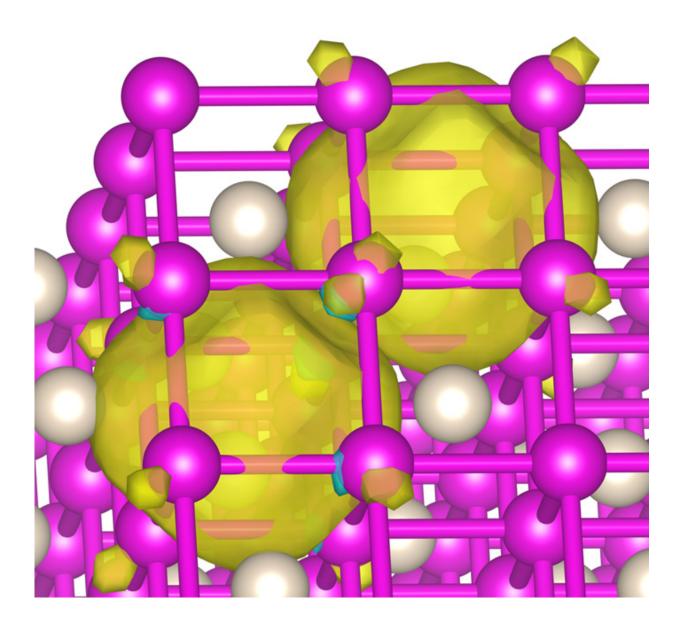


Up, up and away: Chemists say 'yes,' helium can form compounds

February 6 2017, by Mary-Ann Muffoletto



Representation of chemical bonding analysis of the Na2He structure via the SSAdNDP method: 8c-2e bond is found inside of every empty Na8 cube. For



clarity, only two such bonds are shown. Credit: Ivan Popov, Utah State University

Can helium bond with other elements to form a stable compound? Students attentive to Utah State University professor Alex Boldyrev's introductory chemistry lectures would immediately respond "no." And they'd be correct – if the scholars are standing on the Earth's surface.

But all bets are off, if the students journey to the center of the Earth, à la Jules Verne's Otto Lidenbrock or if they venture to one of the solar system's large planets, such as Jupiter or Saturn.

"That's because extremely <u>high pressure</u>, like that found at the Earth's core or giant neighbors, completely alters helium's chemistry," says Boldyrev, faculty member in USU's Department of Chemistry and Biochemistry.

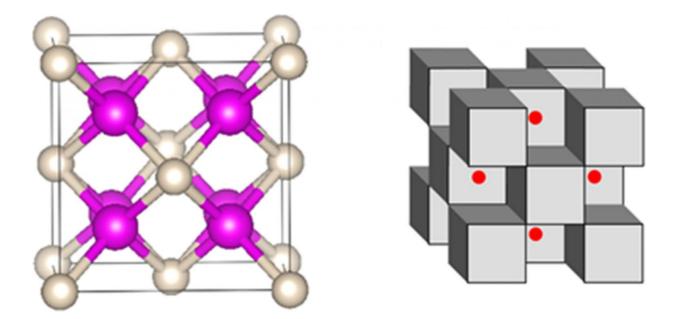
It's a surprising finding, he says, because, on Earth, helium is a chemically inert and unreactive compound that eschews connections with other elements and <u>compounds</u>. The first of the noble gases, helium features an extremely stable, closed-shell electronic configuration, leaving no openings for connections.

Further, Boldyrev's colleagues confirmed computationally and experimentally that sodium, never an earthly comrade to <u>helium</u>, readily bonds with the standoffish gas under high pressure to form the curious Na_2He compound. These findings were so unexpected, Boldyrev says, that he and colleagues struggled for more than two years to convince science reviewers and editors to publish their results.

Persistence paid off. Boldyrev and his doctoral student Ivan Popov, as



members of an international research group led by Artem Oganov of Stony Brook University, published the pioneering findings in the Feb. 6, 2017, issue of *Nature Chemistry*.



Chemical bonding analysis of the Na2He structure via the SSAdNDP method: Ball-and-stick representation, left, and polyhedral representation, right, where half of the Na8 cubes are occupied by He atoms (shown as polyhedra) and haf by two electrons (shown as red spheres). Pink and gray atoms represent Na and He, respectively. Credit: Ivan Popov, Utah State University

Additional authors on the paper include researchers from China's Nankai University, Center for High Pressure Science and Technology, Chinese Academy of Sciences, Northwestern Polytechnical University, Xi'an and Nanjing University; Russia's Skolkovo Institute of Science and Technology, Moscow Institute of Physics and Technology, Sobolev Institute of Geology and Mineralogy and RUDN University; the Carnegie Institution of Washington, Lawrence Livermore National



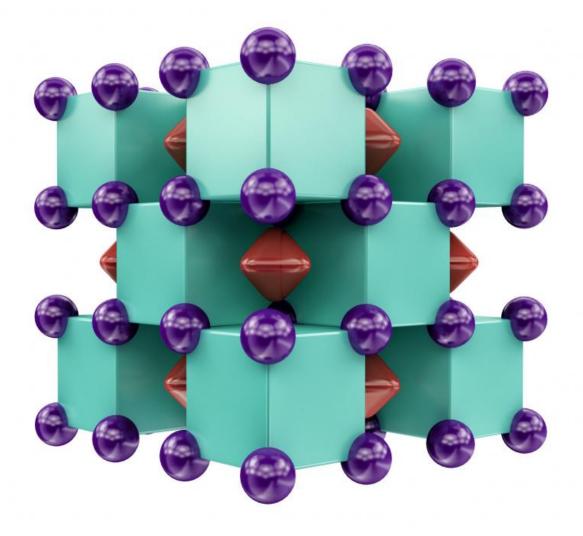
Laboratory, Italy's University of Milan, the University of Chicago and Germany's Aachen University and Photo Science DESY.

Boldyrev and Popov's role in the project was to interpret a chemical bonding in the computational model developed by Oganov and the experimental results generated by Carnegie's Alexander Goncharov. Initially, the Na₂He compound was found to consist of Na₈ cubes, of which half were occupied by <u>helium atoms</u> and half were empty.

"Yet, when we performed <u>chemical bonding</u> analysis of these structures, we found each 'empty' cube actually contained an eight-center, twoelectron bond," Boldyrev says. "This bond is what's responsible for the stability of this enchanting compound."

Their findings advanced the research to another step.





Crystal structure of Na2He, resembling a three-dimensional checkerboard. The purple spheres represent sodium atoms, which are inside the green cubes that represent helium atoms. The red regions inside voids of the structure show areas where localized electron pairs reside. Credit: Artem R. Oganov

"As we explore the structure of this compound, we're deciphering how this bond occurs and we predicted that, adding oxygen, we could create a similar compound," Popov says.



Such knowledge raises big questions about chemistry and how elements behave beyond the world we know. Questions, Boldyrev says, Earth's inhabitants need to keep in mind as they consider long-term space travel.

"With the recent discovery of multiple exoplanets, we're reminded of the vastness of the universe," he says. "Our understanding of chemistry has to change and expand beyond the confines of our own planet."

More information: A stable compound of helium and sodium at high pressure, *Nature Chemistry*, DOI: 10.1038/nchem.2716

Provided by Utah State University

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