

IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS (15) 1925-2052 (2005)



Cover

See R. Graham Cooks *et al.*, page 1950.

Ambient monitoring using desorption electrospray ionization (DESI) showing 5 second RDX mass spectrum and canine acceptance of the new technology.

Image reproduced by permission of Zheng Ouyang, Liang Gao, Bogdan Gologan, Ryan Shreve and Judy Cooks from R. G. Cooks *et al.*, *Chem. Commun.*, 2005, 1950.



Inside cover

See Jonathan L Sessler and Janarthanan Jayawickramarajah, page 1939.

Designing self-assembled structures: a wide range of structures can be stabilized by using functionalized base-pairs (Notepad shown on the cover modified from iband.com).

Image reproduced by permission of Jonathan L. Sessler and Janarthanan Jayawickramarajah from *Chem. Commun.*, 2005, 1939.

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T13

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Chemical Technology

April 2005/Volume 2/Issue 4

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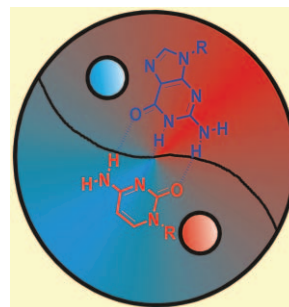
FEATURE ARTICLE

1939

Functionalized base-pairs: versatile scaffolds for self-assembly

Jonathan L. Sessler* and Janarthanan Jayawickramarajah

This article reviews the development of synthetic supramolecular ensembles derived from the association of individual nucleobases. Structures assembled through Watson–Crick, as well as other (such as Hoogsteen) base-pairing modes is discussed.



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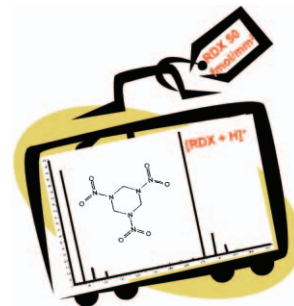
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1950

Direct, trace level detection of explosives on ambient surfaces by desorption electrospray ionization mass spectrometry

Zoltán Takáts, Ismael Cotte-Rodriguez, Nari Talaty, Huanwen Chen and R. Graham Cooks*

Mass spectrum of RDX recorded at a level of 50 fmol mm^{-2} from a non-conducting surface in a time of a few seconds without any sample preparation.

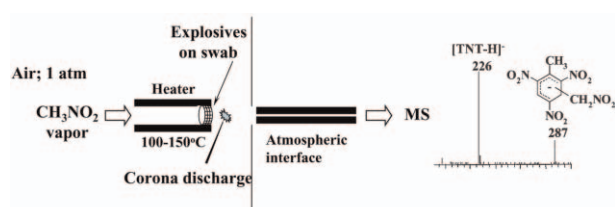


1953

Detection of explosives on solid surfaces by thermal desorption and ambient ion/molecule reactions

Igor A. Popov, Hao Chen, Oleg N. Kharybin, Eugene N. Nikolaev and R. Graham Cooks*

A simple, fast method is presented for detecting traces of solid explosives on cotton swabs or in particulate samples: ions are transferred into a mass spectrometer after thermal desorption and ambient ion/molecule reactions.

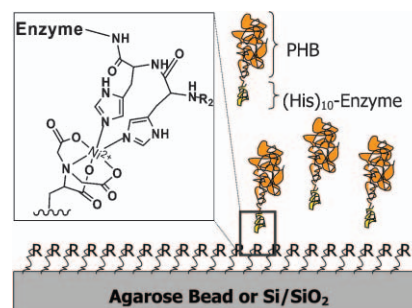


1956

End-functionalization of poly(3-hydroxybutyrate) via genetic engineering for solid surface modification

Hyun-jong Paik, Young-Rok Kim, Reid N. Orth, Christopher K. Ober, Geoffrey W. Coates and Carl A. Batt*

Using genetically engineered PHB synthase fused with a 10x-histidine units at its N-terminus, end-functionalized PHB was synthesized and used for the solid surface modification.

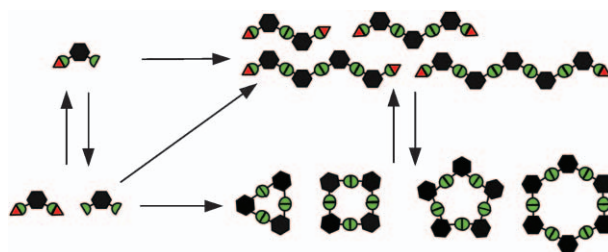


1959

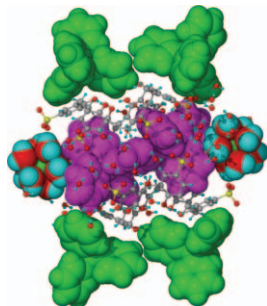
Expanding diversity in dynamic combinatorial libraries: simultaneous exchange of disulfide and thioester linkages

Julien Leclaire, Laurent Vial, Sijbren Otto* and Jeremy K. M. Sanders*

A double-level “communicating” library based on one-pot exchange of disulfide and thioester linkages generates a dynamic mixture of at least eight oligomers of various topologies and functionalities from a single building block. This allows for diversity, not only of the subunits that are linked, but also of the linkage itself.



