Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

cis-1-Benzoyl-2-(2-benzyloxy-5-chlorophenyl)-4-chloropyrrolidine-2-carbonitrile

Rafael Tamazyan,[a]* Levon Matevosyan,[a] Ashot Martirosyan,[b] Sahak Gasparyan[b] and Raymond Schinazi[c]

[a]Molecular Structure Research Center, National Academy of Sciences RA, Azatutyan Avenue 26, 375014 Yerevan, Armenia, [b]Institute of Fine Organic Chemistry, National Academy of Sciences RA, Azatutyan Avenue 26, 375014 Yerevan, Armenia, and [c]Emory University School of Medicine, Veterans Affairs, Medical Center 1670, Clairmont Road, 151-H Decatur, Georgia 30033-4004, USA
Correspondence e-mail: rafael@msrc.am

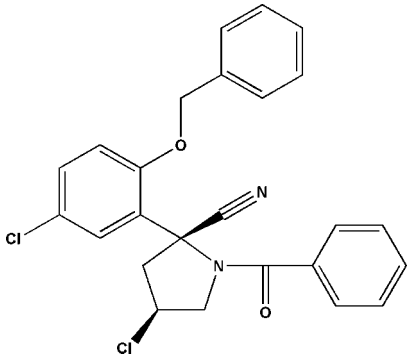
Received 24 August 2007; accepted 7 September 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.131; data-to-parameter ratio = 14.7.

In the title compound, $C_{25}H_{20}Cl_2N_2O_2$, which is a potential anti-human immunodeficiency virus type 1 (HIV-1) non-nucleoside reverse transcriptase inhibitor (NNRTI), the pyrrolidine ring has as envelope conformation. Centrosymmetric dimers of molecules appear to associate *via* short N···Cl interactions [3.205 (2) Å].

Related literature

For synthesis, see: Martirosyan *et al.*, (2000, 2004). For reference structural data, see: Allen *et al.* (1995). For related literature, see: Johnson (1976).



Experimental

Crystal data

$C_{25}H_{20}Cl_2N_2O_2$
M_r = 451.33
Triclinic, $P\overline{1}$
a = 9.803 (2) Å
b = 10.653 (2) Å
c = 12.364 (3) Å
α = 72.12 (3)°
β = 85.82 (3)°
γ = 63.71 (3)°
V = 1098.7 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 293 (2) K
0.35 × 0.28 × 0.22 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
5515 measured reflections
5275 independent reflections
4051 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
3 standard reflections
frequency: 180 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.131
S = 1.02
5275 reflections
360 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Data collection: *CAD-4* (Enraf–Nonius, 1988); cell refinement: *CAD-4*; data reduction: *HELENA* (Meetsma & Spek, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-NT* (Bruker, 2000); software used to prepare material for publication: *SHELXTL-NT*.

The authors are grateful to the Civilian Research and Development Foundation (CRDF) (grant No. ARB2-2701-YE-05).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2520).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1995). *International Tables for Crystallography*, Vol. C, section 9.5, pp. 685–706. Dordrecht: Kluwer Academic Publishers.
Bruker (2000). *SHELXTL-NT*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Enraf–Nonius (1988). *CAD-4 Software*. Enraf–Nonius, Delft, The Netherlands.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Martirosyan, A. O., Gasparyan, S. P., Hovhannesyan, V. E., Mndjoyan, S. L., Alexanyan, M. L., Nikishchenko, M. N. & Babayan, G. S. (2000). *Chem. Heterocycl. C*, **36**, 416–419.
Martirosyan, A. O., Hovhannesyan, V. E., Gasparyan, S. P., Karapetyan, H. A., Panosyan, G. A. & Martirosyan, V. O. (2004). *Chem. Heterocycl. C*, **40**, 1007–1008.
Meetsma, A. & Spek, A. L. (2000). *HELENA*. Utrecht University, The Netherlands.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

 doi:10.1107/S1600536807043875

supplementary materials

Acta Cryst. (2007). E**63**, o4069 [**doi:10.1107/S1600536807043875**]

cis-1-Benzoyl-2-(2-benzyloxy-5-chlorophenyl)-4-chloropyrrolidine-2-carbonitrile

R. Tamazyan, L. Matevosyan, A. Martirosyan, S. Gasparyan and R. Schinazi

Comment

The title compound, (I), (Fig. 1) has potential HIV-1 RT (reverse transcriptase) inhibition properties. These compounds belong to the non-nucleoside reverse transcriptase inhibitor (NNRTI) family.

