

TUU
J80/pa

OCTOBER 3, 2013

VOLUME 117

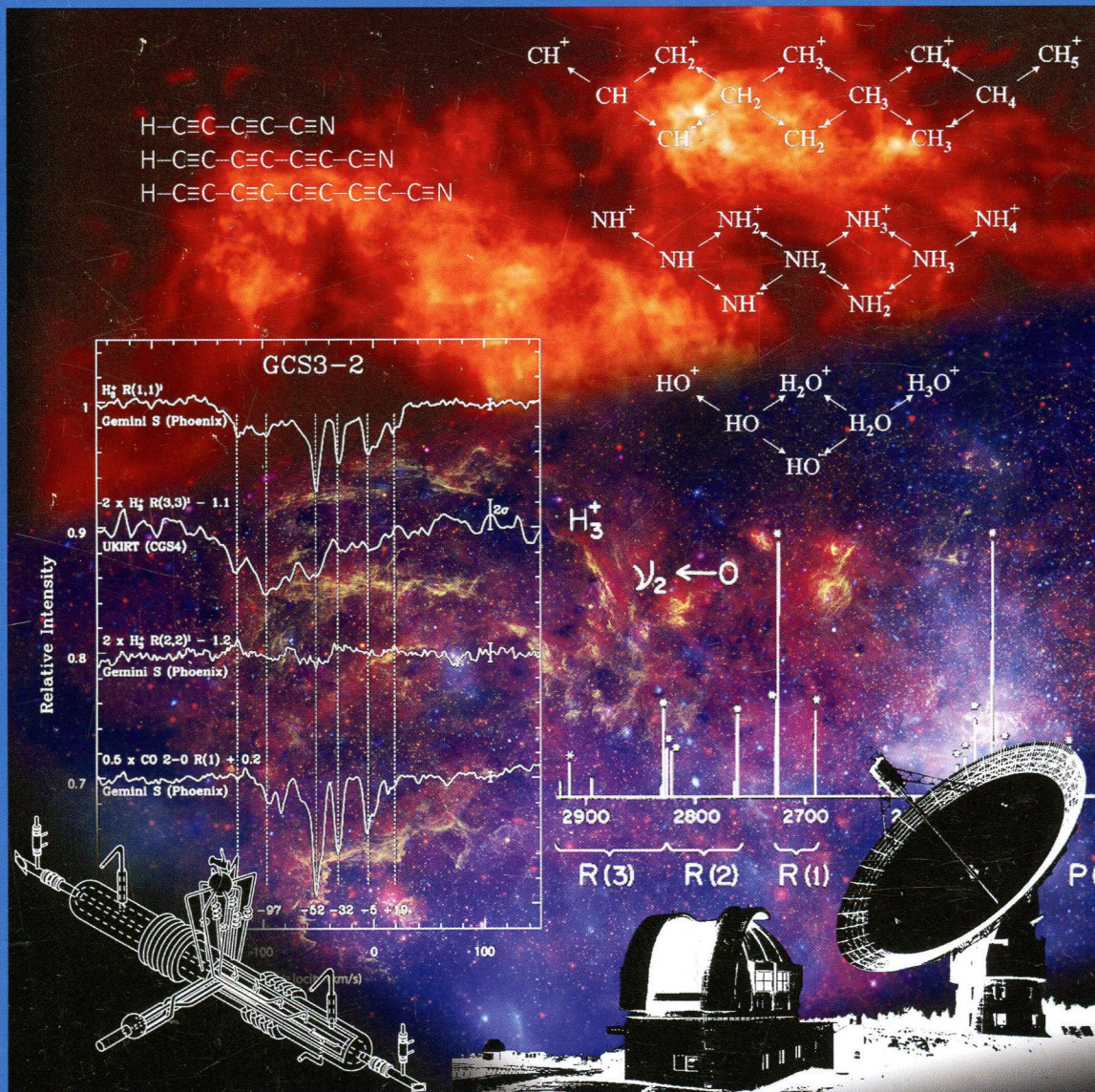
NUMBER 39

pubs.acs.org/JPCA

THE JOURNAL OF PHYSICAL CHEMISTRY

A

Celebrating the
Richness and Beauty
of Terrestrial and
Astronomical Molecular
Spectroscopy
(see page 5A)



**OKA Festschrift:
CELEBRATING 45 YEARS OF ASTROCHEMISTRY**



ACS Publications
MOST TRUSTED. MOST CITED. MOST READ.

www.acs.org

THE JOURNAL OF PHYSICAL CHEMISTRY A

October 3, 2013

Volume 117, Issue 39

Pages 9305-10144

Oka Festschrift: Celebrating 45 Years of Astrochemistry Special Issue Preface

Tribute to Takeshi Oka

Mitchio Okumura , Benjamin J. McCall , Thomas R. Geballe

pp 9305–9307

Publication Date (Web): October 3, 2013 (Special Issue Preface)

