The van der Waals radius for fluorine atoms is normally 1.4 Å, giving 2.8 Å for the F—F distance. Bates[15] has carried out semiempirical calculations for the conformational energy for an isolated PTFE chain. Using "6-exp" terms for the interactions between nonbonded atoms, a dipole–dipole interaction term, and a threefold "intrinsic" torsion potential, he found that a helical arrangement has the least total energy. This helix was close to that experimentally observed from the room temperature x-ray observations and, at the very most, was only 530 cal/mole more stable than the planar zigzag conformation. As a more efficient side-by-side packing can be achieved with the molecule in the planar zigzag conformation, it is reasonable to find that high pressure forces the molecules into this conformation.

The pressure at which the change from helical to planar zigzag takes place is of the order of that occurring in frictional contacts and rolling. Consequently it is possible that some of the polymer is indeed in this planar form during the deformation. However, it has not been possible to observe the changes during deformation because of the reversible nature of the transformation.

The author wishes to thank Dr. D. Tabor, F.R.S., for his interest and encouragement in this work and the Science Research Council for financial support.

References

1. R. I. Beecroft and C. A. Swenson, *J. Appl. Phys.*, **30**, 1793 (1959).
2. G. M. Martin and R. K. Eby, *J. Res. Nat. Bur. Stand.*, **72A**, 467 (1968).
3. E. S. Clark and L. T. Muus, *Z. Krist.*, **117**, 119 (1962).
4. R. G. Brown, *J. Chem. Phys.*, **40**, 2900 (1964).
5. S. Hirakawa and T. Takemura, *Japan J. Appl. Phy*ı, **8**, 635 (1969).
6. B. A. Newman and K. D. Pae, *Bull. Amer. Phys. Soc.*, **15**, 331 (1970).
7. G. J. Piermarini and C. E. Weir, *J. Res. Nat. Bur. Stand.*, **66A**, 325 (1962).
8. C. Weir, S. Block, and G. Piermarini, *J. Res. Nat. Bur. Stand.*, **69C**, 275 (1965).
9. D. L. Decker, *J. Appl. Phys.*, **36**, 157 (1965).
10. J. Matthewman, Crystallography Programs for Titan Computer, 1965.
11. *International Tables for X-ray Crystallography*, Kynoch Press, Birmingham, England, 1962.
12. W. Cochran, F. H. C. Crick, and V. Vand, *Acta Cryst.*, **12**, 171 (1959).
13. H. D. Flack, unpublished results (1971).
14. T. Seto, T. Hara, and K. Tamaka, *Japan J. Appl. Phys.*, **7**, 31 (1968).
15. T. W. Bates, *Trans. Faraday Soc.*, **63**, 1825 (1967).

Received August 6, 1971
Revised December 28, 1971