Preliminary

Characterization of β-(1→4)-D-galactan*1

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Introduction

Over the past few decades, many crystallographic studies have been made on polysaccharides, such as cellulose, amylose[1,2], xylan and mannan. There are many crystallographic studies on high-crystalline polysaccharides, but few on low-crystalline ones. This is mainly because of the difficulty in making single crystals from low-crystalline ones. Furthermore, even high-crystalline ones, their crystallographic reliability factors (R-factors) were around 0.2 and not so reliable from the crystallographic viewpoints.

The purpose of this study is to get the situation better by establishing a new approach: the new molecular modeling method.

Methods

First of all, on our method, the initial structure of β-(1→4)-D-galactan was built up with a molecular building program. The degree of polymerization (D.P.) of this model was 20. The optimized structure of galactan was calculated.

Secondly, the X-ray and electron diffraction data were also collected on galactan experimentally.

Thirdly, comparing the calculated scattering intensity from the optimized structure with the experiment data, R-factors were refined.

Results and Discussion

The optimized structure of galactan was in a six fold left-handed screw symmetry

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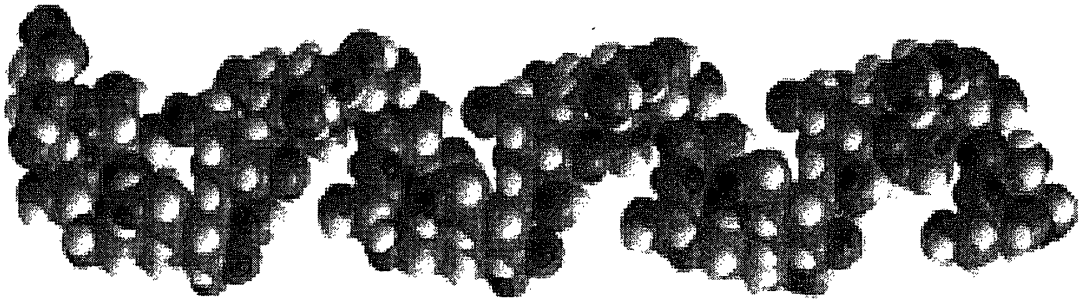

Fig. 1. The optimized β-(1→4)-D-galactan.

(Figure 1). The crystal structure analysis of galactan are still under working, but we found two distinguished advantages on our method rather than usual ones.

One is that, without any experimental data, we can predict the more suitable initial structure in crystallographic analysis than ever. We can also obtain some pieces of information about chain-packing in a unit cell.

Another is that we can expect better R-factors on our method than those on usual methods.

References

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