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Thermodynamic investigation of the AINC and AICN isomers by Knudsen cell mass spectrometry

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Equilibria involving the isomers AINC and AICN above a mixture of aluminum nitride, graphite, and gold contained in a graphite Knudsen cell were investigated with a mass spectrometer. The enthalpies of formation, $\Delta_f H_0^\circ$, and of atomization, $\Delta_a H_0^\circ$, in kJ mol^{-1} , for AINC and AICN, were derived as 281.3 ± 14 and 303.8 ± 14 , and as 1228.1 ± 15 and 1205.6 ± 15 , respectively. © 1999 American Institute of Physics. [S0021-9606(99)01627-X]

INTRODUCTION

In recent years the molecule AINC/AICN has received considerable attention by theorists¹⁻⁵ and spectroscopists,⁴⁻⁸ because it is suspected to be the carrier of some of the unidentified spectral lines in the circumstellar envelope of the carbon star IRC+10216.^{1,2} Related molecules such as NaCN,⁹ MgNC,¹⁰ and MgCN,¹¹ as well as AlCl and AlP,^{12,13} have already been observed in this star. The latter two are of interest in view of the pseudohalogen character of the CN radical. Theoretical calculations^{1,5,14} have predicted a linear geometry and a $^1\Sigma^+$ ground state for both isomers, AINC and AICN, AINC being the more stable isomer by several kcal mol^{-1} .

The first observation of AINC/AICN and the presence of comparable concentrations of the two isomers in the vapor above $\text{AlN}(s) + \text{graphite}$ has been reported by Gingerich¹⁵ from Knudsen effusion mass spectrometric measurements, and an estimate of its atomization energy, $\Delta_a H_{298}^\circ$ of 1255 kJ mol^{-1} , obtained from a second-law treatment. K.A.G. wishes to correct the percentage of fragmentation of AINC (AICN) to AlN^+ and AlC^+ in Ref. 15. It should read 0.5% instead of 5% using 30 V electrons. Additional mass spectrometric measurements yielded a preliminary third-law $\Delta_a H_{298}^\circ$ value of $(1243 \pm 21) \text{ kJ mol}^{-1}$ for this molecule.¹⁶

In the present investigation we report the thermodynamic evaluation of the AINC and AICN isomers from mass spectrometric equilibrium measurements coupled with a fragmentation analysis and utilization of theoretical transi-

tion energies. Thermal functions have been calculated from experimental and theoretical molecular parameters of both isomers.

EXPERIMENT

The measurements were performed with a Nuclide Corporation 12-90 HT mass spectrometer. Additional design features of the instrument and the general experimental procedure have been described previously.¹⁷ The graphite Knudsen cell was charged with finely powdered AlN and graphite; gold was added for calibration purposes. The gold was present during the measurements of AINC/AICN and served also as a liquid metal vaporization catalyst,^{18,19} since $\text{AlN}(s)$ has a low vaporization coefficient of 2.0×10^{-3} .^{20,21} The energy of the ionizing electrons was 30 eV, the emission current 1 mA, the acceleration energy was 3 kV, and the voltage at the entrance shield of the multiplier was 1.5 kV. Temperatures were measured with a calibrated optical pyrometer. Identification of the vapor species was accomplished by their mass-to-charge ratio, shutter effect, ionization efficiency curves, and isotopic intensity distribution. Appearance potentials, in eV, were measured by the extrapolated voltage differences method²² as 8.1 ± 0.5 for AlNC^+ or AlCN^+ , 16.3 ± 0.6 for AlN^+ , and 15.8 ± 0.6 for AlC^+ . The electron energy scale was calibrated with Au (9.22 eV)²³ and N_2 (15.58 eV).²³ Previous experimental values¹⁵ for $\text{AlNC}^+/\text{AlCN}^+$ ($7.4 \pm 0.3 \text{ eV}$), AlC^+ , and AlN^+ (approximately 15 eV) are lower, but still within the error limits

TABLE I. Measured ion currents, in A, over AlN-Au-graphite system.

