

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+}

Pogil Chemistry Polyatomic Ions

Aharon Loewenschuss, Y. Marcus



Pogil Chemistry Polyatomic Ions:

Higher Excited States of Polyatomic Molecules V2 Melvin Robin, 2012-12-02 Higher Excited States of Polyatomic Molecules Volume II focuses on a higher level of activity in vacuum ultraviolet spectroscopy This book explores the Rydberg states in atoms and molecules Comprised of five chapters this volume starts with an overview of the two center unsaturated molecules that usually display sharp Rydberg transitions originating with the pi electrons This book then discusses the unsaturated double bond that adds another dimension to the spectrum Other chapters explore the optical spectrum of the amide group which is the basic chromophoric unit in polypeptides This text further discusses the all electron calculations of the electronic structure of the amide group that is performed in Gaussian orbital basis sets This book considers as well the prominent characteristic of Rydberg excitations in benzene The final chapter deals with the biological molecules that are polyfunctional in general Analytical chemists photochemists molecular spectroscopists and researchers will find this book extremely useful Radiationless Transitions in Polyatomic Molecules Emile S. Medvedev, Vladimir I. Osherov, 1995 Radiationless transitions comprise an important class of physical phenomena occurring in the excited states of molecules They affect the lifetimes of the excited states and govern primary photochemical and photophysical processes Much effort has been devoted to the understanding of radiationless transitions Still owing to recent advances the field continues to attract attention The demand for a book on the theory of these processes naturally arises in attempting to comprehend a large body of literature as the famous review article by K F Freed and the book by R Englman do not encompass some issues of current interest Our intent is to highlight the underlying physical principles and methods in such a way that the book both in its content and its presentation is instructive for a wide audience The basic ideas are treated in simple mathematical terms intelligible to experimentalists and to readers unfamiliar with the field Complicated theoretical methods are always expounded from first principles so that a knowledge of quantum mechanics and mathematics at the graduate student level will enable the reader to easily follow the derivations Experts will find efficient methods of calculating the transition rates as well as new applications of quasiclassical methods and fresh treatments of standard problems Details of measurements are not discussed and experimental data are only invoked to illustrate the theory *Radiationless Transitions in Polyatomic Molecules* Émil' Samuilovich Medvedev, Vladimir Iosifovich Osherov, 1995 Radiationless Transitions in Polyatomic Molecules treats the dynamics of electronically excited states and the transition probabilities of electronic relaxation processes Based on a simple and transparent yet rigorous presentation of the basic physical concepts the mathematical methods required are developed in detail from first principles and new light shed on the treatment of traditional issues *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

Time-Resolved Photoionisation Studies of Polyatomic Molecules Martin Alex Bjørnholst, 2020-08-03 This book explores how structure impacts the dynamics of organic molecules in an extensive and impressive range of femtosecond time resolved experiments that are combined with state of the art theoretical approaches It explores an area of molecular dynamics that remains largely uncharted and provides an extraordinary overview along with novel insights into the concept of the dynamophore the functional group of ultrafast science Divided into four parts this book outlines both experimental and computational studies on the VUV photoinduced dynamics of four cyclic ketones and one linear ketone the ring opening and dissociative dynamics of cyclopropane and the potential ultrafast intersystem crossing in three methylated benzene derivatives Model systems for the disulfide bond and the peptide bond both of which are related to the structure of proteins are also investigated This highly informative and carefully presented book offers a wealth of scientific insights for all scholars with an interest in molecular dynamics

Higher Excited States of Polyatomic Molecules Melvin Robin, 1974-05-28 Higher Excited States of Polyatomic Molecules Volume I focuses on the spectra in the vacuum ultraviolet region between 50 000 and 100 000 cm⁻¹ This book explores the higher excitations in molecules beyond 50 000 cm⁻¹ Organized into three chapters this volume starts with an overview of the excited state properties of a molecule and the excited state ionization potential This book then proceeds with a discussion of the original classification of the properties as well as the types of excitations observed in the vacuum ultraviolet Other chapters discuss photoelectron spectroscopy which is an independent self sustaining branch of molecular spectroscopy This text examines as well the distinction between valence shell and Rydberg excitations The final chapter deals with several topics including the saturated molecules that are classified as having all valence electrons the alkene absorption spectra and the spectroscopic data on boron compounds Analytical chemists photochemists molecular spectroscopists and researchers will find this book extremely useful

