

A triphenylmethanol–pyridinium chloride (1/1) adduct containing a one-dimensional ionic substructure

Richard E. Sykora and Eugene A. Cioffi*

Department of Chemistry, University of South Alabama, Mobile AL 36688-0002, USA

Correspondence e-mail: ecioffi@jaguar1.usouthal.edu

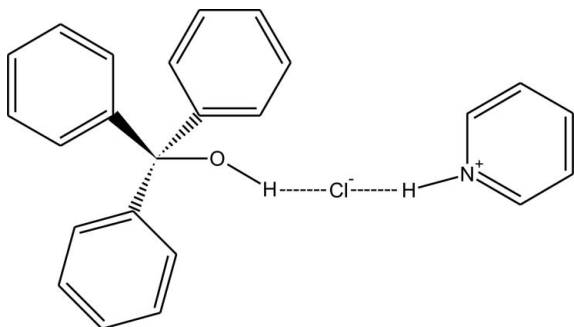
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 Key indicators: single-crystal X-ray study; $T = 290$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.036; wR factor = 0.109; data-to-parameter ratio = 14.8.

The title compound, $(\text{C}_6\text{H}_5)_3\text{COH}\cdot\text{C}_5\text{H}_6\text{N}^+\cdot\text{Cl}^-$, was surprisingly obtained as a precipitate during the dissolution (and unexpected hydrolysis reaction) of chlorotriphenylmethane with a recently opened ‘silylation-grade’ bottle of pyridine. A one-dimensional pyridinium chloride substructure is observed in the crystal structure which exhibits hydrogen bonding between the pyridinium cation and the chloride anion. The donation of the hydroxyl hydrogen to the chloride ion produces a hydrogen-bonding interaction that links the triphenylmethanol molecules to this substructure. The aromatic rings are not involved in stacking interactions.

Related literature

Triphenylmethanol (Ferguson *et al.*, 1992), as well as a number of clathrates containing it, *e.g.* with methanol (Weber *et al.*, 1989) and 1,4-dioxane (Bourne *et al.*, 1991) among others, have been studied previously. All of these compounds contain neutral solvent molecules while the title adduct contains a pyridinium chloride ionic substructure. For related literature on the preparation of the title compound, see: Chaudhary & Hernandez (1979) and Hanessian & Staub (1973).



Experimental

Crystal data

$\text{C}_{19}\text{H}_{16}\text{O}\cdot\text{C}_5\text{H}_6\text{N}^+\cdot\text{Cl}^-$
 $M_r = 375.88$
 Triclinic, $P\bar{1}$
 $a = 8.7991$ (10) Å
 $b = 8.916$ (2) Å
 $c = 14.1665$ (7) Å
 $\alpha = 88.991$ (9)°
 $\beta = 82.109$ (6)°

$\gamma = 63.998$ (11)°
 $V = 988.3$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.21$ mm⁻¹
 $T = 290$ (2) K
 $1.0 \times 0.45 \times 0.42$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
 Absorption correction: analytical (XPREP; Bruker, 2000)
 $T_{\min} = 0.909$, $T_{\max} = 0.928$
 3886 measured reflections

3632 independent reflections
 2945 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$
 3 standard reflections
 frequency: 120 min
 intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.110$
 $S = 1.03$
 3632 reflections

246 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.20$ e Å⁻³
 $\Delta\rho_{\min} = -0.19$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1B}\cdots\text{Cl1}$	0.86	2.16	3.0077 (18)	169
$\text{O1}-\text{H1A}\cdots\text{Cl1}$	0.85	2.32	3.1338 (12)	162
$\text{C3}-\text{H3A}\cdots\text{Cl1}^{\text{i}}$	0.93	2.84	3.577 (2)	137
$\text{C15}-\text{H15A}\cdots\text{Cl1}^{\text{ii}}$	0.93	2.84	3.7299 (19)	161
$\text{C1}-\text{H1C}\cdots\text{Cl1}^{\text{iii}}$	0.93	2.87	3.517 (2)	128

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

Data collection: *CAD-4-PC* (Enraf–Nonius, 1993); cell refinement: *CAD-4-PC*; data reduction: *XCAD4-PC* (Harms, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXP97* (Sheldrick, 1997); software used to prepare material for publication: *pubCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2020).