All the bond lengths and angles in (I) are in good agreement with their reference values (Allen *et al.*, 1995), expect the C1—C20 bond length [1.491 (2) Å], which is shorter than its mean value. The arbitrarily chosen asymmetric molecule is chiral (C1 S, C4 *R* configuration) but crystal symmetry generates a racemic mixture.

Most features of the packing for (I) (Fig. 2) can be ascribed to Van der Vaals interactions. However, the interatomic distance N21···Cl31 [3.205 (2) Å] is slightly shorter than the sum of Van der Vaals radii of N and Cl atoms (3.30 Å) and might be considered as the linker in a weakly bonded centrosymmeric dimmer (Fig. 3).

We believe that shortening of the C1—C20 bond length and the short N···Cl intermolecular distance could be explained by some polarization effects caused by the triple C20 ≡N21 bond.

Experimental

The title compound was synthesized by cycloalkylation of 2-benzyloxy-5-chloro-1-cyano[2,3-dichloropropyl(phenyl)carboxamido]methylbenzene in phase-transfer catalysis condition as described by Martirosyan *et al.* (2000, 2004). The compound as synthesized is a racemate. Colourless prisms of (I) were grown from an ethanol solution.

Refinement

The H atom positions were determined from difference maps and their positions and U_{iso} values were freely reifned.

Figures

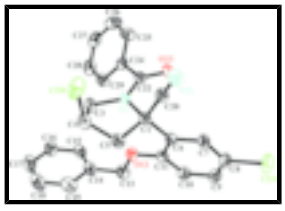


Fig. 1. The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level (H atoms omitted for clarity).

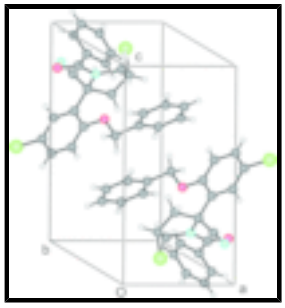


Fig. 2. Unit cell packing for (I).

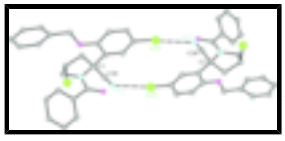


Fig. 3. A centrosymmeric dimer connected *via* N···Cl interactions. Symmetry code: (i) −*x*, 3 − *y*, 1 − *z*.

