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Knudsen cell mass spectrometric investigation of the B_2N molecule

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High-temperature Knudsen cell mass spectrometry has been used to study the equilibria involving the B_2N molecule over the Si–BN system. Thermal functions needed in the evaluation of the mass spectrometric equilibrium data have been calculated from available experimental and theoretical molecular parameters. The enthalpy changes for the reactions $2B(g) + Si_2N(g) = B_2N(g) + 2Si(g)$, and $BN(s) + B(g) = B_2N(g)$ have been measured. The following atomization enthalpy, $\Delta_a H_0^o$, and enthalpy of formation, $\Delta_f H_{298.15}^o$, in kJ mol^{-1}, of 1045.5 ± 18 and 551.3 ± 18 for the B_2N molecule have been determined from these reaction enthalpies. Atomization energies of similar molecules have been compared and discussed. © *2000 American Institute of Physics.* [S0021-9606(00)01044-8]

INTRODUCTION

Boron–nitrogen clusters have been extensively investigated because of their importance to gain a deeper insight in boron nitride thin film formation through chemical vapor deposition (CVD) and to understand the interactions between the solid and gas phase during the thin film formation. This is essential for improving the processes of deposition of boron nitride. In addition, boron–nitrogen clusters have received attention recently because of the existence of fullerenes analogues involving boron and nitrogen atoms.[1,2] In fact boron nitride is a structural analog to carbon, exhibiting bond length, long-order parameters, and lattice constants to be very similar to those of carbon.[3,4]

Boron nitride (BN) is a ceramic material mainly used as surface coating. BN exists in several allotropic forms including graphitelike α-BN, and diamondlike β-BN. The β form, or cubic phase, has significant technological potential for thin film application[5] and rivals diamond in extreme hardness. It also has a number of highly desirable mechanical, thermal, electrical, and optical properties.[4,5]

Different techniques have been applied to study boron-nitrogen containing molecules. Becker *et al.*[6,7] used laser ionization mass spectrometry to study the formation of $B_nN_m^+$ clusters ions in a laser plasma. They observed that for $B_nN_{n-1}^+$ and $B_nN_{n-2}^+$ cluster ions there is an alternating abundance distribution with the higher intensities of the cluster ions with the odd number of atoms. Andrews and co-workers reacted boron and nitrogen atoms in nitrogen[8] or argon[9] matrices. They identified BBNN, cyclic B_2N, BNB, NNBN, and BNBN from mixed isotopic patterns, and isotopic shifts, using Fourier transform infrared spectroscopy and *ab initio* calculations. Knight *et al.*[10] used a laser vaporization matrix isolation electron spin resonance (ESR) apparatus to study the BNB radical. They found that BNB has an $X\,^2\Sigma_u^+$ ground electronic state with a linear centrosymmetric

structure. Roland and Wynne[11] described photoionization and photofragmentation of B_xN_y clusters generated by laser vaporization of boron nitride followed by supersonic expansion. Thompson *et al.*[12,13] studied the infrared (IR) spectra of reaction products of laser ablated boron atoms with ammonia, during condensation with excess argon at 10 K. They observed cyclic and symmetric linear B_2N together with a series of hydrogen–boron–nitrogen containing species. Asmis *et al.*[14–17] employed a negative ion tandem TOF (time-of-flight) photoelectron spectrometer to determine adiabatic detachment energies and vibrational frequencies for several low-lying electronic states of BN, B_2N, and B_3N. In particular Asmis *et al.*[16] found no evidence for a low-lying cyclic isomer of B_2N. They reassigned the matrix IR spectra of Andrews and co-workers[9,12,13] to the $X\,^2\Sigma_u^+$ ground state of linear B_2N.

A large number of theoretical studies have been carried out on BN,[18–23] and polyatomic boron–nitrogen clusters.[16,24–31] The main aim of the computations on boron–nitrogen clusters was to optimize their structures, to calculate the relative stability of different isomers, the vibrational frequencies, the ionization energies and the electron affinities, and to estimate the atomization energies.

In continuation of our recent investigations on small nitrogen containing group 13 and 14 clusters,[32–37] we employed the Knudsen cell mass spectrometric method to perform the first equilibrium study on B_2N and to determine its atomization energy and enthalpy of formation. A preliminary value for the atomization energy of B_2N has previously been reported.[32]

THEORETICAL INVESTIGATIONS

Ab initio calculations were carried out utilizing the GAUSSIAN 98 program package[38] in order to gain information about the ionization energy (IE), electron affinity (EA), and atomization enthalpy ($\Delta_a H_0^o$) of the ground state of B_2N. The calculations were performed at the density-functional level of theory using the Becke three-parameter exchange functional with the Lee, Yang, and Parr correlational func-

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TABLE I. Comparison between our calculations and the experimental molecular parameters, electron affinity (EA), ionization energy (IE), and atomization enthalpy ($\Delta_a H_0^o$) of the $X\,^2\Sigma_u^+$ B_2N molecule and of the $X\,^2\Pi_g$ Si_2N molecule.

