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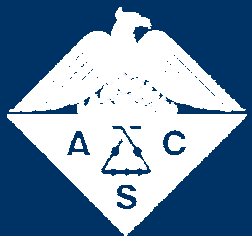
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...of the **American Chemical Society** is to encourage in the broadest and most liberal manner the advancement of the chemical enterprise and its practitioners.

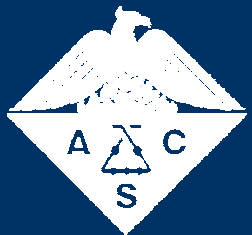
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- ◆ 30 Electronic Journals, 3 Magazines
- ◆ Most Cited Journals in Chemistry
- ◆ Cover all scientific disciplines and consistently rank among the highest impact journals in science

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- ◆ 72% increased in Impact Factor from 1999 to 2000
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- ◆ JACS cited 188,117 times in 2000

*Analytical Chemistry, Chemical Reviews, Environmental Chemistry, Inorganic Chemistry, Journal of Agricultural and Food Chemistry, Journal of the American Chemical Society, Macromolecules, The Journal of Organic Chemistry, and The Journal of Physical Chemistry* are all #1 in their respective fields.



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From Page 1 of *JACS* (c.1879) to **ASAP**  
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## THE AMERICAN CHEMICAL SOCIETY.

### I.—PROCEEDINGS.

#### *Regular Meeting, January 2nd, 1879.*

THE meeting was called to order at 8 o'clock, by Mr. Nichols, in the absence of the President and Vice-Presidents. Dr. Alsberg was elected Chairman. The minutes of the last meeting were read and adopted.

The resignation of Prof. Barker was read and accepted.

Messrs. H. M. McIntyre and G. W. Wigner were elected Members.

Messrs. F. W. P.  
Herbert Hazard w  
Wingate and E. W.  
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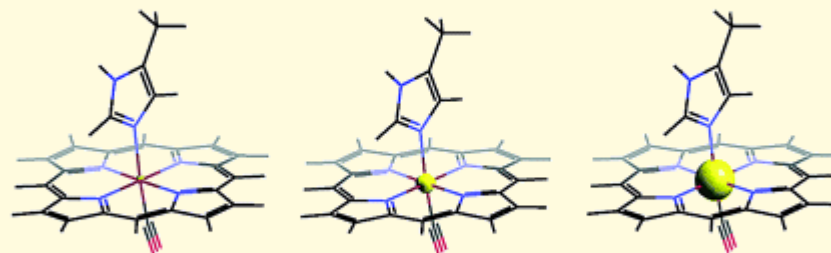
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### <sup>57</sup>Fe Mössbauer Isomer Shifts of Heme Protein Model Systems: Electronic Structure Calculations

Yong Zhang, Junhong Mao, and Eric Oldfield

Web Release Date: 06-Jun-2002; DOI: [10.1021/ja011583v](https://doi.org/10.1021/ja011583v)



$$\delta_{\text{Fe}} = E_{\text{A}} - E_{\text{Fe}} = \frac{2\pi}{3} Ze^2 \left( \langle R^2 \rangle^* - \langle R^2 \rangle \right) \left( |\psi(0)_{\text{A}}|^2 - |\psi(0)_{\text{Fe}}|^2 \right)$$

[Abstract](#) Full: [HTML](#) / [PDF](#) (134K)



# To today's breakthrough articles...

## NANO LETTERS

### Molecular Conductance of Wires

C. Kalyanaraman and D. G. Evans\*

Department of Chemistry and the Albuquerque High Performance Computing Center  
University of New Mexico, Albuquerque, New Mexico 87131

Journal of  
currents **proteome**  
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ACS PUBLICATIONS

Volume 1, Number 3, p203.

