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Complexations of 2-Aminofluorene and 2-N,N′-Dimethylaminofluorene to b-Cyclodextrin in Presence of Sodium Perchlorate in Aqueous Solution

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Abstract — The complexations of 2-aminofluorene (2-AF) and 2-N,N′-dimethylaminofluorene (DMAF) to b-cyclodextrin (b-CD) have been studied in phosphate buffer (pH = 7.4) in presence of varying concentrations of sodium perchlorate ($NaClO_4$) in aqueous solution using absorption and fluorescence spectroscopy. In case of DMAF, association constant is about four times higher than that of 2-AF in absence of $NaClO_4$. The association constant of 2-AF passes through a maximum at around 0.01 M $NaClO_4$ with increasing concentration of $NaClO_4$. However, in case of DMAF there is a continuous decrease of association constant with an increase in the concentration of $NaClO_4$. The variation of association constants with the change in concentration of $NaClO_4$ for both the molecules is consistent with the variation of fluorescence quantum yields with the change in concentration of $NaClO_4$. Structures of 2-AF–b-CD and DMAF–b-CD inclusion complexes have been proposed. Aromatic ring without $-NH_2$ group in case of 2-AF and the same without $-N(CH_3)_2$ group in case of DMAF enter first into the b-CD cavity from the side of larger rim. The stability of ternary complex formed in the low concentration range of $NaClO_4$ depends on the hydrogen bond donor ability of the functional group(s) of the substrate explained with the help of the values of total atomic charges on the hydrogen atoms of $-NH_2$ group of 2-AF molecule obtained from ab initio quantum mechanical calculations by Restricted Hartree-Fock (RHF) method using 6-31G** basis set.