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Thermodynamic properties and the behavior of H_2O in Fe- and Mg-cordierite

E. Dachs (1), **C.A. Geiger** (2)

1. Department of Material Science & Physics, University of Salzburg, Austria (edgar.dachs@sbg.ac.at)
2. Institute for Geosciences, University of Kiel, Germany (chg@min.uni-kiel.de)

Cordierite, ideal formula $(Mg,Fe)_2Al_4Si_5O_{18}n(H_2O,CO_2)$, is a key volatile-bearing phase in many metamorphic rocks. Thus, knowledge of its thermodynamic properties is necessary for a variety of investigations on the nature of fluids in Earth's crust. In order to enable more quantitative thermodynamic calculations, heat capacity measurements between 5 and 300 K were carried out on synthetic samples of anhydrous low Fe-cordierite (Fe-Cd), as well as on anhydrous and hydrous low Mg-cordierite (Mg-Cd), using heat-pulse calorimetry (HPC).

From our HPC results, the standard entropy valuesat 298.15 K for anhydrous Fe-Cd, and anhydrous and hydrous Mg-Cd were calculated as 460.5 $\pm$ 0.5, 406.1 $\pm$ 0.4 and 450.9 $\pm$ 0.5 J/(mol·K), respectively. Heat capacity (C_p) polynomials for anhydrous and hydrous Fe- cordierite and anhydrous Mg-cordierite at T $>$ 270 K are:

C_p^{Fe-Cd} = 911.1 ($\pm$9.7) - 5829.2 ($\pm$363)·$T^{-0.5}$ - 13.9424 ($\pm$2.522) ·10^6 ·T^{-2}+

1470.4 ($\pm$454.84) ·10^6 ·T^{-3},

C_p^{hFe-Cd} = 967.3 ($\pm$9.7) - 6070.4 ($\pm$363)·$T^{-0.5}$ -13.9389 ($\pm$2.522) ·10^6 ·T^{-2}+

1470.4 ($\pm$454.84) ·10^6 ·T^{-3},

C_p^{Mg-Cd} = 882.0 ($\pm$4.9) - 5155.8 ($\pm$167)·$T^{-0.5}$ - 20.7584 ($\pm$0.806) ·10^6 ·T^{-2}+

2736.0 ($\pm$112.73) ·10^6 ·T^{-3},

as derived from the HPC data and published DSC data. Based on the data of Paukov et al. (2007), a C_p-polynomial for H_2O in hydrous Mg-cordierite was derived as:

$C_{p,H2O}^{hMg-Cd}$ = 56.17 ($\pm$0.44) - 241.2 ($\pm$4.5)·$T^{-0.5}$ + 3473.5 ($\pm$272.1)·T^{-2}-

11658.7 ($\pm$1420.3)·T^{-3}.

Using phase equilibrium data for the reaction 3 Fe-Cd·H_2O = 2 almandine + 4 sillimanite + 5 quartz + 3H_2O (Mukhopadhyay & Holdaway 1994), $\Delta_f H^o$ = -8448.26 kJ/mol was obtained for anhydrous Fe-Cd and the values $\Delta_f H^o$ = -8750.23 kJ/mol and S^o = 520.6 J/(mol·K) were derived for hydrous Fe-Cd. Phase relations in the FeO-Al_2O_3-SiO_2-H_2O system and isohydrons for H_2O in Fe-Cd were calculated and the phase diagrams constructed.

References

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