Photochemical reaction of 6H-benzo[cd]pyren-6-one (naphthanthrone)

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This paper describes the photochemical reaction of naphthanthrone, 6*H*-benzo[*cd*]pyren-6- one, with solvent, leading to a specific feature of fluorescence. After irradiation of naphthanthrone indegassed ethanol solution with light it absorbs, the fluorescence spectrum of the solution was blue-shifted by 20nm and the intensity was increased by a factor of about 100 of that before irradiation. Irradiation in its aerated solution, however, gave rise to only very small change in the spectrum. The enhancement of fluorescence on pre-irradiation was observed in benzene, but not in tetrachloromethane. Detailed spectroscopic measurements showed the followings: (1) The absorption spectra of irradiated ethanol and benzene solution exhibited new bands in shorter wavelengths and reduced original bands of naphthanthrone. (2) The excitation spectrum for enhancement fluorescence bands were different from that for original ones of naphthanthrone. (3) When the irradiated solution was stood in the dark at room temperature, the fluorescence intensity was decreased to 1/2 in 200s; on the other hand, the intensity stayed almost constant during 10min at 77K. (4) The phosphorescence of naphthanthrone was decreased gradually against irradiation. These findings suggest that naphthanthrone in degassed solution undergoes photochemical reaction to provide new species that is fluorescent and short-lived in room temperature. Since no fluorescence enhancement occurs in tetrachloromethane that has no hydrogen, hydrogen abstraction is thought to be involved as a primary step. It is highly likely that naphthanthrone excited in the triplet state abstracts hydrogen from the solvent to form radicals. Molecular orbital calculations showed that the absorption of a naphthanthrone radical is blue-shifted compared with that of the parent molecule. We are now going to perform ESR measurements to conform the formation of radicals on irradiation.