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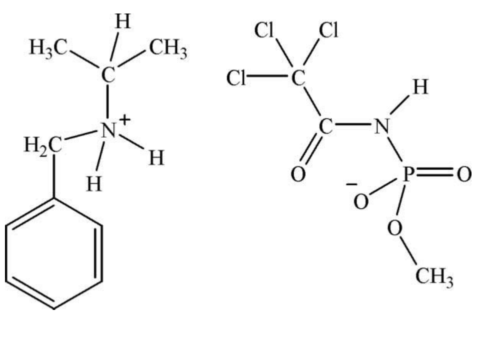
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.076; data-to-parameter ratio = 18.0.

The title compound, $C_{13}H_{20}Cl_3N_2O_4P$, was prepared by the reaction of *N*-isopropylbenzylamine and $CCl_3C(O)N(H)$-$P(O)Cl_2$, followed by crystallization from CH_3OH and CH_3CN. Centrosymmetric dimers of anions are hydrogen-bonded to neighbouring cations (*via* –P—O···H—N– and –C=O···H—N– hydrogen bonds) in a one-dimensional polymeric chain. Furthermore, a Cl···Cl interaction (3.242 Å) and a C—H···π short contact are present in the crystal structure, the former between two adjacent anions and the latter between two neighbouring cations.

Related literature

For related literature, see: Amirkhanov *et al.* (1997); Gholivand & Pourayoubi (2004); Gholivand *et al.* (2005); Kirsanov & Makitra (1956); Wisser & Janiak (2007); Ślepokura & Lis (2006).



Experimental

Crystal data

$C_{13}H_{20}Cl_3N_2O_4P$
M_r = 405.63
Triclinic, $P\bar{1}$
a = 9.5690 (7) Å
b = 9.7554 (7) Å
c = 10.5083 (7) Å
α = 78.757 (1)°
β = 73.902 (1)°
γ = 83.115 (2)°
V = 922.14 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.60 mm^{-1}
T = 120 (2) K
0.35 × 0.20 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; (Bruker, 2005) T_{min} = 0.817, T_{max} = 0.889
7569 measured reflections
4012 independent reflections
3317 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.076
S = 1.03
4012 reflections
223 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

Cg is the centroid of the C5–C10 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4B···Cg^{i}	0.99	2.86 (2)	3.635 (2)	135
N1—H1N···O2^{ii}	0.86 (2)	1.88 (2)	2.743 (2)	175 (2)
N2—H2NB···O1	0.93 (2)	1.95 (2)	2.811 (2)	153 (2)
N2—H2NA···O1^{iii}	0.89 (2)	1.84 (2)	2.727 (2)	173 (2)
N2—H2NB···O4	0.93 (2)	2.35 (2)	2.930 (2)	120 (2)

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2005); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2024).

References

Amirkhanov, V. M., Ochynnikov, V. A. & Galowiak, T. (1997). *Z. Naturforsch. Teil B*, **52**, 1331–1336.
Bruker (2005). *APEX2* (Version 2.0-1), *SAINT* (Version 7.23A), *SADABS* (Version 2004/1) and *SHELXTL* (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.
Gholivand, K. & Pourayoubi, M. (2004). *Z. Kristallogr. New Cryst. Struct.* **219**, 314–316.
Gholivand, K., Pourayoubi, M., Shariatinia, Z. & Molani, S. (2005). *Z. Kristallogr. New Cryst. Struct.* **220**, 387–389.
Kirsanov, A. V. & Makitra, R. G. (1956). *Zh. Obshch. Khim.* **26**, 905–907.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Ślepokura, K. & Lis, T. (2006). *Carbohydr. Res.* **341**, 507–524.
Wisser, B. & Janiak, C. (2007). *Acta Cryst.* E**63**, o2871–o2872.

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supplementary materials

Acta Cryst. (2007). E**63**, o4366 [**doi:10.1107/S1600536807050428**]

N-Benzyl-2-propanaminium *O*-methyl trichloroacetamidophosphate

M. Pourayoubi and F. Sabbaghi

Comment

Phosphate derivatives (XYP(O)O^-, where *X*, Y = O^-, OH, OR, OAr, NRR', halide ion,···) have attracted significant attention due to their utility in supramolecular chemistry and crystal engineering and their ability as the metal complexing agents (Wisser & Janiak, 2007; Ślepokura & Lis, 2006). There is a little reports on *N*-acylated phosphate derivatives, RC(O)N(H)P(O)R^1O^- (Gholivand *et al.*, 2005) but the investigation about this area are of special interest in this context: 1) having an ionic structure and possibility the exchange of cation to obtain desirable solubility and hydrophobicity which is required to bio-study 2) bearing a close structural resemblance to the *β*-diketone frame, 3) usually acting as effective chelating groups (Amirkhanov *et al.*, 1997). In previous works, we report on the structure of phosphate compounds containing $PO_2Cl_2^-$ (Gholivand & Pourayoubi, 2004) and $CF_3C(O)N(H)P(O)(O)[NH(tert,-C_4H_9)]^-$ anions (Gholivand *et al.*, 2005).