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A triphenylmethanol-pyridinium chloride (1/1) adduct containing a one-dimensional ionic substructure

R. E. Sykora and E. A. Cioffi

Comment

The bulky triphenylmethyl group is used to selectively protect primary hydroxyl groups in carbohydrates, nucleosides, *etc.* by reaction of chlorotriphenylmethane/pyridine (Chaudhary & Hernandez, 1979) with the substrate to afford a triphenylmethyl ether. This selectivity is attributed to the overall rapid kinetic rate of ether formation with a primary hydroxyl group *versus* a much slower rate of reaction with a secondary alcohol (Hanessian & Staub, 1973). The reaction is generally conducted under scrupulously anhydrous conditions, as chlorotriphenylmethane is prone to undergo rapid hydrolysis to triphenylmethanol (+HCl). The title adduct (I) was surprisingly obtained as a precipitate during the dissolution (and unexpected hydrolysis reaction) of chlorotriphenylmethane with a recently opened "silylation-grade" bottle of pyridine. In order to confirm the identity of the adduct, and to obtain detailed information on the structural features of the adduct, its crystal structure determination has been carried out.

The molecular structure of (I) along with the atomic labeling scheme is shown in Fig. 1. Fig. 1 also shows the two short hydrogen bonding interactions that are observed in the structure. One of these interactions is between the hydroxyl hydrogen of the triphenylmethanol group and the chloride anion (2.32 Å) while the second involves donation of the pyridinium hydrogen to the chloride anion (2.16 Å). The relatively short hydrogen bonding interaction (N—H \cdots Cl) between the pyridinium ring and the chloride anion as well as two longer C—H \cdots Cl interactions (2.84 to 2.87 Å) result in the formation of an ionic, one-dimensional pyridinium chloride substructure in the compound that propagates along the crystallographic *b* axis as shown in Fig. 2. The ionic substructure consists of two columns of alternating pyridinium and chloride units that are linked together through hydrogen bonding interactions resulting in one-dimensional chains. The triphenylmethanol molecules are strongly hydrogen bonded to the chloride anions of the chains through their hydroxyl H atoms and in addition a weaker C—H \cdots Cl interaction is also present. Because of the absence of hydrogen bonding or π -stacking interactions between the aromatic rings of the triphenylmethanol molecules, these molecules serve to effectively terminate two sides of the one-dimensional chains and do not make significant contributions to the intermolecular bonding in the compound. The intramolecular bond distances and angles for triphenylmethanol are typical of those in other known compounds (Bourne *et al.*, 1991; Ferguson *et al.*, 1992; Weber *et al.*, 1989).

Experimental

A flame-dried 100 ml flask containing a Teflon-coated stir bar was charged with 25 ml of "silylation-grade" pyridine under an Ar blanket. To the stirred solvent, 3.07 g (0.011 mol) of chlorotriphenylmethane was added quickly in two portions until dissolution was complete. The resultant golden-yellow solution began to very slowly cloud-up with formation of a white crystalline precipitate. Stirring (under Ar) was continued overnight, and the next day the murky suspension was allowed to settle resulting in the formation of large X-ray quality crystals of I. After decantation of the solvent from the crystalline mass, the resultant colorless crystals were carefully washed with 3 x 10 ml ice-cold Et₂O, and dried overnight under vacuum (<10.0 Pa). The crystals of I did not cleave very well and several attempts to break or cut them were unsuccessful. Therefore

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a larger than standard crystal (1 mm max. dimension) was used for this study. The X-ray beam that was used was large enough (2 mm i.d.) to ensure that the crystal was completely inside of the beam during the diffraction experiment.

Refinement

H atoms were placed in calculated positions and allowed to ride during subsequent refinement, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ and C—H distances of 0.93 Å for H atoms attached to the C atoms of the aromatic rings, $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$ and an N—H distance of 0.86 Å for the pyridinium H atom, and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ and an O—H distance of 0.85 Å for the hydroxyl H atom.

