THE NEAR-INFRARED SPECTRUM OF CH_2^+

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The molecular ion CH_2^+ is of special theoretical interest because it is both quasi-linear and exhibits a strong Renner-Teller interaction between its ground and first-excited electronic states. At linearity, the ground state is a $^2\Pi_u$ state that splits into $\tilde{X}^2A_1$ and $\tilde{A}^2B_2$ states as the molecule bends. The $\tilde{A}$ state is linear, while the $\tilde{X}$ is quasi-linear with a barrier to linearity of only 1089 cm^{-1}. Thus, only the ground vibrational state is bound by the barrier to linearity.

The spectrum of CH_2^+ in the region 11,000–13,000 cm^{-1} has been recorded with our Ti:sapphire laser spectrometer. This spectrometer couples velocity modulation with heterodyne detection for near shot-noise-limited sensitivity. Since our initial letter on this spectrum,[a] we have selectively rescanned portions of this spectrum with improved signal-to-noise. As a result, we have been able to assign the $\tilde{A}(0,3,0)^3 \leftarrow \tilde{X}(0,0,0)^2$ band and detect the $\tilde{X}(0,9,0)^2 \leftarrow \tilde{X}(0,0,0)^1$ band, whose assignment is in progress. A more detailed analysis of the entire spectrum, including spin splitting, is underway.

[a] J. L. Gottfried and T. Oka, *J. Chem. Phys.* **121**, 11527 (2004).