Here, we report the crystal structure of the title compound, *N*-Benzyl-2-propanaminium *O*-methyl trichloroacetamidophosphate (Fig. 1). Phosphorus atom in the anion of title compound has a distorted tetrahedral geometry. Centrosymmetric dimmers of anions which is produced *via* two equal N1—H1N···$O2^{ii}$ hydrogen bonds (Table 1 and Fig. 2) are hydrogen bonded to neighboring cations in a one-dimensional polymeric chain. Furthermore, the crystal packing is stabilized by Cl···Cl (distance 3.242 Å) electrostatic interaction and C—H···π short contact between a hydrogen of the C4 and the phenyl group (Table 1 and Fig. 2, the centroid of the C5–C10 phenyl ring and the symmetry codes are as in Fig. 2).

Experimental

N-isopropylbenzylamine (1.133 g, 7.594 mmol) was added to a solution of $CCl_3C(O)N(H)P(O)Cl_2$ (0.530 g, 1.899 mmol) (Kirsanov & Makitra, 1956) in CCl_4 (20 ml) and stirred at 273 K. After 12 h, the solvent removed and the residue that formed was stirred with H_2O. After drying, the solid was recrystallized from CH_3OH and CH_3CN.

Refinement

The hydrogen atoms of NH and NH_2 groups were located in difference Fourier maps and the all parameters were freely refined. All H atoms of C were geometrically located in ideal positions and refined using a riding model, with C—H = 0.95 Å for aromatic H atoms, 0.98 Å for methyl H atoms, and 0.99 Å for methylene H atoms, and with $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic and methylene H atoms and 1.5Ueq(C) for methyl H atoms.

Figures

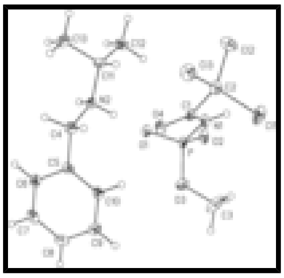

Fig. 1. Structure of title compound showing the atom-labeling scheme with thermal ellipsoid at 50% probability.

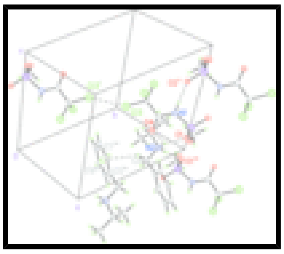

Fig. 2. The N—H···O hydrogen bonds, Cl···Cl and C—H···π interations (dotted lines) in the title compound. [Symmetry code: (i) −*x* + 1, −*y* + 1, −*z* + 1; (ii) −*x* + 2, −*y* + 2, −*z* + 1; (iii) −*x* + 2, −*y* + 2, −*z*; (iv) −*x* + 2, −*y* + 1, −*z*.]

N-Benzyl-2-propanaminium *O*-methyl trichloroacetamidophosphate

Crystal data

$C_{13}H_{20}Cl_3N_2O_4P$	$Z = 2$
$M_r = 405.63$	$F_{000} = 420$
Triclinic, $P\overline{1}$	$D_x = 1.461$ Mg m^{-3}
Hall symbol: -P 1	Mo *K*α radiation λ = 0.71073 Å
a = 9.5690 (7) Å	Cell parameters from 511 reflections
b = 9.7554 (7) Å	θ = 3–27º
c = 10.5083 (7) Å	μ = 0.60 mm^{-1}
α = 78.757 (1)º	*T* = 120 (2) K
β = 73.902 (1)º	Prism, colourless
γ = 83.115 (2)º	0.35 × 0.20 × 0.20 mm
V = 922.14 (11) Å^3	

Data collection

Bruker APEXII CCD area-detector diffractometer	4012 independent reflections
Radiation source: fine-focus sealed tube	3317 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 27.0$º
T = 120(2) K	$\theta_{min} = 2.1$º
ω scans	*h* = −12→12
Absorption correction: multi-scan (SADABS; Sheldrick, 1999)	*k* = −12→12
$T_{min} = 0.817$, $T_{max} = 0.889$	*l* = −13→13

