

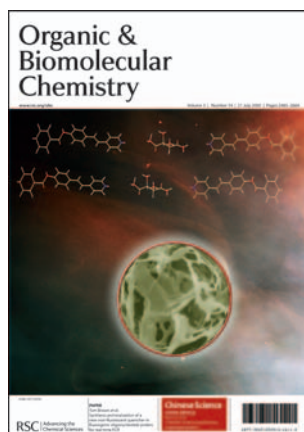
In this issue...

From α -helix to β -sheet

Modelling neurodegenerative diseases by showing how metal ions can be used to change the secondary structure of proteins. See B. Kokschi *et al.* pp. 2500–2502



Chemical biology articles published in this journal also appear in the *Chemical Biology Virtual Journal*: www.rsc.org/chembiol



Cover

See Chunyan Bao, Ran Lu, Ming Jin, Pengchong Xue, Changhui Tan, Guofa Liu and Yingying Zhao, pp. 2508–2512. Strongly enhanced fluorescence is generated due to the formation of self-assembly in tartaric acid-assisted binary organogel.

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EDITORIAL

2499

Chemical Science in China

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Chinese
Science

COMMUNICATIONS

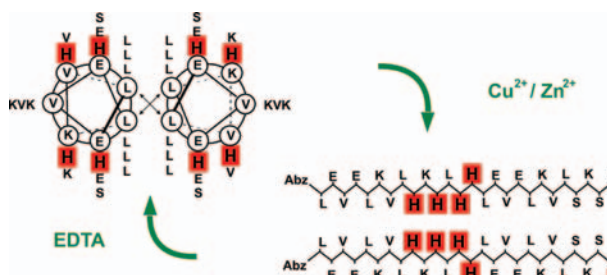
2500



From α -helix to β -sheet – a reversible metal ion induced peptide secondary structure switch

Kevin Pagel, Toni Vagt, Tibor Kohajda and Beate Kokschi*

The influence of metal ions on secondary structure formation can be studied by a *de novo* designed peptide model.



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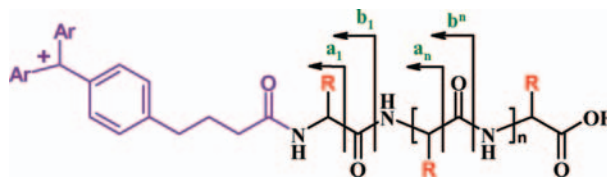
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A new charge derivatization procedure for peptide sequencing

Denekamp Chagit,* Emilia Rabkin and Alexander Tsoglin

Derivatization of peptides by a trityl cation-containing group followed by mass measurements results in informative spectra for peptide sequencing.

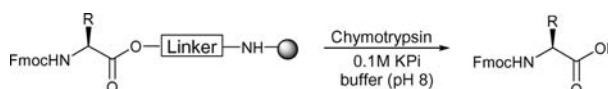


2505

Enzyme-cleavable linkers for peptide and glycopeptide synthesis

Beatrice A. Maltman, Mallesham Bejugam and Sabine L. Flitsch*

Commonly used ester linkers are cleaved by chymotrypsin from PEGA₁₉₀₀ support in quantitative yields; the method is applicable to a wide range of amino acids (R = charged, polar, hydrophobic), peptides and glycopeptides.



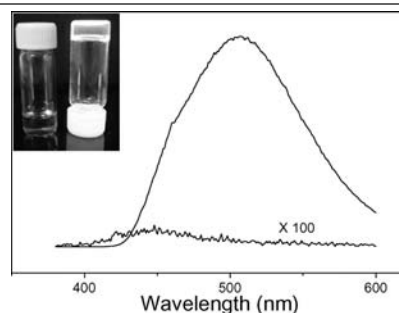
ARTICLES

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L-Tartaric acid assisted binary organogel system: strongly enhanced fluorescence induced by supramolecular assembly

Chunyan Bao, Ran Lu,* Ming Jin, Pengchong Xue, Changhui Tan, Guofa Liu and Yingying Zhao

L-Tartaric assisted binary organogels generated strongly enhanced fluorescence due to the formation of the self-assembly.

