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Studies on the doubly charged cluster ions of sodium and potassium nitrates by electrospray ionization tandem mass spectrometry

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Abstract

Doubly charged cluster ions, besides singly charged cluster ions, from sodium and potassium nitrates were produced evidently under normal source capillary temperature of 200 °C in both positive and negative ion electrospray ionization (ESI) ion trap mass spectrometry. The fragmentation pathways for doubly charged cluster ions were studied in detail using ESI tandem mass spectrometry and two pathways were observed depending on the cluster sizes of alkali metal nitrates. In addition, factors that affect the formation of cluster ions were also interrogated.

Keywords: Cluster; Electrospray ionization tandem mass spectrometry; Sodium nitrate; Potassium nitrate; Collision induced dissociation

1. Introduction

The study of clusters has attracted substantial attention during the past two decades and cluster science has become an increasingly active discipline. This is due to the fact that the physical properties of these weakly bounded species are different from those of other states. Cluster studies are important because cluster ions span the chemical and physical gap between discrete atoms or molecules and solid materials, and provide clues to the transitions between the condensed and gaseous states of matter [1]. Understanding of phase transition, crystal growth, chemical catalysis, and thin film preparation [2,3] may all benefit from the study of clusters. In addition, naturally occurring clusters are also of significance to the environment [4].

Although many analytical technologies are employed in cluster research [5–8], the relatively gentle nature of electrospray ionization (ESI) and the ability to create ions directly from solution, make ESI an attractive approach for studying the property of clusters where other methods may be overly destructive. ESI mass spectrometry cannot only determine the molecular weight of clusters, but also can infer structural information through tandem mass spectrometry. Hao et al. investigated the influence of experimental conditions such as ionic radius, instrument settings and solution pH on the formation of cluster ions from alkali chloride and sodium salts by ESI [9,10]. In some studies salts of the alkali metals have been used to probe the electrospray ion formation mechanism [11,12]. Other researchers have reported that cluster ions could act as a calibration standard for ESI mass spectrometry [13,14]. It is also found that doubly charged cluster ions could be produced from ESI and collision induced dissociation (CID) was employed to determine their fragmentation pattern [15,16]. However, the doubly charged cluster ions were mostly generated in the positive ion mode. Recently, Van Stipdonk et al. used ESI to generate distributions of gas phase cluster ions from solutions of sodium and potassium tetrafluoroborate, which is hard to investigate by other methods [17].

The majority of literature on clusters dealt with singly charged cluster ions, only a few studied doubly charged cluster ions [15,16], even few studied in the negative ion mode [9,10]. Alkali metal nitrates are widely used in industry and of great importance to the environment. In our former study, we found that potassium nitrates can form singly charged cluster ions under ESI conditions [18]. In this paper, we investigated sodium and potassium nitrates systematically using ESI

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ion trap mass spectrometer. Doubly charged cluster ions of alkali metal nitrates, in addition to singly charged cluster ions, were produced evidently under normal source capillary temperature (200 °C), and their fragmentation pathway upon CID as well as factors that affect their formation was studied in detail.

2. Experimental

2.1. Reagents and preparation of the samples

Alkali metal nitrates are of analytical grade from Beijing Chemicals Factory (Beijing, China). Methanol is HPLC grade from Fisher Scientific (Fair Lawn, NJ, USA). Water is from Milli-Q water purification system (Millipore, El Paso, TX, USA).

Certain samples were weighed and prepared to 1.0 mol/L stock solution in 1:1 methanol–water (v:v). The 1.0 mol/L solution were diluted to 0.1, 0.01, 0.001, and 0.0001 mol/L using 1:1 methanol–water (v:v) before analyzing by mass spectrometry.

2.2. Apparatus and conditions

A Finnigan MAT LCQ^{TM} mass spectrometer (San Jose, CA, USA) was used in all experiments. The mass spectrometer was equipped with an ESI source, and ESI parameters were: spray voltage 4.0 kV, temperature of the heated capillary 200 °C, capillary voltage ±14 V, tube lens offset ±35 V, N_2 sheath gas flow 40 (arbitrary units). Maximum injection time of the trap analyzer was 200 ms. The mass to charge (*m*/*z*) range of the instrument is 50–2000. During collision induced dissociation (CID) experiments, mass-selected cluster ions were isolated in the ion trap and collisionally activated with 10–50% ejection RF-amplitude depending on the cluster sizes at standard He pressure. The ESI conditions are maintained constant unless they are specified again. The sample solution was introduced with a syringe pump at a flow rate of 3.0 μL/min, and the spectra represented 20 scans averaged data.

