First principles study of the high temperature partition function and heat capacity of the OH - anion

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Abstract

First principles study of the partition function and heat capacity of OH - anion is conducted at high temperatures (2000K-10,000K). Firstly, with the quantum chemical ab inito methods (RASSCF with CASPT2 correction) were used to cal- culate potential energy curves of the ground and excited electronic states; the energy points were fitted to analytical representation of the curves. Secondly, the statistical thermodynamics calculations with the classical method with the quantum Wigner-Kirkwood correction were performed to obtain partition func- tion and heat capacity. Thermochemical tables and datasets usually give quantities up to 6000K (sometimes even more) and often are not reliable at the highest temperatures, it is shown that in particular electronic excited states could be missing. Parti- tion function is compared with the only available Barklem and Collet dataset. Discrepancies between heat capacity data (given in NIST-JANAF and Burcat databases) are pointed out - the inclusion of excited electronic states is crucial.

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