Higher Excited States of Polyatomic Molecules Melvin B. Robin, 1974

Structure of Free Polyatomic Molecules Kozo Kuchitsu, 2013-03-09 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

The Elimination of Dependent Coordinates in the Theory of Vibration of Polyatomic Molecules L. S. Mayants, 1953

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 $T_{\text{sub gas}}$ values 4 The work in Chapter 5 could be expanded to include more metals Does the curious correlation between measured $T_{\text{sub gas}}$ and element boiling point persist 5 Investigate non linear correlations to $T_{\text{sub gas}}$ 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 $T_{\text{sub gas}}$ 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

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

Christopher John Proctor, 1981 *Rotation-Vibration of Polyatomic Molecules* Gilbert Amat, 1971 *Polyatomic Ions for Surface Analysis and Modification* Erick Ryan Fuoco, 2003 *Computational Spectroscopy of Polyatomic Molecules* Sergey Yurchenko, 2023 This book provides a detailed description of the modern variational methods available for solving the nuclear motion Schrödinger equation to enable accurate theoretical spectroscopy of polyatomic molecules These methods are currently used to provide important molecular data for spectroscopic studies of atmospheres of astronomical objects including solar and extrasolar planets as well as cool stars This book has collected descriptions of quantum mechanical methods into one cohesive text making the information more accessible to the scientific community especially for young researchers who would like to devote their scientific career to the field of computational molecular physics The book addresses key aspects of the high accuracy computational spectroscopy of the medium size polyatomic molecules It aims to describe numerical algorithms for the construction and solution of the nuclear motion Schrödinger equations with the central idea of the modern computational spectroscopy of polyatomic molecules to include the construction of the complex kinetic energy operators KEO into the computation process of the numerical pipeline by evaluating the corresponding coefficients of KEO derivatives on the fly The book details key aspects of variational solutions of the nuclear motion Schrödinger equations targeting high accuracy including construction of rotational and vibrational basis functions coordinate choice molecular symmetry as well as of intensity calculations and refinement of potential energy functions The goal of this book is to show how to build an accurate spectroscopic computational protocol in a pure numerical manner of a general black box type algorithm This book will be a valuable resource for researchers both experts and not experts working in the area of the computational and experimental spectroscopy PhD students and early career spectroscopists who would like to learn basics of the modern variational methods in the field of computational spectroscopy It will also appeal to astrophysicists and

atmospheric physicists who would like to assess data and perform calculations themselves Key features Supported by the latest research and based on the state of the art computational methods in high accuracy computational spectroscopy of molecules Authored by an authority in the field Accessible to both experts and non experts working in the area of computational and experimental spectroscopy in addition to graduate students

Energy Partitioning and Timescales for the Surface-induced Dissociation of Polyatomic Ions David Garrett Schultz,1999 **Wide-amplitude Rovibrational Bound States in Polyatomic Molecules** Igor N. Kozin,Mark M. Law,Jonathan N. L. Connor,2002

Rotation-vibration of Polyatomic Molecules Gilbert Amat,Harald Herborg Nielsen,Ginette Tarrago,1971 Higher Excited States of Polyatomic Molecules V3 Melvin Robin,2012-12-02 Higher Excited States of Polyatomic Molecules Volume III focuses on higher electronic excitations in polyatomic molecules with emphasis on excitations beyond 50 000 cm⁻¹ This book explores the various transitions on the basis of their orbital characteristics Organized into 22 chapters this volume begins with an overview of the relationships between spectra of different molecules and between the results of various types of spectroscopy This book then discusses the higher excited states involving Rydberg excitation Other chapters explore the higher excited states in all classes of biological organic and inorganic molecules This text further discusses the progress in the area of higher excitations in polyatomic atoms and the technique of multiphoton ionization MPI spectroscopy that yields a remarkable amount of spectroscopic information applicable to the vacuum ultraviolet region The final chapter deals with the vacuum ultraviolet spectroscopy of biological materials Analytical chemists photochemists molecular spectroscopists and researchers will find this book extremely useful

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