

Summary

Spectroscopic Studies of Organic Laser Dyes in Sol-gel Glasses

After the invention of solid state laser the question whether it is possible to make a laser that could be tuned over a large range of frequencies raised. The answer came shortly, in a shape of an organic dye laser, dye lasers are normally liquid organic dyes. The tunability of the dye laser is a consequence of the broadened electronic levels characteristic of organic dyes.

Attempts to incorporate organic dyes into a solid host have, in the past, met with good success. Organic compounds are inherently sensitive to high temperature and can not, for example, withstand the thermal processing conditions by which conventional optical glasses are produced. In 1984, Avnir et al. have reported the preparation and optical properties of alkoxide-derived silica gels doped with rhodamine 6G. They have also demonstrated that other organic molecules can be successfully incorporated into sol-gel matrices.

We can conclude that dye lasers based on liquid dye solutions have valuable properties due to their continuous and wide range tunability, with different dyes, from the near-UV to the near-IR regions of the spectrum.

properties of the dye laser in different matrices. In this thesis work we plan a study of absorption and emission spectra of the dyes, rhodamine 6G, sulforhodamine 640, coumarin 440, keton red, and Nile blue in liquid and sol-gel matrix.

As we are well aware with the cracking problem of the sol-gel silica glass, so there is a need to discuss some precautions to avoid the cracking of these samples. In the chapter second we shall discuss some ideas to overcome the cracking problem along with the detailed procedure of sample preparation. In the last few decades there was a revolutionary change in the availability of computer codes for the electronic structure theory.

There are many powerful standard computer codes based upon the theory like semiempirical, density functional theory, and coupled cluster theory. Many of them are free available on public domain. These theoretical calculations provides good results for the transition state energies of even large molecules. In the theoretical part of this research work, we plan to use some standard computer codes

to calculate the ground state equilibrium geometry, excited state equilibrium geometry, and the first excited state transition energy of all the chosen dyes in gas phase state. Because some of these calculations are very expensive on a single processor and the results are very much dependent on the basis function used in these calculations for the large molecules so we plan to adopt different theoretical approaches for the different dye molecules.

In the chapter three the basic of the theories which we have used shall be presented.

In chapter four we shall present the absorption and emission spectra of all dyes in different matrices.

Chapter four is based on the spectroscopic characterization of all the dyes in different matrix.

The matrix effect on the absorption and emission spectrum will be discussed in detail. The theoretically calculated results of the ground state and excited state including equilibrium geometry will be presented. The ground state equilibrium geometry of large structure dyes were obtained using semiempirical calculation and for the small dye, RHF method was employed. We have also calculated the transition state energy of the first excited singlet state for all the dyes in gas phase using CIS (configuration interaction single-excitation) method. In the calculation of the excited state transition energies, the ground state equilibrium geometry was used.

In this thesis work we have recorded absorption and emission spectra of organic laser dyes in polar liquids and in sol-gel silica. Shifting was observed in absorption as well as in emission spectra on changing matrix. Some dyes show their spectra slightly changed in sol-gel as compared to the spectra in polar liquids while some dyes represent their spectra highly affected in rigid cage of sol-gel silica. These spectral change for all dyes was explained on the basis of their specific interaction in a particular matrix.