3. Results and discussion

3.1. Positive and negative ion mass spectra of cluster of alkali metal nitrates

The mass spectrum of cluster consists of even-spaced mass peaks. The positive and negative ion mass spectra of 0.1 M $NaNO_3$ solution are shown in Fig. 1a and b, respectively. Both singly and doubly charged cluster ions are observed in Fig. 1a. The singly charged cluster ions have the formula $[(NaNO_3)_mNa]^+$ ($m = 2–23$), and form a series of peaks in the mass spectrum differing by one $NaNO_3$ unit; a second series of cluster ions exists in the mass spectrum, as evidenced by ion signals located between each singly charged cluster ion. The second series is doubly charged cluster ions of the form $[(NaNO_3)_pNa_2]^{2+}$ ($p = 17–46$), differing by 0.5 $NaNO_3$ unit in the mass spectrum. In the negative ion mass spectrum (Fig. 1b), singly and doubly charged cluster ions are also present. The singly and doubly charged cluster ions have the formula of $[(NaNO_3)_n(NO_3)]^-$ ($n = 2–22$) and $[(NaNO_3)_q(NO_3)_2]^{2-}$ ($q = 18–45$), respectively. In both positive and negative ion mass spectra because the spacing of doubly charged clusters is half that of their singly charged counterparts, overlapping of the two series occurs at positions where $p = 2m$ (positive ion) and $q = 2n$ (negative ion). Superimposed ion signals due to singly and doubly charged ions are observed when p is even for all values of m (10–22) in Fig. 1a.

The positive and negative ion ESI mass spectra of 0.1 M KNO_3 solution are shown in Fig. 2a and b, respectively. Similar to those of 0.1 M $NaNO_3$ solution, both singly and doubly charged cluster ions are present in the mass spectra. However, the intensity of KNO_3 cluster ions is lower than that of $NaNO_3$ counterparts. In the positive ion mass spectrum (Fig. 2a), singly and doubly charged cluster ions have the formula of $[(KNO_3)_mK]^+$ ($m = 2–19$) and $[(KNO_3)_pK_2]^{2+}$ ($p = 19–38$), respectively; In the negative ion mass spectrum (Fig. 2b), singly and doubly charged cluster ions are in the form of $[(KNO_3)_n(NO_3)]^-$ ($n = 1–19$) and $[(KNO_3)_q(NO_3)_2]^{2-}$ ($q = 18–38$), respectively. Overlapped ion

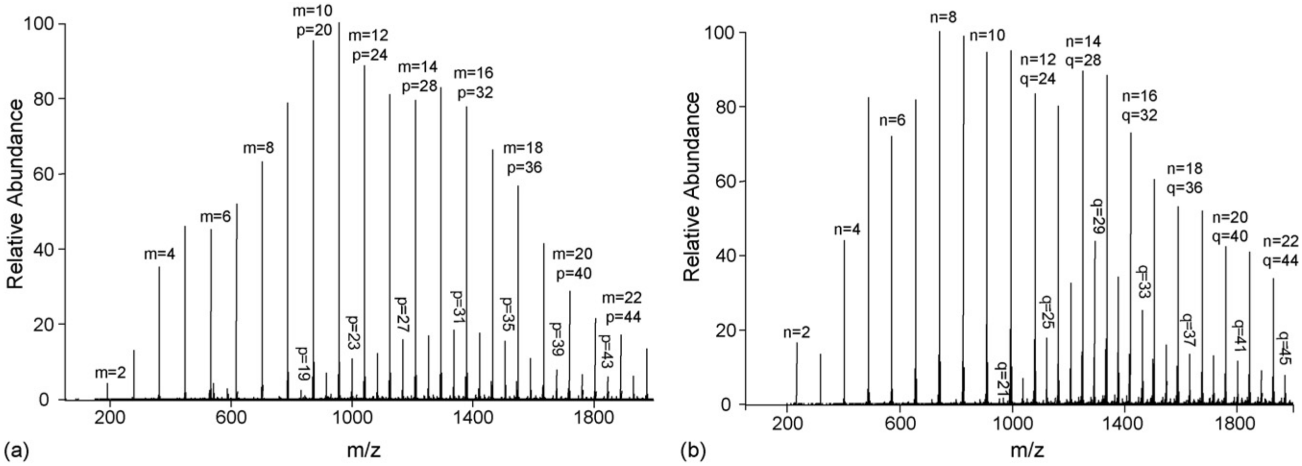


Fig. 1. Full-scan mass spectra of 0.1 M $NaNO_3$ solution under positive (a) and negative (b) ion electrospray conditions. Cluster ions are in the forms of $[(NaNO_3)_mNa]^+$, $[(NaNO_3)_pNa_2]^{2+}$ (a) and $[(NaNO_3)_n(NO_3)]^-$, $[(NaNO_3)_q(NO_3)_2]^{2-}$ (b).

