

Polyatomic Ions

Can a group of atoms have a charge?

Why?

Do you know you eat a lot of "-ates"? Next time you look at a food label, read the ingredients and you will likely find a number of ingredients that end with "-ate," such as sodium phosphate or calcium carbonate. Did you ever wonder what the chemical formulas of these ingredients look like? In this activity we will explore polyatomic ions, which are groups of atoms that carry a charge. These ions are found in our food ingredients, natural waterways, and many other chemical compounds you encounter every day.

Model 1 – Types of Ions

Monatomic Ions	Nitride 	Sulfide 	Chloride 
Polyatomic Ions	Nitrate 	Sulfate 	Ammonium 
	Nitrite 	Sulfite 	Hydroxide 

1. Use Model 1 to complete the table below.

Name of Ion	Nitride	Nitrate	Sulfate	Sulfite	Ammonium
Charge on Ion	-3	-1	-2	-2	+1
Type and Number of Atoms	1 nitrogen	1 nitrogen 3 oxygen	1 sulfur 4 oxygen	1 sulfur 3 oxygen	1 nitrogen 4 hydrogen
Chemical Formula	N^{3-}	NO_3^{1-}	SO_4^{2-}	SO_3^{2-}	NH_4^{1+}

Polyatomic Ions Pogil Answers

Sebastian Brünink

A red circular graphic with a gradient, appearing as a semi-circle or a partial circle, located to the right of the author's name.

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Polyatomic Ions for Surface Analysis and Modification Erick Ryan Fuoco, 2003 **Fragmentation of Diatomic and Polyatomic Ions in the Gas Phase** Christopher John Proctor, 1981 High Resolution Studies of the Origins of Polyatomic Ions in Inductively Coupled Plasma-Mass Spectrometry Jill Wisniewski Ferguson, 2006

The inductively coupled plasma ICP is an atmospheric pressure ionization source. Traditionally the plasma is sampled via a sampler cone. A supersonic jet develops behind the sampler and this region is pumped down to a pressure of approximately one Torr. A skimmer cone is located inside this zone of silence to transmit ions into the mass spectrometer. The position of the sampler and skimmer cones relative to the initial radiation and normal analytical zones of the plasma is key to optimizing the useful analytical signal.

1 The ICP both atomizes and ionizes the sample. Polyatomic ions form through ion molecule interactions either in the ICP or during ion extraction.

1 Common polyatomic ions that inhibit analysis include metal oxides. MO sup adducts with argon the gas most commonly used to make up the plasma and hydride species. While high resolution devices can separate many analytes from common interferences this is done at great cost in ion transmission efficiency a loss of 99% when using high versus low resolution on the same instrument.

2 Simple quadrupole devices which make up the bulk of ICP MS instruments in existence do not present this option. Therefore if the source of polyatomic interferences can be determined and then manipulated this could potentially improve the figures of merit on all ICP MS devices not just the high resolution devices often utilized to study polyatomic interferences.

The Particulate Nature of Polyatomic Ions, 2007 **Investigations Into the Origins of Polyatomic Ions in Inductively Coupled Plasma-mass Spectrometry** Sally M. McIntyre, 2010 **Investigations Into the Origins of Polyatomic Ions in Inductively Coupled Plasma-mass Spectrometry**, 2010

An inductively coupled plasma mass spectrometer ICP MS is an elemental analytical instrument capable of determining nearly all elements in the periodic table at limits of detection in the parts per quadrillion and with a linear analytical range over 8-10 orders of magnitude. Three concentric quartz tubes make up the plasma torch. Argon gas is spiraled through the outer tube and generates the plasma powered by a looped load coil operating at 27.1 or 40.6 MHz. The argon flow of the middle channel is used to keep the plasma above the innermost tube through which solid or aqueous sample is carried in a third argon stream. A sample is progressively desolvated, atomized and ionized. The torch is operated at atmospheric pressure. To reach the reduced pressures of mass spectrometers ions are extracted through a series of two approximately one millimeter wide circular apertures set in water cooled metal cones. The space between the cones is evacuated to approximately one torr. The space behind the second cone is pumped down to or near to the pressure needed for the mass spectrometer MS. The first cone called the sampler is placed directly in the plasma plume and its position is adjusted to the point where atomic ions are most abundant. The hot plasma gas expands through the sampler orifice and in this expansion is placed the second cone called the skimmer. After the skimmer traditional MS designs are employed i.e. quadrupoles, magnetic sectors, time of flight.

