Unusual electron sharing found in cool crystal
30 July 2020, by Yoshihiko Okamoto

The so-called tritungsten molecules were discovered in single crystals of caesium tungsten oxide (CsW$_2$O$_6$) cooled below -58°C. CsW$_2$O$_6$ conducts electricity at room temperature but changes into an insulating material when it is cooled below -58°C. It has been a challenge to study how the atomic structure of this type of material changes in response to temperature. To overcome this, Okamoto and his colleagues in Japan synthesized very pure single crystals of CsW$_2$O$_6$ and bombarded them with X-ray beams at room temperature and -58°C.

The tungsten molecules in the conducting crystal form three-dimensional networks of tetrahedral pyramids connected at their corners, known as a pyrochlore structure. The bonds between the molecules form due to a symmetrical sharing of electrons between them.

However, when the compound is cooled, the electrons re-arrange and two types of tungsten atoms emerge within the tetrahedra, each with a different "valence," or bonding power with other atoms. This, in turn, distorts the lengths of tungsten bonds with oxygen atoms in the compound, leading to a more compressed shape. Importantly, the tungsten atoms with lower valence form small and large triangles on the sides of the tungsten tetrahedra, with the highly unusual tritungsten molecules forming on the small triangles. The three tungsten atoms forming the points of these triangles share only two electrons between them to keep them bonded together.

"To our knowledge, CsW$_2$O$_6$ is the only example where this type of bond formation, where several atoms share only a few electrons, appears as a phase transition," says Okamoto.

The team aims to further investigate compounds with pyrochlore structures, with the ultimate goal of discovering materials with new and interesting properties.
More information: Yoshihiko Okamoto et al. Regular-triangle trimer and charge order preserving the Anderson condition in the pyrochlore structure of CsW$_2$O$_6$, Nature Communications (2020). DOI: 10.1038/s41467-020-16873-7

Provided by Nagoya University

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