First-Principles Prediction of Novel Technetium(IV) Halide Polymeric Compounds

PHILIPPE F. WECK, EUNJA KIM, FREDERIC POINEAU, KENNETH R. CZERWINSKI, University of Nevada Las Vegas — We report the crystal structures of novel technetium tetrahalide polymeric compounds, TcX₄ [X=F,Br,I], as predicted from first-principles calculations. Similar to TcCl₄, TcF₄ and TcBr₄ compounds are orthorhombic with the centro-symmetric space group Pbca, while TcI₄ crystallizes in the space group P2₁/c. The structures consist of distorted octahedral groups of composition TcX₆ linked into endless linear chains. A possible explanation for the differences between these structures is offered in terms of varying degree of bonding within the polymeric chains.

¹This work was supported by the U.S. DOE, agreement no. DE-FG07-01AL67358.