Method/Basis set	$r_{X\text{-}N}$[a] ($X = $ B or Si)	ν_1[b]	ν_2	ν_3	EA[c]	IE	$\Delta_a H_0^o$[d]
B_2N molecule							
B3LYP/cc-pVTZ	1.313	1195	125	1326	2.885	10.67	1102
G1[e]	1.327	1183	153	2392	3.34	8.65	1050
MP4(SDTQ)/6-31G*[f]	1.338						
CCSD(T)/aug-cc-pVTZ[g]	1.328	1143	85	$i1320$	3.139		
APES[h]		1143		855	3.098		
KC-MS[i]						9.7	1046
Si_2N molecule							
B3LYP/cc-pVTZ	1.638	615	223	1066	0.914	6.34	974
CCSD(T)/cc-pVTZ[j]	1.644	614	187	917			
R2PIS[k]	1.640					<8.51	
KC-MS[l]						6.6	1011

[a]The bond lengths are in Å.
[b]ν_1 is the symmetric stretching (σ_g), ν_3 the antisymmetric stretching (σ_u), and ν_2 the bending vibrational mode, in cm^{-1}.
[c]EA and IE are in eV.
[d]$\Delta_a H_0^o$ is in kJ mol^{-1}.
[e]G1 is for GAUSSIAN 1 theory, see Ref. 25.
[f]Reference 10.
[g]Reference 16.
[h]APES is for anion photoelectron spectroscopy, see Ref. 16.
[i]KC-MS is for Knudsen cell mass spectrometry (present investigation).
[j]Reference 39.
[k]R2PI is for resonant two-photon ionization spectroscopy, see Ref. 40.
[l]Reference 34.

tional (B3LYP). The basis set employed for this study was a correlated consistent polarized valence triple-zeta basis set, cc-pVTZ.

From the calculations the lowest lying $^2\Sigma_u^+$ electronic state is found to have the linear symmetric structure in agreement with experimental[10,15,16] and theoretical[9,10,16,24,25] literature data. This result is also in agreement with experimental and theoretical results for similar molecules, Si_2N,[39,40] and Al_2N,[37,41] which too have linear symmetric structures as the most stable ground-state geometry.

The vibrational frequencies for the three vibrational normal modes, the optimized bond lengths, and the physical chemical properties, corrected for the zero-point energies (ZPE), of the $X\,^2\Sigma_u^+$ state for B_2N are listed in Table I, and compared with available experimental and theoretical values. The calculated EA of B_2N at the B3LYP/cc-pVTZ level of theory is about 7% lower than the experimental value of (3.098 ± 0.005) eV.[16]

In order to support our computations, we calculated the bond distances, vibrational frequencies, electron affinity, ionization energy, and atomization enthalpy for the Si_2N molecule at the same level of theory used for B_2N, and compared them with available experimental and theoretical values. The results are reported in Table I. Our computed silicon–nitrogen bond distance practically coincides with the experimental value of (1.6395 ± 0.0014) Å by Brugh and Moorse.[40] The computed IE of 6.34 eV of Si_2N agrees with the value of (6.6 ± 0.5) eV obtained from the linear extrapolation method by Gingerich et al.[34]

Asmis et al.[16] measured the symmetric and antisymmetric vibrational modes of B_2N by anion photoelectron spectroscopy. The calculated symmetric stretching mode agrees with the experimental value of 1143 cm^{-1} at all levels of theory used, B3LYP/cc-pVTZ, Gaussian 1 (G1), and CCSD(T)/aug-cc-pVTZ, but the calculations of the asymmetric stretching mode, ν_3, failed in reproducing the experimental value of 855 cm^{-1}. This problem has been explained by a distortion along the asymmetric stretch coordinate yielding a wave function which is oversimplified and leading to an artifactual structure on the potential energy surface.[16] The surprisingly low experimental value of ν_3 has been attributed to Herzberg–Teller coupling between the $X\,^2\Sigma_u^+$ and the low-lying $A\,^2\Sigma_g^+$ excited state.[16]

EXPERIMENT

The mass spectrometer and experimental procedures used for this work have been described previously.[42] The sample of semiconductor grade silicon powder and Si_3N_4 of 99.9% purity was contained in a boron nitride Knudsen cell, which was inserted into a graphite cell having a molybdenum lid. The molybdenum lid intended to minimize the formation of disilicon carbide, Si_2C, and the overlap of its isotope with those of Si_2N. The Si_3N_4 had decomposed almost completely in the temperature range of present measurements, and the boron nitride served as the source of nitrogen. The liquid silicon also served as a catalyst for the equilibration of BN with the nitrogen containing species,[43] since BN has a low-vaporization coefficient lower than 6×10^{-3}.[44]

