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A new $C^3\Sigma_u^- - X^3\Sigma_g^-$ transition of the V_2 molecule

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The high resolution electronic transition spectrum of the vanadium dimer (V₂) molecule in the visible region between 480 and 528 nm has been observed using laser ablation free jet expansion and laser-induced fluorescence (LIF) spectroscopy. Six vibrational bands have been recorded and analyzed, they belong to two groups of sub-band transitions: $1_u - 1_g$ and $0_u^+ - 0_g^+$, which is very well correspond to a ${}^3\Sigma_u^- - {}^3\Sigma_g^-$ transition. Since the ground state is $X^3\Sigma_g^-$, these bands were assigned to a new $C^3\Sigma_u^- - X^3\Sigma_g^-$ transition.

Rotational analysis has been performed to these bands and the measured line positions were fit by a least squares routine, which yielded molecular constants for the v=0 level of the excited $C^3\Sigma_u^-$ state. The measured vibrational separation, $\Delta G_{1/2}$, and bond length, r_o , of the $C^3\Sigma_u^-$ state are respectively 393.04 cm⁻¹ and 2.029 Å in this work. A molecular orbital energy level diagram has been used to aid the assignment of the newly identified $C^3\Sigma_u^- - X^3\Sigma_g^-$ transition, which is likely to arise from the promotion of an electron from the $d\delta_g$ to the $d\delta_u$ molecular orbitals. Detailed analysis of the electronic structure of the V_2 dimer and a comparison of similar metal dimer molecules will be presented.

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