

STUDY OF SUPRAMOLECULAR INTERACTION OF N-METHYL FULLEROPYRROLIDINE WITH FREE-BASE AND ZINC PORPHYRIN IN SOLUTION

SHIV SANKAR SAHA^a, SUBRATA NAYAK^a, SHALMALI BHATTACHARYA^b,
SRINJAY BID^c, MOUMITA BOSE^d AND SUMANTA BHATTACHARYA^{a*}

The present work reports the non-covalent interaction of N-methyl fulleropyrrolidine (1) with a designed free-base (2) and zinc porphyrin (3) in solution. Appreciable ground state interaction of 1 with 2 and 3 occurs in 1,2-dichlorobenzene (DCB). Steady state fluorescence experiment elicits significant quenching of the fluorescence of both 2 and 3 in presence of 1 in DCB and this phenomenon is nicely utilized to determine the binding constant of 1-2 and 1-3 systems as 8,740 and 15,590 $\text{dm}^3 \times \text{mol}^{-1}$, respectively, in DCB. Time resolved fluorescence experiment reveals that deactivation of the photoexcited 2 and 3 in presence of 1 occurs via static quenching mechanism. Semiempirical PM3 calculations have generated the optimized geometric structure of 1-2 and 1-3 systems in vacuo. Heat of formation values for the said systems, namely, 1-2 and 1-3, evaluated by PM3 calculations corroborate fairly well with the trend in the value of binding constant in DCB.