T (K)	Ion intensities						
	Al^+	N_2^+	$\text{AlNC}^+ + \text{AlCN}^+$	Au^+	AlAu^+	AlNC^{+a}	AlCN^{+a}
1668	1.00e-08	1.33e-09	1.20e-10	1.78e-10	2.90e-10	1.05e-10	1.46e-11
1669	1.05e-08	1.33e-09	1.16e-10	1.78e-10	2.98e-10	1.02e-10	1.42e-11
1697	1.46e-08	1.74e-09	1.72e-10	2.45e-10	4.45e-10	1.51e-10	2.15e-11
1646	6.30e-09	6.62e-10	5.68e-11	1.28e-10	2.15e-10	5.00e-11	6.79e-12
1612	3.60e-09	3.08e-10	2.50e-11	8.25e-11	1.27e-10	2.21e-11	2.89e-12
1558	1.40e-09	8.90e-11	6.00e-12	3.70e-11	5.00e-11	5.34e-12	6.60e-13
1558	1.40e-09	1.08e-10	5.72e-12	3.70e-11	5.00e-11	5.09e-12	6.30e-13
1520	7.61e-10	4.50e-11	2.08e-12	2.20e-11	2.85e-11	1.86e-12	2.20e-13

^aCalculated using ΔE of 1880 cm^{-1} (see text).

TABLE II. The Gibbs energy functions (GEF_0), $(G_T^0 - H_0^0)/T$, in $\text{J K}^{-1} \text{mol}^{-1}$ and the heat content functions (HCF_0), $H_T^0 - H_0^0$, in kJ mol^{-1} for the isomers AINC and AICN.

Species		Temperature (K)				
		298.15	1400	1600	1800	2000
AINC	- GEF_0	212.2	287.4	294.6	301.0	306.9
	HCF_0	13.03	74.86	86.84	98.91	111.1
AICN	- GEF_0	209.9	284.5	291.7	298.1	303.9
	HCF_0	12.77	74.84	86.85	98.95	111.1

given, whereas theoretical values for AINC^+ , 9.64³ and 9.2 eV,⁴ and for AICN^+ , 9.59³ and 9.2 eV,¹⁴ are higher.

The pressure constants were determined from the known $\text{AlAu}(g) = \text{Al}(g) + \text{Au}(g)$ equilibrium, using the measured corresponding ion currents and the known dissociation energy, $D_0^0(\text{AlAu}, g) = (322.2 \pm 6.3) \text{ kJ mol}^{-1}$.²⁴ The multiplier gains, γ_X , for the major species were measured with a 50% transmission grid as 10^5 times 4.10, 1.93, 1.74, 6.24, and 4.36 for Al, Au, AlAu, N_2 , and AINC/AICN, respectively. The relative ionization cross sections used, σ_X , in 10^{-16} cm^2 , were taken from experimental values reported in the literature: Al, 9.71,²⁵ Au, 5.70, by a logarithmic extrapolation;²⁶ AlAu, 11.6, as $0.75 \times (\sigma_{\text{Al}} + \sigma_{\text{Au}})$; AINC/AICN, 9.28, as $0.75 \times (\sigma_{\text{Al}} + \sigma_{\text{C}} + \sigma_{\text{N}})$, where σ_{C} and σ_{N} are taken from Ref. 27; N_2 , 0.998.²⁸ The resulting pressure constants, k_X , in $\text{bar A}^{-1} \text{K}^{-1}$, are 0.841, 3.05, 1.67, 5.42, and 0.840 for Al, Au, AlAu, N_2 , and AINC/AICN, respectively. The uncertainty of the k_X values is estimated to be about 20%.

Table I lists the measured ion currents for the most abundant isotopes of the species pertinent to the present investigation.

