PART II:

Substituted p-Oligophenylenes as Liquid Scintillation Solutes

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The substituted p-oligophenylenes show an extensive fluorescence in dissolved as well as in solid condition. This observation was the reason why they were tested regarding their application as organic scintillation solutes. But not all compounds have as yet been tested.

We used the instrumentation described by Hayes, Ott, Kerr and Rogers (2) in their fundamental work on liquid scintillators. The isotope source was Cs-137, the beakers were made of quartz, practically of the same diameter and height as used in the above mentioned publication. The luminescence was focused by an evaporated aluminum glass reflector and registered by a multichannel analyzer. The scintillator solutes were dissolved in toluene, a reagent of the firm of Merck, Darmstadt, Germany, and compared relatively to a solution of 3 grams per liter PPO in toluene.

The POPOP-TP ratio of the photomultiplier was about 1.2. The optical fluorescence spectra were corrected to give true intensities by means of an especially measured spectral sensitivity curve.

All methyl substituted quaterphenyls shown in Table 1 have a comparable relative pulse height except compound

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TABLE 1

	Compound	RPH	c_{max} (g/l)	s (g/l)	$\bar{\lambda}$ (mμ)	m.p. (°C)
1.	p-Quaterphenyl	0.2	0.2*	0.2	--	320
2.	$2^1,3^4$-dimethyl-p-quaterphenyl	1.26 (1.20)⊗	3.7* (6.3)⊗	3.7 (6.3)	392	213
3.	$2^4,3^1$-dimethyl-p-quaterphenyl	1.26 (0.98)⊗	35 (8.6)⊗	51 (36)	373	150
4.	$2^3,3^2$-dimethyl-p-quaterphenyl	1.23	55	55	400	176
5.	$2^1,2^3,3^2,3^4$-tetramethyl-p-quaterphenyl	1.16	25	>500	390	74
6.	$2^2,2^4,3^1,3^3$-tetramethyl-p-quaterphenyl	~0.1	10-20	490	410	96
7.	$2^1,2^2,3^3,3^4$-tetramethyl-p-quaterphenyl	1.24	16	110	--	139
8.	$2^3,2^4,3^1,3^2$-tetramethyl-p-quaterphenyl	0.90	20	>500	--	84

RPH of 3 g/l PPO equals to unity
s = solubility (toluene 20°C)
* = RPH at the solubility limit
⊗ = as reported by Hayes

No. 6. This is odd since the u.v. spectrum is quite normal (3). The fluorescence spectrum, however, shows almost no intensity.

From a practical point of view compound No. 5 is rather interesting because it is extremely soluble in toluene, more soluble and with higher RPH-value than PPO. There is also an economic advantage: this compound is convenient to synthesize.

The compound No. 3 which is fairly soluble has its mean wave length of the fluorescence spectrum in the same range as p-terphenyl. This was why we tried to add to the optimal concentration 0.5 grams per liter POPOP as a secondary solute. But the efficiency of this secondary solute system was almost the same as we measured for terphenyl with POPOP. Both compounds No. 2 and 3 were earlier tested in Los Alamos. We are sorry, there are some discrepancies in solubility data too (4).

On Table 2 are to be seen the three methyl substituted terphenyls and the phenyl or tolyl substituted fluorenes. The terphenyl derivatives are not as good as the quaterphenyls. Besides they are more difficult to synthesize. The two outer methyl groups, being in m-position to the linking phenylene ring (compound No. 9) show a greater effect than those in p-position (compound No. 10). If the linking phenylene ring is replaced by a cyclohexadiene ring (compound No. 11) the RPH drops to half the value.

The fluorene derivatives No. 14 and 15 were synthesized and measured by Barnett (5) before these compounds were available in our laboratories. However, we found the same relative pulse heights. When our RPH vs. concentration curve for compound No. 15 is extrapolated to a concentration of 0.4 we read exactly the same value.

Number 13 is a good scintillator which is quite soluble in toluene. A better one is compound No. 12 which was unfortunately measured only up to a concentration of 3.5 grams per liter. At this concentration, however, it showed already a relative pulse height of 1.04. This scintillator solute gives reasons for hopeful expectations because at the just mentioned concentration the RPH vs. concentration curve is still rising steeply. These fluorene derivatives are rather easy to prepare.

TABLE 2

	Compound	RPH	c_{max} (g/l)	s (g/l)	$\bar{\lambda}$ (mμ)	m.p. (°C)
9.	$2^1,3^3$-dimethyl-p-terphenyl	1.15	12	49	410	141
10.	$2^3,3^1$-dimethyl-p-quaterphenyl	0.67	10	44	--	145
11.	1,4-di-(m-tolyl)-1,3-cyclohexadiene	0.55	7	very good	--	118
12.	2,7-di-(m-tolyl)-fluorene	1.04	at 3.5	20	--	194
13.	2,7-di-(o-tolyl)-fluorene	1.27	15	85	--	159
14.	2,7-diphenylfluorene	0.95 (0.97)⊗	1.4* (1.0)	1.4	--	285
15.	2,2'-bifluorene	0.45 (0.54)⊗	0.3* (0.4)	0.3	--	307

RPH of 3 g/l PPO equals to unity
s = solubility (toluene 20° C)
⊗ = as reported by Barnett et al.

In Table 3 the compounds No. 16 through 18 are the methoxyl substituted quaterphenyls. Their RPH values are comparable but not better than those for the methyl substituted derivatives. However, their syntheses are more difficult. Compound No. 17 has good solubility. We sent the compounds No. 16 and 17 to Los Alamos and Dr. Hayes was kind enough to have a cross check in his laboratory.

Finally, the compounds No. 17 through 23 are methyl and methoxyl substituted quinqui- and sexiphenyls respectively. The solubility of these substances is poor, and this means the gradient of the RPH vs. concentration curve is limited at the saturated solution. In addition, these compounds are difficult to synthesize.

In summarizing one can say: the quaterphenyl derivatives have the highest RPH values. The attempt to achieve higher pulse heights by a higher degree of condensation has proven useless. The optimal concentrations are, in general, higher than it is the case at the conventional liquid scintillator solutes. In addition these compounds are not as difficult to synthesize.

TABLE 3

	Compound	RPH	c_{max} (g/l)	s (g/l)	$\bar{\lambda}$ (mμ)	m.p. (°C)
16.	$2^2,3^3$-dimethoxy-p-quaterphenyl	1.29 (1.19)⊗	12	18	395	184
17.	$2^1,3^2$-dimethoxy-p-quaterphenyl	1.23 (1.18)⊗	10	207	395	98
18.	$2^1,2^3,3^2,3^4$-tetramethoxy-p-quaterphenyl	1.17	13	22	--	160
19.	$2^1,2^4,3^2,3^5$-tetramethoxy-p-quinquephenyl	0.88	3.5*	3.5	410	165
20.	$2^1,2^5,3^2,3^6$-tetramethoxy-p sexiphenyl	0.49	1.8	2	410	210
21.	$2^1,2^4,3^2,3^5$-tetramethyl-p-quinquephenyl	1.21	7	11	470	186
22.	$2^5,3^1$-dimethyl-p-quinquephenyl	0.76	1.25*	1.25	--	230
23.	$2^1,2^5,3^2,3^6$-tetramethyl-p-sexiphenyl	1.26	26*	26	430	200

RPH of 3 g/l PPO equals to unity
s = solubility (toluene 20° C)
* = RPH at the solubility limit
⊗ = as reported by Hayes

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