Fe- and Mg-cordierite: A calorimetric and thermodynamic study

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Cordierite is a key phase in many metamorphic rocks and it also has important technical applications in industry. Thus, knowledge of its thermodynamic properties is necessary for a variety of investigations. In order to enable more quantitative calculations, heat capacity measurements between 5 and 300 K were carried out on milligram-sized 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 values at 298.15 K for anhydrous Fe-Cd, anhydrous Mg-Cd and hydrous Mg-Cd were calculated as 460.5 ± 0.5, 406.1 ± 0.4 and 450.9 ± 0.5 J/(mol·K), respectively. Heat capacity (Cp) polynomials for anhydrous Fe- and Mg-cordierite at T > 250 K are:

$Cp^{\text{Fe-Cd}} = 911.1\ (\pm 9.7)\ - 5829.2\ (\pm 363)\cdot T^{-0.5}\ -13.9424\ (\pm 2.522)\cdot 10^{6}\cdot T^{-2} + 1470.4\ (\pm 454.84)\cdot 10^{6}\cdot T^{-3}$, and

$Cp^{\text{Mg-Cd}} = 882.0\ (\pm 4.9)\ - 5155.8\ (\pm 167)\cdot T^{-0.5}\ -20.7584\ (\pm 0.806)\cdot 10^{6}\cdot T^{-2} + 2736.0\ (\pm 112.73)\cdot 10^{6}\cdot T^{-3}$,

as derived from the HPC data and published DSC data.

Lattice and non-lattice contributions to the Cp values were modeled for Fe-Cd. The values $S^{o}_{vib} = 447.7$ J/(mol·K) and $S^{o}_{el} = 13.6$ J/(mol·K) were obtained for the vibrational and electronic contributions to the standard third law entropy.

Using phase equilibrium data for the reaction 3Fe-Cd·H_2O = 2almandine + 4sillimanite + 5quartz + $3H_2O$ (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 respective phase diagrams constructed.

References

Mukhopadhyay B., Holdaway, M.J. (1994) *Contrib. Mineral. Petrol.*, **116**, 462-472

Gas-particle partitioning, atmospheric deposition and long range transport of persistent organic pollutants over the oceans

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Gas-particle partitioning of persistent organic pollutants plays an important role on the atmospheric deposition and long range transport potencial of persistent organic pollutants. Aerosol organic and elemental carbon composition has been recognized as important bulk composition parameters controlling the distribution of POPs between gas and aerosol phases. However, sea salt aerosols and desert dust could play a role over some oceanic regions. Furthermore, atmospheric deposition of POPs will also be affected depending on this partitioning processes. On the other hand, trophic status of the ocean does also play a role as controlling factor of gaseous exchange and to lesser extend of dry deposition. In this work, gas-particle partitioning, deposition and long range transport are assessed in terms of aerosol and surface receiving geochemical processes. Results are shown for the tropical Atlantic, the Mediterranean sea and polar (Antarctic) waters.