RELATIVISTIC JAHN-TELLER EFFECTS IN THE QUARTET STATES OF K_3 AND RB_3: A VIBRATIONAL ANALYSIS OF THE $2^4E' \leftarrow 1^4A_2'$ ELECTRONIC TRANSITIONS BASED ON AB INITIO CALCULATIONS

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We apply the Multireference Rayleigh Schrödinger Perturbation Theory of second order to obtain the adiabatic potential energy surface of the $1^4A_2'$ electronic groundstate and the $2^4E'$ excited state of K_3 and Rb_3. Both trimers show a typical E×e Jahn-Teller distortion in their $2^4E'$ state, which is analyzed in terms of the relativistic Jahn-Teller effect theory. Linear, quadratic as well as spin-orbit coupling terms are extracted from the *ab initio* results and used to obtain theoretical spectra for a direct comparison to laser-induced fluorescence and magnetic circular dichroism spectra of alkali-doped helium nanodroplets [Auböck et al. J. Chem Phys. **129** 114501 (2008)].