DOI: 10.1021/jp4079597

My 45 Years of Astrochemistry: Memoirs of Takeshi Oka

Takeshi Oka

pp 9308–9313

Publication Date (Web): October 3, 2013 (Special Issue Preface)

DOI: 10.1021/jp4035826

List of Collaborators of Takeshi Oka

pp 9314–9314

Publication Date (Web): October 3, 2013 (Special Issue Preface)

DOI: 10.1021/jp403580z

Curriculum Vitae of Takeshi Oka

pp 9315–9315

Publication Date (Web): October 3, 2013 (Special Issue Preface)

DOI: 10.1021/jp4042809

Publications of Takeshi Oka

pp 9316–9323

Publication Date (Web): October 3, 2013 (Special Issue Preface)

DOI: 10.1021/jp403581w

Articles

The 1 ³A' HCN and 1 ³A' HCO⁺ Vibrational Frequencies and Spectroscopic Constants from Quartic Force Fields

Ryan C. Fortenberry, Xinchuan Huang, T. Daniel Crawford, and Timothy J. Lee

pp 9324–9330

Publication Date (Web): November 2, 2012 (Article)

DOI: 10.1021/jp309243s

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Photoionization Cross Section of the Propargyl Radical and Some General Ideas for Estimating Radical Cross Sections

Hong Xu and S. T. Pratt

pp 9331–9342

Publication Date (Web): November 26, 2012 (Article)

DOI: 10.1021/jp309874q

 Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Variational Calculations of Vibrational Energies and IR Spectra of trans- and cis-HOCO Using New ab Initio Potential Energy and Dipole Moment Surfaces

Yimin Wang, Stuart Carter, and Joel M. Bowman

pp 9343–9352

Publication Date (Web): November 14, 2012 (Article)

DOI: 10.1021/jp309911w

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Spin–Orbit and Vibronic Coupling in the Ionic Ground State of Iodoacetylene from a Rotationally Resolved Photoelectron Spectrum

Bérenger Gans, Guido Grassi, and Frédéric Merkt

pp 9353–9362

Publication Date (Web): December 11, 2012 (Article)

DOI: 10.1021/jp310241d

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Optomechanical Shutter Modulated Broad-Band Cavity–Enhanced Absorption Spectroscopy of Molecular Transients of Astrophysical Interest

Anton Walsh, Dongfeng Zhao, Wim Ubachs, and Harold Linnartz

pp 9363–9369

Publication Date (Web): December 14, 2012 (Article)

DOI: 10.1021/jp310392n



Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

The Predicted Spectrum and Singlet–Triplet Interaction of the Hypermetallic Molecule SrOSr

B. Ostojčić, Per Jensen, P. Schwerdtfeger, and P. R. Bunker

pp 9370–9379

Publication Date (Web): March 18, 2013 (Article)

DOI: 10.1021/jp310531s



Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Infrared Spectra of Products of the Reaction of H Atoms with O₂ Trapped in Solid Neon: HO₂, HO₂⁺, HOHOH⁻, and H₂O(HO)

Marilyn E. Jacox and Warren E. Thompson

pp 9380–9390

Publication Date (Web): December 7, 2012 (Article)

DOI: 10.1021/jp310849s



Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Microwave Spectra of the Deuterium Isotopologues of cis-Hexatriene and a Semiexperimental Equilibrium Structure

Norman C. Craig, Yihui Chen, Hannah A. Fuson, Hengfeng Tian, Herman van Besien, Andrew R. Conrad, Michael J. Tubergen, Heinz Dieter Rudolph, and Jean Demaison

pp 9391–9400

Publication Date (Web): December 13, 2012 (Article)

DOI: 10.1021/jp311035c



Section:

Physical Organic Chemistry

Two Challenges for Experimenters

R. Stephen Berry

pp 9401–9403

Publication Date (Web): December 4, 2012 (Article)

DOI: 10.1021/jp311106r

 Section:

Electric Phenomena

74 MHz Nonthermal Emission from Molecular Clouds: Evidence for a Cosmic Ray Dominated Region at the Galactic Center

F. Yusef-Zadeh, M. Wardle, D. Lis, S. Viti, C. Brogan, E. Chambers, M. Pound, and M. Rickert

pp 9404–9419

Publication Date (Web): May 1, 2013 (Article)

DOI: 10.1021/jp311240h

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

The Most Diffuse Molecular Gas in the Galaxy

Harvey S. Liszt

pp 9420–9423

Publication Date (Web): February 7, 2013 (Article)

