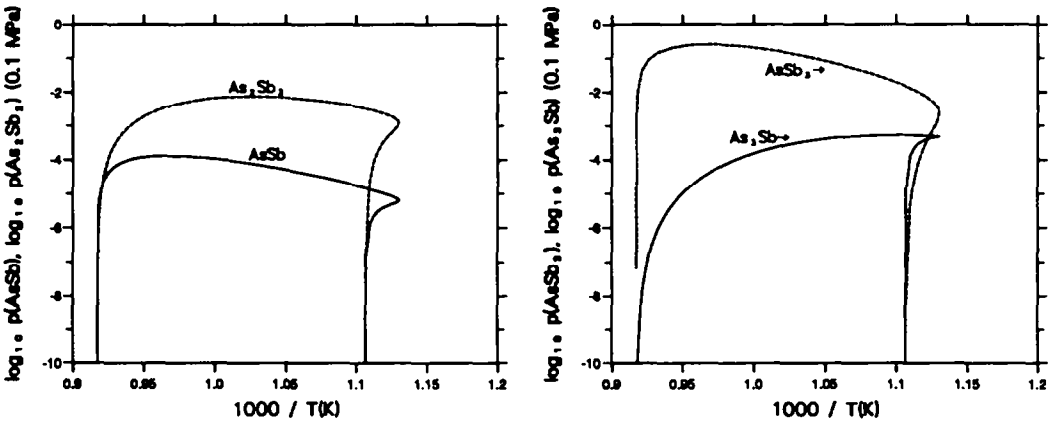

Figure 26: Partial pressures: e) AsSb and As_2Sb_2 , f) As_3Sb and $AsSb_3$.

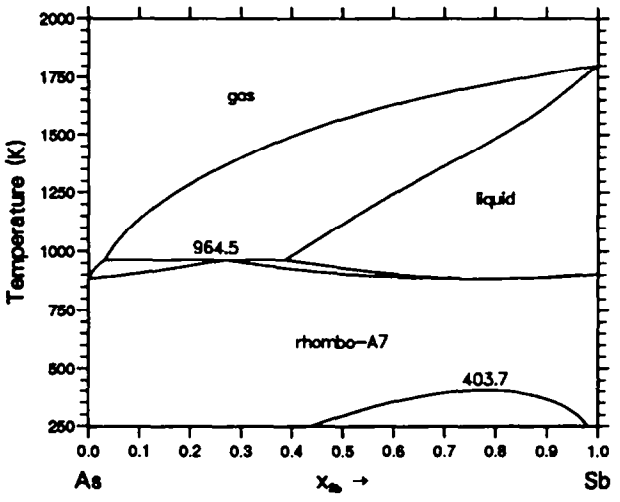

Figure 27: Calculated phase diagram at 0.1 MPa.

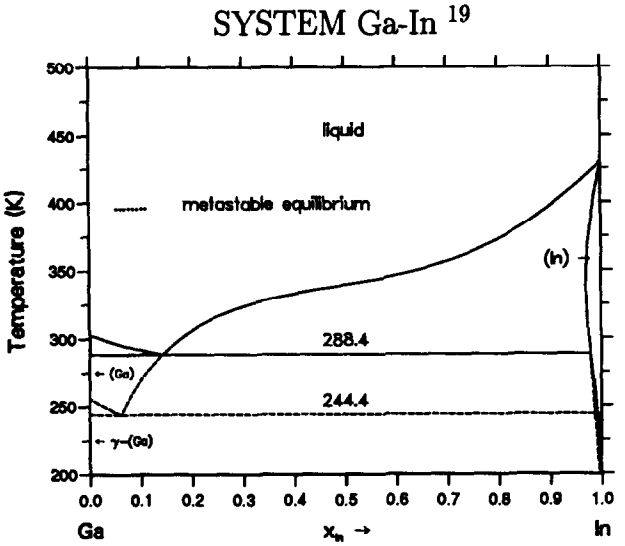

Figure 28: Calculated phase diagram of the Ga–In system.

Invariant Reactions.

Reaction	*Type*	*Compositions* x_{In}			$T(K)$
liquid $\rightleftharpoons$ $(Ga) + (In)$	*Eutectic*	0.142	0.000	0.979	288.4
liquid $\rightleftharpoons$ $(Ga) - \gamma + (In)$ *(metastable)*	*Eutectic*	0.062	0.000	0.987	244.4

Thermodynamic properties of the solution phases in the Ga–In system (J.mol–1)

Phase In (bct-A6)

$${}^{0}L^{bct-A6}_{Ga,In} = 9000.0$$

Phase Liquid

$${}^{0}L^{liq}_{Ga,In} = 4450.0 + 1.19185\ T$$
$${}^{1}L^{liq}_{Ga,In} = 0.25943\ T$$

[19] T.J. Anderson, and I. Ansara, J. Phase Equil., 12, 1, 64-72 (1991)

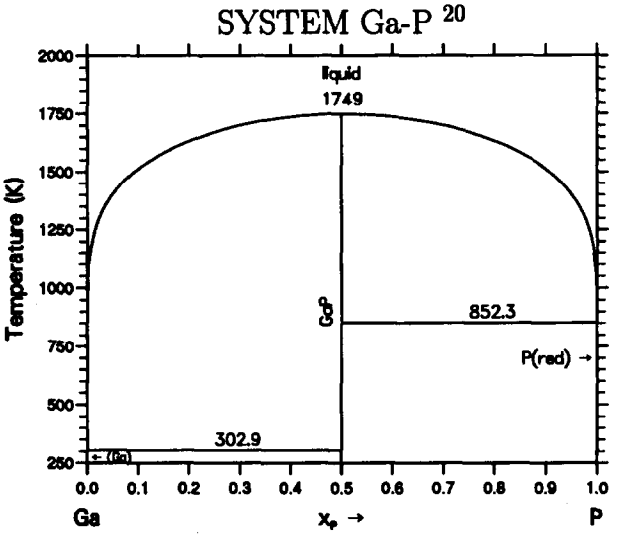

Figure 29: Calculated phase diagram of the Ga–P system.

Invariant Reactions.

Reaction	*Type*	*Compositions* x_P			$T(K)$
liquid $\rightleftharpoons$ *(Ga) + GaP*	*Degenerate*	0.000	0.000	0.500	302.9
liquid $\rightleftharpoons$ *GaP + P(red)*	*Degenerate*	1.000	0.500	1.000	852.3
liquid $\rightleftharpoons$ *GaP*	*Congruent*	0.500	0.500	.....	1749.0

Thermodynamic properties of the solution and compound phases in the Ga–P system ($J.mol^{-1}$)

Phase GaP

$$^{\circ}G^{Zincblende}_{Ga_{0.5}P_{0.5}}(T) - 0.5\ ^{\circ}H^{orthorhombic}_{Ga}(298.15K) - 0.5\ ^{\circ}H^{white}_{P}(298.15K) =$$
$$- 65760.76 + 142.37445\ T - 24.7902\ T\ lnT - 0.7113E\text{-}03\ T^2 + 146440\ T^{-1}$$

Phase Liquid

$$^{0}L^{liq}_{Ga,P} = - 9862$$

[20] I. Ansara, and C. Chatillon, private communication

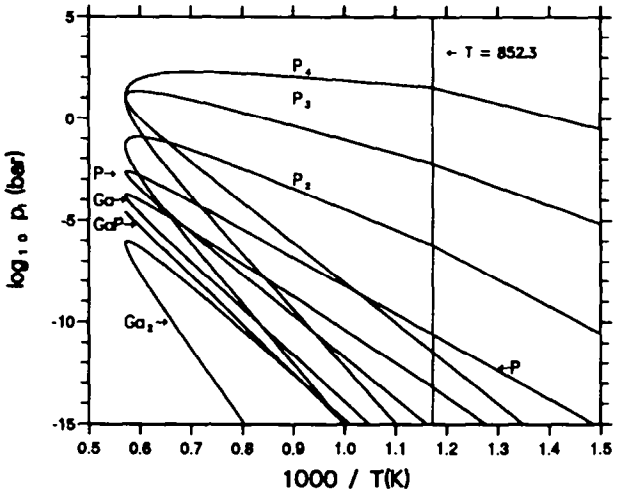

Figure 30: Calculated partial pressures of the various species in the gaseous phase along the equilibrium lines.

