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Theoretical Fit fo Experimental Observations of Energy Level Structure in the Cs₂ $a^{3}\Sigma_{u}^{+}$ State¹ T. BERGEMAN, SUNY Stony Brook, S. SAINIS, Yale, E. TIESINGA, NIST, D. DEMILLE, Yale — Precision measurements [1] on 27 hyperfine/rotational levels from 6 vibrational levels of the Cs₂ $a^{3}\Sigma_{u}^{+}$ state, with binding energies as large as 50 cm⁻¹, have been performed. The objective is to identify suitable transitions to probe the energy difference between a level of a shallow bound state (a) and a level of a more deeply bound state $(X^1\Sigma_q^+)$ to be used ultimately to study the time variation of the electron to proton mass ratio [2]. It is therefore important to characterize the singlet-triplet (X - a) mixing due to hyperfine interactions. We have modeled the energy level structure by using a Hund's case e asymptotic representation for the hyperfine interaction and rotational energy, and a case *a* representation for the Born-Oppenheimer potentials and second-order spin-orbit (SO) interactions, with transformations between the two representations. Potentials and SO effects are adjusted to optimally fit the data. Currently, the rms residual from the fit is about twice the 30 MHz uncertainty for energy differences within each vibrational level.

1. S. Sainis, Ph. D. Thesis, Yale U., 2005.

2. D. DeMille *et al.*, to be published.

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