ture dependence of the molecular inclination ρ is different at the two phase transitions: at T_{12} the change of ρ is small, while at T_{23} it is much larger (see Fig. 10).

Changes in both the inclination of molecules and the O2—C2—O1—C9 torsion angles are consequences of sheer at the structural transformations at T_{12} and T_{23}. This would support the conclusion that the hydrogen bond does not contribute directly to the mechanism of the phase transitions, which are induced mainly by the conformational dynamics at T_{12} and van der Waals interactions between overlapping molecules at T_{23}.

However, it is remarkable that the temperature dependence of the hydrogen-bond dimensions is consistent with the general rules governing the changes of hydrogen-bond geometry depending on the thermodynamic character of the phase transitions (Katrusiak, 1993, 1995, 2001). These characteristic features are a shortening of the O$\cdots$O distance on cooling through the continuous phase transition at T_{12} and a

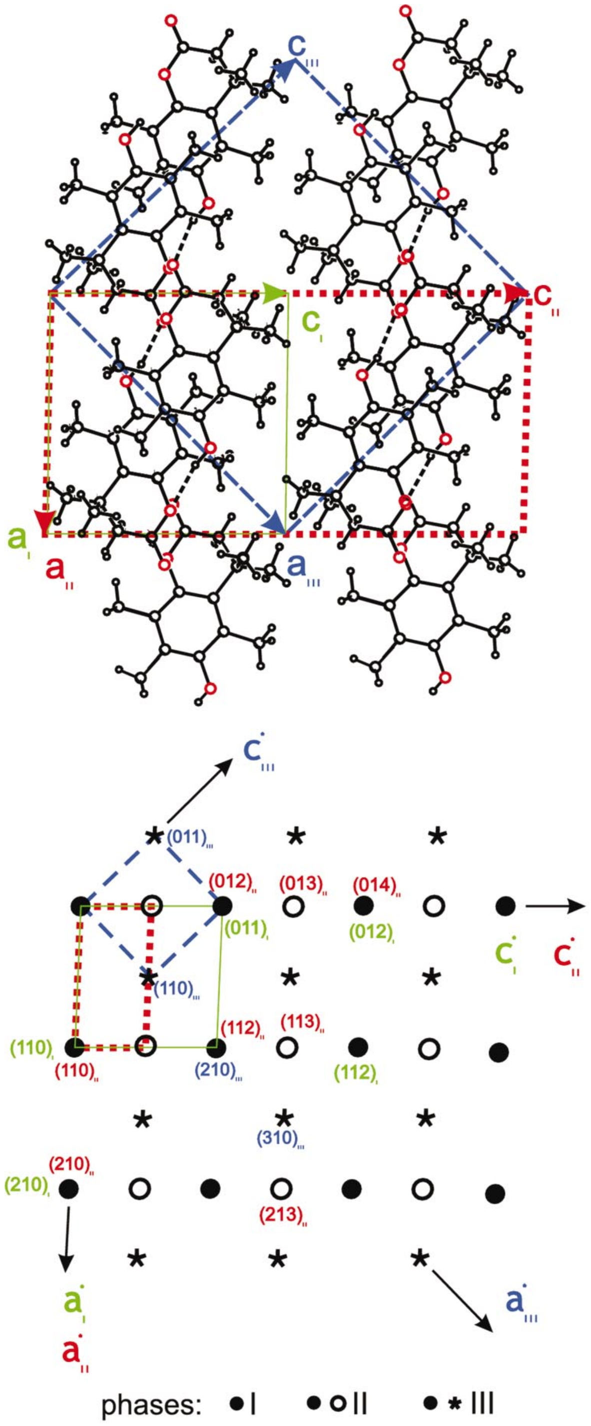

Figure 5
Projection of structure (1) down [010] with indicated unit-cell edges of phases I (thin green line), II (short red dashes) and III (long blue dashes); as well as the corresponding reciprocal spaces nodes: filled circles for phase I, both full and open circles for phase II, and both full circles and asterisks for phase III.