7569 measured reflections

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.076$	$w = 1/[\sigma^2(F_o^2) + (0.0303P)^2 + 0.4098P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
4012 reflections	$\Delta\rho_{max} = 0.40$ e Å^{-3}
223 parameters	$\Delta\rho_{min} = -0.37$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. Spectroscopic analysis: IR (KBr, cm^{-1}) 3417, 3039, 2983, 2940, 2841, 2705, 2434, 1712, 1601, 1469, 1394, 1257, 1233, 1185, 1094, 1057, 865, 810, 749, 676; ^{31}P & ^{1}H-NMR {(D_6)DMSO}: 2.74 (1*P*). ^{1}H-NMR ((D_6)DMSO) 1.27 (6*H*, CH_3), 3.86 (1*H*, CH), 4.09 (2*H*, CH_2), 4.31 (3*H*, OCH_3), 7.10–7.53 (7*H*, 5 Ar—H & 2 NH), 8.82 (1*H*, NH); Anal. Calc.: C 38.49, H 4.97, N 6.91. found: C 38.40, H 4.91, N 6.87.

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 $F^2 > 2\text{sigma}(F^2)$ 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	1.08073 (5)	0.93186 (5)	0.29290 (4)	0.01267 (11)
Cl1	0.80897 (6)	0.61153 (6)	0.65929 (5)	0.02861 (13)
Cl2	0.62282 (5)	0.84713 (5)	0.56791 (5)	0.02585 (12)
Cl3	0.64223 (5)	0.58645 (5)	0.47578 (5)	0.02247 (12)
O1	1.04164 (14)	0.95140 (13)	0.16261 (12)	0.0156 (3)
O2	1.10748 (15)	1.05510 (14)	0.34305 (12)	0.0203 (3)
O3	1.21581 (14)	0.81854 (14)	0.28100 (13)	0.0216 (3)
O4	0.90319 (14)	0.68874 (13)	0.30462 (12)	0.0179 (3)
N1	0.94452 (17)	0.85137 (16)	0.41709 (15)	0.0156 (3)
H1N	0.923 (2)	0.882 (2)	0.492 (2)	0.028 (6)*
N2	0.87102 (16)	0.83093 (15)	0.04059 (15)	0.0120 (3)

