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Abstract

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On the Relationship Between the Chemical Structure of Carbo- and Heterocyclic Compounds and Their Scintillation Activity

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At the present time, in addition to the known inorganic "phosphors," organic "phosphors" in the form of crystalline, liquid, and plastic scintillators have become known and are widely used.

Among organic compounds, the majority of aromatic hydrocarbons and a considerable number of heterocyclic compounds fluoresce; their molecules contain ring structures and conjugated double bonds.

The study of the relationship between the chemical structure of organic compounds and their scintillation activity is of undoubted interest, with the aim of finding regularities that make it possible to create organic scintillators with the best luminescent properties. Such investigations are widely conducted in the study of the properties of crystalline (1) and liquid (2) scintillators, and to a considerably lesser degree in the study of plastic scintillators (3)—despite the fact that there is great interest in them, since they are intended, to a significant extent, to replace crystalline and liquid scintillators in a number of their properties.

We have carried out an investigation of the scintillation activity of substituted anthracenes, polyphenyls, aryl derivatives of dienes, and a number of heterocyclic compounds (60 compounds in all) by introducing them into polystyrene plastic. The indicated substances were introduced into the styrene monomer in amounts corresponding to their maximum efficiencies (1-2 wt. %) and, in the presence of 0.2% benzoyl peroxide, were polymerized with a gradual increase in temperature from 80 to 120° over 4-5 days until transparent solid blocks were obtained, to which the shape of cylinders was imparted. These cylinders were examined for scintillation efficiency with the aid of an apparatus that made it possible to determine the relative magnitude of the voltage amplitude at the output of a photomultiplier (FEU-19). The amplitude of a reference sample (2% terphenyl in polystyrene) at a counting rate of 1000 pulses/min was taken as 100%. If a constant counting rate is maintained for all the samples under investigation by changing the cutoff voltage at the discriminator input, then for each of them we obtain its own cutoff voltage. By comparing these values with the cutoff-voltage value of the reference sample, comparative data for evaluating the samples can be obtained. The voltage-amplitude magnitude of the reference sample is 50% of the amplitude of a stilbene crystal. As a result of the investigation carried out, certain data were obtained indicating the existence of a dependence between the chemical structure of organic compounds and their scintillation efficiency. As can be seen from the data in Table 1, the highest activity in plastics is possessed by 1,4-di-(2-(5-phenyloxazolyl)-benzene) (I) (POPOP), quaterphe-

Table 1

Organic compound	Concentration in polystyrene (wt. %)	Relative pulse magnitude (%)	Organic compound	Concentration in polystyrene (wt. %)	Relative pulse magnitude (%)
1,4-Di-(2-(5-phenyloxazolyl)-benzene) (POPOP)	0.5	105	Dibenzopyrrole	2.0	(2)
Quaterphenyl	0.5	95	Ditolylmethane	2.0	10
9,10-Diphenylanthracene	0.5	80—85	Dixylylmethane	2.0	9
2,5-Diphenyloxazole (PPO)	1.0	105—115	Dinaphthylmethane	2.0	31
2-(α-Naphthyl)-5-phenyloxazole (α-NPO)	1.0	105	9,10-Di-(*p*-methoxyphenyl)-anthracene	2.0	96
2-(ω-Styryl)-5-phenyloxazole	1.0	67	9,10-Di-(*p*-tolyl)-anthracene	2.0	77
2,5-Diphenyloxadiazole	1.0	75	9,10-Di-(*p*-tolyl)-anthracene	2.0	72
1,1,4,4-Tetraphenylbutadiene	1.0	75—85	9,10-Di-(*p*-bromophenyl)-anthracene	2.0	72
1,1,4,4-Tetratolylbutadiene	1.0	70—75	9,10-Di-acetaminoanthracene	2.0	38
p-Terphenyl	2.0	100	9-*n*-Butylanthracene	2.0	52

Organic compound	Concentration in polystyrene (wt. %)	Relative pulse magnitude (%)	Organic compound	Concentration in polystyrene (wt. %)	Relative pulse magnitude (%)
Anthracene	2.0	30	9-*n*-Propylanthracene	2.0	46
Phenanthrene	2.0	15	9-Ethylanthracene	2.0	44
Acenaphthene	2.0	10	9-Methylanthracene	2.0	30
Dibenzofuran	2.0	15	2-Methylanthracene	2.0	35
Dibenzothiophene	2.0	5			

nyl (II), as well as 9,10-diphenylanthracene (III), i.e., hydrocarbons containing 4—5 rings in the molecule and conjugated double bonds.

[structural formula I]

[structural formula II]

[structural formula III]

In the series of oxazoles and oxadiazoles possessing high values of scintillation activity, the latter depends to a considerable degree on the nature of the substituents in positions 2,5. With identical substituents (phenyl), oxazole derivatives IV have greater scintillation activity than oxadiazole derivatives V.

[structural formula IV]

[structural formula V]

These data are in good agreement with the data of Hayes et al. (^4), obtained in the study of liquid scintillators. High scintillation activity is also possessed by 1,1,4,4-tetraarylbutadienes (VI)

[structural formula VI]

$$R = \mathrm{H};\ \mathrm{CH_3};$$

and *p*-terphenyl (VII)

[structural formula VII]

For the group of hydrocarbons with three condensed nuclei, differing from one another in ring structure, number of conjugations, and the presence of various heterocycles (O, S, NH), there also exists a dependence between chemical structure and scintillation activity. Anthracene (VIII) is more effective than phenanthrene (IX) and acenaphthene (X), while in the series of dibenzo derivatives of furan (XI), thiophene (XII), and pyrrole (XIII), the oxygen-containing heterocycle XI has the highest scintillation efficiency.

VIII IX X

XI XII XIII

These results, obtained in the study of plastics, are in agreement with Sangster' s data (^{1}), obtained in the study of the scintillation efficiency of these same substances in the crystalline state. Various diarylmethanes (XIV), in whose molecules the conjugation between the benzene rings is disrupted, have low efficiency:

$$R{-}\langle C_6H_4\rangle{-}CH_2{-}\langle C_6H_4\rangle{-}R \qquad \text{XIV}$$

Only when the number of rings in such a molecule is increased to four, as is the case in dinaphthylmethane, does the scintillation efficiency rise from 9% to 31%. Diphenylmethane likewise has low efficiency in the crystalline state (^{2}).

It should be noted that, when substituents are introduced into the benzene ring of a hydrocarbon, their chemical nature, as well as their isomerism, exerts a noticeable influence on scintillation activity, as we observed for 9-substituted anthracenes:

$$CH_3O > CH_3 > Br > CH_3CONH; \quad m > n,$$

and as Hayes (^{4}) observed for derivatives of oxazoles and oxadiazoles. It is also of interest to note the increase in scintillation activity in 9-substituted anthracenes on going from the methyl radical to the butyl radical.

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