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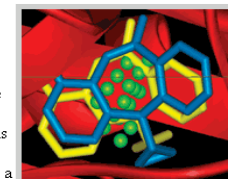
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May/June 2002  
Volume 1, Number 3

### Docking Dilemma

Even as the Protein Database (PDB) fills up with structures of proteins that represent potential drug targets, designing candidate drugs that bind these proteins remains a challenge. No matter how well characterized a protein is, it is still difficult to determine where a ligand might bind. Most docking algorithms start with the assumption that the ligand-binding site has been identified. But to evaluate, de novo, the potential binding sites over the surface of even a small protein is a daunting task for any computer system. To address this problem, Graham Richards and his colleagues at the University of Oxford (U.K.) took a multiscale approach (*J. Am. Chem. Soc.* **2002**, *124*, [2337-2344](#)).



**Real or modeled?** Taking a multiscale approach, researchers predicted the binding of nevirapine to HIV-reverse transcriptase (red). The predicted position (blue) is very close to the position determined by X-ray crystallography (yellow). (*J. Am. Chem. Soc.* **2002**, *124*, [2337-2344](#).)

Their method relies on the application of a scaling factor to the protein surface to generate a multiscale representation of the protein surface.

The predicted position (blue) is very close to the position determined by X-ray crystallography (yellow). (*J. Am. Chem. Soc.* **2002**, *124*, [2337-2344](#).)

The predicted position (blue) is very close to the position determined by X-ray crystallography (yellow). (*J. Am. Chem. Soc.* **2002**, *124*, [2337-2344](#).)

The predicted position (blue) is very close to the position determined by X-ray crystallography (yellow). (*J. Am. Chem. Soc.* **2002**, *124*, [2337-2344](#).)

## Crystal Growth & Design

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2952 WALTER GORDY AND LINUS PAULING Vol. 64

[CONTRIBUTION FROM THE GATES AND CRELLIN LABORATORIES OF CHEMISTRY, CALIFORNIA INSTITUTE OF TECHNOLOGY, No. 934]

## The Molecular Structure of Methyl Isocyanide

BY WALTER GORDY<sup>1</sup> AND LINUS PAULING

[CONTRIBUTION FROM THE RESEARCH LABORATORY, GENERAL ELECTRIC COMPANY]

## Surface Electrification Due to the Recession of Aqueous Solutions from Hydrophobic Surfaces

BY IRVING LANGMUIR

THE RELATION OF PHYSICAL CHEMISTRY TO PHYSICS AND CHEMISTRY<sup>1</sup>

BY J. H. VAN'T HOFF

According to the programme, I have to consider: "General Principles and

## Femtochemistry in Nanocavities: Reactions in Cyclodextrins

A. Douhal,<sup>6,8,9</sup> T. Fiebig,<sup>7,8</sup> M. Chachavilis,<sup>10</sup> and A. H. Zewail<sup>6,8</sup>

Laboratory for Molecular Sciences, Arthur Amos Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, California 91125, and Departamento de Química Física, Facultad de Químicas, Sección de Toledo, Universidad de Castilla-La Mancha, San Lucas 3, 45002 Toledo, Spain

A Convenient Micro Method for the Quantitation of Closed Circular Deoxyribonucleic Acid<sup>†</sup>Peter Beard<sup>‡</sup> and Paul Berg\*

## THE KINETIC TERM IN ELECTROLYTIC CONDUCTANCE

BY RAYMOND M. FUOSS<sup>†</sup> AND LARS ONSAGER

Contribution from the Istituto di Chimico-Fisica dell'Università degli Studi di Roma, Roma, Italy and the Sterling Chemistry Laboratory of Yale University, New Haven, Conn.

Received May 26, 1958

In a previous paper on the conductance of un-associated electrolytes,<sup>1</sup> we mentioned that thecharge can penetrate, if the ions are represented as point charges at the centers of rigid spheres of radius  $a/2$ ; i.e.,  $a$  is the center-to-center distance at contact.) We have as the starting point for the calculation

$$\Delta P = \int \Pi \cdot dS = \int \Pi \cos \theta dS \quad (1)$$

where  $dS = a^2 \sin \theta d\theta d\phi$ . In the absence of an external field, the osmotic pressure due to anions (subscript 2) is

Boron Hydride Valence Structures. A Topological Approach

W. N. Lipscomb\* and I. R. Epstein

Received September 18, 1951

We wish to correct two labeling errors in our previously published paper<sup>1</sup> having the above title and to make two ad-Registry No. B<sub>3</sub>H<sub>3</sub><sup>+</sup>, 12430-13-6; B<sub>2</sub>H<sub>2</sub><sup>+</sup>, 12356-13-7.

