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A CHIMIA Column

A data-driven perspective on the colours of metal-organic frameworks

Kevin M. Jablonka, Seyed M. Moosavi, Mehrdad Asgari, Christopher Ireland, Luc Patiny, and Berend Smit*, Chem. Sci. **2021**, 12, 3587, https://doi.org/10.1039/D0SC05337F Ecole Polytechnique Fédérale de Lausanne (EPFL)

Predicting the colour of a material from first principles is still far beyond the reach of modern quantum chemical methods. Yet, colour is at the heart of chemistry. However, colour is also a key rubric of optoelectronic properties and materials and it is frequently used as a metric to assess the successes of syntheses. In order to achieve greater objectivity and to address the inadequacies of current reporting of the colour of a material, a standardized colour scale was promulgated to predict the colour of compounds. All data was recorded in an objective and standardized form in an electronic lab-book. This process is proposed to be the key to further improve data-driven approaches to chemical research.

Authors' comments:

"When we tried to build a machine learning model to predict the colours of MOFs, we found that our learning was basically limited by the perceptive spread of the chemists. To remedy this, we propose to use a standardized reporting technique and provide the infrastructure to export all data (i.e. all spectra etc.) in FAIR to a repository."

In vitro production of ergothioneine isotopologues

Maria A. Beliaeva, Reto Burn, David Lim, and Florian P. Seebeck*, Angew. Chem. Int. Ed. 2021, 60, 5209-5212, https://doi.org/10.1002/anie.202011096 University of Basel

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The exact role of ergothioneine for a plethora of biological functions (from survival of pathogenic bacteria in the host to mammalian cell homeostasis) is still elusive due to its complex biological interactions. To aid in the study of this molecule, the authors have designed a one-pot enzyme-based synthesis of ergothioneine isotopologues from simple and commercially available isotope materials (histidine or Nα-dimethylhistidine, methyl iodide and elemental sulphur). Inspired by the biosynthesis in strictly anaerobic bacteria, a two-step enzymatic synthesis was designed coupling a histidine-specific S-adenosyl methionine (SAM)methyltransferase and a O₂-independent sulphur transferase. In addition, a halide methyltransferase was added to recycle the SAM and β -mercaptoethanol used to mobilize the sulphur. The fully assembled cascade provides an accessible and efficient synthesis of ergothioneine isotopologues.

Authors' comments:

"We were thrilled to apply methylation biocatalysis developed in our lab as a tool in our research on the biology of ergothioneine."

SUBJECTIVE CHAOS



Insights



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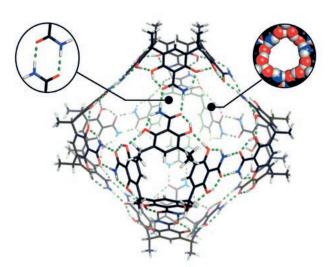
Concentration-dependent self-assembly of an unusually large hexameric hydrogen-bonded molecular Cage

Severin Merget, Lorenzo Catti, Shani Zev, Dan T. Major, Nils Trapp, and Konrad Tiefenbacher*, *Chem. Eur. J.* **2021**, *27*, 4447–4453, https://doi.org/10.1002/chem.202005046 University of Basel

Over the last decades, the self-assembly of molecular capsules and cages using non-covalent interactions (e.g. hydrogen bonds, halogen bonds or hydrophobic interactions) has been intensively studied. In the case of the hydrogen-bond-based systems, the size of the assemblies formed has remained rather modest (largest volumes 1400–2300 Å³). In this work, the authors report a rational design and synthesis of a new hexameric cage with a cavity volume of $\sim 2800 \,\text{Å}^3$. This assembly is larger than any previously known capsule/cage structure relying exclusively on hydrogen bonds. Remarkably, it is held together by only 24 intermolecular hydrogen bonds all based on simple amide-amide dimerization with a porous structure, whereas most other assemblies of this class feature a much more complex hydrogen-bonding network. This work is expected to aid rational development of future systems and provides important lessons for the design of new, more sophisticated assemblies in order to overcome the current limitations.

Authors' comments:

"Although we were able to predict the structure of the hexameric assembly, its host–guest behaviour remains puzzling: in contrast to other hexameric assemblies, it only binds fullerenes. Work to elucidate the reasons for this is ongoing."



- Large Hydrogen-bonded Cage (V ≈ 2800 ų)
- Concentration-dependent Self-assembly
- Encapsulation of Fullerenes

Shear stress-responsive polymersome nanoreactors inspired by the marine bioluminescence of dinoflagellates

Omar Rifaie-Graham, Nikolas F. B. Galensowske, Charlie Dean, Jonas Pollard, Sandor Balog, Micael G. Gouveia, Mohamed Chami, Antoine Vian, Esther Amstad, Marco Lattuada, and Nico Bruns*, *Angew. Chem. Int. Ed.* **2021**, *60*, 904–909, https://doi.org/10.1002/anie.202010099 University of Fribourg

The light emission in response to flowing water is a phenomenon that happens in marine plankton and has been harnessed in this work to activate biocatalytic reactions. Polymersomes were formed from amphiphilic copolymers that carry complementary nucleobases in their membrane. Under turbulent mixing or flow conditions, the nucleobase pairs in the hydrophobic leaflet separate exposing their hydrogen bonding motifs and making the membrane more hydrophilic. Thus, the permeability to water-soluble compounds is highly improved. By encapsulating enzymes, nanoreactors could be generated for a variety of biocatalytic reactions, such as enzymatic polymerisations or chemo luminescence, to be controlled by external stimuli. These results open new opportunities for innovative applications such as 3D printing or force-responsive drug delivery systems.

Authors' comments:

"The work shows a transient activation of polymersome nanoreactors by mechanical forces and is a first example of forceresponsive polymersomes. The ability to switch on enzymatic reactions by shear forces allows to create biocatalytic systems that mimic phenomena and reaction cascades observed in nature."

