Determination of High Pressure Phase Equilibria by Infrared Spectroscopy

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A spectroscopic method for the determination of fluid phase equilibria under high pressure is presented along with some of the results obtained with several binary mixtures of hydrocarbons.

Infrared spectra of binary mixtures were obtained through a variable volume high pressure optical cell. The pressures were imposed by variation of the volume through a piston and ranged up to 200 MPa. The temperature was controlled by a regulated oven and ranged up to 473 K. The cell was filled at near critical composition so that the whole phase envelope could be determined with a single filling of the cell.

The method is based on Beer-Lambert law and yields the concentrations of both compounds in both phases of a mixture by an evaluation of the spectral contribution of each of the compounds on different spectral domains. Other related properties of interest, such as mole fractions, are then calculated from the concentrations. We use a special calibration technique which allows us to get clear of any baseline problem: the results are insensitive to the baseline of the mixture spectrum as well as to the baselines of the calibration spectra.

The coexistence curves at different temperatures including the critical regions of several light-heavy hydrocarbon binary systems, such as squalane-methane and hexatriacontane-methane, have been determined and will be presented here. These results will be compared whenever possible with data previously obtained with other methods.