Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713926090

Liquid crystal properties of 4-*n*-alkylphenyl D-glucopyranosides

Lavinia M. Wingert[a]; George A. Jeffrey[a]; Jahangir[bc]; David C. Baker[b]
[a] Department of Crystallography, University of Pittsburgh, Pittsburgh, Pennsylvania, U.S.A. [b] Department of Chemistry, The University of Tennessee, Knoxville, Tennessee, U.S.A. [c] Syntax Research, Palo Alto, California, U.S.A.

To cite this Article Wingert, Lavinia M. , Jeffrey, George A. , Jahangir and Baker, David C.(1993) 'Liquid crystal properties of 4-*n*-alkylphenyl D-glucopyranosides', Liquid Crystals, 13: 3, 467 — 470
To link to this Article: DOI: 10.1080/02678299308026318
URL: http://dx.doi.org/10.1080/02678299308026318

Liquid Crystals, 1993, Vol. 13, No. 3, 467–470

PRELIMINARY COMMUNICATION

Liquid crystal properties of 4-*n*-alkylphenyl D-glucopyranosides

by LAVINIA M. WINGERT and GEORGE A. JEFFREY*
Department of Crystallography, University of Pittsburgh,
Pittsburgh, Pennsylvania 15260, U.S.A.

JAHANGIR† and DAVID C. BAKER
Department of Chemistry, The University of Tennessee,
Knoxville, Tennessee 37996-1600, U.S.A.

(*Received 13 October 1992; accepted 10 November 1992*)

With a phenyl group positioned between the *n*-alkyl chain and the sugar moiety, 4-*n*-alkylphenyl α- and β-D-glucopyranosides show mesomorphic properties that parallel those of alkyl D-glucopyranosides with longer alkyl chains.

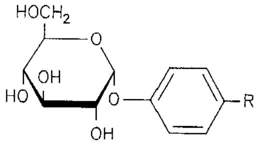
The mesophase behaviour of the amphiphilic 4-*n*-alkylphenyl α- and β-D-glucopyranosides occurs because of conflicting responses of the hydrophilic and hydrophobic moieties of these molecules to changes in temperature and solvation. Inserting a phenyl group between the alkyl and sugar moieties increases the rigidity of the hydrophobic component and shifts the hydrophobic-to-hydrophilic balance of these molecules. In this work, we compare the thermotropic and lyotropic properties of six 4-*n*-alkylphenyl α- and β-D-glucopyranosides **1a–c** and **2a–c** (see structures) with those of a series of mesomorphic *n*-alkyl α- and β-D-glucopyranosides.

Glycosides **1a–c** and **2a–c** were prepared by reaction of a solution of penta-*O*-acetyl-D-glucopyranose with the appropriate *p*-substituted phenol in dichloromethane under catalysis by tin(IV) chloride. By running the reactions under conditions of kinetic control at 20°C, the β-D-glucopyranosides **2a–c** were obtained as the near-exclusive products, after the two step procedure of (1) purification of the acetylated intermediates by column chromatography on silica gel and (2) deacetylation and recrystallization of the final free-hydroxyl products **2a–c**. Compounds **1a–c** were similarly produced by reaction at ~40°C. Both *n*-alkyl α- and β-D-glucosides (structures not shown) were similarly prepared. Yields of products were typically 40–50 per cent for the two step sequence. The products were fully characterized by NMR spectroscopy and, for new substances, by elemental analyses. Known compounds gave optical rotations and melting points that matched values reported in the literature. Details of these syntheses will be reported elsewhere [1]. It is worth noting that various phenyl α- and β-D-glucosides, including **2a**, have been previously synthesized for examination of their antiviral activity; however, their mesomorphic properties were not investigated [2].

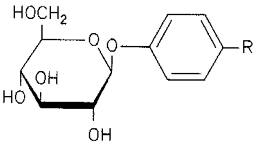
---

* Author for correspondence.

† Present address: Syntax Research, 3401 Hillview Avenue, Palo Alto, California 94304, U.S.A.

