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Editorial

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The *JPC* Periodic Table

In this Virtual Issue, we celebrate the International Year of the Periodic Table by presenting one paper in *JPC* that is concerned with each of the 118 elements. Actually only 116 elements have appeared in *JPC* papers, with elements 109 and 110, meitnerium and darmstadtium, somehow missing as far as we can tell. However, all the rest are there, and the *JPC* editors, including editors of *JPC A*, *B*, *C*, and *Letters*, have all contributed to the list given below, with links to the original articles provided. In choosing these papers, we tried to focus mostly on papers that are well cited and that refer to the element of interest rather than to complex chemistry where the element is one of many involved. However, in many cases the importance of an element is defined by its role in important molecules or materials, so some of the papers are concerned with the physical chemistry of the molecules or materials. Of course, many of the chemical elements have multifaceted personalities when it comes to their physical chemistry, so we apologize that we could only list one paper for each element when, in fact, there were many excellent choices. Near the bottom of the periodic table ($Z > 100$), the number of papers concerned with some elements is quite limited, so the few people brave enough to study these elements receive a lot of publicity in this document.

There are numerous interesting stories that are woven through these papers. We could easily write a story about each element, but to keep this discussion focused, let us only mention a few general issues. It is notable to think about the dates on these papers and when the elements were discovered. The elements with $Z > 92$ were all discovered since 1940, so many of the papers on our list refer to physical property measurements that were done shortly after their discovery. And elements with $Z > 99$ are sufficiently unstable that most of the papers refer to computational studies or empirical models, sometimes done in advance of the discovery of the element (and often before the element had a name, so only the atomic number appears in the paper, or perhaps the name "Eka-X" where X is the corresponding element from the row above on the periodic table). Theory plays an important role with many of the lighter (but still heavy) elements, particularly those that are radioactive ($Z > 83$) and are in low abundance. There have also been several experimental papers concerned with the radioactive properties of these elements. We were not able to include papers going back to the beginning of *JPC* in 1896, but one can find papers by Marie and Pierre Curie and Henri Becquerel that refer to some of the very first measurements on Po, Ra, and other radioactive elements.

Among the elements with $Z < 100$, one theme refers to elements that are gases, including the rare gases (but some of our papers for those refer to liquid or solid forms) and non rare gas molecules that form gaseous diatomics (N_2, O_2, Cl_2, Br_2, I_2). The papers in this case refer to spectroscopic measurements or, in some cases, gas-phase chemical reactions of either neutrals or ions. There are many elements where ions in solution are extremely important (our papers include K^+, Rb^+, Cs^+, Mg^{2+}, Pr^{3+}, Np^{3+}, Cm^{3+}, Bk^{3+}, Cf^{3+}, Es^{3+}, and Fm^{3+}). Many of these ions are important in biophysics, and we also note that our papers on O and S are concerned with biophysics.

Several of the papers are concerned with elemental liquids or solids either as covalent materials (C, Si, Ge, S, Sb, Tl) or as metals (alkalis, noble metals, Fe, Ni, Nb, Pd). Of course, water and solvation are prominently featured (H) and occasionally elements that form molecular liquids (Be). Many of the metals in the table form colloids (noble metals), and then there are the important oxides, sulfides, nitrides, arsenides, etc. that form nanostructures of various types (Ti, Sc, Zr, Cd, Sn, La, Ce, Ir. Pb, Bi, Th, Pa, U, Am), including 2D nanomaterials (F, B, P, As). Battery materials show up in many places (Li, P, Se), and we also find examples of elements that play a crucial role in coordination chemistry (Ru, Rh), catalysis (N, Fe, Sr, Mo, Re, Pt), electronic materials (In,Te, Hf, Ta, W), and intermetallics (Sb, Po). Thermodynamic properties and earth abundance are important in some of papers we cite. Ca, Ba, Tc, At, Fr, Pu, and the lanthanides have their expected roles as emitters, contrast agents, and electronic materials. Finally, we note that the paper we list for Hg involves the use of mercury drop to describe autonomous motion in the presence of a $K_2Cr_2O_7$ crystal.

This discussion amply notes the incredible richness associated with the periodic table that one sees in a list of 116 papers. We are delighted that *JPC* has been able to play (thanks for Cathy Murphy's suggestion) an important role in the dissemination of these scientific discoveries.

(AN#1) - H - Hydrogen

Polarizable Atomic Multipole Water Model for Molecular Mechanics Simulation, Pengyu Ren and Jay W. Ponder

J. Phys. Chem. B **2003**, *107* (24), pp 5933−5947

DOI: 10.1021/jp027815+

Publication Date (Web): May 24, 2003

Introduction of the AMOEBA polarizable force field for water −ABM

(AN#2) - He - Helium

Helium Separation Using Porous Graphene Membranes, Joshua Schrier

J. Phys. Chem. Lett. **2010**, *1* (15), pp 2284−2287

DOI: 10.1021/jz100748x

Publication Date (Web): July 8, 2010

Computational study of He transmission through graphene, exploring the role of quantum tunneling −ABM

(AN#3) - Li - Lithium

Lithium−Air Battery: Promise and Challenges, G. Girishkumar, B. McCloskey, A. C. Luntz, S. Swanson, and W. Wilcke

J. Phys. Chem. Lett. **2010**, *1* (14), pp 2193−2203

DOI: 10.1021/jz1005384

Publication Date (Web): July 2, 2010

Perspective on Li−air batteries that highlights challenges associated with achieving high throughput air-breathing systems

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DOI: 10.1021/acs.jpclett.9b01057
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that pass O_2 and keep out environmental contaminants while assuring electrochemical stability of both the electrolyte and the cathode itself −FZ

(AN#4) - Be - Beryllium

A First-Principles Description of Liquid BeF_2 and Its Mixtures with LiF: 1. Potential Development and Pure BeF_2, Robert J. Heaton, Richard Brookes, Paul A. Madden, Mathieu Salanne, Christian Simon, and Pierre Turq

J. Phys. Chem. B **2006**, *110* (23), pp 11454−11460

DOI: 10.1021/jp061000+

Publication Date (Web): May 24, 2006

A computational study of BeF_2 with comparisons to experiment −ABM

(AN#5) - B - Boron

Soluble, Exfoliated Hexagonal Boron Nitride Nanosheets, Yi Lin, Tiffany V. Williams and John W. Connell

J. Phys. Chem. Lett. **2010**, *1* (1), pp 277−283

DOI: 10.1021/jz9002108

Publication Date (Web): November 30, 2009

Hexagonal boron nitride (h-BN) was functionalized using lipophilic and hydrophilic amine molecules. The functionalization induced the exfoliation of the layered structure of h-BN, resulting in few-layered and monolayered nanosheets. −JB

(AN#6) - C - Carbon

Spectroscopic Insights into Carbon Dot Systems, Marcello Righetto, Alberto Privitera, Ilaria Fortunati, Dario Mosconi, Mirco Zerbetto, M. Lucia Curri, Michela Corricelli, Alessandro Moretto, Stefano Agnoli, Lorenzo Franco, Renato Bozio, and Camilla Ferrante

J. Phys. Chem. Lett. **2017**, *8* (10), pp 2236−2242

DOI: 10.1021/acs.jpclett.7b00794

Publication Date (Web): May 4, 2017

Spectroscopic insights into carbon dot systems −GS

(AN#7) N - Nitrogen

The Influence of Nitrogen Gas upon the Organic Catalysis of Nitrogen Fixation by Azotobacter, Dean Burk

J. Phys. Chem. **1930**, *34* (6), pp 1174−1194

DOI: 10.1021/j150312a005

Publication Date: January 1929

The influence of nitrogen gas upon the organic catalysis of nitrogen fixation by azotobacter −JZ

(AN#8) - O - Oxygen

Lifetime and Diffusion of Singlet Oxygen in a Cell, Esben Skovsen, John W. Snyder, John D. C. Lambert, and Peter R. Ogilby

J. Phys. Chem. B **2005**, *109* (18), pp 8570−8573

DOI: 10.1021/jp051163i

Publication Date (Web): April 8, 2005

Singlet molecular oxygen, created in a single nerve cell upon irradiation of a sensitizer incorporated in the cell nucleus using a focused laser beam, was found to be long-lived and diffuse over appreciable distances including across the cell membrane into the extra-cellular environment. −JZ