H2NB	0.923 (2)	0.844 (2)	0.100 (2)	0.019 (5)*
H2NA	0.896 (2)	0.899 (2)	−0.030 (2)	0.024 (6)*
C1	0.87439 (19)	0.74740 (18)	0.40134 (16)	0.0133 (4)
C2	0.7413 (2)	0.70091 (19)	0.52235 (17)	0.0165 (4)
C3	1.2809 (3)	0.7801 (3)	0.3920 (3)	0.0404 (6)
H3A	1.3707	0.7208	0.3658	0.061*
H3B	1.2126	0.7284	0.4688	0.061*
H3C	1.3038	0.8648	0.4170	0.061*
C4	0.9180 (2)	0.69270 (18)	−0.00419 (18)	0.0166 (4)
H4A	0.8734	0.6864	−0.0772	0.020*
H4B	0.8822	0.6169	0.0718	0.020*
C5	1.0810 (2)	0.67174 (18)	−0.05357 (17)	0.0147 (4)
C6	1.1466 (2)	0.68353 (19)	−0.19101 (18)	0.0181 (4)
H6A	1.0887	0.7080	−0.2534	0.022*
C7	1.2966 (2)	0.6595 (2)	−0.23676 (19)	0.0222 (4)
H7A	1.3409	0.6668	−0.3305	0.027*
C8	1.3821 (2)	0.6250 (2)	−0.14661 (19)	0.0217 (4)
H8A	1.4847	0.6082	−0.1783	0.026*
C9	1.3171 (2)	0.6150 (2)	−0.00961 (19)	0.0205 (4)
H9A	1.3754	0.5918	0.0525	0.025*
C10	1.1677 (2)	0.63857 (18)	0.03649 (18)	0.0164 (4)
H10A	1.1238	0.6321	0.1302	0.020*
C11	0.71066 (19)	0.84825 (19)	0.10844 (18)	0.0164 (4)
H11A	0.6871	0.7726	0.1888	0.020*
C12	0.6802 (2)	0.9887 (2)	0.1561 (2)	0.0227 (4)
H12A	0.7401	0.9921	0.2173	0.034*
H12B	0.5768	1.0006	0.2033	0.034*
H12C	0.7039	1.0641	0.0785	0.034*
C13	0.6198 (2)	0.8340 (2)	0.0142 (2)	0.0236 (4)
H13A	0.6363	0.7388	−0.0066	0.035*
H13B	0.6483	0.9016	−0.0690	0.035*
H13C	0.5163	0.8525	0.0576	0.035*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P	0.0146 (2)	0.0143 (2)	0.0096 (2)	−0.00439 (18)	−0.00358 (17)	−0.00053 (17)
Cl1	0.0312 (3)	0.0351 (3)	0.0186 (2)	−0.0134 (2)	−0.0111 (2)	0.0109 (2)
Cl2	0.0193 (3)	0.0232 (3)	0.0332 (3)	−0.00429 (19)	0.0020 (2)	−0.0118 (2)
Cl3	0.0223 (3)	0.0209 (2)	0.0264 (2)	−0.01088 (19)	−0.00513 (19)	−0.00544 (19)
O1	0.0198 (7)	0.0157 (6)	0.0122 (6)	−0.0049 (5)	−0.0055 (5)	−0.0007 (5)
O2	0.0270 (8)	0.0215 (7)	0.0140 (6)	−0.0128 (6)	−0.0035 (5)	−0.0027 (5)
O3	0.0174 (7)	0.0226 (7)	0.0234 (7)	0.0012 (6)	−0.0071 (6)	0.0003 (6)
O4	0.0233 (7)	0.0167 (7)	0.0145 (6)	−0.0043 (5)	−0.0043 (5)	−0.0039 (5)
N1	0.0201 (8)	0.0174 (8)	0.0102 (7)	−0.0073 (6)	−0.0026 (6)	−0.0027 (6)
N2	0.0141 (8)	0.0103 (7)	0.0118 (7)	−0.0013 (6)	−0.0044 (6)	−0.0008 (6)
C1	0.0147 (9)	0.0129 (8)	0.0126 (8)	−0.0019 (7)	−0.0060 (7)	0.0013 (7)
C2	0.0187 (10)	0.0160 (9)	0.0155 (8)	−0.0053 (7)	−0.0045 (7)	−0.0018 (7)

C3	0.0419 (15)	0.0336 (13)	0.0541 (15)	0.0008 (11)	−0.0358 (13)	0.0048 (11)
C4	0.0175 (9)	0.0127 (9)	0.0211 (9)	−0.0002 (7)	−0.0059 (7)	−0.0059 (7)
C5	0.0157 (9)	0.0095 (8)	0.0192 (9)	−0.0006 (7)	−0.0033 (7)	−0.0055 (7)
C6	0.0218 (10)	0.0168 (9)	0.0173 (9)	0.0001 (8)	−0.0066 (8)	−0.0051 (7)
C7	0.0250 (11)	0.0225 (10)	0.0167 (9)	−0.0021 (8)	0.0005 (8)	−0.0057 (8)
C8	0.0165 (10)	0.0189 (10)	0.0265 (10)	0.0023 (8)	−0.0019 (8)	−0.0036 (8)
C9	0.0196 (10)	0.0188 (10)	0.0237 (10)	0.0020 (8)	−0.0097 (8)	−0.0016 (8)
C10	0.0197 (10)	0.0136 (9)	0.0147 (8)	−0.0007 (7)	−0.0027 (7)	−0.0026 (7)
C11	0.0130 (9)	0.0166 (9)	0.0183 (9)	0.0008 (7)	−0.0029 (7)	−0.0025 (7)
C12	0.0182 (10)	0.0223 (10)	0.0286 (10)	0.0054 (8)	−0.0055 (8)	−0.0117 (8)
C13	0.0172 (10)	0.0255 (11)	0.0318 (11)	0.0014 (8)	−0.0108 (8)	−0.0088 (9)

Geometric parameters (Å, °)

