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# *N*,*N*′-Bis(2-chlorobenzyl)-*N*″-(dichloroacetyl)phosphoric triamide

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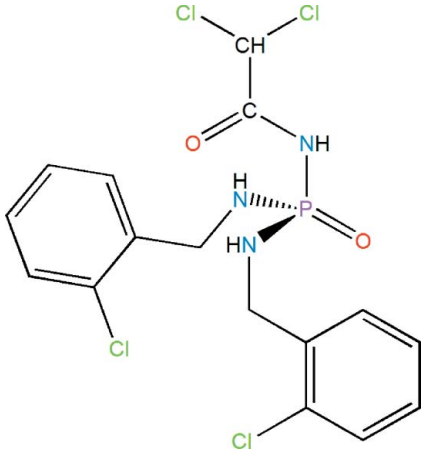
Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.008 Å; $R$ factor = 0.061; $wR$ factor = 0.156; data-to-parameter ratio = 14.9.

In the title compound, $C_{16}H_{16}Cl_4N_3O_2P$, the phosphoryl and carbonyl groups are *anti* to each other. The dihedral angle between the benzene rings is 33.59 (16)°. In the crystal, adjacent molecules are linked *via* N—H···O=P and N—H···O=C hydrogen bonds, into an extended chain running parallel to the *a* axis.

## Related literature

For biologically active organophosphorus compounds, see: Ekstrom *et al.* (2006). For the anticancer activity of compounds with a C(O)NHP(O) skeleton, see: Gholivand *et al.* (2011). For related structures, see: Sabbaghi *et al.* (2010*a*,*b*).




## Experimental

### Crystal data

$C_{16}H_{16}Cl_4N_3O_2P$ $M_r$ = 455.09
Triclinic, $P\overline{1}$
$a$ = 9.901 (1) Å
$b$ = 10.179 (1) Å
$c$ = 12.013 (2) Å
$\alpha$ = 90.403 (5)°
$\beta$ = 112.851 (6)°
$\gamma$ = 114.084 (6)°
$V$ = 998.7 (2) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.69 mm$^{-1}$
$T$ = 295 K
0.22 × 0.12 × 0.11 mm

### Data collection

Oxford Diffraction Xcalibur Sapphire3 Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
$T_{min}$ = 0.978, $T_{max}$ = 1.000
6193 measured reflections
3510 independent reflections
2786 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.018

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.156
$S$ = 1.02
3510 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.96 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.65 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2···O1$^{i}$ | 0.86 | 1.93 | 2.756 (4) | 162 |
| N3—H3···O2$^{ii}$ | 0.86 | 2.24 | 3.024 (4) | 151 |

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+1$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2102).

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# supporting information

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## *N*,*N*′-Bis(2-chlorobenzyl)-*N*′′-(dichloroacetyl)phosphoric triamide

**Mehrdad Pourayoubi, Maryam Toghraee and Vladimir Divjakovic**

### S1. Comment

Organophosphorus compounds are well-known as the biologically active substances (Ekstrom *et al.*, 2006). Among them the anticancer activity of compounds having a C(O)NHP(O) skeleton has been studied (Gholivand *et al.*, 2011). In the previous works, some phosphoric triamides such as P(O)[NHC(O)$C_6H_4$(4-$NO_2$)][$NHC_6H_{11}$]$_2$ (Sabbaghi *et al.*, 2010*a*) and P(O)[NHC(O)$C_6H_4$(4-$NO_2$)][N($CH_3$)($C_6H_{11}$)]$_2$ (Sabbaghi *et al.*, 2010*b*) have been structurally investigated. We report here on the synthesis and crystal structure of P(O)[NHC(O)$CHCl_2$][$NHCH_2$(2-Cl—$C_6H_4$)]$_2$. Single crystals of title compound were obtained from a solution of $CH_3OH$ and $CH_3CN$ after a slow evaporation at room temperature. The phosphoryl and carbonyl groups are *anti* to each other and the phosphorus atom is in a slightly distorted tetrahedral environment (Fig. 1). The bond angles are in the range of 103.08 (16)°-117.84 (17)° around the P atom. The P—N1 and P—N3 (1.616 (3) Å and 1.619 (3) Å) bond lengths are shorter than the P—N2 bond (1.682 (3) Å). The environment of nitrogen atoms is essentially planar. The P═O bond length of 1.471 (3) Å is standard for phosphoramidate compounds.