1962

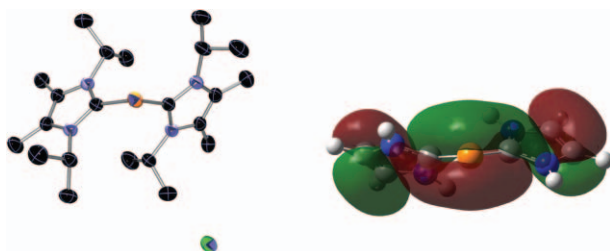


'Molecular capsules' based on *p*-sulfonatocalix[6]arene shrouding two tetraphenylphosphonium cations

Mohamed Makha, Colin L. Raston,*
Alexandre N. Sobolev and Allan H. White

Double cone conformation *p*-sulfonatocalix[6]arene forms 'molecular capsules' with two calixarenes encapsulating an embraced tetraphenylphosphonium cation–cation pair, in association with aquated lanthanide ions and a large array of water molecules.

1965

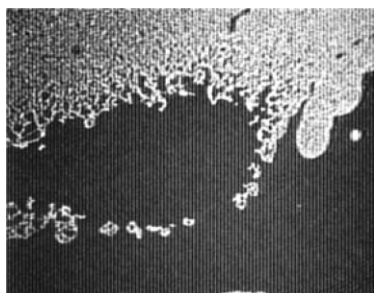


The synthesis, characterisation and electronic structure of *N*-heterocyclic carbene adducts of P^I cations

Bobby D. Ellis, C. Adam Dyker, Andreas Decken and
Charles L. B. Macdonald*

We report new and improved approaches for the synthesis of phosphamethine cyanine salts from *N*-heterocyclic carbenes. Crystallographic and computational investigations are used to elucidate the nature of the bonding in these stable P^I compounds.

1968

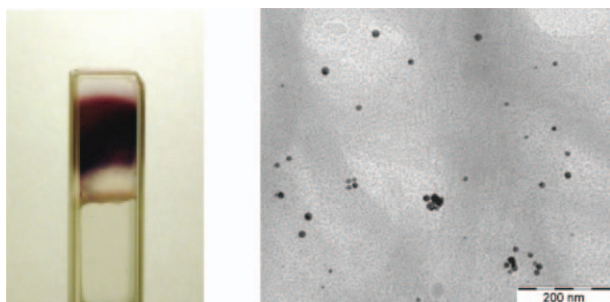


Amphiphilic behavior of an apparently non-polar calixarene

Patrick Shahgaldian, Anthony W. Coleman,*
Srinivasan S. Kuduva and Michael J. Zawrotko

The self-assembly properties of a non-polar calixarene have been investigated at the air–water interface, in water and in the solid state showing that this molecule behaves as an amphiphilic molecule.

1971



Synthesis of gold nanoparticles within a supramolecular gel-phase network

Christine S. Love, Victor Chechik,* David K. Smith,*
Karen Wilson, Ian Ashworth and Colin Brennan

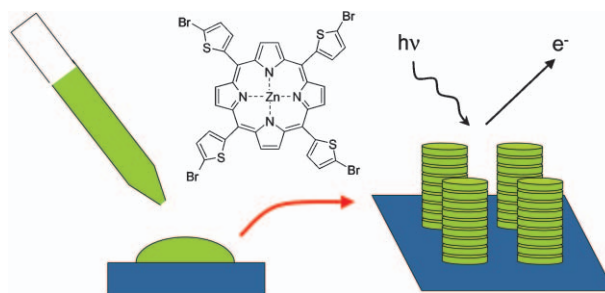
Gold nanoparticles with diameters of *ca.* 13 nm were synthesised by UV irradiation of a supramolecular organogel into which HAuCl₄ and tetraoctylammonium bromide had been diffused. The embedded nanoparticles are stabilised by the gel-phase network.

1974

Solution-processed, highly-oriented supramolecular architectures of functionalized porphyrins with extended electronic states

Rainer Friedlein,* Fredrik von Kieseritzky, Slawomir Braun, Christian Linde, Wojciech Osikowicz, Jonas Hellberg and William R. Salaneck

Thin films of aligned supramolecular architectures built from newly synthesized thiophene-substituted porphyrins have been processed from solution on surfaces.