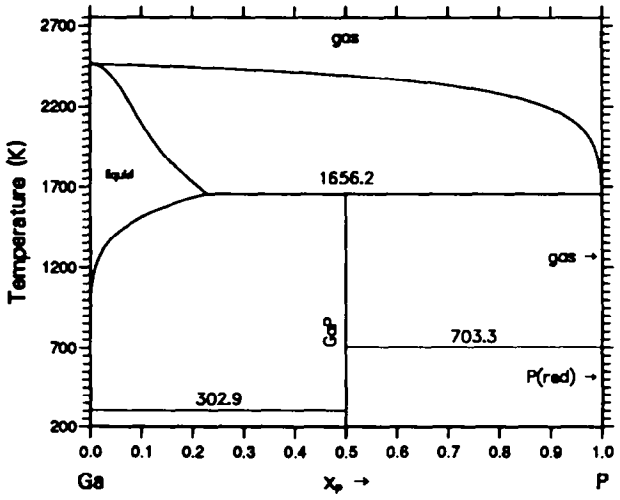

Figure 31: Calculated phase diagram at 0.1 MPa.

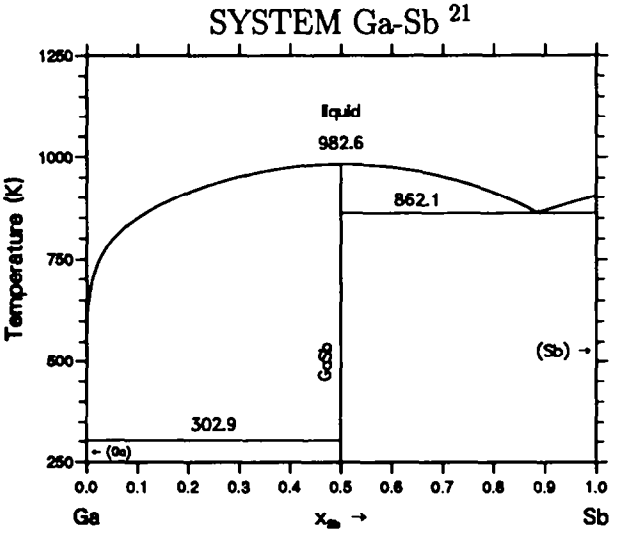

Figure 32: Calculated phase diagram of the Ga–Sb system.

Invariant Reactions.

Reaction	*Type*	*Compositions* x_{Sb}			$T(K)$
liquid ⇌ *(Ga) + GaSb*	*Degenerate*	0.000	0.000	0.500	302.9
liquid ⇌ *GaSb + (Sb)*	*Eutectic*	0.883	0.500	1.000	862.1
liquid ⇌ *GaSb*	*Congruent*	0.500	.....	.....	982.6

Thermodynamic properties of the solution and compound phases in the Ga–Sb system (J.mol^{-1})

Phase GaSb

$${}^{\circ}G^{Zincblende}_{Ga_{0.5}Sb_{0.5}}(T) - 0.5\,{}^{\circ}H^{orthorhombic}_{Ga}(298.15K) - 0.5\,{}^{\circ}H^{rhombo-A7}_{Sb}(298.15K) = 0.5\ GHSER_{Ga} + 0.5\ GHSER_{Sb} - 21738.1 - 10.53764\ T + 2.692876\ T\ lnT - 0.00137791\ T^2$$

Phase Liquid

$${}^{0}L^{liq}_{Ga,Sb} = -\ 13953.8 + 71.07866\ T - 9.6232\ T\ lnT$$

$${}^{1}L^{liq}_{Ga,Sb} = 1722.9 - 1.92588\ T \qquad {}^{2}L^{liq}_{Ga,Sb} = 2128.3$$

[21] T.J. Anderson, private communication

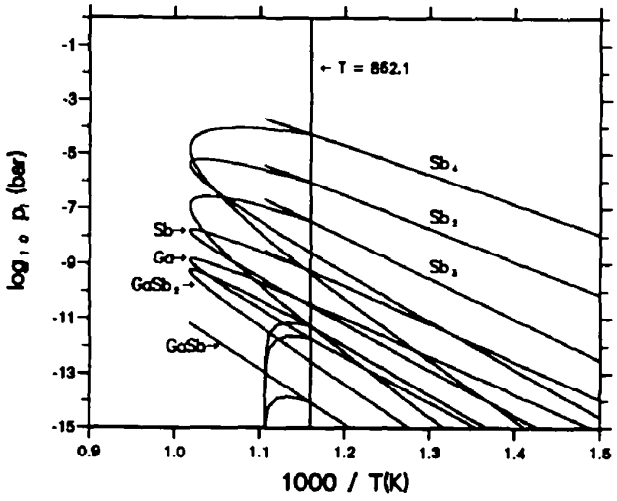

Figure 33: Calculated partial pressures of the various species in the gaseous phase along the equilibrium lines.

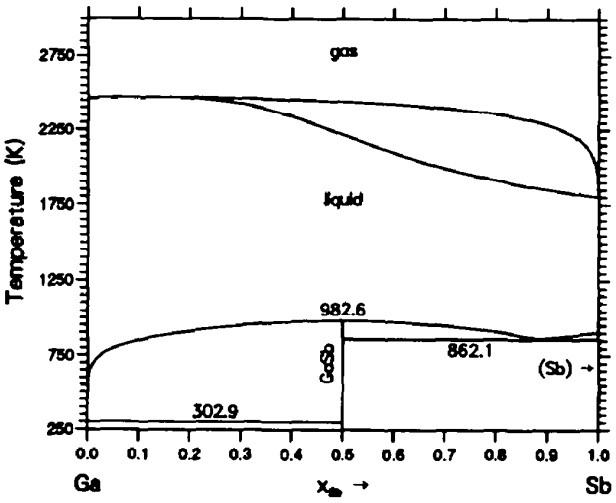

Figure 34: Calculated phase diagram at 0.1 MPa.

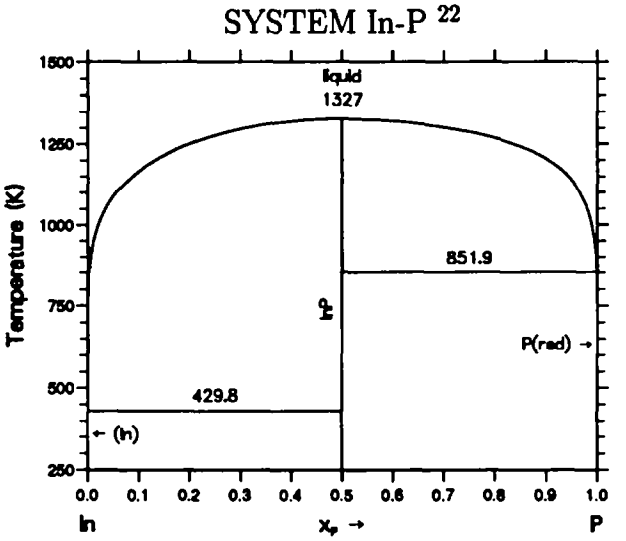

Figure 35: Calculated phase diagram of the In–P system.

Invariant Reactions.

