

Related literature. For earlier studies on phospholes and dibenzophosphole see reviews by Mathey, Fischer & Nelson (1983) and Holah, Hughes & Wright (1975). NMR (^1H , ^{13}C) spectroscopic characterization was reported by Nelson, Affandi, Gray & Alyea (1987). Multinuclear NMR and structural studies of coordination compounds of this ligand are of current interest (Attar, Bearden, Alcock, Alyea & Nelson, 1990; Affandi, Nelson, Alcock, Howarth, Alyea & Sheldrick, 1988; Alyea, Malito & Nelson, 1987). Structural analysis of the corresponding selenide provided an assessment of the steric properties of 1-phenylphosphole (Alyea, Ferguson, Malito & Ruhl, 1986).

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N-(4-Chlorobenzylidene)-2-(4-imidazolyl)ethylamine

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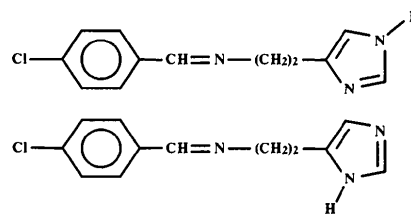
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Abstract. $\text{C}_{12}\text{H}_{12}\text{ClN}_3$, $M_r = 233.7$, triclinic, $P\bar{1}$, $a = 13.768$ (2), $b = 9.947$ (2), $c = 9.825$ (3) Å, $\alpha = 110.98$ (3), $\beta = 105.54$ (2), $\gamma = 94.45$ (3)°, $V = 1187.7$ Å³, $Z = 4$, $D_x = 1.30$ g cm⁻³, $\lambda(\text{Cu K}\alpha) = 1.5418$ Å, $\mu = 26.8$ cm⁻¹, $F(000) = 488$, $T = 296$ K, $R = 0.054$, $wR = 0.057$, $S = 0.58$, for 1438 unique observed reflections. In both molecules of the asymmetric unit the heterocyclic ring is planar and the phenyl ring forms small dihedral angles with respect to the C7,N8,C9 (methylideneaminomethyl) plane [2.8 (5) and 1.1 (6)°]. The two independent molecules form a dimer linked by an NH...N hydrogen bond [N14—H...N14' = 1.93 (10) Å, $\angle\text{N14—H...N14}' = 172$ (8)°]. These dimers are joined to others through N12—H...N12 bonds [N12'—H...N12ⁱ = 1.94 (9) Å, $\angle\text{N12}'\text{—H...N12}^i = 172$ (8)°; (i) = x, y, z + 1].

Experimental. Prismatic crystal 0.11 × 0.23 × 0.37 mm, recrystallized from methanol, mounted on a Siemens AED single-crystal diffractometer equipped with IBM PS2/30 computer (Belletti, Cantoni & Pasquinelli, 1988). Lattice parameters from 24 well centered reflections, $13.7 \leq \theta \leq 39.6^\circ$, one standard

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reflection measured every 50 revealed a decomposition of about 32% during the data-collection time, 4506 reflections collected with a modified version of the Lehmann & Larsen (1974) method, $-14 \leq h \leq 14$, $-11 \leq k \leq 10$, $0 \leq l \leq 11$, θ range 3–70°, 1438 unique observed, $I \geq 2\sigma(I)$, data corrected for the decay and for Lp effects. Structure solved with *SHELXS86* (Sheldrick, 1986), absorption correction following Walker & Stuart (1983) with the program *ABSORB* (Ugozzoli, 1987), 0.722 and 1.268 minimum and maximum correction in φ - μ , 0.956 and 1.103 in θ ; block-matrix least-squares refinement on 396 parameters with *SHELX76* (Sheldrick, 1976), non-H atoms anisotropic, H atoms from ΔF map, $\sum w(\Delta F)^2$ refined. Minimum and maximum peaks in

