Negative thermal bond expansion of a molecular solid, Tc_2O_7

Daniel Mast,[1,2,3] Bradley Childs, [1,2] Keith V. Lawler,[1,3] Frederic Poineau,[1,3] Alfred P. Sattelberger[4], Kenneth R. Czerwinski[1,2] and Paul M. Forster,[1,2,3]

[1] Department of Chemistry and Biochemistry, [2] Radiochemistry Program, [3] High Pressure Science and Engineering Center, University of Nevada Las Vegas, Las Vegas, NV 89154, USA

[4] Energy Engineering and Systems Analysis Directorate, Argonne National Laboratory, Argonne, IL 60439, USA

The binary oxides of group 7 transition metal form a series of unique structures. Two of the three crystallize as molecular solids with two metal centers bridged by a single oxygen. Molecular metal oxides stable under ambient conditions are rare and offer unique insight into the chemistry and physics of materials. The structure of Tc_2O_7 is characterized by centrosymmetric linear molecules with a single bridging oxygen. In a combined computational and experimental investigation, anomalous thermal expansion behavior has been identified between room temperature and 100 K. Using variable temperature single crystal diffraction and Langevin Molecular dynamics we can model the negative thermal bond expansion.