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Note

Capsular polysaccharide of *Klebsiella* type 30: X-ray diffraction results and idealised chain conformation

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X-ray diffraction patterns have been obtained from oriented films of the sodium salt of *Klebsiella* capsular polysaccharide type 30 (K 30) by using methods similar to those reported previously[1] for *Klebsiella* type 57. The quality of the X-ray diffraction patterns (Fig. 1 shows a typical example) was poorer than that obtained for other

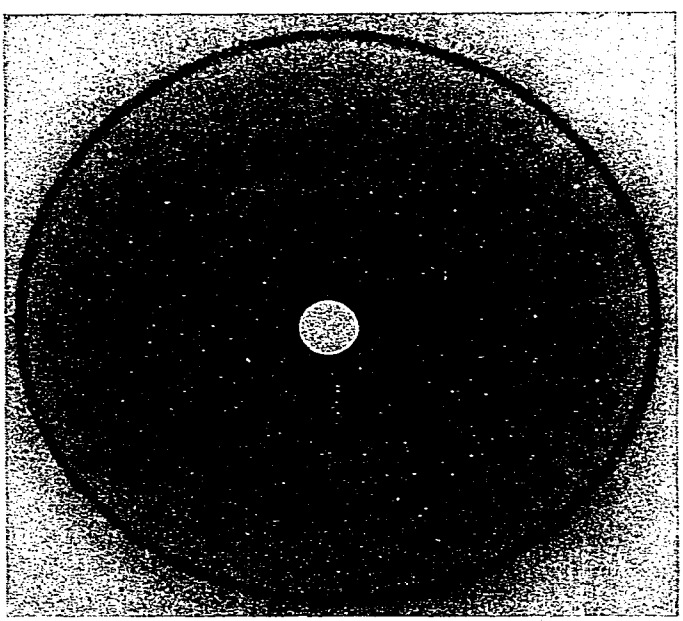

Fig. 1. X-ray diffraction pattern obtained from oriented films of the sodium salt of *Klebsiella* K 30. The chain direction is vertical. The series of meridional reflections (on the vertical bisector) index on a spacing of 1.52 nm, which correlates directly with the trisaccharide backbone-repeat.

