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Global equation of state of a reactive, polyatomic system: application to carbon dioxide[1] PHILIP C. MYINT, CHRISTINE J. WU, DAVID A. YOUNG, PHILIP A. STERNE, Lawrence Livermore National Laboratory — An important topic in high-energy-density science involves developing a global equation of state (EOS) that spans a wide range of pressures and temperatures. One notorious challenge in building a global EOS is the inclusion of chemistry, yet this is essential for modeling many dissociative materials for which the chemical reactions constitute a sizable contribution to the total free energy. We present an EOS for carbon dioxide (CO_2) that accounts for dissociation by capturing the key physics/chemistry present in several relevant pressure–temperature regimes and interpolating between the regimes over the global range in pressure and temperature. We have extended the dissociation methodology proposed by Young and Corey over 25 years ago for diatomic molecules to polyatomic molecules. We use CO_2 as a prototypical polyatomic system, since it is one of the simplest molecular systems beyond diatomic materials, and since a CO_2 EOS would be useful for many applications, including organic synthesis, geochemistry, volcanism, and planetary interiors. We show that while there is still much room for further improvement, taking dissociation into account significantly improves the accuracy of the EOS compared to other global equations of state for CO_2 that neglect chemistry.

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