Prediction of Solid-Liquid-Vapor Phase Equilibria of Noble Gases in Nitrogen

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Supplementary Data File

## Peng Robinson equation of state for calculating fugacity coefficients

The Peng-Robinson equation of state (PR-EoS) [1] is given by

 (S.1)

To find the PR-EoS coefficients for mixtures (i.e., and values), the following mixing rules will be applied:

 (S.2)

 (S.3)

where *kij* is the binary interaction parameter characterizing molecular interactions between molecules *i* and *j*, and is the mole fraction of component *i* in the mixture. The individual component PR-EoS coefficients of component *i* (i.e., and ; and similarly for component *j*) are given by

 (S.4)

 (S.5)

where

 (S.6)

, and are, respectively, the critical pressure, critical temperature and acentric factor of component *i*.

The corresponding fugacity coefficient for component *i* in the mixture (in either vapour or liquid phase) is given by the following equation:

(S.7)

where z is the compressibility factor, and A and B are given by

 (S.8)

 (S.9)

# References

[1] D.-Y. Peng and D. B. Robinson, “A New Two-Constant Equation of State,” *Ind. Eng. Chem. Fundam.*, vol. 15, no. 1, pp. 59–64, Feb. 1976, doi: 10.1021/i160057a011.