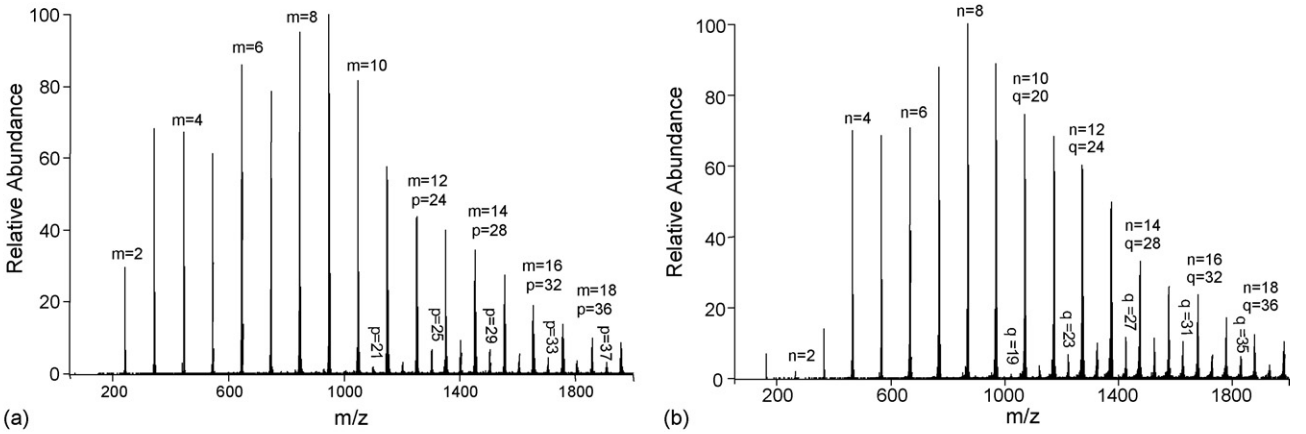


Fig. 2. Full-scan mass spectra of 0.1 M KNO_3 solution under positive (a) and negative (b) ion electrospray conditions. Cluster ions are in the forms of $[(KNO_3)_mK]^+$, $[(KNO_3)_pK_2]^{2+}$ (a) and $[(KNO_3)_n(NO_3)]^-$, $[(KNO_3)_q(NO_3)_2]^{2-}$ (b).

signals due to singly and doubly charged ions are also observed when p or q is even in the mass spectrum.

Note that there is no discontinuity (even in the lower capillary temperature of 100 °C, see Section 3.4) in the cluster size (number) of doubly charged cluster ions of both sodium and potassium nitrates in positive ion ESI mass spectra. This contrasts with that of doubly charged cluster ions of sodium and potassium chloride in positive ion ESI mass spectra [9,15].

3.2. Critical size and magic number

A significant nature of multiply charged clusters is critical size that is defined operationally by the smallest observable multiply charged cluster. It was found that critical size depends on experimental conditions. For instance, doubly charged clusters of alkali halides have been investigated by photoionization methods and a critical size of $m = 18$ was observed for $[(NaI)_mNa_2]^{2+}$ [19], the same value was found for doubly charged KBr and CsI clusters [20]. But when sodium chloride was interrogated by ESI mass spectrometry under source capillary temperature of 120 °C, a critical size of 11 was found for doubly charged cluster ion $[(NaCl)_mNa_2]^{2+}$ [15]. In our experiments when the capillary temperature of ESI source was lowered to 100 °C, the critical size of doubly charged cluster ions for $NaNO_3$ salt was $p = 13$ (relative abundance 6.2%) and $q = 11$ (relative abundance 12%) in positive and negative ion mass spectra, respectively. For KNO_3 salt, the critical size of doubly charged cluster ions was 11 in both positive ($p = 11$, relative abundance 3.8%) and negative ($q = 11$, relative abundance 2.1%) ion mass spectra. When the capillary temperature was lowered further to 75 °C, the critical size of doubly charged cluster ions for both sodium and potassium nitrate did not change (although the intensity of corresponding cluster ion decreased) which indicates that the coulombic repulsion for each of the four critical size ions is just less than the dissociation energy for the corresponding cluster ion.