cis-1-Benzoyl-2-(2-benzyloxy-5-chlorophenyl)-4- chloropyrrolidine-2-carbonitrile

Crystal data

$C_{25}H_{20}Cl_2N_2O_2$	$Z = 2$
$M_r = 451.33$	$F_{000} = 468$
Triclinic, $P\overline{1}$	$D_x = 1.364$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 470 K
$a = 9.803$ (2) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 10.653$ (2) Å	Cell parameters from 24 reflections
$c = 12.364$ (3) Å	$\theta = 8$–19º
$\alpha = 72.12$ (3)º	$\mu = 0.32$ mm^{-1}
$\beta = 85.82$ (3)º	$T = 293$ (2) K
$\gamma = 63.71$ (3)º	Prism, colourless
$V = 1098.7$ (5) Å^3	0.35 × 0.28 × 0.22 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.022$
Radiation source: fine-focus sealed tube	$\theta_{max} = 28.0$º
Monochromator: graphite	$\theta_{min} = 1.7$º
$T = 293(2)$ K	$h = -12 \rightarrow 12$
θ/2θ scans	$k = -13 \rightarrow 14$
Absorption correction: none	$l = 0 \rightarrow 16$
5515 measured reflections	3 standard reflections
5275 independent reflections	every 180 min
4051 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.046$	All H-atom parameters refined
$wR(F^2) = 0.131$	$w = 1/[\sigma^2(F_o^2) + (0.061P)^2 + 0.5189P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
5275 reflections	$\Delta\rho_{max} = 0.29$ e Å^{-3}
360 parameters	$\Delta\rho_{min} = -0.50$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2$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}
Cl31	−0.02327 (7)	1.42050 (6)	0.34471 (6)	0.05911 (19)
Cl30	0.60429 (8)	0.90398 (7)	0.89834 (6)	0.06254 (19)
C1	0.33489 (19)	1.00696 (18)	0.69407 (15)	0.0295 (3)
N2	0.32236 (16)	0.88563 (15)	0.78477 (12)	0.0293 (3)
C3	0.4723 (2)	0.7608 (2)	0.82939 (19)	0.0362 (4)
C4	0.5823 (2)	0.8276 (2)	0.79414 (19)	0.0415 (4)
C5	0.5093 (2)	0.9450 (2)	0.68135 (18)	0.0383 (4)
C6	0.24513 (19)	1.05051 (19)	0.58226 (15)	0.0304 (4)
C7	0.1567 (2)	1.1973 (2)	0.52203 (17)	0.0344 (4)
C8	0.0817 (2)	1.2353 (2)	0.41798 (17)	0.0384 (4)
C9	0.0887 (2)	1.1298 (2)	0.37306 (19)	0.0431 (5)
C10	0.1752 (2)	0.9826 (2)	0.43219 (18)	0.0398 (4)
C11	0.2554 (2)	0.9424 (2)	0.53481 (16)	0.0341 (4)
O12	0.34923 (17)	0.80024 (14)	0.59518 (12)	0.0422 (3)
C13	0.3730 (3)	0.6863 (2)	0.5458 (2)	0.0463 (5)
C14	0.4946 (2)	0.5453 (2)	0.62109 (19)	0.0414 (5)
C15	0.4567 (2)	0.4404 (2)	0.6931 (2)	0.0433 (5)
C16	0.5679 (3)	0.3085 (3)	0.7622 (2)	0.0524 (6)
C17	0.7178 (3)	0.2813 (3)	0.7578 (3)	0.0599 (7)
C18	0.7579 (3)	0.3847 (3)	0.6866 (3)	0.0650 (8)
C19	0.6469 (3)	0.5170 (3)	0.6178 (2)	0.0533 (6)
C20	0.2847 (2)	1.1372 (2)	0.73542 (16)	0.0350 (4)
N21	0.2518 (2)	1.23812 (19)	0.76384 (17)	0.0481 (4)
C22	0.1827 (2)	0.90207 (19)	0.82009 (15)	0.0316 (4)