In the crystal structure, adjacent molecules are linked *via* N–H···O═P and N–H···O═C hydrogen bonds, into an extended chain parallel to the *a* axis.

### S2. Experimental

The reaction of phosphorus pentachloride (16.91 mmol) and $CHCl_2C(O)NH_2$ (16.91 mmol) in dry $CCl_4$ at 358 K (3 h) and then the treatment of formic acid (16.91 mmol) at ice bath temperature leads to $CHCl_2C(O)NHP(O)Cl_2$.

To a solution of $CHCl_2C(O)NHP(O)Cl_2$ (1.04 mmol) in dry $CHCl_3$, a solution of 2-chlorobenzylamine (4.16 mmol) in dry $CHCl_3$ was added dropwise and stirred at 273 K. After 4 h, the solvent was evaporated at room temperature. The solid was washed with $H_2O$. The product was obtained after recrystallization from a methanol/acetonitrile mixture (4:1) after a slow evaporation at room temperature. IR (KBr, $cm^{-1}$): 3392 (NH), 3080 (NH), 2881, 1704 (C═O), 1465, 1203 (P═O), 1072, 887.

### S3. Refinement

All H atoms were placed at calculated positions and were refined riding on the respective carrier atoms.

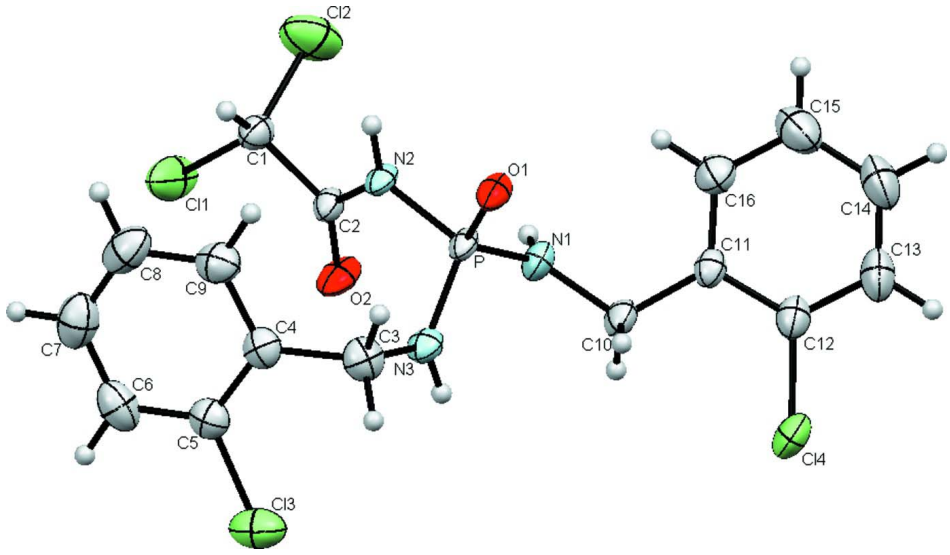


**Figure 1**

An *ORTEP* style plot of title compound. Ellipsoids are given at 30% probability level.

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*Crystal data*

$C_{16}H_{16}Cl_4N_3O_2P$
$M_r = 455.09$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.901$ (1) Å
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$c = 12.013$ (2) Å
$\alpha = 90.403$ (5)°
$\beta = 112.851$ (6)°
$\gamma = 114.084$ (6)°
$V = 998.7$ (2) Å$^3$
$Z = 2$
$F(000) = 464$
$D_x = 1.513$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2802 reflections
$\theta = 3.5$–29.0°
$\mu = 0.69$ mm$^{-1}$
$T = 295$ K
Prism, colourless
0.22 × 0.12 × 0.11 mm

*Data collection*

Oxford Diffraction Xcalibur Sapphire3 Gemini diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.3280 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
$T_{min} = 0.978$, $T_{max} = 1.000$
6193 measured reflections
3510 independent reflections
2786 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 25.0°$, $\theta_{min} = 3.5°$
$h = -11\rightarrow9$
$k = -11\rightarrow12$
$l = -14\rightarrow13$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.156$
$S = 1.02$
3510 reflections
235 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0618P)^2 + 1.5174P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.96$ e Å$^{-3}$
$\Delta\rho_{min} = -0.65$ e Å$^{-3}$