Reaction	*Type*	*Compositions* x_P			$T(K)$
liquid $\rightleftharpoons$ *(In)* + *InP*	*Degenerate*	0.000	0.000	0.500	429.8
liquid $\rightleftharpoons$ *InP* + *P(red)*	*Degenerate*	0.999	0.500	1.000	851.9
liquid $\rightleftharpoons$ *InP*	*Congruent*	0.500	.....	.....	1327.0

Thermodynamic properties of the phases in the In–P system ($J.mol^{-1}$)

Phase InP

$${}^{\circ}G^{Zincblende}_{In_{0.5}P_{0.5}}(T) - 0.5\ {}^{\circ}H^{bct-A6}_{In}(298.15K) - 0.5\ {}^{\circ}H^{white}_{P}(298.15K) =$$
$$- 47600.60 + 179.24993\ T - 31.793475\ T\ lnT + 7.880317E\text{-}03\ T^2 + 220897\ T^{-1} - 1.81522E\text{-}06\ T^3$$

Phase Liquid

$${}^{0}L^{liq}_{In,P} = 14124.08 - 10.17931\ T \qquad {}^{1}L^{liq}_{In,P} = -2900.0$$

[22] I. Ansara, and C. Chatillon, private communication

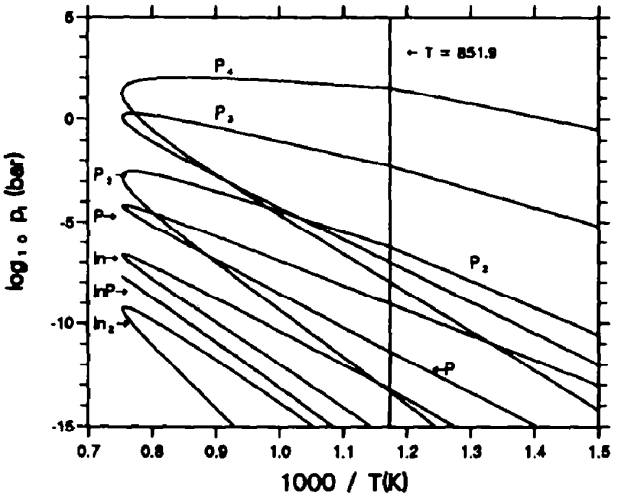

Figure 36: Calculated partial pressures of the various species in the gaseous phase along the equilibrium lines.

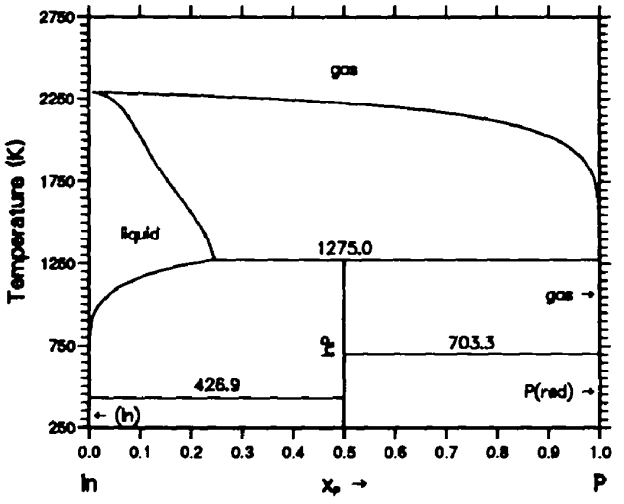

Figure 37: Calculated phase diagram at 0.1 MPa

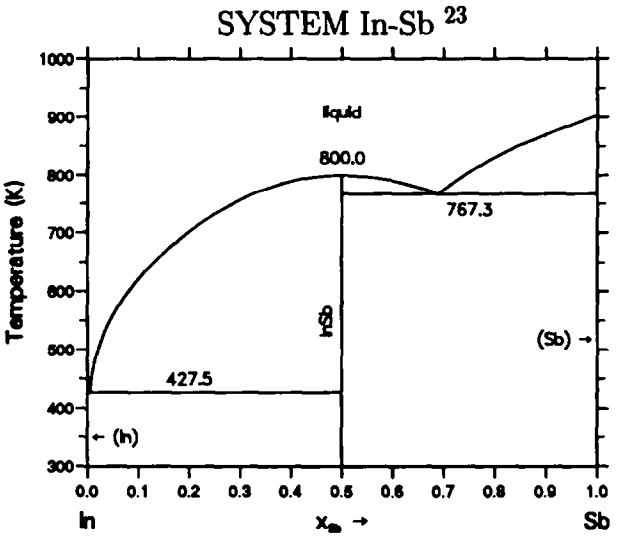

Figure 38: Calculated phase diagram of the In–Sb system.

Invariant Reactions.

Reaction	*Type*	*Compositions* x_{Sb}			$T(K)$
liquid $\rightleftharpoons$ *(In) + InSb*	*Eutectic*	0.000	0.000	0.500	427.5
liquid $\rightleftharpoons$ *InSb + (Sb)*	*Eutectic*	0.688	0.500	1.000	767.3
liquid $\rightleftharpoons$ *InSb*	*Congruent*	0.500	.....	.....	800.0

Thermodynamic properties of the phases in the In–Sb system (J.mol–1)

Phase InSb

$$^{\circ}G^{Zincblende}_{In_{0.5}Sb_{0.5}}(T) - 0.5\ ^{\circ}H^{bct-A6}_{In}(298.15K) - 0.5\ ^{\circ}H^{rhombo-A7}_{Sb}(298.15K) =$$
$$- 15849.3 + 0.293139\ T + 1.293581\ T\ lnT + 0.5\ GHSER_{In} + 0.5\ GHSER_{Sb}$$

Phase Liquid

$$^{0}L^{liq}_{In,Sb} = -25631.2 + 102.9324\ T - 13.45816\ T\ lnT$$
$$^{1}L^{liq}_{In,Sb} = - 2115.4 - 1.31907\ T \qquad ^{2}L^{liq}_{In,Sb} = 2908.9$$

[23] T.J. Anderson, private communication

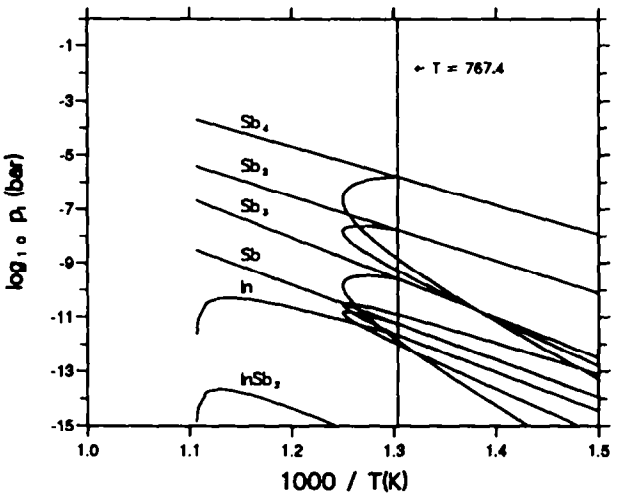

Figure 39: Calculated partial pressures of the various species in the gaseous phase along the equilibrium lines.

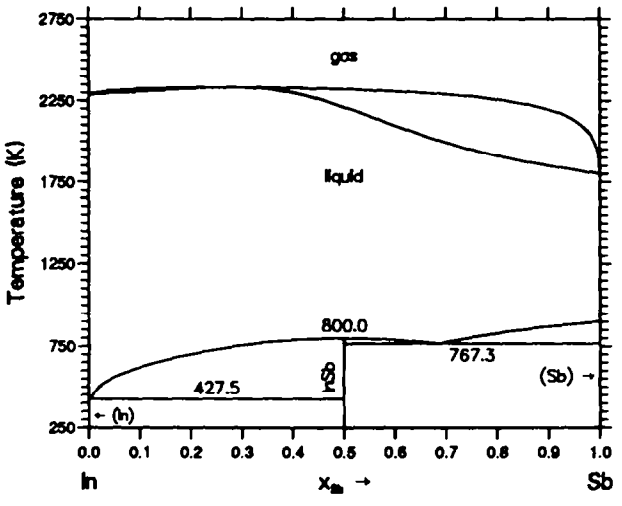

Figure 40: Calculated phase diagram at 0.1 MPa.