RESULTS AND DISCUSSION

The Gibbs energy functions (GEF_0), $(G_T^0 - H_0^0)/T$, and the heat content functions (HCF_0), $H_T^0 - H_0^0$, for AINC and AICN were calculated using the rigid-rotator harmonic-oscillator approximation.²⁹

In our evaluation of the thermal functions we used the experimental values for the vibrational frequencies, in cm^{-1} :

ν_1 , 2069; ν_2 , 549; ν_3 , 100 (2), by Gerasimov *et al.*⁸ for AINC, and those by Fukushima:⁵ ν_1 , 1975.5; ν_2 , 523.5; ν_3 , 132.9 (2), for AICN. The intermolecular distances, in Å, of AINC, $r_{\text{Al-N}} = 1.849$ and $r_{\text{N-C}} = 1.171$, obtained from a millimeter-wave spectrum, were taken from Robinson *et al.*⁶ For AICN, the theoretical values from Ma *et al.*¹ were used: $r_{\text{Al-C}} = 2.014$ and $r_{\text{C-N}} = 1.171$, because Gerasimov *et al.*⁸ found that the rotational constant for the ground state of this molecule, $B = (0.1674 \pm 0.0046) \text{ cm}^{-1}$, is equal to that calculated,¹ $B = 0.1672 \text{ cm}^{-1}$; this means that the intermolecular distances calculated by Ma *et al.*¹ are very close to the experimental value. Electronic excited states of AINC and AICN reported in the literature^{5,8} do not measurably contribute to the thermal functions below 2500 K. Table II lists the thermal functions calculated for AINC and AICN.

The Gibbs energy functions and enthalpy increments for $\text{Al}(g)$, $\text{C}(\text{graph.})$, $\text{AlN}(s)$, and $\text{N}_2(g)$ were taken from Chase *et al.*,³⁰ for $\text{Au}(g)$ from Hultgren *et al.*,³¹ and for $\text{AlAu}(g)$ from Gingerich and Blue.²⁴ The thermal functions of $\text{Au}(g)$ and $\text{AlAu}(g)$ have been adjusted to correspond to the standard pressure $p^\circ = 1 \text{ bar}$ instead of $p^\circ = 1 \text{ atm}$.

During the mass spectrometric investigation, the species AIC^+ and AlN^+ were observed and measured at different temperatures. Their appearance potentials of 15.8 and 16.3 eV indicate that they are fragments of the parent molecules AICN and AINC, respectively. This interpretation is supported by the fact that the difference between the appearance potentials of AlN^+ or AIC^+ and that of 8.1 eV for m/e of 53 (AINC^+ or AICN^+), is about 8.2 or 7.7 eV, respectively, close to the dissociation energy of $\text{CN}(g)$, (7.72 \pm 0.10) eV.³⁰ Possible fragment contributions to AIC^+ from Al_2C_2 and AIC_2 ³² and to AlN^+ from Al_2N are estimated to be less than 5% of the measured fragment ion currents. A peculiar fact, observed already by Gingerich,¹⁵ was that the ion intensities of the two species AIC^+ and AlN^+ were almost the same in the temperature range of the measurements and were about 0.4%–0.5% of the $m/e = 53$ ion intensity; the $I(\text{AIC}^+)/I(\text{AlN}^+)$ ratio was 1.1 ± 0.2 .

The enthalpies of formation, $\Delta_f H_0^0$, and the atomization energies, $\Delta_a H_0^0$, of both the isomers AINC and AICN were evaluated by considering a corrected value of their ion intensities and by utilizing the following reactions:

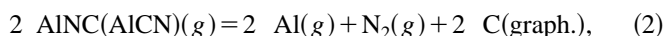
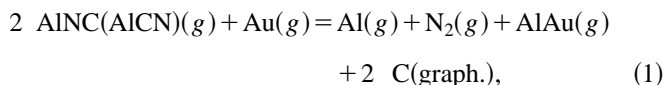
TABLE III. Summary of the enthalpies of reaction, in kJ mol^{-1} , for AINC and AICN.

