



# The following Communications have been judged by at least two referees to be "very important papers" and will be published online at www.angewandte.org soon:

K. Nakano, S. Hashimoto, M. Nakamura, T. Kamada, K. Nozaki\* Synthesis of Stereogradient Poly(propylene carbonate) by Stereoand Enantioselective Copolymerization of Propylene Oxide with Carbon Dioxide

K. Ohmori, T. Shono, Y. Hatakoshi, T. Yano, K. Suzuki\*

An Integrated Synthetic Strategy for Higher Catechin Oligomers

L. Aboshyan-Sorgho, C. Besnard, P. Pattison, K. R. Kittilstved, A. Aebischer, J.-C. Bünzli, A. Hauser,\* C. Piguet\*

Molecular Near-Infrared to Visible Light Upconversion in a Trinuclear d-f-d Complex

C. A. Naini, S. Franzka, S. Frost, M. Ulbricht, N. Hartmann\* Probing the Intrinsic Switching Kinetics of Ultrathin Thermoresponsive Polymer Brushes R. Linser, M. Dasari, M. Hiller, V. Higman, U. Fink, J.-M. d. Amo, S. Markovic, L. Handel, B. Kessler, P. Schmieder, D. Oesterhelt, H. Oschkinat, B. Reif\*

Proton-Detected Solid-State NMR Spectroscopy of Fibrillar and Membrane Proteins

X. Wurzenberger, H. Piotrowski, P. Klüfers\*

A Stable Square-Planar High-Spin-d<sup>6</sup> Molecular Fe<sup>II</sup>O<sub>4</sub> Chromophore From Rare Iron(II) Minerals

I. Piel, M. Steinmetz, K. Hirano, R. Fröhlich, S. Grimme,\* F. Glorius\*

Highly Asymmetric NHC-Catalyzed Hydroacylation of Unactivated Alkenes and Mechanistic Insights

# **Author Profile**

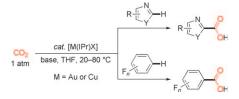
Luis M. Liz-Marzán \_\_\_\_\_\_ 3838

"My greatest achievement has been bringing up two wonderful children.

The biggest problem that scientists face is public awareness about the need for basic research ..."

This and more about Luis M. Liz-Marzán can be found on page 3838.

#### **Obituaries**



CO<sub>2</sub> in a fix: Gold and copper complexes of N-heterocyclic carbenes recently enabled efficient direct carboxylation of (hetero)arenes having moderately acidic C—H bonds under remarkably mild reaction conditions (IPr=1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene).

# Highlights

CO<sub>2</sub> Fixation

L. Ackermann\* \_\_\_\_\_ 3842 - 3844

Transition-Metal-Catalyzed Carboxylation of C-H Bonds

#### Metal-Catalyzed Hydrosilylation

K. Osakada\* \_\_\_\_\_ 3845 – 3846

1,4-Hydrosilylation of Pyridine by Ruthenium Catalyst: A New Reaction and Mechanism Making introductions: A half-sandwich Ru complex catalyzes the hydrosilylation of pyridine derivatives to produce *N*-silyl-3-hydropyridine through a 1,4-addition of the Si–H group (see scheme). The reversibility of the hydrosilylation was suggested based on the experimental results.

$$X \longrightarrow N \qquad \text{Ru cat.} \qquad X \longrightarrow N - \text{SiMe}_2\text{Pl}$$

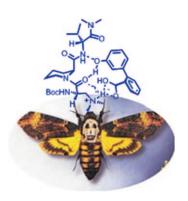
$$X \longrightarrow N - \text{SiMe}_2\text{Pl}$$

#### Organocatalysis

P. G. Cozzi,\* E. Emer,
A. Gualandi \_\_\_\_\_\_\_ **3847 – 3849** 

Atroposelective Organocatalysis

**Spin off:** The synthesis of optically active biaryl compounds using enantioselective organocatalysis is highlighted. Foldamers coupled with organocatalysis, specifically hydrogen-bonding interactions (see scheme; Boc = tert-butoxycarbonyl), can be used to access compounds with a stereogenic axis. New selective syntheses of atropoisomers can be inspired by these findings, thus enhancing the use of atropoisomeric compounds in synthesis and catalysis.