DOI: 10.1021/jp311254w

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Theoretical Studies of the Ground and Excited State Structures of Stilbene

Rajat K. Chaudhuri , Karl F. Freed , Sudip Chattopadhyay , Uttam Sinha Mahapatra

pp 9424–9434

Publication Date (Web): March 26, 2013 (Article)

DOI: 10.1021/jp311493w

 Section:

Physical Organic Chemistry

Vibrationally Hot Bands of the SiCN $\tilde{A}^2\Delta - ^2\Pi$ System

Masaru Fukushima and Takashi Ishiwata

pp 9435–9443

Publication Date (Web): March 5, 2013 (Article)

DOI: 10.1021/jp311684e

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Nonlinear Spectroscopic Theory of Displaced Harmonic Oscillators with Differing Curvatures: A Correlation Function Approach

Andrew F. Fidler and Gregory S. Engel

pp 9444–9453

Publication Date (Web): February 20, 2013 (Article)

DOI: 10.1021/jp311713x

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Chemical Vapor Deposition Synthesis and Raman Spectroscopic Characterization of Large-Area Graphene Sheets

Chun-Da Liao, Yi-Ying Lu, Srinivasa Reddy Tamalampudi, Hung-Chieh Cheng, and Yit-Tsong Chen

pp 9454–9461

Publication Date (Web): March 5, 2013 (Article)

DOI: 10.1021/jp311757r

 Section:

Electric Phenomena

Spectrum of the Autoionizing Triplet Gerade Rydberg States of H_2 and its Analysis Using Multichannel Quantum-Defect Theory

Daniel Sprecher, Christian Jungen, and Frédéric Merkt

pp 9462–9476

Publication Date (Web): February 21, 2013 (Article)

DOI: 10.1021/jp311793t

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Ternary Recombination of H_3^+ and D_3^+ with Electrons in He- H_2 (D_2) Plasmas at Temperatures from 50 to 300 K

R. Johnsen, P. Rubovič, P. Dohnal, M. Hejduk, R. Plašil, and J. Glosík

pp 9477–9485

Publication Date (Web): February 6, 2013 (Article)

DOI: 10.1021/jp311978n

 Section:

Electric Phenomena

Photodissociation and Radiative Association of HeH⁺ in the Metastable Triplet State

J. Loreau, S. Vranckx, M. Desouter-Lecomte, N. Vaeck, and A. Dalgarno

pp 9486–9492

Publication Date (Web): February 25, 2013 (Article)

DOI: 10.1021/jp312007q

 Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Using a Nondirect Product Basis to Compute J > 0 Rovibrational States of H₃⁺

Ralph Jaquet and Tucker Carrington, Jr.

pp 9493–9500

Publication Date (Web): March 14, 2013 (Article)

DOI: 10.1021/jp312027s

 Section:

General Physical Chemistry

Modulated Fluorophore Signal Recovery Buried within Tissue Mimicking Phantoms

Saugata Sarkar, Chaoyang Fan, Jung-Cheng Hsiang, and Robert M. Dickson

pp 9501–9509

Publication Date (Web): May 21, 2013 (Article)

DOI: 10.1021/jp312071n

 Section:

Biochemical Methods

Infrared Spectroscopy of Chloromethyl Radical in Solid Parahydrogen and Its Nuclear Spin Conversion

Yuki Miyamoto, Masaaki Tsubouchi, and Takamasa Momose

pp 9510–9517

Publication Date (Web): March 18, 2013 (Article)

DOI: 10.1021/jp312122p

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Theoretical Investigation of the Infrared Spectra of the H₅⁺ and D₅⁺ Cations

Álvaro Valdés and Rita Prosimiti

pp 9518–9524

Publication Date (Web): February 7, 2013 (Article)

DOI: 10.1021/jp3121947

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Microwave Structure for the Propiolic Acid–Formic Acid Complex

Stephen G. Kukolich, Erik G. Mitchell, Spencer J. Carey, Ming Sun, and Bryan A. Sargus

pp 9525–9530

Publication Date (Web): January 29, 2013 (Article)

DOI: 10.1021/jp312201r

 Section:

Physical Organic Chemistry

Elucidating the Decomposition Mechanism of Energetic Materials with Geminal Dinitro Groups Using 2-Bromo-2-nitropropane Photodissociation

Ryan S. Booth, Chow-Shing Lam, Matthew D. Brynteson, Lei Wang, and Laurie J. Butler

pp 9531–9547

Publication Date (Web): March 15, 2013 (Article)

DOI: 10.1021/jp312248v

 Section:

Propellants and Explosives

Multipass Millimeter/Submillimeter Spectrometer to Probe Dissociative Reaction Dynamics