(AN#9) - F - Fluorine

Difluorophosphorane-Flattened Phosphorene through Di-fluorination, Dmitriy Steglenko, Ruslan M. Minyaev, Vladimir I. Minkin, and Alexander I. Boldyrev

J. Phys. Chem. Lett. **2018**, *9* (24), pp 6963−6966

DOI: 10.1021/acs.jpclett.8b02918

Publication Date (Web): November 27, 2018

Fluorine - a chemical modification of phosphorene by fluorination is proposed for electronics applications −OP

(AN#10) - Ne - Neon

Infrared Spectra of UO_2, UO_2^+, and UO_2^- in Solid Neon, Mingfei Zhou, Lester Andrews, Nina Ismail, and Colin Marsden

J. Phys. Chem. A **2000**, *104* (23), pp 5495−5502

DOI: 10.1021/jp000292q

Publication Date (Web): May 23, 2000

Highly cited paper focusing on the spectroscopy of UO_x compounds in combination with calculation −ABM

(AN#11) - Na - Sodium

An Accurate Electromagnetic Theory Study of Surface Enhancement Factors for Silver, Gold, Copper, Lithium, Sodium, Aluminum, Gallium, Indium, Zinc, and Cadmium, Ellen J. Zeman and George C. Schatz

J. Phys. Chem., **1987**, *91* (3), pp 634−643

DOI: 10.1021/j100287a028

Publication Date: January 1987

Electromagnetic theory study of surface enhancement factors for plasmonic metals −TZ

(AN#12) - Mg - Magnesium

Hydration of Beryllium, Magnesium, Calcium, and Zinc Ions Using Density Functional Theory, Maria Pavlov, Per E. M. Siegbahn, and Magnus Sandström

J. Phys. Chem. A **1998**, *102* (1), pp 219−228

DOI: 10.1021/jp972072r

Publication Date (Web): January 1, 1998

Well cited paper that determined Mg^{+2} hydration energy using DFT −GCS

(AN#13) - Al - Aluminum

Reactions of Laser-Ablated Aluminum Atoms with Cyanogen: Matrix Infrared Spectra and Electronic Structure Calculations for Aluminum Isocyanides $Al(NC)_{1,2,3}$ and Their Novel Dimers, Lester Andrews, Han-Gook Cho, and Yu Gong

J. Phys. Chem. A **2018**, *122* (24), pp 5342−5353

DOI: 10.1021/acs.jpca.8b02036

Publication Date (Web): May 15, 2018

Matrix infrared spectra and electronic calculations discover novel $Al(NC)_{1,2,3}$ dimers and a stable anion $Al(NC)_4^-$ from laser-ablated aluminum reacting with cyanogen. −TC

(AN#14) - Si - Silicon

Doping and Electrical Transport in Silicon Nanowires, Yi Cui, Xiangfeng Duan, Jiangtao Hu, and Charles M. Lieber

J. Phys. Chem. B **2000**, *104* (22), pp 5213−5216

DOI: 10.1021/jp0009305

Publication Date (Web): May 11, 2000

Doping Si nanowires: tuning semiconductor at nanoscale. Nice demonstration! −HZ

(AN#15) - P - Phosphorus

Electrochemical Activity of Black Phosphorus as an Anode Material for Lithium-Ion Batteries, Li-Qun Sun, Ming-Juan Li, Kai Sun, Shi-Hua Yu, Rong-Shun Wang, and Hai-Ming Xie

J. Phys. Chem. C **2012**, *116* (28), pp 14772−14779

DOI: 10.1021/jp302265n

DOI: 10.1021/acs.jpclett.9b01057
J. Phys. Chem. Lett. 2019, 10, 4051−4062

Publication Date (Web): June 18, 2012
Use of black phosphorus as an anode material for lithium ion batteries −AG

(AN#16) - S - Sulfur
Intermolecular Potential Functions and Monte Carlo Simulations for Liquid Sulfur Compounds, William L. Jorgensen
J. Phys. Chem. **1986**, *90* (23), pp 6379−6388
DOI: 10.1021/j100281a063
Publication Date: November 1986
Intermolecular potentials and Monte Carlo simulations for sulfur containing compounds, including sulfur-containing side chains of proteins −ASM

(AN#17) - Cl - Chlorine
The Continuous Absorption Spectra of Chlorine, Bromine, Bromine Chloride, Iodine Chloride, and Iodine Bromide, Daniel J. Seery and Doyle Britton
J. Phys. Chem. **1964**, *68* (8), pp 2263−2266
DOI: 10.1021/j100790a039
Publication Date: August 1964
Absorption spectra of halides −AY

(AN#18) - Ar - Argon
Thermal Energy Charge-Transfer Reactions of Argon Ions (Ar^+ And Ar^{2+}), R. J. Shul, B. L. Upschulte, R. Passarella, R. G. Keesee, and A. W. Castleman
J. Phys. Chem. **1987**, *91* (10), pp 2556−2562
DOI: 10.1021/j100294a022
Publication Date: May 1987
Castleman paper on ion−molecule reactions involving Ar. −BS

(AN#19) - K - Potassium
Hydration of Sodium, Potassium, and Chloride Ions in Solution and the Concept of Structure Maker/Breaker, R. Mancinelli, A. Botti, F. Bruni, M. A. Ricci, and A. K. Soper
J. Phys. Chem. B **2007**, *111* (48), pp 13570−13577
DOI: 10.1021/jp075913v
Publication Date (Web): November 8, 2007
Neutron diffraction experiments challenge the model of ions in aqueous solution as simply either structure makers or breakers. −JS

(AN#20) - Ca - Calcium
The Application of Thermoanalytical Techniques to Reaction Kinetics: The Thermogravimetric Evaluation of the Kinetics of the Decomposition of Calcium Oxalate Monohydrate, Eli S. Freeman and Benjamin Carroll
J. Phys. Chem. **1958**, *62* (4), pp 394−397
DOI: 10.1021/j150562a003
Publication Date: April 1958
A highly cited classic paper on the use of thermoanalytical techniques to study reaction kinetics, with applications here to the decomposition of $CaC_2O_4{\cdot}H_2O$ −JS

(AN#21) - SC - Scandium
Bonding within the Endohedral Fullerenes $Sc_3N@C_{78}$ and $Sc_3N@C_{80}$ as Determined by Density Functional Calculations and Reexamination of the Crystal Structure of $\{Sc_3N@C_{78}\}\cdot Co(OEP)\}\cdot 1.5(C_6H_6)\cdot 0.3(CHCl_3)$, Josep M. Campanera, Carles Bo, Marilyn M. Olmstead, Alan L. Balch, and Josep M. Poblet
J. Phys. Chem. A **2002**, *106* (51), pp 12356−12364
DOI: 10.1021/jp021882m
Publication Date (Web): November 27, 2002
Details of the structure and stability of Sc_3N *in two types of fullerenes* −DC

(AN#22) - Ti - Titanium
The Role of Metal Ion Dopants in Quantum-Sized TiO_2: Correlation between Photoreactivity and Charge Carrier Recombination Dynamics, Wonyong Choi, Andreas Termin, and Michael R. Hoffmann
J. Phys. Chem. **1994**, *98* (51), pp 13669−13679
DOI: 10.1021/j100102a038
Publication Date: December 1994
An impactful paper on TiO_2 *photocatalysis* −JS

(AN#23) - V - Vanadium
Determination of Vanadium−Oxygen Bond Distances and Bond Orders by Raman Spectroscopy, Franklin D. Hardcastle and Israel E. Wachs
J. Phys. Chem. **1991**, *95* (13), pp 5031−5041
DOI: 10.1021/j100166a025
Publication Date: June 1991
A well cited study that uses Raman to determine vanadium−oxygen bond distances and bond orders −EW

