The crystal structure of twinned Cd₅(PO₄)₃Cl, 'cadmium chlorapatite': erratum.

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The bond angles and interatomic distances listed in the original paper [Sudarsanan, Young & Donnay (1973). *Acta Cryst.* B**29**, 808–814] were inadvertently taken from calculations based on a set of temporarily used values of the lattice parameters. The correct values, based on the final lattice-parameter values included in the paper, are given. The largest correction thus made to any distance is 0·3 %, *e.g.*, 0·010 Å in the Cd$_{II}$–O$_I$ distance.

The correct values of the bond angles and interatomic distances listed in Table 4 of the original paper are as follows:

(*a*) Bond angles and their standard deviations

O$_I$—P–O$_{III}$	112·6 (0·1)°
O$_I$—P–O$_{II}$	110·7 (0·1)
O$_{II}$–P–O$_{III}$	107·1 (0·1)
O$_{III}$–P–O$'_{III}$	106·4 (0·1)

(*b*) Interatomic distances and their standard deviations

O$_I$—P	1·525 (1) Å
O$_{II}$—P	1·557 (1)
O$_{III}$–P	1·540 (1)
O$_I$—O$_{II}$	2·536 (2)
O$_{II}$—O$_{III}$	2·490 (2)
O$_I$—O$_{III}$	2·550 (2)
O$_{III}$–O$'_{III}$	2·467 (2)

Cd$_I$–O$_I$	2·310 (1)
Cd$_I$–O$_{II}$	2·376 (1)
Cd$_I$–O$_{III}$	2·871 (2)
Cd$_{II}$–O$_I$	3·148 (2)
Cd$_{II}$–O$_{III}$	2·202 (1)
Cd$_{II}$–O$_{III}$	2·460 (1)
Cd$_{II}$–O$_{II}$	2·246 (2)
Cd$_{II}$–Cl	2·537 (1)

Reference

SUDARSANAN, K., YOUNG, R. A. & DONNAY, J. D. H. (1973). *Acta Cryst.* B**29**, 808–814.

The crystal structures of tropolone and 4-isopropyltropolone: a comparison.

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Comparison of bond lengths determined by X-ray crystal structure analyses indicates that the degree of π-electron delocalization is smaller in 4-isopropyltropolone than in tropolone, but in both molecules it is greater than that predicted by SCF MO calculations.

In a recent paper on the crystal structure of 4-isopropyltropolone (IPT) (Derry & Hamor, 1972), it was noted that the bond lengths did not agree with those observed in the crystal structure of tropolone by Shimanouchi & Sasada (1970), where, apart from a long C(1)–C(2) bond of 1·452 Å, ring bond lengths (mean 1·407 Å) are close to the aromatic value and there is no alternation in length. IPT, in contrast, exhibits bond-length alternation in the sense predicted by the classical valence bond structure, with the C(1)–C(2) length 1·469 Å, close to the C(sp^2)–C(sp^2) single-bond value. The other C–C formal single bonds average 1·416 Å and the double bonds 1·362 Å, respectively shorter and longer than pure single and double bonds, so that the π-electron system is partially delocalized. The carbon-oxygen bonds are also involved in the electron delocalization as indicated by the lengths, C(1)–O(1) = 1·261 and C(2)–O(2) = 1·349 Å. A revised report on the tropolone structure, based on re-measured intensities, has now appeared (Shimanouchi & Sasada, 1973). This indicates that there is in fact bond-length alternation in the ring, in agreement with the situation in IPT. Bond lengths from these three studies are listed in Table 1, with the results of a MO treatment of tropolone (Dewar semi-empirical SCF & Trinajstic, 1970).
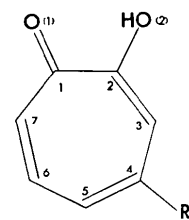
4-Isopropyltropolone R = CHMe₂
Tropolone R = H

Generally, the revised bond lengths for tropolone agree fairly well with those in IPT. A closer examination, however, reveals certain differences which follow a systematic trend. The C(1)–C(2) bond in tropolone is shorter by 0·015 Å than the corresponding bond in IPT and the other formal C–C single bonds average 1·404 Å, shorter by 0·012 Å than the average in IPT. The double bonds average 1·364 Å, very slightly longer than the average in IPT (1·362 Å). The indication, therefore, is that the π-electron system is delocalized to a slightly smaller extent in IPT than in tropolone. Consistent with this, the C(2)–O(2) bond length is shorter by 0·016 Å in tropolone. The C(1)–O(1) lengths are, how-