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Hydrogen-Helium Mixtures at High Pressures MIGUEL A. MORALES, SEBASTIEN HAMEL, KYLE CASPERSEN, ERIC SCHWEGLER, LLNL — We extend our previous work on hydrogen-helium mixtures (Morales, M. A., et. al. PNAS 106, 1324 (2009).) to lower pressures and lower temperatures, across the molecular dissociation regime in hydrogen, to the low pressure molecular liquid. Using density functional theory-based molecular dynamics together with thermodynamic integration techniques, we calculate the Gibbs free energy of the dense liquid as a function of pressure, temperature, and composition. Our work focuses on the mixing properties of the liquid, the optical properties including conductivity and reflectivity, and the creation of accurate mixing models for thermodynamic properties, including pressure and entropy. The resulting models will provide the basis for accurate first-principles equations of state for planetary modeling. Prepared by LLNL under Contract DE-AC52-07NA27344.

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