(AN#24) - Cr - Chromium
Effects of Single Metal-Ion Doping on the Visible-Light Photoreactivity of TiO_2, Jina Choi, Hyunwoong Park, and Michael R. Hoffmann
J. Phys. Chem. C **2010**, *114* (2), pp 783−792
DOI: 10.1021/jp908088x
Publication Date (Web): December 22, 2009
Highly cited paper on how single metal ion doping, including Cr, regulates the visible-light photoactivity of TiO_2 −FG

(AN#25) - Mn - Manganese
Photophysical Properties of ZnS Nanoclusters with Spatially Localized Mn^{2+}, Kelly Sooklal, Brian S. Cullum, S. Michael Angel, and Catherine J. Murphy
J. Phys. Chem. **1996**, *100* (11), pp 4551−4555
DOI: 10.1021/jp952377a
Publication Date (Web): March 14, 1996
A highly cited paper showing that doping ZnS nanoclusters with Mn changes the photophysical properties, and even more specifically that the location of the Mn is responsible for the resulting optical properties −GEMS

(AN#26) - Fe - Iron
Behavior of Metallic Iron Catalysts During Fischer−Tropsch Synthesis Studied with Moessbauer Spectroscopy, X-ray Diffraction, Carbon Content Determination, and Reaction Kinetic Measurements, J. W. Niemantsverdriet, A. M. van der Kraan, W. L. van Dijk, and H. S. van der Baan
J. Phys. Chem. **1980**, *84* (25), pp 3363−3370
DOI: 10.1021/j100462a011
Publication Date: December 1980
Behavior of metallic iron catalysts during Fischer−Tropsch synthesis −GL

(AN#27) - Co - Cobalt
X-ray Absorption Spectroscopic Study of Brønsted, Lewis, and Redox Centers in Cobalt-Substituted Aluminum Phosphate Catalysts, Philip A. Barrett, Gopinathan Sankar, C. Richard A. Catlow, and John Meurig Thomas

DOI: 10.1021/acs.jpclett.9b01057
J. Phys. Chem. Lett. 2019, 10, 4051−4062

J. Phys. Chem. **1996**, *100* (21), pp 8977−8985
DOI: 10.1021/jp953034f
Publication Date (Web): May 23, 1996
The catalytic reactivity of Co centers on the ALPO substrates is characterized using EXAFS spectroscopy. Data acquired as a function of treatment of the porous phases are compared, revealing the local environment of the Co centers, including their oxidation state, coordination environment, and Lewis and Bronsted acid behavior. −GRG

(AN#28) - Ni - Nickel
The Electrolytic Precipitation of Nickel on Nickel, Ralph C. Snowdon
J. Phys. Chem. **1905**, *9* (5), pp 399−401
DOI: 10.1021/j150068a004
Publication Date: January 1904
Study of the electrolytic deposition of Ni on Ni that shows the importance of removing the oxide layer Ni surface −GVH

(AN#29) - Cu - Copper
Removal of Nitrogen Monoxide through a Novel Catalytic Process. 1. Decomposition on Excessively Copper-Ion-Exchanged ZSM-5 Zeolites, Masakazu Iwamoto, Hidenori Yahiro, Kenji Tanda, Noritaka Mizuno, Yosihiro Mine, and Shuichi Kagawa
J. Phys. Chem. **1991**, *95* (9), pp 3727−3730
DOI: 10.1021/j100162a053
Publication Date: May 1991
A highly cited paper on copper zeolites and its role in NO removal −JS

(AN#30) - Zn - Zinc
Preparation and Characterization of Quantum Size Zinc Oxide: A Detailed Spectroscopic Study, Detlef W. Bahnemann, Claudius. Kormann, and Michael R. Hoffmann
J. Phys. Chem. **1987**, *91* (14), pp 3789−3798
DOI: 10.1021/j100298a015
Publication Date: July 1987
Synthesis and spectroscopic characterization of zinc oxide nanoparticles −HF

(AN#31) - Ga - Gallium
Gallium Oxide Nanoribbons and Nanosheets, Z. R. Dai, Z. W. Pan, and Z. L. Wang
J. Phys. Chem. B **2002**, *106* (5), pp 902−904
DOI: 10.1021/jp013228x
Publication Date (Web): January 15, 2002
Highly cited paper on gallium oxide nanoribbons and nanosheets −HG

(AN#32) - Ge - Germanium
Segregation of Impurities during the Growth of Germanium and Silicon, R. N. Hall
J. Phys. Chem. **1953**, *57* (8), pp 836−839
DOI: 10.1021/j150509a021
Publication Date: August 1953
Classic work on determining how to achieve desired doping levels in crystalline semiconductors prepared from the melt −JF

(AN#33) - As - Arsenic
Structural and Electronic Properties of Layered Arsenic and Antimony Arsenide, Liangzhi Kou, Yandong Ma, Xin Tan, Thomas Frauenheim, Aijun Du, and Sean Smith
J. Phys. Chem. C **2015**, *119* (12), pp 6918−6922
DOI: 10.1021/acs.jpcc.5b02096
Publication Date (Web): March 9, 2015
Computational study of 2D materials that includes 2D arsenic −GCS

(AN#34) - Se - Selenium
ZIF-67@Se@MnO_2: A Novel Co-MOF-Based Composite Cathode for Lithium−Selenium Batteries, Wenkai Ye, Weiyang Li, Ke Wang, Weihao Yin, Wenwen Chai, Yi Qu, Yichuan Rui, and Bohejin Tang
J. Phys. Chem. C **2019**, *123* (4), pp 2048−2055
DOI: 10.1021/acs.jpcc.8b10598
Publication Date (Web): December 25, 2018
Selenium is added to a metal−organic-framework as a composite for batteries. −MZ

(AN#35) - Br - Bromine
The Ultraviolet−Visible Absorption Spectrum of Bromine between Room Temperature and 440°, A. A. Passchier, Jerry D. Christian, and Norman W. Gregory
J. Phys. Chem. **1967**, *71* (4), pp 937−942
DOI: 10.1021/j100863a025
Publication Date: March 1967
Classical spectroscopy study of Br_2 from the 1960s −GCS

(AN#36) - Kr - Krypton
A Set of Molecular Models for Symmetric Quadrupolar Fluids, Jadran Vrabec, Jürgen Stoll, and Hans Hasse
J. Phys. Chem. B **2001**, *105* (48), pp 12126−12133
DOI: 10.1021/jp012542o
Publication Date (Web): November 2, 2001
This paper presents a molecular model for 25 pure fluids including krypton. −BM

(AN#37) - Rb - Rubidium
Cesium and Rubidium Ion Equilibriums in Illite Clay, E. Brouwer, B. Baeyens, A. Maes, and A. Cremers
J. Phys. Chem. **1983**, *87* (7), pp 1213−1219
DOI: 10.1021/j100230a024
Publication Date: March 1983
Rubidium cations in solutions exhibit similar properties as the alkali cations in neighboring rows of the periodic table, which makes it a challenge to investigate the corresponding ion exchange processes in Illite clays. −PJ

(AN#38) - Sr - Strontium
Nature of Deficiency in Nonstoichiometric Hydroxyapatites. I. Catalytic Activity of Calcium and Strontium Hydroxyapatites, S. J. Joris and C. H. Amberg
J. Phys. Chem. **1971**, *75* (20), pp 3167−3171
DOI: 10.1021/j100689a024
Publication Date: September 1971
Well-cited paper detailing the catalytic effects of substituting Sr^{2+} for Ca^{2+} in hydroxyapatites for dehydration of alcohol −RD

(AN#39) - Y - Yttrium
Mass Spectroscopic and ESR Characterization of Soluble Yttrium-Containing Metallofullerenes YC_{82} and Y_2C_{82}, Hisanori Shinohara, Hiroyasu Sato, Yahachi Saito, Masato Ohkohchi, and Yoshinori Ando
J. Phys. Chem. **1992**, *96* (9), pp 3571−3573
DOI: 10.1021/j100188a004

Publication Date: April 1992
Solvent soluble, yttrium-containing fullerenes are produced and characterized by mass spectroscopic analysis. −SL