# Correspondence

#### Oxo Complexes

D. Schröder,\* S. Shaik\* \_\_\_\_ 3850 - 3851

Comment on "A Low-Spin Ruthenium(IV)—Oxo Complex: Does the Spin State Have an Impact on the Reactivity" Slippery spin states: When the metal center in a transition-metal complex can adopt multiple spin states, the reactivity of the complex may be influenced. In such

cases, care must be taken that experimental and computational evidence are interpreted correctly.

#### Oxo Complexes

T. Kojima,\* S. Fukuzumi\* \_\_ 3852-3853

Reply

Trust in experiments: As DFT calculations suggest that the hydrogen bonding of water molecules can stabilize a seven-coordinate ruthenium—oxo complex to exhibit a singlet spin state, experiments have shown that the novel seven-coordi-

nate pentaganol-bipyramidal ruthenium oxo complex has a singlet ground state. Nevertheless, it displays the same reactivity as an analogous triplet-state complex.

#### For the USA and Canada:

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individuals who are personal members of a national chemical society prices are available on request. Postage and handling charges included. All prices are subject to local VAT/sales tax.



# X = COOH, COOMe, CH<sub>2</sub>OH OH X OH X Polymers Platform chemicals Detergents Monomers Additives Building blocks

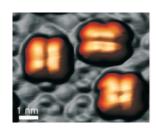
More than just a greasy spoon: Oils and fats are the most important renewable feedstock of the chemical industry. Recent and exciting advances in chemistry and biotechnology were made within the last

10 years concerning their utilization as a chemical feedstock. This progress in organic synthesis, catalysis, and biotechnology using plant oils and their derivatives is highlighted.

#### Reviews

#### Renewable Raw Materials

Oils and Fats as Renewable Raw Materials in Chemistry





**Stacked up:** Use of scanning tunneling microscopy allows manipulation of the upper porphyrin of tris (porphyrinato)

cerium triple-decker complexes, which are obtained by a new synthetic route on a smooth Ag(111) surface (see picture).

### **Communications**

#### Molecular Rotors

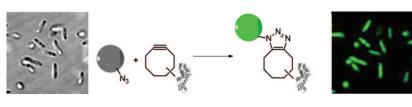
D. Écija,\* W. Auwärter,\*

S. Vijayaraghavan, K. Seufert, F. Bischoff,

K. Tashiro, J. V. Barth \_\_\_\_\_\_ 3872 - 3877

Assembly and Manipulation of Rotatable Cerium Porphyrinato Sandwich Complexes on a Surface





A bright click of life: Strained alkynes are genetically encoded into *E. coli* by use of an engineered pyrrolysine amber suppressor tRNA/synthetase pair from *Methanosarcina mazei*. As a result cyclooctynyl lysine derivatives were incorporated site-

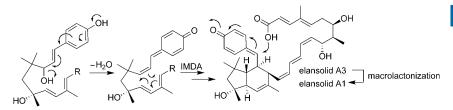
specifically in proteins allowing efficient labeling with fluorogenic azide-bearing dyes by means of a click reaction under physiological conditions in vitro and in vivo (see scheme).

#### In Vivo Protein Labeling

T. Plass, S. Milles, C. Koehler, C. Schultz,\* E. A. Lemke\* \_\_\_\_\_\_\_ **3878 – 3881** 

Genetically Encoded Copper-Free Click Chemistry





**Total control:** The key steps in the biosynthesis of elansolide A1, a new and structurally unique polyketide metabolite from the gliding bacterium *Chitinophaga sancti*, have been elucidated from feeding experiments, by analysis of the biosyn-

thetic gene cluster, and through the synthesis of model substrates. These steps include an unprecedented dehydration reaction, an intramolecular Diels–Alder cycloaddition (IMDA), and an unusual macrolactonization.