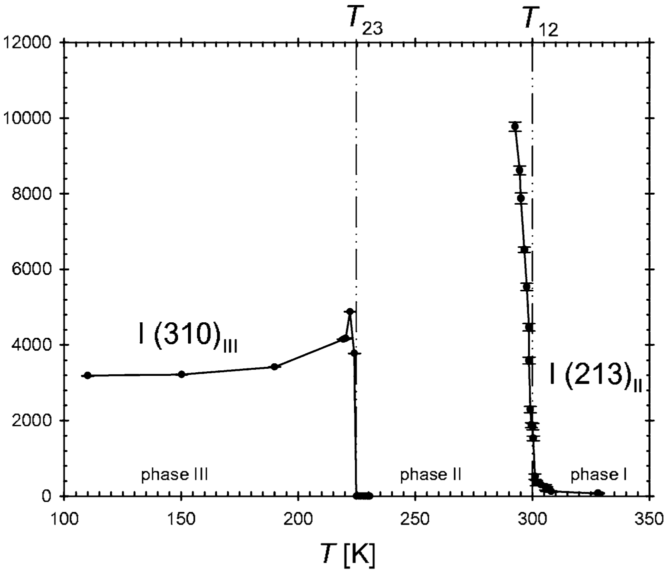

Figure 6
Intensities of reflections $(213)_{\text{II}}$ and $(310)_{\text{III}}$ as a function of temperature.

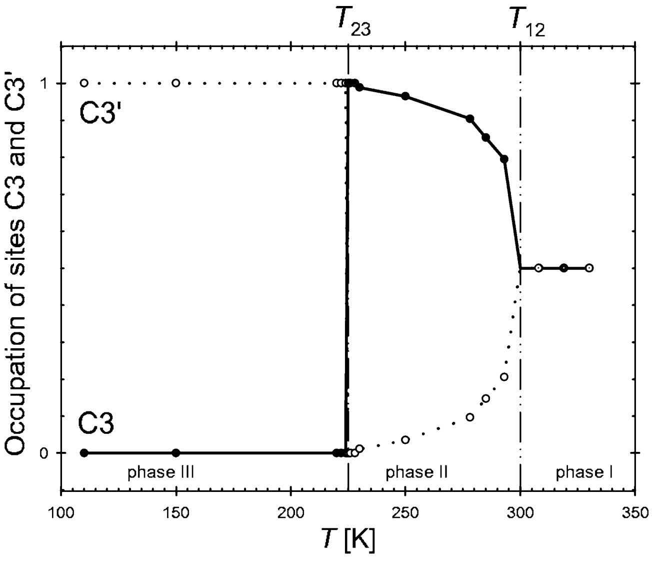

Figure 7
Temperature dependence of the occupancies of C3 (solid line) and C3′ (dotted line).

lengthening of O···O at the discontinuous phase transition at T_{23} (Fig. 11).

4. Conclusions

The phase transitions in crystal (1) are driven by the dynamic disorder and inversions of the molecular lactone ring. The lactone ring disorder at temperatures above T_{12} = 300 K is due to dynamic inversion between two equivalent sofa conformations. Ring-ordering proceeds continuously – begins below T_{12} and continues until T_{23} = 225 K when the molecules become fully ordered. The inversions of the lactone ring at T_{23} allow the molecules to pack more densely, hence the volume change and first-order phase transition. The behaviour of the lactone rings is directly connected to the crystal symmetry.

The main structural transformations at the phase transitions at T_{12} and T_{23} are due to changes in molecular conformation coupled to lattice dynamics of the crystal. Similar effects can occur in much more complex systems and may contribute to the properties and functions of macromolecules.