(AN#40) - Zr -Zirconium
Adsorption of Ordered Zirconium Phosphonate Multilayer Films on Silicon and Gold Surfaces, Haiwon Lee, Larry J. Kepley, Hun Gi Hong, Sohail Akhter, and Thomas E. Mallouk
J. Phys. Chem. **1988**, *92* (9), pp 2597−2601
DOI: 10.1021/j100320a040
Publication Date: May 1988
This was one of the first papers that showed multilayer zirconium phosphonate films can be prepared on silicon and gold substrates via sequential adsorption of their zirconium and phosphonic acid components. −TG

(AN#41) - Nb - Niobium
The Permeability of Niobium to Hydrogen, D. W. Rudd, D. W. Vose, and S. Johnson
J. Phys. Chem. **1962**, *66* (2), pp 351−353
DOI: 10.1021/j100808a038
Publication Date: February 1962
The permeability of niobium metal to hydrogen gas was measured at temperature and pressure ranges of 950−1065 °C and 1.1−2.0 atm, respectively, and it was fit to a simple Arrhenius rate expression with an activation energy of 5.2 kcal/mol −TM

(AN#42) - Mo - Molybdenum
Computational Design of Single-Molybdenum Catalysts for the Nitrogen Reduction Reaction, Qinye Li, Siyao Qiu, Chuangwei Liu, Mingguo Liu, Lizhong He, Xiwang Zhang, and Chenghua Sun
J. Phys. Chem. C **2019**, *123* (4), pp 2347−2352
DOI: 10.1021/acs.jpcc.8b11509
Publication Date (Web): January 4, 2019
Computational design of single-molybdenum catalysts for nitrogen reduction offering overall overpotentials lower than 0.60 V −VB

(AN#43) - Tc - Technetium
Report on the Occurrence of Technetium on the Earth's Crust, G. E. Boyd, and Q. V. Larson
J. Phys. Chem. **1956**, *60* (6), pp 707−715
DOI: 10.1021/j150540a002
Publication Date: June 1956
Hard to prove a negative, but this paper attempts to demonstrate the nonexistence of terrestrial Tc through analysis of geologic samples most likely to contain the element. −WFS

(AN#44) - Ru - Ruthenium
Excited States of Mixed Ligand Chelates of Ruthenium(II) and Rhodium(III), G. A. Crosby and W. H. Elfring Jr.
J. Phys. Chem. **1976**, *80* (20), pp 2206−2211
DOI: 10.1021/j100561a016
Publication Date: September 1976
It has the charming advantage that it was part of a "discussion" so the authors answer questions about it at the end of the paper! −CM

(AN#45) - Rh - Rhodium
Infrared Studies of Carbon Monoxide Chemisorbed on Rhodium, C. Yang and Carl W. Garl
J. Phys. Chem. **1957**, *61* (11), pp 1504−1512
DOI: 10.1021/j150557a013
Publication Date: November 1957
Infrared transmission spectrum of CO on Rh is described as involving three surface species. −XY

(AN#46) - Pd - Palladium
Diffusion and Solubility of Hydrogen in Palladium and Palladium−Silver Alloys, Gerhard L. Holleck
J. Phys. Chem. **1970**, *74* (3), pp 503−511
DOI: 10.1021/j100698a005
Publication Date: February 1970
Pd is a key hydrogenation catalyst and this paper first measures the H diffusion and solubility in Pd and Pd−Ag. −ZPL

(AN#47) - Ag - Silver
The Optical Properties of Metal Nanoparticles: The Influence of Size, Shape, and Dielectric Environment, K. Lance Kelly, Eduardo Coronado, Lin Lin Zhao, and George C. Schatz
J. Phys. Chem. B **2003**, *107* (3), pp 668−677
DOI: 10.1021/jp026731y
Publication Date (Web): December 21, 2002
Feature Article describing the progress made up to 2003 on the theory of nanoparticle optical properties, with emphasis on light scattering from particles of arbitrary shape in complex environments, and discussing spherical and triangular silver particles as an example of particular interest −FZ

(AN#48) - Cd - Cadmium
Two-Dimensional Electronic Spectroscopy Unravels sub-100 fs Electron and Hole Relaxation Dynamics in Cd-Chalcogenide Nanostructures, Tatjana Stoll, Federico Branchi, Julien Réhault, Francesco Scotognella, Francesco Tassone, Ilka Kriegel, and Giulio Cerullo
J. Phys. Chem. Lett. **2017**, *8* (10), pp 2285−2290
DOI: 10.1021/acs.jpclett.7b00682
Publication Date (Web): May 3, 2017
Two-Dimensional electronic spectroscopy unravels sub-100 fs electron and hole relaxation dynamics in Cd-chalcogenide nanostructures −GS

(AN#49) - In - Indium
ITO Interface Modifiers Can Improve V_{OC} in Polymer Solar Cells and Suppress Surface Recombination, Kristina M. Knesting, Huanxin Ju, Cody W. Schlenker, Anthony J. Giordano, Andres Garcia, O'Neil L. Smith, Dana C. Olson, Seth R. Marder, and David S. Ginger
J. Phys. Chem. Lett. **2013**, *4* (23), pp 4038−4044
DOI: 10.1021/jz4021525
Publication Date (Web): November 8, 2013
Linear dependence of the open-circuit voltage of organic photovoltaic devices on the modified indium tin oxide (ITO) work function −JB

(AN#50) - Sn - Tin
Capped Semiconductor Colloids. Synthesis and Photoelectrochemical Behavior of TiO_2 Capped SnO_2 Nanocrystallites, Idriss Bedja and Prashant V. Kamat
J. Phys. Chem. **1995**, *99* (22), pp 9182−9188
DOI: 10.1021/j100022a035
Publication Date: June 1995
An investigation on the effect of TiO_2 capping on SnO_2 colloidal nanocrystallites for photoelectrochemical applications −JZ

(AN#51) - Sb - Antimony
Stability of Free Intermetallic Compound Clusters: Lead/Antimony and Bismuth/Antimony, D. Schild, R. Pflaum, K. Sattler, and E. Recknagel

DOI: 10.1021/acs.jpclett.9b01057
J. Phys. Chem. Lett. 2019, 10, 4051−4062

J. Phys. Chem. **1987**, *91* (10), pp 2649−2653
DOI: 10.1021/j100294a037
Publication Date: May 1987
In the gas phase, antimony atoms form tetrahedra, and this is the starting point for the understanding of lead−antimony and bismuth−antimony clusters. −NS

(AN#52) - Te - Tellurium
Intrinsic Piezoelectricity in Two-Dimensional Materials, Karel-Alexander N. Duerloo, Mitchell T. Ong, and Evan J. Reed
J. Phys. Chem. Lett. **2012**, *3* (19), pp 2871−2876
DOI: 10.1021/jz3012436
Publication Date (Web): September 17, 2012
Tellurium piezoelectricity of two-dimentional $MoTe_2$ and WTe_2 is predicted. (highly cited paper). −OP

(AN#53) - I - Iodine
Photodissociation and Geminate Recombination Dynamics of Iodine (I_2^-) in Mass-Selected Iodine−Carbon Dioxide ($I_2^-(CO_2)_n$) Cluster Ions, John M. Papanikolas, James R. Gord, Nancy E. Levinger, Douglas Ray, Vasil Vorsa, and W. C. Lineberger
J. Phys. Chem. **1991**, *95* (21), pp 8028−8040
DOI: 10.1021/j100174a008
Publication Date: October 1991
I_2-$(CO_2)_n$ cluster photodissociation, geminate recombination −TZ

(AN#54) - Xe - Xenon
Distribution and Dynamic Properties of Xenon Dissolved in the Ionic Smectic Phase of $[C_{16}mim][NO_3]$: MD Simulation and Theoretical Model, Diego Frezzato and Giacomo Saielli
J. Phys. Chem. B **2016**, *120* (9), pp 2578−2585
DOI: 10.1021/acs.jpcb.5b12470
Publication Date (Web): February 5, 2016
Macroscopic transport coefficients are calculated for xenon in an ionic liquid, as it diffuses across the ionic layers of the smectic phase from a hydrophobic, alkyl environment. −TC