Figures



Fig. 1. The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids for non-hydrogen atoms are drawn at the 50% probability level.

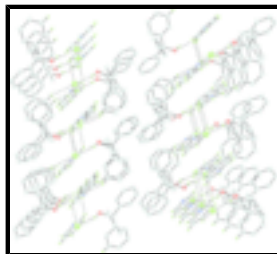


Fig. 2. A depiction of the pyridinium chloride one-dimensional chains that propagate along the *b* axis. The triphenylmethanol molecules are hydrogen bonded to the chains. Phenyl hydrogen atoms not involved in hydrogen bonding are not shown.

triphenylmethanol–pyridinium chloride (1/1)

Crystal data

$\text{C}_{19}\text{H}_{16}\text{O} \cdot \text{C}_5\text{H}_6\text{N}^+ \cdot \text{Cl}^-$

$M_r = 375.88$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 8.7991(10)$ Å

$b = 8.916(2)$ Å

$c = 14.1665(7)$ Å

$\alpha = 88.991(9)^\circ$

$\beta = 82.109(6)^\circ$

$\gamma = 63.998(11)^\circ$

$V = 988.3(3)$ Å³

$Z = 2$

$F_{000} = 396$

$D_x = 1.263$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 25 reflections

$\theta = 8.8\text{--}13.4^\circ$

$\mu = 0.21$ mm⁻¹

$T = 290(2)$ K

Prism, colorless

$1.0 \times 0.45 \times 0.42$ mm

Data collection

Enraf–Nonius CAD-4
diffractometer

$R_{\text{int}} = 0.025$

Radiation source: fine-focus sealed tube	$\theta_{\max} = 25.4^\circ$
Monochromator: graphite	$\theta_{\min} = 2.5^\circ$
$T = 290(2)$ K	$h = 0 \rightarrow 10$
$\theta/2\theta$ scans	$k = -9 \rightarrow 10$
Absorption correction: analytical (XPREP; Bruker, 2000)	$l = -16 \rightarrow 17$
$T_{\min} = 0.909$, $T_{\max} = 0.928$	3 standard reflections
3886 measured reflections	every 120 min
3632 independent reflections	intensity decay: none
2945 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.036$	$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 0.2335P]$
$wR(F^2) = 0.110$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{\max} = 0.001$
3632 reflections	$\Delta\rho_{\max} = 0.20 \text{ e } \text{\AA}^{-3}$
246 parameters	$\Delta\rho_{\min} = -0.19 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97, $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.046 (4)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.72290 (6)	0.25988 (6)	1.00968 (3)	0.05345 (17)
O1	0.59502 (15)	0.19695 (15)	0.82524 (8)	0.0452 (3)
H1A	0.6441	0.2211	0.8661	0.068*
N1	0.7595 (2)	0.5724 (2)	1.04769 (14)	0.0660 (5)
H1B	0.7378	0.4879	1.0436	0.079*
C1	0.6935 (3)	0.6976 (4)	0.99146 (18)	0.0767 (7)

