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Multi-component Mutual Diffusion in the Warm, Dense Matter Regime EDMUND MEYER, CHRISTOPHER TICKNOR, ALEXANDER WHITE, LANL, JEAN CLEROUIN, PHILIPPE ARNAULT, CEA, JOEL KRESS, LEE COLLINS, LANL — We present the formulation of ternary and higher mixtures in the warm, dense matter regime. Binary mixtures have received considerable attention for mass transport, but few studies have addressed the complexities of ternary and higher mixtures. We explicitly examine ternary systems utilizing the Maxwell-Stefan formulation that relates diffusion to gradients in the chemical potential. Trajectories characterized by positions and velocities yield Onsager coefficients, which connect macroscopic diffusion to microscopic particle motions, through various autocorrelation functions (ACF). We use both classical (Yukawa pair-potentials) and orbital-free density functional molecular dynamics simulations to generate long trajectories. We employ the reference-mean form of the ACFs and determine the center-of-mass coefficients through a simple reference-frame-dependent similarity transformation. From the Onsager terms we determine the mutual diffusion coefficients. We compare to the Darken approximation and show that the self-diffusion constants determined in the full mixture (as opposed to the infinite dilution limit) get closer to the Onsager derived value. We present results from mixtures with only light elements (D-Li-C) and highly-asymmetric mass components (H-C-Ag).

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