#### Biosynthesis

R. Dehn, Y. Katsuyama, A. Weber, K. Gerth,

R. Jansen, H. Steinmetz, G. Höfle,

R. Müller,\* A. Kirschning\* \_ **3882 – 3887** 

Molecular Basis of Elansolid Biosynthesis: Evidence for an Unprecedented Quinone Methide Initiated Intramolecular Diels-Alder Cycloaddition/Macrolactonization

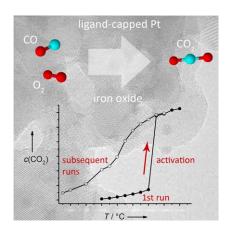


#### Heterogeneous Catalysis

P. Sonström, D. Arndt, X. Wang, V. Zielasek, M. Bäumer\* \_\_\_\_ 3888 – 3891



Ligand Capping of Colloidally Synthesized Nanoparticles: A Way to Tune Metal– Support Interactions in Heterogeneous Gas-Phase Catalysis Better be capped: Ligand-capped, colloidally prepared Pt nanoparticles deposited on nanostructured iron oxide catalyze CO oxidation at unusually low temperatures when compared to the action of identical ligand-free Pt nanoparticles. The ligands efficiently modify the interaction between the metal and the iron oxide support and cause a beneficial strong metal—support interaction. As a result, the limitations resulting from CO poisoning at low temperatures can be overcome.



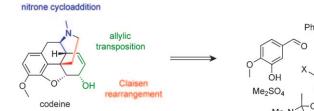
#### **Natural Product Synthesis**

T. Erhard, G. Ehrlich,

P. Metz\* \_\_\_\_\_ 3892 – 3894



A Total Synthesis of ( $\pm$ )-Codeine by 1,3-Dipolar Cycloaddition



**Nitrone cycloaddition** on a dearomatized bicyclic phenol enabled the facile construction of the correctly configured phenanthrene skeleton of codeine. Fur-

ther steps yielded allopseudocodeine in a completely diastereoselective manner and finally  $(\pm)$ -codeine by allylic transposition through the hydrolysis of chlorocodides.

MeNHOH

#### **Orthogonal Cross-Couplings**

N. Hadei, G. T. Achonduh, C. Valente, C. J. O'Brien, M. G. Organ\* 3896-3899



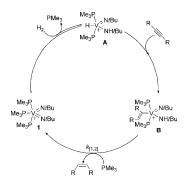
Differentiating C-Br and C-Cl Bond Activation by Using Solvent Polarity: Applications to Orthogonal Alkyl-Alkyl Negishi Reactions



A pot to share: A C<sub>alky</sub>—Cl bond can be rendered "dormant" or "active" in the Negishi alkyl—alkyl cross-coupling by a simple solvent polarity "switch" (see scheme). Adjustment from a 1:2 to a 2:1 solvent ratio of dimethylimidazolidi-

none:tetrahydrofuran enables orthogonal alkyl-alkyl Negishi cross-coupling strategies to be carried out on bifunctional bromochloroalkanes in one pot at room temperature.





Early metal gets the H: Under 1 atm of  $H_2$ , the vanadium complex 1 (PFTB = perfluoro-tert-butoxide) catalytically semihydrogenates alkynes to Z alkenes. Synthetic and DFT studies, in combination with  $H_2/D_2$  and NMR experiments, indicate that  $H_2$  is activated by 1,2-addition to 1. Upon insertion of an alkyne into the V—H bond of **A**, the product alkene and 1 are generated by the 1,2- $\alpha$ -NH-elimination of the alkenyl ligand.

#### Catalytic Hydrogenation

H. S. La Pierre, J. Arnold,\*
F. D. Toste\* \_\_\_\_\_\_ **3900 – 3903** 

Z-Selective Semihydrogenation of Alkynes Catalyzed by a Cationic Vanadium Bisimido Complex



Alkyl—X + Aryl—B 
$$OR$$
  $Cat. Cul$   $Cul$   $Cot. Cul$   $Cot$ 

Non-activated alkyl electrophiles, including alkyl iodides, bromides, tosylates, mesylates, and even chlorides, underwent copper-catalyzed cross-coupling with aryl boron compounds and alkyl 9-BBN reagents (see scheme; 9-BBN = 9-

borabicyclo[3.3.1]nonane). The reactions proceed with practically useful reactivities and thus complement palladium- and nickel-catalyzed Suzuki–Miyaura coupling reactions of alkyl halides.

