

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+}

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Andrey V. Samartsev



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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 Investigations Into the Origins of Polyatomic Ions in Inductively Coupled Plasma-mass Spectrometry Sally M. McIntyre, 2010 *The Particulate Nature of Polyatomic Ions*, 2007 Fragmentation of Diatomic and Polyatomic Ions in the Gas Phase Christopher John Proctor, 1981 *Unimolecular and Collision-induced Dissociation Study of Polyatomic Ions at High Collision Energy* Xuedong Zhou, 2001 **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_{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_{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_{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_{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_{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_{gas} values
- 4 *Standard Thermodynamic Functions of Gaseous Polyatomic Ions at 100-1000 K* Aharon Loewenschuss, Y. Marcus, 1987 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

Sputtering of Indium Under Polyatomic Ion Bombardment Andrey V. Samartsev, 2004
Experimental Studies of Polyatomic Ion Interactions with Clean and Adsorbate Covered Metal Surfaces Samuel B. Wainhaus, 1997

Energy Partitioning and Timescales for the Surface-induced Dissociation of Polyatomic Ions David Garrett Schultz, 1999

Polyatomic Ion-surface Interactions Luke Hanley, 1998 Special issue polyatomic ion surface interactions Luke Hanley, 1998

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