Preliminary Theoretical and Experimental Studies of Al-group14 diatomics

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Two-color photoionization spectroscopy and density functional calculations have been used to investigate the Al-Group14 diatomics, AlSi, AlGe and AlSn. The bond lengths, vibrational frequencies, and dipole moments have been calculated using the DFT formalism for the lowest quartet and doublet of the neutrals, and the lowest singlet and triplet of the cations. The ground electronic state of the neutral is unequivocally the $^4\Sigma^-$ state arising from the $\pi^2\sigma^1$ configuration. Strong band systems lying in the 540-495 nm region have been observed using resonant two photon ionization (R2PI). At low resolution ($0.1cm^{-1}$), one band system appears to be $^4\Pi -^4 \Sigma$ in nature. Higher resolution spectra $0.005cm^{-1}$ should be available at the time of the meeting. Two-color photoionization efficiency spectroscopy yielded accurate ionization potentials. The electronic structure and bonding will be discussed at the meeting.

Time required: 15 min
Session in which paper is recomended for presentation: 2
Comment: this paper could also fit in 8