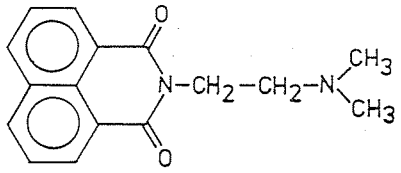
03.3-2 THE STRUCTURE OF THE ANTICANCER COMPOUND N-1'-ETHYL-1,8-NAPHTHALOIMIDE-2'-DIMETHYL AMMONIUM CHLORIDE, AND THE STRUCTURES OF ITS $PtCl_4^{2-}$ AND $PtCl_6^{2-}$ SALTS.

By G.R. Clark and S.B. Hall, Department of Chemistry, University of Auckland, New Zealand.

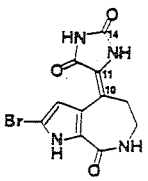
Two important classes of anticancer compounds are the intercalating agents, such as the acridines, and the DNA selective binding agents, such as cis-platin. We have been attempting to synthesise single molecules containing both of these functions - i.e. intercalator-appended derivatives of cis-platin, using the intercalator shown below.



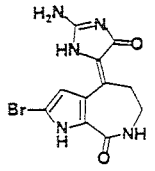
As side-products of these synthetic attempts we have grown crystals of several salts of the title compound. We have determined the crystal structures of the title compound (1), and its $PtCl_4^{2-}$ (2) and $PtCl_6^{2-}$ (3) salts. All three compounds crystallise in the monoclinic space group $P2_1/c$. Cell constants are (1) a=13.261(1), b=12.099(1), c=10.693(2)Å, β=118.02(1)°, n=4; (2) a=12.548(1), b=8.957(1), c=14.829(1)Å, β=105.95(1)°, n=2; (3) a=9.717(1), b=12.748(1), c=14.228(6)Å, β=105.89(1)°, n=2. The structures were determined by Patterson and electron density maps, and refined using SHELX-76 to R values of 0.040, 0.029 and 0.026 for 2531, 2796, and 3162 observed reflections respectively. The geometries of the three compounds will be compared.

03.3-3 AXASTATIN A, AN ANTITUMOR AGENT FROM THE MARINE SPONGE AXANILLA sp., By R.B. Bates,[1] M.A. Bruck,[1] F.A. Camou,[1] C.L. Herald,[2] J.E. Leet,[2] G.R. Pettit[2] and D. Schaufelberger,[2] (1)Department of Chemistry, University of Arizona, Tucson, and (2)Cancer Research Institute, Arizona State University, Tempe, Arizona, USA

An X-ray study shows the title compound to be 1, related to hymenialdisine 2 (Cimino et al., Tetrahedron Lett. 23, 767 (1982); Kitagawa et al., Chem. Pharm. Bull. 31, 2321 (1983)) but having O instead of N at C14, existing as a different tautomer, and having the opposite configuration of the C10-C11 double bond.



1



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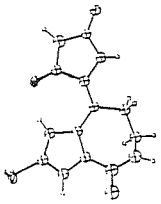

03.3-4 VISNAGIN, $C_{13}H_{10}O_4$(5-METHOXY-2 METHYL-FURO-(9) CHROMEN. By Karimat El-Sayed, A.M. Abd El-Rahman, Department of Physics, Ain-Shams University, Cairo, Egypt, And Herman L. Ammon, Department of Chemistry, Maryland University, U.S.A.

Ammi Visnaga is a perennial herbaceous plant belonging to the family Umbelliferae, growing in the waste lands of the Eastern Mediterranean and particularly in the region of Nile Delta. The Furochromones extracted from the fruits of the plants (Kellin, visnagin and Kellol glucoside) have been the object of an exhaustive pharmacological research (Hutter, C.P. and Dale, E. Chem. Reviews, 1951, 40). The crystal is orthorhombic, space group $p2_12_12_1$ with a = 7.087(6), b = 9.917(15), c = 14.884(17) Å, V = 1046.09(1) Å^3, z = 4, Dx = 1.46 Mgm^{-3}, λ(MOK) = 0.7107 A. The intensities were collected on a CAD-4 computer controled diffractometer with graphite monochromater. The structure was solved by using MITHRIL program, the hydrogen atoms of the three rings shown in Fig.1 are located geometrically, the methyl and methoxyl hydrogen are located on difference map. The structure was refined by block diagonal least squares minimising $\Sigma w(|F_o|-|F_c|)^2$, w = $1/\sigma^2$ F final R is 0.045 (1090 reflections).

The results showed that the Visnagin molecule is planar within ±0.032(1)Å except for C(11) which lies on the opposite side of the plane of O(4), the methoxyl group arrange itself in a zigzag way along z axis. The crystal cohesion is mainly obtained by Wander Waal's force.

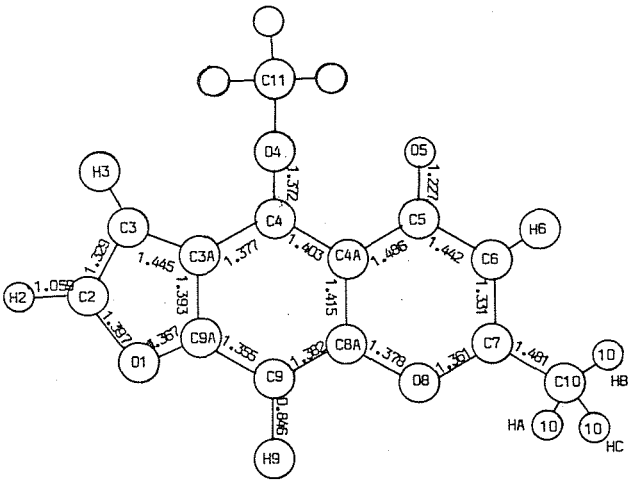

Fig. 1