Jacob C. Laas, Brian M. Hays, and Susanna L. Widicus Weaver

pp 9548–9554

Publication Date (Web): May 16, 2013 (Article)

DOI: 10.1021/jp3122402

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Influence of Molecular Structure on the Laser-Induced Plasma Emission of the Explosive RDX and Organic Polymers

Frank C. De Lucia, Jr. and Jennifer L. Gottfried

pp 9555–9563

Publication Date (Web): July 10, 2013 (Article)

DOI: 10.1021/jp312236h

 Section:

Propellants and Explosives

The Structure and Spectroscopy of Cyanate and Bicarbonate Ions. Astrophysical Implications

M. A. Moreno, B. Maté, Y. Rodríguez-Lazcano, O. Gálvez, P. C. Gómez, V. J. Herrero, and R. Escribano

pp 9564–9573

Publication Date (Web): January 29, 2013 (Article)

DOI: 10.1021/jp3122616

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Electronic Absorption Spectrum of Triacetylene Cation for Astronomical Considerations

S. Chakrabarty, C. A. Rice, F. J. Mazzotti, R. Dietsche, and J. P. Maier

pp 9574–9577

Publication Date (Web): March 5, 2013 (Article)

DOI: 10.1021/jp312294f

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Laser Absorption Spectroscopy of the $d^3\Pi_g \leftarrow c^3\Sigma_u^+$ Transition of C_2

Man-Chor Chan, Shun-Hin Yeung, Na Wang, and A. S.-C. Cheung

pp 9578–9583

Publication Date (Web): March 14, 2013 (Article)

DOI: 10.1021/jp3122769

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Ortho-Para Mixing Hyperfine Interaction in the H_2O^+ Ion and Nuclear Spin Equilibration

Keiichi Tanaka, Kensuke Harada, and Takeshi Oka

pp 9584–9592

Publication Date (Web): March 26, 2013 (Article)

DOI: 10.1021/jp312270u

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Tracing the Physical Conditions in Active Galactic Nuclei with Time-Dependent Chemistry

Rowin Meijerink, Marco Spaans, Inga Kamp, Giambattista Aresu, Wing-Fai Thi, and Peter Woitke

pp 9593–9604

Publication Date (Web): June 10, 2013 (Article)

DOI: 10.1021/jp312289f

 Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

Fundamental and Torsional Combination Bands of Two Isomers of the OCS- CO_2 Complex in the CO_2 ν_3 Region

J. Norooz Olliaee, M. Dehghany, N. Moazzen-Ahmadi, and A. R. W. McKellar

pp 9605–9611

Publication Date (Web): January 16, 2013 (Article)

DOI: 10.1021/jp312339w

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

CO Dimer: The Infrared Spectrum Revisited

Mojtaba Rezaei, S. Sheybani-Deloui, N. Moazzen-Ahmadi, K.H. Michaelian, and A.R.W. McKellar

pp 9612–9620

Publication Date (Web): February 15, 2013 (Article)

DOI: 10.1021/jp312337v

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Electronic Relaxation after Resonant Laser Excitation of Cr in Superfluid Helium Nanodroplets

Andreas Kautsch, Markus Koch, and Wolfgang E. Ernst

pp 9621–9625

Publication Date (Web): February 14, 2013 (Article)

DOI: 10.1021/jp312336m



 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Binary Recombination of H_3^+ and D_3^+ Ions with Electrons in Plasma at 50–230 K

Peter Rubovič, Petr Dohnal, Michal Hejduk, Radek Plašil, and Juraj Glosík

pp 9626–9632

Publication Date (Web): March 27, 2013 (Article)

DOI: 10.1021/jp3123192

 Section:

Electric Phenomena

Calculation of Rotation–Vibration Energy Levels of the Water Molecule with Near-Experimental Accuracy Based on an *ab Initio* Potential Energy Surface

Oleg L. Polyansky, Roman I. Ovsyannikov, Aleksandra A. Kyuberis, Lorenzo Lodi, Jonathan Tennyson, and Nikolai F. Zobov

pp 9633–9643

Publication Date (Web): March 21, 2013 (Article)

DOI: 10.1021/jp312343z

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

High-Resolution Study of $^{13}C^{16}O$ A–X($v' = 0–9$) Bands Using the VUV-FTS at SOLEIL: Revised Term Values

Liseth Gavilan, Jean Louis Lemaire, Michèle Eidelsberg, S. R. Federman, Glenn Stark, Alan N. Heays, Jean-Hugues Fillion, James R. Lyons, and Nelson de Oliveira

pp 9644–9652

Publication Date (Web): April 9, 2013 (Article)

DOI: 10.1021/jp312338z

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Formation of HCN⁺ in Heterogeneous Reactions of N₂⁺ and N⁺ with Surface Hydrocarbons

