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**A statistical-mechanical equation-of-state model for dense chlorine-containing reactive mixtures**<sup>1</sup> SERGEY VICTOROV, Ecole Normale Supérieure de Cachan, France — We present a thermodynamic model of supercritical reactive mixtures containing the elements Cl, C, H, N, and O. The model describes the thermodynamics of a multi-component fluid phase with reliable statistical-mechanical theories and exp-6 intermolecular potentials, and also includes a multi-phase equation of state for carbon nanoparticles. Using the thermochemical TDS code, we show that the model reproduces Hugoniot data on chlorocarbons in good agreement with experiments. To our knowledge, this is the first chemical equilibrium model, which a) yields temperatures of CCl<sub>4</sub>, shock-compressed to pressures over 23 GPa, in good agreement with measurements; b) allows one to reproduce a non-monotonic behavior of the experimental dependence of sound velocity of this material on pressure; c) predicts shock-induced cooling of doubly shocked CCl<sub>4</sub>, an unusual phenomenon detected for CCl<sub>4</sub> experimentally. The reliability of the model is also demonstrated by thermodynamic modeling detonations of Cl- containing liquids.

<sup>1</sup>A part of this work was carried out in Laboratoire de Combustion et de Détonique, UPR 9028 du CNRS, Futuroscope, France.

Prefer Oral Session  
 Prefer Poster Session

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