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| P | 0.84901 (11) | 0.52095 (11) | 0.59850 (8) | 0.0398 (3) |
| Cl1 | 0.4017 (2) | 0.3402 (3) | 0.12756 (12) | 0.1300 (8) |
| Cl2 | 0.5672 (2) | 0.16627 (16) | 0.23126 (18) | 0.1108 (6) |
| Cl3 | 0.65788 (18) | 0.91760 (16) | 0.50769 (15) | 0.0893 (5) |
| Cl4 | 0.77087 (18) | 0.44836 (16) | 1.03178 (11) | 0.0804 (4) |
| O1 | 1.0238 (3) | 0.5568 (3) | 0.6484 (2) | 0.0543 (7) |
| O2 | 0.5072 (3) | 0.4115 (4) | 0.3908 (3) | 0.0670 (9) |
| N1 | 0.7379 (4) | 0.4006 (4) | 0.6531 (3) | 0.0496 (8) |
| H1 | 0.6627 | 0.3184 | 0.6048 | 0.059* |
| N2 | 0.7656 (3) | 0.4413 (3) | 0.4495 (3) | 0.0427 (7) |
| H2 | 0.8279 | 0.4239 | 0.4240 | 0.051* |
| N3 | 0.8251 (4) | 0.6669 (3) | 0.6149 (3) | 0.0481 (8) |
| H3 | 0.7538 | 0.6631 | 0.6405 | 0.058* |
| C1 | 0.5775 (5) | 0.3419 (5) | 0.2368 (4) | 0.0512 (10) |
| H1A | 0.6696 | 0.4058 | 0.2197 | 0.061* |
| C2 | 0.6105 (4) | 0.4020 (4) | 0.3661 (3) | 0.0423 (8) |
| C3 | 0.9204 (5) | 0.8049 (5) | 0.5877 (4) | 0.0611 (11) |
| H3A | 1.0292 | 0.8142 | 0.6081 | 0.073* |
| H3B | 0.9319 | 0.8859 | 0.6395 | 0.073* |
| C4 | 0.8437 (5) | 0.8158 (4) | 0.4545 (4) | 0.0524 (10) |
| C5 | 0.7214 (5) | 0.8603 (4) | 0.4084 (4) | 0.0560 (10) |
| C6 | 0.6453 (6) | 0.8610 (5) | 0.2847 (5) | 0.0741 (14) |
| H6 | 0.5635 | 0.8919 | 0.2570 | 0.089* |
| C7 | 0.6907 (8) | 0.8161 (6) | 0.2034 (5) | 0.0846 (16) |
| H7 | 0.6393 | 0.8155 | 0.1199 | 0.102* |
| C8 | 0.8110 (8) | 0.7727 (6) | 0.2449 (5) | 0.0837 (16) |
| H8 | 0.8424 | 0.7428 | 0.1897 | 0.100* |
| C9 | 0.8878 (6) | 0.7724 (5) | 0.3692 (5) | 0.0678 (12) |
| H9 | 0.9705 | 0.7425 | 0.3960 | 0.081* |
| C10 | 0.7581 (5) | 0.4233 (5) | 0.7789 (4) | 0.0513 (10) |
| H10A | 0.6585 | 0.4211 | 0.7776 | 0.062* |
| H10B | 0.8462 | 0.5203 | 0.8215 | 0.062* |