ICP MS is the leading trace element analysis technique. One of its weaknesses are polyatomic ions. This dissertation has added to the fundamental understanding of some of these polyatomic ions, their origins and behavior. Although mainly continuing the work of others, certain novel approaches have been introduced here. Chapter 2 includes the first reported efforts to include high temperature corrections to the partition functions of the polyatomic ions in ICP MS. This and other objections to preceding papers in this area were addressed. Errors in the measured T_{sub} gas values were found for given errors in the experimental and spectroscopic values. The ionization energy of the neutral polyatomic ion was included in calculations to prove the validity of ignoring more complicated equilibria. Work was begun on the question of agreement between kinetics of the plasma and interface and the increase and depletion seen in certain polyatomic ions. This dissertation was also the first to report day to day ranges for T_{sub} gas values and to use a statistical test to compare different operating conditions. This will help guide comparisons of previous and future work. Chapter 4 was the first attempt to include the excited electronic state 2 in the partition function of ArO as well as the first to address the different dissociation products of the ground and first electronic levels of ArO. Chapter 5 reports an interesting source of memory in ICP MS that could affect mathematical corrections for polyatomic ions. For future work on these topics, I suggest the following experiments and investigations. Clearly not an extensive list, they are instead the first topics curiosity brings to mind.

1. Measurement of T_{sub} gas values when using the flow injection technique of Appendix B. It was believed that there was a fundamental difference in the plasma when the auto sampler was used versus a continuous injection. Is this reflected in T_{sub} gas values?
2. The work of Chapter 3 can be expanded and supplemented with more trials, new cone materials, i.e. copper, stainless steel, and more cone geometries. Some of this equipment is already present in the laboratory; others could be purchased or made.
3. T_{sub} gas values from Chapter 3 could be correlated with instrument pressures during the experiment. Pressures after the skimmer cone were recorded for many days but have yet to be collated with the measured T_{sub} gas values.
4. The work in Chapter 5 could be expanded to include more metals. Does the curious correlation between measured T_{sub} gas and element boiling point persist?
5. Investigate non linear correlations to T_{sub} gas values of the MO memory in Chapter 5. Temperatures along the skimmer walls are not a linear gradient. Ring deposits have been observed on the cone, and photographs of the interface show light intensities shaping a sort of tailing peak along the outside skimmer wall. Is there a physical property of the metals or metal oxides that would give this peak with the T_{sub} gas values?
6. Chemical state speciation of the metal deposits on the skimmers of Chapter 5. There may be a more logical correlation between T_{gas} and a physical property of the depositing chemical if all the metals do not deposit in the same form.
7. A collaboration with our computational colleagues would be most welcome. Newer calculations for ArO and RuO would be very helpful.

Fragmentation of Diatomic and Polyatomic Ions in the Gas Phase Christopher John Proctor, 1981
Standard Thermodynamic Functions of Gaseous Polyatomic Ions at 100-1000 K Aharon Loewenschuss, Y. Marcus, 1987
Unimolecular and Collision-induced Dissociation Study of Polyatomic