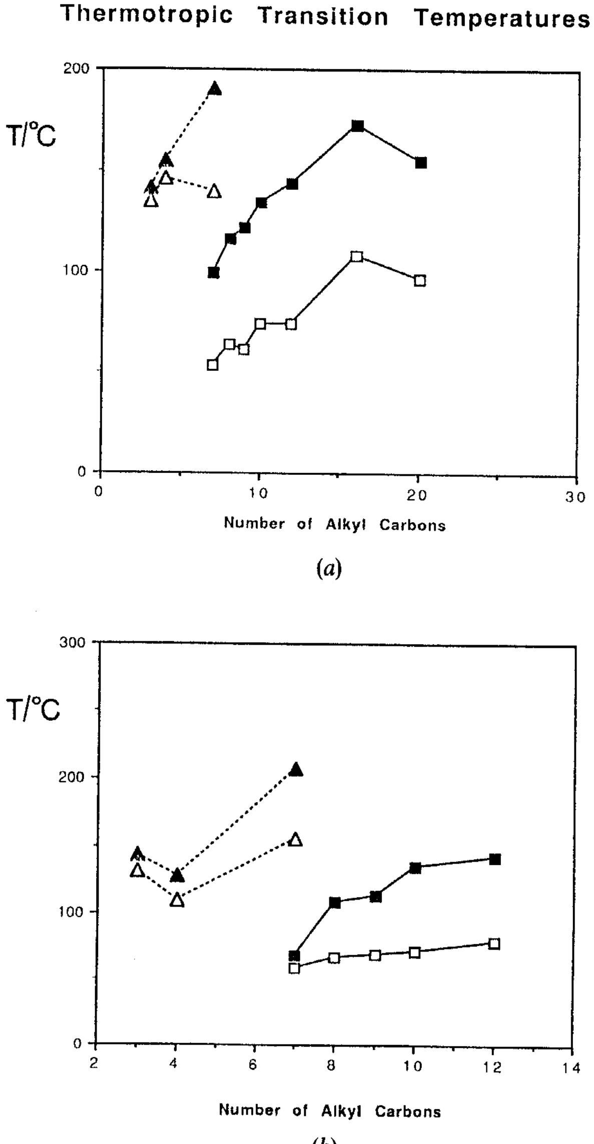


1



2

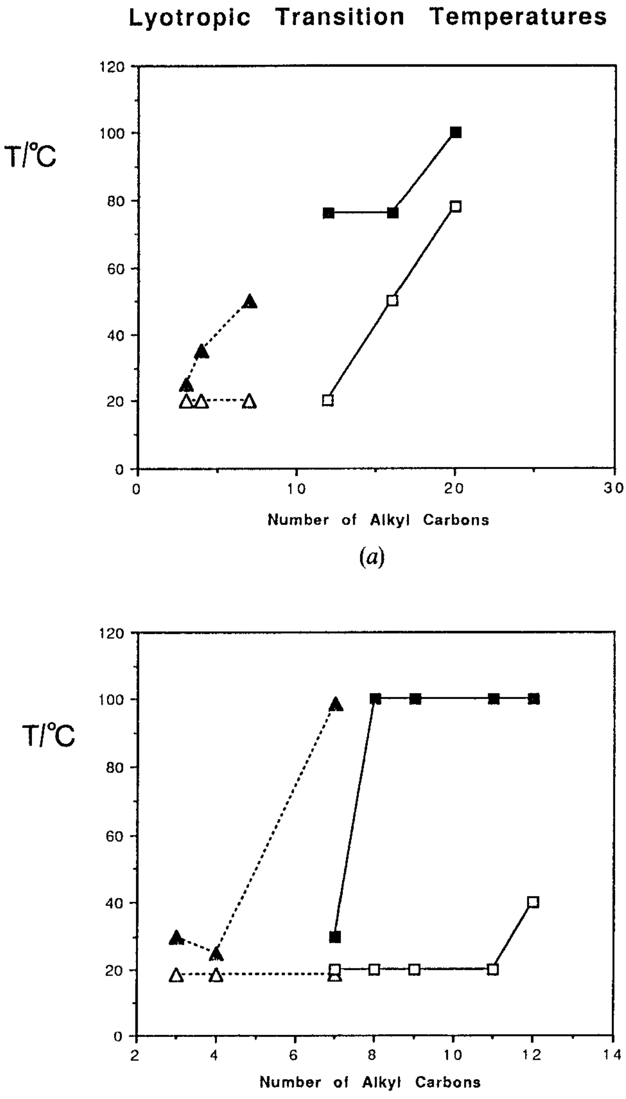
Series: **a**, $R=C_3H_7$; **b**, $R=C_4H_9$; **c**, $R=C_7H_{15}$.



