Physical Chemistry Chemical Physics



See A. Sanov and W. C. Lineberger, pp. 2018-2032. Artist's view of the s&p model treatment of negative-ion photodetachment. The electron waves shown are responsible for the angular anisotropy of the photoelectron images, which are depicted as islands floating among the water waves. The third of the three photoelectron images (islands) corresponds to $400 \,\mathrm{nm}$ photodetachment of $\mathrm{S_2}^-$, while the first and second are obtained in 800 and 267 nm detachment from CS₂⁻ respectively. The molecular orbitals (shown in different lab-frame orientations) on the right are the a_1 HOMO, b_2 (HOMO – 1) and a_2 (HOMO – 2) of the anion. The s and p orbitals on the left represent the s&p-wave expansion of the free (photodetached) electron formed via the a_1^{-1} , b_2^{-1} , and a_2^{-1} photodetachment channels (laser polarization is assumed to be vertical). The corresponding photodetachment bands can be seen in the middle photoelectron image below

Image kindly supplied by A. Sanov, Department of Chemistry, University of Arizona, Tucson, AZ, USA.



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tents



Chemical Science

May 2004/Volume 1/Issue 5 www.rsc.org/chemicalscience

Drawing together the research highlights and news from all RSC publications, *Chemical Science* provides a 'snapshot' of the latest developments across the chemical sciences showcasing newsworthy articles, as well as the most significant scientific advances.



1000 $p/\mathrm{bar}(300\,\mathrm{K})$ 10-10 $/cm^3$ molecule⁻¹ s⁻¹ 300 K 400 K 500 K 600 K 700 K [M] / molecule cm⁻

COMMUNICATIONS

Pressure dependence of the reaction $H + O_2 (+Ar) \rightarrow HO_2$ (+Ar) in the range 1–900 bar and 300–700 K

J. Hahn, L. Krasnoperov, K. Luther and J. Troe

The falloff curves of a central reaction in combustion and supercritical water oxidation were for the first time measured up to very high temperatures and pressures



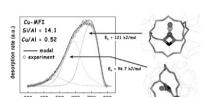
COMMUNICATIONS

Effect of platinum morphology on lean reduction of NO with C₃H₆

Ioan Balint, Akane Miyazaki and Ken-ichi Aika

The relationship between the morphology (size and shape) of alumina supported Pt nanoparticles and catalytic behavior for lean reduction of NO with C₃H₆ is investigated.





Temperature (K)

Localization of Cu⁺ sites and framework Al positions in high-silica zeolites: Combined experimental and theoretical study

Roman Bulánek, Pavel Čičmanec, Petr Knotek, Dana Nachtigallová and Petr Nachtigall

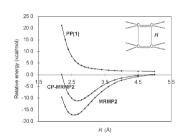
Information about framework Al localization can be obtained from CO-TPD spectra analysis of Cu⁺/ZSM-5.

2008

What is the nature of the long bond in the $TCNE_2^{2-}$ π -dimer?

Yousung Jung and Martin Head-Gordon

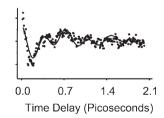
The long C–C bond (2.9 Å) observed in $TCNE_2^{2-}$ π -dimers is due to significant dispersion attractions, as well as their intradimer partial π -bonding interactions.



Observation of low frequency vibrational modes in a mutant of the green fluorescent protein

Konstantin L. Litvinenko and Stephen R. Meech

Ultrafast coherence spectroscopy reveals low frequency modes in a mutant of the green fluorescent protein.

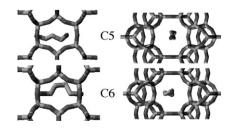




Adsorption of hydrocarbons in zeolites from molecular simulations. The alkane-ferrierite system revisited

P. Pascual and A. Boutin

Linear alkanes adsorption in zeolite ferrierite is reinvestigated with a new simulation model reproducing subtle changes in adsorption sites occupancies.





