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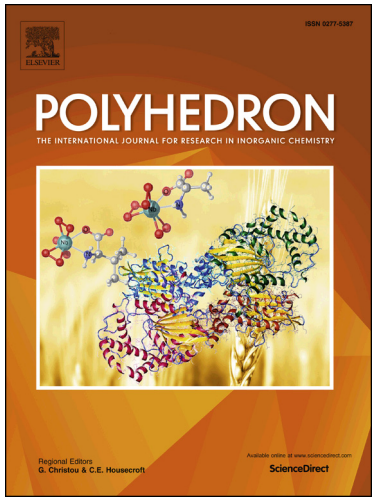

Stability of the $Ti_nF_{4n+1}^-$ and $Ge_nF_{4n+1}^-$ superhalogen anions and the acidity of the HTi_nF_{4n+1} and HGe_nF_{4n+1} (n=1–3) superacids

Iwona Anusiewicz, Sylwia Freza, Piotr Skurski

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Stability of the $Ti_nF_{4n+1}^-$ and $Ge_nF_{4n+1}^-$ superhalogen anions and the acidity of the HTi_nF_{4n+1} and HGe_nF_{4n+1} (n=1-3) superacids

Iwona Anusiewicz*, Sylwia Freza, Piotr Skurski

Laboratory of Quantum Chemistry, Faculty of Chemistry, University of Gdańsk
Wita Stwosza 63, 80-308 Gdańsk, Poland

Abstract

Polynuclear superhalogen anions containing titanium and germanium as the central atoms and fluorine atoms as the ligands were investigated on the basis of ab initio calculations employing the CCSD(T), MP2 and OVGF methods and the 6-311++G(d,p) basis set. The structures of most stable isomers of $Ti_nF_{4n+1}^-$ and $Ge_nF_{4n+1}^-$ (n=1-3) anions, their thermodynamic stability and the vertical electron detachment energies are provided and discussed. The possible existence and stability of the corresponding HTi_nF_{4n+1} and HGe_nF_{4n+1} neutral molecules, obtained by the protonation of the $Ti_nF_{4n+1}^-$ and $Ge_nF_{4n+1}^-$ anions, are also considered. The most important findings include the prediction of large electronic stability of the $Ti_nF_{4n+1}^-$ and $Ge_nF_{4n+1}^-$ anions (exceeding 9.7 eV in all cases and approaching 12 eV for n = 3) and significant acidity of the HTi_nF_{4n+1} and HGe_nF_{4n+1} compounds (manifested by their Gibbs free deprotonation energies in the 258.7-302.6 kcal/mol range).

Keywords: superhalogens, superacids, acidity

*corresponding author: e-mail: iwona.anusiewicz@ug.edu.pl