COMBINED DUNHAM ANALYSIS OF ROTATIONAL AND ELETRONIC TRANSITIONS OF CH+

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A Dunham analysis of the $A^1\Pi-X^1\Sigma^+$ band was carried out by Müller, and predictions of the pure rotational transition frequencies were made.^a More recently, in submillimeter to THz region, several rotational lines were observed for $^{12}\mathrm{CH}^+$, $^{13}\mathrm{CH}^+$, and CD^+ .^{bcd} In this investigation, those newly obtained rotational lines are incorporated in the Dunham analysis. The Λ -doubling splittings in $^1\Pi$ electronic states have been expressed as (1/2)qJ(J+1) in most investigations. However, it should be noted that the e-levels of $^1\Pi$ state interact with $^1\Sigma^+$ states, while the f-levels with $^1\Sigma^-$ states. For CH^+ , the e-levels of $A^1\Pi$ are pushed upward from the interaction with the ground $X^1\Sigma^+$ state. The $^1\Sigma^-$ states are not known experimentally and they, if any, should lie high over the $A^1\Pi$ state. In this analysis, only the f-levels are included in the least-squares analysis by neglecting the Λ -doubling. The mass independent parameters have been obtained, and the conventional spectroscopic parameters are derived for each isotopologue. These results should be useful for determining the potential energies of this fundamental ion.^e

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