β = 108.31(4)°, U = 2401(2) Å^3, space group P2$_1$/n,
D$_m$ = 1.20 g cm^{-3}, D$_c$(Z = 4) = 1.21 g cm^{-3}.

alkylating reagents.
Other interesting fact is the lower stability of these K-salts versus the Na-salts(C. Esteban-Calderón, M. Martínez-Ripoll, to be published elsewhere): The free compounds behave as sequestering agents for Na ions.
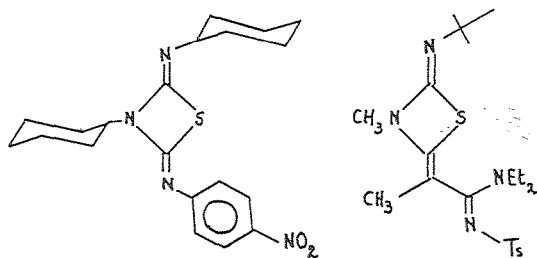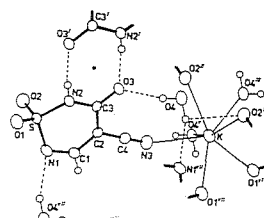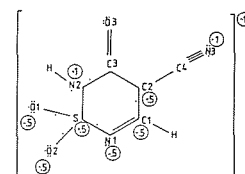

(1)   (2)

These thiazetidine rings are planar and more symmetrical than other published thiazetidine rings because both carbon atoms of the ring have external double bonds (C-S : 1.81 - 1.88 Å and C-N : 1.37 - 1.40 Å).

4CN-K

Fig.1   Fig.3

4NO2-K

Fig.2   Fig.4

09.2-45   MONOPOTASSIUM SALTS OF 4-CYANO AND 4-NITRO-3-HYDROXY-6H-1,2,6-THIADIAZINE 1,1-DIOXIDE.MONOHYDRATE. By C. Esteban-Calderón ,M. Martínez-Ripoll and S. García-Blanco, X-Ray Department, Institute "Rocasolano",Serrano 119, Madrid-6, Spain.

Both compounds have been synthetized by Goya and Stud (J. Heterocyclic Chem.(1978)15, 253-256), as a part of a research project aimed at obtaining substances with biological activity.
Crystal data are:
4CN-K(C$_4$H$_2$N$_3$O$_3$SK.H$_2$O): a=9.811(1);b=7.296(1);c=5.858(1)Å
α=103.06(1);β=94.56(2);γ=100.51(2)°; Z=2; P$\bar{1}$; n°reflex. in refinement 2835.
4NO2-K(C$_3$H$_2$N$_3$O$_5$SK.H$_2$O): a=6.0744(4);b=18.583(2)Å
c=7.497(1)Å;β=91.68(1)°; Z=4; P2$_1$/c; n°reflex. in refinement 2006.
Both structures have been solved by using single crystal data and MoKα radiation, and refined by least-squares analysis to the values of 0.042(R$_w$=0.049) and 0.039 (R$_w$=0.050), respectively.
Major electron distributions are proposed (Fig.3 and 4), according to Linnett's model(Linnett, J.W.(1966). The Electron Structure of Molecules. A New Approach. London. Methuen)
Two facts are relevant in these salt crystal structures, when compared with the structures of both free compounds (C. Esteban-Calderón, M. Martínez-Ripoll and S. García-Blanco, Acta Cryst.(1979),B35,2795-2797) and (C. Esteban-Calderón, M. Martínez-Ripoll, to be published elsewhere):
1) Strong electron modifications occur within the thiadiazine ring, the main alterations being around O(3), C(3), N(2), S and N(1).
2) The diferent location of the H atom, attached to N(2) in these structures, in comparison with the free compounds (where H is attached to N(1), explains the diferent behaviour of both free and salt compounds, versus
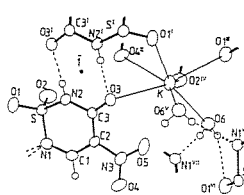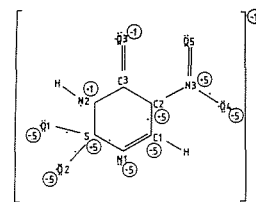
09.2-46   CONFORMATIONAL AND STRUCTURAL RELATIONSHIPS BETWEEN TEN DITERPENOIDS FROM TEUCRIUM SPECIES. By L. Eguren, J. Fayos and A. Perales, X-Ray Department, Instituto "Rocasolano", C.S.I.C., Serrano 119, Madrid-6, Spain.

The chemistry of diterpenoids ocurring in the genus Teucrium, is described in a recent general review (Piozzi, Heterocycles. (1981) in press). The structures of ten of these compounds shown below have been determined by X-Ray diffraction.
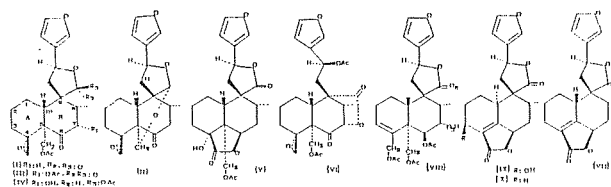
The purpose of this study is to classify these compounds according to the conformation of their rings. Special attention has been devoted to the decaline group. Parameters definition: for this study Cremer's parameters have been used (Cremer and Pople. J.Am.Chem.Soc. (1975) 97(6), 1354-58), θ(°), Φ(°) and Q(Å). Chairs occur for θ=0,180°, and boat or twist for θ=90°. Φ describes the boat form (Φ=0,60,120...) and twist form (Φ=30,90,150..), and Q the puckering. The table shows the experimental X-Ray values for the decaline moieties. τ_A is the internal torsion C1-C10-C5-C4 and τ_B is C6-C5-C10-C9. It is observed that <τ_A+τ_B> is nearly constant: 108° for sp3-sp3 bonds and 53° for sp2-sp3 bonds. The 108° value is diminished by the C5-C9 axial interaction and the oxo substituted C6 in compounds I, IV and VI. For saturated cyclohexane rings Q$_i$ increases with θ_i to reach a maximum at $\theta_i \sim$90° and decreases again towards $\theta_i \sim$180°,