

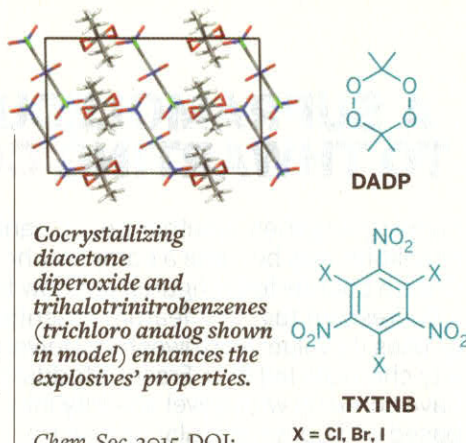
sees similar covalency in a compound with 2,6-pyridinedicarboxylate ligands— $\text{Cf}(\text{HDPa})_3 \cdot \text{H}_2\text{O}$. Several of its properties suggest that the metal-ligand bonds have covalent character, with the ligands donating electron density to the 5f, 6d, 7s, and 7p orbitals of Cf. In particular, the team pins the complex's green photoluminescence on a typically covalent ligand-to-metal charge-transfer transition. The source of the covalency is likely the relative stability of the Cf(II) oxidation state plus effects from the smaller size of Cf(III)—both characteristics that should also lead to covalent bonding in later actinides, the researchers say.—JK

STYRENE PRODUCED IN ONE STEP

A new catalyst makes possible a long-standing research goal—synthesizing styrene from benzene and ethylene in a single step. Styrene, used for fine chemicals synthesis and plastics and elastomer preparation, is currently produced globally in the 20 million-ton-per-year range, so a more efficient method could result in significant cost savings. It's generally made by using AlCl_3 (with HF) or zeolites to convert benzene and ethylene to ethylbenzene, followed by dehydrogenation to styrene. Now, T. Brent Gunnoe of the University of Virginia, Thomas R. Cundari of the University of North Texas, and coworkers have identified a rhodium catalyst that does the trick in one step (*Science* 2015, DOI: 10.1126/science.aaa2260). Their approach converts benzene, ethylene, and a Cu(II) reagent to styrene plus a Cu(I) compound, with 100% styrene selectivity. Although a rhodium catalyst might be too expensive for practical industrial use, Gunnoe believes it's a major step toward a more efficient industrial process and notes that its selectivity is unprecedented. "If they can ultimately recycle the copper oxidant with oxygen, the commercial potential looks high," comments Karen Goldberg of the University of Washington.—SB

COCRYSTALLIZATION IMPROVES EXPLOSIVES

Cocrystallizing pairs of explosive organic compounds is a viable route to improving the compounds' chemical stability, shock sensitivity, and other properties that determine an explosive's usefulness in applications, according to a study (*J. Am.*



Cocrystallizing diacetone diperoxide and trichlorotrinitrobenzenes (trichloro analog shown in model) enhances the explosives' properties.

Chem. Soc. 2015, DOI: 10.1021/jacs.5b00661).

Acetone peroxides are easy to prepare and inexpensive, but they tend to be unstable—exploding unpredictably—and low in density, a property associated with low explosive power. Those factors limit their usefulness as commercial explosives. The University of Michigan's Adam J. Matzger and coworkers may have a way to bypass those limitations. The team formed cocrystals in one-to-one ratios between diacetone diperoxide (DADP) and three trichlorotrinitrobenzenes—the trichloro (TCTNB), tribromo (TBTNB), and triiodo (TITNB) analogs. They found that cocrystallization increased DADP's density and stability. They also found that, compared with DADP, the cocrystal DADP-TCTNB was just as sensitive to impact yet less volatile and higher in density. In contrast, DADP-TITNB exhibited much lower impact sensitivity than either DADP or TITNB, showing for the first time that an energetic cocrystal can be less sensitive to impact than its pure components.—MJ

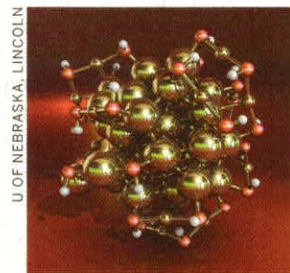
PHOTOSYNTHETIC O₂'S ISOTOPIC SIGNATURE

Photosynthesis imparts a unique isotopic signature to the O₂ it produces via "isotopic clumping," a phenomenon in which molecules accumulate two or more heavy isotopes. Molecules with clumped isotopes are uncommon, but modern mass spectrometers can reliably measure their abundances. Isotope clumping as a field is only 10 years old and has been used to deduce the formation temperatures of minerals. When a system is at chemical equilibrium, isotopic clumps are found more often than random chance would predict. But on the basis of a study of isotopically clumped O₂ (¹⁸O¹⁸O and ¹⁸O¹⁷O) in hyacinth plants, Laurence Yeung, Jeanine Ash, and Edward D. Young of UCLA show that photosynthesis actually produces isotopically clumped O₂ less often

than chance would predict (*Science* 2015, DOI: 10.1126/science.aaa6284). In another investigation, a team lead by David T. Wang and Shuhei Ono of MIT studied isotopically clumped methane, ¹³CH₃D. They showed that its relative abundances can be used to identify methane sources produced by cattle (*Science* 2015, DOI: 10.1126/science.aaa4326). "Clumped isotope anomalies will help place much-needed constraints on biogeochemical sources, sinks, and budgets of O₂ and CH₄," writes Johns Hopkins University's Benjamin H. Passey, in an accompanying commentary.—EKW

PINPOINTING ATOMS IN GOLD NANOCCLUSERS

More than a decade after gold, a model inert metal, showed itself to be catalytically active when prepared as nanosized particles, researchers continue to puzzle over the basis of the metal's surprising activity. Knowing the positions of every atom in a nanocluster, including the organic ligands that typically cap these structures, would enable researchers to understand the relation between the particles' structures and functions. But that level of detail, which could speed development of gold-based catalysts, biomedical sensors, and other applications, has remained elusive. X-ray methods typically require large crystals, and microscopy generally cannot resolve ligand atoms because of their low masses. So Xiao Cheng Zeng of the University of Nebraska, Lincoln, and coworkers combined results of an atomic resolution microscopy analysis of Au₆₈(SH)₃₂ clusters reported last year with a new computational technique and thereby pinpointed the positions of all atoms—heavy and light (*Sci. Adv.* 2015, DOI: 10.1126/sciadv.1400211). The analysis revealed the structures of four highly stable Au₆₈(SH)₃₂ isomers (one shown) and also indicated that these clusters could serve as air-purifying catalysts that convert CO to CO₂.—MJ



This model represents a 1.7-nm-diameter cluster of 68 gold atoms capped with thiolate ligands. Au = gold, S = red, H = white.