HIGH RESOLUTION SPECTROSCOPY OF THE $[18.0]^2\Pi_{3/2}$ - $X^2\Sigma^+$ TRANSITION OF THORIUM NITRIDE, ThN[a]

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Serious draw backs to nuclear power include long-term nuclear waste storage and amelioration of the existing waste. The 4% enriched uranium fuel used in a typical light water reactor is converted to spent nuclear fuel (SNF) made up of 3% fission products, of which $\sim$30% are lanthanides (Ln), and 1% transuranium actinide (Ac) elements Np, Pu, Am and Cm. Partitioning of the Ln from the Ac present in the SNF by developing element-specific ligands for solvent extraction is a one of the most challenging facet of nuclear waste processing.[b] Systematic experimental and theoretical studies of simple Ac and Ln containing molecules is one avenue for garnering insight into element-specific ligation.[c] As part of an effort to establish trends in Th-X bonding, a combined experimental and theoretical study of ThN has been undertaken. High-resolution ($\sim$30MHz) LIF spectroscopy, both field-free and in the presence of static magnetic and electric fields, were recorded. A strong band near 555 nm, which was not previously detected via REMPI spectroscopy [b] has been assigned to a $[18.0]^2\Pi_{3/2}$ - $^2\Sigma^+$ transition. The determined fine structure parameters, electric dipole moments, and magnetic g-factors will be discussed in terms of the present, and previous[b], ab initio predictions.

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[b]Leoncini, A.; Huskens, J.; Verboom, W., Ligands for f-element extraction used in the nuclear fuel cycle. Chem. Soc. Rev. 2017, 46 (23), 7229-7273.

[c]Heaven, M. C.; Barker, B. J.; Antonov, I. O., Spectroscopy and Structure of the Simplest Actinide Bonds. J. Phys. Chem. A 2014, 118 (46), 10867-10881.