

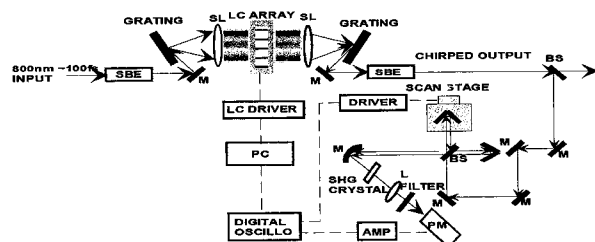
# Laser Research Center for Molecular Science

## VIII-B Developments of Advanced Lasers for Chemical Reaction Controls and ZEKE Photoelectron Spectroscopy

### VIII-B-1 Developments of Liquid Crystal Spatial Light Modulator

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The chemical reaction controls with laser lights are one of the most important subjects of chemistry. The coherence of laser lights has not been considered seriously in the old fashion of the laser controls of chemical reactions. Recent theoretical studies have shown that the more sophisticated controls of chemical reactions. As a first step, we are trying to maximize efficiency of the quantum transition with a chirped ultra short pulsed laser. This technique is based on an adiabatic passage theory of quantum transitions. We are developing a photo waveform shaper of ultra short laser pulses to make an arbitrary shaped pulse, including chirped ones. The spectral components of the incident pulse are spatially dispersed with a grating, modulated or retarded with a liquid crystal array on the Fourier plane and recombined with another grating.



**Figure 1.** Schematic diagram of liquid crystal spatial light modulator.

### VIII-B-2 ZEKE Electron Spectroscopy of Azulene and Azulene-Argon

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Mass-selected ion-current spectra and zero-kinetic-energy (ZEKE) electron spectra were obtained for azulene and its van der Waals (vdW) complex with Ar in supersonic jets by two-photon ( $1 + 1'$ ) resonant ionization through the second singlet electronic excited state ( $S_2$ ). Ab initio calculations were also carried out to study the optimized geometry and vibrational modes for azulene in the neutral and cation ground states ( $S_0$  and  $D_0$ ). Lennard Jones (LJ) potential energy calculations including "charge-charge-induced-dipole interactions" were also made for azulene-Ar. The main results may be summarized as follows. (1) The adiabatic ionization energies have been determined as  $I_a$  (azulene) =  $59781 \pm 5 \text{ cm}^{-1}$  and  $I_a$  (azulene-Ar) =  $59708 \pm 5 \text{ cm}^{-1}$ . The difference in  $I_a$  is  $73 \text{ cm}^{-1}$ . (2) Several vibrational frequencies of (azulene)<sup>+</sup> have been observed and identified on the basis of ab initio theoretical calculations. (3)

vibrational progression with a spacing of  $9\text{--}10 \text{ cm}^{-1}$  in the ZEKE spectra of azulene-Ar has been assigned experimentally and theoretically to the vdW bending vibration  $b_x^{+1}$  along the long axis of azulene. (4) From the calculated LJ potential energy minima, it has been found that Ar is shifted by  $0.10 \text{ \AA}$  along the long axis of azulene from the position in the neutral ground state. (5) The observed vdW vibrational progressions have been reproduced by Franck-Condon calculations, suggesting that Ar is shifted by  $2^\circ$  for (azulene-Ar)<sup>+</sup> with respect to its neutral  $S_2$  state.