

LETTERS TO THE EDITOR

CRYSTALLIZATION AND CRYSTAL
DATA OF ACETAMINOPHEN AND
METAMIZOL

ACETAMINOPHEN (also known as paracetamol) and metamizol (Novalgin) are well-known pain relieving medicines. Acetaminophen is a derivative of acetanilide whereas metamizol is a pyrazole derivative. The crystallization and the preliminary X-ray study of these compounds have been carried out as part of a programme of structural investigations of analgesics and their interactions¹⁻³.

Large, nearly transparent crystals of acetaminophen were crystallized by slow evaporation of its solution in ethanol. Tiny, needle-like crystals of metamizol were grown by vapour diffusion with water as the solvent and ethanol as the precipitant. The space groups and the unit cell dimensions of the crystals were determined from oscillation, Weissenberg and precession photographs taken about crystallographic axes using nickel filtered copper radiation. The densities of the samples were measured by flotation method using a mixture of carbon tetrachloride and benzene. These data are given in Table I.

TABLE I
Crystal data

	Acetaminophen	Metamizol
Space group	P2 ₁ /c	P2 ₁ /c
a in Å	7.12 ± 0.01	9.25 ± 0.01
b in Å	9.40 ± 0.03	49.22 ± 0.02
c in Å	12.88 ± 0.03	7.32 ± 0.02
β in degrees	116.2 ± 0.5	90.5 ± 0.5
Volume of the Unit Cell in Å ³	773.50	3332.69
Molecular formula	C ₈ H ₉ O ₂ N	C ₁₃ H ₁₆ N ₂ NaO ₄ S
Formula weight	151.16	333.35
No. of formula weights in the unit cell	4	8
Measured density in gm/cc	1.294 ± 0.005	1.388 ± 0.005
Number of solvent molecules in the unit cell	..	8 H ₂ O
Calculated density in gm/cc	1.298	1.400

The complete structure determination of the compounds is in progress. The authors thank Prof. P. S. Narayanan for his interest in the work.

Department of Physics,
Indian Institute of Science,
Bangalore-560012,
February 9, 1973.

T. P. SINGH.
T. N. BHAT.
M. VIJAYAN.

1. Vijayan, M., *Curr. Sci.*, 1971, 40, 262.
2. —, *Ibid.*, 1971, 40, 489.
3. Singh, T. P. and Vijayan, M., *Ibid.*, 1972, 41, 700.

ELECTRICAL PROPERTIES OF A NEW
TYPE OF A⁺B⁵⁺B⁶⁺O₆²⁻ COMPOUNDS

RECENTLY¹ the structural properties of a new type of compounds with the general formula A⁺B⁵⁺B⁶⁺O₆²⁻, where A⁺ = Na⁺, K⁺, B⁵⁺ = Nb⁵⁺, Ta⁵⁺ and B⁶⁺ = Mo⁶⁺, W⁶⁺ have been reported. This note summarises the electrical properties of the compositions in the above systems.

The electrical properties like dielectric constant (ε), loss tangent (tan δ) and room temperature resistivities (both a.c. and d.c.) were measured on 12 mm diameter, 1–2 mm thickness circular pellets by the methods described earlier². The results obtained are as follows:

(1) In the system NaNbO₃-WO₃, compositions with 20 mole% WO₃ gave values of ε and tan δ ranging from 25 (ε), 0.12% (tan δ) for pure NaNbO₃ to 200 (ε) and 0.5% (tan δ) for 20 mole% WO₃ incorporation. The compositions are ferroelectric in this region. Appearance of a columbite phase beyond 20 mole% WO₃ incorporation results in semi-conducting properties (order of the dc resistivities 10⁻⁵ ohm. cm). The semi-conducting properties may be attributed to either (1) the Na-Na bonding resulting from the overlapping of the sodium 3p orbitals, (2) W-W or Nb-Nb bonding from the overlapping of tungsten or niobium t_{2g} orbitals or (3) covalent bonding from a mixing of the Na p orbitals and W(Nb) t_{2g} orbitals. Further work is in progress to establish the mechanism of conduction in these compositions. Beyond 35 mole WO₃ addition it was not possible to measure the dielectric constant probably due to the enhanced conduction resulting in lossy samples.

(2) In the system NaTaO₃-WO₃, the values of ε and tan δ varied from 50 (ε) and 0.02% (tan δ) to 500 (ε) and 0.12% (tan δ) as the WO₃ concentration increased. The NaTaO₃ phase exists upto 50 mole% incorporation of WO₃ and shows the ferroelectric properties which tend to disappear beyond 50 mole% WO₃ incorporation. A linear relationship between T_c (transition temperature)