03. CRYSTALLOGRAPHY IN BIOCHEMISTRY AND PHARMACOLOGY C-57

03.3-8 THE CRYSTAL STRUCTURES OF O5-ACETYLMORPHINE AND O5-ACETYLMORPHINE-ETHYL ACETATE COMPLEX.

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The formation of a stable O5-acetylmorphine ethyl acetate complex has been described by Beckstead and Neville (1986) as being rather unique since no such complex is formed for morphine or its closely related derivatives codeine, thebaine, O6-acetylmorphine or heroin. The FT-IR spectra of the complex and its parent substance, O5-acetylmorphine, have been reported (H.D. Beckstead and G.A. Neville, 69th Annual Canadian Chemical Conference, 1986); both crystal structures have been determined by X-ray analyses, for comparison with related derivatives.

O5-acetylmorphine, \( \text{C}_{19}\text{H}_{21}\text{N}_0\text{O}_4 \), is orthorhombic, \( P_2_1_2_1_2_1 \), \( a = 13.141(2), b = 16.714(2), c = 7.47(1) \text{ Å}, R = 0.036 \) and \( wR = 0.041 \) for 1896 observed reflections. The O5-acetylmorphine-ethyl acetate complex, \( \text{C}_{19}\text{H}_{21}\text{N}_0\text{O}_4\cdot\text{C}_4\text{H}_8\text{O}_2 \), is orthorhombic, \( P_2_1_2_1_2_1 \), \( a = 19.943(1), b = 16.352(1), c = 8.098(2) \text{ Å}, R = 0.048 \) and \( wR = 0.060 \) for 2159 observed reflections. In both structures acetamide molecules are linked by \( O-H...N \) hydrogen bonds to form chains. In the complex (see Fig.1), the solvate is accommodated in the channels between the chains, without any hydrogen bonding.

The dihedral angle between the two strictly planar rings is 89.6(2)º, so that the rings are virtually perpendicular to each other, as shown in Fig. 2.

This conformational feature resembles that found in the two phenoxy-phenoxy herbicidally active species: methyl \( 2-[4-(2,4-	ext{dichlorophenoxy})	ext{phenoxy}] 