Martina Harnisch, Alan Keim, Paul Scheier, and Zdenek Herman

pp 9653–9660

Publication Date (Web): April 24, 2013 (Article)

DOI: 10.1021/jp312307a

 ACS AuthorChoice

 Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

Ortho-to-Para Ratio in Interstellar Water on the Sightline toward Sagittarius B2(N)

Dariusz C. Lis, Edwin A. Bergin, Peter Schilke, and Ewine F. van Dishoeck

pp 9661–9665

Publication Date (Web): May 8, 2013 (Article)

DOI: 10.1021/jp312333n

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Organic Synthesis in the Interstellar Medium by Low-Energy Carbon Irradiation

E. J. McBride, T. J. Millar, and J. J. Kohanoff

pp 9666–9672

Publication Date (Web): May 10, 2013 (Article)

DOI: 10.1021/jp312342v

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Conversion of Nuclear Spin Isomers of Ethylene

P. L. Chapovsky, V. V. Zhivonitko, and I. V. Koptug

pp 9673–9683

Publication Date (Web): July 8, 2013 (Article)

DOI: 10.1021/jp312322f

 Section:

Magnetic Phenomena

Spectroscopic and Theoretical Investigations of UF and UF⁺

Ivan O. Antonov and Michael C. Heaven

pp 9684–9694

Publication Date (Web): January 29, 2013 (Article)

DOI: 10.1021/jp312362e

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

FHF⁻ Isotopologues: Highly Anharmonic Hydrogen-Bonded Systems with Strong Coriolis Interaction

Peter Sebald, Arne Bargholz, Rainer Oswald, Christopher Stein, and Peter Botschwina

pp 9695–9703

Publication Date (Web): February 19, 2013 (Article)

DOI: 10.1021/jp3123677

 Section:

General Physical Chemistry

Potential Curves for the Dissociative Recombination of CO⁺

Steven L. Guberman

pp 9704–9711

Publication Date (Web): March 21, 2013 (Article)

DOI: 10.1021/jp312359c

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Matrix Isolation Spectroscopy and Nuclear Spin Conversion of NH₃ and ND₃ in Solid Parahydrogen

Mahmut Ruzi and David T. Anderson

pp 9712–9724

Publication Date (Web): March 22, 2013 (Article)

DOI: 10.1021/jp3123727

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Identifying Single Molecular Ions by Resolved Sideband Measurements

James E. Goeders, Craig R. Clark, Grahame Vittorini, Kenneth Wright, C. Ricardo Viteri, and Kenneth R. Brown

pp 9725–9731

Publication Date (Web): April 5, 2013 (Article)

DOI: 10.1021/jp312368a

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Terahertz Spectroscopy of ^{25}MgH ($X^2\Sigma^+$) and ^{67}ZnH ($X^2\Sigma^+$): Bonding in Simple Metal Hydrides

Matthew P. Bucchino and Lucy M. Ziurys

pp 9732–9737

Publication Date (Web): March 21, 2013 (Article)

DOI: 10.1021/jp3123743

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Study of the Q Branch Structure of the ^{14}N and ^{15}N Isotopologues of the ν_4 Band of Ammonia Using Frequency Chirped Quantum Cascade Lasers

Geoffrey Duxbury, David Wilson, Kenneth Hay, and Nigel Langford

pp 9738–9745

Publication Date (Web): April 12, 2013 (Article)

DOI: 10.1021/jp3123665

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Theoretical Prediction of the Structures and Energies of Olympicene and its Isomers

Andrew J. S. Valentine and David A. Mazziotti

pp 9746–9752

Publication Date (Web): March 19, 2013 (Article)

DOI: 10.1021/jp312384b

 Section:

Physical Organic Chemistry

***Microwave Studies on 1,4-Pentadiene: CH₂=CH-CH₂-CH=CH₂;
Transformations among the Three Rotational Isomers***

Eizi Hirota , Ryo Watanabe and Yoshiyuki Kawashima , Toshiaki Shigemune, Juichi Matsumoto, and Kenji Murakami , Asao Mizoguchi and Hideto Kanamori , Masakazu Nakajima and Yasuki Endo , Yoshihiro Sumiyoshi

pp 9753–9760

Publication Date (Web): March 14, 2013 (Article)

DOI: 10.1021/jp3124023

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Rydberg States of Triatomic Hydrogen and Deuterium

Jia Wang and Chris H. Greene

pp 9761–9765

Publication Date (Web): April 4, 2013 (Article)

DOI: 10.1021/jp312462a

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Ortho/Para Ratio of H₂O⁺ Toward Sagittarius B2(M) Revisited