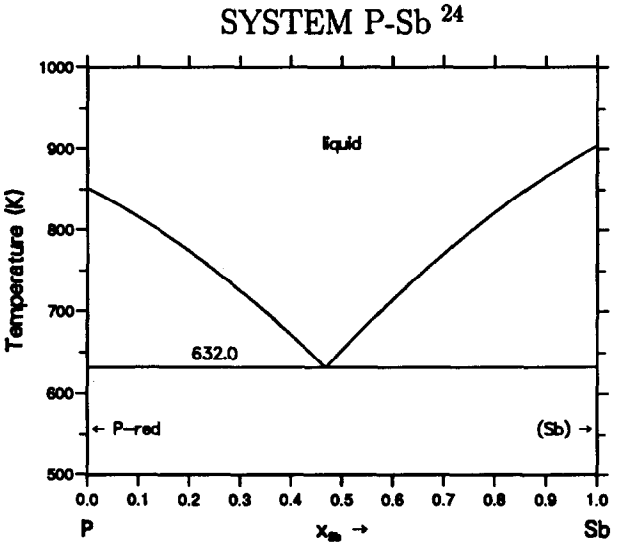

Figure 41: Calculated phase diagram of the P–Sb system.

Invariant Reactions.

Reaction	*Type*	*Compositions* x_{Sb}			$T(K)$
$liquid(2) \rightleftharpoons P-red + rhombo-A7$	*Eutectic*	0.468	0.000	1.000	632.0

Thermodynamic properties of the liquid phase in the P–Sb system ($J.mol^{-1}$)

Phase Liquid

$${}^{0}L^{liq}_{P,Sb} = -7000.0$$

[24] I. Ansara, and C. Chatillon, private communication

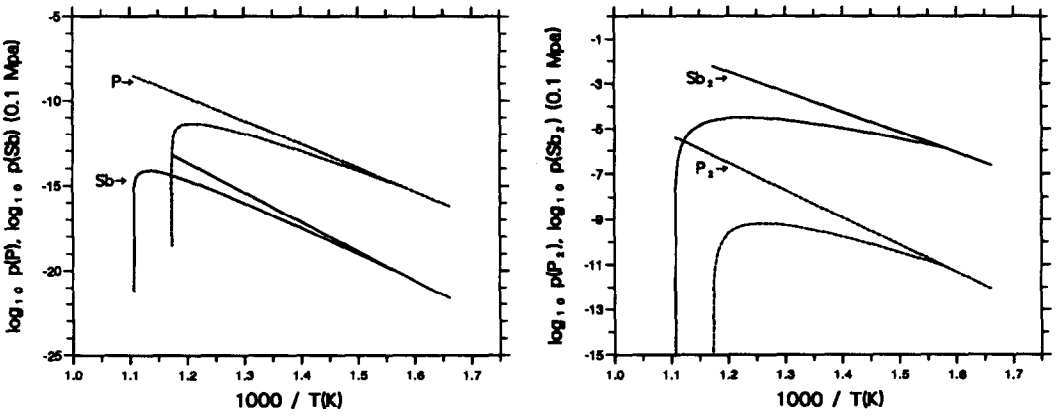

Figure 42: Partial pressures: a) P and Sb, b) P_2 and Sb_2.

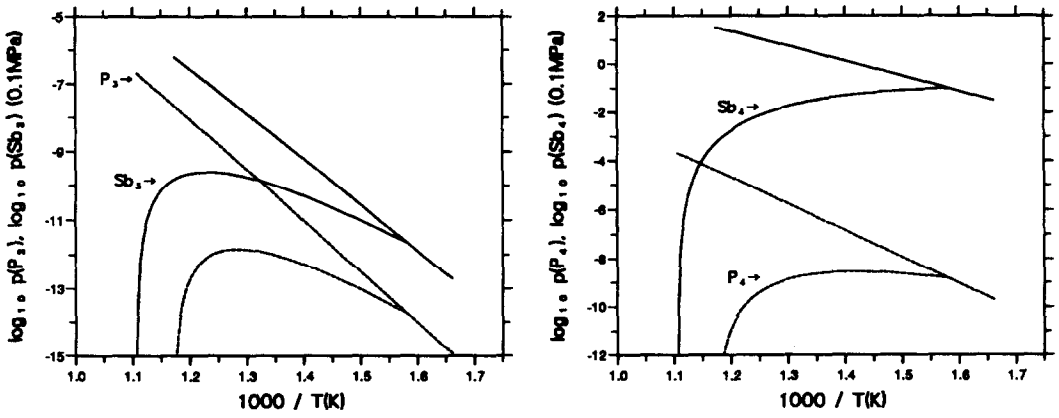

Figure 43: Partial pressures: c) P_3 and Sb_3 d) P_4 and Sb_4.

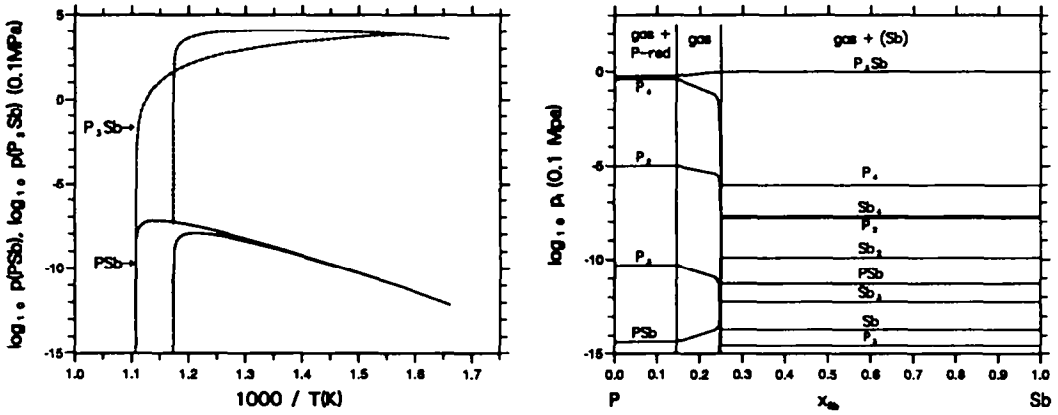

Figure 44: Partial pressures: e) PSb and Pb_3Sb. f) P_iSb_j at 675K

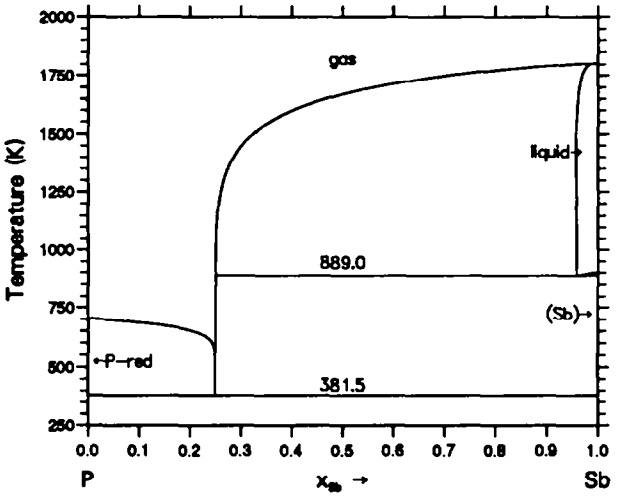

Figure 45: Calculated phase diagram at 0.1 MPa.