(AN#55) - Cs - Cesium
Many-Body Effects Determine the Local Hydration Structure of Cs^+ in Solution, Debbie Zhuang, Marc Riera, Gregory K. Schenter, John L. Fulton, and Francesco Paesani
J. Phys. Chem. Lett. **2019**, *10* (3), pp 406−412
DOI: 10.1021/acs.jpclett.8b03829
Publication Date (Web): January 10, 2019
MD simulations of Cs^+ hydration demonstrate the importance of polarization effects. −HZ

(AN#56) - Ba - Barium
Structures of the Ferroelectric Phases of Barium Titanate, G. H. Kwei, A. C. Lawson, S. J. L. Billinge, and S. W. Cheong
J. Phys. Chem. **1993**, *97* (10), pp 2368−2377
DOI: 10.1021/j100112a043
Publication Date: March 1993
Structure of ferroelectric phases of $BaTiO_3$ determined by Rietveld refinement using powder diffraction data collected at a spallation neutron source −AG

(AN#57) - La - Lanthanum
Fullerenes with Metals Inside, Yan Chai, Ting Guo, Changming Jin, Robert E. Haufler, L. P. Felipe Chibante, Jan Fure, Lihong Wang, J. Michael Alford, and Richard E. Smalley
J. Phys. Chem. **1991**, *95* (20), pp 7564−7568
DOI: 10.1021/j100173a002
Publication Date: October 1991
Letter reports the observation of fullerenes with single lanthanum atoms caged inside −ASM

(AN#58) - Ce - Cerium
Direct Evidence for Hydroxyl Radical Scavenging Activity of Cerium Oxide Nanoparticles, Ying Xue, Qingfen Luan, Dan Yang, Xin Yao, and Kebin Zhou
J. Phys. Chem. C **2011**, *115* (11), pp 4433−4438
DOI: 10.1021/jp109819u
Publication Date (Web): March 1, 2011
Studies the mechanism of antioxidant behavior of cerium oxide nanoparticles −AY

(AN#59) - Pr - Praseodymium
The Effect of $LiClO_4$, LiCl, and LiBr on the Polarographic Behavior and Ultraviolet Spectrum of Praseodymium(III) in Ethanol, Sheldon H. Cohen, Reynold T. Iwamoto, and Jacob Kleinberg
J. Phys. Chem. **1963**, *67* (6), pp 1275−1278
DOI: 10.1021/j100800a027
Publication Date: June 1963
Paper on effects of different anions on Pr(III) in solution −BS

(AN#60) - Nd - Neodymium
Enhanced Emission of Deuterated Tris(hexafluoroacetylacetonato)neodymium(III) Complex in Solution by Suppression of Radiationless Transition via Vibrational Excitation, Yasuchika Hasegawa, Yasutaka Kimura, Kei Murakoshi, Yuji Wada, Jeong-Ho Kim, Nobuaki Nakashima, Tatsuhiko Yamanaka, and Shozo Yanagida
J. Phys. Chem. **1996**, *100* (24), pp 10201−10205
DOI: 10.1021/jp960290z
Publication Date (Web): June 13, 1996
A study of the impact of various deuterated solvents on a Nd^{3+} complex (150 citations) −DC

(AN#61) - Pm - Promethium
Calorimetric Determination of the Mean β-Energy and Half-Life of Promethium-147, E. J. Wheelwright, D. M. Fleming, and F. P. Roberts
J. Phys. Chem. **1965**, *69* (4), pp 1220−1223
DOI: 10.1021/j100888a021
Publication Date: April 1965
The authors determine the mean β-particle energy and the half-life of promethium 147. −EW

(AN#62) - Sm - Samarium
The Near Infrared Transitions of the Trivalent Lanthanides in Solution. I. Praseodymium(III), Neodymium(III), Samarium-(III), and Europium(III) Ions, W. T. Carnall, D. M. Gruen, and R. L. McBeth
J. Phys. Chem. **1962**, *66* (11), pp 2159−2164
DOI: 10.1021/j100817a020
Publication Date: November 1962
Report of NIR transitions of molten trivalent lanthanides −FG

(AN#63) - Eu - Europium
Hierarchical Emergence and Dynamic Control of Chirality in a Photoresponsive Dinuclear Complex, Yuichiro Hashimoto,

Takuya Nakashima, Miku Yamada, Junpei Yuasa, Gwénaël Rapenne, and Tsuyoshi Kawai
J. Phys. Chem. Lett. **2018**, *9* (9), pp 2151−2157
DOI: 10.1021/acs.jpclett.8b00690
Publication Date (Web): April 11, 2018
Hierarchical emergence and dynamic control of chirality in a photoresponsive dinuclear complex −GS

(AN#64) - Gd - Gadolinium
Water-Exchange, Electronic Relaxation, and Rotational Dynamics of the MRI Contrast Agent [Gd(DTPA-BMA)(H_2O)] in Aqueous Solution: A Variable Pressure, Temperature, and Magnetic Field Oxygen-17 NMR Study, Gabriel Gonzalez, D. Hugh Powell, Veronique Tissieres, and Andre E. Merbach
J. Phys. Chem. **1994**, *98* (1), pp 53−59
DOI: 10.1021/j100052a010
^{17}O NMR longitudinal and transverse relaxation rates and chemical shifts were measured for a gadolinium complex as a measure of the efficacy as a magnetic resonance imaging contrast agent. −GEMS

(AN#65) - Tb - Terbium
Rare Earths. II. A Mass Spectrometric Determination of the Heats of Sublimation (or Vaporization) of Neodymium, Praseodymium, Gadolinium, Terbium, Dysprosium, Holmium, Erbium and Lutetium, David White, Patrick N. Walsh, Harold W. Goldstein, and David F. Dever
J. Phys. Chem. **1961**, *65* (8), pp 1404−1409
DOI: 10.1021/j100826a030
Publication Date: August 1961
Initial measurement of mass spectrometry determination of heat of sublimation of seven rare earth metals including terbium, holmium, erbium, and lutetium −GL

(AN#66) - Dy - Dysprosium
Synthesis, Structure, Photoluminescence, and Electroluminescence Properties of a New Dysprosium Complex, Zhe-Feng Li, Liang Zhou, Jiang-Bo Yu, Hong-Jie Zhang, Rui-Ping Deng, Ze-Ping Peng, and Zhi-Yong Guo
J. Phys. Chem. C **2007**, *111* (5), pp 2295−2300
DOI: 10.1021/jp064749t
Publication Date (Web): January 17, 2007
A new dysprosium complex was synthesized, and its structural and photophysical properties were evaluated. The energy transfer mechanism between the ligand and central Dy^{3+} ion is discussed, and a series of electroluminescent devices were built. Emission at both yellow (572 nm) and blue (480 nm) wavelengths was observed. Appropriate choice of the yellow/blue intensity ratio is proposed to be tunable to achieve white luminescent emission. −GRG

(AN#67) - Ho - Holmium
Amplifying Excitation-Power Sensitivity of Photon Upconversion in a $NaYbF_4$:Ho Nanostructure for Direct Visualization of Electromagnetic Hotspots, Bing Chen, Yong Liu, Yao Xiao, Xian Chen, Yang Li, Mingyu Li, Xvsheng Qiao, Xianping Fan, and Feng Wang
J. Phys. Chem. Lett. **2016**, 7 (23), pp 4916−4921
DOI: 10.1021/acs.jpclett.6b02210
Publication Date (Web): November 15, 2016
Holmium ion doped nanoparticles produce upconverted luminescence that can be used for imaging hot-spots in plasmonic materials. −GVH

(AN#68) - Er - Erbium
Highly Efficient Multicolor Up-Conversion Emissions and Their Mechanisms of Monodisperse $NaYF_4$:Yb,Er Core and Core/Shell-Structured Nanocrystals, Hao-Xin Mai,Ya-Wen Zhang, Ling-Dong Sun, and Chun-Hua Yan
J. Phys. Chem. C **2007**, *111* (37), pp 13721−13729
DOI: 10.1021/jp073920d
Publication Date (Web): August 24, 2007
Synthesis of highly efficient erbium doped phosphors and their mechanism of efficient up-conversion −HF