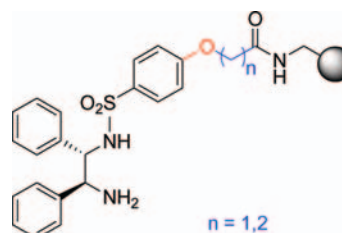


2513

Preparation of polymer-supported Ru-TsDPEN catalysts and use for enantioselective synthesis of (S)-fluoxetine

Yangzhou Li, Zhiming Li, Feng Li, Quanrui Wang* and Fanggang Tao

Reusable polymer-supported chiral ligands in combination with [RuCl₂(*p*-cymene)]₂ were applied for the asymmetric synthesis of fluoxetine.



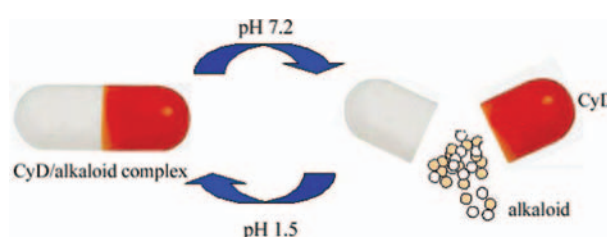
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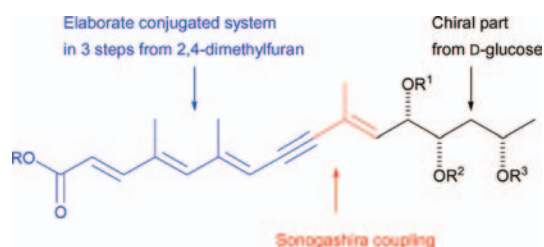
Cyclodextrins as carriers for cinchona alkaloids: a pH-responsive selective binding system

Yu Liu,* Guo-Song Chen, Yong Chen, Fei Ding and Jing Chen

The inclusion complexation behavior of some β -CyD derivatives with four cinchona alkaloids has been investigated at pH 7.2 and 1.5; the results showed that CyDs could enhance the water-solubilities of these alkaloids.



2524

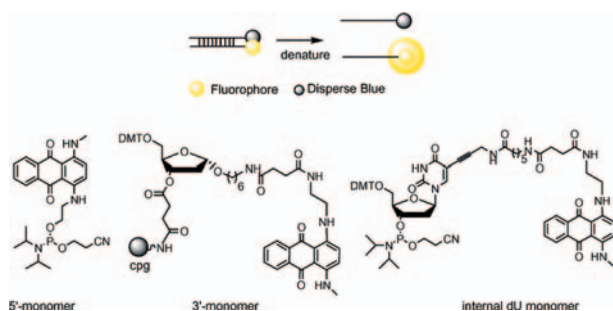


New approaches towards the synthesis of the side-chain of mycolactones A and B

Ruben P. van Summeren, Ben L. Feringa* and Adriaan J. Minnaard*

The fast and convergent synthesis of an 8,9-dehydro analogue of the side-chain of mycolactones A and B was achieved by Sonogashira coupling of a chiral building block to a conjugated chain. The key elements in our strategy were the rapid assembly of an elaborate conjugated system in only 3 steps and the synthesis of the chiral part with complete stereocontrol by modification of naturally occurring monosaccharides.

2534

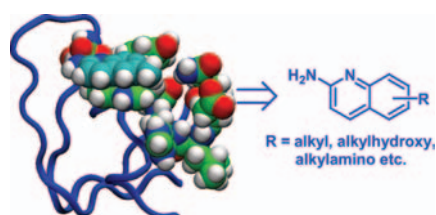


Synthesis and evaluation of a new non-fluorescent quencher in fluorogenic oligonucleotide probes for real-time PCR

Jonathan P. May, Lynda J. Brown, Ian van Delft, Nicola Thelwell, Kate Harley and Tom Brown*

Three Disperse Blue quencher monomers for incorporation into oligonucleotide probes have been synthesised, and assessed by fluorimetry and real-time PCR.

2543

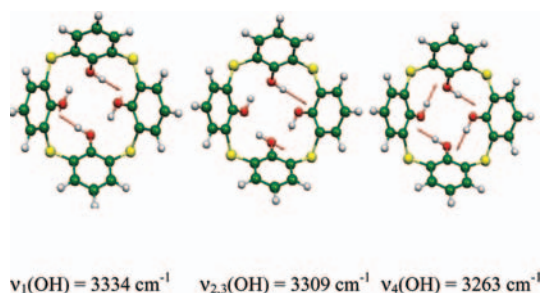


Synthesis of 5-, 6- and 7-substituted-2-aminoquinolines as SH3 domain ligands

Steven Inglis, Rhiannon Jones, Daniel Fritz, Cvetan Stojkoski, Grant Booker and Simon Pyke*

Synthesis of a range of new 5-, 6- and 7-substituted-2-aminoquinolines, and their binding studies with the Tec SH3 domain is presented.