Ions at High Collision Energy Xuedong Zhou, 2001 *Energy Partitioning and Timescales for the Surface-induced Dissociation of Polyatomic Ions* David Garrett Schultz, 1999 **Sputtering of Indium Under Polyatomic Ion Bombardment** Andrey V. Samartsev, 2004 **Structure of Free Polyatomic Molecules** K. Kuchitsu, Kozo Kuchitsu, 1998-09-10 This volume *Structure of Free Polyatomic Molecules Basic Data* contains frequently used data from the corresponding larger Landolt B rNSTEIN handbooks in a low price book for the individual scientists working in the laboratory Directories link to the more complete volumes in the library The book contains important information about a large number of semiconductors **Polyatomic Ion Impact on Solids and Related Phenomena** Y Le Beyec, Y Hoppilliard, H Bernas, 1994 **Polyatomic Ion-surface Interactions** Luke Hanley, 1998 *Structure Data of Free Polyatomic Molecules* K. Kuchitsu, 1995-11-27 Since the publication of Volumes II 7 in 1976 and its supplements II 15 in 1987 and II 21 in 1992 the information on the structure of free molecules in the ground state and in excited electronic states has increased considerably Therefore this volume II 23 contains data from 148 inorganic and 498 organic polyatomic free molecules including free radicals and molecular ions published between 1990 and 1993 inclusively and a small number of structures published 1994 All experimental methods for the determination of structural data of free molecules have been considered all data obtained by these methods have been critically evaluated and compiled The structural data for more than 3400 polyatomic free molecules can be completely surveyed and easily retrieved by means of this volume **Experimental Studies of Polyatomic Ion Interactions with Clean and Adsorbate Covered Metal Surfaces** Samuel B. Wainhaus, 1997 *Special issue polyatomic ion surface interactions* Luke Hanley, 1998 Determination of Optimum Conditions for Distinguishing the Pulse Height Distributions of Atomic and Polyatomic Ions M. J. Kristo, 2006 This work explored the use of pulse height distributions PHD from multiplier type detectors as a means of detecting and eliminating the effects of polyatomic interferences in secondary ion mass spectrometry SIMS We explored the behavior of PHD for sup 235 U sup sup 208 Pb sup 27 Al sup and sup 207 Pb sup 28 Si sup all with a nominal mass to charge ratio of 235 In every case the distribution for the atomic ion sup 235 U sup was clearly shifted relative to the distributions for sup 208 Pb sup 27 Al sup and sup 207 Pb sup 28 Si sup When the first surface of the detector is metallic in character the polyatomic ions are shifted to larger pulse heights relative to the atomic ion When the first surface of the detector is oxide in character the atomic ion is shifted to larger pulse heights relative to the polyatomic ions The relative positioning appear to be stable for a given detector over time at the same secondary ion impact energy Consequently it appears to be feasible to use PHD data to detect interfering polyatomic ions and eliminate their deleterious effects using peak deconvolution techniques Consequently the updated Ultrafast RAE detector will be designed to make the pulse height information available to the data acquisition system *High Resolution Studies of the Origins of Polyatomic Ions in Inductively Coupled Plasma-Mass Spectrometry*, 2006 The inductively coupled plasma ICP is an atmospheric pressure ionization source Traditionally the plasma is sampled via a sampler cone A supersonic

jet develops behind the sampler and this region is pumped down to a pressure of approximately one Torr. A skimmer cone is located inside this zone of silence to transmit ions into the mass spectrometer. The position of the sampler and skimmer cones relative to the initial radiation and normal analytical zones of the plasma is key to optimizing the useful analytical signal.¹ The ICP both atomizes and ionizes the sample. Polyatomic ions form through ion-molecule interactions either in the ICP or during ion extraction.¹ Common polyatomic ions that inhibit analysis include metal oxides. MO adducts with argon, the gas most commonly used to make up the plasma, and hydride species. While high-resolution devices can separate many analytes from common interferences, this is done at great cost in ion transmission efficiency: a loss of 99% when using high versus low resolution on the same instrument.² Simple quadrupole devices, which make up the bulk of ICP-MS instruments in existence, do not present this option. Therefore, if the source of polyatomic interferences can be determined and then manipulated, this could potentially improve the figures of merit on all ICP-MS devices, not just the high-resolution devices often utilized to study polyatomic interferences.

Calculated Angular Distribution of Fragment Ions from Polyatomic-ion Collisions, 1982. The angular distribution of ion fragments from dissociation collisions of ions with molecular ions is discussed, and results are given for the fragments of nitromethane molecular ion. WHK.

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