Reaction	Second-law		Third-law	
	$\Delta_r H_{(T)}^0$	$\Delta_r H_0^0$	$\Delta_r H_0^0$	$\Delta_r H_0^0$ selected
$2\text{AINC}(g) + \text{Au}(g) = \text{Al}(g) + \text{N}_2(g) + \text{AlAu}(g) + 2\text{C}(\text{graph.})$	-229.1 ± 17.8^a	-218.2 ± 17.8	-255.7 ± 2.5	-243.2 ± 6.0
$2\text{AINC}(g) = 2\text{Al}(g) + \text{N}_2(g) + 2\text{C}(\text{graph.})$	113.1 ± 19.3	114.3 ± 19.3	66.3 ± 3.0	82.3 ± 6.6
$\text{AlN}(s) + \text{C}(\text{graph.}) = \text{AINC}(g)$	568.2 ± 12.7	572.5 ± 12.7	587.9 ± 1.6	582.8 ± 4.3
$2\text{AICN}(g) + \text{Au}(g) = \text{Al}(g) + \text{N}_2(g) + \text{AlAu}(g) + 2\text{C}(\text{graph.})$	-274.1 ± 17.8	-262.9 ± 17.8	-300.7 ± 2.5	-288.8 ± 6.0
$2\text{AICN}(g) + 2\text{Al}(g) + \text{N}_2(g) + 2\text{C}(\text{graph.})$	68.0 ± 19.3	69.4 ± 19.3	21.3 ± 3.0	37.3 ± 6.6
$\text{AlN}(s) + \text{C}(\text{graph.}) = \text{AICN}(g)$	590.8 ± 12.7	594.9 ± 12.7	610.4 ± 1.6	605.2 ± 4.3
$2\text{AINC}(\text{AICN})(g) + \text{Au}(g) = \text{Al}(g) + \text{N}_2(g) + \text{AlAu}(g) + 2\text{C}(\text{graph.})$	-234.4 ± 17.8	-223.4 ± 17.8	-252.4 ± 2.3	-242.7 ± 6.0
$2\text{AINC}(\text{AICN})(g) = 2\text{Al}(g) + \text{N}_2(g) + 2\text{C}(\text{graph.})$	107.9 ± 19.2	109.1 ± 19.3	69.6 ± 2.8	82.8 ± 6.6
$\text{AlN}(s) + \text{C}(\text{graph.}) = \text{AINC}(\text{AICN})(g)$	570.8 ± 12.7	575.1 ± 12.7	586.2 ± 1.5	582.5 ± 4.3

^aThe error terms are standard deviations.

TABLE IV. Selected experimental results, in kJ mol^{-1} , for AINC and AICN, compared to theoretical literature values.

Species	Present investigation				G2 Theory ^a	
	$\Delta_f H_0^\circ$	$\Delta_a H_0^\circ$	$\Delta_f H_{298}^\circ$	$\Delta_a H_{298}^\circ$	$\Delta_f H_0^\circ$	$\Delta_a H_0^\circ$
AINC	281.3 ± 14	1228.1 ± 15	278.2 ± 14	1234.8 ± 15	266 ± 10	1246 ± 10
AICN	303.8 ± 14	1205.6 ± 15	300.9 ± 14	1212.5 ± 15	293 ± 10	1223 ± 10
AINC ^b	281.0 ± 14	1228.3 ± 15	277.9 ± 14	1235.0 ± 15		

^aReference 3.^bUsing total ion current of $m/e=53$ (see text).

The reaction enthalpies were calculated for AINC(*g*) and AICN(*g*) separately after proportioning the total measured ion current for m/e of 53 on the basis of the theoretically predicted energy difference of 1880 cm^{-1} between the two isomers. The value of 1880 cm^{-1} is the average between that calculated by Ma *et al.*¹ (1924 cm^{-1}), and that by Fukushima⁵ (1831 cm^{-1} at the CCD/6-311 G(*d*) level). Using the Gibbs energy functions of the isomers (see Table II) and the equation for the third-law enthalpy of the isomerization reaction, $\text{AINC}(g) = \text{AICN}(g)$, $\Delta H_0^\circ = -RT \ln K_p - T\Delta[(G_T^\circ - H_0^\circ)/T]$, the equilibrium constant of the isomerization reaction was calculated,^{33,34} and from that the ratio of AICN to AINC. The corresponding ion currents of AICN⁺ and AINC⁺ obtained from this ratio for each data set have been included in Table I.

The enthalpy changes, $\Delta_f H_0^\circ$, for the reactions (1)–(3) were calculated from the equilibrium data by the second-law method, based on a least-squares analysis of $\ln K_p$ vs $1/T$ plots, and by the third-law method. Table III lists the results of the second-law and third-law evaluations. To obtain a selected $\Delta_f H_0^\circ$ value for each reaction, the third-law value was given twice the weight of the second-law value.

