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ADDITIONS AND CORRECTIONS

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Correction to "Molecular Modeling of the Vapor−Liquid Equilibrium Properties of the Alternative Refrigerant 2,3,3,3-Tetrafluoro-1-propene (HFO-1234yf)"

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In Figure 4 of the above-referenced Letter, we presented the radial distribution functions (RDFs) of two different fluorine atom types around the HC hydrogens in HFO-1234yf at 298.15 and 1 MPa. The RDF of the FCT fluorines of the CF_3 group around the HC hydrogens exhibited distinctive peaks, from which we suggested that hydrogen bonding interactions exist between the FCT fluorine and the HC hydrogen.

However, a further analysis of the simulation data discloses that these peaks result from both intermolecular and intramolecular (1−5) interactions between the FCT and HC atoms. When only intermolecular interactions are considered in the analysis, neither the FCM-HC nor the FCT-HC RDF shows a distinctive peak, as illustrated by the corrected Figure 4 given in this note.

From this, it can be concluded that no hydrogen bonding interactions occur in pure HFO-1234yf.

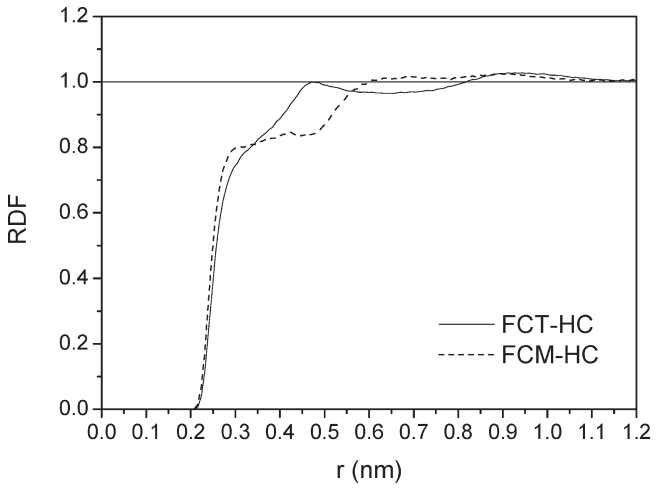

Figure 4. Intermolecular RDF for HFO-1234yf in the liquid phase at 298.15 K and 1 MPa.

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