

Correction to Spectroscopy and Structure of the Simplest Actinide Bonds

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In the discussion of the results for the ThF^+ ion, we presented evidence in support of the assignment of the ground state as $X^1\Sigma^+$. The evidence consisted of a rotationally resolved vibronic band that appears to exhibit an $R(0)$ line (Figure 7). The viable alternative assignments for the ground state are $^1\Sigma^+$ and $^3\Delta_1$. Observation of the $R(0)$ line indicates that the former is correct. However, high-resolution spectra recorded by Gresh et al.¹ now show definitively that the ground state is $X^3\Delta_1$. We have subsequently reinvestigated the origin of the rotational line that we had assigned as $R(0)$. We find that this can be reasonably reassigned as the $R(21)$ line. Although the rotational temperature of the low-energy rotational levels was on the order of 20 K, additional modeling shows that the population of the higher J levels was not consistent with a Boltzmann distribution due to the kinetic limitations of jet cooling. The population residing in $J = 21$ was sufficient to produce a significant feature at the $R(0)$ position. We are therefore in agreement with Gresh et al.'s¹ reassignment of the ground state as $X^3\Delta_1$.

■ REFERENCES

(1) Gresh, D. N.; Cossel, K. C.; Zhou, Y.; Ye, J.; Cornell, E. "Broadband velocity modulation spectroscopy of ThF^+ for use in a measurement of the electron electric dipole moment" *J. Mol. Spectrosc.* Submitted.

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