The Knudsen cell was heated by radiation from a tungsten coil resistor and the temperatures were measured with a calibrated Leeds and Northrup optical pyrometer focused

TABLE II. Measured relative ion currents, in A, over the Si–BN system, and third-law values, in kJ mol^{-1}, of the $\Delta_r H_0^o$ and $\Delta_a H_0^o$ of B_2N.

| T (K)	Ion intensities				$\Delta_r H_0^o$ Reaction (1)	$\Delta_a H_0^o$	$\Delta_r H_0^o$ Reaction (2)	$\Delta_a H_0^o$
	B^+	Si_2N^+	Si^+	B_2N^+				
2066	1.10E−12	2.70E−12	2.04E−10	5.30E−15	−35.72	1046.3	238.2	1040.6
2082	1.55E−12	3.80E−12	2.75E−10	9.54E−15	−38.71	1049.3	235.7	1043.1
2119	1.88E−12	8.20E−12	3.12E−10	2.10E−14	−37.36	1047.9	229.4	1049.4
2146	2.32E−12	1.27E−12	1.87E−10	1.68E−14	−41.33	1051.9	240.0	1038.8
2095	8.71E−13	3.43E−13	9.30E−11	2.88E−15	−42.28	1052.8	248.0	1030.8
2052	8.69E−13	2.94E−13	6.10E−11	3.87E−15	−34.81	1045.4	237.9	1040.9
2135	1.92E−12	6.65E−13	1.12E−10	1.91E−14	−43.11	1054.0	233.1	1045.7
					−39.1±3.3[a]	1049.7±3.3	237.5±5.9	1041.3±5.9

[a]The error terms are standard deviations.

onto a black body hole at the bottom of the graphite cell. Appropriate window and prism corrections were applied. The ions were produced with ionizing electrons and electron emission current of 12 eV and 10 mA, respectively. The acceleration voltage used was 4.5 kV and the electron multiplier was operated at −3 kV.

The ions pertinent to the present investigation were B^+, Si^+, Si_2N^+, and B_2N^+. The ions were identified by their mass-to-charge ratio, isotopic abundance, and ionization efficiency curves. At each measurement a movable slit was interposed into the molecular beam to distinguish between ions produced from species in the beam and from residual gases with the same mass-to-charge ratio in the ionization region of the mass spectrometer. The electron impact energy was calibrated against the first ionization energy of B (8.296 eV)[45] and Si (8.149 eV).[45] The appearance potential of (9.7 ±0.5) eV was measured for B_2N by the linear extrapolation method. The measured appearance potential is 9% lower than our computed value of 10.67 eV (see Table I), and 12% higher than the G1 value of 8.65 eV.[25]

The ion current data of the species pertinent to this investigation are listed in Table II. In the case of B_2N the ion intensities at mass 35 were measured due to better signal-to-noise ratio; for all other species the maximum intensity peaks were recorded. The ion intensity of Si_2N^+ in Table II has been corrected for a small contribution due to Si_2C; the maximum correction was 10% at $m/e = 70$.

RESULTS AND DISCUSSION

For the determination of the enthalpy of formation, $\Delta_f H_0^o$, and the enthalpy of atomization, $\Delta_a H_0^o$, of B_2N, the enthalpy changes of the following reactions:

$$2B(g) + Si_2N(g) = B_2N(g) + 2Si(g), \qquad (1)$$

$$BN(s) + B(g) = B_2N(g), \qquad (2)$$
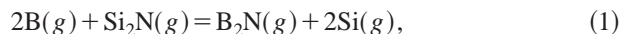
were evaluated according to the third-law method, using the relation $\Delta_r H_0^o = -RT \ln K_p - T\Delta[(G_T^o - H_0^o)/T]$.

The Gibbs energy functions, $(G_T^o - H_0^o)/T$ (GEF$_0$), and the heat content functions, $H_T^o - H_0^o$ (HCF$_0$), needed in the evaluation of the reactions enthalpies were taken from literature for B(g),[46] Si(g) (Ref. 46, Vol. 2), BN(s),[46] and $Si_2N(g)$.[34] Those for $B_2N(g)$ were computed according to statistical thermodynamic procedures, using the rigid-rotor

harmonic-oscillator approximation[47] and the molecular constants computed at the CCSD(T)/aug-cc-pVTZ level of theory by Asmis et al.,[16] bond distance of 1.328 Å and bending vibrational mode of 85 cm^{-1} for which there are no experimental values. These values have been preferred to those calculated at the B3LYP/cc-pVTZ level of theory because of the higher level of theory used. For the asymmetric and symmetric vibrational frequencies the experimental values of 855 and 1143 cm^{-1}, respectively, were used.[16] The $A\,^2\Sigma_g^+$ excited state with the transition energy (T_e) of 6330 cm^{-1} (Ref. 16) was also considered. Table III lists the thermal functions of B_2N.

