ACCIDENTAL CONICAL INTERSECTIONS IN MIXED TRIMERS OF POTASSIUM AND RUBIDIUM: A VIBRONIC ANALYSIS OF THE 4^4B_2 AND 3^4A_1 STATES

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We compare the 3^4A_1 and 4^4B_2 states of homonuclear and heteronuclear alkali trimers formed of potassium and rubidium. The Multireference Rayleigh Schrödinger Perturbation Theory of second order is applied to obtain the corresponding adiabatic potential energy surfaces. In the case of homonuclear trimers these pairs of states correspond to the two branches of the E$\times$e Jahn-Teller distorted $2^4E'$ state. For heteronuclear trimers, the vibrational modes Q_x and Q_y are no longer degenerate, but the two electronic states still show a conical intersection at obtuse (KRb_2) or acute (K_2Rb) isosceles geometries. Spectroscopic consequences of this situation are discussed, vibronic spectra are predicted and compared to LIF spectra obtained in helium droplet isolation spectroscopy experiments of our group[b,c].

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