An intriguing mass spectrometric result in the study of clusters is magic number effect that refers to the irregularity in intensity as a function of cluster size. Cluster abundance distributions are considered a direct reflection of their relative stabilities so magic number clusters have special stable structure. From Figs. 1 and 2, the intensity of both doubly and singly charged cluster ions is not uniform with the increase in cluster size, which indicates that magic numbers are present. Because of the overlap of signals due to singly and doubly charged clusters when p or q is even, the relative abundance of the overlapped singly and doubly charged cluster ions cannot be determined unambiguously from above conditions. However, by using energetic instrumental conditions, less stable clusters could decompose and more stable clusters could be emphasized [16]. Hence we increased the capillary temperature from 200 to 300 °C (the upper temperature limit of the instrument), the prominent magic number clusters were observed and shown in Table 1.

The magic numbers of singly charged potassium nitrate clusters are consistent with those of our former study [18], and $n = 4$, 9 in the negative ion mode are also magic numbers in sodium and potassium chloride [9]. The magic number of sodium nitrate clusters is a little bigger than corresponding magic number of potassium nitrate clusters and this discrepancy may be due to different radius between sodium and potassium ion. The prominent magic number (29, 33, 35) of doubly charged nitrate salts is one number smaller than corresponding magic number (30, 34, 36) of doubly charged sodium chloride reported by Zhang and Cooks [15]. Because the magic number cluster is stable, a regular structure is usually preferred. In the doubly charged magic number clusters of sodium nitrate, the two sodium ions in excess may be attached to nitrate ions and separated as far as possible to minimize coulombic repulsion.

Table 1
The prominent magic numbers of clusters of sodium and potassium nitrates

	$NaNO_3$		KNO_3	
	Positive ion	Negative ion	Positive ion	Negative ion
Singly charged (m/n)	6, 10	5, 11	3, 6	4, 9
Doubly charged (p/q)	33	35	29	33

3.3. ESI tandem mass spectrometry of doubly charged cluster ions

Because collision induced dissociation (CID) is an excellent way to study the structure of gas phase ions, CID has been used to probe the structure, stability, and fragmentation behavior of cluster ions produced from sodium and potassium nitrates.

3.3.1. Cluster ions from sodium nitrate

For positively charged cluster ions from sodium nitrate, the authors firstly selected the doubly charged cluster ions of odd number because they were not overlapped by signals from singly charged cluster ions. Because the intensity of $p = 17$ doubly charged cluster ion was too low to trap, we began with $p = 19$ (*m*/*z* 830.5) cluster ion and the product ions of it are mainly singly charged cluster ions generated by charge separation in 20% collision energy CID (Fig. 3a). However, some neutral losses (up to two $NaNO_3$ units) and the inceptive dication $p = 17$ can also be seen; For $19 < p \leq 27$, the fragmentation pathways observed in low energy CID are those of charge separation into singly charged cluster ions and the loss of neutral $NaNO_3$ units (up to five) to form doubly charged cluster ions of lower mass/charge ratio (Fig. 3b). With the increase in cluster size in above range the relative abundance of product singly charged cluster ions is decreasing compared to that of corresponding doubly charged cluster ions, hence the fragmentation pathway of neutral $NaNO_3$ units losses is increasing. For $p > 27$, the sole fragmentation pathway becomes the loss of neutral $NaNO_3$ molecules (up to nine) to form doubly charged cluster ions of lower mass/charge ratio (Fig. 3c). The larger precursor clusters might be more stable to the fission-type of reaction (which can be related to the ability to separate the cations and minimize coulombic repulsion), and thus favor the elimination of one or more $NaNO_3$ units. In addition, the relative collision energy (which was employed to generate smaller than 30% of the relative abundance of the precursor ion) used to dissociate cluster ions was plotted as a function of cluster size (odd cluster number) (Fig. 4, line with square) and it can be seen that as a whole the larger cluster requires more relative collision energy than the smaller one does. The most abundant ion in the product ions is highly stable and usually a magic number ion (for instance, $m = 18$, $p = 22$, $p = 33$ in Fig. 3a–c, respectively).

Secondly, we selected the doubly charged cluster ions of even-number to be interrogated by CID. Because of the overlapping of doubly charged cluster ion and singly charged counterpart at cluster number $p = 2m$, a mixture of the two types