Peter Schilke, Dariusz C. Lis, Edwin A. Bergin, Ronan Higgins, and Claudia Comito

pp 9766–9769

Publication Date (Web): May 28, 2013 (Article)

DOI: 10.1021/jp312364c

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Cooling by H₃⁺ Emission

Steve Miller, Tom Stallard, Jonathan Tennyson, and Henrik Melin

pp 9770–9777

Publication Date (Web): July 16, 2013 (Article)

DOI: 10.1021/jp312468b

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

***State-to-State Quantum Mechanical Calculations of Rate Coefficients for the
D⁺ + H₂ → HD + H⁺ Reaction at Low Temperature***

P. Honvault and Y. Scribano

pp 9778–9784

Publication Date (Web): March 1, 2013 (Article)

DOI: 10.1021/jp3124549

 Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

Experimental Observation and Quantum Chemical Characterization of the $S_1 \leftarrow S_0$ Transition of Protonated Naphthalene–Argon Clusters

Alexander Patzer, Markus Schütz, Christophe Jouvét, and Otto Dopfer

pp 9785–9793

Publication Date (Web): March 8, 2013 (Article)

DOI: 10.1021/jp312581v

 Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Profound Isotope Effect in Dissociation of Triatomic Hydrogen

P. C. Fechner, K. Mozer, and H. Helm

pp 9794–9799

Publication Date (Web): July 18, 2013 (Article)

DOI: 10.1021/jp312560t

 Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

Nuclear-Spin Selection Rules in the Chemistry of Interstellar Nitrogen Hydrides

Claire Rist, Alexandre Faure, Pierre Hily-Blant, and Romane Le Gal

pp 9800–9806

Publication Date (Web): March 5, 2013 (Article)

DOI: 10.1021/jp312640a

 Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

Photodissociation Structural Dynamics of TrirutheniumDodecacarbonyl Investigated by X-ray Transient Absorption Spectroscopy

Michael R. Harpham, Andrew, B. Stickrath, Xiaoyi, Zhang, Jier Huang, Michael W. Mara, Lin X. Chen, and Di-Jia Liu

pp 9807–9813

Publication Date (Web): May 22, 2013 (Article)

DOI: 10.1021/jp312663q

 Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Accurate High-N Rest Frequencies for CO⁺, an Ideal Tracer of Photon-Dominated Regions

Silvia Spezzano, Sandra Brünken, Holger S. P. Müller, Gabriele Klapper, Frank Lewen, Karl M. Menten, and Stephan Schlemmer

pp 9814–9818

Publication Date (Web): July 1, 2013 (Article)

DOI: 10.1021/jp312616u

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Sub-Doppler Electronic Spectra of Benzene-(H₂)_n Complexes

Masato Hayashi and Yasuhiro Ohshima

pp 9819–9830

Publication Date (Web): May 28, 2013 (Article)

DOI: 10.1021/jp312754v

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Anomalous ¹³C Isotope Abundances in C₃S and C₄H Observed toward the Cold Interstellar Cloud, Taurus Molecular Cloud-1

Nami Sakai, Shuro Takano, Takeshi Sakai, Shoichi Shiba, Yoshihiro Sumiyoshi, Yasuki Endo, and Satoshi Yamamoto

pp 9831–9839

Publication Date (Web): June 21, 2013 (Article)

DOI: 10.1021/jp3127913

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Neutral and Ionized Hydrides in Star-Forming Regions. Observations with Herschel/HIFI

Arnold O. Benz, Simon Bruderer, Ewine F. van Dishoeck, Pascal Stäuber, and Susanne F. Wampfler

pp 9840–9847

Publication Date (Web): July 17, 2013 (Article)

DOI: 10.1021/jp312813a



 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Solid-State Nuclear Magnetic Resonance Measurements of HIV Fusion Peptide ^{13}C to Lipid ^{31}P Proximities Support Similar Partially Inserted Membrane Locations of the α Helical and β Sheet Peptide Structures

Charles M. Gabrys, Wei Qiang, Yan Sun, Li Xie, Scott D. Schmick, and David P. Weliky

pp 9848–9859

Publication Date (Web): February 18, 2013 (Article)

DOI: 10.1021/jp312845w

 Section:

General Biochemistry

Electronic Spectroscopy and Electronic Structure of Copper Acetylide, CuCCH

Maria A. Garcia and Michael D. Morse

pp 9860–9870

Publication Date (Web): February 19, 2013 (Article)

DOI: 10.1021/jp312841q

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Vibrating H_3^+ in a Uniform Magnetic Field

Héctor Medel Cobaxin and Alexander Alijah

pp 9871–9881

Publication Date (Web): March 5, 2013 (Article)

DOI: 10.1021/jp312856s

 Section:

Magnetic Phenomena

FTIR Spectroscopy of Three Fundamental Bands of H_2F^+

R. Fujimori, Y. Hirata, I. Morino, and K. Kawaguchi

pp 9882–9888

Publication Date (Web): February 22, 2013 (Article)

DOI: 10.1021/jp312863e

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Rotation and Rotation–Vibration Spectroscopy of the $0^+–0^-$ Inversion Doublet in Deuterated Cyanamide

Zbigniew Kisiel, Adam Kraśnicki, Wolfgang Jabs, Eric Herbst, Brenda P. Winnewisser, and Manfred Winnewisser

pp 9889–9898

Publication Date (Web): March 20, 2013 (Article)

DOI: 10.1021/jp3128687

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Hot Band Spectroscopy of the Formyl Cation, $H^{12}C^{16}O^+$

Christopher F. Neese, Peter S. Kreyenin, and Takeshi Oka

pp 9899–9907

Publication Date (Web): March 14, 2013 (Article)

DOI: 10.1021/jp312879f

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

High-Resolution Near-Infrared Spectroscopy of CH_2^+ and Its Deuterated Isotopologues

Haiming Wang, Christopher F. Neese, Christopher P. Morong, Maria Kleshcheva, and Takeshi Oka

pp 9908–9918

Publication Date (Web): August 19, 2013 (Article)

DOI: 10.1021/jp3128803

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

H_3^+ Spectroscopy and the Ionization Rate of Molecular Hydrogen in the Central Few Parsecs of the Galaxy

Miwa Goto, Nick Indriolo, T. R. Geballe, and T. Usuda

pp 9919–9930

Publication Date (Web): April 25, 2013 (Article)

DOI: 10.1021/jp400017s

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Further Insight into the Nature of Ball-Lightning-Like Atmospheric Pressure Plasmoids

David M. Friday, Peter B. Broughton, Tanner A. Lee, Garrett A. Schutz, Jeremiah N. Betz, and C. Michael Lindsay

pp 9931–9940

Publication Date (Web): June 14, 2013 (Article)

DOI: 10.1021/jp400001y

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Resonant States of the H_3^- Molecule and Its Isotopologues D_2H^- and H_2D^-

M. Ayouz, O. Dulieu, and J. Robert

pp 9941–9949

Publication Date (Web): May 20, 2013 (Article)

DOI: 10.1021/jp4000279

 Section:

General Physical Chemistry

On the Symmetry and Degeneracy of H_3^+

Kyle N. Crabtree and Benjamin J. McCall

pp 9950–9958

Publication Date (Web): March 28, 2013 (Article)

DOI: 10.1021/jp400080j

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

CH_2D^+ , the Search for the Holy Grail

Evelyne Roueff, Maryvonne Gerin, Dariusz C. Lis, Alwyn Wootten, Nuria Marcelino, Jose Cernicharo, and Belen Tercero

pp 9959–9967

Publication Date (Web): April 29, 2013 (Article)

DOI: 10.1021/jp400119a

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Detection of Nitrogen-Protonated Nitrous Oxide (HNNO⁺) by Rotational Spectroscopy

Michael C. McCarthy, Oscar Martinez, Jr., Kyle N. Crabtree, Valerio Lattanzi, Stewart E. Novick, and Sven Thorwirth

pp 9968–9974

Publication Date (Web): April 10, 2013 (Article)

DOI: 10.1021/jp4002065

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

High-Resolution Spectroscopy of CH₂D⁺ in a Cold 22-Pole Ion Trap

Sabrina Gärtner, Jürgen Krieg, André Klemann, Oskar Asvany, Sandra Brünken, and Stephan Schlemmer

pp 9975–9984

Publication Date (Web): April 26, 2013 (Article)

DOI: 10.1021/jp400258e

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

(H₂O)₂₀ Water Clusters at Finite Temperatures

P. Parkkinen, S. Riikonen, and L. Halonen

pp 9985–9998

Publication Date (Web): June 3, 2013 (Article)

DOI: 10.1021/jp4003092

 Section:

General Physical Chemistry

Dissociative Recombination of CH₄⁺

Richard D. Thomas, Iryna Kashperka, E. Vigren, Wolf D. Geppert, Mathias Hamberg, Mats Larsson, Magnus af Ugglas, and Vitali Zhaunerchyk

pp 9999–10005

Publication Date (Web): May 7, 2013 (Article)

DOI: 10.1021/jp400353x

 Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Cavity Ringdown Spectroscopy of the Hydroxy-Methyl-Peroxy Radical

Matthew K. Sprague, Laura A. Mertens, Heather N. Widgren, and Mitchio Okumura, Stanley P. Sander, Anne B. McCoy

pp 10006–10017

Publication Date (Web): May 3, 2013 (Article)