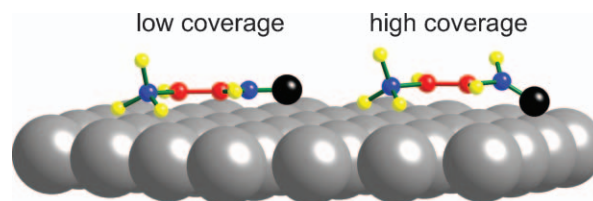


1977

Adsorbate conformation determines catalytic chemoselectivity: crotonaldehyde on the Pt(111) surface

Andrew J. Urquhart, Federico J. Williams, Owain P. H. Vaughan, Rachael L. Cropley and Richard M. Lambert*

Chemoselectivity in the heterogeneous catalytic hydrogenation of unsaturated aldehydes is determined by coverage-dependant adsorption geometry.

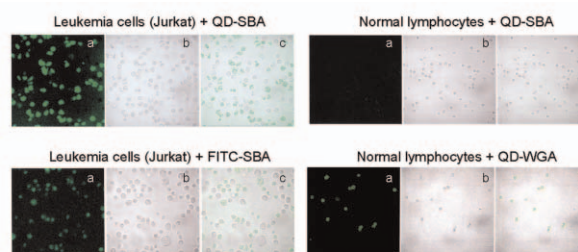


1980

Fabrication of quantum dot–lectin conjugates as novel fluorescent probes for microscopic and flow cytometric identification of leukemia cells from normal lymphocytes

Zhivko Zhelev, Hideki Ohba,* Rumiana Bakalova,* Rajan Jose, Satoshi Fukuoka, Toshimi Nagase, Mitsuru Ishikawa and Yoshinobu Baba

The present study describes a “home-lab” synthesis of QD–lectin conjugates appropriate for microscopic identification of leukaemia cells and visualization of cytoagglutination activity of lectins.

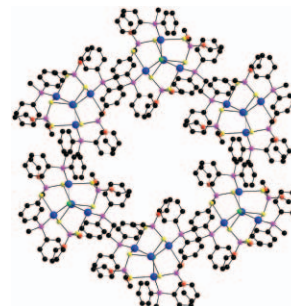


1983

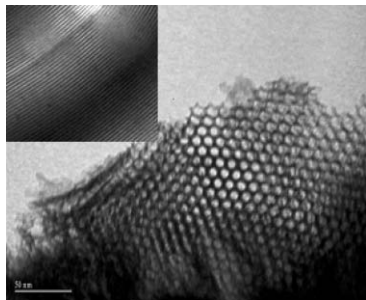
A 2D honeycomb-shaped network based on a starburst cluster: $[Ag_4(\mu_3-Cl)(PPh_2(CH_2)_2PPh_2)_{1.5}\{S_2P(OR)_2\}_3]$ (R = Et, Pr)

C. W. Liu,* Ben-Jie Liaw, Lin-Shou Liou and Ju-Chun Wang

The 42-atom macrocycle (see picture, Ag: blue, Cl: green, S: yellow, P: pink, O: red, C: black), which consists of 24 silver(I) atoms, is generated by six tetranuclear silver clusters, $[Ag_4(\mu_3-Cl)\{S_2P(OR)_2\}_3]$, linked together by six dppc ligands in an alternating up and down fashion.



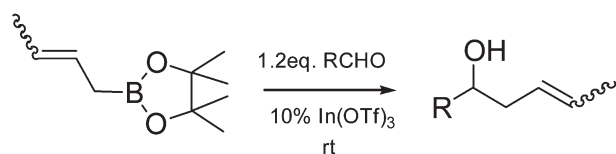
1986

**Sol-gel synthesis of ordered mesoporous alumina**

Krisztian Niesz, Peidong Yang and Gabor A. Somorjai*

Well-ordered mesoporous Al₂O₃ with high surface area and narrow pore size distribution was synthesized using a sol-gel based self assembly technique.

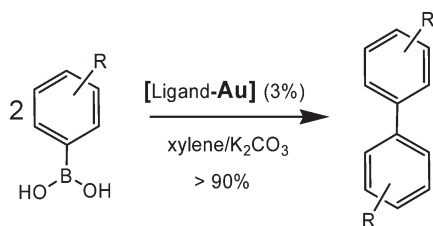
1988

**Synthesis of 4-substituted homoallylic alcohols via a one-pot tandem Lewis-acid catalyzed crotylboration-[3,3]-sigmatropic rearrangement**

P. Veeraghavan Ramachandran,* Debarshi Pratihari and Debanjan Biswas

Crotylboration of aldehydes with *E*- or *Z*-crotylboronates in the presence of catalytic amounts of indium triflate provides the corresponding 4-substituted homoallylic alcohols.