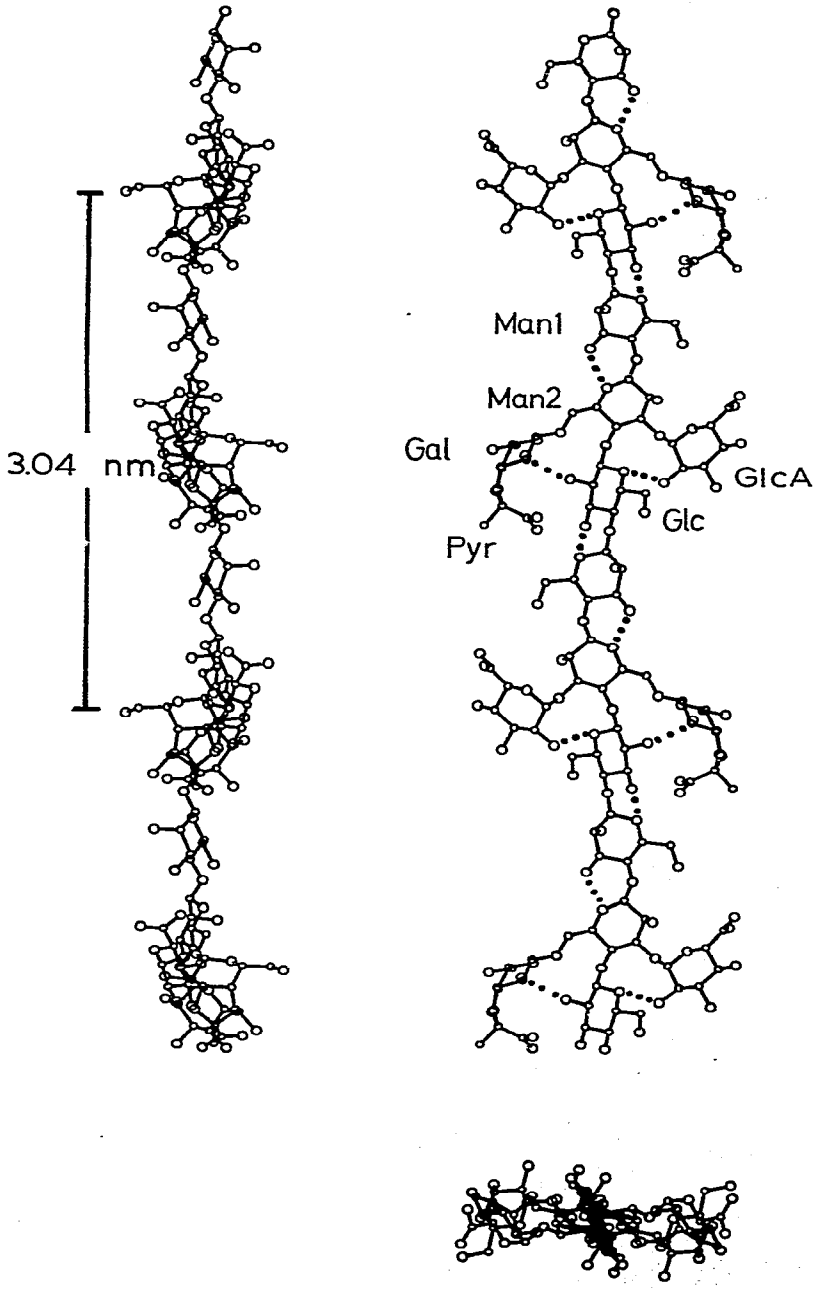

Fig. 2. Computer-drawn projections of the idealized, two-fold, helical model for *Klebsiella* K 30. Intrachain hydrogen-bonds are shown dotted. The incorporation of non-stoichiometric *O*-acetyl groups will upset the true repeat of $2 \times 1.52 = 3.04$ nm.

Klebsiella serotypes[2], but was sufficient to provide a series of clearly defined, meridional arcs. These arcs relate to repeats along the polysaccharide chain, and index on a one-dimensional lattice with spacing 1.52 $\pm$0.01 nm.

The chemical structure of *Klebsiella* K 30 is given in the preceding paper by Lindberg *et al.*[3]. The three residues in the backbone, one β-D-glucosyl and two β-D-mannosyl, would be expected to exist in the condensed phase in the normal $^4C_1$ conformation. Thus, all glycosidic linkages in the backbone would be 1,4-di-equatorially arranged in common with the simpler homopolymers; namely, cellulose, mannan, and chitin. These polymonosaccharides exist as almost fully extended, helical chains in the condensed phase with an axial advance per saccharide (h_s) in the range 0.515–0.505 nm[4-6]. The asymmetric backbone-repeat in K 30 is a tri-saccharide, and therefore the value of the average advance per saccharide is 1.52/3 = 0.507 nm, which is nearly identical with the reported values of h_s for the extended two-fold helices, with ribbon-like appearance, of cellulose and mannan. Thus, we assert that the limited X-ray evidence supports a trisaccharide backbone-repeat with all glycosidic linkages disposed 1,4-diequatorial. Furthermore, the torsion angles about each glycosidic bond cannot be too far from that found in the cellulose, mannan, and chitin group of polymonosaccharides. If they were, a decrease in the value of h_s would be expected, similar to that observed in the three-fold helical structures of (1→4)-linked β-D-xylan[7] and *Watsonia primidata*[8], and the five-fold helical structures of xanthan gum[9]. Thus, successive saccharide residues may be imagined to be rotated by 180° about the chain (helix) axis; because there are three different saccharide residues (one mannosyl residue has side-appendages that distinguish it structurally from the other mannosyl residue) in *Klebsiella* K 30, the final result is to produce a two-fold helix, with ribbon-like appearance, as illustrated by the idealized conformation shown in Fig. 2. This two-fold, ribbon-like, helical conformation is expected to occur for the fully extended chain in any 1,4-diequatorially linked polysaccharide containing an odd number of saccharide residues in the chemical repeating-unit for the backbone.

