DEBYE-EINSTEIN MODELS FOR HEAT CAPACITIES OF CRYSTALLINE SOLIDS

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Low temperature experimental data of the heat capacities of carbonates (e.g. BISSENGALIYEVA et al., 2012), molybdates (e.g. MORISHITA et al., 2016) and hollandites (WU et al., 2016) are assessed by means of semi-empirical models. Previous studies frequently present fit functions with a large amount of coefficients resulting in almost perfect agreement with experimental data. It is, however, demonstrated in this work by both local and global minimization tools that special care is required to avoid overfitting. The temperature dependent heat capacities are described by relatively simple Debye-Einstein integrals with sufficient accuracy. In case that experimental data below 50K are lacking heat capacities can be extrapolated reasonably well to lower temperatures, i.e. from 50K to absolute zero by the Debye-Einstein integral (GAMSJÄGER et al., 2016). It is suggested to establish the Debye Einstein integral fit as standard method to describe molar heat capacities in the low temperature range between almost 0K and 300K. Thereby, the derived thermodynamic functions are obtained on the same theory-related semi-empirical basis.

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