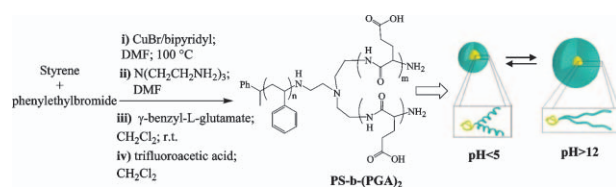
1990

**Homogeneous and heterogenized Au(III) Schiff base-complexes as selective and general catalysts for self-coupling of aryl boronic acids**

C. González-Arellano, A. Corma,* M. Iglesias and F. Sánchez

A series of homogeneous and heterogenized gold metal complexes presents high activity and selectivity for the homocoupling of a large variety of aryl boronic acids, showing general utility for the synthesis of C₂-symmetric biaryls.

1993

**Towards an easy access to amphiphilic rod-coil miktoarm star copolymers**

Jérôme Babin, Céline Leroy, Sébastien Lecommandoux,* Redouane Borsali, Yves Gnanou and Daniel Taton*

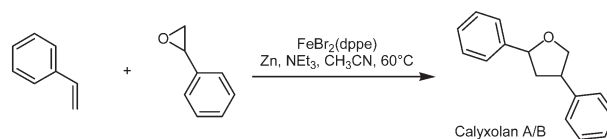
Water-soluble stimuli-responsive AB₂ miktoarm star copolymers were prepared by atom transfer radical polymerisation of styrene followed by chain-end modification, polymerisation of γ -benzyl-L-glutamate *N*-carboxyanhydride and a final step of hydrolysis.

1996

An iron-catalysed chemo- and regioselective tetrahydrofuran synthesis

Gerhard Hilt,* Patrick Bolze and Iris Kietlsch

An intermolecular ring expansion of styrene oxide with various alkenes is discussed and is used in the one step synthesis of racemic calyxolanes with good diastereoselectivity.

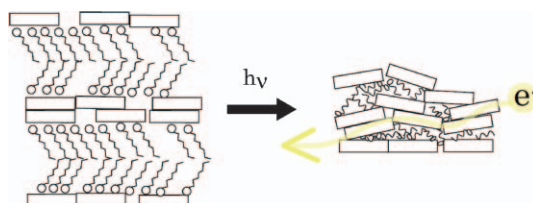


1999

Evidence for the role of organic layers in photoconductivity of organic/inorganic hybrid nanosheets as prepared by Langmuir–Blodgett methods

Kazuko Saruwatari,* Hisako Sato, Jun Kameda, Akihiko Yamagishi and Kazunari Domen

A hybrid film of layered niobate and octadecylammonium undergoes an insulator-to-photoconductor transition during photo-modification treatment by UV light.



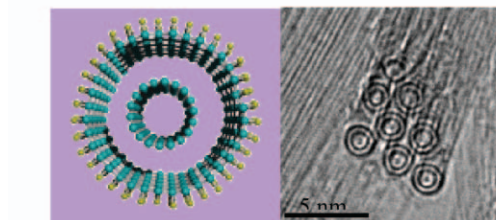
2002

Fluorination of double-walled carbon nanotubes

H. Muramatsu, Y. A. Kim,* T. Hayashi, M. Endo, A. Yonemoto, H. Arikai, F. Okino and H. Touhara*

Fluorination of double-walled carbon nanotubes (DWNTs) using elemental fluorine at 200°C was carried out for the first time. Fluorine atoms were selectively attached to the sidewall of the outer shell of DWNTs without disrupting the double-layered morphology.

Fluorinated double-walled carbon nanotubes

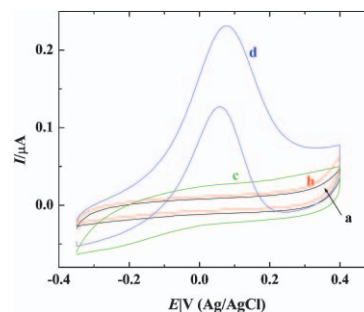


2005

Efficient electrocatalytic oxidation of NADH at gold nanoparticles self-assembled on three-dimensional sol-gel network

C. Retna Raj* and Bikash Kumar Jena

Nanosized gold (Au) particles self-assembled on a sol-gel derived silicate network efficiently catalyze the electrochemical oxidation of NADH in the absence of electron transfer mediator.



