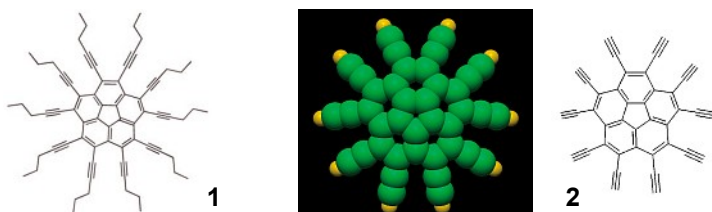


Science Concentrates

Synthesis, Structure, and Isomerization of Decapentynylcorannulene: Eneidyne Cyclization/ Interconversion of $C_{40}R_{10}$ Isomers

T. Hayama, Y.-T. Wu, A. Linden, K. K. Baldrige,* and J. S. Siegel*, *J. Am. Chem. Soc.* **2007**, *129*, 12612
University of Zurich

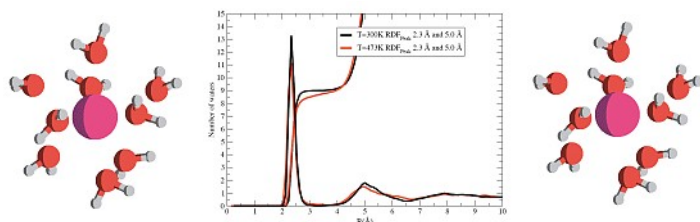
Per-alkynyl-polynuclear aromatic hydrocarbons, such as **2**, are high-energy carbon-rich compounds. A concise synthesis of decapentynylcorannulene **1**, an alkyl derivative of **2**, proceeds efficiently *via* aryl-alkyne coupling chemistry starting from decachlorocorannulene and trimethylstannyl pentyne. During the synthesis of **1**, an eneidyne cyclization occurs and forms a diradical intermediate, which ring-opens to a novel biscumulenyl [10]annulene. An alternative fate for the diradical could in principle result in the formation of a monodispersed single-walled carbon-based nanotube. Computational predictions for the structure of **2**, which resembles the crystal structure of **1**, predict that the nanotube structure lies over 1 mega Joule lower in energy. Chemistry toward nanotube synthesis is on-going.



A Quantum Chemical and Molecular Dynamics Study of the Coordination of Cm(III) in Water

D. Hagberg, E. Bednarz, N.M. Edelstein, and L. Gagliardi*, *J. Am. Chem. Soc.* **2007**, *129*, 14136
University of Geneva

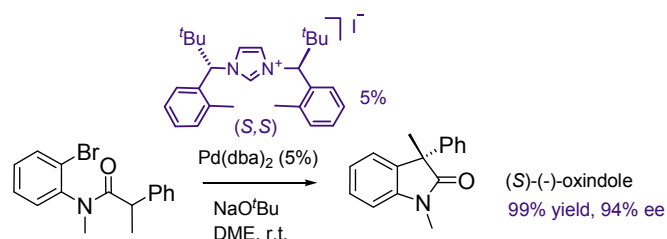
Molecular dynamics simulation of Cm(III) in water were performed at two temperatures ($T = 300$ K and $T = 473$ K) and fully *ab initio* intermolecular potentials were employed. The study reveals that at lower temperature nine molecules of water coordinate the Cm(III) ion in the first coordination sphere, while at higher temperature the preferred coordination number is eight. For the second coordination sphere the number of the molecules of water is probably 16, but that is not uniquely defined.



Bulky Chiral Carbene and Their Application in the Palladium-Catalyzed Asymmetric Intramolecular α -Arylation of Amides

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University of Geneva

The enantioselective Pd-catalyzed intramolecular α -arylation of amides is an interesting entry route to the formation of oxindole alkaloids that constitutes a large family of natural products with significant biological activities. In this article the authors describe the preparation of new C_2 -symmetric bulky N-heterocyclic carbenes and their use as enantiopure ligands for the title reaction which affords oxindoles with excellent yields (up to 99%) and excellent enantioselectivity (up to 95%, dba = *trans,trans*-dibenzylideneacetone).



1,3-Dipolar Cycloaddition: Click Chemistry for the Synthesis of 5-Substituted Tetrazoles from Organoaluminum Azides and Nitriles

V. Aureggi and G. Sedelmeier,* *Angew. Chem., Int. Ed.* **2007**, *46*, 8440
Novartis Pharma AG

Tetrazoles are a class of heterocycles with a wide range of applications but conventional methods to prepare these moieties employ dangerous, toxic reagents. In this article, the authors describe a new route to these heterocycles that uses inexpensive and nontoxic dialkyl aluminum azides. The cycloaddition occurs under mild conditions and tolerates a variety of functional groups. This new methodology is significant with respect to safety, economy, ecology, and diversity of substrates.