APPENDIX I: THERMODYNAMIC PROPERTIES OF THE ELEMENTS ($J.mol^{-1}$)

NOTE: The Gibbs energies of formation at T are relative to the enthalpy of the Standard Element Reference (HSER) at 298.15K

Aluminium

$GHSER_{Al} = {}^{\circ}G_{Al}^{fcc-A1}(T) - {}^{\circ}H_{Al}^{fcc-A1}(298.15K) =$

298.15 <T< 700.00 :
$-7976.15 + 137.093038\ T - 24.3671976\ T\ lnT - 1.884662E{-}3\ T^2 - 0.877664E{-}6\ T^3 + 74092\ T^{-1}$

700.00 <T< 933.47 :
$-11276.24 + 223.048446\ T - 38.5844296\ T\ lnT + 18.531982E{-}3\ T^2 - 5.764227E{-}6\ T^3 + 74092\ T^{-1}$

933.47 <T< 2900.00 :
$-11277.378 + 188.684153\ T - 31.748192\ T\ lnT - 1231.0E25\ T^{-9}$

${}^{\circ}G_{Al}^{liquid}(T) - {}^{\circ}H_{Al}^{fcc-A1}(298.15K) =$

298.15 <T< 933.47 :
$+11005.029 - 11.841867\ T + 7.934E{-}20\ T^7 + GHSER_{Al}$

933.47 <T< 2900.00 :
$+10482.382 - 11.253974\ T + 1.231E{+}28\ T^{-9} + GHSER_{Al}$

Arsenic

$GHSER_{As} = {}^{\circ}G_{As}^{rhombo-A7}(T) - {}^{\circ}H_{As}^{rhombo-A7}(298.15K) =$

298.15 <T< 1090.00 :
$-7270.447 + 122.211069\ T - 23.3144\ T\ lnT - 2.71613E{-}3\ T^2 + 11600\ T^{-1}$

1090.00 <T< 3000.00 :
$-10454.913 + 163.457433\ T - 29.216037\ T\ lnT$

${}^{\circ}G_{As}^{liquid}(T) - {}^{\circ}H_{As}^{rhombo-A7}(298.15K) = 24442.9 - 22.424679\ T + GHSER_{As}$

${}^{\circ}G_{As}^{red}(T) - {}^{\circ}H_{As}^{rhombo-A7}(298.15K) = 5782.0 - 3.85466\ T + GHSER_{As}$

${}^{\circ}G_{As}^{AsP}(T) - {}^{\circ}H_{As}^{rhombo-A7}(298.15K) = 6377.0 + 4.2516\ T + GHSER_{As}$

Gallium

$GHSER_{Ga} = {}^{\circ}G_{Ga}^{orthorhombic}(T) - {}^{\circ}H_{Ga}^{orthorhombic}(298.15K) =$

200.00 <T< 302.92 :
$-21312.331 + 585.263691\ T - 108.2287832\ T\ lnT + 227.155636E{-}3\ T^2 - 118.575257E{-}6\ T^3 + 439954\ T^{-1}$

302.92 <T< 4000.00 :
$-7055.643 + 132.73019\ T - 26.0692906\ T\ lnT + 0.1506E{-}3\ T^2 - 0.040173E{-}6\ T^3 - 118332\ T^{-1} + 164.5E21\ T^{-9}$

$^{\circ}G_{Ga}^{bct-A6}(T) - {}^{\circ}H_{Ga}^{orthorhombic}(298.15K) = 3500.0 - 10.0\ T + GHSER_{Ga}$

$^{\circ}G_{Ga}^{fcc-A1}(T) - {}^{\circ}H_{Ga}^{orthorhombic}(298.15K) = 3800.0 - 10.20\ T + GHSER_{Ga}$

$^{\circ}G_{Ga}^{7}(T) - {}^{\circ}H_{Ga}^{orthorhombic}(298.15K) = 3089.8 - 8.71535\ T + GHSER_{Ga}$

$^{\circ}G_{Ga}^{liquid}(T) - {}^{\circ}H_{Ga}^{orthorhombic}(298.15K) =$

$200.00 < T < 302.92 : + 5491.298 - 18.073995\ T - 7.017E{-}17\ T^{7} + GHSER_{Ga}$

$302.92 < T < 4000.00 : + 5666.455 - 18.681147\ T - 1.645E{+}23\ T^{-9} + GHSER_{Ga}$

Indium

$GHSER_{In} = {}^{\circ}G_{In}^{bct-A6}(T) - {}^{\circ}H_{In}^{bct-A6}(298.15K) =$

$298.15 < T < 429.75 : - 6978.89 + 92.338115\ T - 21.8386\ T\ lnT - 5.72566E{-}3\ T^{2} - 2.120321E{-}6\ T^{3} - 22906\ T^{-1}$

$429.75 < T < 3800.00 : - 7033.516 + 124.476588\ T - 27.4562\ T\ lnT + 0.54607E{-}3\ T^{2} - 0.08367E{-}6\ T^{3} - 211708\ T^{-1} + 353.0E20\ T^{-9}$

$^{\circ}G_{In}^{fcc-A1}(T) - {}^{\circ}H_{In}^{bct-A6}(298.15K) = 123.0 - 0.1988\ T + GHSER_{In}$

$^{\circ}G_{In}^{liquid}(T) - {}^{\circ}H_{In}^{bct-A6}(298.15K) =$

$298.15 < T < 429.75 : + 3282.092 - 7.63686\ T - 5.59E{-}20\ T^{7} + GHSER_{In}$

$429.75 < T < 2500.00 : + 3283.706 - 7.640804\ T - 3.53E{+}22\ T^{-9} + GHSER_{In}$

Phosphorus

$GHSER_{P} = {}^{\circ}G_{P}^{white}(T) - {}^{\circ}H_{P}^{white}(298.15K) =$

$250.00 < T < 317.30 : - 43821.799 + 1026.693886\ T - 178.426\ T\ lnT + 290.708E{-}3\ T^{2} - 104.022667E{-}6\ T^{3} + 1632695\ T^{-1}$

$317.30 < T < 1000.00 : - 9587.448 + 152.341487\ T - 28.7335301\ T\ lnT + 1.715669E{-}3\ T^{2} - 0.22829E{-}6\ T^{3} + 172966\ T^{-1}$

$1000.00 < T < 3000.00 : - 8093.075 + 135.87631\ T - 26.326\ T\ lnT$

$^{\circ}G_{P}^{red}(T) - {}^{\circ}H_{P}^{white}(298.15K) =$

$250.00 < T < 317.30 : - 25976.559 + 148.672002\ T - 25.55\ T\ lnT + 3.4121E{-}3\ T^{2} - 2.418867E{-}6\ T^{3} + 160095\ T^{-1}$

$500.00 < T < 852.35 : - 21723.721 + 77.671736\ T - 14.368\ T\ lnT - 9.57685E{-}3\ T^{2} + 0.393917E{-}6\ T^{3} - 141375\ T^{-1}$

$852.35 < T < 1500.00 - 119408.413 + 1026.02962\ T - 149.4495562\ T\ lnT + 67.272364E{-}3\ T^{2} - 6.651929E{-}6\ T^{3} + 12495943\ T^{-1}$

$1500.00 < T < 3000.00 - 24524.119 + 153.839181\ T - 26.326\ T\ lnT$

$^{\circ}G_P^{liquid}(T) - {}^{\circ}H_P^{white}(298.15K) =$

250.00 <T< 317.30 : $-26316.111 + 434.930931\ T - 70.7440584\ T\ lnT - 2.898936E{-}3\ T^2 + 39.049371E{-}6\ T^3 + 1141147\ T^{-1}$

317.30 <T< 3000.00 : $-7232.449 + 133.291873\ T - 26.326\ T\ lnT$

$^{\circ}G_P^{rhombo-A7}(T) - {}^{\circ}H_P^{white}(298.15K) = -188.0 + 0.12527\ T + GHSER_P$

$^{\circ}G_P^{AsP}(T) - {}^{\circ}H_P^{white}(298.15K) = 10210.3 + 6.80686\ T + GHSER_P$

Antimony

$GHSER_{Sb} = {}^{\circ}G_{Sb}^{rhombo-A7}(T) - {}^{\circ}H_{Sb}^{rhombo-A7}(298.15K) =$

298.15 <T< 903.78 : $-9242.858 + 156.154689\ T - 30.5130752\ T\ lnT + 0.007748768\ T^2 - 3.003415E{-}06\ T^3 + 100625\ T^{-1}$

903.78 <T< 6000.00 : $-11738.83 + 169.485872\ T - 31.38\ T\ lnT + 1.61682E{+}27\ T^{-9}$

