

## Gas Adsorption

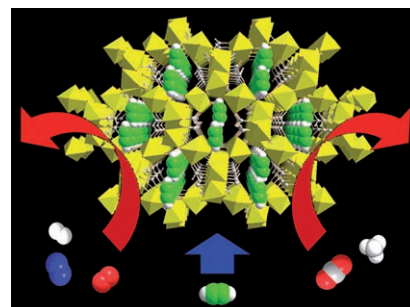
D. G. Samsonenko, H. Kim, Y. Sun,  
G.-H. Kim, H.-S. Lee, K. Kim\*

### Microporous Magnesium and Manganese Formates for Acetylene Storage and Separation

*Chem. Asian J.*

DOI: 10.1002/asia.200600390

**Exclusive entry:** Microporous magnesium and manganese formates show not only a high capacity for acetylene sorption but also remarkable selectivity over CO<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub>, O<sub>2</sub>, and H<sub>2</sub> at room temperature. The single-crystal X-ray structure analysis of the acetylene-adsorbed metal formates reveals two acetylene sorption sites.



## Solid-state NMR Spectroscopy

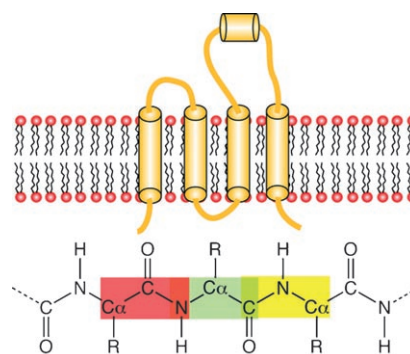
Y. Li, D. A. Berthold, H. L. Frericks,  
R. B. Gennis, C. M. Rienstra\*

### Partial <sup>13</sup>C and <sup>15</sup>N Chemical-Shift Assignments of the Disulfide-Bond-Forming Enzyme DsbB by 3D Magic-Angle Spinning NMR Spectroscopy

*ChemBioChem*

DOI: 10.1002/cbic.200600484

**Another piece of the puzzle.** A 20 kDa integral membrane protein DsbB has been studied by 2D and 3D solid-state NMR. Partial chemical-shift assignments have been made in the transmembrane helices.



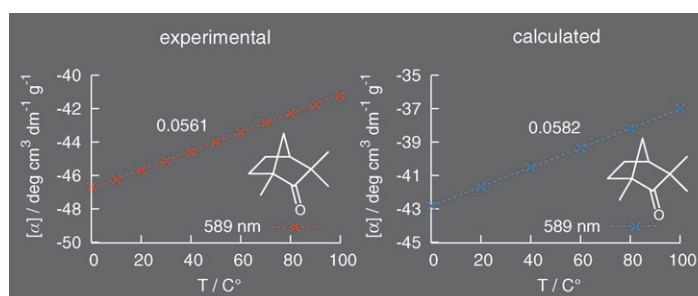
## Optical Rotation

B. C. Mort, J. Autschbach\*

### Temperature Dependence of the Optical Rotation in Six Bicyclic Organic Molecules Calculated by Vibrational Averaging

*ChemPhysChem*

DOI: 10.1002/cphc.200600757



**Accurate predictions:** A computational model which includes vibrational corrections is used to compute optical rotations in bicyclic molecules. The inclusion

of temperature effects in the vibrational averaging elucidates the temperature dependence (see figure) of the optical rotation from a purely vibrational effect.

