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New, simple inorganic species

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Abstract

Ab initio quantum chemistry and isoeletronic thinking can be used to predict new inorganic species. A recent example [1] are the surprisingly stable Group-4 tetra-azides $M(N_3)_4$, which are lower-lying isomers to the $(N_5)M(N_7)$; M=Ti,Zr,Hf,Th, predicted earlier. They present a unique structural feature, namely the M-N-N-N fragments are linear.

Our new insights to heavy-element chemistry include the prediction of the existence of the a series of tetrahedral molecules with general formula $M(Au)_4$; M=Ti,Zr,Hf,Th,U [2]. They correspond to Au in the formal valence state -1 and indicate that gold can act as a ligand similar to the halogen series. Of the $M(Au)_4$ species studied, $U(Au)_4$, the first predicted mixed gold uranium compound, has a short M-Au bond, 2.71 Å, which would locate Au between Br and I from the bond length point of view in the U-tetra-halide series. Energetically, the U-Au bond is weaker than the corresponding U-Br and U-I bonds.

[1] L. Gagliardi and P. Pyykkö Inorg. Chem. 42, 3074-3078 (2003).

[2] L. Gagliardi J. Am. Chem. Soc., web release (2003).

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