

ABSTRACT

The thesis comprises of crystallographic studies of acridinediones and triazolothienopyrimidine derivatives. Since both the group of molecules are of biological and pharmacological interest, crystal and molecular structure determination of seven acridinedione and four triazolothienopyrimidine derivatives were carried out.

First chapter of the thesis gives the general introduction about acridine, acridinedione and triazolothienopyrimidine derivatives and their various biological and pharmacological applications. In addition to it, a brief description of the crystal structure determination procedure using X-ray diffraction is also presented.

The second chapter comprises of crystal structures of three acridinedione monomers. All the three structures were solved by direct methods and refined by full matrix least-squares technique. The final residual factor R1 is 0.043, 0.039 and 0.062 respectively. The exterior rings of the acridinedione moiety adopt sofa conformation and the central ring adopts boat conformation. Of the three monomers, one of the structures possesses a water molecule which forms O-H...O hydrogen bonds for structure stability. The other two structures are stabilised by N-H...O and C-H...O hydrogen bonds. The dihedral angles between the exterior rings (the buckling angle) are $21.06(2)^\circ$, $36.8(1)^\circ$ and $40.0(1)^\circ$ respectively for the three mono acridinediones.

The third chapter describes the crystal structure determination of two acridinedione dimers. Both the structures were solved by direct methods and refined by full matrix least-squares technique and the final R1 values are 0.067 and 0.049. Both the dimers possess half a molecule per asymmetric unit and in one case a water molecule is present in the lattice to form O-H...O hydrogen bonds. The crystal structures are stabilised by O-H...O and C-H...O hydrogen bonds.

Fourth chapter describes the crystal structure of an acridinedione trimer which has twinned lattice. The hkl reflections from one individual is overlapped with khl reflections from the other such that the resulting diffraction pattern is pseudo-hexagonal. The structure was solved in monoclinic space group $P2_1$ consisting of one full molecule in an asymmetric unit. The structure was refined considering two inversely related twinning components; the final residual factor is 0.111. The crystal structure is stabilised by C-H...O hydrogen bonds.

The fifth chapter carries the crystal structure determination of a (nitrogen replaced by sulphur in the acridinedione moiety) thiapyranedione. The structural features of this compound are compared with all other acridinedione structures presented in this thesis. The sixth chapter deals with the spectroscopic studies on the interaction of thiapyranedione and a bis-acridinedione with ct-DNA. The spectral changes are observed which show the formation of molecular aggregation.

The seventh chapter gives the crystal structures of two triazolothienopyrimidine derivatives which differs from one another by a single methyl group substitution. The cyclohexane ring is disordered with two conformers for both the structures and favours more of a half-chair conformation than sofa. The structures are stabilised by N-H...N hydrogen bonds and S...S short contacts.

The eighth chapter comprises of two pyrimidone crystal structures; one is triazolothienopyrimidone and the other one is a pyrazolopyrimidone derivative. The pyrazolopyrimidone possesses two molecules per asymmetric unit and they have different orientations of the substituted ring systems. The crystal structures of both the compounds are stabilised by N-H...N and C-H...O hydrogen bonds.

All the structures presented in the thesis are solved by direct methods using the program SHELXS86 and refined by full matrix least-squares technique using the program SHELXL93. The geometrical parameters are calculated using PARST program. To compile the thesis within the limitations, the observed and calculated structure factors are not included in the thesis. The same are available with the author for any clarification and reference. The last chapter gives an overall conclusion of the thesis in an explicit manner.