

Protection/Deprotection-Free Syntheses and Structural Analysis of (Keto-aryl)diynes.

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Streszczenie

The reactions of precursors 4-BrC₆H₄COR with TMSCCH (Sonogashira coupling) followed by in situ deprotection and subsequent dimerization gave thermally stable dimeric ketodiyne RCOC₆H₄(CC)₂C₆H₄COR (8–11) as yellow powders

in 25–85% yields without the necessity of carbonyl group protection/deprotection steps. Compounds 8–11 were also synthesized by an alternative method that utilized α-haloalkynes previously obtained directly from TMS-protected 4-RCOC₆H₄CCTMS alkynes. The resulting diynes were characterized by spectroscopic methods and in most cases by X-ray crystallography. Careful analysis of the crystal data revealed a surprisingly high degree of chain curvature. Moreover, compounds 9 (R = Me) and 10 (R = Et) were extremely flat, which greatly facilitates electronic communication throughout the whole molecule. Deeper analysis of the packing motifs showed 9 to have a great potential for topochemical 1,4-polymerization.

Słowa kluczowe

Polyynes, Homocoupling, Dimerization, Halogenation, Alkynes

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