Strychnine crystallises with a variety of anions in two structural types (Fig. 2).

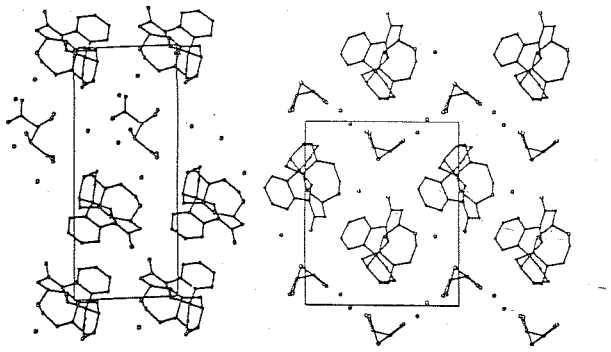


Fig. 2. Packing in strychnine (+) tartrate and strychnine (-) bitartrate.

They may both be described as bilayers with the strychnine molecules projecting hydrophilic portions toward one surface or the other. The bilayers differ in the extent of "grooving" to accommodate hydrophobic parts of counterions.

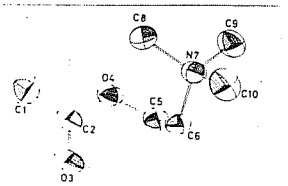
Brucine complexes are more widely used in resolutions than strychnine ones, and show greater variety. They can, however, normally be classed as corrugated monolayers of three types: channelled head-to-head, channelled head-to-tail, and offset head-to-tail. A range of examples will be presented and discussed.

03.4-8 MODELS FOR THE BINDING TO DNA OF CIS-PLATINUM DERIVATIVES CONTAINING BIDENTATE TERTIARY AMINES. By Max R. Taylor, Sally L. Birch, Sharon E. Lawton, Lisa J. Keefe and Louise M. Vilkins, School of Physical Sciences, The Flinders University of South Australia, Bedford Park, S.A. 5042, Australia, and John D. Orbell, St. Vincents Institute of Medical Research, 41 Victoria Pde., Fitzroy, Victoria, 3065, Australia.

The binding of the cis-$A_2Pt(II)$ cationic moiety (A = a monodentate amine or A_2 = a bidentate amine) to two adjacent guanine residues on the same strand of DNA, i.e. the formation of an intrastrand crosslinkage, is a leading hypothesis concerning the mode of action of cis-platinum antitumour agents. The effectiveness of these drugs is strongly influenced by the nature of the amine ligands(s) A or A_2. For example, the cytotoxic activity of these compounds is found to decrease along the series $A = NH_3 \approx NH_2R > NHR_2 > NR_3$. This may be wholly or in part due to intramolecular steric effects which would be expected to influence the formation and subsequent geometry of cis-platinum adducts with DNA.
To date, crystallographic investigations of model systems for an intrastrand cross linkage have involved compounds where two nucleobase derivatives are cis-coordinated to $A_2Pt(II)$, where A or A_2 are primary amines; representative of effective oncolytic agents. There is a paucity of structural information on model systems for cis-platinum derivatives which are ineffective due to the amines being secondary or tertiary - this requires the presence of relative bulky substituents on the coordinated nitrogen atoms.
The complexes
cis-[(TMED)Pt(9-methylguanine)$_2$]$(PF_6)_2$.$2H_2O$,
cis-[(TMED)Pt(9-ethylguanine)$_2$]$(ClO_4)_2$.$2H_2O$,
cis-[(TMED)Pt(1,3-dimethylxanthine)$_2$]$(PF_6)_2$.$4H_2O$ and
cis-[(TMED)Pt(1,3,9-trimethylxanthine)$_2$]$(PF_6)_2$.$\times H_2O$ where TMED = N,N,N^1,N^1-tetramethylethylenediamine have been prepared and structurally characterised by x-ray methods. Least-squares refinement has given R values of 0.020, 0.045, 0.059 and 0.09 respectively. Each [(TMED)Pt(Base)$_2$]$^{2+}$ cation shows square-planar geometry with the two crystallographically independent purine ligands coordinated through N(7) and arranged in a head-to-tail conformation so that the cation has approximately C_2 symmetry.
The structures are compared with each other and with related compounds in terms of their base/base and base/coordination plane dihedral angles, and their different crystalline environments.

03.5-1 PICRATES OF ACETYLCHOLINE AND METHOXYCARBONYLCHOLINE. By Karla Frydenvang and Birthe Jensen, Department of Chemistry BC, The Royal Danish School of Pharmacy, Universitetsparken 2, DK-2100 Copenhagen, Denmark.

The title compounds have been studied at 105 K as part of a series of salts of acetylcholine and related compounds. A very clear correlation is found between conformation and geometry. The magnitude of the angle O4-C5-C6 varies from ∿100° in a fully extended choline ester to ∿113° in the most folded conformers.



Packing patterns in crystals may reveal preferred types of interaction between choline derivatives and neighbouring groups. Acetylcholine as well as methoxycarbonylcholine form a great number of contacts to oxygen atoms. Contacts from the quaternary ammonium group do not seem to be of greater importance than contacts from the acetyl- or methoxycarbonyl-moiety. Direct contacts between aromatic rings and the quaternary ammonium group in acetylcholine have been observed by NMR-techniques (Minch et al., J. Org. Chem., 1979, 44, 3247-3252). This type of contact is not found in the picrates. Their possible importance in crystals is being studied, based on data retrieved from the Cambridge Database (Allen et al., Acc. Chem. Res., 1983, 16, 146-155).