Table 1. Atomic fractional coordinates ($\times 10^4$) and U_{eq} values ($\times 10^4 \text{ \AA}^2$)

| | Molecule 1 | | | | Molecule 2 | | | |
|-----|------------|-----------|-----------|----------|------------|------------|------------|----------|
| | x | y | z | U_{eq} | x | y | z | U_{eq} |
| C1 | 1479 (2) | 9293 (2) | 887 (2) | 932 (12) | -6821 (2) | 12197 (2) | 20553 (2) | 986 (13) |
| C1 | 899 (7) | 8887 (7) | 2086 (9) | 639 (41) | -6135 (7) | 11302 (8) | 19365 (9) | 667 (42) |
| C2 | -152 (9) | 8634 (10) | 1685 (11) | 788 (47) | -6647 (7) | 10109 (9) | 18021 (10) | 746 (46) |
| C3 | -631 (7) | 8270 (8) | 2602 (10) | 690 (47) | -6103 (7) | 9440 (10) | 17098 (11) | 734 (48) |
| C4 | -75 (6) | 8122 (6) | 3912 (8) | 540 (36) | -5066 (6) | 9910 (8) | 17454 (9) | 662 (43) |
| C5 | 993 (7) | 8415 (8) | 4281 (10) | 658 (47) | -4591 (7) | 11123 (9) | 18790 (10) | 765 (49) |
| C6 | 1467 (7) | 8783 (8) | 3387 (10) | 680 (46) | -5108 (7) | 11836 (10) | 19762 (11) | 760 (46) |
| C7 | -584 (7) | 7714 (7) | 4879 (10) | 629 (42) | -4450 (7) | 9200 (10) | 16483 (12) | 802 (47) |
| N8 | -123 (5) | 7521 (6) | 6065 (7) | 654 (33) | -4833 (5) | 8101 (8) | 15218 (9) | 857 (39) |
| C9 | -764 (7) | 7109 (9) | 6862 (10) | 670 (47) | -4119 (9) | 7517 (11) | 14364 (14) | 931 (66) |
| C10 | -584 (7) | 5652 (11) | 6972 (13) | 729 (49) | -4127 (9) | 5971 (11) | 14147 (14) | 872 (58) |
| C11 | -1359 (5) | 5043 (7) | 7530 (9) | 533 (39) | -3479 (6) | 5272 (8) | 13196 (8) | 634 (36) |
| N12 | -2329 (5) | 4338 (7) | 6535 (7) | 625 (36) | -2842 (5) | 4410 (6) | 13596 (7) | 618 (33) |
| C13 | -2795 (8) | 3962 (9) | 7372 (11) | 687 (49) | -2376 (6) | 3926 (8) | 12526 (8) | 601 (40) |
| N14 | -2223 (5) | 4369 (6) | 8803 (8) | 629 (36) | -2670 (5) | 4419 (7) | 11455 (7) | 672 (31) |
| C15 | -1284 (7) | 5081 (8) | 8929 (10) | 598 (44) | -3366 (6) | 5275 (9) | 11890 (9) | 706 (49) |

Table 2. Bond distances (\AA), bond angles ($^\circ$) and selected torsion angles ($^\circ$)

