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EPR and ENDOR of two axial Fe³⁺ centers in stoichiometric lithium tantalate VALENTIN GRACHEV, GALINA MALOVICHKO, ROBERT PETERSEN, Physics Department, Montana State University, CHRISTOFF BAEUMAN, Department of Physics, University of Osnabrück, D-49069, Osnabrück, Germany — The determination of structures of centers in oxide crystals created by impurity ions, including those of transition metals and rare- earth elements, is one of the most important tasks in defect study. The iron ions play a key-role in the photovoltaic and photorefractive effects, holographic records and many other physical properties of lithium tantalate. The axial Fe³⁺ center, Fe1 with the crystal field parameter $b_2^0 \approx 0.313$ 1/cm is well studied in congruent lithium tantalate crystals. Using the EPR we have discovered and investigated a new axial Fe³⁺ center, Fe2 in stoichiometric samples prepared by vapor transport equilibrium treatment. The crystal field parameter of the Fe2 center $b_2^0 \approx 0.205$ 1/cm is significantly smaller than for Fe1. The ENDOR measurements have shown that hyperfine interactions of the Fe³⁺ electrons with the surrounding Li nuclei for Fe2 are stronger than for Fe1. Therefore, the conclusion was made that in the case of Fe2 center the iron ion substitutes for Ta and has Li nuclei in the nearest neighborhood, whereas in the case of Fe1 it substitutes for Li, has Ta nuclei as nearest neighbors and Li nuclei in the second shell only.

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