Cluster anions: Structure, interactions, and dynamics in the sub-nanoscale regime

Andrei Sanov and W. Carl Lineberger

RESEARCH PAPERS

Properties of Molecules



Cyclopent[b,c]acenaphthylene: An elusive isomer of pyracylene with the ring currents of an annelated pentalene

Remco W. A. Havenith, Leonardus W. Jenneskens, Patrick W. Fowler and Erich Steiner



Construction of planar graphs for IPR fullerenes using 5- and 6-fold rotational symmetry: some eigenspectral analysis

Bholanath Mandal, Manas Banerjee and Asok K. Mukherjee



Density functional studies of the luminescence of Si₂₉H₃₆

Dage Sundholm



Rydberg Matter as the diffuse interstellar band (DIB) carrier in interstellar space: the model and accurate calculations of band centres

Leif Holmlid



The effect of local approximations in coupled-cluster wave functions on dipole moments and static dipole polarisabilities

Tatiana Korona, Klaus Pflüger and Hans-Joachim Werner



Optical bands of dodecanuclear compounds H₄PVMo₁₁O₄₀·yH₂O with Keggin structure. Semiclassical vibronic model

S. Klokishner, J. Melsheimer, F. S. Jentoft and R. Schlögl



A density functional study of the dimerization mechanisms of molybdenum(vi) in aqueous solution

Sabri Messaoudi, Eric Furet, Régis Gautier, Eric Le Fur and Jean-Yves Pivan



Solute relaxation on the solvatochromism of *ortho*-betaine dyes. A sequential Monte Carlo/quantum mechanics study

Marcelo Zaldini Hernandes, Ricardo Longo, Kaline Coutinho and Sylvio Canuto



Neutral excited radicals formed by ethylene photodissociation in the 8-24 eV region

Koutayba Alnama, Séverine Boyé, Stéphane Douin, Fabrizio Innocenti, John O'Reilly, Anne-Lise Roche, Niloufar Shafizadeh, Lucia Zuin and Dolores Gauyacq





Rotational isomers of lactic acid: first experimental observation of higher energy forms

Ana Borba, Andrea Gómez-Zavaglia, Leszek Lapinski and R. Fausto



O-H Bond dissociation enthalpies in hydroxyphenols. A time-resolved photoacoustic calorimetry and quantum chemistry study

Catarina F. Correia, Rita C. Guedes, Rui M. Borges dos Santos, Benedito J. Costa Cabral and José A. Martinho Simões



Paramagnetic relaxation of cyclohexane radical cation in solution as measured by the method of time-resolved magnetic field effect

V. I. Borovkov and Yu. N. Molin



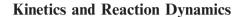
Conformational stabilities of dicyclopropyl ketone determined from variable temperature infrared spectra of xenon solutions and *ab initio* calculations

Charles J. Wurrey, Chao Zheng, Gamil A. Guirgis and James R. Durig



X-ray and neutron diffraction studies and molecular dynamics simulations of liquid DMSO

Usa Onthong, Tünde Megyes, Imre Bakó, Tamás Radnai, Tamás Grósz, Kersti Hermansson and Michael Probst





Temperature-dependent kinetics study of the reactions of O(1D2) with N2 and O2

R. S. Strekowski, J. M. Nicovich and P. H. Wine



Kinetic studies of the reactions of O(1D) with several atmospheric molecules

Edward J. Dunlea and A. R. Ravishankara



Laser induced fluorescence studies of the reactions of $O(^1D_2)$ with N_2 , O_2 , N_2O , CH_4 , H_2 , CO_2 , Ar, Kr and n- C_4H_{10}

Mark A. Blitz, Terry J. Dillon, Dwayne E. Heard, Michael J. Pilling and Ian D. Trought



Reaction of O(³P) with the alkyl iodides: CF₃I, CH₃I, CH₂I₂, C₂H₅I, 1-C₃H₇I and 2-C₃H₇I