| | | | | |
|---|---|---|---|---|
| C11 | 0.7950 (4) | 0.3128 (4) | 0.8509 (3) | 0.0458 (9) |
| C12 | 0.8030 (5) | 0.3159 (5) | 0.9693 (4) | 0.0571 (11) |
| C13 | 0.8391 (6) | 0.2189 (6) | 1.0401 (5) | 0.0745 (14) |
| H13 | 0.8461 | 0.2247 | 1.1196 | 0.089* |
| C14 | 0.8644 (7) | 0.1145 (7) | 0.9923 (6) | 0.0904 (17) |
| H14 | 0.8875 | 0.0476 | 1.0391 | 0.108* |
| C15 | 0.8562 (7) | 0.1062 (6) | 0.8740 (6) | 0.0893 (17) |
| H15 | 0.8733 | 0.0343 | 0.8414 | 0.107* |
| C16 | 0.8225 (6) | 0.2060 (5) | 0.8060 (5) | 0.0657 (12) |
| H16 | 0.8182 | 0.2013 | 0.7273 | 0.079* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| P | 0.0347 (5) | 0.0643 (6) | 0.0311 (5) | 0.0268 (5) | 0.0192 (4) | 0.0135 (4) |
| Cl1 | 0.1450 (15) | 0.226 (2) | 0.0426 (7) | 0.1471 (16) | −0.0041 (8) | −0.0079 (9) |
| Cl2 | 0.1193 (13) | 0.0728 (9) | 0.1247 (14) | 0.0485 (9) | 0.0318 (11) | −0.0113 (9) |
| Cl3 | 0.0902 (10) | 0.0832 (9) | 0.1143 (12) | 0.0446 (8) | 0.0567 (9) | 0.0103 (8) |
| Cl4 | 0.1089 (10) | 0.1091 (10) | 0.0488 (7) | 0.0593 (9) | 0.0469 (7) | 0.0242 (6) |
| O1 | 0.0390 (14) | 0.097 (2) | 0.0371 (14) | 0.0384 (15) | 0.0170 (12) | 0.0138 (14) |
| O2 | 0.0404 (15) | 0.119 (3) | 0.0490 (17) | 0.0405 (17) | 0.0219 (13) | 0.0053 (16) |
| N1 | 0.0538 (19) | 0.060 (2) | 0.0360 (17) | 0.0223 (16) | 0.0241 (15) | 0.0118 (14) |
| N2 | 0.0367 (16) | 0.069 (2) | 0.0332 (16) | 0.0281 (15) | 0.0206 (13) | 0.0093 (14) |
| N3 | 0.0443 (17) | 0.062 (2) | 0.0473 (19) | 0.0251 (16) | 0.0272 (15) | 0.0121 (15) |
| C1 | 0.050 (2) | 0.064 (2) | 0.041 (2) | 0.029 (2) | 0.0177 (18) | 0.0055 (18) |
| C2 | 0.0390 (19) | 0.060 (2) | 0.0346 (19) | 0.0248 (18) | 0.0187 (16) | 0.0131 (16) |
| C3 | 0.050 (2) | 0.058 (3) | 0.061 (3) | 0.018 (2) | 0.017 (2) | 0.008 (2) |
| C4 | 0.048 (2) | 0.045 (2) | 0.060 (3) | 0.0138 (18) | 0.025 (2) | 0.0131 (18) |
| C5 | 0.052 (2) | 0.047 (2) | 0.065 (3) | 0.0174 (19) | 0.027 (2) | 0.012 (2) |
| C6 | 0.062 (3) | 0.059 (3) | 0.084 (4) | 0.024 (2) | 0.018 (3) | 0.022 (3) |
| C7 | 0.089 (4) | 0.073 (3) | 0.067 (3) | 0.019 (3) | 0.029 (3) | 0.016 (3) |
| C8 | 0.103 (4) | 0.075 (3) | 0.078 (4) | 0.024 (3) | 0.058 (3) | 0.013 (3) |
| C9 | 0.069 (3) | 0.062 (3) | 0.086 (4) | 0.029 (2) | 0.046 (3) | 0.021 (2) |
| C10 | 0.058 (2) | 0.068 (3) | 0.041 (2) | 0.031 (2) | 0.0303 (19) | 0.0182 (19) |
| C11 | 0.039 (2) | 0.059 (2) | 0.041 (2) | 0.0201 (18) | 0.0203 (17) | 0.0160 (17) |
| C12 | 0.050 (2) | 0.075 (3) | 0.047 (2) | 0.027 (2) | 0.0222 (19) | 0.021 (2) |
| C13 | 0.070 (3) | 0.092 (4) | 0.059 (3) | 0.034 (3) | 0.027 (2) | 0.038 (3) |
| C14 | 0.095 (4) | 0.097 (4) | 0.090 (4) | 0.056 (4) | 0.036 (3) | 0.053 (3) |
| C15 | 0.097 (4) | 0.088 (4) | 0.112 (5) | 0.059 (3) | 0.053 (4) | 0.046 (3) |
| C16 | 0.069 (3) | 0.077 (3) | 0.066 (3) | 0.038 (3) | 0.038 (2) | 0.022 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| P—O1 | 1.471 (3) | C5—C6 | 1.382 (7) |
| P—N1 | 1.616 (3) | C6—C7 | 1.367 (8) |
| P—N3 | 1.619 (3) | C6—H6 | 0.9300 |
| P—N2 | 1.682 (3) | C7—C8 | 1.354 (8) |
| Cl1—C1 | 1.718 (4) | C7—H7 | 0.9300 |

