$$H_{3/2}=\left(\frac{z}{2\pi}\right)^{1/2}\left(1+\frac{2}{z^2}\right)-\left(\frac{2}{\pi z}\right)^{1/2}\left(\sin z+\frac{\cos z}{z}\right)$$

$$\therefore R_3=\frac{3\sqrt{(2\pi)}}{z^{3/2}}\left\{\left(\frac{z}{2\pi}\right)^{1/2}\left(1+\frac{2}{z^2}\right)-\left(\frac{2}{\pi z}\right)^{1/2}\left(\sin z+\frac{\cos z}{z}\right)\right\}$$

$$=3\left\{\frac{1}{z}\left(1+\frac{2}{z^2}\right)-\frac{2}{z^2}\left(\sin z-\frac{\cos z}{z}\right)\right\}$$

$$=3\left\{\frac{1}{z}+\frac{2}{z^3}-\frac{2}{z^2}\left(z-\frac{z^3}{6}+\ldots\ldots+\frac{1}{z}-\frac{z}{2}+\frac{z^3}{24}-\ldots\right)\right\}\simeq\tfrac{3}{4}z.$$

These values are so nearly the same that it is reasonable to say

$$R\simeq z=\pi\Delta r_x s_{\max}\,.$$

Since only low order reflexions would normally be used a value of $s_{\max}\sim 0{\cdot}5$ would be reasonable; and since, in a centrosymmetric structure the value of R for a randomly wrong structure is 0·828 (Wilson, 1949) it would be reasonable to take $\sim\frac{1}{4}$ of this value as the maximum change to the tolerated within the interval of calculation.

i.e.

$$R=0{\cdot}20=\pi\Delta r_x s_{\max}$$

$$\Delta r_x=\frac{0{\cdot}2}{\pi s_{\max}}\simeq 0{\cdot}07/s_{\max}$$

If $s_{\max}$ is taken as 0·5 then $\Delta r_x\sim 0{\cdot}13$ Å .

This means that an 8 Å cell edge should bedivided into 60ths which is a much finer interval than might at first be expected at this stage of the crystal structure determiation.

References

BHUIYA, A. K. & STANLEY, E. (1964). *Acta Cryst.* In the press.

WATSON, G. N. (1922). *Theory of Bessel Functions.* Cambridge Univ. Press.

WILSON, A. J. C. (1949). *Acta Cryst.* **2**, 318.

Acta Cryst. (1964). **17**, 610

Crystallographic data for some cyclobutene derivatives.

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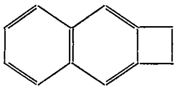
Naphtho[*b*]*cyclobutene*: (I) (Cava & Shirley, 1960)

Colourless plates with (100) developed; twinning on (100) is common.



I

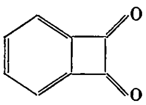
$C_{12}H_{10}$; $M=154{\cdot}2$; m.p. 84·5–86 °C. *Monoclinic,*

$$a=18{\cdot}04\pm0{\cdot}02,\ b=5{\cdot}91\pm0{\cdot}01,$$
$$c=8{\cdot}13\pm0{\cdot}01\text{ Å};\ \beta=92\ {}^\circ0'\pm6'.$$
$$U=866{\cdot}3\text{ Å}^3.\ D_m=1{\cdot}19,\ Z=4,\ D_x=1{\cdot}18\text{ g.cm}^{-3}.$$

$F(000)=328$. Absent spectra: hkl when $h+k$ is odd, $h0l$ when l is odd. Space group Cc ($C2/c$ being excluded since it requires the twofold symmetry axis of the molecule (of length $\sim$ 6 Å) to be parallel to b).

Benzocyclobutadienoquinone: (II) (Cava & Napier, 1957)

Yellow prisms bounded by {100}, with {110} also developed.



II

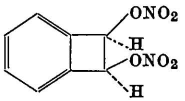
$C_6H_4(CO)_2$; $M=132.1$; m.p. 132·5 °C. *Orthorhombic,*

$$a=10{\cdot}72\pm0{\cdot}01,\ b=7{\cdot}94\pm0{\cdot}01,$$
$$c=7{\cdot}15\pm0{\cdot}01\text{ Å}.\ U=608{\cdot}6\text{ Å}^3.$$
$$D_m=1{\cdot}45,\ Z=4,\ D_x=1{\cdot}44\text{ g.cm}^{-3}.\ F(000)=272.$$

Absent spectra: $h0l$ when h is odd, $0kl$ when l is odd. Space group is $Pca2_1$ or $Pcam$.

cis-1,2-*Benzocyclobutenediol dinitrate*: (III) (Cava & Napier, 1957)

Colourless prisms elongated along a, with (010) and (001) developed.



III

$C_6H_4(CHONO_2)_2$; $M=226{\cdot}1$; m.p. 110 °C. *Monoclinic,*

$$a=7{\cdot}41\pm0{\cdot}01,\ b=15{\cdot}71\pm0{\cdot}02,$$
$$c=8{\cdot}14\pm0{\cdot}01\text{ Å};\beta=98\ {}^\circ2'\pm5'.$$
$$U=938{\cdot}3\text{ Å}^3.\ D_m=1{\cdot}57,\ Z=4,\ D_x=1{\cdot}60\text{ g.cm}^{-3}.$$

$F(000)=464$. Absent spectra: $h0l$ when $h+l$ is odd, $0k0$ when k is odd. Space group is $P2_1/n$.

No further work on these compounds is planned. The authors are indebted to Dr M. P. Cava for the crystal samples, and to the National Research Council of Canada for financial support and for the award of a studentship (to T.C.W.M.).

References

CAVA, M. P. & NAPIER, D. R. (1957). *J. Amer. Chem. Soc.* **79**, 3606.

CAVA, M. P. & SHIRLEY, R. L. (1960). *J. Amer. Chem. Soc.* **82**, 654.