

THE CLASSIFICATION OF POLYMERS ACCORDING TO THEIR
SYMMETRY PROPERTIES

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The present work is a part of an extensive investigation of the symmetries of stereoregular polymers|1-3|, in relation with their physical properties and processes involving such systems. The line group theory has been applied to investigation of the vibrational|4| and the electronic|2,5| spectra of macromolecules. These investigations are aimed at enabling one to infer as much as possible about the physical behaviour of a polymer, once its related line group is known.

A complementary but not less important part of this research programme is to determine the corresponding line groups for as many polymers as possible. To this task the present work is devoted. We have already collected relevant experimental data for 82 polymers, making use of which we were able to determine unambiguously the line groups for 31 of them. The type of the screw axis can be assigned for further 22 polymers, while the data for the rest of them are incomplete, inconclusive or contradictory. A part of this classification is given in the Table 1 below.

Table 1

| <u>Polymer</u> | <u>Fibre period (in Å)</u> | <u>Line group</u> | <u>Space group</u> |
|---------------------------|----------------------------|----------------------|------------------------------|
| Poly(tetrafluoroethylene) | 16.8 | $\underline{L}13_22$ | |
| Poly(oxyethylene) | 17.30 | $\underline{L}9_22$ | C_3^2 or C_3^3 |
| Poly(isobutene) | 18.63 | $\underline{L}8_522$ | $P2_1^2 2_1^2 2_1^2 = D_2^4$ |
| Poly(oxyethylene) | 19.39 | $\underline{L}7_4^2$ | |
| Poly(ethylene glycol) | 19.5 | $\underline{L}7_4^2$ | |

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|----------------------------------|-------|--|----------------------------------|
| Isotactic Poly(propylene) | 6.5 | $\underline{L}3_12$ or $\underline{L}3_22$ | $P3_121=D_3^4$ or $P3_221=D_3^6$ |
| Poly(ethylene) | 2.534 | $\underline{L}2_1/mcm$ | $Pnma=D_{2h}^{16}$ |
| 1-4-cis-poly(isoprene) | 8.10 | $\underline{L}2_1/m$ | $P2_1/b=C_{2h}^5$ |
| Poly(vynil alcohol) | 5.51 | $\underline{L}2_1/m$ | $P2_1/m=C_{2h}^2$ |
| 1-4-cis-poly(butadiene) | 8.60 | $\underline{L}1c$ | $B2/b=C_{2h}^6$ |
| Poly(allene) | 3.88 | $\underline{L}2_1/mcm$ | $Pnan=D_{2h}^6$ |
| Poly(vynil chloride) | 5.1 | $\underline{L}2_1/mcm$ | $Pbcm=D_{2h}^{11}$ |
| Syndiotactic poly(acrylonitrile) | 5.10 | $\underline{L}2mc$ | $Ama2=C_{2v}^{16}$ |

The symbols for the line groups adopted here follows closely the International crystallographic notation. L denotes translational periodicity along a line, n_k , $k=0,1,\dots, n-1$ is a screw axis, "2" after the main axis symbol denotes additional horizontal order-two rotation axis; m and c are a mirror and a glide plane respectively.

The complete classification will be published elsewhere.

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