2558

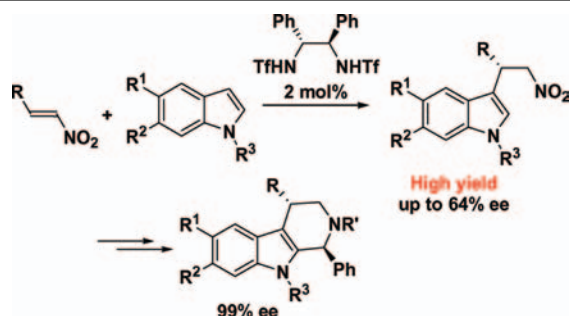


Vibrational spectra, co-operative intramolecular hydrogen bonding and conformations of calix[4]arene and thiacalix[4]arene molecules and their *para-tert*-butyl derivatives

Sergey Katsyuba,* Valeri Kovalenko, Alla Chernova, Elena Vandyukova, Vladislav Zverev, Roald Shagidullin, Igor Antipin, Svetlana Solovieva, Ivan Stoikov and Alexander Konovalov

The IR and Raman spectra, conformations and hydrogen bonding of calix[4]arene, thiacalix[4]arene and their *p-tert*-butyl derivatives have been analysed within the framework of scaled quantum mechanics (SQM).

2566



Enantioselective Friedel-Crafts type addition of indoles to nitro-olefins using a chiral hydrogen-bonding catalyst – synthesis of optically active tetrahydro- β -carboline

Wei Zhuang, Rita G. Hazell and Karl Anker Jørgensen*

The enantioselective and high-yielding Friedel-Crafts addition of indoles to nitro-olefins using chiral hydrogen-bonding bis-sulfonamides as the catalysts has been developed.

2572

Two structural types of 1,3-alternate tetrapropoxycalix[4]arene derivatives in the solid state

Jan Sýkora,* Jan Budka, Pavel Lhoták, Ivan Stibor and Ivana Čisarová

Only two different cavity shapes were found in the crystal structures of 1,3-alternate calix[4]arene derivatives.

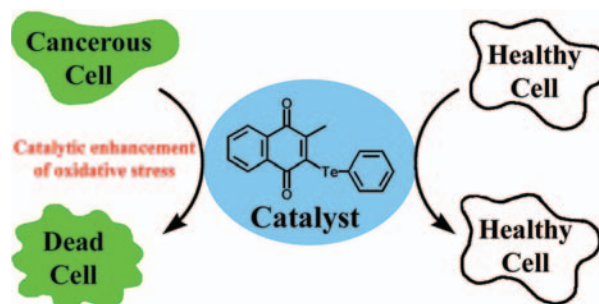


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Multifunctional redox catalysts as selective enhancers of oxidative stress

Fiona H. Fry, Andrea L. Holme, Niroshini M. Giles, Gregory I. Giles, Catriona Collins, Kim Holt, Sandra Pariagh, Thomas Gelbrich, Michael B. Hursthouse, Nick J. Gutowski and Claus Jacob*

Redox catalysts containing a chalcogen and a quinone redox centre selectively target cultured cancer cells under oxidative stress.

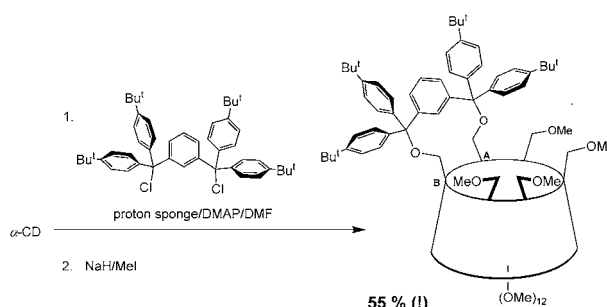


2588

A new approach to A,B-difunctionalisation of cyclodextrins using bulky 1,3-bis[bis(aryl)chloromethyl]benzenes as capping reagents

Dominique Armspach,* Laurent Poorters, Dominique Matt,* Belkacem Benmerad, Fadila Balegroune and Loic Toupet

1,3-Bis[bis(4-*tert*-butylphenyl)chloromethyl]benzene and 1,3-bis[bis(anisyl)chloromethyl]benzene were employed as efficient regioselective capping reagents for the preparation of C-6^A, C-6^B-bridged permethylated α - and β -CD derivatives.



