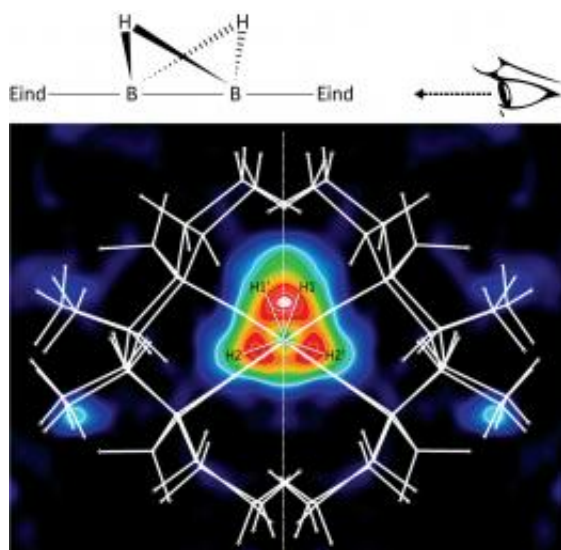


Bulky molecules trap boron compounds into a never-before-seen structural arrangement

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X-ray measurements (bottom) reveal that a butterfly-shaped boron compound (top left) has an intense electron distribution in its B₂H₂ core (red areas) that is stabilized by exterior bulky ligands (white lines). The human eye (top right) shows the direction from which you look at the electron density map. Reproduced from Ref. 1 © 2010 Yoshiaki Shoji et al.

When it comes to chemical bonding, boron has a reputation for being unconventional. While covalent bonds are usually formed by sharing two electrons between two atoms, some compounds—including diboranes (B₂H₆)—contain B–H–B bonds in which an electron pair is distributed over three sites. The electron-deficient nature of these ‘3-center, 2-electron’ bonds can generate a variety of distinct chemical structures,

some of which—such as triple-bonded diborane derivatives—have only been seen theoretically.

Kohei Tamao and colleagues from the RIKEN Advanced Science Institute in Wako and Kyoto University, Japan, have now isolated the first stable diborane molecule with butterfly-shaped B–H–B bonds and a boron–boron link with triple bond characteristics. This discovery unlocks new insights into the workings of 3-center, 2-electron boron interactions and puts scientists one step closer to synthesizing the elusive boron–boron triple bond.

The key to this approach is a bulky molecule known as ‘Eind’ that contains a rigid core of fused hydrocarbon rings covered with ethyl side chains. Previously, the researchers used Eind ligands to stabilize heavy elements into multiply bonded species. This time, the team hoped to generate a neutral boron–boron double bond by substituting Eind groups for hydrogen [atoms](#) in diborane.

However, after characterizing the structure of the diborane–Eind compound—a difficult task requiring synchrotron x-rays to detect hydrogen atom positions—the researchers saw a previously unidentified arrangement at the B₂H₂ core: a central boron–boron connection nearly as short as a theoretical triple bond, flanked by two symmetric B–H–B ‘wings’ (Fig. 1). “We did not expect this butterfly-shaped structure at first, and finding it was a kind of serendipity,” says co-author Yoshiaki Shoji.

Quantum computations revealed that the Eind ligands enforced a linear bonding geometry upon the boron atoms, creating molecular energy levels closely related to the triple-bond species. Furthermore, the bridging hydrogen atoms enhanced the multiple bonding characteristics. “Based on this analysis, it is possible to consider triple bonding interactions between the two [boron](#) atoms,” says team-member Tsukasa

Matsuo.

Matsuo notes that the butterfly-shaped molecule already displays unique chemical reactivity, and the insights gained from this new structure could lead to additional multiply-bonded diboranes. “We may be able to synthesize a more triply bonded species in the near future by replacing the bridging hydrogen atoms with alkali metals,” he says. “At the moment, this compound is just a dream but I think we have a chance to obtain it.”

More information:

-- Shoji, Y, et al. A stable doubly hydrogen-bridged butterfly-shaped diborane(4) compound. *Journal of the American Chemical Society* 132, 8258–8260 (2010). [Article](#)

-- Li, B., et al. π -Conjugated phosphasilenes stabilized by fused-ring bulky groups. *Journal of the American Chemical Society* 131, 13222–13223 (2009) [Article](#)

Provided by RIKEN

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