ELECTRONIC SPECTROSCOPY OF Be_2: EXPERIMENTAL AND THEORETICAL RESULTS

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Low-lying electronic states of Be_2 have been examined using laser excitation techniques. The dimer was formed by pulsed laser ablating Be into a free-jet expansion. Dimer formation was enhanced by liquid nitrogen cooling of the nozzle assembly.

Dispersed fluorescence spectra were recorded following excitation of various vibrational levels of the $B\ ^1\Sigma_u^+$ state. These spectra revealed bands of the previously unobserved $B\ ^1\Sigma_u^+ \longrightarrow A'\ ^1\Pi_g$ transition. The term energy (T_0=13,942$\pm$20cm^{-1}) and vibrational interval $\Delta G_{1/2}$ =717$\pm$20cm^{-1}) for the A' state were determined for the first time.

Potential energy curves and electronic transition moments for Be_2 were calculated using EOM coupled cluster and MRSDCI levels of theory with a (12s6p3d2f1g)/[5s4p3d2f1g] basis set. The properties of low-lying singlet, triplet, and quintet states were predicted. The MRSDCI results were found to be in excellent agreement with experimental observations[a]

[a] V. E. Bondybey, Chem. Phys. Lett. **109**, 436 (1984)