(AN#69) - Tm - Thulium
The Electronic and Vibrational Structure of Endohedral $Tm_3N@C_{80}$ (I) Fullerene - Proof of an Encaged Tm^{3+}, Matthias Krause, Xianjie Liu, Joanna Wong, Thomas Pichler, Martin Knupfer, and Lothar Dunsch
J. Phys. Chem. A **2005**, *109* (32), pp 7088−7093
DOI: 10.1021/jp0525080
Publication Date (Web): July 23, 2005
Characterization of encaged Tm^{3+} in C_{80} fullerene −HG

(AN#70) - Yb - Ytterbium
Visible Upconversion in Rare Earth Ion-Doped Gd_2O_3 Nanocrystals, Hai Guo, Ning Dong, Min Yin, Weiping Zhang, Liren Lou, and Shangda Xia
J. Phys. Chem. B **2004**, *108* (50), pp 19205−19209
DOI: 10.1021/jp048072q
Publication Date (Web): November 20, 2004
A landmark paper in the rare-earth upconversion literature −JF

(AN#71) - Lu - Lutetium
Electrical and Magnetic Properties of Liquid Crystalline Molecular Materials: Lithium and Lutetium Phthalocyanine Derivatives, Z. Belarbi, C. Sirlin, J. Simon, and Jean Jacques Andre
J. Phys. Chem. **1989**, *93* (24), pp 8105−8110
DOI: 10.1021/j100361a026
Publication Date: November 1989
Double decker lutetium phthalocyanine based liquid crystalline molecular materials with interesting properties and applications −KB

(AN#72) - Hf - Hafnium
Atomic Layer Deposition of Hafnium Oxide from Tetrakis-(ethylmethylamino)hafnium and Water Precursors, Wei Chen, Qing−Qing Sun, Min Xu, Shi-Jin Ding, David Wei Zhang, and Li-Kang Wang
J. Phys. Chem. C **2007**, *111* (17), pp 6495−6499
DOI: 10.1021/jp070362u
Publication Date (Web): April 6, 2007
Thermodynamics of halfnium calculated to predict atomic layer deposition processes. - MZ

(AN#73) - Ta - Tantalum
Quantum-Sized PbS, CdS, Ag_2S, Sb_2S_3, and Bi_2S_3 Particles as Sensitizers for Various Nanoporous Wide-Bandgap Semiconductors, R. Vogel, P. Hoyer, and H. Weller
J. Phys. Chem. **1994**, *98* (12), pp 3183−3188
DOI: 10.1021/j100063a022
Publication Date: March 1994
Paper investigates the sensitization of nanoporous oxides (including tantalum oxide) by quantum-sized metal sulfides. −BM

DOI: 10.1021/acs.jpclett.9b01057
J. Phys. Chem. Lett. 2019, 10, 4051−4062

(AN#74) - W - Tungsten

Photoelectrochemistry of Quantized Tungsten Trioxide Colloids: Electron Storage, Electrochromic, and Photoelectrochromic Effects, Idriss Bedja, Surat Hotchandani, and Prashant V. Kamat

J. Phys. Chem. **1993**, *97* (42), pp 11064−11070

DOI: 10.1021/j100144a027

Publication Date: October 1993

Tungsten oxide (WO_3) colloidal particles have been shown to act as electron-relay systems with potential for construction of solar energy conversion and storage devices. −PJ

(AN#75) - Re - Rhenium

Surface Catalytic Sites Prepared from $[HRe(CO)_5]$ and $[H_3Re_3(CO)_{12}]$: Mononuclear, Trinuclear, and Metallic Rhenium Catalysts Supported on Magnesia, P. S. Kirlin, F. B. M. van Zon, D. C. Koningsberger, and Bruce C. Gates

J. Phys. Chem. **1990**, *94* (22), pp 8439−8450

DOI: 10.1021/j100385a017

Publication Date: November 1990

Spectroscopic and structural characterization of various heterogeneous Re catalysts on MgO, providing a better understanding of catalytic activity −RD

(AN#76) - Os - Osmium

Application of the Energy Gap Law to Excited-State Decay of Osmium(II)−Polypyridine Complexes: Calculation of Relative Nonradiative Decay Rates from Emission Spectral Profiles, Edward M. Kober, Jonathan V. Caspar, Richard S. Lumpkin, and Thomas J. Meyer

J. Phys. Chem. **1986**, *90* (16), pp 3722−3734

DOI: 10.1021/j100407a046

Publication Date: July 1986

Radiative and nonradiative decay rates of the metal-to-ligand charge-transfer excited states for osmium complexes scale in accordance with the Einstein law for spontaneous emission and the energy gap law, respectively −SL

(AN#77) - Ir - Iridium

A High Yield Synthesis of Ligand-Free Iridium Oxide Nanoparticles with High Electrocatalytic Activity, Yixin Zhao, Emil A. Hernandez-Pagan, Nella M. Vargas-Barbosa, Jennifer L. Dysart, and Thomas E. Mallouk

J. Phys. Chem. Lett. **2011**, *2* (5), pp 402−406

DOI: 10.1021/jz200051c

Publication Date (Web): February 7, 2011

Synthesis and characterization of IrO_x nanoparticles, which are highly active for water oxidation −GCS

(AN#78) - Pt - Platinum

Platinum Black Catalysts. I, G. B. Taylor, G. B. Kistiakowsky, and J. H. Perry

J. Phys. Chem. **1930**, *34* (4), pp 748−752

DOI: 10.1021/j150310a007

Publication Date: January 1929

Platinum black was prepared by three methods, and its catalytic activity to several oxidation and reduction reactions was correlated with particle size, with the smaller particle size showing higher catalytic activity. −TM

(AN#79) - Au - Gold

Adsorption and Surface-Enhanced Raman of Dyes on Silver and Gold Sols, P. C. Lee and D. Meisel

J. Phys. Chem. **1982**, *86* (17), pp 3391−3395

DOI: 10.1021/j100214a025

Publication Date: August 1982

Classic paper on colloidal gold (and silver) −CM

(AN#80) - Hg - Mercury

Mercury Drop "Attacks" an Oxidant Crystal, Satoshi Nakata, Haruhisa Komoto, Kumiko Hayashi, and Michael Menzinger

J. Phys. Chem. B **2000**, *104* (15), pp 3589−3593

DOI: 10.1021/jp9936502

Publication Date (Web): March 3, 2000

A mercury drop "attacks" a $K_2Cr_2O_7$ crystal placed ∼10 mm apart. The circular Hg drop began to elongate and to move toward the crystal with a shape and motion related to the anisotropy of the interfacial tension. −VB

(AN#81) - Tl - Thallium

Viscosity and Self-Diffusion of Liquid Thallium from Its Melting Point to About 1300 K, J. A. Cahill and A. V. Grosse

J. Phys. Chem. **1965**, *69* (2), pp 518−521

DOI: 10.1021/j100886a026

Publication Date: February 1965

Great example of how physical property measurements were at one time an important part of the journal, here in the context of a less common element −WFS

(AN#82) - Pb - Lead

Interband and Intraband Optical Studies of PbSe Colloidal Quantum Dots, Brian L. Wehrenberg, Congjun Wang, and Philippe Guyot-Sionnest

James Franck Institute, The University of Chicago, 5640 South Ellis Avenue, Chicago, Illinois 60637

J. Phys. Chem. B **2002**, *106* (41), pp 10634−10640

DOI: 10.1021/jp021187e

Publication Date (Web): September 24, 2002

Interband and intraband optical studies of PbSe colloidal quantum dots −XY

(AN#83) - Bi - Bismuth

The Bismuth−Bismuth Tribromide and Bismuth−Bismuth Triiodide Systems, S. J. Yosim, L. D. Ransom, R. A. Sallach, and L. E. Topol

J. Phys. Chem. **1962**, *66* (1), pp 28−31

DOI: 10.1021/j100807a006

Publication Date: January 1962

Paper concerned with industrial applications −CM

(AN#84) - Po - Polonium

The Preparation and Identification of Some Intermetallic Compounds of Polonium, W. G. Witteman, A. L. Giorgi, and D. T. Vier