2593

Synthesis of profluorescent isoindoline nitroxides via palladium-catalysed Heck alkenylation

Daniel J. Keddie, Therese E. Johnson, Dennis P. Arnold and Steven E. Bottle*

A new structural class of isoindoline nitroxides (aminoxyls) is accessible via palladium-catalysed Heck coupling with alkenes.

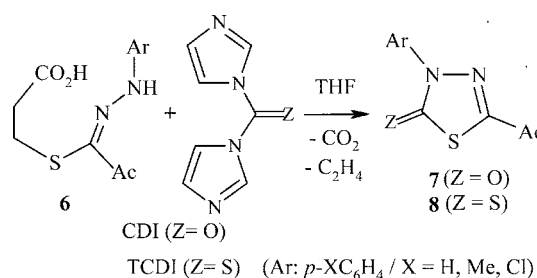


2599

3-Mercaptopropionic acid–nitrile imine adducts. An unprecedented cyclization into 1,3,4-thiadiazol-2(3H)-ones and -2(3H)-thiones

Jalal A. Zahra, Bassam A. Abu Thaher, Mustafa M. El-Abadelah* and Roland Boese

Interaction of 3-mercaptopropionic acid–nitrile imine acyclic adducts (**6**) with 1,1'-carbonyldiimidazole (CDI) and with TCDI yielded the respective 1,3,4-thiadiazol-2-(3H)-ones (**7**) and their -thione analogs (**8**), with ultimate elimination of the propionate moiety.



2604

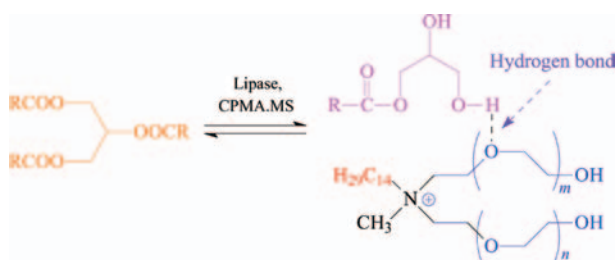


Kinetics of oxidation of benzyl alcohols by the dication and radical cation of ABTS. Comparison with laccase-ABTS oxidations: an apparent paradox

Barbara Branchi, Carlo Galli* and Patrizia Gentili*

The possible structure of the oxidised form(s) of mediator ABTS, produced from preliminary interaction with the enzyme laccase, is investigated.

2615

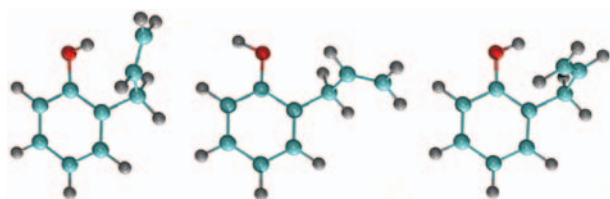


New opportunity for enzymatic modification of fats and oils with industrial potentials

Zheng Guo and Xuebing Xu*

An amphiphilic tetraammonium-based ionic liquid creates a compatible system for glycerol and oil, yielding high productivity of monoglyceride by shifting the equilibrium.

2620



Spectroscopic and theoretical studies on intramolecular OH-π hydrogen bonding in 4-substituted 2-allylphenols

Paul Rademacher,* Levan Khelashvili and Klaus Kowski

Intramolecular OH-π hydrogen bonding in 4-substituted 2-allylphenols has been studied by photoelectron and infrared spectroscopy in combination with B3LYP calculations.

2626

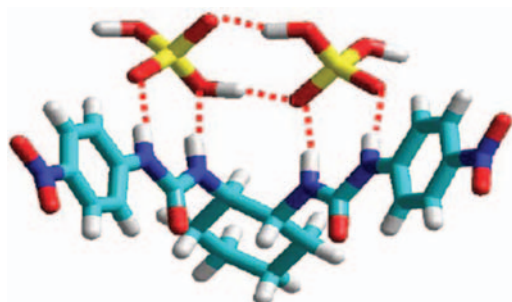


Asymmetric syntheses of (-)-lentiginosine and an original pyrrolizidinic analogue thereof from a versatile epoxyamine intermediate

Tahar Ayad, Yves Génisson* and Michel Baltas

(-)-Lentiginosine and its pyrrolizidinic analogue have been prepared in a straightforward 5-step sequence from a versatile chiral *cis* α,β -epoxyamine.

