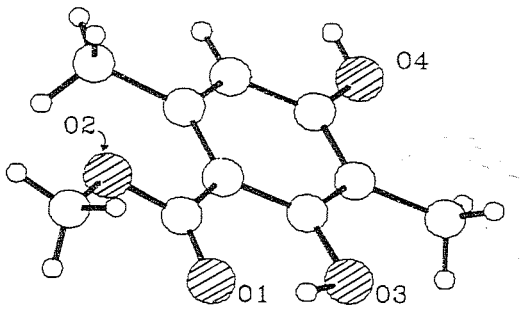
programs and algorithms. Detailed results of (both) structures will be presented, along with conclusions about the solution method(s) for [17].

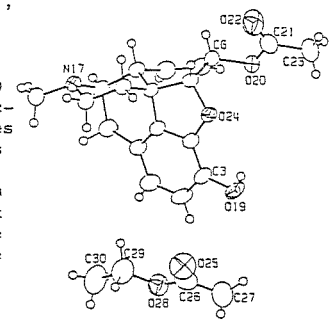
Structure [5]



03.3-8 THE CRYSTAL STRUCTURES OF O^6-ACETYLMORPHINE AND O^6-ACETYLMORPHINE-ETHYL ACETATE COMPLEX.
By F.R. Ahmed, Division of Biological Sciences, National Research Council of Canada, Ottawa, Canada K1A OR6

The formation of a stable O^6-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, O^6-acetylmorphine or heroin. The FT-IR spectra of the complex and its parent substance, O^6-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.

O^6-acetylmorphine, $C_{19}H_{21}NO_4$, is orthorhombic, $P2_12_12_1$, $a = 13.141(2)$, $b = 16.714(2)$, $c = 7.474(1)$ Å, $R = 0.036$ and $wR = 0.041$ for 1896 observed reflections. The O^6-acetylmorphine-ethyl acetate complex, $C_{19}H_{21}NO_4.C_4H_8O_2$, is orthorhombic, $P2_12_12_1$, $a = 15.943(3)$, $b = 16.332(3)$, $c = 8.098(2)$ Å, $R = 0.048$ and $wR = 0.060$ for 2159 observed reflections. In both structures acetylmorphine molecules are linked by O-H···N hydrogen bonds to form chains. In the complex (see Fig.), the solvate is accommodated in the channels between the chains, without any hydrogen bonding.



03.3-9 STRUCTURE OF THE COGNITION ACTIVATOR 3-PHENOXY--PYRIDINIUM HYDROGENSULFATE. By G.Bandoli, U.Casellato, M.Nicolini and G.C.Pappalardo, Department of Pharmaceutical Sciences, Via Marzolo 5 - University of Padova , Italy; CNR - ICTR - Padova, Italy

In vitro and in vivo studies indicated that the title compound may exert its cognition function-enhancing properties (D.E.Butler,B.P. H.Poschel and J.G.Mariott, J.Med.Chem.,1981,24,346-350) by increasing DA neuronal function (T.A.Pugsley and R.B.Schwarz, IVth World Cong.Biol.Psychiatr.,Philadelphia,1985,abst.151.4). To gain insight into the structure/activity relationship of this and related compounds, a structural investigation has now been initiated.
Crystal data. $(C_{11}H_{10}NO)^+(HSO_4)^-$; monoclinic, $P2_1/c$, $a=7.967(4)$, $b=5.899(4)$, $c=25.480(10)$Å, $\beta=96.90(5)°$; $Z=4$; $M_r=269.3$, $D_c=1.50gcm^{-3}$, $R=0.048$ for 1307 observed reflexions.
The structure (Fig.1) is built up from 3-phenoxy-pyridinium cation and hydrogensulfate counter anion, which are linked by a rather strong hydrogen bond N-H---O (2.72Å).
The dimensions of the compound show no abnormal values.

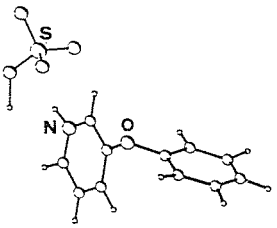


Fig. 1

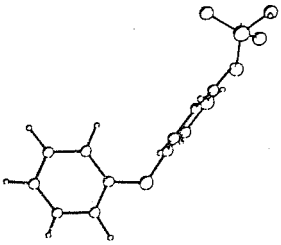


Fig. 2

The dihedral angle between the two strictly planar rings is 89.6(2)° 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-dichlorophenoxy)phenoxy]propionate (81.9°) (G.Smith, C.H.L.Kennard, A.H.White and B.W.Skelton, J.Agr.Food Chem., 1981, 29, 1046-1049) and 2-[2-(phenoxy)phenoxy]-2-methylpropionic acid (104.5°) (A.Wagner and G.Malmros, Acta Cryst., 1979, B35, 2222-2225).