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The crystal structure of ammonium tris(pentasulfido)platinum(IV) dihydrate. Erratum.

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In *Acta Cryst.* (1969), B**25**, 745, the value for β used was 87·26° rather than 92·74°.

In an article by Jones and Katz (1969), the monoclinic angle was specified as 92·74°. However, a review of the calculations reveals that, albeit unintentionally, the authors did not follow convention, and chose β acute rather than obtuse. The value of β which corresponds to the indices, atomic parameters, and bond lengths and angles is 87·26°.

The authors are grateful to Dr Keith Butler of the University of Adelaide, South Australia, for discovering this error.

References

Jones, P. E. & Katz, L. (1969). *Acta Cryst.* B**25**, 745.

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The structure of barium silicon niobium oxide, $Ba_3Si_4Nb_6O_{26}$: a compound with linear silicon-oxygen-silicon groups. Erratun.

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A corrected atomic position parameter is given for the paper in *Acta Cryst.* (1970). B**26**, 105.

The atomic parameters listed in an article by Shannon & Katz (1970) do not correspond to the same cycle of refinement for which R and the interatomic distances and angles are given. The differences are of course small – less than σ for atoms other than oxygen and less than 2σ for oxygen – but the correct atomic parameters are available on request. However, there was a serious transcription error in the x parameter for barium, which should be 0·59952 ± 0·00014 (rather than 0·59334 ± 0·00012).

We are grateful to Professor Werner Baur, of the University of Illionis at Chicago Circle, for calling our attention to discrepancies between the published atomic parameters and the distances and angles.

References

Shannon, J. & Katz, L. (1970). *Acta Cryst.* B**26**, 105.

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An X-ray investigation of octafluoronaphthalene.

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Crystals of octafluoronaphthalene have been examined by X-ray methods. They crystallize in the monoclinic system (space group $P2_1/c$, with $a = 7{\cdot}585$, $b = 5{\cdot}004$, $c = 12{\cdot}007$ Å and $\beta = 96{\cdot}75°$) and show remarkable continuous diffuse scattering. The molecular orientation in the crystal was determined by Patterson's method and by the diffuse-scattering intensity distribution.

Octafluoronaphthalene is a commercially available compound which can be prepared in good yield by defluorination of perfluorodecalin over heated nickel or iron (Gething, Patrick, Stacey & Tatlow, 1959).

Single crystals were grown from light petroleum solutions as colourless prisms, elongated along the [010] direction and with an oblique cross-section. From Weissenberg and precession photographs of zero and upper layers the crystal symmetry and the unit-cell dimensions were determined; the unit cell chosen proved to be reduced (Buerger, 1957). The crystal density was measured by flotation in ZnI_2 solution.

From the crystallographic data, reported in Table 1, it may be derived that the octafluoronaphthalene molecule has a point group symmetry $\bar{1}$ in the crystal. It is interesting to remember also that naphthalene crystallizes in the same space group $P2_1/c$ with molecular symmetry $\bar{1}$ (Abrahams, Robertson & White, 1949); furthermore if the reduced cell is chosen ($a=8{\cdot}080$, $b=6{\cdot}003$, $c=8{\cdot}235$ Å, $\beta=115{\cdot}9°$) the values of the lattice constants of naphthalene and octafluoronaphthalene (Table 1) are comparable.

Table 1. *Crystallographic data*

M.W.	272
m.p.	87–88°C
Crystal system	monoclinic
Space group	$P2_1/c$ (C^5_{2h})
a	$7{\cdot}585 \pm 7$ Å
b	$5{\cdot}004 \pm 5$
c	$12{\cdot}007 \pm 10$
β	$96{\cdot}75 \pm 0{\cdot}2°$
V	$452{\cdot}7$ Å^3
D_x	$1{\cdot}99$ g.cm^{-3}
D_m	$1{\cdot}98$
Z	2
$F(000)$	264
$\mu_{\mathrm{Cu}K\alpha}$	$22{\cdot}3$ cm^{-1}
$\mu_{\mathrm{Mo}K\alpha}$	$2{\cdot}6$

Equi-inclination Weissenberg photographs were taken of $h0l$, $h1l$, $h2l$ and $h3l$ with Ni-filtered Cu $K\alpha$ radiation and multiple-film packs. Intensities of 503 independent reflexions were measured by a recording microdensitometer.

Interlayer scaling was carried out through the $hk0$ and $0kl$ precession photographs.

The relative intensities, corrected for Lorentz and polarization factors, were converted to an approximately absolute scale by Wilson's statistical method, which also gave an approximate value of the overall temperature factor. No corrections were made for absorption or extinction.

All processing of data and crystallographic calculations were carried out on an IBM 7094/7040 DCS computer with the X-ray 63 system (1965). By a close inspection of the Patterson map it was possible to deduce the molecular orientation in the unit cell: the molecular plane is approximately parallel to the ($\bar{1}12$) crystallographic plane.

It is interesting to note that the crystals of octafluoronaphthalene show remarkable continuous diffuse scattering, characteristic of molecular compounds (Amoros & Amoros, 1968); a very intense diffuse spot associated with Bragg reflexions and continuous weak diffuse-scattering regions, which spread over areas between reciprocal lattice points, even through lattice points forbidden by space group symmetry.

At the same time the Bragg intensities fall off very rapidly with increasing order, the overall temperature factor having a high value around 10 Å^2. It therefore appears that octafluoronaphthalene, like other planar molecules joined only by weak Van der Waals forces (naphthalene, anthraquinone anthracene *etc.*) (Amoros & Amoros, 1968) exhibit thermal diffuse scattering due to the thermal vibrations of its molecules.

It is well known (Amoros & Amoros, 1968) that the close relationship existing between continuous diffuse scattering and the shape and orientation of the molecules building up the crystal enable us to use such information in the early stages of crystal structure determination of a molecular crystal. Equi-inclination Weissenberg photographs were therefore taken of $h\frac{1}{2}l$, $h\frac{3}{2}l$, $h\frac{5}{2}l$ and $h\frac{7}{2}l$ with Ni-filtered Cu $K\alpha$ radiation and multiple-film packs. In this way it was possible to get a good picture of the continuous diffuse scattering intensity distribution.

As the continuous diffuse scattering contains the mean features of the molecular intensity Fourier transform (Hoppe, 1956; Wooster, 1962) the possibility of using the information of continuous diffuse scattering in crystal structure determination is an extension of the molecular Fourier transform method (Taylor & Lipson, 1965).

A method developed by Mackay (1962) has therefore been applied to the continuous diffuse scattering intensity distribution of octafluoronaphthalene. This method enables one to study the continuous diffuse scattering function of molecules containing benzene rings.

In this way the orientation of the octafluoronaphthalene molecule in the crystal was determined; the result agrees well with that obtained from Patterson's method.

No further work is contemplated.

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