Isobaric heat capacity data of orthorhombic FePO$_4$ in the temperature range between 223 K to 773 K

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The orthorhombic iron(III)-phosphate (FePO$_4$) with the space group $Pnma$ reversibly intercalates lithium ions under reducing conditions. Hence, FePO$_4$ raised a lot of attention since 1997 [1] because of its potential application as cathode material in lithium ion batteries (LIB). Despite its huge relevance to industry and research the availability of reliable thermodynamic data of FePO$_4$ is presently limited to the low temperature range of 2 K to 300 K.

This contribution focuses on the experimental determination of precise isobaric heat capacity values $c_p$ between 223 K and 773 K using two different types of calorimeters. A power compensation twin-type calorimeter DSC 8000 from PerkinElmer equipped with the external cooling unit IntraCooler II was applied in the temperature range from 223 K to 553 K. The sample was pressed manually to a flat pellet in order to gain a good thermal conductivity inside the sample. The measurement was continuously performed in intervals of 100 K each. In the temperature range between 298 K and 773 K the heat flux calorimeter Sensys DSC from Setaram was utilised and the sample was densely packed into a stainless steel crucible, which was tightly crimped with a nickel sealing ring. In contrast to the measurement with the DSC 8000, the heat capacity was determined via the $c_p$-by-step approach with temperature steps $\Delta T$ of 10 K. Prior to the measurements, both calorimeters were calibrated with a sapphire standard.

The resulting $c_p$-data of both calorimeters are identical within the experimental error of 1 % to 2 % and fit perfectly to the low temperature heat capacity data of Woodfield et al. [2]. Consequently, the presented results for $c_p$ of orthorhombic FePO$_4$ are very reliable and can improve the quality of further CALPHAD calculations in the temperature interval from 300 K to 773 K.