Aluminum triple bond made for first time

September 27, 2018

Chemists have discovered elusive species containing triple aluminum-aluminum bond via combined photoelectron spectroscopy and *ab initio* studies

The Science

Through a close collaboration between experimentalists and theorists at the Theoretical Division of Los Alamos National Laboratory, Nankai University (NU), Utah State University (USU), Johns Hopkins University (JHU) and Karlsruhe Institute of Technology (KIT), researchers have theoretically designed and experimentally observed gas-phase $Na_3Al_2^-$ cluster exhibiting unprecedented chemical bonding features. Scientists report an Al#Al classical triple bond in the designer $Na_3Al_2^-$ cluster, which was predicted *in silico* and subsequently generated by pulsed arc discharge, and further characterized by mass spectrometry and photoelectron spectroscopy. Excellent agreement between the experimental and calculated vertical detachment energies of the most stable isomer of $Na_3Al_2^-$ confirm the proposed structure. Presence of the triple bond in $Na_3Al_2^-$ is supported by its reproducibly intense mass peak among the neighboring clusters, which indicates an unusually high stability. Similarity of the canonical molecular orbitals of the P#P molecule with $Na_3Al_2^-$ and Na_4Al_2, along with the Adaptive Natural Density Partitioning results, further confirm that Na atoms can "transmutate" Al into P, and therefore, aid in the formation of the Al#Al triple bonds.

The Impact

The discovery of the Al#Al classical triple bond represents a fundamental chemical bonding issue. Similar to the valence-isoelectronic triple bonded C_2^{2-} species functioning as building blocks of a large family of carbide compounds, the Al^{2-}#Al^{2-} core found in $Na_3Al_2^-$ and Na_4Al_2 also holds potential to be realized in periodically extended solid-state compounds, which can possess unique properties.

Summary

The discovery of homodinuclear multiple bonds composed of Group 13 elements represents one of the most challenging frontiers in modern chemistry. A classical triple bond such as N#N and HC#CH contains one s bond and two p bonds constructed from the *p* orbitals perpendicular to the s bond. However, the traditional textbook triple bond between two Al atoms has so far remained elusive. Scientists at LANL, NU, USU, JHU, and KIT have succeeded in creating such compounds by performing a joint photoelectron spectroscopy and theoretical study. They have computationally designed and experimentally verified geometric and electronic structure of the mixed aluminum-sodium cluster, i.e., $Na_3Al_2^-$, which possesses unprecedented Al#Al classical triple bond. The researchers found that the Al atoms, which are considered as Al^{2-} due to the electron donation from Na atoms, undergo a double electronic transmutation into Group 15 elements, thus the Al^{2-}#Al^{2-} kernel mimics the P#P and N#N molecules.

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Funding: I.A.P. acknowledges the support from a Director's Postdoctoral Fellowship and J. Robert Oppenheimer Distinguished Postdoctoral Fellowship at Los Alamos National Laboratory. Los Alamos National Laboratory is operated by Los Alamos National Security, LLC, for the National Nuclear Security Administration of U.S. Department of Energy (Contract DEAC52-06NA25396). X.Z. acknowledges the Thousand Talents Program of China and the College of Chemistry at Nankai University for the start funding. The theoretical work was supported by the National Science Foundation (CHE-1664379 to A.I.B.). This material is based upon work supported by the Air Force Office of Scientific Research (AFOSR) under grant number FA9550-15-1-0259 (K.H.B.).

Publications: Zhang, I. A. Popov, K. A. Lundell, H. Wang, C. Mu, W. Wang, H. Schöckel, A. I. Boldyrev, K. H. Bowen, *Angew. Chem. Int. Ed.*, 2018, DOI:10.1002/anie.201806917.

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