M. A. Teruel, T. J. Dillon, A. Horowitz and J. N. Crowley



Dynamics study of CIO + O2 collisions and their role in the chemistry of stratospheric ozone

O. B. M. Teixeira, J. M. C. Marques and A. J. C. Varandas



A potential energy surface and a trajectory study of photodynamics and strong-field alignment of CIF molecule in rare gas (Ar,Kr) solids

Toni Kiljunen, Matias Bargheer, Markus Gühr and Nikolaus Schwentner



Effect of translational energy on the reaction Li + HF(v = 0) \rightarrow LiF + H

O. Höbel, R. Bobbenkamp, A. Paladini, A. Russo and H. J. Loesch



Unraveling the chemical dynamics of bimolecular reactions of ground state boron atoms, $B(^2P_j)$, with acetylene, $C_2H_2(X^{-1}\Sigma_g^{-1})$

R. I. Kaiser, N. Balucani, N. Galland, F. Caralp, M. T. Rayez and Y. Hannachi



Absolute rate coefficients of the reactions of $CF_2(\tilde{a}\ ^3B_1)$ with C_3H_8 , C_3H_6 , iso- C_4H_8 and C_3H_4 between 295 and 550 K

Bart Dils, Raviraj Mahabaleshwar Kulkarni, Jozef Peeters and Shaun Avondale Carl



Kinetics of the reaction of vinyl radicals with NO: Ab initio theory, master equation predictions, and laser absorption measurements

Frank Striebel, Leonard E. Jusinski, Askar Fahr, Joshua B. Halpern, Stephen J. Klippenstein and Craig A. Taatjes



Rate coefficients and production of vibrationally excited HCl from the reactions of chlorine atoms with methanol, ethanol, acetaldehyde and formaldehyde

Paul W. Seakins, John J. Orlando and Geoffrey S. Tyndall



A kinetic study of the reaction of Cl with a series of linear and ramified ketones as a function of temperature

Carlos A. Cuevas, Alberto Notario, Ernesto Martínez and José Albaladejo



On the role of s-cis conformers in the reaction of dienes with OH radicals

Misaela Francisco-Márquez, J. Raúl Alvarez-Idaboy, Annia Galano and Annik Vivier-Bunge



Gas phase oxidation of benzene: Kinetics, thermochemistry and mechanism of initial steps

Séverine Raoult, Marie-Thérèse Rayez, Jean-Claude Rayez and Robert Lesclaux



Switched external magnetic field CIDNP studies of coupling reaction of carbon-centered radicals with TEMPO

N. V. Lebedeva, D. P. Zubenko, E. G. Bagryanskaya, R. Z. Sagdeev, G. S. Ananchenko, S. Marque, D. Bertin and P. Tordo



Dynamic solvent effects on the fading of a merocyanine formed from a spironaphthoxazine. A case of a strong coupling between chemical and medium coordinate

Hiroharu Kono, Hiroyuki Osako, Makoto Sasaki, Toru Takahashi, Yasushi Ohga, Tsutomu Asano, Michael Hildebrand and Noham N. Weinberg



Free electron transfer mirrors rotational conformers of substituted aromatics: Reaction of benzyltrimethylsilanes with n-butyl chloride parent radical cations

Ortwin Brede, Ralf Hermann, Sergej Naumov, Antonios K. Zarkadis, Gerasimos P. Perdikomatis and Michael G. Siskos



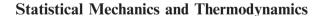
Intramolecular charge transfer in bipolar molecules for electron and hole transporting materials

R. Karpicz, V. Gulbinas, A. Undzenas, J. V. Grazulevicius and R. Lygaitis



Proton transfer in 1,4-dioxane/ammonia hydrogen bond clusters

Tujin Shi, Dalin Yang, Qihe Zhu, Jianhong Ge, Peng Bai, Liusi Sheng, Guohua Wu and Yunwu Zhang





