Fluorite-Type Solid Solutions in the System Y-Ta-O-N: A Nitrogen-Rich Analogue to Yttria-Stabilized Zirconia (YSZ)

H. Schilling[a], H. Wolff[b], R. Dronskowski[b], and M. Lerch[a]

[a] Institut für Chemie, TU Berlin, Straße des 17. Juni 135, D-10623 Berlin
[b] Institut für Anorganische Chemie, RWTH Aachen, Landoldtweg 1, D-52056 Aachen

Reprint requests to Prof. Dr. M. Lerch. E-mail: Lerch@chem.tu-berlin.de

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Fluorite-type phases in the system Y-Ta-O-N have been prepared by ammonolysis of Y-Ta-O precursors. X-ray powder patterns show unusual asymmetrical reflection profiles explained by DFT and MD methods. The anion vacancy concentration of some of these oxynitrides is similar to that of yttria-doped zirconia, commercially used as solid electrolyte in fuel cells. Hence, these compounds are interesting candidates for mixed oxygen-nitrogen superion conductors.

Key words: Tantalum Oxynitride, Fluorite-Type Structure, Synthesis, Computational Chemistry