pyrazole derivative, but also the *Z* configuration of the side chain and the intramolecular hydrogen bond. The distance between O8 and O19 is 2·523 Å (2·518 Å), that between O19 and H19 is 0·984 Å (1·081 Å) and the O8-to-H19 non-bonding distance is 1·560 Å (1·452 Å); the figures in parentheses are the Laue-data-determined values. The extent of conjugation from O8 through C7, C9, C10, C17, C18 to O19 is apparent from the bond lengths listed in Table 2.

Concluding remarks

In this study the X-ray crystal structure analyses by monochromatic or Laue methods indentified the tautomeric form of an organic molecule. The 20 hydrogen atoms were identified in the respective difference Fourier syntheses after anisotropic refinement of the non-hydrogen atoms. Clearly the Laue data set was almost as sensitive to the hydrogen-atom scattering effects as the monochromatic data. This study gives confidence in the Laue method and the associated data-processing procedures being able to give data capable of discriminating between alternative, chemically possible, structures in the same way as the monochromatic method, at least, for a crystal with effectively absent anomalous-dispersion effects.

The total exposure time for the Laue data was 2s *versus* at least 72 h for this diffractometer data. The analysis of the Laue data took approximately 1–2 weeks *versus* a few hours for the diffractometer data. Clearly, the main advantage of the synchroton Laue method lies in kinetic studies and utilization of small crystals or for the solution of other special crystallographic problems rather than routine structure solving.

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Acta Cryst. (1989). B**45**, 596–597

3,17-Dioxo-19-norandrost-4-ene-7β-butyric Acid. Corrigendum.

By ROGER A. LALANCETTE,* PAUL B. SLIFER and HUGH W. THOMPSON, *Carl A. Olsons Memorial Laboratories, Department of Chemistry, Rutgers University, Newark, NJ*07102, *USA*

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Abstract

The crystalline (monoclinic, $P2_1$) cell parameters for the title compound, $C_{22}H_{30}O_4$, described [Precigoux, Busetta & Hospital (1977). *Acta Cryst.* B**33**, 566–568] as a = 9·099 (5), b = 16·407 (8), c = 6·564 (4) Å, β = 98·59 (10)°, Z = 2 should be a = 9·099 (5), b = 6·564 (4), c = 16·407 (8) Å, β = 98·59 (10)°, Z = 2. A projection is presented which makes unambiguously clear the helical catemeric hydrogen-bonding pattern.

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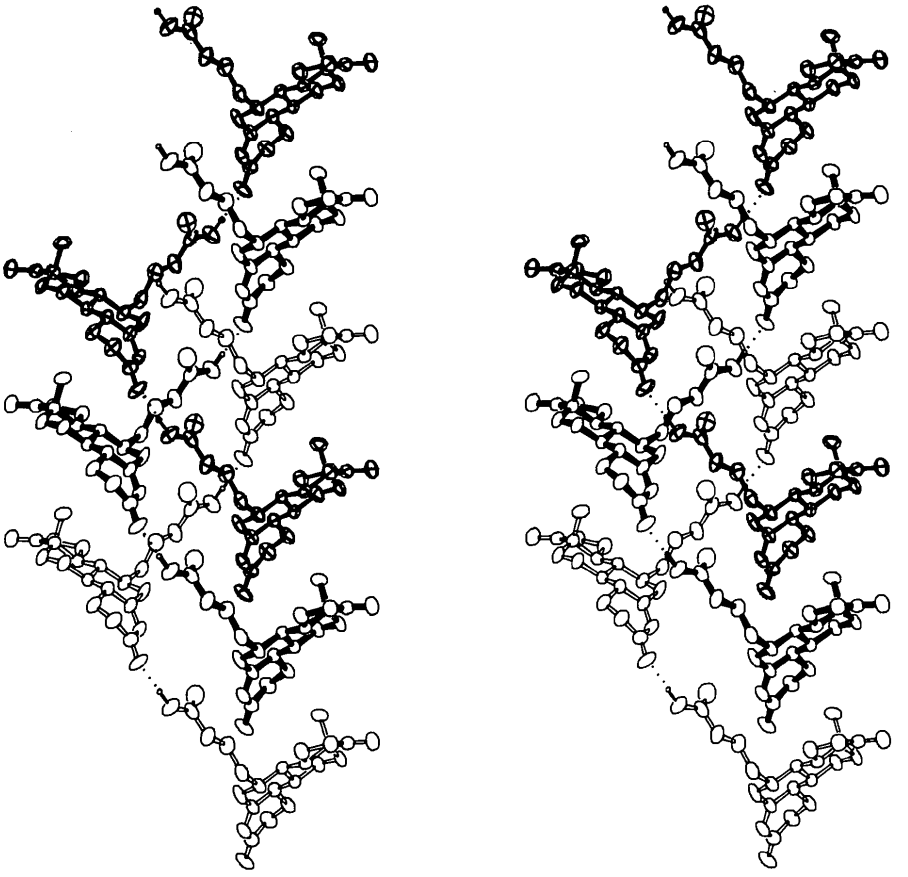

Fig. 1. Stereoscopic *ORTEP*II (Johnson, 1976) diagram perpendicular to the 2_1 screw axis. The entire bundle resembles a three-stranded rope; each of the identical intercoiled strands is a helical catemer linked by COOH···O=C hydrogen bonds. For differentiation, the strands of the triple helix have been independently highlighted.

All relevant numerical information is contained in the *Abstract*, and has also been noted in the *Atlas of Steroid Structure* (Griffin, Duax & Weeks, 1984) and the Cambridge Structural Database (Allen *et al.*, 1979; Refcode: DXANBU 770722).

The original article (Precigoux, Busetta & Hospital, 1977) correctly described an intermolecular hydrogen bond from the butyryl carboxyl to the ring-*A* ketone with a 2·70 Å O—O distance, and spoke of 'blocs helicoïdaux'. However, the projection which was presented (along the *b* axis) is ambiguous in this regard and appears to show these intermolecular hydrogen bonds in a mutually dimeric arrangement. The projection shown in Fig. 1 makes clear that the pattern is a helical catemer linked by COOH···O=C hydrogen bonds.

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