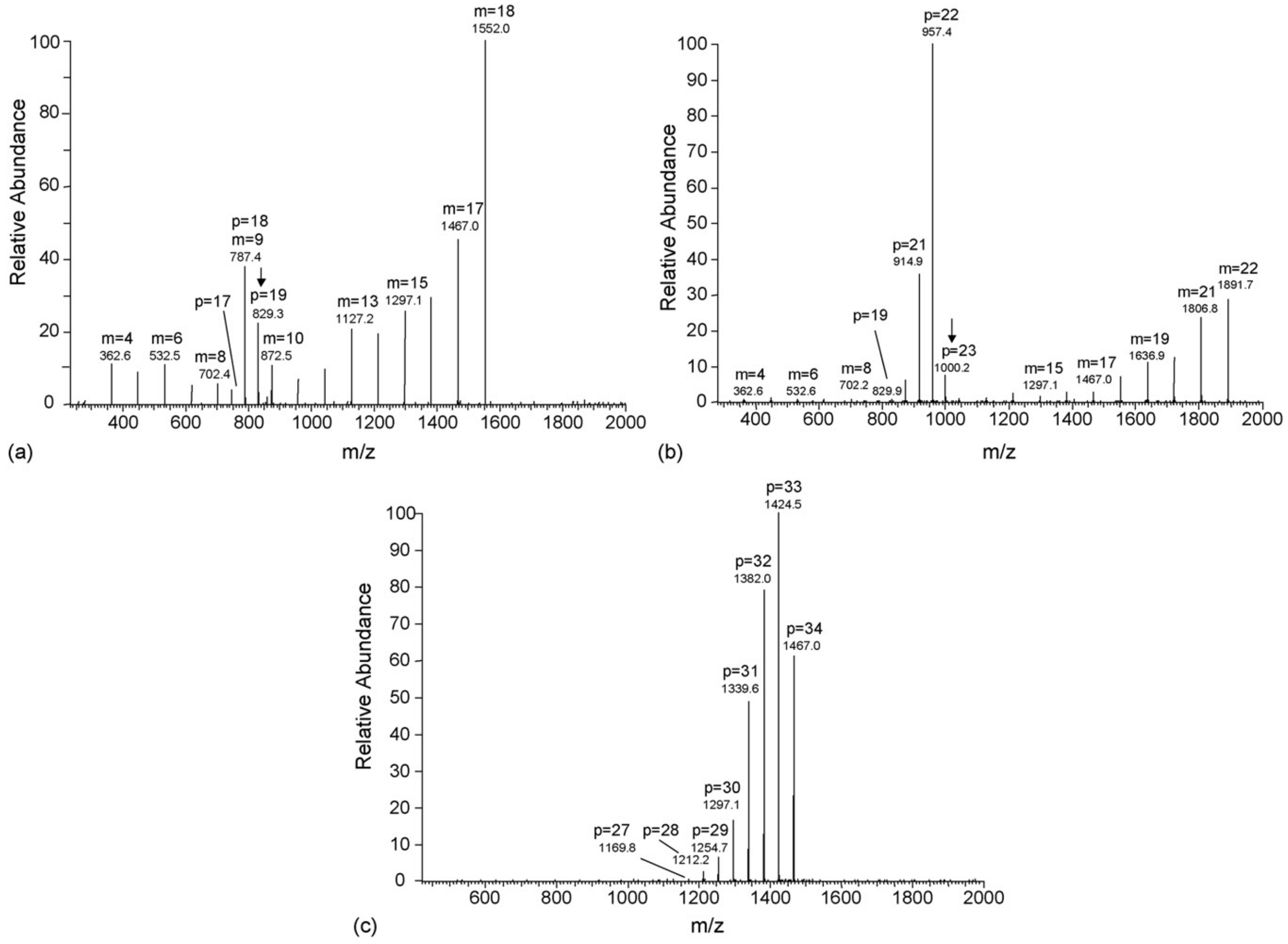


Fig. 3. MS/MS mass spectra of doubly charged clusters in the form of $[(NaNO_3)_pNa_2]^{2+}$ in odd cluster number: (a) $p = 19$ (*m*/*z* 830.5, relative collision energy 20%); (b) $p = 23$ (*m*/*z* 1000.2, relative collision energy 21%); (c) $p = 35$ (*m*/*z* 1510, relative collision energy 32%).

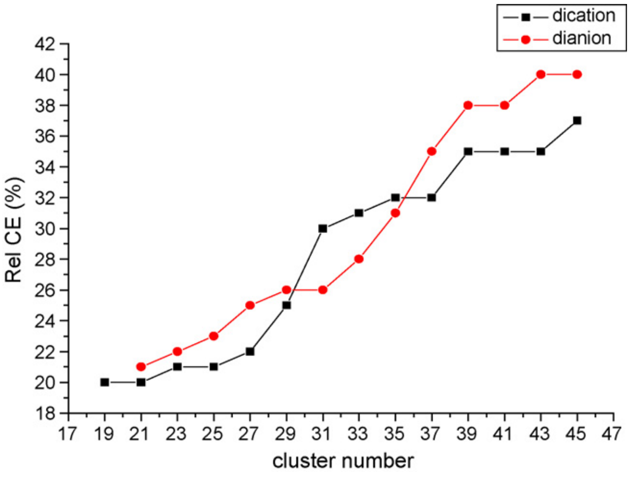
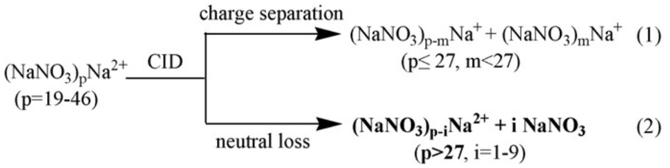