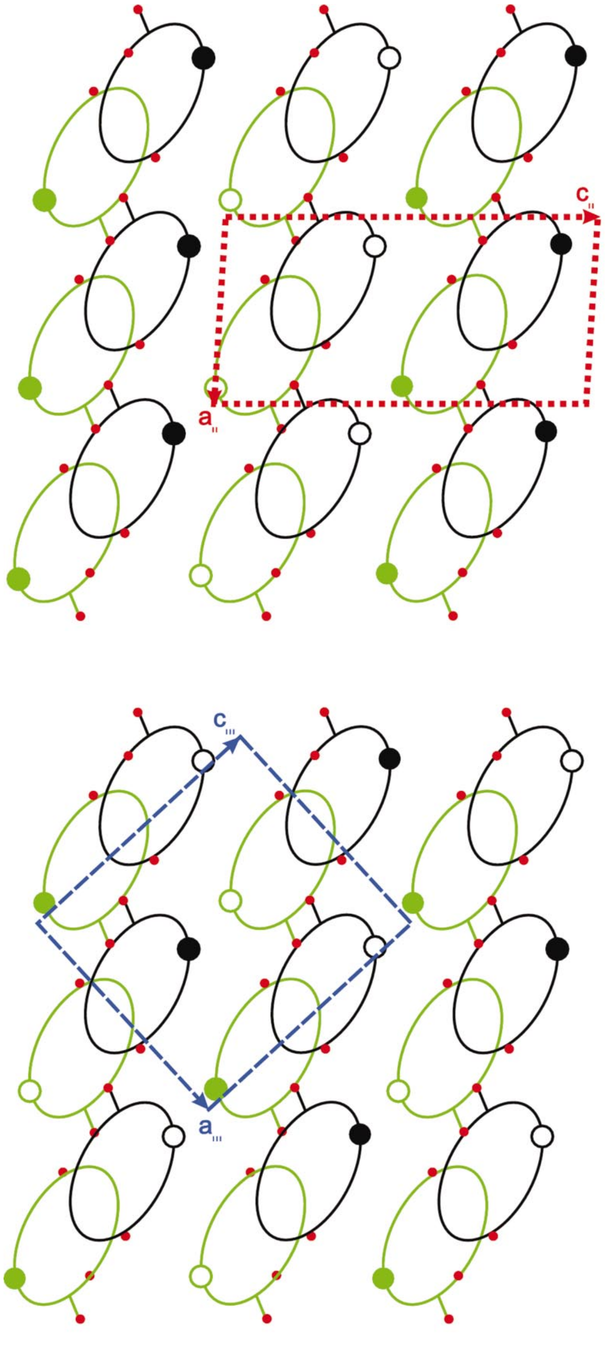

Figure 8
Schematic drawing of two sheets of molecules viewed down [101] in phases II and III (*cf.* Figs. 4 and 5). The molecules are represented as ovals; the large circles show methylene C3 directed upward (shaded) or downward (open); small red dots indicate the lactone O atoms and site of the hydroxyl groups. The molecules in the lower sheet are shown in green.

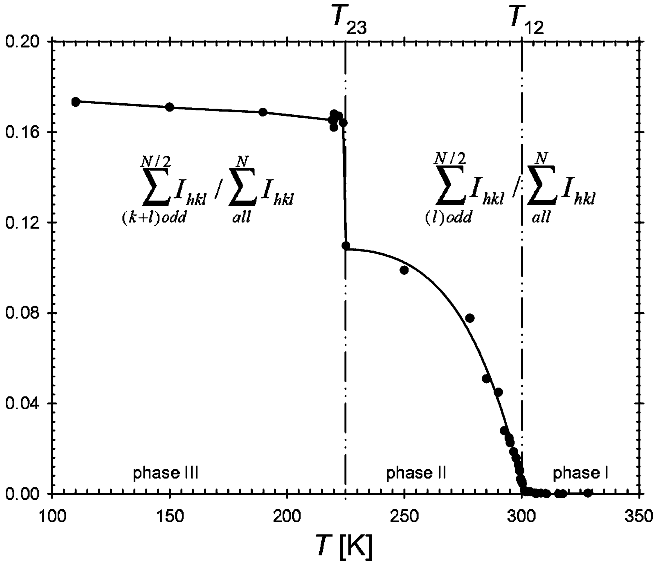

Figure 9
Temperature dependence of the ratio of the sum of intensities of reflections extinguished in phase I (see open circles and asterisks for phases II and III, respectively, in Fig. 5) to the sum of intensities of all reflections. The e.s.d.'s are smaller than the plotted symbols.

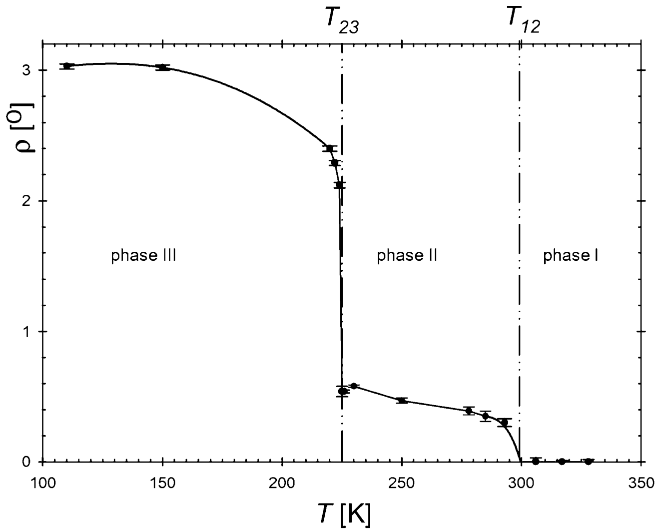

Figure 10
The temperature dependence of the inclination of the least-squares mean planes fitted to six C5–10 atoms to the crystal plane (010).