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Cell dimensions and space groups of some carbocyclic compounds.

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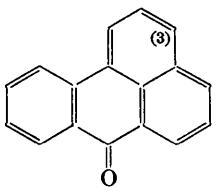
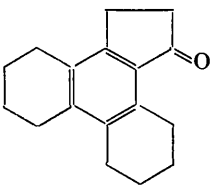
In connection with studies on benzanthrone (I) which are being pursued in this department both as crystal-



(I)



(II)

structure and as molecular-orbital investigations, the cell dimensions and space groups of the 3-chloro- and 3-bromo- derivatives were determined in the hope of finding morphological relationships to the parent compound as well as of being able to use the heavy-atom technique of structure analysis. Such relationships were not, however, recognized and as further study of the derivatives has had to be postponed it seems worth while to publish for these two compounds the crystallographic and optical results at present available; corresponding measurements on the parent compound are added for comparison.

Similar information on 1′-keto-9:10-*cyclo*penteno-1:2:3:4:5:6:7:8-octahydrophenanthrene (II) has been included.

Benzanthrone, $C_{17}H_{10}O$

Mol.wt. = 230·08; m.p. = 170° C.; $d_{calc.}$ = 1·372, $d_{obs.}$ = 1·371 g.cm.$^{-3}$. Orthorhombic, class 222: a = 14·57±0·01, b = 15·00±0·02, c = 5·07±0·01 Å. Volume of unit cell = 1107·6 Å^3. Absent spectra: {*hkl*}, {*hk*0}, {*h*0*l*}, {0*kl*} no general halvings; {00*l*}, {0*k*0}, {*h*00} absent when *l*, *k*, *h* odd respectively. Space group: $P2_12_12_1$ uniquely determined. Molecules per unit cell: 4; molecular symmetry: none. Electrons per unit cell: F(000) = 480. Absorption coefficient for Cu $K\alpha$ radiation = 7·9 cm.$^{-1}$.

The crystals, which were most successfully grown from solution in nitrobenzene, are rather hard for a compound having no obvious hydrogen or ionic bonds. They form yellowish needles elongated parallel to *c*, bounded by *a*{100} and *r*{120} and terminated by *c*{001} though often fractured.

Refractive indices: 1·62 < α < 1·74 parallel to *a*, β = 1·79 parallel to *c*, $\gamma \approx$ 1·9 (estimated) parallel to *b*.

3-Chlorobenzanthrone, $C_{17}H_9OCl$

Mol.wt. = 264·54; m.p. = 182° C.; $d_{calc.}$ = 1·46, $d_{obs.}$ = 1·49 g.cm.$^{-3}$. Monoclinic, class 2/*m*: a = 14·40±0·02, b = 11·56±0·01, c = 7·27±0·01 Å.; β = 93° 37′. Volume of unit cell = 1205 Å^3. Absent spectra: {*hkl*} no general halvings; {*h*0*l*} absent when *h*+*l* odd, {0*k*0} absent when *k* odd. Space group $P2_1/n$ uniquely determined. Molecules per unit cell: 4; molecular symmetry: none. Electrons per unit cell: F(000) = 544. Absorption coefficient for Cu $K\alpha$ radiation = 27·5 cm.$^{-1}$.

The crystals were yellow laths tabular on *a*{100} and elongated parallel to *c*[001] with *m*{110} as prism faces. The best specimens were recrystallized from glacial acetic acid or nitrobenzene but there is a marked tendency to form twins.

It was impossible to make a complete optical characterization of the crystals but the refractive index for vibrations parallel to *c* is 1·51 and that for vibrations parallel to *b* is approximately 1·8.

3-Bromobenzanthrone, $C_{17}H_9OBr$

Mol.wt. = 309·00; m.p. = 170° C.; $d_{calc.}$ = 1·696, $d_{obs.}$ = 1·695 g.cm.$^{-3}$. Orthorhombic, class *mmm*: a = 15·65, b = 16·11, c = 9·57 Å. Volume of unit cell = 2410 Å^3, Absent spectra: {*hkl*} no general halvings; {*hk*0}, {*h*0*l*}. {0*kl*} absent when *h*, *l*, *k* odd respectively. Space group *Pbca* uniquely determined. Molecules per unit cell: 8; molecular symmetry: none. Electrons per unit cell: F(000) = 616. Absorption coefficient for Cu $K\alpha$ radiation = 47·9 cm.$^{-1}$.

Excellent pale yellow needles were obtained from solution in nitrobenzene.

1′-Keto-9:10-*cyclo*penteno-1:2:3:4:5:6:7:8-octahydrophenanthrene, $C_{17}H_{20}O$

Mol.wt. = 240·16; m.p. = 196 C.; $d_{calc.}$ = 1·23, $d_{obs.}$ = 1·21 g.cm.$^{-3}$. Monoclinic, probably class 2/*m*: a = 7·42±0·02, b = 18·01±0·02, c = 19·33±0·02 Å; β = 95° 30′. Volume of unit cell = 2488 Å^3. Absent spectra: {*hkl*} absent when *h*+*k*+*l* odd, {*h*0*l*} absent when *h* or *l* odd, {0*k*0} absent when *k* odd. Space group *I*2/*a* or *Ic*; since the latter requires only four asymmetric units per cell while the former requires eight (the number actually observed), *I*2/*a* seems the more likely.

The colourless crystals are usually long needles of almost square section bounded by *b*{010} and *c*{001} and terminated by *a*{100}. Plates elongated parallel to *a* [100] are, however, also formed and show marked cleavage parallel to *b*{010}, thus breaking down into the acicular crystals.

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