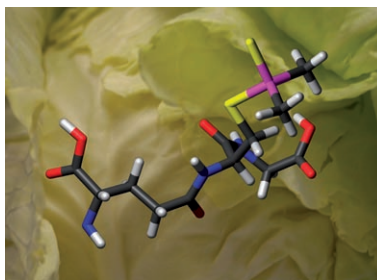
## Bioinorganic Chemistry

A. Raab, S. H. Wright, M. Jaspars,  
A. A. Meharg, J. Feldmann\*

### Pentavalent Arsenic Can Bind to Biomolecules

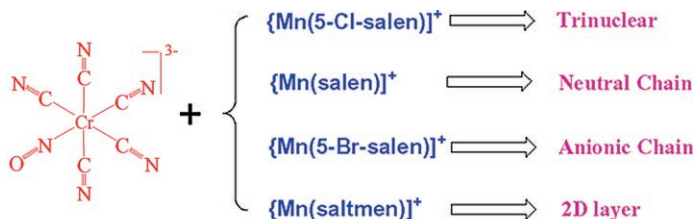
*Angew. Chem. Int. Ed.*

DOI: 10.1002/anie.200604805



**As biomolecules go:** By identifying the dimethylarsinothioyl glutathione complex in arsenic-exposed cabbage, it was shown that pentavalent arsenic can bind to biomolecules when it is activated by sulfide (see picture; As<sup>V</sup> purple, S yellow, O red, N blue). The result highlights that sulfide reactions may play a role in the reactivity of arsenic intermediates and the metabolic pathway of arsenic in organisms.

## Heterodimetallic Complexes



Four cyanido-bridged complexes derived from the  $[Cr(CN)_5(NO)]^{3-}$  anion and  $Mn^{III}$  Schiff-base cations have been synthesized with trinuclear, 1D chain or

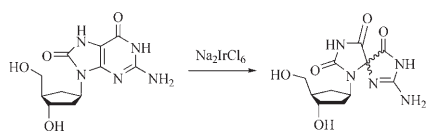
2D layered molecular structures. Antiferromagnetic  $Mn^{III}-Cr^I$  coupling has been exclusively observed in these complexes.

Z.-H. Ni, Lei Zheng, L.-F. Zhang, A.-L. Cui, W.-W. Ni, C.-C. Zhao, H.-Z. Kou\*

**Cyanido-Bridged Dimetallic Complexes Derived from Manganese(III) Schiff Bases and Pentacyanonitrosyl-chromate(I): Synthesis, Crystal Structure and Magnetic Properties**

*Eur. J. Inorg. Chem.*

DOI: 10.1002/ejic.200600958



Carbocyclic DNA lesion analogs provide a powerful tool for the investigation of the recognition of DNA lesions by DNA glycosylases. Here, we report the synthesis of carbocyclic analogs of the DNA lesions 7,8-dihydro-8-oxo-2'-deoxyguanosine and spiroiminodihydantoin as a nucleoside as well as in single-stranded DNA.

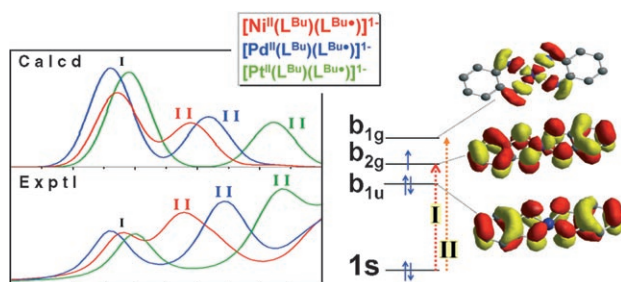
H. Müller, T. Carell\*

**A Carbocyclic Analog of the Oxidatively Generated DNA Lesion Spiroiminodihydantoin**

*Eur. J. Org. Chem.*

DOI: 10.1002/ejoc.200600982

## Coordination Modes



A new methodology based on quasi-relativistic time-dependent density functional theory (TD-DFT) has been applied in order to interpret experimental cova-

lencies from the S K-edge pre-edge intensities obtained for a series of transition-metal dithiolene complexes (see example in diagram).

K. Ray, S. DeBeer George, E. I. Solomon, K. Wieghardt,\* F. Neese\*

**Description of the Ground-State Covalencies of the Bis(dithiolato) Transition-Metal Complexes from X-ray Absorption Spectroscopy and Time-Dependent Density-Functional Calculations**

*Chem. Eur. J.*

DOI: 10.1002/chem.200601425



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