(*a*)

(*b*)

Figure 1. A comparison of the thermotropic melting and clearing points for (*a*) the alkylphenyl-1-*O*-α-glucosides (··· △ ···, melting; ··· ▲ ···, clearing) and the alkyl-1-*O*-α-glucosides (–□–, melting; –■–, clearing) and (*b*) the alkylphenyl-1-*O*-β-glucosides (··· △ ···, melting; ··· ▲ ···, clearing) and the alkyl-1-*O*-β-glucosides (–□–, melting; –■–, clearing) versus the number of alkyl carbons.



(*a*)

(*b*)

Figure 2. A comparison of the temperatures of penetration and clearing for (*a*) the alkylphenyl-1-*O*-α-glucosides (··· △ ···, penetration; ··· ▲ ···, clearing) and the alkyl-1-*O*-α-glucosides (–□–, penetration; –■–, clearing) and (*b*) the alkyl-1-*O*-β-glucosides (··· △ ···, penetration; ··· ▲ ···, clearing) and the alkyl-1-*O*-β-glucosides (–□–, penetration; –■–, clearing) versus the number of alkyl carbons.

Studies have been carried out by both differential scanning calorimetry (DSC) and optical microscopy. The DSC was performed at a heating rate of 5 K min^{-1} using a Mettler TA-4000 system. The microscopy was carried out using a Leitz Wetzlar Laborlux 12 Pol polarized-light microscope equipped with a Leitz 350 heated stage and a West 2050 programmable temperature controller.

The thermotropic melting and clearing points for the 4-*n*-alkylphenyl D-glucopyranosides are compared with those for the *n*-alkyl D-glucopyranosides [3, 4] in figure 1. The transition temperatures are higher, particularly for the melting points of the α series. There is, however, a correspondence in the temperature increments per hydrophobic carbon atom, when the phenyl group is equated to four or five alkyl carbons. The mesophases are enantiotropic and identical in texture to the S_A phases of the *n*-alkyl D-glucopyranosides.

All six 4-*n*-alkylphenyl D-glucopyranosides form lyotropic liquid crystals with water at room temperature (20°C). This is in contrast to the *n*-alkyl α-D-glucopyranosides with alkyl chains shorter than C_9H_{19}, which are sparingly soluble in water and do not form lyotropic liquid crystals at room temperature. The temperatures of penetration and clearing for the α and β series of these compounds, with and without the phenyl ring, are given in figure 2.

As with the *n*-alkylpropane-1,2-diol series of amphiphiles [5], the introduction of a rigid phenyl group into the hydrophobic region of a molecule [6] does not greatly affect its liquid crystal properties, except for increasing the temperatures at which the thermotropic transitions occur.

References

[1] Jahangir, and Baker, D. C. (unpublished result).
[2] Arita, H., Sugita, K., Nomura, A., Sato, K., and Kawanami, J., 1978, *Carbohydr. Res.*, **62,** 143.
[3] Vill, V., Böcker, T., Thiem, J., and Fischer, F., 1989, *Liq. Crystals*, **6,** 349.
[4] Jeffrey, G. A., and Wingert, L. M., 1992, *Liq. Crystals*, **12,** 179.
[5] Van Doren, H. A., Van der Geest, R., Kellogg, R. M., and Wynberg, H. L., 1990, *Recl Trav. Chim. Pays-Bas*, **109,** 197.
[6] Tschierske, C., Hentrich, F., Joachime, D., Agent, O., and Zaschke, H., 1991, *Liq. Crystals*, **9,** 571.