LETTERS TO THE EDITOR

COMMENT ON ACTA PHYS. POL. B 32 (2001) 3303 PAPER BY A.M. OLEŚ "MAGNETIC ORDER IN TRANSITION METAL OXIDES WITH ORBITAL DEGREES OF FREEDOM"

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We argue that the $^3A_2$ state considered by Oleś in *Acta Phys. Pol. B* **32**, 3303 (2001) for the d^2 system occurring in the V^{3+} ion in V_2O_3 and $LaVO_3$ as well as in Ti^{2+} ion in TiO and in many other oxides is wrong. The proper ground state is $^3T_{1g}$ — its 9-fold degeneracy is further split in a crystal by intra-atomic spin-orbit interactions and lattice distortions.

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Oleś in *Acta Phys. Pol. B* **32**, 3303 (2001) [1] presents in Fig. 1 excitations spectra for d^8, d^5, d^2 and d^3 systems. According to Fig. 1(b) excitations spectra in cubic transition metal oxides for d^2 ions have the ground state $^3A_2$ and higher states $^1T_2$, ^1E and $^1A_1$. According to us this ground state is wrong. For the d^2 system in the octahedral anion surrounding the ground state is $^3T_{1g}$ [2, 3]. The state $^3T_{1g}$ is completely different from the Oleś ground state $^3A_2$ — the latter has 3-fold degeneracy whereas the former — 9-fold degeneracy. The state $^3A_2$ is the orbital singlet whereas $^3T_{1g}$ is an orbital triplet. This difference is of fundamental importance in modern solid-state physics owing to widely discussed properties of V_2O_3, $LaVO_3$ and

YVO_3 not mention TiO or CrO_2. Behind these states is completely different physics. By this Comment we would like to clarify the ground state of the V^{3+} and Ti^{2+} ions in the octahedral crystal field as it becomes at present a subject of strong discussion.

The ${}^3T_{1g}$ state as the ground state in the d^2 system occurring in V_2O_3 has been calculated by us for the SCES-02 Conference [5]. This ground state in the solid compound (3d ions form the crystallographic lattice) is in agreement with the ground state discussed in Ref. [4] for the d^2 ions dissolved in a lattice as impurities. For the scientific honesty we have to say that there is at present much more scientists who came out to completely different description of $3d$ electrons ignoring the atomic integrity of the $3d$ ion, what is visible in no using the atomic many-electron notation. In a recent paper by Horsch *et al.* [6], of which Oles is the coauthor, a state ${}^3T_2$ is mentioned to be the ground state of V^{3+} ions in V_2O_3. However, there was no explanation for the change of the ground state compared to the commented paper.

In conclusion, we argue that the ${}^3A_2$ state considered by Oleś in the commented paper for d^2 system occurring in the V^{3+} ion in V_2O_3 and $LaVO_3$ as well as in Ti^{2+} ion in TiO and in many other oxides is wrong. The proper ground state for the octahedral crystal field is ${}^3T_{1g}$ — its 9-fold degeneracy is further split in a crystal by intra-atomic spin-orbit interactions and lattice distortions.

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