

OF

CHEMICAL PHYSICS

John Light, Editor Donald Levy, Associate Editor

J. W. Stout, Consulting Editor

Editorial Board

Term ending 31 December 1988

Bruce J. Berne

Robert W. Field

Jon T. Hougen

Jiri Jonas

Charles S. Parmenter

Richard E. Smalley

Term ending 31 December 1989

Graham R. Fleming

Sandra C. Greer

Yoshitsugu Oono

Joe Paldus

William P. Reinhardt

Jurgen Troe

Term ending 31 December 1990

C. A. Angell

L. E. Brus

Michael D. Fayer

David M. Golden

Herbert L. Strauss

Ahmed H. Zewail

Managing Editor: Kathleen Strum; Chief Copy Editors: Deborah McHone, Mary Ellen Mormile

The Journal of Chemical Physics is published semimonthly by the American Institute of Physics (AIP). Its purpose is to bridge a gap between journals of physics and journals of chemistry. The artificial boundary between physics and chemistry has now been in actual fact completely eliminated, and a large and active group is engaged in research which is as much the one as the other. It is to this group that the Journal is rendering its principal service and makes its greatest appeal, both as a prompt and efficient medium for publication of research and as a convenient and carefully edited assemblage of pertinent information.

Information for Contributors

Submit manuscripts in duplicate to John Light, Editor, *Journal of Chemical Physics*, Department of Chemistry, 5735 S. Ellis Avenue, The University of Chicago, Chicago, IL 60637. Submission is a representation that the manuscript has not been published previously nor currently submitted for publication elsewhere. The manuscript should be accompanied by a statement transferring copyright from the authors (or their employers— whoever holds the copyright) to AIP; a suitable form for copyright transfer is occasionally printed in the back of this journal and is available from the Editor's office or AIP. This written transfer of copyright, which previously was assumed to be implicit in the act of submitting a manuscript, is necessary under the 1978 U.S. copyright law in order for AIP to continue disseminating physics research results as widely as possible. Further information may be obtained from AIP.

Publication Charge: To support the cost of wide dissemination of research results through publication of journal pages and production of a data base of articles, the author's institution is requested to pay a *page charge* of \$45 per page (with a one-page minimum) and an *article charge* of \$20 per article. The page charge (if honored) entitles the author to 100 free reprints. For **Errata** the minimum page charge is \$10, with no article charge and no free reprints. Nonpayment of the publication charge may lead to delays in publication.

All mathematical expressions and formulas, insofar as possible, should be typed, with unavailable Greek letters or symbols inserted neatly in ink. Distinguish between capital and small letters. Avoid complicated superscripts and subscripts. Avoid repetition of a complicated expression by representing it as a symbol. Identify in the margin handwritten Greek letters and unusual symbols. Use fractional exponents instead of root signs.

References should appear as consecutively numbered footnotes. Literature citations of technical journals should be in the form indicated in the *AIP Style Manual* (price \$7.50 prepaid from American Institute of Physics, Dept. BN, 335 East 45th Street, New York, NY 10017).

Tables may be typewritten on sheets separate from the running text. Each table must have a caption that will make the data in the table intelligible without reference to the text. Avoid complicated column headings.

Figures should, whenever practicable, be planned for reproduction in one-column width (8 cm). Line drawings should be in India ink on white paper or high-quality tracing cloth. The original drawing or a high-quality glossy print should be submitted. To facilitate mailing and handling, original drawings should not exceed 22 by 28 cm in size. Lettering, preferably drawn with a mechanical set, should be of a size so that when reduced the smallest lower-case letters will not be less than about 1.5 mm. Avoid gross disparities in lettering size on a drawing. Consult the *AIP Style Manual* for further discussion of figures. Type figure captions on a separate sheet of paper. Number figures consecutively. Identify each original drawing or photograph with the figure number and authors' names, written where they will not be reproduced.

AIP's **Physics Auxiliary Publication Service (PAPS)** is a low-cost depository for material that is part of and supplementary to a published paper, but is too long to be included in the journal; inquire of the Editor.

Proofs and all correspondence concerning papers in the process of publication should be addressed to: Editorial Supervisor, *The Journal of Chemical Physics*, American Institute of Physics, 335 East 45th Street, New York, NY 10017. In all correspondence, reference should be made to title, author, journal, and scheduled date of issue. A limited number of **alterations in proof** are unavoidable, but the cost of making extensive alterations after the article has been set in type will be charged to the author.

Copyright 1988, American Institute of Physics. Individual teachers, students, researchers, and libraries acting for them are permitted to make copies of articles in this journal for their own use in research or teaching, including multiple copies for classroom or library reserve use, provided such copies are not sold. Copying for sale is subject to payment of copying fees. (See "Copying Fees" paragraph elsewhere in this journal.) Permission is granted to quote from this journal with the customary acknowledgment of the source. To reprint a figure, table, or other excerpt requires in addition the consent of one of the original authors and notification to AIP. Reproduction for advertising or promotional purposes, or republication in any form, is permitted only under license from AIP, which will normally require that the permission of one of the authors also be obtained. Direct inquiries to Office of Rights and Permissions, American Institute of Physics, 335 East 45th Street, New York, NY 10017.

