

Inspired by these results, Philippe Poizot, at the University of Picardie Jules Vernes in France, and co-workers have investigated the tetralithiated oxocarbon salt $\text{Li}_4\text{C}_6\text{O}_6$. The researchers prepared the salt directly from tetrahydroxybenzoquinone, which can itself be made in aqueous solution from sugar found in plants. Alternatively, the salt could also be obtained by annealing the dilithium salt ($\text{Li}_2\text{C}_6\text{O}_6$) under an inert atmosphere. This solid-state disproportionation reaction, which occurred with sodium and potassium as well as with lithium, is unusual with organic compounds.

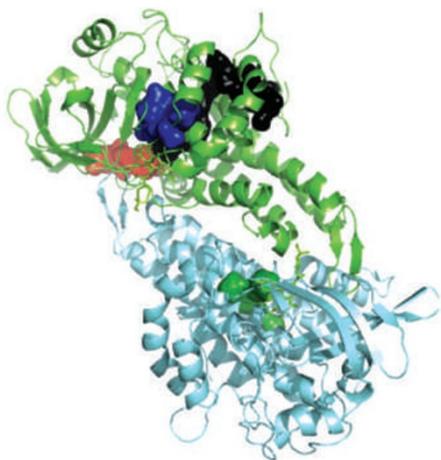
When it was tested as a material for the positive electrode in a lithium-ion battery, the $\text{Li}_4\text{C}_6\text{O}_6$ salt showed good electrochemical performance and reversibility. Furthermore, because it can be both reduced to $\text{Li}_2\text{C}_6\text{O}_6$ and oxidized to $\text{Li}_6\text{C}_6\text{O}_6$, it could also be used to construct a symmetrical lithium-ion cell. Although the operating voltage of this device is too low to be practical, chemical substitution offers various possibilities to tune the oxidation and reduction potentials.

ENZYMOLGY

Directing diffusion

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Flavoenzymes take part in many cellular processes and have a central role in aerobic metabolism. As their name suggests they contain a flavin cofactor, and its reaction with oxygen is a key step in many of these processes. Exactly how oxygen molecules arrive at the enzyme active site is currently under debate: is it simply passive diffusion or is it guided by the protein? If it is guided, then can the molecule take just one pathway or several?

Now Riccardo Baron, from the University of California at San Diego,

and colleagues have studied the diffusion pathways of oxygen in examples of two types of flavoenzymes: a monooxygenase and an oxidase. Using molecular dynamics they simulated 500 oxygen trajectories for each enzyme and found multiple pathways for both. In each enzyme the pathways led to the same defined active-site entry points, showing that oxygen diffusion is indeed guided by the protein using funnelling architectures.

The active-site entry points in each enzyme are made up of specific sets of residues that direct oxygen to the flavin cofactor. The importance of the environment local to the flavin was confirmed through understanding differences in reaction rates when key residues in each enzyme were replaced to create mutants.

BERYLLIUM DIMER

Elusive bond elucidated

Science 324, 1548–1551 (2009)

Theoretical calculations can predict the structure and properties of increasingly large molecules — yet understanding the electronic ground state of the beryllium dimer, with its eight electrons, has remained challenging. Numerous models have suggested different bond lengths and dissociation energies, but the few samples obtained experimentally could not provide sufficient information to elucidate the dimer's structure. Now, Michael Heaven, at Emory University in Atlanta, and co-workers have measured all the bound vibrational energies of the electronic ground state by stimulated emission spectroscopy.

The researchers used a pulsed laser to populate a single rotational–vibrational level of a particular electronically excited state ($A^1\Pi_u$), from which transitions to the vibrationally excited levels of the ground state are favoured. The relaxation of the system is then induced by a second laser, and the resulting fluorescence is recorded.

Subsequent analysis enabled the determination of the dissociation energy and the unusually shaped potential energy curve of the dimer for Be–Be distances shorter than 8.5 Å. Theoretical analyses agreed well with experiment and showed a fine balance between the chemical and physical interactions of the beryllium atoms. The study revealed a weak Be–Be bond but with a length close to that of a conventional covalent bond.

The definitive versions of these Research Highlights first appeared on the *Nature Chemistry* website, along with other articles that will not appear in print. If citing these articles, please refer to the web version.

blogroll

Not to be sniffed at

Advice on dealing with malodorous molecules, how programming is like hot dogs, and a twittering lord.

Derek Lowe's series of posts on 'Things I won't work with' normally feature extremely hazardous compounds "that explode with bizarre violence even in laughably small amounts". The latest post on In the Pipeline (<http://bit.ly/Mb3rC>), however, warns readers away from thioacetone. Not because it's dangerous, but because "it merely stinks. But it does so relentlessly and unbearably." Lowe goes on to relate some of the historical responses to this odiferous chemical, including from its earliest appearance in Freiburg. *Chemische Berichte* reported in 1889 "an offensive smell which spread rapidly over a great area of the town causing fainting, vomiting and a panic evacuation". *Chemistry and Industry* from 1967 carries the smelly mantle, where Esso researchers reported that a single drop was detectable up to a quarter of a mile away "in seconds". Fortunately, they offered some advice for dealing with it, but as that involved nitrous fumes and destroying all residues by fire, Lowe doesn't recommend it.

Prof-like Substance (<http://bit.ly/umtx6>) came to a sad realization recently: "I need to learn some programming." He goes on to explain "I was hoping that I could leave that to students or technicians, but I know that I won't feel comfortable with the meal I am served unless I understand what goes into the recipe. It's why I don't eat hotdogs." There were several comments on the post, with the majority recommending the Python programming language as a good starting point.

The world of 'Web 2.0' and social networking has even reached the dusty corridors of power in the UK's Houses of Parliament. The science minister Lord Drayson (@lorddrayson) is a user of the micro-blogging site Twitter and hosted an "impromptu question and answer session" on the recent reorganization that saw science under the control of the Department for Business, Innovation and Skill. Drayson offered the reassurance that science funding was "safe and sound" and that he will "continue to advocate for science".