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Phase behaviour of neopentylglycol up to 700 MPa^{*}

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In 1990, Suenaga, Matsuo and Suga [1] published the heat capacities and phase transitions of neopentylglycol (2,2-dimethyl-1,3-propanediol) at low temperatures and pressures; here a solid-solid phase transition $(s_3 \rightarrow s_2)$ was observed at 60.4 K. In the present study, the phase behaviour of neopentylglycol was measured by high-pressure DTA in the temperature range 300-370 K at normal pressure and at pressures up to 700 MPa. The apparatus and measuring method have been described elsewhere [2-4]. The neopentylglycol was obtained from Aldrich (purity 99%) and used without further purification.

Fig. 1 shows three typical thermograms of neopentylglycol at approx. 440, 640 and 666 MPa as obtained in the present investigations. Fig. 2 shows the temperature (T)-pressure (p) phase diagram that results from the measurements.

The transition temperature for $s_2 \rightarrow s_1$ was found to be 315 K at normal pressure. As the apparatus is not suitable for low temperature measurements, the transition temperature for $s_3 \rightarrow s_2$ could not be determined at normal pressure. The s_2 phase is pressure-limited. It is destabilized at a triple point where the three solid phases, s_1 , s_2 and s_3 , coexist (363 K, 646 MPa); the triple-point data were obtained from extrapolations of the experimental T(p) curves by third-degree polynomials.

The investigations are continuing [5].

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Fig. 1. Original DTA thermograms of neopentylglycol at approximately constant pressure [5]; ΔT between reference and sample is plotted against *T*. During heating, the pressure increases slightly; the material was obtained from Aldrich (purity 99%); sample cell, closed, no contact with furnace atmosphere; reference cell, empty; heating rate 1 K min⁻¹; peaks correspond to endothermic phase transitions. (a) Phase transitions $s_3 \rightarrow s_2$ (306 K) and $s_2 \rightarrow s_1$ (353 K) at a pressure of about 440 MPa. (b) Phase transitions $s_3 \rightarrow s_2$ (361 K) and $s_2 \rightarrow s_1$ (363 K) at a pressure of about 640 MPa. (c) Phase transition $s_3 \rightarrow s_1$ (365 K) at a pressure of about 666 MPa.



Fig. 2. Temperature (T)-pressure (p) phase diagram of neopentylglycol [5].

Acknowledgement

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