Spectroscopy and Light Scattering

Vibrationally hot emission and electronic relaxation of CO in Ne matrix Johannes Bahrdt and Nikolaus Schwentner	2869
Infrared laser spectroscopy of the $a^3\Sigma_g^+ - c^3\Pi_u$ system of H₂ and D₂ Paul B. Davies, Michael A. Guest, and Simon A. Johnson	2884
Observation and characterization of a new $c(2)^3\Sigma^+$ electronic state using Stark effect and perturbation analysis in NaK($B^1\Pi$) J. Derouard and N. Sadeghi	2891
Monte Carlo simulations of structural properties and infrared spectra of SF₆-(Ar)_n clusters Dieter Eichenauer and Robert J. Le Roy	2898
Effect of metal ion perturbers on the triplet state of naphthalene in naphthalene crown ether-metal ion complexes. II. Stark effect Sanjib Ghosh, Michael Petrin, August H. Maki, and Lynn R. Sousa	2913
Rotational spectra and structures of small clusters: The Ar₄-H/DF pentamers H. S. Gutowsky, Carl Chuang, T. D. Klots, Tryggvi Emilsson, R. S. Ruoff, and Karl R. Krause	2919
Differentiation between resonance Raman scattering and single vibrational level fluorescence 5100 cm⁻¹ above the $^1B_{2u}$ origin in benzene vapor by means of excitation profiles Paul A. Harmon and Sanford A. Asher	2925
The effect of the exchange mode dynamics on vibrational phase relaxation at surfaces Willeeta Green-Johnson	2939
The core hole decay of N₂O following core to bound state excitations F. P. Larkins, W. Eberhardt, In-Whan Lyo, R. Murphy, and E. W. Plummer	2948
$S_n \leftarrow S_1$ and $S_1 \rightarrow S_0$ resonance CARS spectra of perylene in the S_1 state Satoshi Matsunuma, Naotoshi Akamatsu, Toshio Kamisuki, Yukio Adachi, Shiro Maeda, and Chiaki Hirose	2956
Photophysical properties of matrix-isolated Mg₂: Evidence for efficient predissociation John G. McCaffrey and Geoffrey A. Ozin	2962
Observation of strong Rydberg-valence mixing in the $E^3\Sigma_u^-$ state of O₂ by 3+1 MPI photoelectron spectroscopy Paul J. Miller, Leping Li, William A. Chupka, and Steven D. Colson	2972
Static and dynamical properties of D₁⁰ (Li) in MgO:Li studied by EPR: Isotope effects V. M. Orera, M. L. Sanjuán, and M. M. Abraham	2976

(Continued)

Subscription Prices (1988)	Optional air freight			
	U.S.A. & Poss.	Foreign (incl. Can. & Mex.)	Europe, Mideast, N. Africa	Asia and Oceania
Members (affiliated & member societies)	\$ 110.00	\$ 160.00	\$ 245.00	\$ 245.00
All other	\$1165.00	\$1215.00	\$1300.00	\$1300.00

Back number prices: Single copies: \$50.00.

The Journal of Chemical Physics (ISSN: 0021-9606) is published semimonthly by the American Institute of Physics. Second-class postage rates paid at Woodbury, NY and at additional mailing offices. POSTMASTER: Send address changes to *Journal of Chemical Physics*, 500 Sunnyside Blvd., Woodbury, NY 11797.

Subscriptions, renewals, address changes, and single-copy orders should be addressed to *AIP Subscription Fulfillment Division*, 335 East 45th St., New York, NY 10017. Allow at least six weeks advance notice. For address changes please send both old and new addresses and, if possible, include a mailing label from the wrapper of a recent issue. For your convenience a **change of address form is included in every issue of *Physics Today*; please use it.** Requests from subscribers for missing journal issues will be honored without charge only if received within six months of the issue's actual date of publication; otherwise, the issue may be purchased at the single-copy price. (AIP Headquarters are located at 335 East 45th St., New York, NY 10017; Subscription Fulfillment offices are located at 500 Sunnyside Blvd., Woodbury, NY 11797.)

Reprints of individual articles in this journal may be ordered singly at \$10.00 per article copy (postage included) for articles up to 20 pages. Beyond 20 pages there is a surcharge of \$0.20 per page. Air mail delivery available. Orders are filled in 24 hours. Send orders to the American Institute of Physics, *Current Physics Reprints*, 335 East 45th St., New York, NY 10017.

Copying Fees: The code that appears on the first page of articles in this journal gives the fee for each copy of the article made beyond the free copying permitted by AIP. (See statement under "Copyright" elsewhere in this journal.) If no code appears, no fee applies. The fee for pre-1978 articles is \$0.25 per copy. With the exception of copying for advertising and promotional purposes, the express permission of AIP is not required provided the fee is paid through the *Copyright Clearance Center, Inc. (CCC)*, 21 Congress Street, Salem, MA 01970. Contact the CCC for information on how to report copying and remit payment.

Microfilm editions of back volumes of *The Journal of Chemical Physics* are available on 16 mm and 35 mm. Special discounts for the complete backfile of journals published by AIP are also available. *The Journal of Chemical Physics* appears on a monthly basis in *Current Physics Microform (CPM)* along with 26 other journals published by the American Institute of Physics and its member societies. A *Microfilm Catalog* is available on request. *The Journal of Chemical Physics* is indexed quarterly in *Current Physics Index*, a subject and author index (with abstracts) to all journals published by AIP and its member societies.