P—O2	1.478 (1)	C4—H4B	0.9900
P—O1	1.489 (1)	C5—C10	1.393 (2)
P—O3	1.591 (1)	C5—C6	1.394 (2)
P—N1	1.709 (2)	C6—C7	1.388 (3)
Cl1—C2	1.772 (2)	C6—H6A	0.9500
Cl2—C2	1.768 (2)	C7—C8	1.386 (3)
Cl3—C2	1.764 (2)	C7—H7A	0.9500
O3—C3	1.437 (2)	C8—C9	1.390 (3)
O4—C1	1.212 (2)	C8—H8A	0.9500
N1—C1	1.340 (2)	C9—C10	1.383 (3)
N1—H1N	0.86 (2)	C9—H9A	0.9500
N2—C4	1.492 (2)	C10—H10A	0.9500
N2—C11	1.507 (2)	C11—C12	1.518 (3)
N2—H2NB	0.93 (2)	C11—C13	1.522 (2)
N2—H2NA	0.89 (2)	C11—H11A	1.0000
C1—C2	1.568 (2)	C12—H12A	0.9800
C3—H3A	0.9800	C12—H12B	0.9800
C3—H3B	0.9800	C12—H12C	0.9800
C3—H3C	0.9800	C13—H13A	0.9800
C4—C5	1.503 (3)	C13—H13B	0.9800
C4—H4A	0.9900	C13—H13C	0.9800
O2—P—O1	119.68 (7)	C10—C5—C6	119.34 (17)
O2—P—O3	111.84 (8)	C10—C5—C4	120.82 (16)
O1—P—O3	105.46 (7)	C6—C5—C4	119.83 (16)
O2—P—N1	105.49 (8)	C7—C6—C5	120.01 (17)
O1—P—N1	108.94 (7)	C7—C6—H6A	120.0
O3—P—N1	104.44 (8)	C5—C6—H6A	120.0
C3—O3—P	118.41 (14)	C8—C7—C6	120.40 (18)
C1—N1—P	123.40 (13)	C8—C7—H7A	119.8
C1—N1—H1N	121.3 (15)	C6—C7—H7A	119.8
P—N1—H1N	115.3 (15)	C7—C8—C9	119.67 (18)
C4—N2—C11	113.87 (13)	C7—C8—H8A	120.2
C4—N2—H2NB	110.0 (13)	C9—C8—H8A	120.2
C11—N2—H2NB	108.1 (13)	C10—C9—C8	120.13 (17)
C4—N2—H2NA	109.0 (14)	C10—C9—H9A	119.9

C11—N2—H2NA	110.7 (14)	C8—C9—H9A	119.9
H2NB—N2—H2NA	104.8 (18)	C9—C10—C5	120.43 (17)
O4—C1—N1	126.73 (16)	C9—C10—H10A	119.8
O4—C1—C2	118.51 (15)	C5—C10—H10A	119.8
N1—C1—C2	114.75 (15)	N2—C11—C12	108.21 (14)
C1—C2—Cl3	109.39 (12)	N2—C11—C13	110.70 (15)
C1—C2—Cl2	110.96 (12)	C12—C11—C13	112.64 (16)
Cl3—C2—Cl2	108.20 (10)	N2—C11—H11A	108.4
C1—C2—Cl1	108.37 (12)	C12—C11—H11A	108.4
Cl3—C2—Cl1	109.21 (10)	C13—C11—H11A	108.4
Cl2—C2—Cl1	110.69 (10)	C11—C12—H12A	109.5
O3—C3—H3A	109.5	C11—C12—H12B	109.5
O3—C3—H3B	109.5	H12A—C12—H12B	109.5
H3A—C3—H3B	109.5	C11—C12—H12C	109.5
O3—C3—H3C	109.5	H12A—C12—H12C	109.5
H3A—C3—H3C	109.5	H12B—C12—H12C	109.5
H3B—C3—H3C	109.5	C11—C13—H13A	109.5
N2—C4—C5	112.12 (14)	C11—C13—H13B	109.5
N2—C4—H4A	109.2	H13A—C13—H13B	109.5
C5—C4—H4A	109.2	C11—C13—H13C	109.5
N2—C4—H4B	109.2	H13A—C13—H13C	109.5
C5—C4—H4B	109.2	H13B—C13—H13C	109.5
H4A—C4—H4B	107.9		