J. Phys. Chem. **1960**, *64* (4), pp 434−440

DOI: 10.1021/j100833a014

Publication Date: April 1960

The finding of Po-forming solid alloy with other elements −ZPL

(AN#85) - At - Astatine

Astatine Standard Redox Potentials and Speciation in Acidic Medium, J. Champion, C. Alliot, E. Renault, B. M. Mokili, M. Chérel, N. Galland, and G. Montavon

J. Phys. Chem. A **2010**, *114* (1), pp 576−582

DOI: 10.1021/jp9077008

Publication Date (Web): December 16, 2009

DOI: 10.1021/acs.jpclett.9b01057
J. Phys. Chem. Lett. 2019, 10, 4051−4062

A combined experimental and theoretical study that shows that At can be present in aqueous solution in three forms, namely, At^-, At^+, and AtO^+, in the 1−2 pH range, and that the oxidation state 0 cannot exist −FZ

(AN#86) - Rn - Radon

Adsorption of Radon on Metal Surfaces: A Model Study for Chemical Investigations of Elements 112 and 114, R. Eichler and M. Schädel

J. Phys. Chem. B **2002**, *106* (21), pp 5413−5420

DOI: 10.1021/jp015553q

Publication Date (Web): April 27, 2002

There are more highly cited papers, but they usually include radon with a bunch of other noble gases. −CM

(AN#87) - Fr - Francium

First Experimentally Determined Thermodynamic Values of Francium: Hydration Energy, Energy of Partitioning, and Thermodynamic Radius, Lætitia H. Delmau, Jérôme Moine, Saed Mirzadeh, and Bruce A. Moyer

J. Phys. Chem. B **2013**, *117* (31), pp 9258−9261

DOI: 10.1021/jp401880f

Publication Date (Web): July 12, 2013

Experimental measurement of Fr^+ ionic radius resulted in a smaller radius than previously thought. −GCS

(AN#88) - Ra - Radium

Structures and Heats of Formation of Simple Alkaline Earth Metal Compounds II: Fluorides, Chlorides, Oxides, and Hydroxides for Ba, Sr, and Ra, Monica Vasiliu, J. Grant Hill, Kirk A. Peterson, and David A. Dixon

J. Phys. Chem. A **2018**, *122* (1), pp 316−327

DOI: 10.1021/acs.jpca.7b09056

Publication Date (Web): December 14, 2017

Relativistic coupled cluster theory has been used to calculate heats of formation of compounds of Ra. −KB

(AN#89) - Ac - Actinium

Capped Semiconductor Colloids. Synthesis and Photoelectrochemical Behavior of TiO_2 Capped SnO_2 Nanocrystallites, Idriss Bedja and Prashant V. Kamat

J. Phys. Chem. **1995**, *99* (22), pp 9182−9188

DOI: 10.1021/j100022a035

Publication Date: June 1995

The volatility of actinium was measured through volatilization experiments at high temperature. −JZ

(AN#90) - Th - Thorium

Making and Breaking Bonds in the Solid State: The Thorium Chromium Silicide ($ThCr_2SI_2$) Structure, Roald Hoffmann and Chong Zheng

J. Phys. Chem. **1985**, *89* (20), pp 4175−4181

DOI: 10.1021/j100266a007

Publication Date: September 1985

Highly cited feature article by Roald Hoffman on crystal structures for which $ThCr_2Si_2$ is a prototype −JF

(AN#91) - Pa - Protactinium

Theoretical Study on Molecular Property of Protactinium(V) and Uranium(VI) Oxocations: Why Does Protactinium(V) Form Monooxo Cations in Aqueous Solution? Takashi Toraishi, Takao Tsuneda, and Satoru Tanaka

J. Phys. Chem. A **2006**, *110* (49), pp 13303−13309

DOI: 10.1021/jp0641435

Publication Date (Web): November 15, 2006

Electronic structure calculations of the Pa(V) oxocation in aqueous solution clearly support from an energetic point of view the experimental result that monooxo protactinyl cation, PaO_3^+ is a preferable species for $Pa(V)_{aq}$. −PJ

(AN#92) - U - Uranium

The Uranium−Oxygen System: $UO_{2.5}$ to U_3O_8, H. R. Hoekstra, S. Siegel, L. H. Fuchs, and J. J. Katz

J. Phys. Chem. **1955**, *59* (2), pp 136−138

DOI: 10.1021/j150524a010

Publication Date: February 1955

Uranium−oxygen system: $UO_{2.5}$ to U_3O_8 −TZ

(AN#93) - U - Neptunium

Measurement of the Absorption Spectra of Neptunium Ions in Heavy Water Solution from 0.35 to 1.85 μ, W. C. Waggener

J. Phys. Chem. **1958**, *62* (3), pp 382−383

DOI: 10.1021/j150561a050

Publication Date: March 1958

Examines the adsorption spectrum of neptunium in heavy water −AG

(AN#94) - Pu - Plutonium

The Kinetics of the Reaction between Plutonium(VI) and Iron(II), T. W. Newton and F. B. Baker

J. Phys. Chem. **1963**, *67* (7), pp 1425−1432

DOI: 10.1021/j100801a005

Publication Date: July 1963

Classic 1962 study of rates and thermodynamics of the oxidation−reduction reaction of plutonium and iron −ASM

(AN#95) - Am - Americium

Americium Organometallic Ions Produced by Laser Ablation of AmO_2 in Polyimide, John K. Gibson

J. Phys. Chem. A **1998**, *102* (24), pp 4501−4508

DOI: 10.1021/jp981145j

Publication Date (Web): May 20, 1998

Americium organometallic ions produced by laser ablation of AmO_2 in polyimide −AY

(AN#96) - Cm - Curium

Hydration Shell Structure and Dynamics of Curium(III) in Aqueous Solution: First Principles and Empirical Studies, Raymond Atta-Fynn, Eric J. Bylaska, Gregory K. Schenter, and Wibe A. de Jong

J. Phys. Chem. A **2011**, *115* (18), pp 4665−4677

DOI: 10.1021/jp201043f

Publication Date (Web): April 18, 2011

Simulation paper on the structure of Cm(III) in aqueous solution −BS

(AN#97) - Bk - Berkelium

Electron-Transfer Spectra and the II−III Oxidation Potentials of Some Lanthanide and Actinide Halides in Solution, Leonard J. Nugent, R. D. Baybarz, and J. L. Burnett

J. Phys. Chem. **1969**, *73* (4), pp 1177−1178

DOI: 10.1021/j100724a084

Publication Date: April 1969

Includes calculated absorption maximum and oxidation potential of BkBr −DC

DOI: 10.1021/acs.jpclett.9b01057
J. Phys. Chem. Lett. 2019, 10, 4051−4062

(AN#98) - Cf - Californium

Radiolysis of 0.4 M Sulfuric Acid Solutions with Fission Fragments from Dissolved Californium-252. Estimated Yields of Radical and Molecular Products that Escape Reactions in Fission Fragment Tracks, Ned E. Bibler

J. Phys. Chem. **1975**, *79* (19), pp 1991−1995

DOI: 10.1021/j100586a002

Publication Date: September 1975

A study of the radiolysis of sulfuric acid solution, with and without Fe^{2+} and Ce^{4+} ions, using dissolved californium-252 −EW

(AN#99) - Es - Einsteinium

Intramolecular Energy Transfer and Sensitized Luminescence in Actinide(III) β-Diketone Chelates, Leonard J. Nugent, J. L. Burnett, R. D. Baybarz, George Knoll Werner, S. P. Tanner, J. R. Tarrant, and O. L. Keller, Jr.