\*To whom correspondence should be addressed at Harvard University.

- (1) I. R. Epstein and W. N. Lipscomb, *Inorg. Chem.*, **10**, 1921 (1971).
- (2) M. Gielen, *Bull. Soc. Chim. Belg.*, **90**, 501 (1981).
- (3) J. Albara, *J. Am. Chem. Soc.*, **100**, 3339 (1978).

DITHIOTOSYLATES

*J. Org. Chem.*, Vol. 36, No. 8, 1971 1137Dithiotosylates as Reagents in Organic Synthesis<sup>1</sup>R. B. WOODWARD, IRWIN J. PACTHER, AND MONTE L. SCHEINBAUM\*<sup>2</sup>

Converse Memorial Laboratories, Harvard University, Cambridge, Massachusetts 02138, and the Department of Chemistry, East Tennessee State University, Johnson City, Tennessee 37601

## Nobel Laureates Found in the ACS Journal Archives

- ◆ Linus Pauling – *JACS* and *J Phys Chem*
- ◆ Irving Langmuir – *JACS*
- ◆ Jacobus Van't Hoff (1<sup>st</sup> Nobel Prize recipient in 1901) – published in *JACS* in 1905
- ◆ Ahmed Zewail – *JACS* and *J Phys Chem*
- ◆ Paul Berg – *JACS* and *Biochemistry*
- ◆ Lars Onsager – *JACS* and *J Phys Chem*
- ◆ William N. Lipscomb – *Inorganic Chemistry*
- ◆ Robert Burns Woodward – *The Journal of Organic Chemistry*

- Over the course of the 100 years the Nobel Prize has been awarded, a total of 94 recipients in Chemistry have published in ACS journals
- In the last 30 years, 51 of the 59 Nobel recipients have published in ACS journals



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- Manual checks by ACS technical staff/chemists
- Computerized tests
  - Polarity
  - Skewing
- Solicited help from Library Advisory Group to critique output



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## ◆ Complete IT Environment Redesign

- Integration of 2.5 Million New Pages
- Revised Interface – Search and TOC Layers
- Cross Journal Searching

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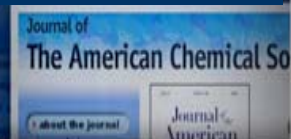
## ◆ Redundancy

- Two T-3 lines (Easy to Increase)
- ISPs
- Load-Balanced Oracle Web Servers
- 10 Terabyte Storage Array

## ◆ Disaster Recovery Provisions

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<b>Print</b>	\$40,000	<b>\$40,000</b>	\$40,000	\$40,000	\$40,000	\$40,000	\$0	\$0
<b>Web</b>	\$0	<b>\$36,000</b>	\$10,000	\$10,000	\$6,000	\$6,000	\$40,000	\$40,000
<b>Archive One Large Site</b>						\$2,250	\$2,250	\$4,500
<b>Grand Total</b>	\$40,000	<b>\$76,000</b>	\$50,000	\$50,000	\$46,000	\$48,250	\$42,250	\$44,500
<b>#of Articles</b>	20,000	<b>60,000</b>	60,000	80,000	100,000	120,000	640,000	660,000
<b>Web Content</b>	None	<b>3 Years (1996- 1998)</b>	3 Years (1996- 1998)	4 Years (1996- 1999)	5 Years (1996- 2000)	124 Years (1996- 2002)	124 Years (1879- 2002)	<b>125 Years (1879- 2003)</b>
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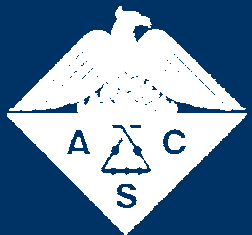
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**Matthew J. Price**

**202.452.8918**

**[m\\_price@acs.org](mailto:m_price@acs.org)**

**Dean J. Smith**

**202.872.8063**

**[d\\_smith@acs.org](mailto:d_smith@acs.org)**