2008

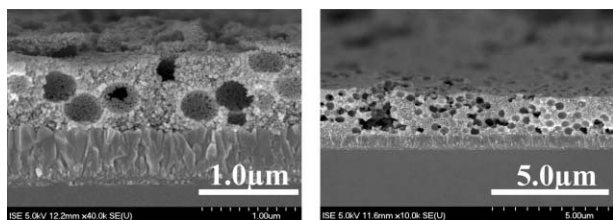


Intramolecular iodoarylation reaction of alkynes: easy access to derivatives of benzofused heterocycles

José Barluenga,* Mónica Trincado, María Marco-Arias, Alfredo Ballesteros, Eduardo Rubio and José M. González

A series of benzofused heterocycles was prepared by the intramolecular iodoarylation of ω -arylalkynes. The first study of the reaction to be carried out in water is presented.

2011

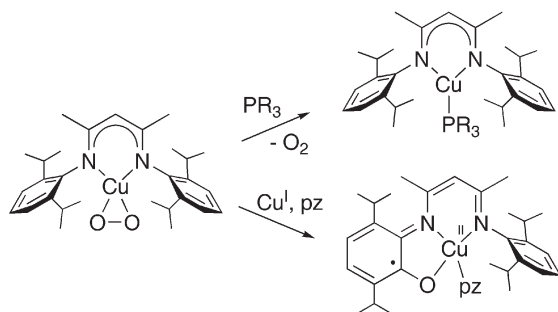


Scattering spherical voids in nanocrystalline TiO₂ – enhancement of efficiency in dye-sensitized solar cells

Sarmimala Hore,* Peter Nitz, Carmen Vetter, Christof Prahl, Michael Niggemann and Rainer Kern

Spherical voids in TiO₂ films in Dye Solar Cells enhance light trapping in the device and support diffusion of ions in the electrolyte. Overall efficiency (η) of 6.7% has been reached on areas of 2.5 cm².

2014

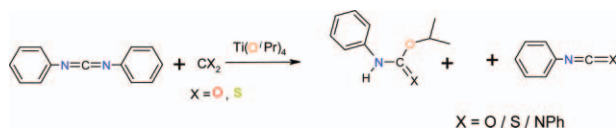


Reactivity of a 1:1 copper–oxygen complex: isolation of a Cu(II)-*o*-iminosemiquinonato species

Anne M. Reynolds, Elizabeth A. Lewis, Nermeen W. Aboeella and William B. Tolman*

Reactivity studies of a 1:1 Cu/O₂ adduct reveal displacement of O₂ by phosphines and a novel internal ligand oxidation/rearrangement upon addition of a Cu(I) salt.

2017



Catalytic metathesis of carbon dioxide with heterocumulenes mediated by titanium isopropoxide

Rajshekhkar Ghosh and Ashoka G. Samuelson*

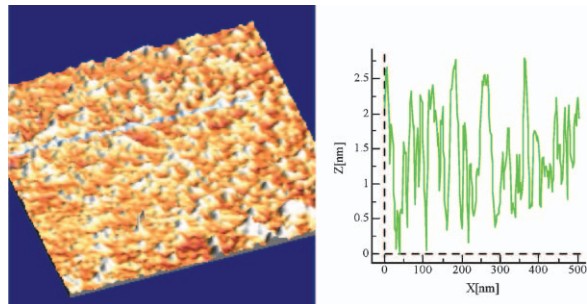
Multiple insertion of heterocumulenes into the Ti–O bond in titanium isopropoxide in a head to head fashion, followed by an extrusion reaction at elevated temperatures results in metathesis.

2020

A new approach to grafting a monolayer of oriented Mn₁₂ nanomagnets on silicon

Benoit Fleury, Laure Catala,* Vincent Huc, Christophe David, Wang Zhao Zhong, Pascale Jegou, Laurent Baraton, Serge Palacin, Pierre-Antoine Albouy and Talal Mallah*

The functionalisation of a Si(100) silicon wafer allows for the oriented grafting of a monolayer of Mn₁₂ nanomagnets using a two-step procedure.

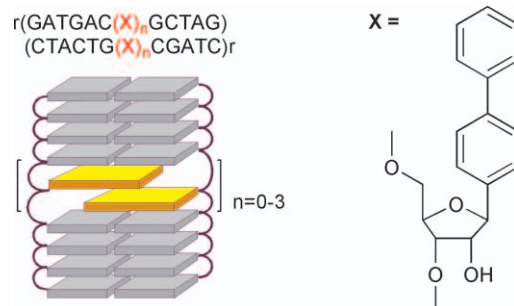


2023

RNA duplexes with biphenyl substituents as base replacements are less stable than DNA duplexes

Christine Brotschi and Christian J. Leumann*

The nature of the backbone (DNA vs. RNA) can dramatically influence the stability of hydrophobic, non-hydrogen bonding base-pairs that recruit their interaction energy mostly from interstrand stacking interactions.

