Study of the Phase Diagram of the (Carbon Dioxide + Caffeine) System at High Pressures by Combined Transitiometry and Thermodynamic Modeling

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Caffeine is not only interesting as a drug; it has been studied by crystallographers because of the unusually high disorder in its solid phases. The phase behaviour of the (carbon dioxide-caffeine) system is important for the industrial decaffeination of coffee beans, and has therefore been the objective of many publications. But still, the agreement of thermodynamic data of caffeine between different literature sources is moderate. We report new measurements of the solid-solid transition and the melting pressure curve up to 300 MPa. Furthermore, transitiometric scans were performed on the (CO_2-caffeine) system up to about 550 K and 100 MPa, which give evidence of several phase transitions. The system - fluid as well as both solid phases - was then modeled by (several) equations of state. Comparison of the experimental transitiometer traces and simulated traces from the thermodynamic model made it possible to identify the transitiometer peaks and to construct a thermodynamically consistent phase diagram of the system.

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