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Spectroscopic studies of Th-containing molecules relevant to physics and chemistry¹

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ThO[1]: The current upper limit for the magnitude of the electron electric dipole moment (eEDM), $|d_e|$, is 8.710^{-29} e-cm and has been determined in an experiment involving the $H^3\Delta_1(v=0)$ state of thorium oxide, ThO [2]. An improved determination of the upper limit for $|d_e|$ would be an effective route for assessing extensions to the Standard Model; many such extensions predict a $|d_e|$ of approximately 10^{-29} e-cm. Here we will report on the spectroscopic characterization of an electronic transition that will be used in a new optical pumping and detection schemes to search for $|d_e|$. **Th₂[3]:** Understanding the chemistry of the early to middle actinide elements (Th-Cm) is critical to the nuclear energy industry for the development of efficient enrichment methods as well as methods for waste remediation. Given the hazards of dealing with these elements, computational chemistry is often used to predict their properties. Such predictions can only be tested by comparison with experimental data available for small gas-phase, Th-containing molecules. Bonding in Th₂, and other actinides dimers, has been theoretically investigated using multiconfiguration wave function based methods (CASSCF/CASPT2) [4] to predict twelve electronic states all within 1 eV of the ground state. These 12 states give rise to 29 spin-orbit components. Here we report on the first observation of resonant transitions of thorium dimer, Th₂, and evaluate the theoretical predictions. **ThS[5]:** Thorium monosulfide (ThS) is an ideal model system for studies of the interactions between an actinide and a soft donor ligand. Here we report on the results of a separated field, pump/probe microwave optical double resonance measurement of the pure rotational transitions of Th³²S $X^1\Sigma^+$. This is the first example of a microwave study of an actinide compound that is not an oxide. The versatility and precision of the spectroscopic method will be outlined.

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References

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