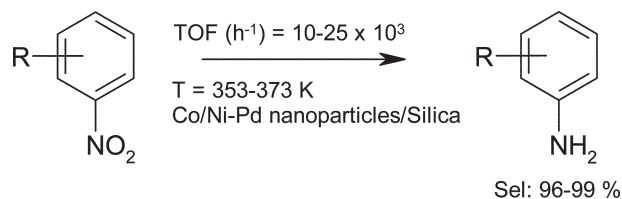


2026

Highly efficient catalysts for the hydrogenation of nitro-substituted aromatics

Robert Raja,* Vladimir B. Golovko, John M. Thomas, Angel Berenguer-Murcia, Wuzong Zhou, Songhai Xie and Brian F. G. Johnson

Nanoparticles of Co and NiPd, supported on non-ordered mesoporous silica, are highly efficient heterogeneous catalysts for the hydrogenation of nitro-substituted aromatics under mild conditions.

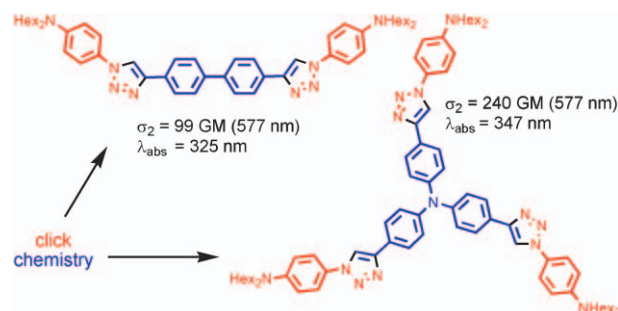


2029

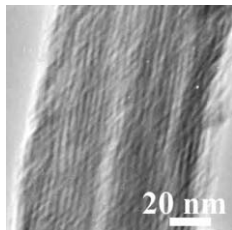
New chromophores from click chemistry for two-photon absorption and tuneable photoluminescence

Manuel Parent, Olivier Mongin, Kenji Kamada, Claudine Katan and Mireille Blanchard-Desce*

Multipolar derivatives that combine full transparency and strong TPA in the visible region, as well as excited-state lifetimes that can be lengthened by playing on the solvent, have been designed for optical limiting in the visible region.



2032

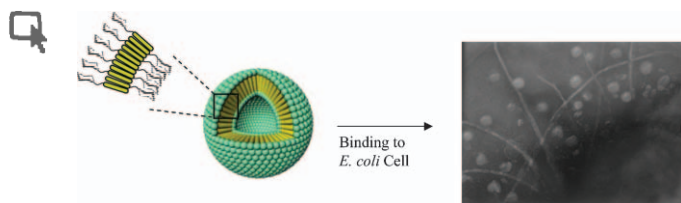


Nanofiberization of inner helical mesoporous silica using chiral gelator as template under a shear flow

Yonggang Yang, Masahiro Suzuki, Hirofusa Shirai, Akio Kurose and Kenji Hanabusa*

Aligned nanofibers consisting of inner-helical mesoporous silica were synthesized using the self-assembly of chiral gelator as template under basic conditions and a shear flow.

2035

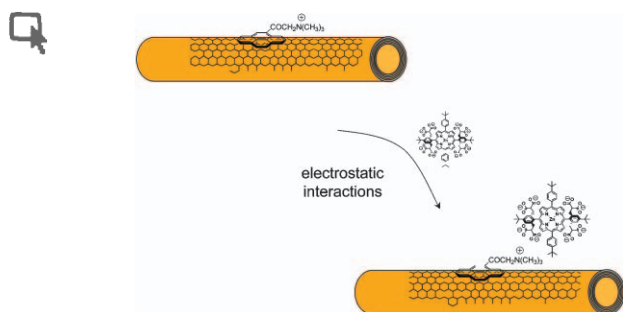


Carbohydrate-coated nanocapsules from amphiphilic rod-coil molecule: binding to bacterial type 1 pili

Byung-Sun Kim, Won-Young Yang, Ja-Hyoung Ryu, Yong-Sik Yoo and Myongsoo Lee*

Stable carbohydrate-coated nanocapsules designed as multivalent nanoscaffolds for selective interactions with receptors are able to encapsulate guest molecules within their interior and to bind efficiently to FimH adhesin of bacterial type 1 pili.