#### **Cross-Coupling Reactions**

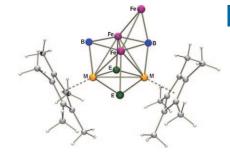
C.-T. Yang, Z.-Q. Zhang, Y.-C. Liu, L. Liu\* \_\_\_\_\_\_\_ **3904 – 3907** 

Copper-Catalyzed Cross-Coupling Reaction of Organoboron Compounds with Primary Alkyl Halides and Pseudohalides



Metal-rich metallaboranes: An exo-Fe(CO)<sub>3</sub> moiety linked to a cubane core is the most prominent feature of complexes [(Cp\*M)<sub>2</sub>( $\mu_3$ -E)<sub>2</sub>B<sub>2</sub>H( $\mu$ -H){Fe(CO)<sub>2</sub>}<sub>2</sub>-Fe(CO)<sub>3</sub>] (M = Mo, E = S, Se; M = Ru, E = CO; Cp\*=  $\eta^5$ -C<sub>5</sub>Me<sub>5</sub>), which are the first heterobimetallic cubane-type clusters

with a boride unit (see structure).



#### Cluster Compounds

K. Geetharani, S. K. Bose, S. Sahoo, S. Ghosh\* \_\_\_\_\_\_\_ **3908 – 391**1

A Family of Heterometallic Cubane-Type Clusters with an *exo*-Fe(CO)<sub>3</sub> Fragment Anchored to the Cubane



Clever boxing: A cyclization-carbonylation-cyclization-coupling reaction of propargyl acetates 1 or amides 2 in the presence of a palladium(II)-bisoxazoline (box) catalyst afforded symmetrical ketones of types 3 and 4, respectively,

containing two heterocyclic groups in moderate to excellent yields (see scheme; tfa = trifluoroacetate). Compounds **3** were converted into ketones containing two 3(2H)-furanone rings.

#### **Domino Reactions**

Cyclization—Carbonylation—Cyclization Coupling Reactions of Propargyl Acetates and Amides with Palladium(II)— Bisoxazoline Catalysts

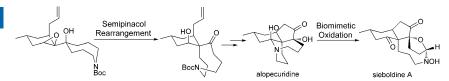


#### Alkaloid Synthesis

X.-M. Zhang, Y.-Q. Tu,\* F.-M. Zhang, H. Shao, X. Meng \_\_\_\_\_\_ **3916-3919** 



Total Synthesis of  $(\pm)$ -Alopecuridine and Its Biomimetic Transformation into  $(\pm)$ -Sieboldine A



The features you need: The first total synthesis of lycopodium alkaloid alope-curidine has been achieved in 13 steps in the longest linear sequence, and its biomimetic conversion into sieboldine A has been validated through a two-step

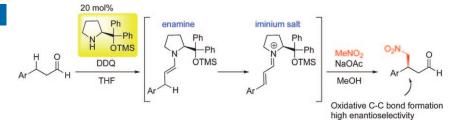
oxidation. The synthesis features a semipinacol rearrangement of a functionalized medium-sized ring and an intramolecular pinacol coupling mediated by SmI<sub>2</sub> (see scheme; Boc = tert-butoxycarbonyl).

#### Asymmetric Catalysis

Y. Hayashi,\* T. Itoh,
H. Ishikawa \_\_\_\_\_\_ **3920 – 3924** 



Oxidative and Enantioselective Cross-Coupling of Aldehydes and Nitromethane Catalyzed by Diphenylprolinol Silyl Ether



**Synthetically important** β-substituted γ-nitro aldehydes have been synthesized with excellent enantioselectivity by the cross-coupling reaction of β-aryl substituted aldehydes or γ,δ-unsaturated alde-

hydes and nitromethane using 2,3-dichloro-5,6-dicyanoquinone (DDQ) and diphenylprolinol silyl ether as an oxidant and catalyst, respectively (see scheme; TMS = trimethylsilyl).