O23	0.07083 (15)	1.02139 (14)	0.78492 (13)	0.0446 (4)
C24	0.1688 (2)	0.7713 (2)	0.89974 (15)	0.0325 (4)
C25	0.0677 (3)	0.7920 (3)	0.9841 (2)	0.0472 (5)
C26	0.0475 (3)	0.6741 (3)	1.0559 (2)	0.0579 (6)
C27	0.1249 (3)	0.5373 (3)	1.0421 (2)	0.0537 (6)
C28	0.2208 (3)	0.5165 (2)	0.9567 (2)	0.0509 (5)
C29	0.2441 (2)	0.6330 (2)	0.88615 (19)	0.0410 (4)
H1	0.356 (3)	0.458 (2)	0.6938 (19)	0.038 (6)*
H2	0.143 (3)	1.273 (3)	0.555 (2)	0.045 (6)*
H3	0.497 (2)	0.687 (2)	0.7912 (17)	0.028 (5)*
H4	0.544 (2)	1.021 (3)	0.6607 (19)	0.039 (6)*
H5	0.679 (3)	0.757 (3)	0.787 (2)	0.049 (6)*
H6	0.474 (3)	0.721 (2)	0.907 (2)	0.040 (6)*
H7	0.533 (2)	0.896 (2)	0.6244 (19)	0.037 (5)*
H8	0.011 (3)	0.888 (3)	0.984 (2)	0.058 (7)*
H9	0.668 (3)	0.589 (3)	0.566 (2)	0.063 (8)*
H10	0.305 (3)	0.619 (2)	0.8272 (19)	0.037 (6)*
H11	0.104 (3)	0.461 (3)	1.088 (2)	0.068 (8)*
H12	0.793 (3)	0.196 (3)	0.804 (3)	0.068 (8)*
H13	0.270 (3)	0.682 (3)	0.539 (2)	0.049 (6)*
H14	0.182 (3)	0.916 (3)	0.403 (2)	0.048 (7)*
H15	0.266 (3)	0.425 (3)	0.942 (2)	0.068 (8)*
H16	0.542 (3)	0.239 (3)	0.815 (2)	0.063 (8)*
H17	0.407 (3)	0.715 (3)	0.469 (2)	0.052 (7)*
H18	−0.018 (3)	0.690 (3)	1.108 (3)	0.071 (9)*
H19	0.035 (3)	1.158 (3)	0.306 (2)	0.051 (7)*
H20	0.851 (4)	0.373 (3)	0.681 (3)	0.077 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl31	0.0534 (3)	0.0406 (3)	0.0619 (4)	−0.0149 (2)	−0.0160 (3)	0.0080 (2)
Cl30	0.0710 (4)	0.0549 (3)	0.0636 (4)	−0.0323 (3)	−0.0220 (3)	−0.0077 (3)
C1	0.0280 (8)	0.0250 (8)	0.0329 (9)	−0.0100 (6)	0.0045 (7)	−0.0088 (7)
N2	0.0265 (7)	0.0229 (6)	0.0323 (7)	−0.0076 (5)	0.0022 (6)	−0.0055 (6)
C3	0.0290 (9)	0.0270 (8)	0.0430 (11)	−0.0061 (7)	−0.0027 (8)	−0.0065 (8)
C4	0.0292 (9)	0.0368 (10)	0.0516 (12)	−0.0097 (8)	−0.0020 (8)	−0.0111 (9)
C5	0.0282 (9)	0.0382 (10)	0.0442 (11)	−0.0127 (8)	0.0065 (8)	−0.0110 (9)
C6	0.0277 (8)	0.0278 (8)	0.0325 (9)	−0.0105 (7)	0.0051 (7)	−0.0084 (7)
C7	0.0305 (9)	0.0283 (9)	0.0389 (10)	−0.0116 (7)	0.0036 (7)	−0.0054 (7)
C8	0.0307 (9)	0.0323 (9)	0.0417 (10)	−0.0115 (7)	−0.0008 (8)	−0.0003 (8)
C9	0.0356 (10)	0.0510 (12)	0.0386 (11)	−0.0195 (9)	−0.0018 (8)	−0.0069 (9)
C10	0.0399 (10)	0.0414 (10)	0.0400 (10)	−0.0187 (9)	0.0039 (8)	−0.0142 (9)
C11	0.0326 (9)	0.0315 (9)	0.0352 (9)	−0.0118 (7)	0.0064 (7)	−0.0110 (7)
O12	0.0503 (8)	0.0267 (6)	0.0417 (8)	−0.0060 (6)	−0.0035 (6)	−0.0155 (6)
C13	0.0565 (13)	0.0316 (10)	0.0500 (13)	−0.0131 (9)	0.0006 (10)	−0.0207 (9)
C14	0.0409 (10)	0.0326 (9)	0.0527 (12)	−0.0102 (8)	0.0025 (9)	−0.0249 (9)
C15	0.0390 (11)	0.0368 (10)	0.0538 (12)	−0.0117 (8)	0.0042 (9)	−0.0216 (9)

C16	0.0558 (13)	0.0375 (11)	0.0572 (14)	−0.0129 (10)	−0.0011 (11)	−0.0164 (10)
C17	0.0494 (13)	0.0444 (13)	0.0717 (17)	−0.0015 (11)	−0.0134 (12)	−0.0244 (12)
C18	0.0349 (12)	0.0729 (18)	0.094 (2)	−0.0149 (12)	0.0007 (12)	−0.0468 (17)
C19	0.0502 (13)	0.0527 (13)	0.0699 (16)	−0.0275 (11)	0.0123 (11)	−0.0304 (12)
C20	0.0355 (9)	0.0285 (9)	0.0378 (10)	−0.0133 (7)	0.0027 (7)	−0.0074 (7)
N21	0.0558 (11)	0.0355 (9)	0.0549 (11)	−0.0203 (8)	0.0063 (9)	−0.0169 (8)
C22	0.0313 (8)	0.0284 (8)	0.0341 (9)	−0.0115 (7)	0.0056 (7)	−0.0117 (7)
O23	0.0309 (7)	0.0294 (7)	0.0593 (9)	−0.0059 (5)	0.0102 (6)	−0.0081 (6)
C24	0.0332 (9)	0.0323 (9)	0.0320 (9)	−0.0153 (7)	0.0018 (7)	−0.0086 (7)
C25	0.0523 (12)	0.0499 (12)	0.0497 (12)	−0.0291 (11)	0.0201 (10)	−0.0229 (10)
C26	0.0654 (15)	0.0761 (17)	0.0443 (13)	−0.0452 (14)	0.0204 (12)	−0.0171 (12)
C27	0.0549 (13)	0.0520 (13)	0.0500 (13)	−0.0336 (11)	−0.0065 (10)	0.0076 (10)
C28	0.0491 (12)	0.0346 (11)	0.0648 (15)	−0.0206 (10)	−0.0013 (11)	−0.0054 (10)
C29	0.0418 (10)	0.0345 (10)	0.0455 (11)	−0.0163 (8)	0.0070 (9)	−0.0128 (8)

