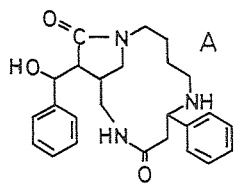
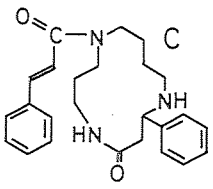
fractometer-measurement intensities and refined by full-matrix least-squares to R = 0.07. All the hydrogen atoms have been located as dominant peaks on a difference electron density map and refined isotropically. Bond lengths and angles agree well with those of analogous compounds. The S - C(1), C(1) - N(1) and C(1) - N(2) distances of 1.666(5), 1.374(7) and 1.321(7) indicate the effect of the thiourea resonance system. The tetrahydrofurane ring is in the envelope conformation, the best least-square mean shows the spirocarbon out of the plane of the other atoms in the same way as in some similar compounds (Bron, Cottier, Descortes, Faure & Loiseleur, Acta Cryst., 1983). The imidazolidine ring is nearly planar (maximum diviation 0.106 Å) and the phenyl group is completely planar (maximum deviation 0.007 Å). The dihedral angle between the two main ring is 90.8° and between the phenyl and imidazolidine rings is 86.5°. There is an intermolecular hydrogen bond between atoms O(3) and O(4) (O(3)....O(4) = 2.679(7) Å and H....O(4) = 1.727 Å). All other intermolecular contacts are van der Waals contacts.

03.5–11 X-RAY INVESTIGATIONS OF CAESALPININE A AND C, NOVEL SPERMIDINE ALKALOIDS FROM CAESALPINIA DIGYNA ROTTL. By S.B. Mahato and N.P. Sahu, Indian Institute of Chemical Biology Jadavpur, Calcutta, India, and E. Müller and P. Luger, Institut für Kristallographie, Freie Universität Berlin, Berlin, West-Germany.

Caesalpinia digyna Rottl. (Leguminosae) is a prickly scandent shrub growing in eastern India, Burma, and Ceylon. It has the reputation for pharmacological use in phthisis, scrofula and diabetes. ("The Wealth of India, Raw Materials"; CSIR, 1950;VOL.II,4). Chemical investigations of the plant have led to the isolation of caesalpinine, a novel macrocyclic spermidine alkaloid having a new skeleton. Three forms of caesalpinine have so far been distinguished, named A, B, and C. Caesalpine A (Mahato,Sahu,Luger, J.Am.Chem.Soc.(1983)105, 4441) and C could be crystallized and their structures were established by means of single crystal X-ray analysis. Caesalpinine A possesses a 13-membered lactam ring fused to a five membered lactam ring, in Caesalpinine C the five membered ring is no longer present. Structural details of the analyses will be presented and the biogenetic pathway of formation will be outlined.





03.5–12 LOW ENERGY PHOSPHATES: GLUCOSE 1-PHOSPHATE HAS DIFFERENT CONFORMATIONS IN ITS POTASSIUM AND SODIUM SALTS By N.Narendra, T.P.Seshadri and M.A.Viswamitra, Department of Physics and ICMR Centre on Genetics and Cell Biology, Indian Institute of Science, Bangalore - 560 012, India.

Glucose 1-phosphate plays an important role as a low energy phosphate in glycolysis.

$G1Pk_2$ crystallizes in the space group $P2_1$ with a = 10.447(1); b = 9.019(1); c = 7.523(1) Å, β = 110.44(1)°; Z = 2, D_m = 1.85, D_x = 1.86 Mgm^{-3}. CuK_α diffractometer data were collected and final R for 1520 unique reflections is 0.075. $G1PNa_2$ belongs to monoclinic space group C2 with a = 8.429(1); b = 10.184(2); c = 16.570(2) Å; β = 99.18(1)°; Z = 4, D_m = 1.73, D_x = 1.74 Mgm^{-3}. The final R for 1531 unique CuK_α reflections is 0.069.

The conformation about the C(5)-C(6) exocyclic bond is gauche-trans in $G1Pk_2$, in contrast to gauche-gauche observed in the crystal structures of $G1PNa_2$ and G6PBa (Katti, Seshadri and Viswamitra, Acta Cryst. (1982) B38, 1136-1140).

The pyranose sugar ring in both the structures however, has the $^4C_1$ chair conformation a geometry also found in the low energy phosphate G6PBa. The phosphate ester bond lengths in $G1PNa_2$ and $G1Pk_2$ are 1.641(6) and 1.630(5) Å respectively somewhat higher compared to the P ~ O bond length of 1.612 Å found in the high energy phosphate, monopotassium salt of phosphoenolpyruvate (Hosur and Viswamitra, Acta Cryst. (1981), B37, 839-843).