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Crystallographic data for testosterone hydrate and anhydrate.

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Testosterone hydrate crystallizes in the space group $P2_12_12_1$ with four molecules in a unit cell having the dimensions $a=13{\cdot}63$, $b=15{\cdot}95$ and $c=7{\cdot}94$ Å. Anhydrous testosterone crystallizes in the space group $P2_1$ with four molecules in the unit cell. The proper cell dimensions are $a=14{\cdot}45$, $b=11{\cdot}09$, $c=10{\cdot}88$ Å and $\beta=110{\cdot}5°$.

In a previous study on the solution behavior of testosterone in aqueous media, conversion of the anhydrate form to a hydrate was reported (Thakkar & Hall, 1969). Since testosterone is a natural hormone and exists in an aqueous environment, characterization of this form is important. We wish to report here the crystallographic parameters of the hydrate.

Small single-crystals were grown by a continuous fall method from saturated aqueous solution cooled from 33·0 to 29·5 °C at 0·1 °C per hour. Elemental analysis, Karl Fischer titration and thermogravimetric analysis showed this crystalline form to be the monohydrate.

From Weissenberg and precession photographs taken with Cu $K\alpha$ radiation the space group has been found to be $P2_12_12_1$ (systematic absences: $h00$, $0k0$, and $00l$ for h, k or l odd); there are four molecules in a unit-cell having the dimensions $a=13{\cdot}63$, $b=15{\cdot}95$ and $c=7{\cdot}94$ Å. The density measured by displacement is 1·181 g.cm^{-3}, which agrees well with the calculated density for $C_{19}H_{28}O_2.H_2O$ of 1·179 g.cm^{-3}.

For comparison we have measured the crystal parameters for anhydrous testosterone and have obtained values which differ from those reported by Bernal & Crowfoot (1936). The space group is $P2_1$ with four molecules in a unit-cell having the dimensions $a=14{\cdot}73$, $b=11{\cdot}09$, $c=10{\cdot}88$ Å and $\beta=113{\cdot}3°$, which agree fairly well with the values given by Ohrt, Haner & Norton (1965). There is, however, an alternative cell with β closer to 90°. The dimensions for this proper cell are $a=14{\cdot}45$, $b=11{\cdot}09$, $c=10{\cdot}88$ Å and $\beta=110{\cdot}5°$. These cells give a calculated density of 1·173 g.cm^{-3}, which is identical with the experimentally measured value given by Bernal & Crowfoot.

The indexed powder data for these two forms of testosterone will be submitted for inclusion in the *ASTM Powder Diffraction File.*

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Crystal data of $BaSrFe_4O_8$.

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The dimensions of the orthorhombic unit cell of $BaSrFe_4O_8$, which contains two formula units, are $a=5{\cdot}516$, $b=8{\cdot}265$, $c=9{\cdot}188$ Å. The sapce group is *Pnna*.

A previous report on the phase equilibrium diagram, BaO–SrO–Fe_2O_3, shows that a new stable compound, having the composition $BaSrFe_4O_8$, may occur as a single phase above 1100 ± 10 °C (Batti, 1962). It undergoes thermal transformation at about 1200 °C and melts incongruently at 1240 ± 10 °C. A further investigation by Barbariol & Batti (1968) established that this new phase forms a solid solution with the binary compound $BaFe_2O_4$, which is reported to be orthorhombic (Okazaki, Mori & Mitsuda, 1963; DoDinh & Bertaut, 1965). They display complete solubility above 1200 °C whereas at lower temperatures a solid-solution gap of increasing width was reported.

Single crystals of $BaSrFe_4O_8$ were grown, by solid-state reaction, from a pressed pellet mixture of 1 $BaCO_3$: 1 $SrCO_3$: 2 Fe_2O_3 which was heated on a platinum strip in a resistance furnace to about 950 °C. The sintered pellet was reground and refired to assure complete reaction. The microcrystalline specimen was brought to 1200 °C and left in the furnace