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Theoretical Chemistry

Element 126

As-yet-unsynthesized superheavy atom should form a stable diatomic molecule with fluorine

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Element 126 (E126) should readily form a stable diatomic molecule with fluorine, according to a theoretical study of the chemical properties of the as-yet-unsynthesized superheavy element (*J. Chem. Phys.* **2006,** *124*, 071102).

The molecule (E126F) is unique in that it contains an atom with a g atomic orbital that is predicted to be occupied with valence electrons in the atom's ground state. The study further predicts that the g-orbital electrons are involved in forming molecular orbitals, a bonding configuration that may impart distinct chemical properties.

Decades-old predictions of enhanced stability of E126 relative to other transactinide nuclides suggest that, if atoms of the element (with 126 protons and 184 neutrons) can be synthesized, they may persist long enough for their chemical properties to be probed experimentally.

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is studying E126 computationally. Using relativistic methods, he finds the molecule's dissociation energy to be about 7.5 eV, 3 eV less than he finds with nonrelativistic methods. This result highlights the effects of relativity, which can strongly alter the properties of heavy elements.

Cautioning that the conclusions need to be verified by additional studies, Walter D. Loveland, a professor of nuclear chemistry at Oregon State University, Corvallis, describes the work as "noteworthy." The "promise of g-electron chemistry adds to the interest in the formidable task of synthesizing the element," Loveland remarks. "Studies like this of 'relativity in a test tube' extend the frontiers of both chemistry and physics."

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