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Crystal data of 'three-pyraphene' and of some derivatives of 'dipyraphene'.

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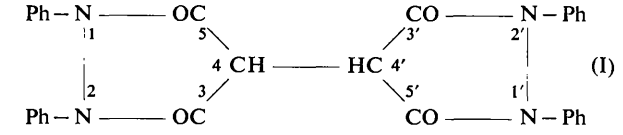
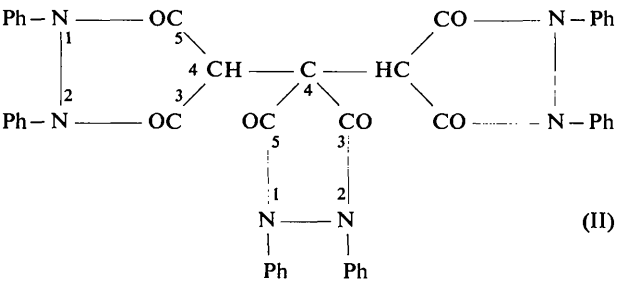
The chemical constitution of 'dipyraphene' (1,2,1′,2′-tetraphenyl-3,5,3′,5′-tetraoxo-4,4′-dipyrazolidinyl)



and of 'three-pyraphene' (1,2-diphenyl-3,5-dioxo-4,4- bis-(1,2-diphenyl-3,5-dioxo-4-pyrazolidinyl) pyrazolidine)



has been determined by Cardani & co-workers (Cardani, Scaramuzza, Mondelli & Merlini, 1963; Mondelli, Merlini, Bovis & Cardani, 1964).

The dipotassium and disodium salts of compound (I) are very likely derived from the dienolic form of (I), 1,2,1′,2′-tetraphenyl-3,3′-dienol-5,5′-dioxo-4,4′-dipyrazolidinyl.

The crystals of these compounds have been examined and the crystal data determined.

Compound (I). Dipyraphene, $C_{30}H_{22}N_4O_4$.
Crystal shape: Very fine needles, easily altered by light.

Compound (II). Three-pyraphene, $C_{45}H_{32}N_6O_6$.
Crystal shape: very fine needles; [001] parallel to the elongation axis.

Compound (III). Dipotassium dipyraphene, $C_{30}H_{20}N_4O_4K_2$.
Crystal shape: thick plates, monoclinic, [010] parallel to the longest edges.

Compound (IV). Disodium dipyraphene, $C_{30}H_{20}N_4O_4Na_2$.
Crystal shape: flat plates with rhomboidal faces; [010] parallel to the shorter diagonal of the basal rhomboid.

The unit-cell constants obtained with Cu $K\alpha$ radiation are shown in Table 1.

Table 1. *Crystal data*

Compound	II	III	IV
a	14·92 ± 0·01	16·39 ± 0·01	14·77 ± 0·01 Å
b	24·80 ± 0·03	12·36 ± 0·03	14·28 ± 0·01 Å
c	12·28 ± 0·01	15·50 ± 0·01	15·65 ± 0·01 Å
β	110° 46′ ± 18′	116° 22′ ± 11′	104° 25′ ± 14′
U	4241	2818	3198 Å^3
Space group	$P2_1/c$	$P2_1/a$	$P2_1/c$
Molecular units per unit cell	4	4	4
ϱ calc.	1·18	1·37	1·14 g.cm^{-3}

Crystals of compound (I) are altered very rapidly by light.

The crystals of the dipotassium and disodium salts of 'dipyraphene' are not isostructural.

In the photographs of these compounds, the reflexions become very weak at moderate values of θ owing to thermal motion.

The determination of the crystal structure of dipotassium dipyraphene is in progress.

We wish to thank Prof. C. Cardani of the Polytechnic of Milan who kindly supplied the crystals and the Consiglio Nazionale delle Ricerche, Rome for financial aid.

References

CARDANI, C., SCARAMUZZA, A., MONDELLI, R. & MERLINI, L. (1963). *Gazz. chim. ital.* **93**, 1353.

MONDELLI, R., MERLINI, L., BOVIS, G. & CARDANI, C. (1964). *Gazz. chim. ital.* **94**, 306.

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Improved approximation for incoherent X-ray scattering*.

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The incoherent or modified part of the X-ray intensity scattered by an atom, neglecting exchange terms, is given (James, 1958, p. 462) by

$$I_{\text{inc}} = Z - \sum_{1}^{z} f_K^2 \qquad (1)$$

where Z is the atomic number and f_K is the scattering factor corresponding to individual electronic wave functions. f_K is unity at zero angle of scatter and decays to oscillation about zero for increasing $\sin\theta/\lambda$.

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