Geometric parameters (Å, °)

Cl31—C8	1.735 (2)	C13—H13	1.04 (3)
Cl30—C4	1.791 (2)	C13—H17	0.99 (3)
C1—N2	1.474 (2)	C14—C15	1.374 (3)
C1—C20	1.491 (2)	C14—C19	1.386 (3)
C1—C6	1.524 (3)	C15—C16	1.391 (3)
C1—C5	1.552 (2)	C15—H1	0.92 (2)
N2—C22	1.358 (2)	C16—C17	1.366 (4)
N2—C3	1.473 (2)	C16—H16	0.94 (3)
C3—C4	1.510 (3)	C17—C18	1.371 (4)
C3—H3	0.97 (2)	C17—H12	0.92 (3)
C3—H6	0.92 (2)	C18—C19	1.391 (4)
C4—C5	1.518 (3)	C18—H20	0.86 (3)
C4—H5	0.94 (2)	C19—H9	0.93 (3)
C5—H4	0.96 (2)	C20—N21	1.137 (3)
C5—H7	0.96 (2)	C22—O23	1.226 (2)
C6—C7	1.389 (3)	C22—C24	1.495 (3)
C6—C11	1.408 (3)	C24—C29	1.384 (3)
C7—C8	1.383 (3)	C24—C25	1.384 (3)
C7—H2	0.97 (2)	C25—C26	1.384 (3)
C8—C9	1.373 (3)	C25—H8	0.93 (3)
C9—C10	1.387 (3)	C26—C27	1.372 (4)
C9—H19	0.91 (3)	C26—H18	0.88 (3)
C10—C11	1.388 (3)	C27—C28	1.364 (4)
C10—H14	0.87 (3)	C27—H11	0.93 (3)
C11—O12	1.367 (2)	C28—C29	1.382 (3)
O12—C13	1.444 (2)	C28—H15	0.95 (3)
C13—C14	1.503 (3)	C29—H10	0.91 (2)
N2—C1—C20	109.20 (14)	O12—C13—C14	106.96 (17)
N2—C1—C6	114.02 (14)	O12—C13—H13	109.4 (13)
C20—C1—C6	109.83 (14)	C14—C13—H13	113.1 (13)
N2—C1—C5	102.64 (14)	O12—C13—H17	106.6 (14)
C20—C1—C5	108.75 (16)	C14—C13—H17	111.2 (14)