Fig. 4. The relative collision energy (the collision energy was to generate smaller than 30% of the relative abundance of the precursor ion) (Rel CE, %) during CID for doubly charged cluster ions of sodium nitrate in odd cluster number measured as a function of cluster size.

of cluster ions was isolated. Nevertheless, we can gain enough information from the CID of the even-number cluster ions. For $18 \leq p \leq 26$ and $9 \leq m \leq 13$, the main fragmentation profile is the loss of $NaNO_3$ units to form singly charged cluster ions of lower mass/charge ratio in low energy CID (Fig. 5a, $p = 22$ and $m = 11$), which shows that singly charged cluster ion is dominant in the precursor ion mixture. For $p > 26$ and $m > 13$, because of the increased contribution of doubly charged cluster ion signal to the precursor ion signal, the product ions are of lower mass/charge ratio due to the loss of $NaNO_3$ units from both singly and doubly charged cluster ions, respectively (Fig. 5b, $p = 30$ and $m = 15$). From the mass spectrum in Fig. 5b, it was observed that the relative abundance of the doubly charged cluster ions with even-number is higher than their neighboring odd-number counterparts. This may be due to two reasons: one is that in the precursor ion mixture the quantity of singly charged cluster ion is larger than that of doubly charged counterpart, and produced more singly charged product ions; the other is that the relative abundance of the doubly charged cluster ion with even-number is an addition of the abundance of singly and doubly charged product ions in the same mass/charge ratio.



Scheme 1. Fragmentation pathways of positively charged cluster ions of sodium nitrate $[(NaNO_3)_pNa_2]^{2+}$ (where bold form shows the fragmentation pathway of cluster ions of $p > 27$).

In the positive ion mass spectrum, the non-overlapped singly charged cluster ions ($m < 9$) lose a series of $NaNO_3$ units to form singly charged ions of lower mass/charge ratio in low energy CID.

In brief summary, for the positively charged cluster ions of sodium nitrate, $[(NaNO_3)_pNa_2]^{2+}$, where $19 \leq p \leq 27$, the fragmentation pathways observed are those of charge separation into singly charged cluster ions and the loss of neutral $NaNO_3$ units to form doubly charged cluster ions of lower mass/charge ratio (Scheme 1, pathway 1 and 2). This behavior contrasts with that of NaCl dications (containing smaller than 35 NaCl molecules) which generated only charge separation product ions [15]. For the positively charged cluster ions, $[(NaNO_3)_pNa_2]^{2+}$, where $p > 27$, the sole fragmentation pathway becomes the loss of neutral $NaNO_3$ molecules to form doubly charged cluster ions of lower mass/charge ratio (Scheme 1, pathway 2). With the increase in cluster size and the distance between two excess cations, the coulombic repulsion becomes less and the doubly charged cluster ion becomes more stable.

In the negative ion mode, for doubly charged cluster ions of sodium nitrate, $[(NaNO_3)_q(NO_3)_2]^{2-}$, the fragmentation pathways are similar to those of positively charged cluster ions. For $21 \leq q \leq 25$, the fragmentation pathways observed are those of charge separation into singly charged cluster ions and the loss of neutral $NaNO_3$ units to form doubly charged cluster ions of lower mass/charge ratio. From $q > 25$ on, loss of neutral $NaNO_3$ units becomes the only fragmentation pathway observed.