The literature values for the enthalpies of formation, $\Delta_f H_0^\circ$, in kJ mol^{-1} , used to obtain the final values for the enthalpy of formation and atomization of AINC/AICN were: 327.3 ± 4.2 ,³⁰ 322.2 ± 6.3 ($D_0^\circ(\text{AlAu}, g)$),²⁴ -313.0 ± 2.5 ,³⁰ 711.2 ± 0.5 ,³⁰ 470.8 ± 0.1 ,³⁰ for Al(*g*), AlAu(*g*), AlN(*s*), C(*g*), and N(*g*), respectively. From the selected $\Delta_f H_0^\circ$ values (see Table III) and these auxiliary literature data, the respective $\Delta_f H_0^\circ$ and $\Delta_a H_0^\circ$ values were derived for each reaction. By giving the same weight to the reactions (1)–(3), we propose for the $\Delta_f H_0^\circ(\text{AINC}, g)$, $\Delta_f H_0^\circ(\text{AICN}, g)$, $\Delta_f H_{298}^\circ(\text{AINC}, g)$, $\Delta_f H_{298}^\circ(\text{AICN}, g)$, $\Delta_a H_0^\circ(\text{AINC}, g)$, $\Delta_a H_0^\circ(\text{AICN}, g)$, $\Delta_a H_{298}^\circ(\text{AINC}, g)$, and $\Delta_a H_{298}^\circ(\text{AICN}, g)$, in kJ mol^{-1} , the values 281.3 ± 14 , 303.8 ± 14 , 278.2 ± 14 , 300.9 ± 14 , 1228.1 ± 15 , 1205.6 ± 15 , 1234.8 ± 15 , and 1212.5 ± 15 , respectively. Here the uncertainties are the overall error obtained as discussed in Schmude *et al.*³⁵

Table IV lists our results together with the theoretical values of Petrie³ predicted by the GAUSSIAN-2 level of theory.

The theoretical values for the atomization energies of AINC and AICN are slightly higher than our experimental ones but agree within the error limits given.

Our value for the atomization energy of AINC/AICN, based on the total ion current of $m/e=53$, $\Delta_a H_0^\circ = (1228.3 \pm 15) \text{ kJ mol}^{-1}$ or $\Delta_a H_{298}^\circ = (1235.0 \pm 15) \text{ kJ mol}^{-1}$, can also be compared to the previous result of $\Delta_a H_{298}^\circ = (1243 \pm 21) \text{ kJ mol}^{-1}$,¹⁶ as reported, obtained by a third-law evaluation. Correcting the literature value of the atomization energy for the thermal functions of AINC(*g*) and the k_X values used in the present investigation, gives $\Delta_a H_0^\circ = (1212 \pm 21) \text{ kJ mol}^{-1}$ or $\Delta_a H_{298}^\circ = (1219 \pm 21) \text{ kJ mol}^{-1}$.

The upper value for the atomization energy, $\Delta_a H_0^\circ$, of $(1278 \pm 27) \text{ kJ mol}^{-1}$ reported by L'vov and Pelieva³⁶ has been determined by electrothermal atomic absorption spectrometry under the assumption that the observed decrease of absorption of elemental Al in the presence of nitrogen, N₂, inside a graphite furnace at high temperatures (e.g., 2700 K) in comparison with that in an argon atmosphere, to be solely due to the formation of gaseous aluminum monocyanide. The difference of 50 kJ mol^{-1} with our value suggests that molecular carbides such as Al₂C₂, AlC₂ are formed by interaction of aluminum with graphite at 2700 K in addition to AINC(AICN).

Our proportioning of the $m/e=53$ primary ion current to I(AINC⁺) and I(AICN⁺) has been based on the energy difference of 1880 cm^{-1} between the two isomers AINC and AICN predicted by the most advanced theoretical calculations.^{1,5} If we assume the same percentage of fragmentation for AINC yielding AlN⁺ and AINC yielding AIC⁺, our observation of approximately equal concentrations suggests that this energy difference would be smaller than the theoretical one and may even be reversed (AICN possibly being the more stable isomer).

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