The poor crystallinity, lack of any well-defined layer lines, and very small, inter-chain, interference effects indicate that *Klebsiella* K 30 chains have been captured in an extended conformation, similar to the idealized model in Fig. 2, but with un-co-ordinated variations about this "average" conformation. Our inability to crystallize this polysaccharide, using our annealing techniques[10], indicates that the penta-saccharide repeating-unit[3] is idealized; in fact, Lindberg *et al.*[3] obtained poorly resolved n.m.r. spectra, and suggested that such a repeat only accounts for a proportion of the polymer. Only when the polysaccharide was *O*-deacetylated did the n.m.r. spectrum improve. A non-stoichiometric arrangement of *O*-acetyl groups would impair crystallinity, and would also be expected to perturb the model shown in Fig. 2 in a small, but random, fashion and destroy the precise two-fold nature of the helix. Thus Fig. 2, the atomic co-ordinates of which are given in Table I, should be thought of as the idealized model without *O*-acetyl groups attached.

TABLE I

CARTESIAN CO-ORDINATES OF THE MODEL SHOWN IN FIG. 2

Atom	*x (nm)*	*y (nm)*	*z (nm)*	*Atom*	*x (nm)*	*y (nm)*	*z (nm)*
β-D-Mannose (1)				*β-D-Mannose (2)*			
C-1	0.0492	−0.0173	−0.1246	C-1	0.0779	−0.0941	−0.6353
C-2	0.1261	0.0663	−0.2261	C-2	0.0710	−0.2059	−0.7385
C-3	0.0748	0.0399	−0.3668	C-3	0.1297	−0.1598	−0.8711
C-4	0.0761	−0.1095	−0.3964	C-4	0.0634	−0.0303	−0.9160
C-5	0.0030	−0.1856	−0.2863	C-5	0.0689	0.0732	−0.8042
C-6	0.0108	−0.3357	−0.3041	C-6	−0.0056	0.2005	−0.8386
O-1	0.1080	0.0000	0.0000	O-1	0.0115	−0.1361	−0.5207
O-2	0.2645	0.0339	−0.2192	O-2	−0.0646	−0.2447	−0.7576
O-3	0.1569	0.1086	−0.4615	O-3	0.1099	−0.2610	−0.9700
O-4	0.0115	−0.1361	−0.5207	O-4	0.1302	0.0227	−1.0303
O-5	0.0612	−0.1556	−0.1585	O-5	0.0085	0.0205	−0.6850
O-6	−0.0471	−0.3775	−0.4277	O-6	0.0481	0.2634	−0.9549
H-1	−0.0569	0.0118	−0.1260	H-1	0.1830	−0.0680	−0.6164
H-2	0.1166	0.1729	−0.2006	H-2	0.1248	−0.2941	−0.7008
H-3	−0.0279	0.0783	−0.3762	H-3	0.2379	−0.1436	−0.8596
H-4	0.1801	0.1447	−0.4026	H-4	−0.0415	−0.0501	−0.9427
H-5	−0.1031	−0.1568	−0.2860	H-5	0.1736	0.0996	−0.7837
β-D-Glucose				*α-D-Glucuronic acid (side-group)*			
C-1	0.0513	0.0488	−1.1417	C-1	0.2259	−0.3275	−1.0164
C-2	0.1426	0.0886	−1.2569	C-2	0.1954	−0.3878	−1.1529
C-3	0.0625	0.1044	−1.3853	C-3	0.0889	−0.4957	−1.1409
C-4	−0.0195	−0.0211	−1.4122	C-4	0.1294	−0.5989	−1.0364
C-5	−0.1022	−0.0573	−1.2893	C-5	0.1647	−0.5300	−0.9053
C-6	−0.1773	−0.1877	−1.3057	C-6	0.2198	−0.6259	−0.8019
O-1	0.1302	0.0227	−1.0303	O-1	0.1099	−0.2610	−0.9700
O-2	0.2097	0.2097	−1.2241	O-2	0.1532	−0.2847	−1.2414
O-3	0.1514	0.1283	−1.4946	O-3	0.0710	−0.5596	−1.2674
O-4	−0.1080	0.0000	−1.5220	O-4	0.0224	−0.6900	−1.0125
O-5	−0.0167	−0.0724	−1.1749	O-5	0.2650	−0.4312	−0.9277
O-6	−0.2680	−0.1831	−1.4158	O-6a	0.3383	−0.6521	−0.7890
H-1	−0.0223	0.1285	−1.1238	O-6b	0.1275	−0.6800	−0.7250
H-2	0.2197	0.0115	−1.2710	H-1	0.3064	−0.2545	−1.0254
H-3	−0.0048	0.1910	−1.3762	H-2	0.2872	−0.4313	−1.1951
H-4	0.0479	−0.1044	−1.4369	H-3	−0.0068	−0.4498	−1.1120
H-5	−0.1758	0.0221	−1.2699	H-4	0.2104	−0.6556	−1.0726
				H-5	0.0748	−0.4821	−0.8636
3,4-O-(1-Carboxyethylidene)-β-D-galactose (side-group)							
C-1	0.0043	0.3925	−0.9813	H-1	0.0272	0.4627	−0.8997
C-2	0.0705	0.4405	−1.1098	H-2	0.0524	0.3674	−1.1900
C-3	0.0151	0.5760	−1.1510	H-3	0.0457	0.6521	−1.0777
C-4	−0.1370	0.5709	−1.1584	H-4	−0.1764	0.6723	−1.1744
C-5	−0.1940	0.5153	−1.0283	H-5	−0.1711	0.5842	−0.9457
C-6	−0.3442	0.4969	−1.0336	C-7	−0.0495	0.5672	−1.3798
O-1	0.0481	0.2634	−0.9549	C-8	−0.0841	0.4366	−1.4504
O-2	0.2113	0.4473	−1.0903	O-8a	0.0168	0.3835	−1.5164
O-3	0.0563	0.5920	−1.2869	O-8b	−0.1942	0.3842	−1.4474
O-4	−0.1584	0.5997	−1.2964	C-9	−0.0434	0.6629	−1.4926
O-5	−0.1372	0.3864	−1.0005	H-9a	−0.1368	0.6574	−1.5504
O-6	0.4118	0.6202	−1.0583	H-9b	−0.0305	0.7649	−1.4535
				H-9c	0.0415	0.6376	−1.5577