2038

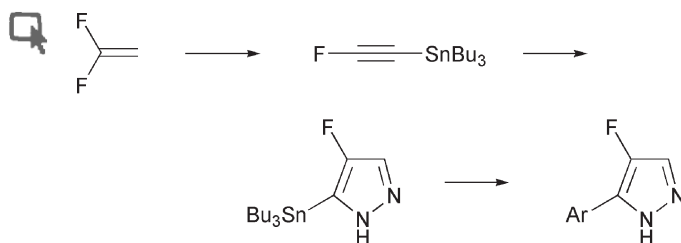


Multiwalled carbon nanotubes in donor-acceptor nanohybrids—towards long-lived electron transfer products

Dirk M. Guldi,* G. M. A. Rahman, Norbert Jux,* Domenico Balbinot, Nikos Tagmatarchis and Maurizio Prato*

Novel multiwalled carbon nanotube/metalloporphyrin nanohybrids are devised and probed as versatile donor-acceptor hybrids.

2041



Palladium catalyzed cross-coupling reaction of 5-tributylstannyl-4-fluoropyrazole

Takeshi Hanamoto,* Yukinori Koga, Eisaku Kido, Toshio Kawanami, Hiroshi Furuno and Junji Inanaga

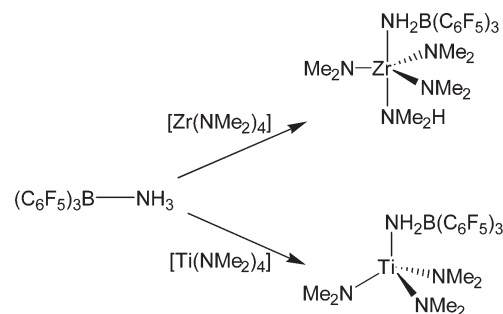
The palladium catalyzed cross-coupling reactions of aryl iodides and 5-tributylstannyl-4-fluoropyrazole prepared from fluoro(tributylstannyl)acetylene proceeded smoothly giving the corresponding 5-aryl-4-fluoropyrazole in good yields.

2044

New titanium and zirconium complexes with M–NH₂ bonds formed by facile deprotonation of H₃N·B(C₆F₅)₃

Andrew J. Mountford, William Clegg,
Ross W. Harrington, Simon M. Humphrey and
Simon J. Lancaster*

The first reported reactions of H₃N·B(C₆F₅)₃, with [M(NMe₂)₄] (M = Zr or Ti), proceed through facile deprotonation and yield the novel M–NH₂–B(C₆F₅)₃ containing complexes [Zr(NMe₂)₃{NH₂B(C₆F₅)₃}(HNMe₂)] and [Ti(NMe₂)₃{NH₂B(C₆F₅)₃}].

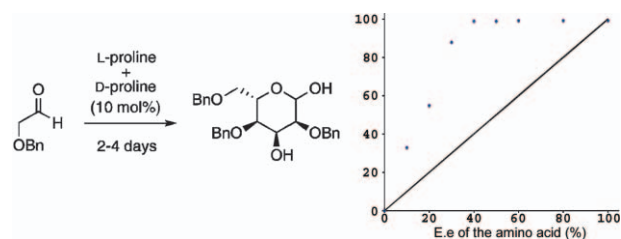


2047

Plausible origins of homochirality in the amino acid catalyzed neogenesis of carbohydrates

Armando Córdova,* Magnus Engqvist, Ismail Ibrahim,
Jesús Casas and Henrik Sundén

The intrinsic ability of amino acids to catalyze the asymmetric formation of hexose carbohydrates, which enzymes have mediated for millions of years, with significant amplification of enantiomeric excess is presented.