C6—C1—C5	112.09 (15)	H13—C13—H17	109 (2)
C22—N2—C3	128.35 (15)	C15—C14—C19	118.7 (2)
C22—N2—C1	119.22 (14)	C15—C14—C13	120.3 (2)
C3—N2—C1	112.36 (14)	C19—C14—C13	121.0 (2)
N2—C3—C4	103.58 (15)	C14—C15—C16	121.2 (2)
N2—C3—H3	110.8 (12)	C14—C15—H1	119.0 (14)
C4—C3—H3	107.1 (12)	C16—C15—H1	119.9 (14)
N2—C3—H6	110.3 (14)	C17—C16—C15	119.7 (3)
C4—C3—H6	113.4 (14)	C17—C16—H16	118.8 (17)
H3—C3—H6	111.4 (18)	C15—C16—H16	121.5 (17)
C3—C4—C5	103.64 (16)	C16—C17—C18	120.0 (2)
C3—C4—Cl30	111.10 (16)	C16—C17—H12	121.4 (18)
C5—C4—Cl30	111.88 (15)	C18—C17—H12	118.6 (18)
C3—C4—H5	111.3 (15)	C17—C18—C19	120.4 (2)
C5—C4—H5	112.2 (15)	C17—C18—H20	124 (2)
Cl30—C4—H5	106.8 (15)	C19—C18—H20	116 (2)
C4—C5—C1	105.15 (16)	C14—C19—C18	120.1 (3)
C4—C5—H4	113.8 (13)	C14—C19—H9	115.8 (17)
C1—C5—H4	112.5 (13)	C18—C19—H9	124.1 (17)
C4—C5—H7	106.9 (13)	N21—C20—C1	176.5 (2)
C1—C5—H7	108.0 (13)	O23—C22—N2	120.07 (17)
H4—C5—H7	110.1 (19)	O23—C22—C24	121.38 (17)
C7—C6—C11	118.25 (17)	N2—C22—C24	118.54 (15)
C7—C6—C1	121.17 (16)	C29—C24—C25	118.98 (19)
C11—C6—C1	120.52 (15)	C29—C24—C22	122.17 (17)
C8—C7—C6	120.49 (18)	C25—C24—C22	118.63 (17)
C8—C7—H2	120.0 (14)	C24—C25—C26	120.0 (2)
C6—C7—H2	119.5 (14)	C24—C25—H8	115.9 (16)
C9—C8—C7	121.24 (18)	C26—C25—H8	123.9 (16)
C9—C8—Cl31	120.22 (16)	C27—C26—C25	120.2 (2)
C7—C8—Cl31	118.54 (16)	C27—C26—H18	121.2 (19)
C8—C9—C10	119.2 (2)	C25—C26—H18	118.6 (19)
C8—C9—H19	119.1 (15)	C28—C27—C26	120.5 (2)
C10—C9—H19	121.6 (16)	C28—C27—H11	120.9 (18)
C9—C10—C11	120.3 (2)	C26—C27—H11	118.4 (18)
C9—C10—H14	119.2 (16)	C27—C28—C29	119.7 (2)
C11—C10—H14	120.4 (16)	C27—C28—H15	120.7 (18)
O12—C11—C10	123.82 (17)	C29—C28—H15	119.3 (18)
O12—C11—C6	115.78 (16)	C28—C29—C24	120.6 (2)
C10—C11—C6	120.39 (17)	C28—C29—H10	118.8 (14)
C11—O12—C13	117.91 (16)	C24—C29—H10	120.4 (14)
C20—C1—N2—C22	64.0 (2)	C7—C6—C11—C10	−1.9 (3)
C6—C1—N2—C22	−59.3 (2)	C1—C6—C11—C10	−179.10 (17)
C5—C1—N2—C22	179.22 (16)	C10—C11—O12—C13	3.8 (3)
C20—C1—N2—C3	−113.25 (17)	C6—C11—O12—C13	−175.28 (18)
C6—C1—N2—C3	123.48 (16)	C11—O12—C13—C14	172.84 (18)
C5—C1—N2—C3	2.02 (19)	O12—C13—C14—C15	105.1 (2)
C22—N2—C3—C4	−157.32 (18)	O12—C13—C14—C19	−76.2 (3)
C1—N2—C3—C4	19.6 (2)	C19—C14—C15—C16	0.4 (3)