| | Molecule 1 | Molecule 2 | | Molecule 1 | Molecule 2 |
|--------------|------------|-------------|----------------|-------------|------------|
| C1—C1 | 1.727 (11) | 1.738 (10) | N8—C9 | 1.451 (14) | 1.480 (16) |
| C1—C2 | 1.371 (15) | 1.378 (9) | C9—C10 | 1.526 (16) | 1.474 (16) |
| C1—C6 | 1.352 (13) | 1.369 (13) | C10—C11 | 1.502 (16) | 1.493 (16) |
| C2—C3 | 1.376 (17) | 1.354 (15) | C11—N12 | 1.377 (8) | 1.354 (11) |
| C3—C4 | 1.375 (12) | 1.375 (12) | C11—C15 | 1.337 (14) | 1.334 (13) |
| C4—C5 | 1.397 (12) | 1.374 (9) | N12—C13 | 1.301 (15) | 1.340 (11) |
| C4—C7 | 1.465 (14) | 1.474 (14) | C13—N14 | 1.308 (12) | 1.298 (12) |
| C5—C6 | 1.353 (16) | 1.371 (15) | N14—C15 | 1.378 (12) | 1.383 (11) |
| C7—N8 | 1.257 (12) | 1.267 (10) | | | |
| C1—C1—C6 | 120.8 (7) | 119.1 (6) | C7—N8—C9 | 116.2 (7) | 116.7 (8) |
| C1—C1—C2 | 119.2 (6) | 119.1 (7) | N8—C9—C10 | 110.2 (8) | 109.4 (10) |
| C2—C1—C6 | 120.0 (9) | 121.8 (8) | C9—C10—C11 | 112.2 (8) | 112.6 (10) |
| C1—C2—C3 | 120.1 (9) | 118.3 (9) | C10—C11—C15 | 130.2 (8) | 133.5 (9) |
| C2—C3—C4 | 121.2 (9) | 122.5 (9) | C10—C11—N12 | 120.0 (7) | 121.4 (7) |
| C3—C4—C7 | 121.3 (8) | 123.8 (8) | N12—C11—C15 | 109.7 (7) | 105.1 (7) |
| C3—C4—C5 | 116.3 (7) | 117.2 (8) | C11—N12—C13 | 104.3 (7) | 108.1 (6) |
| C5—C4—C7 | 122.3 (7) | 118.9 (8) | N12—C13—N14 | 113.5 (9) | 111.6 (7) |
| C4—C5—C6 | 122.6 (8) | 122.5 (8) | C13—N14—C15 | 106.4 (7) | 104.2 (6) |
| C1—C6—C5 | 119.7 (9) | 117.8 (8) | C11—C15—N14 | 106.0 (7) | 111.0 (7) |
| C4—C7—N8 | 124.4 (8) | 122.9 (9) | | | |
| C5—C4—C7—N8 | -3.6 (14) | -178.3 (10) | N8—C9—C10—C11 | -169.8 (8) | 176.0 (9) |
| C3—C4—C7—N8 | 177.9 (9) | 1.1 (16) | C9—C10—C11—N12 | 78.7 (11) | 136.1 (10) |
| C4—C7—N8—C9 | -179.5 (8) | 179.4 (9) | C9—C10—C11—C15 | -100.0 (12) | -44.8 (16) |
| C7—N8—C9—C10 | 122.2 (9) | 120.9 (11) | | | |

the final ΔF map were -0.25 and 0.20 e \AA^{-3} , respectively, maximum $\Delta/\sigma = 0.88$, scattering factors of *SHELX76*, $R = 0.054$, $wR = 0.057$, $w = 0.5154/(\sigma^2 F + 0.00319F^2)$, $S = 0.58$. All calculations performed on an IBM PS2/80 personal computer with the *CRYSRULER* package (Rizzoli, Sangermano, Cales-tani & Andreotti, 1987). Positional and equivalent isotropic thermal parameters (Hamilton, 1959) of the non-H atoms are in Table 1,* bond lengths and angles are in Table 2. A drawing of the molecules with the atomic labeling is in Fig. 1. Packing of the molecules in the crystal with the hydrogen-bonding scheme is shown in Fig. 2.

Related literature. The structure of the title compound was determined as part of studies on the

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54796 (11 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: PA0238]

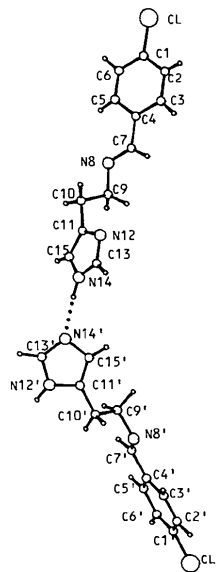


Fig. 1. The molecular geometry and hydrogen-bonding scheme of the compound. The dotted line indicates a hydrogen bond.

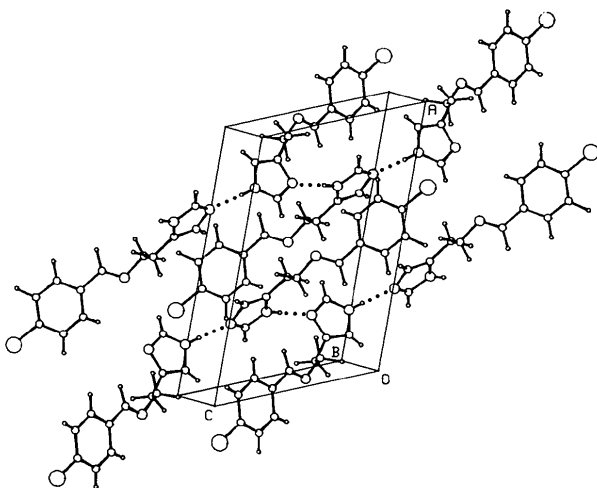


Fig. 2. Packing of the molecules.

reactivity of imidazole-containing compounds. Derivatives with a similar molecular skeleton have not been reported so far in the Cambridge Structural Database files.

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