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Reactive Monte Carlo Validation of Thermochemical Equations of State of High Explosives JEFFERY LEIDING, CHRISTOPHER TICKNOR, STEPHEN ANDREWS, DARIO PANICI, CURTIS PETERSON, Los Alamos National Laboratory — LANL has developed a new thermochemical equation of state code called "Magpie." Magpie uses Ross' soft-sphere perturbation theory to calculate the equations of state of chemical equilibrium mixtures. We will present benchmark atomistic reactive Monte Carlo calculations of the equations of state of high-explosive product mixtures (the exact result given a set of pair potentials) and compare these to results from Magpie. We will study results for several quantities of interest to high explosives, such as the CJ state and overdriven Hugoniot. These results will quantify the errors of the perturbation theory implementation and mixing rules employed in Magpie, as well as test commonly used chemical equilibrium solvers

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