N2—C3—C4—C5	−33.1 (2)	C13—C14—C15—C16	179.1 (2)
N2—C3—C4—Cl30	87.23 (17)	C14—C15—C16—C17	−0.8 (3)
C3—C4—C5—C1	35.1 (2)	C15—C16—C17—C18	0.9 (4)
Cl30—C4—C5—C1	−84.71 (17)	C16—C17—C18—C19	−0.6 (4)
N2—C1—C5—C4	−22.87 (19)	C15—C14—C19—C18	−0.1 (3)
C20—C1—C5—C4	92.73 (19)	C13—C14—C19—C18	−178.8 (2)
C6—C1—C5—C4	−145.63 (16)	C17—C18—C19—C14	0.2 (4)
N2—C1—C6—C7	135.27 (17)	C3—N2—C22—O23	169.57 (18)
C20—C1—C6—C7	12.3 (2)	C1—N2—C22—O23	−7.1 (3)
C5—C1—C6—C7	−108.67 (19)	C3—N2—C22—C24	−11.9 (3)
N2—C1—C6—C11	−47.6 (2)	C1—N2—C22—C24	171.39 (15)
C20—C1—C6—C11	−170.52 (16)	O23—C22—C24—C29	136.3 (2)
C5—C1—C6—C11	68.5 (2)	N2—C22—C24—C29	−42.2 (3)
C11—C6—C7—C8	−0.3 (3)	O23—C22—C24—C25	−38.3 (3)
C1—C6—C7—C8	176.90 (17)	N2—C22—C24—C25	143.23 (19)
C6—C7—C8—C9	1.9 (3)	C29—C24—C25—C26	2.4 (3)
C6—C7—C8—Cl31	−178.36 (14)	C22—C24—C25—C26	177.2 (2)
C7—C8—C9—C10	−1.3 (3)	C24—C25—C26—C27	−1.5 (4)
Cl31—C8—C9—C10	178.97 (16)	C25—C26—C27—C28	−0.9 (4)
C8—C9—C10—C11	−0.9 (3)	C26—C27—C28—C29	2.3 (4)
C9—C10—C11—O12	−176.54 (19)	C27—C28—C29—C24	−1.3 (3)
C9—C10—C11—C6	2.5 (3)	C25—C24—C29—C28	−1.0 (3)
C7—C6—C11—O12	177.23 (16)	C22—C24—C29—C28	−175.61 (19)
C1—C6—C11—O12	0.0 (2)		

