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Biphenyl and 1,2-Diphenylethane Derivatives Containing Two Terminal Alkynyl Groups

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BIPHENYL AND 1,2-DIPHENYLETHANE DERIVATIVES CONTAINING TWO TERMINAL ALKYNYL GROUPS

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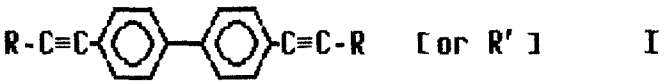
ABSTRACT

Synthesis and mesomorphic properties of biphenyl and 1,2-diphenylethane derivatives, containing two terminal alkynyl groups, are presented.

RESULTS AND DISCUSSION

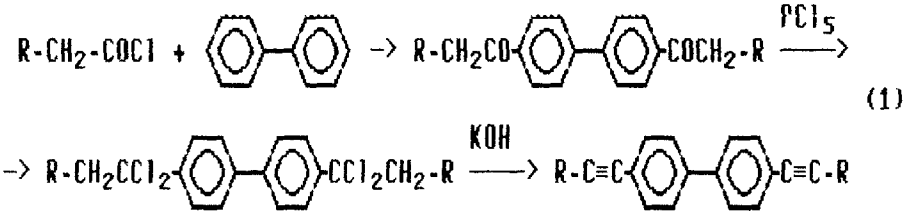
Tolans and diacetylenes are well known mesogens possessing high values of optical birefringence. Many types of nematogens have been described which contain one acetylenic linkage along with another bridge group of different type. In this work we wanted to evaluate the properties of compounds, obtained by a connection of two alkynyl groups with biphenyl either 1,2-diphenylethane core:



I

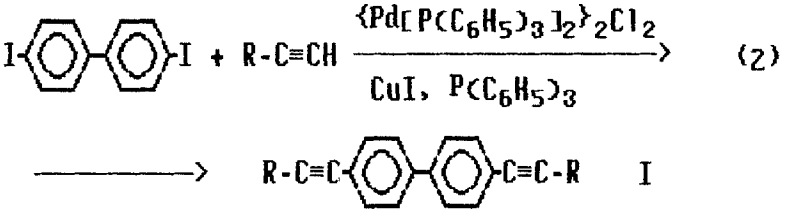
II

For the first we tried to synthesize compounds I according the following scheme:



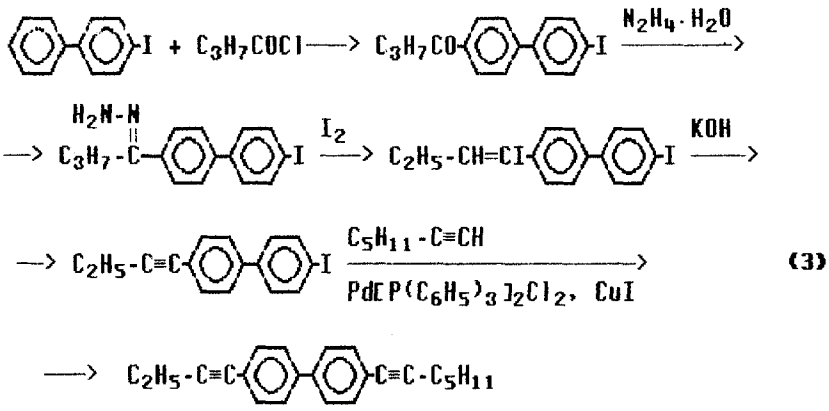
(1)

We did not manage to get pure compounds by this route, as all the attempts led to a rather complicated mixtures. Symmetrically substituted compounds I were obtained via 4,4'-diiodobiphenyl and 1-alkynes:



(2)

A similar route, starting from 1,2-bis-(4iodophenyl)ethane, led to compounds II. The situation was more complicated in the case of compounds I, containing different size alkynyl substituents. Our attempts to obtain 4-alkynyl-4'-iodobiphenyl by changing the ratio of reagents in the scheme (2) were not successful - we managed to isolate disubstituted product only. Similarly, we could not obtain a pure assymmetric product by combining schemes (1) and (2), e.g., acylation- action of phosphorous pentachloride- dehydrochlorination of 4-iodobiphenyl either 4-bromobiphenyl. To our estimation, an optimal route to assymmetric 4,4'-di-alkynylbiphenyl was the following:



(3)

An idea for this synthesis was taken from [1]. This route led to pure product with considerable yields (60-50%) at all stages.
The purity of all the compounds was checked by TLC, all the structures were confirmed by elemental analysis and NMR H^1 spectra. The phase transition temperatures of obtained compounds (I, II) are given below.

Table 1. Phase transition temperatures of 4,4'-di-alkynylbiphenyls (I) and 4,4'-di-alkynyl-1,2-diphenylethanes (II).

Compound	R	R'	Cryst.-Smectic	Smectic - Isotrope
I	C_5H_{11}	C_5H_1	67.5	86
I	C_7H_{15}	C_7H_{15}	(59.0)	73
I	C_5H_{11}	C_2H_5	98.0	-
II	C_5H_{11}	C_5H_{11}	80.5	-
II	C_7H_{15}	C_7H_{15}	76.5	-

Compounds I form smectic state (non-identified high viscous mesophase), whilst compounds II are nonmesomorphic. Evidently, the presence of two acetylenic linkages connected to an aromatic core creates too rigid molecular structure, which is not favorable for mesophase formation.

REFERENCES

1. A.M.Krubiner, N.Gotttfried and E.P.Oliveto, J.Org.Chem., 34 (11), 3502-5 (1969).