Short Communication

Rotamers in 2-styrylnaphthalene

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2-Styrylnaphthalene (I) has been shown to exist in solution as a mixture of two modifications, called S and L, differing in their emission spectra and decay rates [1]. It was suggested that these modifications be assigned the conformations IA and IB:



A recent note by Saltiel and Eaker [2] provides excellent and clear-cut evidence for the assignment of conformation IA to the L modification of compound I. It also shows that *no* good correlation exists between the two emission spectra, characterizing the two postulated rotamers, and the two decay times, 3.5 ns and 22 ns, observed [1 - 3] for the bi-exponential decay of this compound's emission.

In view of our extensive work on rotamerism in this and related compounds [4], I wish to make the following remarks.

In our earlier paper [1] describing the evidence for rotamers in compound I and in 1,2-di(2-naphthyl)ethylene (II)



we showed (without stressing this point) that with I no correlation exists between room temperature emission *spectra* and emission *decay* results: for longer excitation wavelengths, say 355 nm, the spectra clearly indicate a mixture of the S and L modifications, with the S modification still predominating, while in the bi-exponential decay the ratio between the contributions of τ_1 and τ_2 approaches infinity, indicating a mixture consisting mainly of one modification characterized by τ_1 (ref. 1, Table III and Fig. 2a). More-

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over, the effect of oxygen quenching on the shape of the emission spectra is small, in fact much smaller than with compound II ($\tau_1 = 2$ ns, $\tau_2 = 7.3$ ns), although one would expect the reverse. With II, a good correlation exists between the S and L spectra and τ_2 and τ_1 respectively, *i.e.* the L modification is characterized by the shorter τ . This agrees with the observed effect of oxygen on the shape of the emission spectra, which can be explained by preferential quenching of the long-lived emission. Table II in our paper [1] illustrates the good agreement between the composition of the rotamer mixtures obtained from the effect of oxygen on the spectral shape and from the pre-exponentials of the bi-exponential decay. Finally, time-resolved emission spectra of II by Ghiggino [5] showed that the emission spectrum "immediately" after excitation is a superposition of L and S, while that after some 30 ns is quite similar to S. Very similar results were obtained [6, 7] with several analogous 2-anthryl derivatives III



both with regard to the correlation between the spectra and the lifetimes and with regard to the effect of preferential quenching by oxygen. Furthermore, time-resolved emission spectra obtained with a solution of III by the PRS method of SLM Inc. are almost identical with the S and L spectra [7]. Results obtained with 3-phenanthryl analogues of II, e.g. IV



IV

although less detailed, indicate a similar situation [8].

It thus appears that compound I may present a rather special and complex case necessitating further study, and it is regrettable that research has focused extensively on this particular compound. In any case, decay measurements should obviously be carried out also at low temperatures where photoselective excitation of the S and L forms is so much better, to the extent that an almost pure L spectrum may be obtained [1].

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