ELECTRONIC SPECTRUM OF THE AlC₂ RADICAL

EVAN B. JOCHNOWITZ, EGOR CHASOVSKIKH, EUNSOOK KIM, and JOHN P. MAIER, Department of Chemistry, University of Basel, Klingelbergstrasse 80, CH-4056 Basel, Switzerland; ISABELLE NAVIZET, Laboratoire de Chimie Théorique, Université de Marne-la-Vallée, F-77454 Champs sur Marne, France.

An electronic transition of the AlC₂ radical (C₃ᵥ structure) has been observed using laser induced fluorescence spectroscopy. The molecule was prepared in a supersonic expansion using laser ablation of an aluminum rod in the presence of acetylene gas. A spectrum was recorded and assigned to the $\hat{C} \ 2B₂ - \hat{X} \ 2A₁$ system based on a rotational analysis and agreement with calculated molecular parameters and excitation energies. Ab initio results are in accord with previous theoretical studies which conclude that AlC₂ possesses a triangular $C₃v \ 2A₁$ geometry, with the linear $C_{∞v} \ 2Σ^+$ AlCC isomer 0.70 eV higher in energy. A spectral fit yields molecular constants both in the ground and electronically excited states.