J. Phys. Chem. **1969**, *73* (5), pp 1540−1549

DOI: 10.1021/j100725a060

Publication Date: May 1969

First measurements of Es(III) chelate lifetimes from the transuranium laboratory at ORNL −FG

(AN#100) - Fm - Fermium

Electron-Transfer Spectra and the II−III Oxidation Potentials of Some Lanthanide and Actinide Halides in Solution, Leonard J. Nugent, R. D. Baybarz, and J. L. Burnett

J. Phys. Chem. **1969**, *73* (4), pp 1177−1178

DOI: 10.1021/j100724a084

Publication Date: April 1969

Calculated oxidation potential (II−III) and lowest charge-transfer band for a Fermium bromide. −GEMS

(AN#101) - Md - Mendelevium

Role of Atomic Electronics in f-Element Bond Formation: Bond Energies of Lanthanide and Actinide Oxide Molecules, John K. Gibson

J. Phys. Chem. A **2003**, *107* (39), pp 7891−7899

DOI: 10.1021/jp035003n

Publication Date (Web): August 22, 2003

This paper makes estimates of the bond dissociation enthalpies of all the actinide monoxides. −GCS

(AN#102) - No - Nobelium

Role of Atomic Electronics in f-Element Bond Formation: Bond Energies of Lanthanide and Actinide Oxide Molecules, John K. Gibson

J. Phys. Chem. A **2003**, *107* (39), pp 7891−7899

DOI: 10.1021/jp035003n

Publication Date (Web): August 22, 2003

The bond dissociation energy of NoO cannot be estimated with confidence. −GCS

(AN#103) - Lr - Lawrencium

Redox Reactions for Group 5 Elements, Including Element 105, in Aqueous Solutions, G. V. Ionova, V. Pershina, E. Johnson, B. Fricke, and M. Schaedel

J. Phys. Chem. **1992**, *96* (26), pp 11096−11101

DOI: 10.1021/j100205a086

Publication Date: December 1992

Calculation of ionization potentials using the multiconfiguration Dirac−Fock method, showing that the maximum oxidation state of Lr is more stable than the higher mass group 5 elements −GVH

(AN#104) - Rf - Rutherfordium

Total Energy Calculations of $RfCl_4$ and Homologues in the Framework of Relativistic Density Functional Theory, S. Varga, B. Fricke, M. Hirata, T. Baştuğ, V. Pershina, and S. Fritzsche

J. Phys. Chem. A **2000**, *104* (27), pp 6495−6498

DOI: 10.1021/jp993980m

Publication Date (Web): June 16, 2000

Demonstration that a four-component, fully relativistic density functional method could provide accurate values for the formation and binding energies of $RfCl_4$ −HF

(AN#105) - Db - Dubnium

Thermochemical Characterization of Seaborgium Compounds in Gas Adsorption Chromatography, B. Eichler, A. Türler, and, H. W. Gäggeler

J. Phys. Chem. A **1999**, *103* (46), pp 9296−9306

DOI: 10.1021/jp9917751

Publication Date (Web): October 30, 1999

Dubnium is mentioned in this paper, but no experimental data are reported. −HG

(AN#106) - Sg - Seaborgium

Ionization Potentials of Seaborgium, E. Johnson, V. Pershina, and B. Fricke

J. Phys. Chem. A **1999**, *103* (42), pp 8458−8462

DOI: 10.1021/jp9903211

Publication Date (Web): October 4, 1999

This is the first paper to attempt to calculate the ionization potentials of seaborgium, which was officially only 2 years old at the time. −JF

(AN#107) - Bh - Bohrium

On the Stability and Volatility of Group 8 Tetroxides, MO_4 (M = Ruthenium, Osmium, and Hassium (Z = 108)), Christoph E. Düllmann, Bernd Eichler, Robert Eichler, Heinz W. Gäggeler, and Andreas Türle

J. Phys. Chem. B **2002**, *106* (26), pp 6679−6684

DOI: 10.1021/jp0257146

Publication Date (Web): June 8, 2002

Bohrium is briefly mentioned in a study that mostly refers to Hs. −KB

(AN#108) - Hs - Hassium

On the Stability and Volatility of Group 8 Tetroxides, MO_4 (M = Ruthenium, Osmium, and Hassium (Z = 108)), Christoph E. Düllmann, Bernd Eichler, Robert Eichler, Heinz W. Gäggeler, and Andreas Türle

J. Phys. Chem. B **2002**, *106* (26), pp 6679−6684

DOI: 10.1021/jp0257146

Publication Date (Web): June 8, 2002

The adsorption behavior of HsO_4 on quartz surfaces is predicted on the basis of its chemical stability. −MZ

(AN#109) - Mt - Meitnerium

N/A

(AN#110) - DS - Darmstadtium

N/A

DOI: 10.1021/acs.jpclett.9b01057
J. Phys. Chem. Lett. 2019, 10, 4051−4062

(AN#111) - Rg - Roentgenium

Predicted Properties of the Superheavy Elements. II. Element 111, Eka-Gold, O. L. Keller, Jr., C. W. Nestor, Jr., Thomas A. Carlson, and Burkhard Fricke

J. Phys. Chem. **1973**, *77* (14), pp 1806−1809

DOI: 10.1021/j100633a017

Publication Date: July 1973

Early (1973) electronic structure study comparing Rg and Au −TG

(AN#112) - Cn - Copernicium

Atomic and Molecular Properties of Elements 112, 114, and 118, Clinton S. Nash

J. Phys. Chem. A **2005**, *109* (15), pp 3493−3500

DOI: 10.1021/jp050736o

Publication Date (Web): March 26, 2005

Theoretical calculations of atoms and diatomic molecules of elements 112, 114, and 118 were conducted, and the effects of spin−orbit coupling on the expected chemistry were examined. Element 112 (copernicium) is similar in most respects to Hg, but the complex valence shell structure makes it intermediate in behavior between 6d and 7p transactinides. −TM

(AN#113) - Nh - Nihonium

Atomic Properties of Element 113 and Its Adsorption on Inert Surfaces from ab Initio Dirac−Coulomb Calculations, V. Pershina, A. Borschevsky, E. Eliav, and U. Kaldor

J. Phys. Chem. A **2008**, *112* (51), pp 13712−13716

DOI: 10.1021/jp8061306

Publication Date (Web): December 2, 2008

Dirac−Coulomb calculations with comparison with Tl −GCS

(AN#114) - Fl - Flerovium

Taming the Electronic Structure of Lead and Eka-lead (Flerovium) by the Relativistic Coupled Cluster Method, Rajat K. Chaudhuri, Sudip Chattopadhyay, and Uttam Sinha Mahapatra

J. Phys. Chem. A **2013**, *117* (36), pp 8555−8567

DOI: 10.1021/jp402376b

Publication Date (Web): May 7, 2013

For the very heaviest elements, trends in atomic properties (here ionization potential and excitation energies) are most readily probed with first-principles calculations. −WFS

(AN#115) - Mc - Moscovium

Predicted Properties of The Superheavy Elements. III. Element 115, Eka-Bismuth, O. L. Keller, Jr., C. W. Nestor, Jr., and Burkhard Fricke

J. Phys. Chem. **1974**, *78* (19), pp 1945−1949

DOI: 10.1021/j100612a015

Publication Date: September 1974

Computational study comparing Mc with Bi - XY

(AN#116) - Lv - Livermorium

An Anomalous Bond Angle in (116)H_2. Theoretical Evidence for Supervalent Hybridization, Clinton S. Nash and Wesley W. Crockett

J. Phys. Chem. A **2006**, *110* (14), pp 4619−4621

DOI: 10.1021/jp060888z

Publication Date (Web): March 18, 2006

Theoretical calculation shows the interesting structure of LvH_2 structure due to spin−orbit coupling. −ZPL

(AN#117) - Ts - Tennessine

Spin−Orbit Effects on the Electronic Structure of Heavy and Superheavy Hydrogen Halides: Prediction of an Anomalously Strong Bond in H[117], Clinton S. Nash and Bruce E. Bursten

J. Phys. Chem. A **1999**, *103* (5), pp 632−636

DOI: 10.1021/jp9843407

Publication Date (Web): January 13, 1999

MRCI and CCSD(T) calculations of the bond energy and bond length of HTs show that the 8s orbital contributes significantly to bonding due to spin−orbit effects. −GCS

(AN#118) - Og - Oganesson

Atomic and Molecular Properties of Elements 112, 114, and 118, Clinton S. Nash

J. Phys. Chem. A **2005**, *109* (15), pp 3493−3500

DOI: 10.1021/jp050736o

Publication Date (Web): March 26, 2005

CCSD(T) study of Og suggests that it is much more reactive than Rn, with a Og_2 bond energy of 0.062 eV, compared to 0.016 eV for Rn_2. −GCS

Table 1. Editor Abbreviations

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Notes

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