

Transferable potentials for Phase Equilibria: 7. Primary, secondary, and tertiary amines, nitro alkanes and nitro benzene, nitriles, amides, pyridine, and pyrimidine

Collin D. Wick,^{1,2} John M. Stubbs,^{1,3} Neeraj Rai,¹ and J. Ilja Siepmann^{1,*}

¹ *Departments of Chemistry and of Chemical Engineering and Material Science,
University of Minnesota, 207 Pleasant Street SE, Minneapolis, Minnesota 55455-0431*

² *School of Chemical Engineering, Department of Materials Science and Engineering,
National Technical University of Athens, 9 Heron Polytechniou Street,
Zografou Campus, 15780 Athens, Greece*

³ *Department of Chemistry, Grinnell College,
1116 8th Avenue, Grinnell, IA 50112-1690*

Abstract

The transferable potentials for phase equilibria (TraPPE) force field is extended to amine, nitro, nitrile and amide functionalities and to pyridine and pyrimidine. In many cases, the same parameters for a functional group are used for both united-atom and explicit-hydrogen representations of alkyl tails. Following the TraPPE philosophy, the non-bonded interaction parameters were fitted to the vapor–liquid coexistence curves for selected one-component systems. Coupled-decoupled configurational-bias Monte Carlo simulations in the Gibbs ensemble were applied to neat (methyl, dimethyl, trimethyl, ethyl, diethyl, or triethyl) amine, nitro methane, nitro ethane, nitro benzene, acetonitrile, propionitrile, acetamide, propanamide, butanamide, pyridine, and pyrimidine. Excellent agreement with experimental results was found with the mean unsigned errors being less than 1% for both the critical temperature and the normal boiling temperature. Similarly, the liquid densities at low reduced temperatures are reproduced to within 1%, while the deviation for the critical densities is about 4%. Additional simulations were performed for the binary mixtures of methyl amine + *n*-hexane, diethyl ether + acetonitrile, 1-propanol + acetonitrile, and nitro ethane + ethanol. With the exception of the methyl amine/*n*-hexane mixture for which the separation factor is substantially overestimated, agreement with experiment for the other three mixtures is very satisfactory.

* Corresponding author: siepmann@chem.umn.edu