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Electronic and Vibrational Properties of Ultra-Low Ionization Potential Molecules. NASRIN MIRSALEH KOHAN, University of Tennessee, WESLEY ROBERTSON, Emory University, JEFF STEILL, JOHN TURNER, CHARLES FEIGERLE, RICHARD PAGNI, ROBERT COMPTON — The ionization potentials (IPs) of the tetrakis(dimethylamino)ethylene($C_{10}H_{24}N_4$, TDAE) molecule and the recently synthesized 1,2,3,4,5,6,7,8-octahydro-2a,4a,6a,8a-tetraazacyclopenta[fg]acenaphthylene ($C_{10}H_{16}N_4$,OTCA) molecules are comparable to that of some alkali atoms making them useful in a number of applications. High resolution electron impact ionization of TDAE was studied using a trochoidal electron monochromator mated to a linear time-of-flight mass spectrometer. The energy threshold for the formation of the parent ion was found to be 5.3 $\pm$ 0.2 eV, in close agreement with an earlier low resolution photoionization result, $<$ 5.36$\pm$ 0.2 eV, (Chem.Phys. Lett., 1971, 9, 615). Energy onsets for some of the fragment ions, i.e. loss of CH_3, $N(CH_3)_2$, ($C_5H_{12}N_2$) etc. from the parent ion will also be presented. Fragment ions were observed to be more dominate than that of the parent ion for electron energies above $\sim$40eV. We will report further information (REMPI, Raman, and FTIR) as well as supporting theoretical studies on these fascinating molecules. For example, the Raman spectrum for OTCA at 780 nm is simplified by the high symmetry and calculations provide an accurate description of the vibrational modes.

Nasrin Mirsaleh Kohan
Departments of Physics ,University of Tennessee

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