THE $\tilde{A}(0,8,0)^1 \leftarrow \tilde{X}(0,0,0)^2$ AND $\tilde{A}(0,8,0)^3 \leftarrow \tilde{X}(0,0,0)^2$ BANDS OF CH_2^+

CHRISTOPHER F. NEESE, JENNIFER L. GOTTFRIED, and TAKESHI OKA, *Department of Chemistry, Department of Astronomy & Astrophysics, and the Enrico Fermi Institute, The University of Chicago, Chicago IL, 60637, USA*.

The methylene 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 $\tilde{X}$ state is quasi-linear with a barrier to linearity of only 1089 cm^{-1}.

Recently, the spectrum of CH_2^+ in the region 10,700–11,000 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. In this new spectrum we have assigned the $\tilde{A}(0,8,0)^1 \leftarrow \tilde{X}(0,0,0)^2$ and $\tilde{A}(0,8,0)^3 \leftarrow \tilde{X}(0,0,0)^2$ bands.[a] These bands are the first high-resolution detection of $K_a = 2$ levels for the ground state. In addition, the $\tilde{A}(0,8,0)^1 \leftarrow \tilde{X}(0,0,0)^2$ can be combined with the previously studied $\tilde{A}(0,8,0)^1 \leftarrow \tilde{X}(0,0,0)^0$ band[b] to produce $K_a = 2 - 0$ combination differences for the ground state. These combination differences provide the first high-resolution information about the ground state A rotational constant.

[a] The $\tilde{X}$ state is labeled using bent notation and the $\tilde{A}$ state is labeled using linear notation.

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