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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.

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Chemistry is the scientific discipline involved with elements and compounds composed of atoms, molecules and ions: their composition, structure, properties, behavior and the changes they undergo during a reaction with other substances.

### **Chemistry - Wikipedia**

Room-Temperature Activation of the C-H Bond in Methane over Terminal Zn II "Oxyl Species in an MFI Zeolite: A Combined Spectroscopic and Computational Study of the Reactive Frontier Molecular Orbitals and Their Origins

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Metallocenophanes of p-block elements are somewhat unexplored compared to their transition metal analogues. A number of disila-bridged metallocenophanes with the group 14 elements silicon, germanium, tin, and lead, and the group 15 element antimony as central atoms were prepared and structurally characterized, expanding this little-explored class of compounds.

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Humans have 60-70 2OG-dependent oxygenases, of which some are important therapeutic targets. A priority in the development of oxygenase inhibitors is to identify scaffolds selective for a particular enzyme, made challenging by the highly conserved oxygenase active sites.

**Chemistry – A European Journal: Early View**

Complete Chemistry for Cambridge IGCSE (2nd Edition) is written by RoseMarie Gallagher and Paul Ingram; published by Oxford University Press in 2011 and endorsed by University of Cambridge, UK.

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