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An experimental investigation of n-hexane at high temperature and pressure

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Abstract At present, no high temperature experiments on phase change are reported. In this study, we have measured the Raman bands $v_s(CH_3)$, $v_s(CH_2)$, $v_{as}(CH_3)$, and $v_{as}(CH_2)$ of *n*-hexane in a hydrothermal diamond cell up to 588 K. We determined that the liquid–solid phase transition pressure of *n*-hexane is 1.17 GPa, and we also gave a number of high temperatures and pressures data on phase change which are not reported previously. In addition, we defined the solidus of *n*-hexane which can be represented by the equation $P = 8.581T\text{-}1550.16$, and the relation $dP/dT = 8.581$ which can be used to calculate the thermodynamic parameters for *n*-hexane in the liquid–solid phase transition. For all we know, the above two equations are presented here for the first time. Furthermore, it is the first report here in a graphic way on high-temperature phase change in *n*-hexane, and it is also the first to be shown in the 3-D figure.

Keywords *n*-Hexane; Phase diagram; High temperature; Thermodynamic parameter; Hydrothermal diamond anvil cell; Raman spectroscopy

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