#### Frustrated Lewis Pairs

C. Appelt, H. Westenberg, F. Bertini, A. W. Ehlers, J. C. Slootweg,

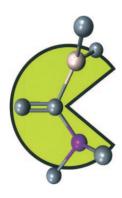
K. Lammertsma,\* W. Uhl\* \_ 3925-3928



Geminal Phosphorus/Aluminum-Based Frustrated Lewis Pairs:

C−H versus C≡C Activation and CO<sub>2</sub>
Fixation

Catch it! Geminal phosphorus/aluminum-based frustrated Lewis pairs (FLPs) are easily obtained by hydroalumination of alkynylphosphines. These FLPs can activate terminal acetylenes by two competitive pathways, which were analyzed by DFT calculations, and they can bind carbon dioxide reversibly. Therefore, alongside polyfluorinated boranes, alanes are also ideal Lewis acids for FLP chemistry.



#### Switchable Pores

K. K. R. Datta, D. Jagadeesan, C. Kulkarni, A. Kamath, R. Datta,

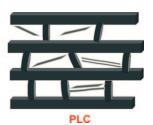
M. Eswaramoorthy\* \_\_\_\_\_ 3929 – 3933



Observation of Pore-Switching Behavior in Porous Layered Carbon through a Mesoscale Order–Disorder Transformation







A structural chameleon: A porous layered carbon material (PLC) containing nanographene domains was prepared by graphitizing glucose within the nanoscopic voids of an aminoclay template. The size of the pores in the PLC was

altered reversibly by a mesoscale order—disorder transformation brought about by an applied mechanical force (see picture). This pore flexibility was exploited for the size-selective separation of dye molecules.



An oxygenation pathway: The title transformation involves a two-step process: a selective oxygenation step to generate

aldehyde intermediates and a subsequent condensation step to afford the imine products (see scheme).

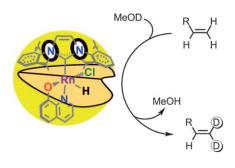
#### **Photocatalysis**



X. Lang, H. Ji, C. Chen, W. Ma, J. Zhao\* \_\_\_\_\_\_ **3934-3937** 

Selective Formation of Imines by Aerobic Photocatalytic Oxidation of Amines on TiO<sub>2</sub>





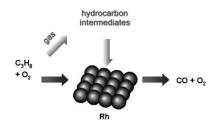
#### Pacman bites selectively! Stable

rhodium(III)—N-heterocyclic carbene—hydride complexes (Pacman-like catalysts) are highly active and selective catalysts for H/D exchange at the  $\beta$  position of aromatic  $\alpha$ -olefins (see picture). The interplay between bulky N-heterocyclic carbene and quinolinate ligands determines the size of the steric window responsible for this selectivity.

#### H/D Exchange

Mild and Selective H/D Exchange at the  $\beta$  Position of Aromatic  $\alpha\text{-Olefins}$  by N-Heterocyclic Carbene-Hydride-Rhodium Catalysts





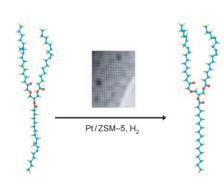
By land or by air: Ultrafast catalytic processes for converting hydrocarbons at short contact times are characterized by extremely severe operating conditions. In situ sampling and detailed modeling of surface and gas-phase kinetics allowed the elucidation of the complex interplay between heterogeneous and homogenous pyrolytic routes to H<sub>2</sub> and CO in the catalytic partial oxidation (CPO) of C<sub>3</sub>H<sub>8</sub>.

#### Hydrocarbon Conversion



Synergy of Homogeneous and Heterogeneous Chemistry Probed by In Situ Spatially Resolved Measurements of Temperature and Composition

Well tuned: ZSM-5 with platinum nanoparticles preferably hydrogenates *trans* fatty acids over *cis* isomers in model triacylglycerols for geometric reasons. The central fatty acid chain reacts faster, pointing to pore mouth adsorption in a tuning fork conformation (see picture). This conformation induces stepwise hydrogenation, resulting in fast removal of the unstable central triene, while formation of saturated chains is limited.