The continuity and family concepts: Useful tools in fluid phase science

Gerhard M. Schneider



Liquid-liquid phase equilibria in nitrobenzene-hexane critical mixture under negative pressure

A. Drozd-Rzoska, S. J. Rzoska and A. R. Imre



High pressure phase behavior of carbon dioxide + heptadecafluorodecyl acrylate and carbon dioxide + heptadecafluorodecyl methacrylate systems

Won Bae, Hyunsoon Shin and Hwayong Kim



Global phase diagrams of the van der Waals-Dieterici and the BMCSL-Dieterici equations of state

Jan Bumba and Jiří Kolafa

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Barotropic phenomena in complex phase behaviour

Sergio E. Quiñones-Cisneros



On the classification and representation of ternary phase diagrams: The yin and yang of a T-x approach

José N. Canongia Lopes



Homotopy continuation based prediction of azeotropy in binary and multicomponent mixtures through equations of state

Naveed Aslam and Aydin K. Sunol



Kinetics of solid hydrate formation by carbon dioxide: Phase field theory of hydrate nucleation and magnetic resonance imaging

B. Kvamme, A. Graue, E. Aspenes, T. Kuznetsova, L. Gránásy, G. Tóth, T. Pusztai and G. Tegze



Accurate equation of state of the hard sphere fluid in stable and metastable regions

Jiří Kolafa, Stanislav Labík and Anatol Malijevský



Simple analytical approximation of the longitudinal electronic relaxation rate of Gd(III) complexes in solutions

Elie Belorizky and Pascal H. Fries



A study of tri-phasic behavior of ionic liquid-methanol-CO₂ systems at elevated pressures

Zhaofu Zhang, Weize Wu, Zhimin Liu, Buxing Han, Haixiang Gao and Tao Jiang

Macromolecules and Soft Matter



Hydrodynamic parameters of hydrated macromolecules: Monte Carlo calculation

M. Bánó, J. Marek and M. Stupák



Structural changes in CTAB/H₂O mixtures using a rheological approach

Luigi Coppola, Raffaella Gianferri, Isabella Nicotera, Cesare Oliviero and Giuseppe Antonio Ranieri



Thermal diffusion in a critical polymer blend

W. Enge and W. Köhler



Adsorbed layer structure of a weak polyelectrolyte studied by colloidal probe microscopy and QCM-D as a function of pH and ionic strength

Shannon M. Notley, Simon Biggs, Vincent S. J. Craig and Lars Wågberg

Nanosciences



Evidence of ultrafast optical switching behaviour in individual single-walled carbon nanotubes

H. Hippler, A.-N. Unterreiner, J.-P. Yang, S. Lebedkin and M. M. Kappes



Effects of ultrasound on the microenvironment in reverse micelles and synthesis of nanorods and nanofibers

Jianling Zhang, Buxing Han, Dongxia Liu, Jing Chen, Zhimin Liu, Tiancheng Mu, Rui Zhang and Guangying Yang



Photoexcited triplets of nitrodiphenylpolyenes hosted in channel cavities. A time resolved EPR study

Antonio Barbon, Marco Bortolus, Marina Brustolon, Anna Lisa Maniero and Roberto Zanrè

Interfaces, Electrochemistry



The solid-state reaction of a functionalised polypyrrole; analysis using high resolution X-ray photoelectron spectroscopy

J. M. Cooper, A. Glidle, A. R. Hillman, M. D. Ingram, C. Ryder and K. S. Ryder



Self-motion of a camphor disk coupled with convection

Hiroyuki Kitahata, Shin-ichi Hiromatsu, Yukie Doi, Satoshi Nakata and Mohammed Rafiqul Islam



Probing possible structural models at the air/H₂SO₄(aq) interface: a second harmonic generation study

A. J. Fordyce, W. J. Bullock, R. D. Spencer-Smith and J. G. Frey



Reversible aggregation, precipitation and re-dissolution of rhodamine 6G in aqueous sodium dodecyl sulfate

