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Volume dependence of the transit contribution in the vibration-transit theory of liquids[1] ERIC CHISOLM, NICOLAS BOCK, DUANE WALLACE, Los Alamos National Laboratory — Previously, we created a model for the transit contribution to the thermodynamic functions of a liquid [Phys. Rev. **E** 81, 041201 (2010)]. The model modifies the potential surface in which atoms in the liquid state move. The two parameters of the model are χ, the maximum transit entropy, and $\theta_{\rm tr}$, a characteristic temperature near (but not equal to) the melt temperature. Using a combination of experimental data and density functional theory results, we calculate the volume derivatives of these parameters, thus giving the first-order volume dependence of the model.

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Eric Chisolm
Los Alamos National Laboratory

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