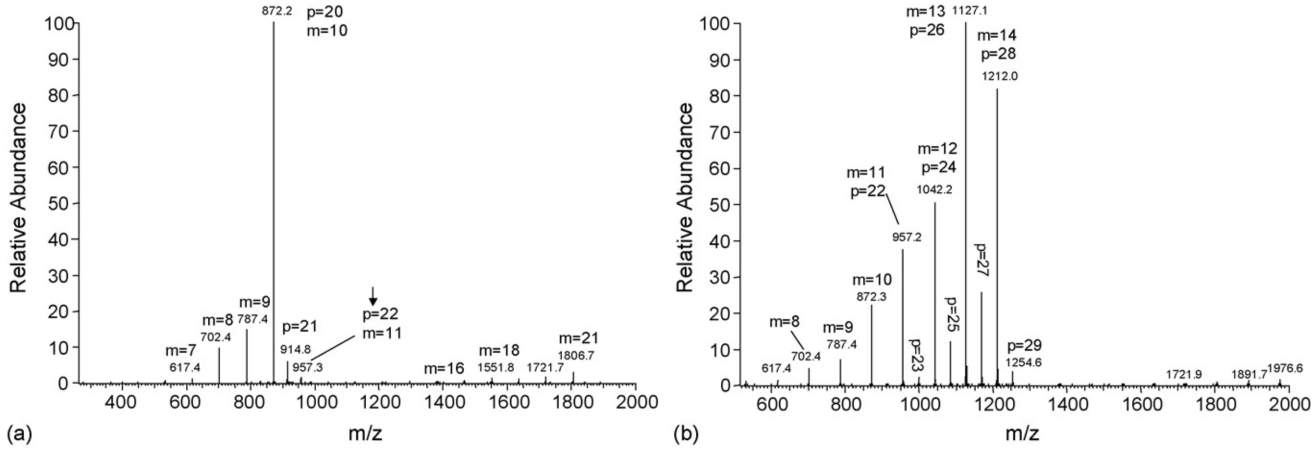


Fig. 5. MS/MS mass spectra of singly and doubly charged clusters in the form of $[(NaNO_3)_mNa]^+$ and $[(NaNO_3)_pNa_2]^{2+}$: (a) $m = 11$and $p = 22$ (m/z 957.5, relative collision energy 20%) and (b) $m = 15$ and $p = 30$ (m/z 1297.6, relative collision energy 40%).

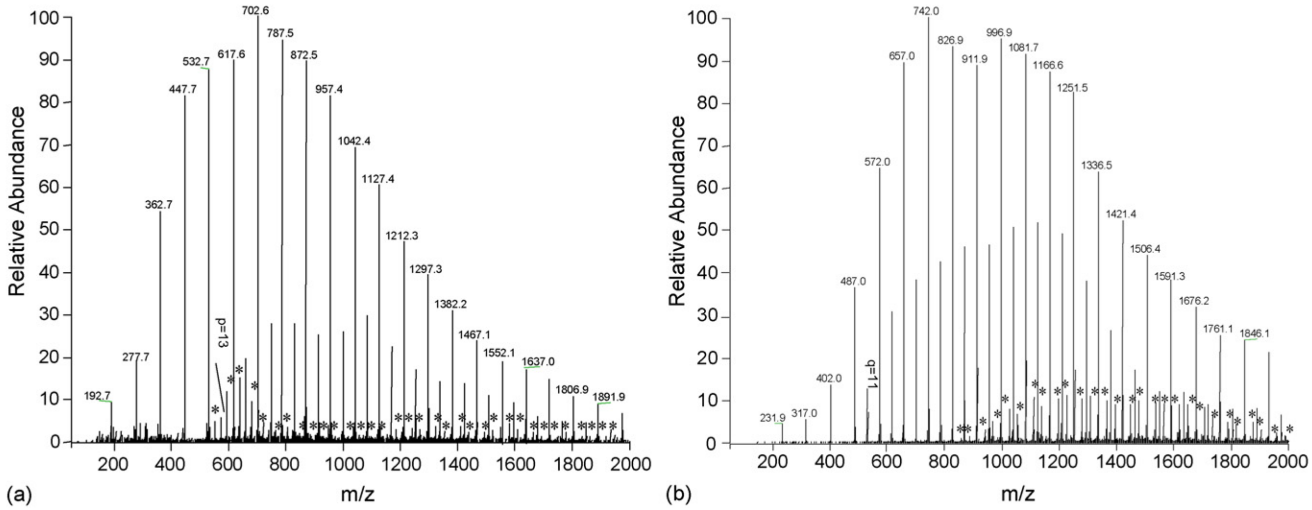


Fig. 6. ESI positive (a) and negative (b) ion mass spectrum of 0.1 mol/L $NaNO_3$ solution at capillary temperature of 100 °C (where '*' indicates triply charged cluster ions).

In the negative ion mode, the fragmentation pathway of the non-overlapped singly charged cluster ions ($n < 9$) is similar to their positively charged counterparts in the low energy CID.

