2D16 **Magnetic Field Effects on the Laser-Induced Movement of Photochromic Compound in Benzene Solution**

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【Introduction】 Dynamics of thermal convection of benzene solution in high magnetic fields are studied by using a thermally stable photochromic compound, 1,2-dicyano-1,2-bis(2,4,5-trimethyl-3-thienyl) ethane (CMTE). CMTE undergoes photo-isomerization reaction by UV-irradiation and its color changes from pale yellow to red. The excess photon energy will be used for local heating of the photo-isomer (PI) solution.

【Experimental】 CMTE and benzene were used as received. The experiments were carried out at room temperature in a quartz cell with dimensions of 10×10×40 mm (Fig. 1). The diameter of the hole on a copper shade below the vessel was 6 mm. The cell was placed in a 40-mm bore tube of a superconducting magnet (JASTEC, LH15T40, 15 T, 1500 T^2m^{-1}, vertical field) and irradiated from its bottom by a UV light from an XeCl excimer laser. The movement of the PI solution was observed using a CCD camera and recorded by a video camera. Molecular energies were calculated by *Gaussian 03,* DFT, B3LYP method with a base set of 6-31g and diamagnetic susceptibilities of CMTE and its photo-isomer were calculated by a Gaussian 03 CSGT method.

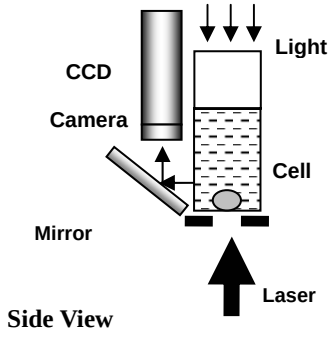

Fig. 1. Experimental setup

【Results and Discussion】 After the laser shot, a thin layer of CMTE benzene solution at the bottom of the vessel changes its color to red due to its photo-isomer (PI) and the PI solution starts to move. Figure 2 shows the movement of the PI solution generated by the laser-irradiation. The PI solution moves upwards at 0 T (0 T^2m^{-1}) and 10T (-1300 T^2m^{-1}). The movement at 14T (0 T^2m^{-1}) and 2 T (0 T^2m^{-1}) are very similar to that at 0T (0T^2m^{-1}), indicating the magnetic field flux density does not affect significantly the movement of the PI solution. At 11T (+1000 T^2m^{-1}), the PI solution moves up and then moves down at a 20 s delay after laser excitation. The movement of the PI solution will be divided into two steps. The first is departure from the bottom of the vessel.

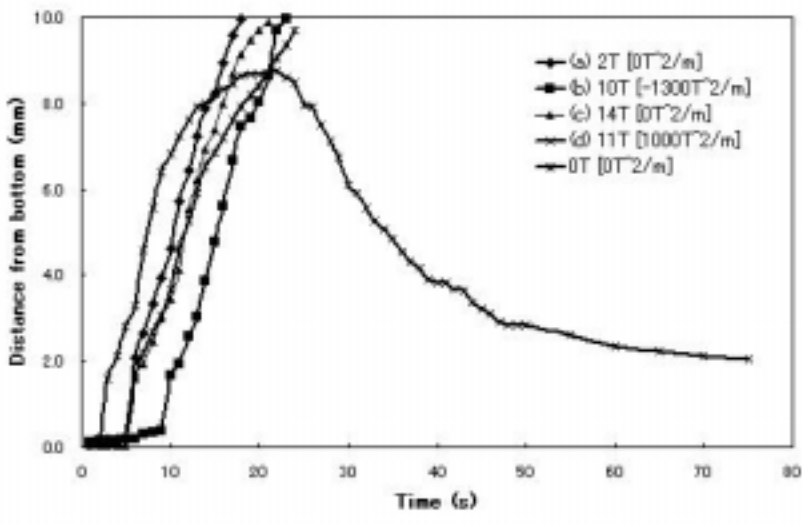

Fig. 2. Movement of the PI solution in magnetic fields.

Second is the motion in bulk solution after the departure. At zero field, the PI solution removes from the bottom surface of the vessel at a 5 s delay after laser excitation and moves upwards. At -1300 T^2m^{-1}, the solution starts to depart at a 9 s delay and then moves upwards. At +1000 T^2m^{-1}, it leaves from the bottom at a 3 s delay, moves upwards slowly, and finally it returns to lower part of the solution. By laser irradiation, the photon energy is partly used to initiate the isomerization reaction and the rest is used to heat the solution. The temperature of the PI solution increases due to the heat absorbed from the laser light, and, at the same time, its density and magnetic susceptibility are also changed. The results shown in Fig. 2 will be explained in terms of the magnetic force acting on the CMTE/PI solutions.

The movements of the PI solution shown in Fig. 2 will be divided into two stages. The first step is the departure of the solution from the bottom surface of the vessel. The second is the movement of the solution after the removal from the surface. Now let us consider the 1st step of the movement. The removal of the PI solution from the bottom surface will be explained by taking into account of the pressure in solution. The pressure difference of the bulk CMTE solution and the PI solution can be calculated by the following equation,

$$\Delta P = (\Delta\rho_{solution})gh + (\Delta\chi_{benzene})(1/\mu_0)hB\partial B/\partial z + (\chi_{PI} - \chi_{CMTE})\, c(1/\mu_0)hB\partial B/\partial z \quad (1)$$

where, $\Delta\rho_{solution}$ is the density change of the solution, $\Delta\chi_{benzene}$ is the magnetic susceptibility change of benzene induced by the temperature jump, h is the height of the PI solution, g is gravity, μ_0 is magnetic permeability of vacuum, B is the magnetic flux density and $\partial B/\partial z$ is its gradient to z direction which is vertical, respectively, χ_{PI} and χ_{CMTE} are magnetic susceptibilities of PI and CMTE, and c is the concentration of the solute. The first term of the right-hand side of eq. 1 is the density change of the solution induced by photoirradiation. The second is the susceptibility change of benzene due to temperature change and the third is the susceptibility change of solute due to photo-isomerization.

All the parameters appeared in eq. 1 are estimated by using parameters obtained experimentally and those from literatures. The ΔP values are calculated to be $5.88h$, $0.41h$, and $10.09h$ Nm^{-2} at 0, -1300 and +1000 T^2/m, respectively. At -1300 T^2m^{-1} ΔP is about one order of magnitude smaller than that at zero field, whereas at +1000 T^2m^{-1} it is about 1.7 times larger than that at zero field. At zero field, the value of ΔP only depends on the first term of the right-hand in eq. 1 and the departure time is about 5 s. In magnetic fields, the second and third terms must be taken into account. At -1300 T^2m^{-1}, the upward magnetic force almost balances with gravity and, therefore, ΔP is too small to push the PI solution upward immediately after laser irradiation, as the departure time is about 9 s. At +1000 T^2m^{-1}, the magnetic force is downward and the sum of gravity and magnetic force is roughly estimated to be 1.7 times larger than that of gravity. ΔP is large enough to remove the PI solution shortly after laser irradiation, as the departure time is about 3 s. This is why the departure time of the PI solution is different in three cases.

The movement of the PI solution floating in the bulk solution is also discussed analogously.