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## The unit cell and space group of L-tyrosine.

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The space group of L-tyrosine is $P2_12_12_1$, and there are four molecules in a unit cell having $a=6{\cdot}921\pm0{\cdot}002$, $b=21{\cdot}146\pm0{\cdot}006$, $c=5{\cdot}835\pm0{\cdot}001$ Å.

The space group *Pnam* was assigned to L-tyrosine by Khawas & Krishna Murti (1969*a*) on the basis of indexing of powder photographs, and of fiber patterns obtained from clusters of very fine acicular crystals: they had been unable to obtain good single crystals. The unit-cell dimensions were given as $a=13{\cdot}89$, $b=21{\cdot}08$, and $c=5{\cdot}842$ Å, with $Z=8$. After it was pointed out to them by Dr Gerald Strahs that a centric space group was not possible for L-tyrosine, they (Khawas & Krishna Murti, 1969*b*) withdrew *Pnam* and remarked 'No acentric space group can be assigned to L-tyrosine satisfying the apparent systematic extinctions of X-ray reflection. Presumably the extinctions are accidental.', the implication being that the space group is thus *P*222, the one assigned by them in the same communication to L-tryptophan. Because we considered this space group unlikely, and because of continuing interest in these laboratories in amino acid structures, we undertook a reinvestigation of the space group.

After numerous attempts, one single crystal was obtained by evaporation of saturated aqueous solutions. It proved to be orthorhombic, and the only systematic absences observed on precession photographs are *h*00 with *h* odd, 0*k*0 with *k* odd, and 00*l* with *l* odd. The space group is thus uniquely determined as the ubiquitous $P2_12_12_1$. These photographs also showed that the *a* axis of Khawas & Krishna Murti must be halved, giving 4 molecules per unit cell, a not unusual number for this space group. Unfortunately, shortly after the precession photographs had been obtained, the crystal became detached from the glass fiber and was lost.

We recorded the powder pattern of L-tyrosine in a Philips 11·46 cm camera using Cr$K\alpha$ radiation. This pattern matches that published by Khawas & Krishna Murti (1969*a*), except that we did not observe a line at $d=6{\cdot}237$ Å (*vw*), which they indexed as 130, nor at 2·336 Å (*vvw*), which they indexed as 332. Of the 39 other *hkl* having *h* odd in their Table 1 only 7 do not have spacings coinciding with other *hkl* having *h* even. These 7 are 1·10·0, 720, 581–731, 313, 760, and 513. However, these may be indexed as 291, 490, 602–233–043–0·11·1, 472, 4·10·1–810, and 273 respectively, which had been overlooked by the previous authors. The powder pattern is accordingly consistent with the halving of *a*.

The fiber pattern, Table 2 of Khawas & Krishna Murti, includes 14 *hkl* having *h* odd, 5 of which do not coincide with *h* even reflections. These are 360, 111, 171, 361, and 142, which may be indexed as 470, 021, 441, 271, and 232 respectively, likewise previously overlooked. The fiber pattern is thus also consistent with the halving of *a*.

We have obtained revised values of the lattice constants by least-squares treatment of 42 resolved lines in our powder pattern. If there was any suspicion that a line was composite it was omitted from the calculations. The results are $a=6{\cdot}921\pm0{\cdot}002$, $b=21{\cdot}146\pm0{\cdot}006$, and $c=5{\cdot}835\pm0{\cdot}001$ Å, where the stated uncertainties are 10 times those obtained from the least-squares calculations, which we feel are unrealistic.

If we succeed in obtaining another crystal suitable for recording intensity data a full structure determination will be initiated.

It is worth mentioning that the danger of basing a unit cell on powder data only has recently been pointed out by Lester & Lipson (1970).

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