

PHOTOIONISATION STUDIES OF TANTALUM-CARBON CLUSTERS

G.F. Metha, G.M. Stewart and M.A. Buntine

Department of Chemistry, University of Adelaide, South Australia 5005.

The laser ablation method has revolutionised the synthesis of refractory element containing molecules. In combination with supersonic expansions, this has become a powerful and versatile method for producing diatomic transition-metal carbides such as CoC, FeC and NbC for spectroscopic investigation. Recently, larger metal-carbon cluster molecules have been generated and studied such as Nb<sub>3</sub>C<sub>2</sub> [1] and Y<sub>3</sub>C<sub>2</sub> [2]. The method involves reacting laser ablated transition-metals with a selected precursor gas (*e.g.* CH<sub>4</sub> or C<sub>2</sub>H<sub>2</sub>) seeded in helium or argon. Many complex reactions occur forming various exotic molecules and radical species which are then introduced into a vacuum chamber whereby the molecules undergo supersonic expansion. The rapidity of this expansion ensures that even species with extremely short lifetimes become isolated from one another in their lowest internal energy states. The usual probes for these molecules involve ionisation techniques like Resonance Enhanced Multi Photon Ionisation (REMPI) and Pulsed Field Ionisation-Zero Electron Kinetic Energy (PFI-ZEKE).

Recently, we have generated neutral tantalum-carbon clusters of the form Ta<sub>n</sub>C<sub>m</sub> (*n* ≥ 1, *m* ≥ 1) following the reaction of laser ablated tantalum and acetylene. Similar ionic clusters have been observed previously in a Fourier transform ion cyclotron mass spectrometer [3]. The neutral species are subsequently ionised by laser initiated non-resonant multi-photon ionisation at 532 and 355 nm and injected into a reflectron time of flight mass spectrometer. By measuring the intensity of each species as a function of laser power, it is possible to determine an energy range for the ionisation potential (IP) of each species. Although the ionisation potentials generally decrease with cluster size, there are some marked deviations such as TaC which shows an unusually high IP. Work is currently underway utilising a tunable dye laser to accurately determine the IP of each tantalum-carbon species.

[1] D.-S. Yang, M. Zgierski, A. Berces, P. Hackett, P-N Roy, A. Martinez, T. Carrington, D. Salahub, R. Fournier, T. Pang and C. Chen, *J. Chem. Phys.*, **105**, 10663-10671 (1996)

[2] D.-S. Yang, M. Zgierski and P. Hackett, *J. Chem. Phys.*, **108**, 3591-3597 (1998)

[3] S. McElvany and C. Cassady, *J. Amer. Chem. Soc.*, **94**, 2057-2062 (1990)