

ISOPLETHS OF ALKALI HYDRIDES

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The aim of present scientific work is the theoretical investigation of isopleths (the $\ln P$ dependence on inverse temperature $1/T$ at the constant limiting concentration S of hydrogen) of alkali hydrides, the calculation of formula for P-T-S curves, the substantiation and explanation of existing experimental data by change of isopleths slope and level, by coincidence of isopleths for some concentrations of MeH phase and also the prediction of possibility of new effects manifestation - the isopleths curvature. For that the calculation of thermodynamic potential of metals hydrides of B1 structure of NaCl type has been performed by the method of average energies. The pressure dependence of crystal volume, activity of hydrogen atoms and their interaction energies with nearest atoms of metal has been taken into account. The equilibrium equation has been investigated, the possible character of functional dependence of isopleths of hydrogen solubility in metals has been elucidated. It has been ascertained the physical parameters, which characterize the level, slope, confluence, non-linearity of isopleths.

The calculation results have been compared with experimental isopleths for LiH, KH, NaH hydrides, the constructed figures show good agreement between the obtained equation and the experimental data.

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