$^{\circ}G_{Sb}^{liquid}(T) - {}^{\circ}H_{Sb}^{rhombo-A7}(298.15K) =$

298.15 <T< 903.78 : $+19822.329 - 21.923164\ T - 1.7485E{-}20\ T^7 + GHSER_{Sb}$

903.78 <T< 2500.00 : $19914.189 - 22.029886\ T - 1.61682E{+}27\ T^{-9} + GHSER_{Sb}$

APPENDIX II: THERMODYNAMIC PROPERTIES OF THE GASEOUS SPECIES PRESENT IN BINARY III-V SYSTEMS ($J.mol^{-1}$)

NOTE: The Gibbs Energies of Formation at T are relative to the Enthalpy of the Standard Element Reference (HSER) at 298.15K

Al<g>

$${}^{\circ}G^{gas}_{Al}(T) - {}^{\circ}H^{fcc-A1}_{Al}(298.15K) =$$

298.15 <T< 3700.00 :
$$+ 323947.58 - 25.1480948\ T - 20.859\ T\ lnT + 4.5665E\text{-}05\ T^2 - 3.942E\text{-}09\ T^3 - 24275.5\ T^{-1} + RT\ lnP$$

Al_2<g>

$${}^{\circ}G^{gas}_{Al_2}(T) - 2\ {}^{\circ}H^{fcc-A1}_{Al}(298.15K) =$$

298.15 <T< 900.00 :
$$+ 496408.232 + 35.479739\ T - 41.6397\ T\ lnT + 2.49636E\text{-}03\ T^2 - 4.9050733E\text{-}07\ T^3 + 85390.3\ T^{-1} + RT\ lnP$$

900.00 <T< 2800.00 :
$$+ 497613.221 + 17.368131\ T - 38.85476\ T\ lnT - 2.249805E\text{-}04\ T^2 - 9.4900316E\text{-}09\ T^3 - 5287.23\ T^{-1} + RT\ lnP$$

AlAs<g>

$${}^{\circ}G^{gas}_{AlAs}(T) - {}^{\circ}H^{fcc-A1}_{Al}(298.15K) - {}^{\circ}H^{rhombo-A7}_{As}(298.15K) =$$

298.15 <T< 1100.00 :
$$+ 404737.869 - 1.72226943\ T - 35.91797\ T\ lnT - 0.0011864985\ T^2 + 1.73145833E\text{-}07\ T^3 + 112834.1\ T^{-1} + RT\ lnP$$

1100.00 <T< 2500.00 :
$$+ 403941.515 + 8.13583179\ T - 37.38697\ T\ lnT - 8.51444E\text{-}06\ T^2 + 5.04172E\text{-}10\ T^3 + 193267.35\ T^{-1} + RT\ lnP$$

AlP<g>

$${}^{\circ}G^{gas}_{AlP}(T) - {}^{\circ}H^{fcc-A1}_{Al}(298.15K) - {}^{\circ}H^{white}_{P}(298.15K) =$$

298.15 <T< 3000.00 :
$$+ 418432.069 + 24.5561614\ T - 37.19604\ T\ lnT - 1.730803E\text{-}04\ T^2 + 6.83827167E\text{-}09\ T^3 + 98823.05\ T^{-1} + RT\ lnP$$

AlP_2 <g>

$$^{\circ}G^{gas}_{AlP_2}(T) - {}^{\circ}H^{fcc-A1}_{Al}(298.15K) - 2\ {}^{\circ}H^{white}_{P}(298.15K) =$$

298.15 <T< 1100.00 :
$+ 313726.626 + 124.763317\ T - 56.8823\ T\ lnT - 0.004231306\ T^2 + 6.07965333E{-}07\ T^3 + 248956.4\ T^{-1} + RT\ lnP$

1100.00 <T< 3000.00 :
$+310708.208 + 160.951753\ T - 62.25089\ T\ lnT - 3.015459E{-}05\ T^2 + 1.58303E{-}09\ T^3 + 569151.5\ T^{-1} + RT\ lnP$

AlSb<g>

$$^{\circ}G^{gas}_{AlSb}(T) - {}^{\circ}H^{fcc-A1}_{Al}(298.15K) - 2\ {}^{\circ}H^{rhombo-A7}_{Sb}(298.15K) =$$

298.15 <T< 3000.00 :
$+ 373326.483 - 2.64789254\ T - 37.1519\ T\ lnT - 1.464158E{-}04\ T^2 + 8.22252333E{-}09\ T^3 + 106454.3\ T^{-1} + RT\ lnP$

As<g>

$$^{\circ}G^{gas}_{As}(T) - {}^{\circ}H^{rhombo-A7}_{As}(298.15K) =$$

298.15 <T< 1800.00 :
$272027.85 - 32.2533338\ T - 21.21551\ T\ ln\ T + 4.3891495E{-}04\ T^2 - 7.393995E{-}08\ T^3 + 9666.555\ T^{-1} + RT\ lnP$

1800.00 <T< 3700.00 :
$293094.184 - 133.732322\ T - 8.281945\ T\ lnT - 0.002703715\ T^2 + 3.43112833E{-}08\ T^3 - 6025190\ T^{-1} + RT\ lnP$

As_2 < g >

$$^{\circ}G^{gas}_{As_2}(T) - 2\ {}^{\circ}H^{rhombo-A7}_{As}(298.15K) =$$

298.15 <T< 2200.00 :
$179351.548 + 10.5519715\ T - 37.35966\ T\ ln\ T - 5.61806E{-}05\ T^2 - 2.13098E{-}08\ T^3 + 104881.15\ T^{-1} + RT\ lnP$

2200.00 <T< 3700.00 :
$190396.109 - 11.4088459\ T - 35.19088\ T\ ln\ T + 8.55731E{-}04\ T^2 - 1.59161083E{-}07\ T^3 - 5169920\ T^{-1} + RT\ lnP$

As_3 < g >

$$^{\circ}G^{gas}_{As_3}(T) - 3\ {}^{\circ}H^{rhombo-A7}_{As}(298.15K) =$$

298.15 <T< 3700.00 :
$237070.283 + 72.1949142\ T - 58.15764\ T\ ln\ T - 1.097306E{-}05\ T^2 + 4.391665E{-}10\ T^3 + 95566.7\ T^{-1} + RT\ lnP$

As_4 <g>

$^{\circ}G^{gas}_{As_4}(T) - 4\ ^{\circ}H^{rhombo-A7}_{As}(298.15K) =$

298.15 <T< 3700.00 : 129731.745 + 230.754352 T - 83.04465 T ln T
- 2.5148475E-05 T^2 + 1.00444733E-09 T^3 + 252728.45 T^{-1}
+ RT lnP

AsGa<g>

$^{\circ}G^{gas}_{AsGa}(T) - {}^{\circ}H^{rhombo-A7}_{As}(298.15K) - {}^{\circ}H^{orthorhombic}_{Ga}(298.15K) =$

298.15 <T< 2000.00 : + 351178.641 - 7.5681515 T - 37.3627 T lnT
- 2.986345E-05 T^2 + 3.00181333E-09 T^3
+ 40854.26 T^{-1} + RT lnP

AsIn<g>

$^{\circ}G^{gas}_{AsIn}(T) - {}^{\circ}H^{rhombo-A7}_{As}(298.15K) - {}^{\circ}H^{bct-A6}_{In}(298.15K) =$

298.15 <T< 2500.00 : + 316678.645 - 13.5079581 T - 37.3342504 T lnT
- 3.935052E-05 T^2 + 3.30605733E-09 T^3
+ 57665.98 T^{-1} + RT lnP

AsP<g>

$^{\circ}G^{gas}_{AsP}(T) - {}^{\circ}H^{rhombo-A7}_{As}(298.15K) - {}^{\circ}H^{P-white}_{P}(298.15K) =$