O2—P—O3—C3	46.85 (16)	C11—N2—C4—C5	−172.01 (14)
O1—P—O3—C3	178.48 (14)	N2—C4—C5—C10	76.1 (2)
N1—P—O3—C3	−66.75 (16)	N2—C4—C5—C6	−104.87 (18)
O2—P—N1—C1	169.64 (15)	C10—C5—C6—C7	1.3 (3)
O1—P—N1—C1	39.97 (17)	C4—C5—C6—C7	−177.78 (17)
O3—P—N1—C1	−72.32 (16)	C5—C6—C7—C8	−0.6 (3)
P—N1—C1—O4	6.3 (3)	C6—C7—C8—C9	−0.3 (3)
P—N1—C1—C2	−173.17 (12)	C7—C8—C9—C10	0.4 (3)
O4—C1—C2—Cl3	−9.6 (2)	C8—C9—C10—C5	0.4 (3)
N1—C1—C2—Cl3	169.95 (13)	C6—C5—C10—C9	−1.2 (3)
O4—C1—C2—Cl2	−128.87 (15)	C4—C5—C10—C9	177.87 (16)
N1—C1—C2—Cl2	50.65 (18)	C4—N2—C11—C12	176.53 (14)
O4—C1—C2—Cl1	109.40 (16)	C4—N2—C11—C13	−59.6 (2)
N1—C1—C2—Cl1	−71.08 (17)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4B···Cg^{i}	0.99	2.86 (2)	3.635 (2)	135
N1—H1N···O2^{ii}	0.86 (2)	1.88 (2)	2.743 (2)	175 (2)
N2—H2NB···O1	0.93 (2)	1.95 (2)	2.811 (2)	153 (2)
N2—H2NA···O1^{iii}	0.89 (2)	1.84 (2)	2.727 (2)	173 (2)
N2—H2NB···O4	0.93 (2)	2.35 (2)	2.930 (2)	120 (2)

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

Fig. 1

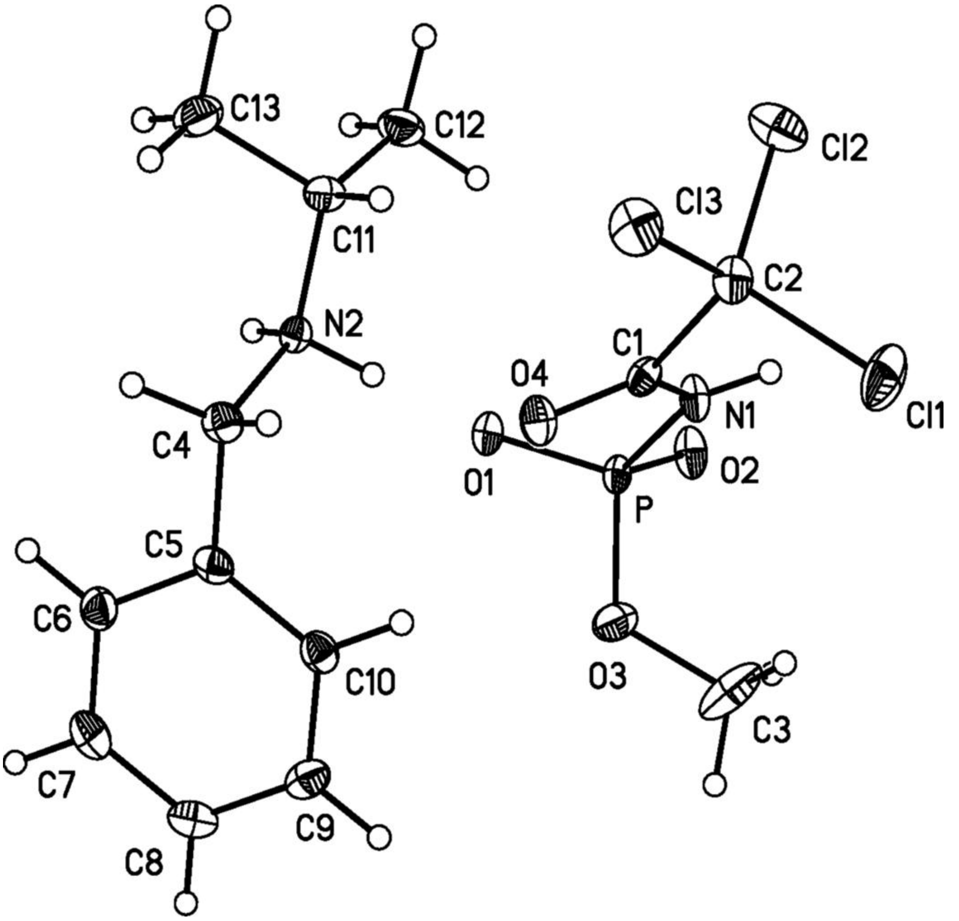
C13
C12
Cl2
Cl3
C11
C2
N2
C1
O4
N1
Cl1
C4
O1
O2
P
C5
C6
C10
O3
C3
C7
C9
C8

Fig. 2