2632



Chiral receptors for phosphate ions

Valeria Amendola, Massimo Boiocchi, David Esteban-Gómez, Luigi Fabbrizzi and Enrico Monzani

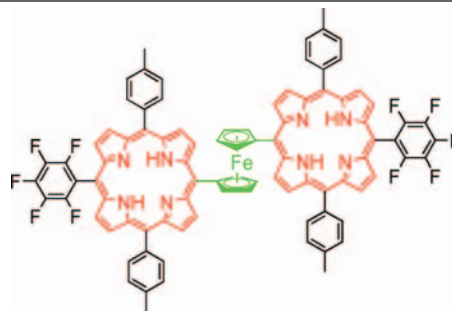
The *R,R* and *S,S* forms of a neutral bis-urea receptor bind in MeCN solution a pair of H-bond linked H_2PO_4^- ions and display enantioselective recognition of D-2,3-diphosphoglycerate.

2640

The synthesis and properties of bis-1,1'-(porphyrinyl)-ferrocenes

Beata Koszarna, Holger Butenschön* and Daniel T. Gryko*

Complex dynamic processes occur in novel, efficiently synthesized ferrocene-bridged bisporphyrins, which probably involve conformers, formation of H-aggregates and tautomers.

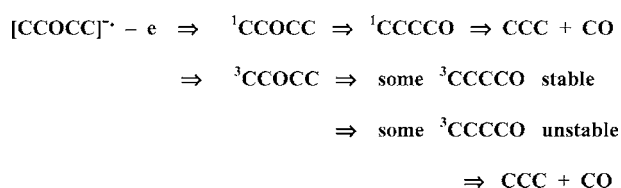


2646

One-electron oxidation of [CCOCC]^{-•} in the gas phase forms stable and decomposing forms of CCCC

Mark Fitzgerald, Suresh Dua and John H. Bowie*

Franck–Condon one-electron vertical oxidation of [CCOCC]^{-•} is demonstrated to give both singlet and triplet CCOCC neutrals which rearrange over small energy barriers to produce neutral CCCC.

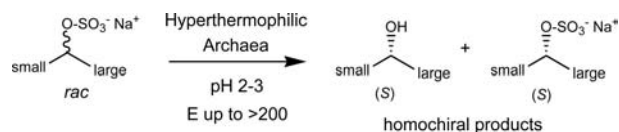


2652

Highly enantioselective stereo-inverting *sec*-alkylsulfatase activity of hyperthermophilic *Archaea*

Sabine R. Wallner, Bettina M. Nestl and Kurt Faber*

Enantioselective hydrolysis of *rac-sec*-alkyl sulfate esters using whole cells of *Sulfolobus* spp. proceeded with inversion of configuration to furnish homochiral products.

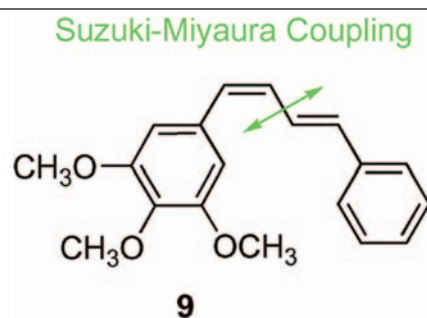


2657

Synthesis and biological evaluation of vinylogous combretastatin A-4 derivatives

Julia Kaffy, Renée Pontikis,* Jean-Claude Florent and Claude Monneret

An improved synthesis of dienic analogues of combretastatin A-4 is described. Phenyl derivative **9** had shown to have potent antitubulin activity with reduced cytotoxicity.



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Thibaud Coradin, David Eglin, M. M. Giraud-Guille, Jacques Livage and Gervaise Mosser

Papers

Effect of guest capture modes on molecular recognition by a dynamic cavity array at the air–water interface: soft vs. tight and fast vs. slow

Katsuhiko Ariga, Takashi Nakanishi, Jonathan P. Hill, Yukiko Terasaka, Daisuke Sakai and Jun-ichi Kikuchi

A small-angle neutron scattering study of biologically relevant mixed surfactant micelles comprising 1,2-diheptanoyl-sn-phosphatidylcholine and sodium dodecyl sulfate or dodecyltrimethylammonium bromide

Peter C. Griffiths, Alison Paul, Zeena Khayat, Richard K. Heenan, Radha Ranganathan and Isabelle Grillo