3.3.2. Cluster ions from potassium nitrate

Although there may be structural difference between potassium nitrate and sodium nitrate crystals [21,22], there was not marked difference between the fragmentation pathways of cluster ions of the two nitrate salts. However, because the effect of potassium nitrate isotopic peak is bigger than that of sodium nitrate counterpart in the mass spectrum, in the MS/MS experiment the maximum isolation window of potassium nitrate we used is 8.0 *m*/*z*, larger than that of sodium nitrate we used (3.0 *m*/*z*), in order to obtain enough isolation efficiency. The fragmentation pathways of potassium nitrate cluster ions are summarized in the following: In the positive ion mass spectrum, for $[(KNO_3)_pK_2]^{2+}$, where $21 \le p \le 27$, the fragmentation pathways observed are those of charge separation into singly charged cluster ions and the loss of KNO_3 molecules (up to five) to form doubly charged cluster ions of lower mass/charge ratio. From $p > 27$ on, loss of neutral KNO_3 units (up to eight) becomes the only fragmentation pathway observed. In the negative ion mass spectrum, for $[(KNO_3)_q(NO_3)_2]^{2-}$, where $19 \le q \le 25$, the fragmentation pathways observed are those of charge separation into singly charged cluster ions and the loss of KNO_3 molecules (up to five) to form doubly charged cluster ions of lower mass/charge ratio. From $p > 25$ on, loss of neutral KNO_3 units (up to seven) becomes the only fragmentation pathway observed.

The fragmentation pathway of the non-overlapped singly charged cluster ions of potassium nitrate is similar to that of their sodium nitrate counterparts in positive or negative ion mode in the low energy CID.

3.4. The effect of solution concentration and capillary temperature on the formation of cluster ions

The effects of sample concentration, capillary temperature of the ESI source, and spray voltage on the formation of cluster ions are investigated. The sample concentration plays an important role in the formation of cluster ions, especially in that of the doubly charged cluster ions. By varying the concentration of alkali nitrates from 10^{-4} to 10^{-1} mol/L (the instrumental parameters are maintained constant), we found that singly charged cluster ions appear at about 10^{-3} mol/L, while doubly charged cluster ions begin to form at 10^{-2} mol/L. But the cluster ions (singly and/or doubly charged) produced from "onset concentration" are very small in size and low in intensity, and the signal-to-noise ratio is low. Solutions above 10^{-1} mol/L can block the heated capillary by salt crystallization. The temperature of the heated capillary also influences the distribution of cluster ions formed. At a fixed concentration of 0.1 mol/L $NaNO_3$ solution, the capillary temperature was changed from 75 to 300 °C (the upper temperature limit of the instrument) in steps of 25 °C, and it was observed that (1) at 75–100 °C the intensity of the doubly charged cluster ions decreased sharply (compared to that of these ions at normal temperature of 200 °C), and the critical size of these ions appeared. In addition, triply charged cluster ions were produced in both positive and negative ion mode (Fig. 6a and b '*'), and may reflect the initial distribution of nascent gaseous cluster ions [9], (2) at 200 °C triply charged cluster ions disappeared and the signal-to-noise ratio is the highest, and (3) at 300 °C the intensity of doubly charged cluster ions was very low, some doubly charged cluster ions of lower mass/charge ratio vanished. The increment in the capillary temperature affected the singly charged cluster ions formed together, and the most abundant cluster ion shifted to smaller size. Finally, the effect of the spray voltage on the formation of the cluster ions was also investigated and found to have limited influence.

4. Conclusions

The clusters of sodium and potassium nitrates formed under positive and negative ion ESI conditions were studied, and doubly charged cluster ions were generated evidently under normal source capillary temperature (200 °C) together with singly charged cluster ions. Critical sizes of doubly charged cluster ions were observed. Magic number clusters were present in the mass spectra and prominent magic numbers were underlined by using energetic instrumental condition.

The fragmentation pathways of doubly charged cluster ions were investigated in detail by tandem mass spectrometry and two pathways were observed depending on the cluster size. The fragmentation pathways of smaller ($p \leq 27$ or $q \leq 25$) cluster ions are those of charge separation into singly charged ions and the loss of neutral nitrate units to form doubly charged cluster ions of lower mass/charge ratio, whereas the sole fragmentation pathway of larger cluster ($p > 27$ or $q > 25$) ions becomes the loss of neutral nitrate molecules. With the increase in cluster size, the doubly charged cluster ion becomes more stable. In the product ions the most prominent ion is highly stable and usually a magic number ion.

The influence of sample concentration, capillary temperature of the ESI source, and spray voltage on the formation of cluster ions was also interrogated. Only the sample concentration and the capillary temperature have a marked effect. Triply charged cluster ions were produced under low capillary temperature of 75–100 °C.

Acknowledgments

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