more experimental evidences. The simulation of energy levels structure of Sm^{3+} ions in $SmAl_2$ for orbital–only ordering mechanism is shown on fig.7.

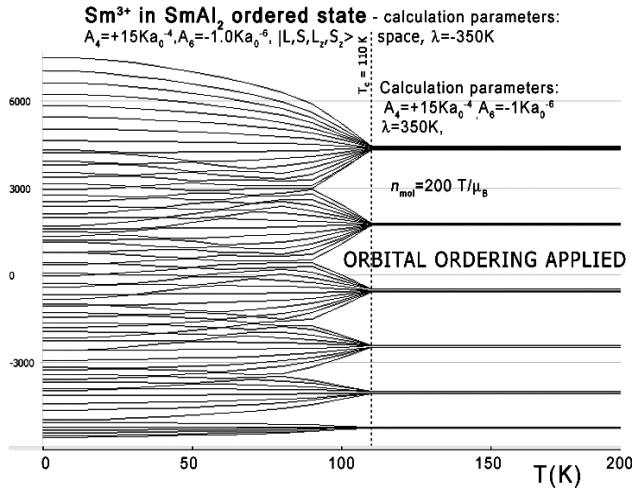

Fig.7. The result of calculations of energy levels structure vs. temperature $4f^5$ electronic system of Sm^{3+} in $SmAl_2$ calculated according to orbital coupling in $|LS,L_z,S_z>$ space.

5 Conclusions

We performed calculations for $SmAl_2$ electronic and magnetic properties using the ATOMIC MATTERS MFA computation system. The local symmetry of the Sm ions is cubic, which significantly simplifies the analyses and gives chance to evaluate calculation methodology itself. Very good agreement of obtained magnetic properties and experimental data confirms the effectiveness of our theoretical approach. Working with ATOMIC MATTERS MFA revealed its high usefulness. The visual form of calculationresults, full 3D interactive CEF potential visualization, intuitive tools for convention and unit recalculation, and the ability to compare data results all allow the user to utilize the power of the application very effectively. In conclusion, we confirm that ATOMIC MATTERS MFA is a unique application that combines a package of tools for correctly describing the physical properties of atomic-like electron systems subjected to electromagnetic interactions in real materials. This is an accurate tool for calculating properties of ions under the influence of the electrostatic potential of definable symmetry and both external and inter-ionic magnetic fields taken as a mean field approximation in magnetically ordered state. This paper is our 4th in a series devoted to the RAl_2 (R=rare earth) compounds family.

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