Considering the approximate nature of the method of linear combination of atomic orbitals, this surprisingly close agreement must, of course, be regarded as fortuitous. However, calculations based on data given in the literature seem to support the general validity of the proposed relation between bond order and restoring coefficient: It may, therefore, be useful also for calculations of potential functions as for control of approximations used in the method itself.

A detailed report will be published in *Acta Chem. Scand.*

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X-Ray Analysis of the Swelling of Wood Pulp in Sodium Hydroxide Solution

Investigations[1] on the hydrolysis and water-regaining properties of wood pulp, cotton and cotton linters swelled in sodium hydroxide solutions of varying concentrations showed that, whereas for wood pulps a low constant-limit degree of polymerization and high constant water-regain were reached by swelling in an 8 per cent lye, it was necessary to swell cotton and cotton linters in a 10 per cent solution in order to obtain a similar result. These differences between swollen samples of the two fibres might be due to easier mercerizing, that is, transformation of the cellulose I lattice into the cellulose II lattice, in the case of the wood pulp as compared with the cotton linters.

The mercerizing of cotton fibres has been subject to a number of investigations[2,3,4], and at the temperature employed in our work the cotton will show a mixed cellulose I – cellulose II X-ray diffraction pattern when swelled in sodium hydroxide solutions of between 9·5 and 10·5 per cent. Below this range cellulose I, and above this range cellulose II, patterns are observed. Few investigations have been carried out on wood pulp fibres. Katz and Seiberlich[5] found at 18° C. that the mercerizing strength of sodium hydroxide was 15 per cent for cotton and only 11·25 per cent for wood pulps. They claim that fibres with a higher degree of polymerization are more difficult to mercerize than those of lower degree of polymerization, thus accounting for this difference between wood pulps and cotton fibres.

It was thought to be of interest to compare the X-ray diffraction patterns of pulp samples swelled in the range of sodium hydroxide solutions where the rather abrupt changes in the hydrolysis and water-regains are observed. Two sodium chlorite bleached pulps, 1,556 and 1,597, with degrees of polymerization of 1,700 and 1,300, respectively, were swelled in sodium hydroxide solutions varying in concentration between 5·5 and 8·0 weight per cent at 3° C. as described by Jörgensen[1]. For the X-ray diffraction work the fibres were carefully arranged to give complete random orientation and irradiated in a Debye-camera in a hydrogen atmosphere with a copper $K\alpha$ beam.

The X-ray diffraction diagram of pulp 1,556 swelled in 5·5 per cent lye exhibits an unchanged cellulose I pattern, whereas the diagram for that from 6 per cent lye shows partial mercerization. The formation of cellulose II at the expense of cellulose I is indicated from the decrease of the intensities of the 101 and $10\bar{1}$ interferences of cellulose I and from the increase in the intensity of the 121 interference of cellulose I caused by the superposition of the $10\bar{1}$ interference of cellulose II. For samples swelled in 7 and 7·5 per cent lye a steady increase in the amount of cellulose II is indicated by the appearance of the 101 interference of cellulose II and further decrease in the intensities of the 101 and 101 interferences of cellulose I. The 8 per cent sample exhibits the pure cellulose II diagram.

The mercerizing of pulp 1,597 is retarded as compared with 1,556, as the 6 per cent sample gives an X-ray diagram showing very little change towards cellulose II. Again, the 6·5 and 7·5 per cent samples show diffraction diagrams of the mixed cellulose I and cellulose II patterns, and the 8 per cent sample has a pure cellulose II diagram.

Limit D.P., Water-Regain and X-Ray Evidence for Wood Pulps Swelled in Alkaline Solutions of Varying Concentrations

Swelling solution (weight % NaOH)	Pulp 1,556 (D.P. = 1,700)			Pulp 1,597 (D.P. = 1,300)		
	Water-regain (%)	Limit D.P.	X-ray evidence	Water-regain (%)	Limit D.P.	X-ray evidence
0	6·5	240	Cell. I	6·6	225	Cell I
5·5	6·6	140	Cell. I	7·7	115	Cell. I
6·0	8·3	95	Cell. I & II	8·1	75	Cell. I
7·0	8·4	80	Cell. I & II	8·3	75	Cell. I & II
7·5	8·7	75	Cell. I & II	8·7	65	Cell. I & II
8·0	8·8	55	Cell. II	8·8	55	Cell. II

The accompanying table shows that the X-ray analysis of the two pulps is in full agreement with the hydrolysis and water-absorption properties, which are seen to be sensitive indicators of any intracrystalline swelling. Note that the limit degree of polymerization may drop to half its original value without change in the X-ray diffraction pattern.

Wood pulps are undoubtedly more easily mercerized than cotton and cotton linters[1]. This difference cannot be explained on the basis of the lower degree of polymerization of the pulps[5], because the 1,556 pulp had a degree of polymerization similar to that of cotton linters. It seems to be more plausible to base an explanation on a possible difference in crystallite dimensions. The pulp of lower degree of polymerization (1,597) seemed to be more difficult to mercerize partially than the material of higher degree of polymerization (1,556). This indicates that the transition of cellulose I to cellulose II is dependent also upon the intercrystalline network, in that long cellulose chains extending through and connecting the crystallites facilitate the transformation to the cellulose II lattice. Details of this work will be published elsewhere.

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