Scaling of Nonclassical Nucleation Rates of Methanol GERALD
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bid, Jordan — Nonclassical gradient theory (GT) calculations of nucleation rates
are presented for methanol, an associating vapor system. The calculations use the
SAFT-0 equation of state (EOS) that accounts for the effects of molecular associa-
tion based on the statistical association fluid theory (SAFT). Calculated rates were
compared to the experimental rates of Strey, et al. [*J. Chem. Phys.* **1986**, 84,
2325]. The GT nucleation rates showed improved T and Sdependence compared to
classical nucleation theory (CNT). The GT rates were also improved by factors of
100-1000 compared to CNT. Despite these improvements, GT does not describe the
reported T and S dependence of the nucleation rates. To explore this further, the
GT and experimental rates were analyzed using Hale's scaled model [*J. Chem. Phys.*
2005, 122, 204509]. This analysis reveals an inconsistency between the predictions
of GT, which scale relatively well, and the experimental data, which do not scale. It
also shows that the measured rate data have an anomalous T and S dependence. A
likely source of this anomaly is the inadequate thermodynamic data base for small
cluster properties that was used originally to correct the raw rate data for the effects
of association.

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