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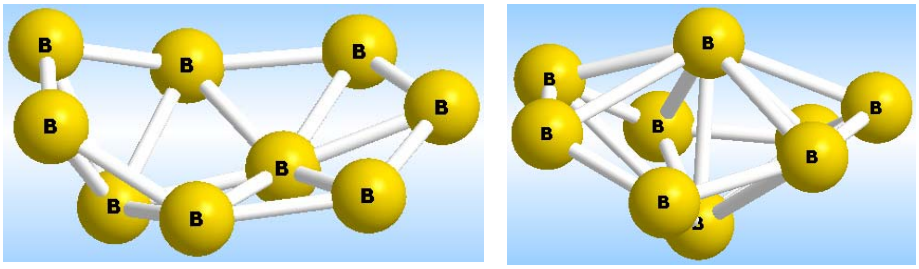
EMSL Science Made Possible

Researchers Discover Two Isomers of 9-boron Clusters

EMSL supercomputer instrumental for complex calculations



Isomers of B_9^-. *These two forms were recently discovered.*

Two new isomers of negatively charged 9-atom boron clusters, which could be vital in designing storage devices for the hydrogen economy, were discovered, thanks to careful research and the use of the supercomputer at the Department of Energy's EMSL. The EMSL users, from Tsinghua University in China, Washington State University, and Pacific Northwest National Laboratory, performed complex calculations and simulations on experimental spectra obtained with EMSL's photoelectron spectroscopy capabilities in 2003 to search for the isomers. The 2003 data showed the B_9^- forms a stable planar wagon-wheel structure, but minor features in the photoelectron spectra hinted at other structures. However, the density functional theory calculations used at the time indicated the other structures were not feasible.

So, the research team of Li-Li Pan, Jun Li, and Lai-Sheng Wang used EMSL's 11.8-teraflop supercomputer to run Car–Parrinello molecular dynamics calculations followed by simulated annealing and extensive geometry optimizations at various levels of DFT and *ab initio* theory, all in search of other isomers. Without the supercomputer, these calculations would not have been possible. The researchers' work revealed two more isomers: a convex quasiplanar structure (right) and a distorted heptagonal bipyramid (left). The latter was found to be present in the experiment and provided a complete interpretation of the 2003 photoelectron data.

Scientific impact: The new work allowed a deeper understanding into the molecular structures and energetics of B_9^- clusters. Selecting the right level of theory for computer simulations is imperative when studying conformational isomers. As this work showed, current computational methods can be relied on to accurately simulate experimental results. This work is part of EMSL's ongoing efforts to obtain fundamental molecular understanding of chemical systems of environmental and energy importance by linking theory and computation with experimental research.

Societal impact: Because boron reacts with every element on the periodic chart, understanding the structures and energetics of small boron clusters could provide insights into devices that safely store and release hydrogen to power vehicles.

For more information, contact EMSL Communications Manager Mary Ann Showalter (509-371-6017).

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