298.15 <T< 1300.00 : + 148893.997 + 5.32607457 T - 35.58733 T ln T
- 0.001438031 T^2 + 1.68080667E-07 T^3
+ 129056.95 T^{-1} + RT lnP
1300.00 <T< 3000.00 : + 142966.673 + 46.9791261 T - 41.2751 T ln T
+ 0.001175498 T^2 - 8.15693333E-08 T^3
+ 1333588.5 T^{-1} + RT lnP

AsP_3 <g>

$^{\circ}G^{gas}_{AsP_3}(T) - {}^{\circ}H^{rhombo-A7}_{As}(298.15K) - 3.0\ {}^{\circ}H^{P-white}_{P}(298.15K) =$

298.15 <T< 1600.00 : 70396.2694 + 244.805285 T - 80.93279 T ln T
- 0.00140404 T^2 + 1.57551383E-07 T^3
+ 455746.3 T^{-1} + RT lnP
1600.00 <T< 3000.00 : 69005.5067 + 259.786787 T - 83.10146 T ln T
- 1.202009E-05 T^2 + 0.22268333E-10 T^3
+ 614865 T^{-1} + RT lnP

As_2P_2 <g>

$$^{\circ}G^{gas}_{As_2P_2}(T) - 2.0\ ^{\circ}H^{rhombo-A7}_{As}(298.15K) - 2.0\ ^{\circ}H^{P-white}_{P}(298.15K) =$$

298.15 <T< 2000.00 : + 88683.199 + 187.422353*T82383.199 T – 73.6591 T ln T
– 6.375555E–04 T^2 + 5.98925167E–08 T^3
+ 343146.95 T^{-1} + RT lnP

2000.00 <T< 3000.00 : + 87688.4754 + 196.329213 T – 74.91212 T ln T
+ 2.271923E–05 T^2 – 1.1587775E–09 T^3
+ 496108.7 T^{-1} + RT lnP

As_3P<g>

$$^{\circ}G^{gas}_{As_3P}(T) - 3.0\ ^{\circ}H^{rhombo-A7}_{As}(298.15K) - \ ^{\circ}H^{P-white}_{P}(298.15K) =$$

298.15 <T< 3000.00 : 116273.164 + 231.440504 T – 82.63698 T ln T
– 2.19418E–04 T^2 + 1.58954167E–08 T^3
+ 338394.15 T^{-1} + RT lnP

AsSb<g>

$$^{\circ}G^{gas}_{AsSb}(T) - \ ^{\circ}H^{rhombo-A7}_{As}(298.15K) - \ ^{\circ}H^{rhombo-A7}_{Sb}(298.15K) =$$

298.15 <T< 1700.00 : 211663.042 – 1.92474626 T – 37.59641 T ln T
+ 1.256325E–04 T^2 – 6.23121667E–08 T^3
+ 79822.7 T^{-1} + RT lnP

1700.00 <T< 3000.00 : 214598.477 – 4.44994282 T – 37.60442 T ln T
+ 0.0011372535 T^2 – 2.101E– 07 T^3
– 1176163 T^{-1} + RT lnP

$AsSb_3$ <g>

$$^{\circ}G^{gas}_{AsSb_3}(T) - \ ^{\circ}H^{rhombo-A7}_{As}(298.15K) - 3.0\ ^{\circ}H^{rhombo-A7}_{Sb}(298.15K) =$$

298.15 <T< 3000.00 : 176316.699 + 194.150775 T – 83.07418 T ln T
– 2.6862745E–05 T^2 + 1.7468E–09 T^3
+ 150929.4 T^{-1} + RT lnP

As_2Sb_2 <g>

$$^{\circ}G^{gas}_{As_2Sb_2}(T) - 2.0\ ^{\circ}H^{rhombo-A7}_{As}(298.15K) - 2.0\ ^{\circ}H^{rhombo-A7}_{Sb}(298.15K) =$$

298.15 <T< 3000.00 : 163893.813 + 199.185739 T – 83.02444 T ln T
– 4.860865E–05 T^2 + 3.28926667E–09 T^3
+ 186090.9 T^{-1} + RT lnP

As_3Sb<g>

$^{\circ}G^{gas}_{As_3Sb_2}(T) - 3.0\ {}^{\circ}H^{rhombo-A7}_{As}(298.15K) - {}^{\circ}H^{rhombo-A7}_{Sb}(298.15K) =$

298.15 <T< 3000.00 : 147770.924 + 210.970771 T - 82.97471 T lnT
- 7.03545E-05 T^2 + 4.83173333E-09 T^3
+ 221252.45 T^{-1} + RT lnP

Ga<g>

$^{\circ}G^{gas}_{Ga}(T) - {}^{\circ}H^{orthorhombic}_{Ga}(298.15K) =$

298.15 <T< 600.00 : + 259072.279 +88.0130701 T - 38.71057 T lnT
+ 0.01053784 T^2 - 9.86907833E-07 T^3
600.00 <T< 1400.00 : + 263812.519 + 33.4871429 T - 30.75007 T lnT
+ 0.00537745 T^2 - 5.46534E-07 T^3
- 150942.65 T^{-1} + RT lnP
1400.00 <T< 2700.00 + 270292.502 - 28.1810499 T - 21.9834 T lnT
+ 3.192416E-04 T^2 - - 1.46299133E-08 T^3
- 992093 T^{-1} + RT lnP

Ga_2 <g>

$^{\circ}G^{gas}_{Ga_2}(T) - 2\ {}^{\circ}H^{orthorhombic}_{Ga}(298.15K) =$

298.15 <T< 1100.00 : + 422882.385 - 36.0787973 T - 33.72863 T lnT
- 0.009368525 T^2 + 7.62775167E-07 T^3
- 19520.385 T^{-1} + RT lnP
1100.00 <T< 2500.00 : + 419324.178 + 8.33965897 T - 40.33555 T lnT
- 0.004185412 T^2 + 2.679565E-08 T^3
+ 312119.6 T^{-1} + RT lnP

GaP<g>

$^{\circ}G^{gas}_{GaP}(T) - {}^{\circ}H^{orthorhombic}_{Ga}(298.15K) - {}^{\circ}H^{white}_{P}(298.15K) =$

298.15 <T< 2500.00 : + 338723.188 + 4.12127639 T - 37.21519 T lnT
- 9.81506E-05 T^2 + 8.251335E-09 T^3
+ 85392.45 T^{-1} + RT lnP

GaSb<g>

$^{\circ}G^{gas}_{GaSb}(T) - {}^{\circ}H^{orthorhombic}_{Ga}(298.15K) - {}^{\circ}H^{rhombo-A7}_{Sb}(298.15K) =$

298.15 <T< 2000.00 : + 338661.848 - 16.2870454 T - 37.39532 T lnT
- 9.362025E-05 T^2 + 1.13351083E-09 T^3
+ 26904.44 T^{-1} + RT lnP

$GaSb_2$<g>

$^{\circ}G^{gas}_{GaSb_2}(T) - {}^{\circ}H^{orthorhombic}_{Ga}(298.15K) - 2\ {}^{\circ}H^{rhombo-A7}_{Sb}(298.15K) =$

298.15 <T< 2000.00 : + 287059.147 + 102.311273 T – 62.26559 T lnT
– 5.332025E–05 T^2 + 5.37548E–09 T^3
+ 85257.85 T^{-1} + RT lnP

In<g>

$^{\circ}G^{gas}_{In}(T) - {}^{\circ}H^{bct-A6}_{In}(298.15K) =$

298.15 <T< 600.00 : + 236267.082 – 68.7705736 T – 15.35206 T lnT
: – 0.00527185 T^2 – -3.98269833E-07 T^3
– -94520.0 T^{-1} + RT lnP
600.00 <T< 1100.00 : + 237868.024 – 110.524313 T – 8.405227 T lnT
: – 0.0156847 T^2 + 2.21196333E–06 T^3
- 110674.05 T^{-1} + RT lnP
1100.00 <T< 2900.00 : + 214982.499 + 118.641772 T – 41.36283 T lnT
: + 0.00521457 T^2 – 2.526305E-07 T^3
+ 2837067 T^{-1} + RT lnP