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H1C	0.6232	0.6947	0.9489	0.092*
C2	0.7295 (3)	0.8321 (3)	0.99634 (19)	0.0759 (7)
H2A	0.6839	0.9213	0.9573	0.091*
C3	0.8318 (3)	0.8327 (3)	1.05850 (19)	0.0707 (6)
H3A	0.8585	0.9222	1.0620	0.085*
C4	0.8959 (3)	0.7035 (3)	1.11591 (17)	0.0725 (6)
H4A	0.9660	0.7045	1.1592	0.087*
C5	0.8578 (3)	0.5731 (3)	1.10998 (17)	0.0687 (6)
H5A	0.9006	0.4843	1.1496	0.082*
C6	0.6764 (2)	0.20135 (19)	0.73120 (11)	0.0358 (3)
C7	0.54903 (19)	0.20884 (18)	0.66523 (11)	0.0373 (4)
C8	0.4547 (2)	0.1192 (2)	0.68622 (14)	0.0493 (4)
H8A	0.4662	0.0589	0.7412	0.059*
C9	0.3431 (2)	0.1187 (3)	0.62596 (17)	0.0629 (6)
H9A	0.2810	0.0576	0.6406	0.076*
C10	0.3241 (3)	0.2076 (3)	0.54522 (16)	0.0633 (6)
H10A	0.2482	0.2081	0.5054	0.076*
C11	0.4171 (3)	0.2961 (3)	0.52316 (15)	0.0603 (5)
H11A	0.4052	0.3555	0.4678	0.072*
C12	0.5287 (2)	0.2974 (2)	0.58286 (13)	0.0488 (4)
H12A	0.5907	0.3585	0.5675	0.059*
C13	0.84447 (19)	0.04172 (18)	0.70852 (11)	0.0354 (3)
C14	0.9482 (2)	-0.0243 (2)	0.77860 (12)	0.0446 (4)
H14A	0.9135	0.0272	0.8394	0.054*
C15	1.1025 (2)	-0.1654 (2)	0.75948 (14)	0.0536 (5)
H15A	1.1708	-0.2073	0.8073	0.064*
C16	1.1556 (2)	-0.2441 (2)	0.67028 (15)	0.0541 (5)
H16A	1.2589	-0.3395	0.6576	0.065*
C17	1.0543 (2)	-0.1803 (2)	0.60014 (13)	0.0513 (4)
H17A	1.0893	-0.2328	0.5396	0.062*
C18	0.9003 (2)	-0.0383 (2)	0.61877 (12)	0.0421 (4)
H18A	0.8335	0.0040	0.5704	0.051*
C19	0.70802 (19)	0.35789 (18)	0.72392 (11)	0.0352 (3)
C20	0.5804 (2)	0.5085 (2)	0.76513 (13)	0.0469 (4)
H20A	0.4791	0.5122	0.7971	0.056*
C21	0.6024 (3)	0.6528 (2)	0.75918 (14)	0.0565 (5)
H21A	0.5153	0.7529	0.7866	0.068*
C22	0.7521 (3)	0.6495 (2)	0.71307 (14)	0.0558 (5)
H22A	0.7671	0.7465	0.7101	0.067*
C23	0.8789 (2)	0.5022 (2)	0.67159 (14)	0.0537 (5)
H23A	0.9799	0.4993	0.6398	0.064*
C24	0.8567 (2)	0.3564 (2)	0.67694 (12)	0.0439 (4)
H24A	0.9433	0.2570	0.6484	0.053*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0683 (3)	0.0509 (3)	0.0517 (3)	-0.0344 (2)	-0.0136 (2)	-0.00025 (19)