Intrinsic viscosity of dendrimers via equilibrium molecular dynamics

Philip M. Drew and David B. Adolf

Structure and rheology of aqueous micellar solutions and gels formed from an associative poly(oxybutylene)–poly(oxyethylene)–poly(oxybutylene) triblock copolymer


V. Castelletto, I. W. Hamley, X.-F. Yuan, A. Kelarakis and C. Booth

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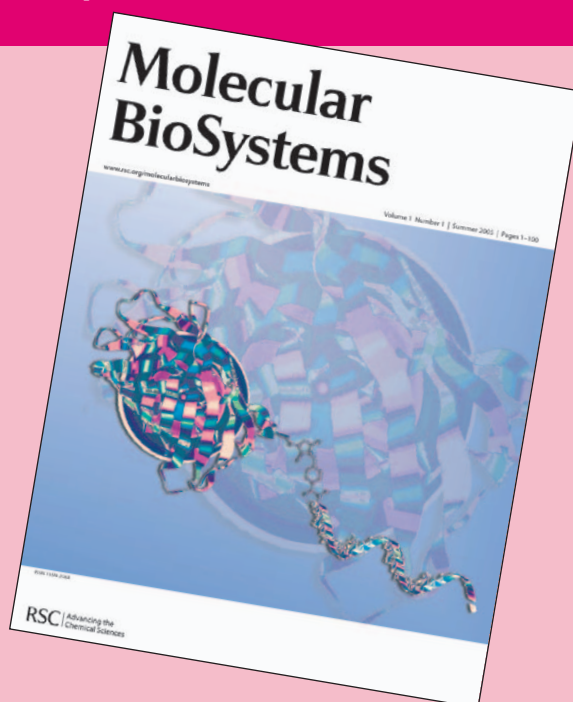
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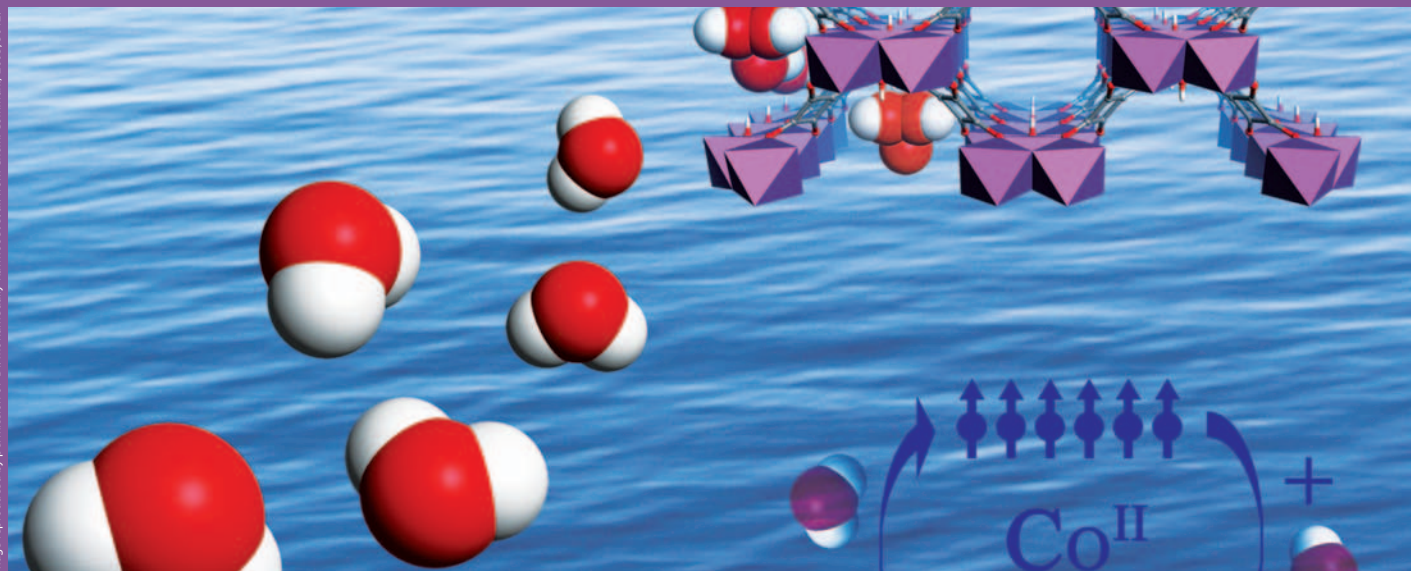
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