Abstract Submitted
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First-Principles Prediction of Novel Technetium(IV) Halide Polymeric Compounds[1] 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, TcX_4 [X=F,Br,I], as predicted from first-principles calculations. Similar to $TcCl_4$, TcF_4 and $TcBr_4$ compounds are orthorhombic with the centro-symmetric space group *Pbca*, while TcI_4 crystallizes in the space group $P2_1/c$. The structures consist of distorted octahedral groups of composition TcX_6 linked into endless linear chains. A possible explanation for the differences between these structures is offered in terms of varying degree of bonding withing the polymeric chains.

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