J. C. Micheau, G. V. Zakharova and A. K. Chibisov

Biophysical Chemistry



First principles electrochemical study of redox events in DNA bases and chemical repair in aqueous solution

Jorge Llano and Leif A. Eriksson



Conformation a l determination of [Leu] enkephalin based on theoretical and experimental VA and VCD spectral analyses

S. Abdali, K. J. Jalkanen, X. Cao, L. A. Nafie and H. Bohr



Partial molar isentropic and isothermal compressibilities of some N-acetyl amino acid amides in aqueous solution at 298.15 K

Gavin R. Hedwig and Harald Høiland

Solids and Materials Science



Structure and dynamics of interlayer species in a hydrated Zn-vermiculite. A molecular dynamics study

Mehdi Arab, Daniel Bougeard and Konstantin S. Smirnov



Evidence for C_{60} dimerisation in the fulleride $[Cr(C_9H_{12})_2]^+C_{60}^-$

Andreas Hönnerscheid, Leo van Wüllen, Robert Dinnebier, Martin Jansen, Jürgen Rahmer and Michael Mehring



 $Formation \ of \ cyanide-functionalized \ SBA-15 \ and \ its \ transformation \ to \ carboxylate-functionalized \ SBA-15$

Chia-min Yang, Yanqin Wang, Bodo Zibrowius and Ferdi Schüth



Surface chemical functionalities in bioactive glasses. The gas/solid adsorption of acetonitrile

Marta Cerruti, Vera Bolis, Giuliana Magnacca and Claudio Morterra



Structure and bonding in single- and two-phase alumina-based glasses

Richard Weber, Chris J. Benmore, Joan Siewenie, Jacob Urquidi and Thomas S. Key



A rhenium carbonyl bonded to highly dealuminated zeolite Y: structure determination by infrared and X-ray absorption spectroscopies

Bryan Enderle and Bruce C. Gates



A calorimetric and statistical mechanics study of ammonia adsorption in zeolite NaY

Bruno Boddenberg, Gairat U. Rakhmatkariev, Aneta Wozniak and Stefan Hufnagel

Catalysis



Formation of carboxy species at CO/Al₂O₃ interfaces. Impacts of surface hydroxylation, potassium alkalization and hydrogenation as assessed by *in situ* FTIR spectroscopy

Alexandra Iordan, Mohamed I. Zaki and Charles Kappenstein



Acidity of sulfated oxides: Al₂O₃, TiO₂ and SiO₂. Application of test reactions

Marek Marczewski, Agnieszka Jakubiak, Hanna Marczewska, Anna Frydrych, Małgorzata Gontarz and Anna Śnieguła



Elucidation of the local structure of active titanium(IV) sites on silica-based phase-boundary catalysts for alkene epoxidation with aqueous hydrogen peroxide

Keita Ikeue, Shigeru Ikeda, Atsushi Watanabe and Bunsho Ohtani



Measurement of the relative acid strength and acid amount of solid acids by argon adsorption

Hiromi Matsuhashi and Kazushi Arata



Anomalous valence changes and specific dinitrogen adsorption features of copper ion exchanged in ZSM-5 zeolite prepared from an aqueous solution of $[Cu(NH_3)_2]^+$

Yasushige Kuroda, Atsushi Itadani, Ryotaro Kumashiro, Tomomi Fujimoto and Mahiko Nagao

ADDITIONS AND CORRECTIONS



Structure and the conductive behaviour of hydrate melt coexisting with porous solid materials—α-Al₂O₃ powder/ZnCl₂ hydrate melt coexisting system

Minoru Mizuhata, Yasushi Sumihiro and Shigehito Deki



A comparison of water adsorption on ordered and disordered silica substrates

Joël Puibasset and Roland J.-M. Pellenq



Electronic supplementary information is available on http://www.rsc.org/esi: see article for further information.

^{*} Indicates the author for correspondence: see article for details.