Fig. 1

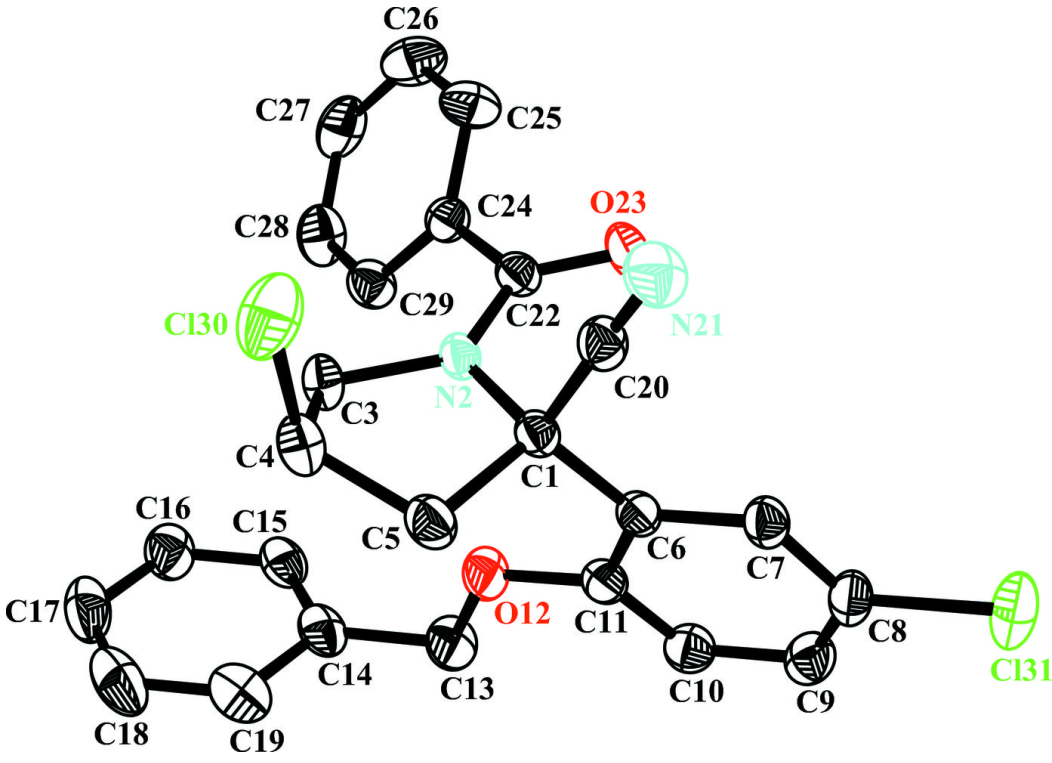

C26
C27
C25
C28
C24
O23
C29
C22
N21
Cl30
N2
C20
C3
C4
C1
C16
C15
C5
C6
C7
O12
C11
C8
C17
C14
C13
C10
C9
Cl31
C18
C19

Fig. 2

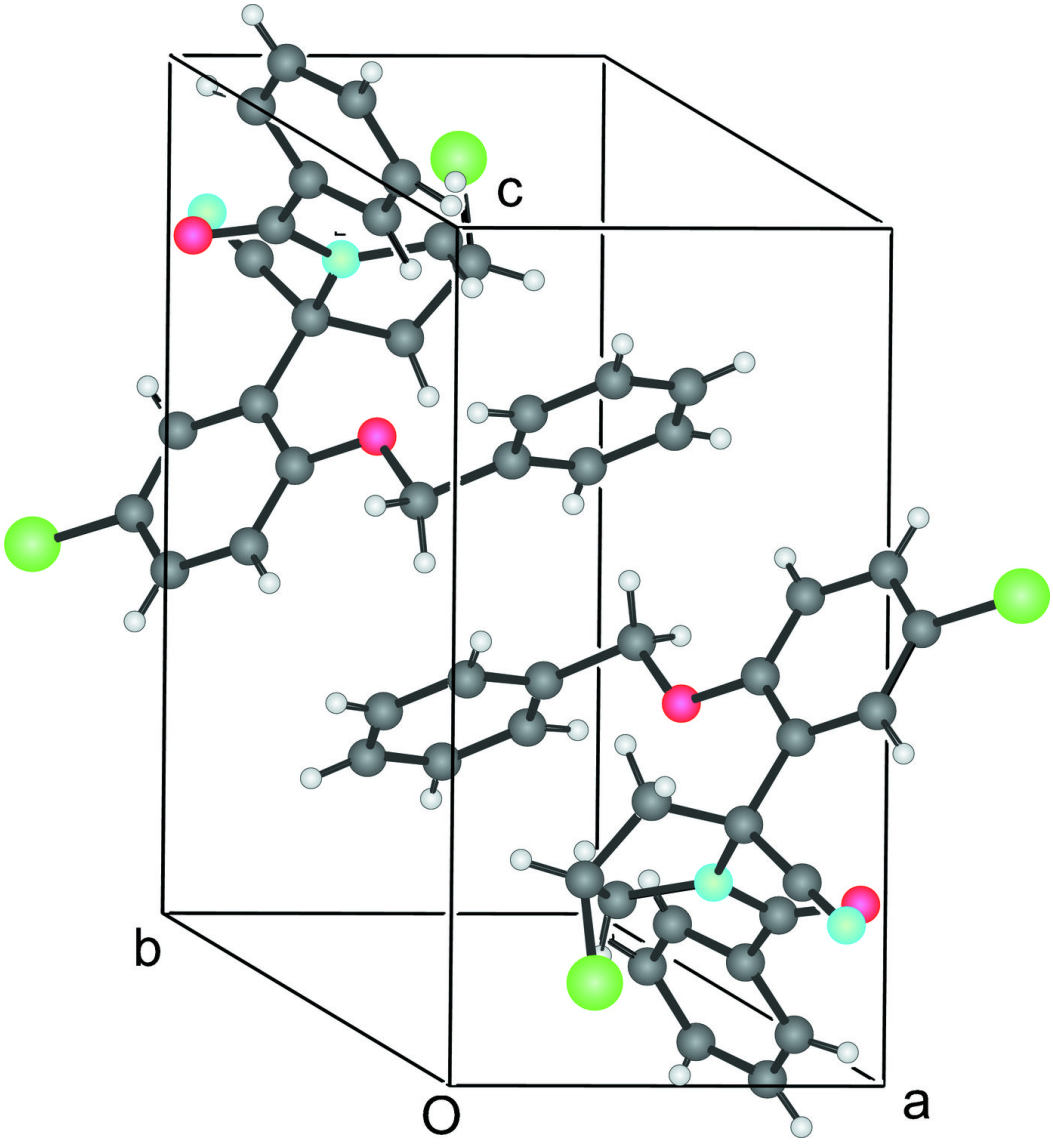


Fig. 3