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### **Chemistry - 101science.com**

Computational chemistry is a branch of chemistry that uses computer simulation to assist in solving chemical problems. It uses methods of theoretical chemistry, incorporated into efficient computer programs, to calculate the structures and properties of molecules and solids. It is necessary because, apart from relatively recent results concerning the hydrogen molecular ion (dihydrogen cation ...

### **Computational chemistry - Wikipedia**

The first step in solving a quantum chemical problem is usually solving the Schrödinger equation (or Dirac equation in relativistic quantum chemistry) with the electronic molecular Hamiltonian. This is called determining the electronic structure of the molecule.

### **Quantum chemistry - Wikipedia**

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### **The Journal of Physical Chemistry A (ACS Publications)**

An Introduction to Chemistry by Mark Bishop. There are two versions of this current textbook, both containing the same information but organized differently: the "Chemistry-first" version begins with actual "chemistry" — that is, chemical equations and reactions.

### **General Chemistry for Students - Steve Lower's Web pages**

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Going for gold: The mono- and di-chloroform solvates of  $[Au_2(\mu_4-1,2-bis(diphenylarsino)ethane)_2](AsF_6)_2$  undergo single-crystal-to-single-crystal transformations that result in gain or loss of only one chloroform molecule and changes in the structure and luminescence of the digold cation.

### **Chemistry — A European Journal: Early View**

Student Alternative Conceptions in Chemistry (Originally: Student Misconceptions and Preconceptions in Chemistry) Christopher Horton Worcester, MA 01602

### **Student Alternative Conceptions in Chemistry - Daisley.net**

Theoretical chemistry is a branch of chemistry, which develops theoretical generalizations that are part of the theoretical arsenal of modern chemistry, for example, the concept of chemical bonding, chemical reaction, valence, the surface of potential energy, molecular orbitals, orbital interactions, molecule activation et cetera.

## **Home : Science Journal of Chemistry**

Papers in Press. These articles have been fully reviewed and editorially accepted, and are formally published as of the date of release listed. These articles have not been copyedited or published in an issue.

## **Papers in Press - The Journal of Biological Chemistry**

Molecular modelling, drawing, molecular mechanics, Semi-empirical calculations, structure display

## **Chemdraw ultra: Molecular modelling, structure drawing**

In 1993 Gehring, Leroy and Guéron disclosed that DNA sequences containing stretches of cytosines can form intercalated, quadruple-helical structures under acidic conditions. 7 The tetrameric structure consisted of two parallel duplexes combined in an antiparallel fashion by forming intercalated hemiprotonated cytosine-cytosine base pairs ( $C^+ \cdot C$ ). Due to the unusual nature of the configuration ...

## **i-Motif DNA: Structure, stability and targeting with ligands**

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