#### Fatty Acid Hydrogenation

A. Philippaerts, S. Paulussen, A. Breesch, S. Turner, O. I. Lebedev, G. Van Tendeloo, B. Sels,\* P. Jacobs \_\_\_\_\_\_\_\_ **3947 – 3949** 

Unprecedented Shape Selectivity in Hydrogenation of Triacylglycerol Molecules with Pt/ZSM-5 Zeolite

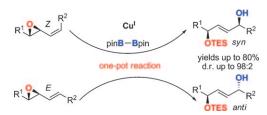


#### Asymmetric Synthesis

M. Tortosa\* \_\_\_\_\_ 3950 - 3953



Synthesis of syn and anti 1,4-Diols by Copper-Catalyzed Boration of Allylic Epoxides



Two sides of the same coin: Syn and anti 1,4-diols have been synthesized through the regio- and diastereoselective Cu<sup>1</sup>-catalyzed boration of allylic epoxides (see scheme; pin = pinacolato, TES = triethyl-

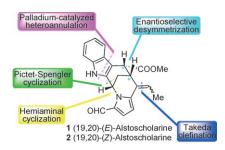
silyl). In situ protection of the alcohol allows isolation of *syn* and *anti* 1,4-silyloxyboronates. Monoprotected 1,4-diols can be prepared by a one-pot addition—protection—oxidation sequence.

#### Natural-Product Synthesis

- T. Gerfaud, C. Xie, L. Neuville,\*
  J. Zhu\* \_\_\_\_\_\_ 3954 3957

Protecting-Group-Free Total Synthesis of (*E*)- and (*Z*)-Alstoscholarine

Looking for hidden symmetry: The first asymmetric total synthesis of pentacyclic compounds 1 and 2 has been accomplished starting from a cyclic *meso*-anhydride. The absolute configuration of the final products was set by an organocatalytic desymmetrization of the *meso*-anhydride. The economic synthesis is protecting-group-free and confirms the assigned absolute configuration.

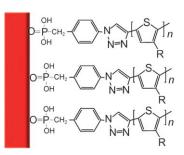


#### Semiconductor Nanocomposites

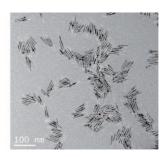
L. Zhao, X. Pang, R. Adhikary, J. W. Petrich, Z. Lin\* \_\_\_\_\_\_\_ **3958 – 3962** 



Semiconductor Anisotropic Nanocomposites Obtained by Directly Coupling Conjugated Polymers with Quantum Rods



Semiconductor organic-inorganic nanocomposites were synthesized by a catalyst-free click reaction of ethynyl-terminated polythiophene) with azide-functionalized CdSe nanorods. Such rationally



designed nanocomposites possess a welldefined interface between polymer and nanorods, thereby facilitating electronic interaction.

#### **Asymmetric Catalysis**

T. Shibuya, Y. Shibata, K. Noguchi, K. Tanaka\* \_\_\_\_\_\_ 3963 – 3967



Palladium-Catalyzed Enantioselective Intramolecular Hydroarylation of Alkynes To Form Axially Chiral 4-Aryl 2-Quinolinones



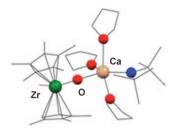


up to 98% ee

A long-awaited asymmetric version of the intramolecular hydroarylation of alkynes to form fused ring systems has been developed. A cationic palladium(II)/(S)-xyl-H<sub>8</sub>-binap complex was used to catalyze

an enantioselective hydroarylation of alkynes at room temperature to furnish axially chiral 4-aryl 2-quinolinone derivatives in good yields with good enantioselectivity (see scheme; Bn = benzyl).





One for two: A zirconium compound combined with a main-group alkaline earth metal through an oxygen bridge has been synthesized. A number of primary and secondary aminoalkenes were successfully converted into cyclic products using this heterobimetallic complex as catalyst. The calcium center activates primary aminoalkenes, and the zirconium center activates secondary aminoalkenes.