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REFERENCES

1 D. H. ISAAC, K. H. GARDNER, E. D. T. ATKINS, U. ELSASSER-BEILE, AND S. STIRM, *Carbohydr. Res.*, 66 (1978) 43–52.
2 E. D. T. ATKINS, D. H. ISAAC, AND H. F. ELLOWAY, in R. C. W. BERKELEY, G. W. GOODAY, AND D. C. ELLWOOD (Eds.), *Microbial Polysaccharides and Polysaccharases*, Academic Press, London, 1979, pp. 161–189.
3 B. LINDBERG, F. LINDH, J. LÖNNGREN, AND I. W. SUTHERLAND, *Carbohydr. Res.*, 76 (1979) 281–284.
4 K. H. GARDNER AND J. BLACKWELL, *Biopolymers*, 14 (1974) 1975–2001.
5 I. A. NIEDUSZYNSKI AND R. H. MARCHESSAULT, *Can. J. Chem.*, 50 (1972) 2130–2138.
6 R. MINKE AND J. BLACKWELL, *J. Mol. Biol.*, 120 (1978) 167–181.
7 I. A. NIEDUSZYNSKI AND R. H. MARCHESSAULT, *Biopolymers*, 11 (1972) 1335–1344.
8 C. LELLIOTT, E. D. T. ATKINS, J. W. F. JURITZ, AND A. M. STEPHEN, *Polymer*, 19 (1978) 363–367.
9 R. MOORHOUSE, M. D. WALKINSHAW, W. T. WINTER, AND S. ARNOTT, in J. C. ARTHUR (Ed.), *Cellulose Chemistry and Technology, ACS Symp. Ser.*, 48 (1977) 133–152.
10 E. D. T. ATKINS AND W. MACKIE, *Biopolymers*, 11 (1972) 1685–1691.