| | | | |
|---|---|---|---|
| Cl2—C1 | 1.748 (4) | C8—C9 | 1.388 (7) |
| Cl3—C5 | 1.741 (5) | C8—H8 | 0.9300 |
| Cl4—C12 | 1.733 (5) | C9—H9 | 0.9300 |
| O2—C2 | 1.208 (4) | C10—C11 | 1.500 (5) |
| N1—C10 | 1.450 (5) | C10—H10A | 0.9700 |
| N1—H1 | 0.8600 | C10—H10B | 0.9700 |
| N2—C2 | 1.349 (4) | C11—C16 | 1.376 (6) |
| N2—H2 | 0.8600 | C11—C12 | 1.394 (5) |
| N3—C3 | 1.461 (5) | C12—C13 | 1.375 (6) |
| N3—H3 | 0.8600 | C13—C14 | 1.358 (8) |
| C1—C2 | 1.525 (5) | C13—H13 | 0.9300 |
| C1—H1A | 0.9800 | C14—C15 | 1.392 (8) |
| C3—C4 | 1.509 (6) | C14—H14 | 0.9300 |
| C3—H3A | 0.9700 | C15—C16 | 1.373 (7) |
| C3—H3B | 0.9700 | C15—H15 | 0.9300 |
| C4—C5 | 1.381 (6) | C16—H16 | 0.9300 |
| C4—C9 | 1.392 (6) | | |

| | | | |
|---|---|---|---|
| O1—P—N1 | 117.84 (17) | C7—C6—C5 | 119.7 (5) |
| O1—P—N3 | 110.86 (18) | C7—C6—H6 | 120.1 |
| N1—P—N3 | 106.48 (17) | C5—C6—H6 | 120.1 |
| O1—P—N2 | 106.38 (15) | C8—C7—C6 | 119.7 (5) |
| N1—P—N2 | 103.08 (16) | C8—C7—H7 | 120.2 |
| N3—P—N2 | 112.03 (16) | C6—C7—H7 | 120.2 |
| C10—N1—P | 123.7 (3) | C7—C8—C9 | 120.7 (5) |
| C10—N1—H1 | 118.2 | C7—C8—H8 | 119.7 |
| P—N1—H1 | 118.2 | C9—C8—H8 | 119.7 |
| C2—N2—P | 126.3 (2) | C4—C9—C8 | 121.3 (5) |
| C2—N2—H2 | 116.9 | C4—C9—H9 | 119.3 |
| P—N2—H2 | 116.9 | C8—C9—H9 | 119.3 |
| C3—N3—P | 122.2 (3) | N1—C10—C11 | 114.6 (3) |
| C3—N3—H3 | 118.9 | N1—C10—H10A | 108.6 |
| P—N3—H3 | 118.9 | C11—C10—H10A | 108.6 |
| C2—C1—Cl1 | 111.5 (3) | N1—C10—H10B | 108.6 |
| C2—C1—Cl2 | 109.2 (3) | C11—C10—H10B | 108.6 |
| Cl1—C1—Cl2 | 111.2 (2) | H10A—C10—H10B | 107.6 |
| C2—C1—H1A | 108.3 | C16—C11—C12 | 117.0 (4) |
| Cl1—C1—H1A | 108.3 | C16—C11—C10 | 123.2 (4) |
| Cl2—C1—H1A | 108.3 | C12—C11—C10 | 119.7 (4) |
| O2—C2—N2 | 123.9 (3) | C13—C12—C11 | 122.2 (5) |
| O2—C2—C1 | 123.1 (3) | C13—C12—Cl4 | 118.4 (4) |
| N2—C2—C1 | 113.0 (3) | C11—C12—Cl4 | 119.4 (3) |
| N3—C3—C4 | 113.0 (3) | C12—C13—C14 | 119.0 (5) |
| N3—C3—H3A | 109.0 | C12—C13—H13 | 120.5 |
| C4—C3—H3A | 109.0 | C14—C13—H13 | 120.5 |
| N3—C3—H3B | 109.0 | C15—C14—C13 | 120.8 (5) |
| C4—C3—H3B | 109.0 | C15—C14—H14 | 119.6 |
| H3A—C3—H3B | 107.8 | C13—C14—H14 | 119.6 |