In_2 <g>

$^{\circ}G^{gas}_{In_2}(T) - 2\ {}^{\circ}H^{bct-A6}_{In}(298.15K) =$

298.15 <T< 1800.00 : + 407673.852 – 41.5349385 T – 35.82134 T lnT
: – 0.00654889 T^2 + 2.03928167E–08 T^3
– 20133.6055 T^{-1} + RT lnP
1800.00 <T< 3000.00 : + 397374.677 + 2.12494681 T – 41.1879 T lnT
: – 0.00591436 T^2 + 8.15535516E–08 T^3
+ 3047627 T^{-1} + RT lnP

InP<g>

$^{\circ}G^{gas}_{InP}(T) - {}^{\circ}H^{bct-A6}_{In}(298.15K) - {}^{\circ}H^{white}_{P}(298.15K) =$

298.15 <T< 1700.00 : + 346990.994 - 3.97062442 T – 36.93928 T lnT
– 2.9085075E–04 T^2 + 3.12684333E–08 T^3
+ 100083.35 T^{-1} + RT lnP
1700.00 <T< 2500.00 + 346687.715 – 0.757786205 T – 37.40245 T lnT
– 3.47272E–06 T^2 + 1.90372E–10 T^3
+ 134967.45 T^{-1} + RT lnP

InSb<g>

$^{\circ}G^{gas}_{InSb}(T) - {}^{\circ}H^{bct-A6}_{In}(298.15K) - {}^{\circ}H^{rhombo-A7}_{Sb}(298.15K) =$

298.15 <T< 2500.00 : + 345845.335 + 11.5111691 T – 37.37164 T lnT
– 6.74135E–04 T^2 + 1.80797167E–09 T^3
+ 43601.51 T^{-1} + RT lnP

$InSb_2$ <g>

$^{\circ}G^{gas}_{InSb_2}(T) - {}^{\circ}H^{bct-A6}_{In}(298.15K) - 2\ {}^{\circ}H^{rhombo-A7}_{Sb}(298.15K) =$

298.15 <T< 2500.00 : + 325396.384 + 94.4051815 T − 62.2438 T lnT
− 5.688785E−05 T^2 + 4.79559667E−09 T^3
+ 95531 T^{-1} + RT lnP

P<g>

$^{\circ}G^{gas}_{P}(T) - {}^{\circ}H^{white}_{P}(298.15K) =$

298.15 <T< 1900.00 : + 310152.015 − 21.3997117 T − 21.18864 T lnT
+ 3.9907815E−04 T^2 − 6.467185E−08 T^3
+ 9337.96 T^{-1} + RT lnP
1900.00 <T< 3400.00 : + 332461.723 − 123.51155 T − 8.27475 T lnT
− 0.0025407355 T^2 + 2.77886167E−08 T^3
− 6752450 T^{-1} + RT lnP

P_2<g>

$^{\circ}G^{gas}_{P_2}(T) - 2\ {}^{\circ}H^{white}_{P}(298.15K) =$

298.15 <T< 900.00 : + 133357.682 − 0.182114286 T − 32.02798 T lnT
− 0.004670767 T^2 + 7.28558667E−07 T^3
+ 106826.35 T^{-1} + RT lnP
900.00 <T< 3500.00 : + 128832.659 + 49.3136334 T − 39.23087 T lnT
+ 7.156115E−04 T^2 − 6.82824333E−08 T^3
+ 666443.5 T^{-1} + RT lnP

P_3<g>

$^{\circ}G^{gas}_{P_3}(T) - 3\ {}^{\circ}H^{white}_{P}(298.15K) =$

298.15 <T< 1000.00 : + 191023.012 + 115.134798 T − 55.58992 T lnT
− 0.00549647 T^2 + 8.37126667E−07 T^3
+ 291982.3 T^{-1} + RT lnP
1000.00 <T< 3000.00 : + 187367.887 + 160.09545 T − 62.29736 T lnT
− 1.1488665E−05 T^2 + 3.82699333E−10 T^3 + 671571.5 T^{-1}
+ RT lnP

P_4<g>

$^{\circ}G^{gas}_{P_4}(T) - 4\ {}^{\circ}H^{white}_{P}(298.15K) =$

298.15 <T< 1100.00 : + 31689.2276 + 246.976571 T − 77.33235 T lnT
− 0.0046207025 T^2 + 6.76817E−07 T^3
+ 563393 T^{-1} + RT lnP
1100.00 <T< 3000.00 : + 28520.4465 + 285.801741 T − 83.11153 T lnT
− 6.057165E−06 T^2 + 1.99865333E−10 T^3 + 890230 T^{-1}
+ RT lnP

PSb<g>

$^{\circ}G^{gas}_{PSb}(T) - {}^{\circ}H^{P-white}_{P}(298.15K) - {}^{\circ}H^{rhombo-A7}_{Sb}(298.15K) =$

298.15 <T< 2000.00 : + 214229.594 + 5.02994959 T - 36.85219 T ln T
- 4.3537175E-04 T^2 +2.308895E-08 T^3
+ 119774 T^{-1} + RT lnP

2000.00 <T< 3000.00 : + 183283.753 + 167.479175 T - 57.97816 T ln T
+ 0.0060526 T^2 - 3.56568333E-07 T^3
+ 8691045 T^{-1} + RT lnP

P_3Sb<g>

$^{\circ}G^{gas}_{P_3Sb}(T) - 3.0\ {}^{\circ}H^{P-white}_{P}(298.15K) - {}^{\circ}H^{rhombo-A7}_{Sb}(298.15K) =$

298.15 <T< 1800.00 : - 4776.72 + 240.89347 T - 81.5624 T ln T
- 9.284325E-04 T^2 + 9.50185333E-08 T^3
+ 429544.1 T^{-1} + RT lnP

1800.00 <T< 3000.00 : - 5846.21775 + 251.80766 T - 83.12543 T ln T
- 4.4852385E-06 T^2 + 1.89597167E-10 T^3
+ 558737.5 T^{-1} + RT lnP

Sb<g>

$^{\circ}G^{gas}_{Sb}(T) - {}^{\circ}H^{rhombo-A7}_{Sb}(298.15K) =$

298.15 <T< 1500.00 : + 260807.82 - 37.9550038 T - 21.27672 T lnT
+ 5.524195E-04 T^2 - 1.05228767E-07 T^3
+ 9996.235 T^{-1} + RT lnP

1500.00 <T< 2000.00 : + 277520.519 - 132.229974 T - 8.970999 T lnT
- 0.0030704565 T^2 + 5.21558333E-08 T^3
- 3997436 T^{-1} + RT lnP

Sb_2<g>

$^{\circ}G^{gas}_{Sb_2}(T) - 2\ {}^{\circ}H^{rhombo-A7}_{Sb}(298.15K) =$

298.15 <T< 1700.00 : + 225644.034 - 1.64062093 T - 38.03868 T ln T
+ 5.08568E-04 T^2 - 1.31408217E-07 T^3
+ 60968.15 T^{-1} + RT lnP

1700.00 <T< 3200.00 +231514.886-6.69092891 T - 38.05471 T ln T
+ 0.00253181 T^2 - 4.26984E-07 T^3
- 2451004 T^{-1} + RT lnP

Sb_3<g>

$^{\circ}G^{gas}_{Sb_3}(T) - 3\ {}^{\circ}H^{rhombo-A7}_{Sb}(298.15K) =$

298.15 <T< 2000.00 : 277165.227 + 46.0530737 T - 58.19257 T ln T
- 2.0866265E-06 T^2 + 8.316025E-11 T^3
+ 43601.08 T^{-1} + RT lnP

Sb_4<g>

$^{\circ}G^{gas}_{Sb_4}(T) - 4\ {}^{\circ}H^{rhombo-A7}_{Sb}(298.15K) =$

298.15 <T< 3000.00 : 192849.585 + 194.765811 T - 83.12392 T ln T
- - 5.116865E-06 T^2 + 2.043415E-10 T^3
+ 115767.85 T^{-1} + RT lnP