THE $^1\Pi$ STATES OF NaCs: SPECTROSCOPY, LIFETIMES, PERMANENT AND TRANSITION DIPOLE MOMENTS.

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The NaCs molecule is one of the prospective objects for production of ultracold polar molecules. LIF Fourier transform spectroscopy study is presented for the $(1,3)^1\Pi$ states with 0.03 cm^{-1} resolution. Potential energy curves (PECs) are obtained by the Inverted Perturbation Approach reproducing $(3)^1\Pi$ state[a] energies for R = 3 to 11 Å. In the $B(1)^1\Pi$ state we accounted for numerous $B(1)^1\Pi \sim c^3\Sigma^+$ perturbations by omitting perturbed levels for the fit to construct the PEC for R = 2.6 to 8.4 Å.
The permanent electric dipole moments d and the Λ-splitting were measured[b] by dc Stark mixing and electric RF-optical double resonance methods yielding d within 5 - 8 D for $(3)^1\Pi$ and $d \sim 1$ D for the $D(2)^1\Pi$ ($v < 3$) state. The radiative lifetimes τ were measured from LIF kinetics as τ = 29 to 21 ns for $(3)^1\Pi$ (v = 3 to 25) and τ = 37 ns for $D(2)^1\Pi$ (v = 0).
The measured data are supported by electronic structure calculations for the $(1\text{-}3)^1\Pi$ states[b] by many-body multipartitioning perturbation theory of PECs, permanent and transition dipole moments, as well as angular coupling matrix elements for the lowest singlet states. The predicted d values reproduce their experimental counterparts within the measurement errors. Lifetimes for the $(1\text{-}3)^1\Pi$-states have been calculated in Hund's "a" coupling case using the approximate sum rule over the lower vibronic states. The spectra and formation rates of ultracold NaCs in the $X^1\Sigma^+$ (v = 0, J = 0) state were simulated for the optical cycle $a^3\Sigma^+ \rightarrow B(1)^1\Pi \sim c^3\Sigma^+ \sim b^3\Pi \rightarrow X^1\Sigma^+$.
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[a] O. Docenko et al *J. Chem. Phys.*, **124**, 174310, 2006.
[b] J. Zaharova et al *J. Chem. Phys.*, **124**, 184318, 2006.