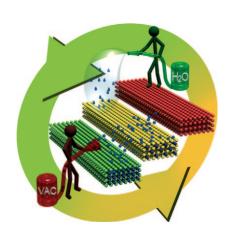
#### Heterobimetallic Catalysis

A. Mukherjee, S. Nembenna, T. K. Sen, S. P. Sarish, P. K. Ghorai, H. Ott, D. Stalke, S. K. Mandal,\*

H. W. Roesky\* \_\_\_\_\_\_ 3968 – 3972

Assembling Zirconium and Calcium Moieties through an Oxygen Center for an Intramolecular Hydroamination Reaction: A Single System for Double Activation



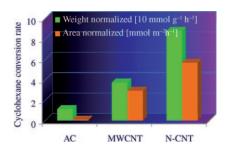


Stairway to heaven: An  $\rm Mn_2Nb$  coordination framework shows huge switching of the magnetic ordering temperature in two well-defined steps, finally reaching 100 K in its anhydrous form. The switching, controlled by removal/uptake of guest molecules, is related to an intraskeletal molecular rearrangement involving reversible formation/breaking of molecular bridges and translocation of an organic ligand on dehydration (see picture;  $\rm VAC = vacuum$ ).

#### Switchable Materials

Double Switching of a Magnetic Coordination Framework through Intraskeletal Molecular Rearrangement





Putting the N in nanotube: Carbon nanotubes (CNTs) catalyze the aerobic oxidation of cyclohexane into cyclohexanol, cyclohexanone, and adipic acid with excellent activity and controllable selectivity. The catalytic activity is further enhanced by nitrogen dopants in the nanotube (see diagram; AC = activated carbon, MWCNT = multiwalled CNT, N-CNT = nitrogen-doped CNT).

#### Heterogeneous Catalysis

Selective Catalysis of the Aerobic Oxidation of Cyclohexane in the Liquid Phase by Carbon Nanotubes





**Elegant control**: A DNA actuator based on the most fundamental motif in DNA nanotechnology, the double crossover tile, has a linear sliding-gauge type of motion among eleven different states (see pic0 S1 S2 S3 S4 S5 S6 S7 S8 S9 S10



ture). The actuator has the ability to finetune the distances between attached components (resolution of less than 1 nm) for both physical studies and chemical control.

#### **DNA** Actuator

Z. Zhang, E. M. Olsen, M. Kryger, N. V. Voigt, T. Tørring, E. Gültekin, M. Nielsen, R. MohammadZadegan, E. S. Andersen, M. M. Nielsen, J. Kjems, V. Birkedal, K. V. Gothelf\* \_\_\_ 3983 - 3987

A DNA Tile Actuator with Eleven Discrete States

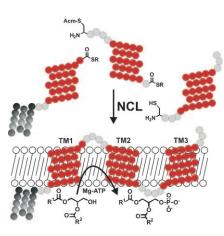


#### Synthetic Enzymes

S. Lahiri, M. Brehs, D. Olschewski, C. F. W. Becker\* \_\_\_\_\_\_ **3988 – 3992** 



Total Chemical Synthesis of an Integral Membrane Enzyme: Diacylglycerol Kinase from *Escherichia coli* 



From the ground up: Chemical synthesis provided direct access to a catalytically active membrane-embedded kinase with three transmembrane domains (TMs). Three key segments formed from the individual amino acids (represented by red and gray balls) by solid-phase peptide synthesis were connected by native chemical ligation (NCL; see picture); the synthetic protein underwent spontaneous folding in detergent micelles. ATP = adenosine 5'-triphosphate.

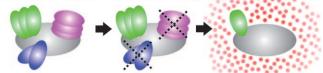
#### NMR Spectroscopy

T. Madl, T. Güttler, D. Görlich, M. Sattler\* \_\_\_\_\_\_ **3993 – 3997** 



Structural Analysis of Large Protein Complexes Using Solvent Paramagnetic Relaxation Enhancements





The solvent helps out: Conventional protocols for structural analysis of protein complexes often fail if only sparse experimental data are available. NMR-spectroscopy-derived solvent paramagnetic relaxation enhancements (PREs) from a

soluble spin label (picture) significantly improve the structural quality of a 150 kDa protein complex. This general protocol is an efficient approach for structural analysis of large protein complexes in solution.

#### **Natural Products**

L. Radtke, M. Willot, H. Sun, S. Ziegler,

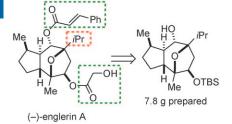
S. Sauerland, C. Strohmann, R. Fröhlich,

P. Habenberger, H. Waldmann,

M. Christmann\* \_\_\_\_\_ 3998 - 4002



Total Synthesis and Biological Evaluation of (–)-Englerin A and B: Synthesis of Analogues with Improved Activity Profile



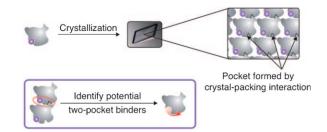
The large-scale synthesis of englerin A (see scheme) and subsequent structure-activity relationship studies have led to the discovery of highly potent analogues. TBS = tert-butyldimethylsilyl.