| | | | |
|---|---|---|---|
| C5—C4—C9 | 116.2 (4) | C14—C15—C16 | 118.9 (5) |
| C5—C4—C3 | 123.2 (4) | C14—C15—H15 | 120.6 |
| C9—C4—C3 | 120.5 (4) | C16—C15—H15 | 120.6 |
| C4—C5—C6 | 122.5 (4) | C11—C16—C15 | 122.0 (5) |
| C4—C5—Cl3 | 119.7 (4) | C11—C16—H16 | 119.0 |
| C6—C5—Cl3 | 117.8 (4) | C15—C16—H16 | 119.0 |
| | | | |
| O1—P—N1—C10 | 66.5 (4) | C4—C5—C6—C7 | 0.1 (7) |
| N3—P—N1—C10 | −58.7 (3) | Cl3—C5—C6—C7 | −179.6 (4) |
| N2—P—N1—C10 | −176.8 (3) | C5—C6—C7—C8 | −0.6 (8) |
| O1—P—N2—C2 | −174.1 (3) | C6—C7—C8—C9 | 0.4 (8) |
| N1—P—N2—C2 | 61.3 (4) | C5—C4—C9—C8 | −0.7 (6) |
| N3—P—N2—C2 | −52.8 (4) | C3—C4—C9—C8 | 175.8 (4) |
| O1—P—N3—C3 | 44.0 (3) | C7—C8—C9—C4 | 0.3 (8) |
| N1—P—N3—C3 | 173.4 (3) | P—N1—C10—C11 | −121.2 (3) |
| N2—P—N3—C3 | −74.6 (3) | N1—C10—C11—C16 | 5.6 (6) |
| P—N2—C2—O2 | −4.7 (6) | N1—C10—C11—C12 | −174.5 (4) |
| P—N2—C2—C1 | 176.0 (3) | C16—C11—C12—C13 | 1.0 (6) |
| Cl1—C1—C2—O2 | 17.2 (5) | C10—C11—C12—C13 | −178.9 (4) |
| Cl2—C1—C2—O2 | −106.1 (4) | C16—C11—C12—Cl4 | 179.6 (3) |
| Cl1—C1—C2—N2 | −163.5 (3) | C10—C11—C12—Cl4 | −0.3 (5) |
| Cl2—C1—C2—N2 | 73.2 (4) | C11—C12—C13—C14 | −1.4 (7) |
| P—N3—C3—C4 | 87.6 (4) | Cl4—C12—C13—C14 | 179.9 (4) |
| N3—C3—C4—C5 | 83.3 (5) | C12—C13—C14—C15 | 0.8 (9) |
| N3—C3—C4—C9 | −93.0 (5) | C13—C14—C15—C16 | 0.2 (9) |
| C9—C4—C5—C6 | 0.5 (6) | C12—C11—C16—C15 | 0.1 (7) |
| C3—C4—C5—C6 | −175.9 (4) | C10—C11—C16—C15 | 180.0 (5) |
| C9—C4—C5—Cl3 | −179.7 (3) | C14—C15—C16—C11 | −0.7 (8) |
| C3—C4—C5—Cl3 | 3.9 (5) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2···O1$^{i}$ | 0.86 | 1.93 | 2.756 (4) | 162 |
| N3—H3···O2$^{ii}$ | 0.86 | 2.24 | 3.024 (4) | 151 |

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1.