

EXCITED STATES OF THE DIATOMIC MOLECULE CrHe

JOHANN V. POTOTSCHNIG, MARTIN RATSCHKEK, ANDREAS W. HAUSER and WOLFGANG E. ERNST, *Institute of Experimental Physics, TU Graz, Petersgasse 16, 8010 Graz, Austria.*

Chromium (Cr) atoms embedded in superfluid helium nanodroplets (He_N) have been investigated by laser induced fluorescence, beam depletion and resonant two-photon ionization spectroscopy in current experiments at our institute. Cr is found to reside inside the He_N in the a^7S ground state. Two electronically excited states, z^7P and y^7P , are involved in a photoinduced ejection process which allowed us to study Fano resonances in the photoionisation spectra^a. The need for a better understanding of the experimental observations triggered a theoretical approach towards the computation of electronically excited states via high-level methods of computational chemistry. Two well-established, wave function-based methods, CASSCF and MRCI, are combined to calculate the potential energy curves for the three states involved. The character of the two excited states z^7P and y^7P turns out to be significantly different. Theory predicts the ejection of the Cr atom in the case of an y^7P excitation as was observed experimentally^b. The quasi-inert helium environment is expected to weaken spin selection rules, allowing a coupling between different spin states especially during the ejection process. We therefore extend our theoretical analysis to the lowest state in the triplet- and quintet- manifold. Most of these alternative states show very weak bonding of only a few cm^{-1} .

^aA. Kautsch, M. Hasewend, M. Koch and W. E. Ernst, *Phys. Rev. A* 86, 033428 (2012).

^bA. Kautsch, M. Koch and W. E. Ernst, *J. Phys. Chem. A*, accepted, doi:10.1021/jp312336m