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Title:	Scholl reaction of hexaphenylbenzenes with hexakis-alkoxy substituents
Authors:	Setia, S. (/jspui/browse?type=author&value=Setia%2C+S.) Adhikari, D. (/jspui/browse?type=author&value=Adhikari%2C+D.) Pal, S.K. (/jspui/browse?type=author&value=Pal%2C+S.K.)
Keywords:	Hexakis-alkoxy substituted Described Investigated HBC
Issue Date:	2019
Publisher:	Taylor and Francis Online
Citation:	Liquid Crystals, 46(3).pp 430-441.
Abstract:	The hexakis-alkoxy substituted hexa-peri-hexabenzocoronene (HBC) discotic core is desirable aiming at strong π - π interactions in columns, electronic tuning of the core and better processability. The feasibility of synthesising a new hexakis-alkoxy substituted HBC core is investigated and described in this report. Experimentally, it has been found that when two alkoxy substituents in a peripheral aromatic ring are placed meta to each other, the Scholl reaction results in fully cyclised HBC product. Surprisingly, when the alkoxy groups are ortho to each other, cyclodehydrogenation results in the formation of a partially fused product. This partially-fused ring formation happens under varying reaction conditions and irrespective of the differing alkyl chain lengths. Most plausibly, the considerable strain in the fully fused molecule from 1,2 isomer is the reason to cease the reaction at the partially fused stage. Further quantum-mechanical calculations at the B3LYP/6-31G(d) level of theory also support the hypothesis. The incorporation of two electron donating groups has also reduced the band gap compared to its mono alkoxy analogue. Reduced band gap values are promising feature of these molecules for finding future applications of discotic liquid crystals in organic electronics.
Description:	Only IISERM authors are available in the record.
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