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 Albouy, Pierre-Antoine, 2020
 Arikai, H., 2002
 Ashworth, Ian, 1971
 Baba, Yoshinobu, 1980
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 Bakalova, Rumiana, 1980
 Balbinot, Domenico, 2038
 Ballesteros, Alfredo, 2008
 Baraton, Laurent, 2020
 Barluenga, José, 2008
 Batt, Carl A., 1956
 Berenguer-Murcia, Angel, 2026
 Biswas, Debanjan, 1988
 Blanchard-Desce, Mireille, 2029
 Bolze, Patrick, 1996
 Borsali, Redouane, 1993
 Braun, Slawomir, 1974
 Brennan, Colin, 1971
 Brotschi, Christine, 2023
 Casas, Jesús, 2047
 Catala, Laure, 2020
 Chechik, Victor, 1971
 Chen, Hao, 1953
 Chen, Huanwen, 1950
 Clegg, William, 2044
 Coates, Geoffrey W., 1956
 Coleman, Anthony W., 1968
 Cooks, R. Graham, 1950, 1953
 Córdova, Armando, 2047
 Corma, A., 1990
 Cotte-Rodriguez, Ismael, 1950
 Cropely, Rachael L., 1977
 David, Christophe, 2020
 Decken, Andreas, 1965
 Domen, Kazunari, 1999
 Dyker, C. Adam, 1965
 Ellis, Bobby D., 1965
 Endo, M., 2002
 Engqvist, Magnus, 2047
 Fleury, Benoit, 2020
 Friedlein, Rainer, 1974
 Fukuoka, Satoshi, 1980
 Furuno, Hiroshi, 2041
 Ghosh, Rajshekhar, 2017
 Gnanou, Yves, 1993
 Golovko, Vladimir B., 2026
 González, José M., 2008
 González-Arellano, C., 1990
 Guldi, Dirk M., 2038
 Hanabusa, Kenji, 2032
 Hanamoto, Takeshi, 2041
 Harrington, Ross W., 2044
 Hayashi, T., 2002
 Hellberg, Jonas, 1974
 Hilt, Gerhard, 1996
 Hore, Sarmimala, 2011
 Huc, Vincent, 2020
 Humphrey, Simon M., 2044
 Ibrahim, Ismail, 2047
 Iglesias, M., 1990
 Inanaga, Junji, 2041
 Ishikawa, Mitsuru, 1980
 Jayawickramarajah, Janarthanan, 1939
 Jegou, Pascale, 2020
 Jena, Bikash Kumar, 2005
 Johnson, Brian F. G., 2026
 Jose, Rajan, 1980
 Jux, Norbert, 2038
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 Kameda, Jun, 1999
 Katan, Claudine, 2029
 Kawanami, Toshio, 2041
 Kern, Rainer, 2011
 Kharybin, Oleg N., 1953
 Kido, Eisaku, 2041
 Kieltisch, Iris, 1996
 Kim, Byung-Sun, 2035
 Kim, Y. A., 2002
 Kim, Young-Rok, 1956
 Koga, Yukinori, 2041
 Kuduva, Srinivasan S., 1968
 Kurose, Akio, 2032
 Lambert, Richard M., 1977
 Lancaster, Simon J., 2044
 Leclaire, Julien, 1959
 Lecommandoux, Sébastien, 1993
 Lee, Myongsoo, 2035
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 Leumann, Christian J., 2023
 Lewis, Elizabeth A., 2014
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 Linde, Christian, 1974
 Liou, Lin-Shou, 1983
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 Love, Christine S., 1971
 Macdonald, Charles L. B., 1965
 Makha, Mohamed, 1962
 Mallah, Talal, 2020
 Marco-Arias, María, 2008
 Mongin, Olivier, 2029
 Mountford, Andrew J., 2044
 Muramatsu, H., 2002
 Nagase, Toshimi, 1980
 Niesz, Krisztian, 1986
 Niggemann, Michael, 2011
 Nikolaev, Eugene N., 1953
 Nitz, Peter, 2011
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 Okino, F., 2002
 Orth, Reid N., 1956
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 Paik, Hyun-jong, 1956
 Palacin, Serge, 2020
 Parent, Manuel, 2029
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 Pratihari, Debarshi, 1988
 Prato, Maurizio, 2038
 Rahman, G. M. A., 2038
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 Raja, Robert, 2026
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 Reynolds, Anne M., 2014
 Rubio, Eduardo, 2008
 Ryu, Ja-Hyoung, 2035
 Salaneck, William R., 1974
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 Sánchez, F., 1990
 Sanders, Jeremy K. M., 1959
 Saruwatari, Kazuko, 1999
 Sato, Hisako, 1999
 Sessler, Jonathan L., 1939
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 Shirai, Hirofusa, 2032
 Smith, David K., 1971
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 Somorjai, Gabor A., 1986
 Soudén, Henrik, 2047
 Suzuki, Masahiro, 2032
 Tagmatarchis, Nikos, 2038
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 Talaty, Nari, 1950
 Taton, Daniel, 1993
 Thomas, John M., 2026
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 Toudara, H., 2002
 Trincado, Mónica, 2008
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 Vaughan, Owain P. H., 1977
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 Vial, Laurent, 1959
 von Kieseritzky, Fredrik, 1974
 Wang, Ju-Chun, 1983
 White, Allan H., 1962
 Williams, Federico J., 1977
 Wilson, Karen, 1971
 Xie, Songhai, 2026
 Yamagishi, Akihiko, 1999
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 Yang, Won-Young, 2035
 Yang, Yonggang, 2032
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 Yoo, Yong-Sik, 2035
 Zaworotko, Michael J., 1968
 Zhao Zhong, Wang, 2020
 Zhelev, Zhivko, 1980
 Zhou, Wuzong, 2026

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