DOI: 10.1021/jp400390y

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Determination of the Ortho to Para Ratio of H_2Cl^+ and H_2O^+ from Submillimeter Observations

Maryvonne Gerin, Massimo de Luca, Dariusz C. Lis, Carsten Kramer, Santiago Navarro, David Neufeld, Nick Indriolo, Benjamin Godard, Franck Le Petit, Ruisheng Peng, Thomas G. Phillips, and Evelyne Roueff

pp 10018–10026

Publication Date (Web): July 19, 2013 (Article)

DOI: 10.1021/jp4004533

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

New Potential Energy Surface Features for the $Li + HF \rightarrow LiF + H$ Reaction

Qunchao Fan, Huidong Li, Hao Feng, Weiguo Sun, Tongxiang Lu, Andrew C. Simmonett, Yaoming Xie, and Henry F. Schaefer, III

pp 10027–10033

Publication Date (Web): April 15, 2013 (Article)

DOI: 10.1021/jp400541a

 Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

Indirect Rotational Spectroscopy of HCO^+

Brian M. Siller, James N. Hodges, Adam J. Perry, and Benjamin J. McCall

pp 10034–10040

Publication Date (Web): June 12, 2013 (Article)

DOI: 10.1021/jp400570m

 Section:

Physical Organic Chemistry

Millimeter-Wave Spectroscopy of S₂Cl₂: A Candidate Molecule for Measuring Ortho-Para Transition

Zeinab Tafti Dehghani, Shinji Ota, Asao Mizoguchi, and Hideto Kanamori

pp 10041–10046

Publication Date (Web): May 1, 2013 (Article)

DOI: 10.1021/jp400632g

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

High-Resolution Rovibrational Spectroscopy of Jet-Cooled Phenyl Radical: The ν_{19} Out-of-Phase Symmetric CH Stretch

Grant T. Buckingham, Chih-Hsuan Chang, and David J. Nesbitt

pp 10047–10057

Publication Date (Web): March 28, 2013 (Article)

DOI: 10.1021/jp400702p

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Size Effects on Cation Heats of Formation. II. Methyl Substitutions in Oxygen Compounds

Sydney Leach

pp 10058–10067

Publication Date (Web): March 18, 2013 (Article)

DOI: 10.1021/jp400736y

 Section:

Thermodynamics, Thermochemistry, and Thermal Properties

State Specific Stabilization of H⁺ + H₂(j) Collision Complexes

D. Gerlich, R. Plašil, I. Zymak, M. Hejduk, P. Jusko, D. Mulin, and J. Glosík

pp 10068–10075

Publication Date (Web): March 15, 2013 (Article)

DOI: 10.1021/jp400917v

 Section:

General Physical Chemistry

Isotopic Spectra of the Hydroxyl Radical

Brian J. Drouin

pp 10076–10091

Publication Date (Web): May 1, 2013 (Article)

DOI: 10.1021/jp400923z

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

R2PI Spectroscopy of Aromatic Molecules Produced in an Ethylene-Rich Flame

Yvain Carpentier, Thomas Pino, and Philippe Bréchnignac

pp 10092–10104

Publication Date (Web): July 18, 2013 (Article)

DOI: 10.1021/jp400913n

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Nuclear Spin Symmetry Conservation and Relaxation in Water ($^1\text{H}_2^{16}\text{O}$) Studied by Cavity Ring-Down (CRD) Spectroscopy of Supersonic Jets

Carine Manca Tanner, Martin Quack, and David Schmidiger

pp 10105–10118

Publication Date (Web): May 13, 2013 (Article)

DOI: 10.1021/jp400958f

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Ground State of the H_3^+ Molecular Ion: Physics Behind

A. V. Turbiner and J. C. Lopez Vieyra

pp 10119–10128

Publication Date (Web): April 12, 2013 (Article)

DOI: 10.1021/jp401439c

 Section:

General Physical Chemistry

Molecular Relativistic Corrections Determined in the Framework Where the Born–Oppenheimer Approximation is Not Assumed

Monika Stanke and Ludwik Adamowicz

pp 10129–10137

Publication Date (Web): May 16, 2013 (Article)

DOI: 10.1021/jp4020492

 Section:

General Physical Chemistry

Geometry and Microwave Rotational Spectrum of the $FC^{16}O^{18}O\cdot$ Radical

Jan Koucký, Patrik Kania, Tereza Uhlíková, Lucie Kolesníková, Helmut Beckers, Helge Willner, and Štěpán Urban

pp 10138–10143

Publication Date (Web): September 4, 2013 (Article)

DOI: 10.1021/jp4054549

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties