

Note

Comment on S. Bobbo, L. Fedele, M. Scattolini, and R. Camporese, *Int. J. Thermophys.* 21:781 (2000): Vapor + Liquid Equilibrium Measurements and Correlation of the Binary Refrigerant Mixtures Difluoromethane (HFC-32) + 1,1,1,2,3,3-Hexafluoropropane (HFC-236a) and Pentafluoroethane (HFC-125) + 1,1,1,2,3,3-Hexafluoropropane (HFC-236a) at 288.6, 303.2, and 318.2 K

U. K. Deiters¹

The authors of the cited article spared no efforts to obtain high-quality chemicals for their work and to ensure their purity. Their experimental work on the binary mixtures (difluoromethane + hexafluoropropane) and (pentafluoroethane + hexafluoropropane) was carried out very well, and the resulting experimental data show remarkably little scatter.

From a purist's point of view, however, it must be stated that 1,1,1,2,3,3-hexafluoropropane is a chiral compound: the carbon atom 2 is a center of asymmetry. The 1,1,1,2,3,3-hexafluoropropane used for this work was therefore probably not a pure compound but a mixture of two enantiomers, characterized by opposite optical activities. Hence, the mixtures studied in the cited article were not binary but ternary.

Does this have any consequences for measurements or calculations of thermodynamic properties?

Usually one would expect chiral refrigerants to come as racemic mixtures, i.e., mixtures of equal amounts of the two enantiomers, which therefore have no optical activity. As long as the enantiomer ratio remains the same during a change of state, such mixtures behave like pure compounds, and the existence of enantiomers has no influence on VLE calculations.

¹ Institute of Physical Chemistry, University at Cologne, Luxemburger Str. 116, D-50939 Köln, Germany. E-mail: ukd@xenon.pc.uni-koeln.de

The mixtures studied in the cited publication can therefore be regarded as exactly pseudobinary.

However, it is well known that the melting points of racemic mixtures often differ considerably from those of the pure enantiomers, and this may be the case for other thermodynamic properties, too; it has been argued that enantiomer mixtures might have nonvanishing excess properties. Authors of publications involving chiral compounds should therefore make clear whether their measurements apply to racemic mixtures or to pure enantiomers.

Furthermore, it is possible that a chiral compound was produced from material of biological origin or that the enantiomer ratio of a racemic mixture was shifted by contact with such material (e.g., filters or chromatography column packings derived from dextrose or cellulose). The latter is not very likely, but nevertheless, it is better to check the optical activity of chiral compounds like 1,1,1,2,3,3-hexafluoropropane before using them.

None of the points raised here diminish in any way the usefulness of the experimental data or the correlational work of the cited publication; but future work involving 1,1,1,2,3,3-hexafluoropropane or other chiral compounds might eventually be impaired if stereochemical properties of compounds are ignored.

REFERENCES

1. U. K. Deiters, *Fluid Phase Equil.* **132**:265 (1997).
2. J. F. Kenney and U. K. Deiters, *Phys. Chem. Chem. Phys.* **2**:3163 (2000).