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Preliminary X-ray data of 1,4-dinaphthoquinone.

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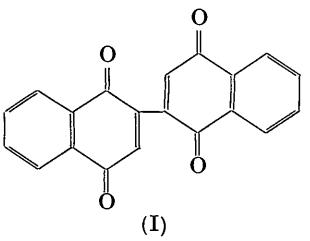
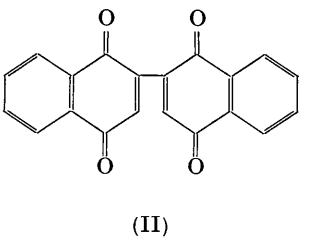
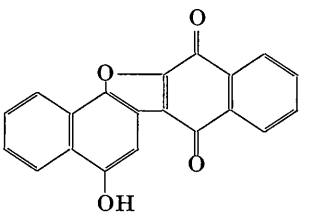
Chemical considerations lead to the following possible molecular configurations for 1,4-dinaphthoquinone (Cohen, 1961):



(I)



(II)



(III)

Dinaphthoquinone forms brilliant yellow needles elongated about the [*b*] axis. The following unit-cell dimensions were obtained from oscillation and Weissenberg photographs about the [*b*] axis:

$$a = 13{\cdot}22,\ b = 3{\cdot}80,\ c = 16{\cdot}29\ \text{Å};\ \beta = 118{\cdot}7°.$$

The space group is uniquely determined as $P2_1/a$ by the systematic absences, $h0l$ absent for h odd, $0k0$ absent for k odd. The calculated density of 1·46 g.cm.$^{-3}$, assuming 2 molecules in the unit cell, is in agreement with the observed density of 1·48 g.cm.$^{-3}$ obtained by the floatation method in carbon tetrachloride–benzene mixtures. The molecular symmetry is therefore $\bar{1}$ and the *trans* configuration (I) is the only acceptable structure consistent with the chemistry. The short [*b*] axis requires an almost planar molecule with a tilt not exceeding 30° from (010).

I am grateful to Dr T. Cohen of the Chemistry Department, University of Pittsburgh for suggesting the problem and Dr T. Tsuji of the same department for providing the crystals. The writer wishes to thank Prof. G. A. Jeffrey for his interest, and the U.S. Public Health Service, National Institutes of Health for the support of this research under Grant E-1423.

Reference

COHEN, T. (1961). Private communication.

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Unit cell and space groups of $Ni[SC(NH_2)_2]_6(NO_3)_2$ and $Ni[SC(NH_2)_2]_6(ClO_4)_2$.

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The green crystals of $Ni[SC(NH_2)_2]_6(NO_3)_2$ and olive-green crystals of $Ni[SC(NH_2)_2]_6(ClO_4)_2$ were prepared by Šramko (1961). From rotating-crystal photographs, taken with Cu $K\alpha$ radiation and calibrated with aluminium, and from Weissenberg and precession photographs the following results were obtained.

$Ni[SC(NH_2)_2]_6(NO_3)_2$ is monoclinic with

$$a = 22{\cdot}48,\ b = 9{\cdot}28,\ c = 16{\cdot}35\ \text{Å};\ \beta = 129{\cdot}8°.$$

The calculated density $\varrho_c = 1{\cdot}64$ g.cm.$^{-3}$; the measured density $\varrho_o = 1{\cdot}62$ g.cm.$^{-3}$.

There are four molecules in the unit cell.

The conditions for the presence of reflections are:

$$hkl:\ h + k = 2n$$
$$h0l:\ l = 2n\ .$$

which leads to two possible space groups: Cc–C_s^4 and $C2/c$–C_{2h}^6.

$Ni[SC(NH_2)_2]_6(ClO_4)_2$ is tetragonal with

$$a = 9{\cdot}68,\ c = 29{\cdot}47\ \text{Å}\ .$$

The calculated density $\varrho_c = 1{\cdot}74$ g.cm.$^{-3}$; the measured density $\varrho_o = 1{\cdot}72$ g.cm.$^{-3}$.

There are four molecules in the unit cell.

The conditions for the presence of reflections are:

$$hkl:\ \text{no conditions}$$
$$00l:\ l = 4n$$
$$h00:\ h = 2n\ ,$$

which leads to two possible space groups: $P4_12_12$–D_4^4 and $P4_32_12$–D_4^8.

Reference

ŠRAMKO, T. (1961). *Chem. zvesti.* (In press.)