Reactions (1) and (2) are pressure independent, therefore, the measured ion intensities listed in Table II were utilized directly to calculate the equilibrium constant of the reactions (1) and (2), after correcting them for the isotopic abundance and ionization cross sections. For the multiplier gains cancellation of mass and molecular effects was assumed. The isotopic abundance of the atomic species was taken from Kiser,[48] and those of the molecular species were calculated from the isotopic abundance of the constituent elements. The relative ionization cross section used, σ, in 10^{-16} cm^2, were taken from experimental values reported in the literature, except for B, where a calculated value was used: B, 0.72;[49] Si, 3.34;[50] N, 0.05;[51] Si_2N, 5.69 as $0.75 \times (2\sigma_{Si} + \sigma_N)$; B_2N, 1.12 as $0.75 \times (2\sigma_B + \sigma_N)$.

The literature values for the enthalpies of formation, $\Delta_f H_0^o$, in kJ mol^{-1}, used to obtain the final values for the enthalpy of formation and atomization of B_2N were: 559.9±5.0,[46] 445.7±8.0,[46] −248.1±1.0,[46] 351.6±14.8,[34] and 470.8±0.1[52] for B(g), Si(g), BN(s), $Si_2N(g)$, and N(g), respectively. From the $\Delta_r H_0^o$ values, see Table II, and

TABLE III. The Gibbs energy functions, $(G_T^o - H_0^o)/T$ (GEF$_0$), in J K^{-1} mol^{-1}, and the heat content functions, $H_T^o - H_0^o$ (HCF$_0$), in kJ mol^{-1}, for the B_2N molecule.

Species		Temperature (K)					
		298.15	1400	1600	1800	2000	2200
B_2N	−GEF$_0$	201.8	277.4	284.7	291.3	297.3	302.7
	HCF$_0$	12.91	76.51	88.87	101.4	114.0	126.7

these auxiliary literature data the respective $\Delta_f H_0^o$ and $\Delta_a H_0^o$ were derived, using the following relations: for reaction (1), $\Delta_f H_0^o(B_2N, g) = \Delta_r H_0^o - 2\Delta_f H_0^o(Si, g) + 2\Delta_f H_0^o(B, g) + \Delta_f H_0^o(Si_2N, g)$ and $\Delta_a H_0^o(B_2N, g) = 2\Delta_f H_0^o(B, g) + \Delta_f H_0^o(N, g) - \Delta_f H_0^o(B_2N, g)$; for reaction (2), $\Delta_f H_0^o(B_2N, g) = \Delta_r H_0^o + \Delta_f H_0^o(B, g) + \Delta_f H_0^o(BN, s)$.

By giving the same weight to both reactions employed in the present investigation, we obtain the values, in kJ mol^{-1}: 1045.5 ± 18, 1051.4 ± 18, 545.2 ± 18, and 551.3 ± 18 for $\Delta_a H_0^o$, $\Delta_a H_{298.15}^o$, $\Delta_f H_0^o$, and $\Delta_f H_{298.15}^o$ of $B_2N(g)$, respectively. Here the uncertainties are the overall errors obtained as discussed by Schmude et al.[53]

Our computed $\Delta_a H_0^o(B_2N, g)$ value of 1102 kJ mol^{-1} is about 5% higher than the experimental value, and the scaled CCD+STD(CCD)/6-31G* value of 1109 kJ mol^{-1} (Ref. 24) is about 6% higher than our experimental value. The G1 $\Delta_a H_0^o(B_2N, g)$ value of 1050 kJ mol^{-1} (Ref. 25) is in good agreement with our experimental value.

It is interesting to compare the thermodynamic stability of similar molecules. The atomization energy, in kJ mol^{-1}, of B_2N, B_2C,[46] B_2O,[25] Al_2N,[37] Al_2C,[54] Al_2O[46] are: 1045 ± 18, 1060 ± 30, 1211 ± 8, 783 ± 15, 852 ± 42, and 1050 ± 20, respectively. The $\Delta_a H_0^o$ of Al_2C was estimated by Gurvich et al.[54] from the relative abundance of Al_2C^+ observed by Chupka et al.[55] For B_2O the theoretical value based on the G1 method has been used since no reliable experimental value is available.

The thermodynamic stability of the B_2–X and Al_2–X type molecules (X=N, C, and O) increases with the replacement of N by C and C by O, B_2O and Al_2O being the most stable. B_2N and B_2C, as well as Al_2N and Al_2C, have comparable stability.

ACKNOWLEDGMENTS

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