

0.521 (1) Å above and P(1) 0.331 (1) Å below the plane. The short C(3)–C(7) and C(4)–N(9) single bonds, together with the long C(3)–C(4) double bond indicate considerable π -electron delocalization over the C(7)–C(3)–C(4)–N(9) fragment.

The phenyl group is axial to the hetero ring with the projection of its plane almost parallel to the P(1)–C(2) bond [the torsion angle C(2)–P(1)–C(10)–C(11) is *ca* 166.6 (3)°]. The steric crowding imposed by this configuration results in a slight displacement [0.135 (1) Å] of the P atom from the phenyl-group mean plane, and the phenyl group itself departs from D_{6h} symmetry, primarily because of the closure of the C(15)–C(10)–C(11) bond angle [117.2 (2)°]. This type of behavior has been discussed by Domenicano & Vaciago (1975) who concluded that the internal angles at the *ipso* C atoms are sensitive to the nature of the phenyl-ring substituents.

An examination of intermolecular contacts revealed only one distance which is significantly less than the sum of the relevant van der Waals radii.* This contact, of magnitude 2.31 (3) Å, is between N(8) of one molecule and H(92') in an adjacent, glide-plane-related molecule, with an N(8)–N(9') distance of 3.108 (2) Å and the N(8)…H(92')–N(9') angle equal to 170 (3)°. The structure is thus built up of $C_{12}H_{13}N_2P$ moieties hydrogen-bonded through N(8)…H(92')–N(9') links,

* van der Waals radii were taken from Pauling (1967) except for H, which is taken from Bauer (1972).

forming infinite molecular chains extending along **c** (Fig 3).*

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* See deposition footnote.

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Notes for Authors

Revised *Notes for Authors* for *Acta Crystallographica* and *Journal of Applied Crystallography* have been published in the January 1983 issue of *Acta Crystallographica*, Section A, pages 174–186. Reprints of these directions may be obtained on request from any of the Editors. These *Notes* give information on submission procedures, categories of contributions and details of format for all parts of a paper. However, for the use of contributors to *Acta Crystallographica*, Section C, Appendix I, which gives the criteria for papers to be published in Sections B and C and the format for papers to be published in Section C, is reprinted below.

APPENDIX I

Criteria for publication in *Acta Crystallographica*, Sections B and C, and format for papers to be published in Section C

Papers will only be considered for publication in Section B of *Acta Crystallographica* if they meet the following three criteria:

1. The paper must contain a major structural element. This component may be an original determination of one or more structures (a single structure should generally have been studied under more than one condition of temperature or pressure), a theoretical structural investigation including new methodology, or a study of structural relationships based on a search of the literature. The calibre of this component should be at least as high as was previously required for acceptance in Section B up to 1982.

2. The paper should also present an experimental and/or theoretical contribution to one of the natural sciences that is novel, original and of high quality.

3. The paper should combine these two types of contribution to provide new structural insight for that science or for crystallography.

Papers which present the results of a crystal structure determination or of several such determinations, but are concerned with the crystal and molecular structure alone, will only satisfy the first of these criteria and will therefore be considered for publication in Section C.

Subject to the Co-editor's discretion, papers submitted for consideration in *Acta Cryst.*, Section C should conform with the following arrangement [*Acta Cryst.* (1981), **B38**, 699–700]:

The *Title* will consist of the name of the substance and the

chemical formula; a qualification such as 'Structure of . . .', 'New Form of . . .', 'from Minas Gerais' etc. may be added.

The *Abstract* will consist of the information given in Table 3(a) (in abbreviated telegraphic form and preferably in the order given there).

The *Introduction* will briefly state the reason for undertaking the structure determination and its chemical, physical, biological or other interest. If organic, or containing complicated organic ligands, a display of the structural formula of the material studied should be given, in accordance with IUPAC convention.

The *Experimental* section will include the information given in Table 3(b), given in tabular or abbreviated telegraphic form. Any further details, say of refinement, should be treated as normal text, but kept as brief as possible.

The *Discussion* will generally include two tables and two figures as described in § 2.1, although bond distances and angles may be shown on a figure if this is reasonably compact (see also § 5.1). Additional tables and figures may be deposited. If the table of bond distances and angles is very long, this will be deposited and only values that are unusual and relevant to the discussion will be given for publication. Comment should be made on any unusual features of coordination, bonding, bond lengths, bond angles, thermal vibrations, etc.

Any nonroutine measurement of physical properties (magnetic susceptibility, dielectric permittivity, elastic moduli, etc.) should be mentioned in the *Abstract* and the numerical values quoted there if possible. If the numerical values are too lengthy to be given in the *Abstract*, they should be given in a suitably headed paragraph in the paper, normally preceding the *Discussion*.

Tables of structure factors, anisotropic thermal parameters, least-squares planes and hydrogen-atom coordinates if not refined must be submitted in triplicate with the paper, but will not normally be published. After acceptance of the paper they will be deposited along with any other extensive tables or figures, in accordance with the Union's procedures (see § 11).

Table 3. *Information required in (a) the Abstract and (b) the Experimental section of papers in Acta Crystallographica Section C*

(a) *Abstract*

Formula weight
Space group
Unit cell dimensions
Volume of unit cell (\AA^3)
 Z
Measured and calculated densities D_m , D_x
Radiation and wavelength
Linear absorption coefficient
 $F(000)$
Temperature of measurement
Final value of $R = [\sum (|F_o| - |F_c|)^2 / \sum |F_o|^2]$ and number of unique reflections
Source of material
+ such other material (especially structural) as can be conveyed in about 50 further words.

(b) *Experimental section*

Method of measuring D_m
Crystal shape and size
Diffractometer used
Number and θ range of reflections used for measuring lattice parameters
Absorption correction applied (with maximum and minimum values)
Maximum value of $(\sin \theta / \lambda)$ reached in intensity measurements
Range of h , k and l
Standard reflections and their intensity variation throughout experiment
Number of reflections measured
Number of unique reflections
Value of $R_{\text{int}} = [\sum (I - \langle I \rangle)^2 / \sum I]$, from merging equivalent reflections
Number of unobserved reflections
Criterion for recognizing unobserved reflections [$I < n\sigma(I)$]
Method used to solve structure
Use of F or F^2 magnitudes in least-squares refinement
Methods of locating and refining H atoms if applicable
Parameters refined
Values of $R = \sum (|F_o| - |F_c|)^2 / \sum F_o^2$, $wR = [\sum w(|F_o| - |F_c|)^2 / \sum wF_o^2]^{1/2}$ and $S = [\sum w(|F_o| - |F_c|)^2 / (m - n)]^{1/2}$ (or the F^2 equivalents)
Method used to calculate w
Ratio of maximum least-squares shift to error in final refinement cycle
Maximum and minimum height in final difference Fourier synthesis
Secondary extinction value (if used)
Source of atomic scattering factors and f' , f'' values
All computer programs used.