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Synopsis The electronic structures of nicotine, nicotinic acid and nicotinamide have been studied by valence photoemission spectroscopy (PES), core X-ray photoelectron spectroscopy (XPS), and near-edge X-ray absorption fine structure (NEXAFS) and interpreted with the aid of quantum chemical calculations. Nicotinamide and nicotinic acid are closely related and show correspondingly similar spectral features, while nicotine is both structurally and spectroscopically diverse.

We report results on three biologically important derivatives of pyridine: nicotine ($C_{10}H_{14}N_2$, m=162 u), nicotinic acid ($C_6H_5NO_2$, m=123 u), and nicotinamide ($C_6H_6N_2O$, m=122 u). They are pharmacologically important chemicals for their psycho-active properties (nicotine), and as vitamins (nicotinic acid, vitamin B3, and nicotinamide, provitamin B3)

The ionization potentials and outermost valence ionic states of nicotinic acid and nicotinamide [1, 2] as well as calculations of the valence bands [2, 3] have been reported. No gas phase core level spectra are available so far and we report them here.

We have measured valence band (VB) photoelectron spectra (Figure 1), as well as core level carbon, nitrogen, and oxygen 1s X-ray photoemission and near edge X-ray absorption fine structure spectra. In addition, we have carried out quantum chemical calculations using the OVGF model for the valence bands and Core Electron Binding Energy model for the core levels [4]. XPS probes the chemical state of the molecule because the binding energy shifts depend on the chemical environment of the atom that is ionized, while VB spectra and NEXAFS provide complementary information about the occupied and unoccupied valence states. Measurements were performed at the GasPhase Photoemission beamline of Elettra-Sincrotrone Trieste, Italy. Results and their interpretation in the light of our quantum chemical calculations will be presented.

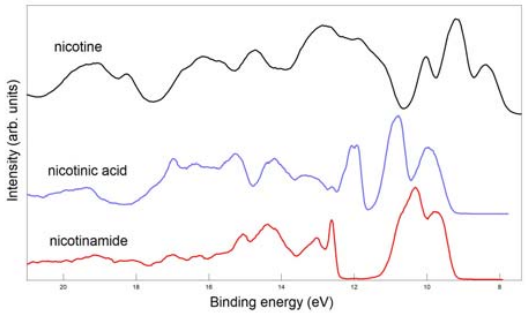

Figure 1. Valence band photoelectron spectra of nicotine, nicotinic acid, and nicotinamide measured at 100 eV photon energy [5].

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