#### **Molecular Recognition**

P. Śledź, C. J. Stubbs, S. Lang, Y.-Q. Yang, G. J. McKenzie, A. R. Venkitaraman, M. Hyvönen, C. Abell\* \_\_\_\_\_ 4003 – 4006



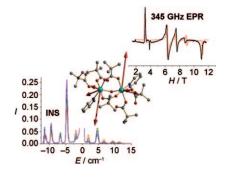
From Crystal Packing to Molecular Recognition: Prediction and Discovery of a Binding Site on the Surface of Polo-Like Kinase 1



**Picking the pocket**: Crystal-packing interactions are present in every macromolecular structure solved with X-ray methods; however, they have not been extensively used to gain insight into molecular rec-

ognition. A novel approach is described to utilize these packing interactions for the discovery of a flexible binding site and ligands recognized by it (see picture).





#### Structurally similar, magnetically diverse:

The exchange and Zeeman parameters of two dimetallic, six-coordinate cobalt(II) compounds—i.e., with orbitally degenerate metal ions—have been determined by a combination of high-resolution EPR and INS spectroscopies, together with ab intio calculations. It is suggested that the correlation between the local crystal field about the Co<sup>II</sup> centers and the superexchange pathway controls the magnetic interaction.

#### Molecular Magnets

A. B. Boeer, A.-L. Barra, L. F. Chibotaru, D. Collison, E. J. L. McInnes,\* R. A. Mole, G. G. Simeoni, G. A. Timco, L. Ungur, T. Unruh, R. E. P. Winpenny 4007 – 4011

A Spectroscopic Investigation of Magnetic Exchange Between Highly Anisotropic Spin Centers











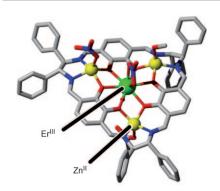


#### Gels

N. Kumano, T. Seki, M. Ishii, H. Nakamura, Y. Takeoka\* \_ 4012-4015

A porous gel exhibiting angle-independent structural color was obtained by a facile self-assembly approach. The porous swollen gel changes color reversibly in response to changes in solvent composition and temperature as a result of changes in the wavelength dispersions of the refractive indices of the gel portion and the solvent portion in the pores. Tunable Angle-Independent Structural Color from a Phase-Separated Porous Gel





Designer SMM: An Er<sup>III</sup>-based single-molecule magnet (SMM) was synthesized by designing the ligand-field anisotropy around an Er<sup>III</sup> ion in an equatorial arrangement of donors using a rigid and planar macrocyclic Schiff base ligand including three Zn<sup>III</sup> ions. The resulting Er<sup>III</sup>Zn<sup>III</sup><sub>3</sub> complex (see picture; C gray, O red, N blue) behaves as a SMM with an energy barrier of 24.6(9) K for flipping of the molecular magnetic moment.

#### Single-Molecule Magnets

A. Yamashita, A. Watanabe, S. Akine, T. Nabeshima,\* M. Nakano, T. Yamamura, T. Kajiwara\* \_\_\_\_\_\_ 4016 – 4019

Wheel-Shaped Er<sup>III</sup>Zn<sup>II</sup><sub>3</sub> Single-Molecule Magnet: A Macrocyclic Approach to Designing Magnetic Anisotropy





Supporting information is available on www.angewandte.org (see article for access details).



A video clip is available as Supporting Information on www.angewandte.org (see article for access details).



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Issue 10: February 24 · Issue 11: March 2 · Issue 12: March 8 · Issue 13: March 15 · Issue 14: March 22

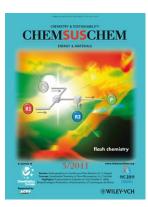
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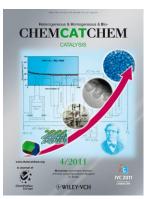
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