O1	0.0513 (7)	0.0531 (7)	0.0380 (6)	-0.0306 (6)	-0.0008 (5)	-0.0001 (5)
N1	0.0725 (12)	0.0605 (11)	0.0751 (12)	-0.0459 (10)	0.0188 (10)	-0.0198 (9)
C1	0.0649 (14)	0.113 (2)	0.0685 (14)	-0.0530 (14)	-0.0110 (11)	-0.0014 (14)
C2	0.0615 (13)	0.0692 (14)	0.0955 (18)	-0.0284 (12)	-0.0105 (12)	0.0247 (13)
C3	0.0693 (14)	0.0531 (12)	0.0984 (17)	-0.0371 (11)	-0.0028 (13)	-0.0057 (11)
C4	0.0798 (15)	0.0804 (16)	0.0739 (14)	-0.0481 (13)	-0.0188 (12)	0.0011 (12)
C5	0.0732 (14)	0.0571 (12)	0.0722 (14)	-0.0284 (11)	-0.0004 (12)	0.0083 (10)
C6	0.0398 (8)	0.0356 (8)	0.0356 (8)	-0.0203 (7)	-0.0042 (6)	0.0004 (6)
C7	0.0347 (8)	0.0323 (8)	0.0448 (9)	-0.0146 (6)	-0.0055 (7)	-0.0040 (6)
C8	0.0451 (10)	0.0472 (10)	0.0615 (11)	-0.0256 (8)	-0.0080 (8)	0.0024 (8)
C9	0.0510 (11)	0.0626 (12)	0.0888 (15)	-0.0359 (10)	-0.0135 (10)	-0.0072 (11)
C10	0.0519 (11)	0.0657 (13)	0.0762 (14)	-0.0241 (10)	-0.0263 (10)	-0.0107 (11)
C11	0.0672 (13)	0.0625 (12)	0.0573 (11)	-0.0291 (10)	-0.0263 (10)	0.0043 (9)
C12	0.0548 (10)	0.0501 (10)	0.0507 (10)	-0.0291 (9)	-0.0157 (8)	0.0048 (8)
C13	0.0392 (8)	0.0330 (8)	0.0404 (8)	-0.0216 (7)	-0.0070 (6)	0.0047 (6)
C14	0.0514 (10)	0.0428 (9)	0.0422 (9)	-0.0219 (8)	-0.0112 (7)	0.0028 (7)
C15	0.0530 (11)	0.0481 (10)	0.0585 (11)	-0.0180 (9)	-0.0209 (9)	0.0114 (8)
C16	0.0463 (10)	0.0408 (9)	0.0669 (12)	-0.0116 (8)	-0.0084 (9)	0.0038 (8)
C17	0.0512 (10)	0.0472 (10)	0.0496 (10)	-0.0176 (8)	-0.0020 (8)	-0.0048 (8)
C18	0.0457 (9)	0.0418 (9)	0.0397 (8)	-0.0192 (7)	-0.0090 (7)	0.0031 (7)
C19	0.0404 (8)	0.0343 (8)	0.0353 (8)	-0.0192 (7)	-0.0107 (6)	0.0025 (6)
C20	0.0466 (9)	0.0401 (9)	0.0535 (10)	-0.0198 (8)	-0.0031 (8)	-0.0002 (7)
C21	0.0691 (12)	0.0348 (9)	0.0617 (11)	-0.0199 (9)	-0.0071 (10)	-0.0027 (8)
C22	0.0742 (13)	0.0427 (10)	0.0645 (12)	-0.0364 (10)	-0.0177 (10)	0.0069 (8)
C23	0.0550 (11)	0.0529 (11)	0.0653 (12)	-0.0351 (9)	-0.0079 (9)	0.0084 (9)
C24	0.0444 (9)	0.0387 (9)	0.0518 (10)	-0.0215 (7)	-0.0054 (7)	0.0006 (7)

Geometric parameters (Å, °)

O1—C6	1.4316 (18)	C11—C12	1.386 (2)
O1—H1A	0.8500	C11—H11A	0.9300
N1—C5	1.320 (3)	C12—H12A	0.9300
N1—C1	1.321 (3)	C13—C18	1.386 (2)
N1—H1B	0.8600	C13—C14	1.386 (2)
C1—C2	1.373 (4)	C14—C15	1.383 (2)
C1—H1C	0.9300	C14—H14A	0.9300
C2—C3	1.344 (3)	C15—C16	1.374 (3)
C2—H2A	0.9300	C15—H15A	0.9300
C3—C4	1.352 (3)	C16—C17	1.373 (3)
C3—H3A	0.9300	C16—H16A	0.9300
C4—C5	1.351 (3)	C17—C18	1.385 (2)
C4—H4A	0.9300	C17—H17A	0.9300
C5—H5A	0.9300	C18—H18A	0.9300
C6—C7	1.534 (2)	C19—C24	1.378 (2)
C6—C13	1.535 (2)	C19—C20	1.389 (2)
C6—C19	1.538 (2)	C20—C21	1.382 (2)
C7—C12	1.385 (2)	C20—H20A	0.9300
C7—C8	1.386 (2)	C21—C22	1.376 (3)
C8—C9	1.388 (3)	C21—H21A	0.9300

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C8—H8A	0.9300	C22—C23	1.370 (3)
C9—C10	1.367 (3)	C22—H22A	0.9300
C9—H9A	0.9300	C23—C24	1.396 (2)
C10—C11	1.369 (3)	C23—H23A	0.9300
C10—H10A	0.9300	C24—H24A	0.9300
C6—O1—H1A	109.5	C7—C12—C11	120.72 (17)
C5—N1—C1	122.00 (19)	C7—C12—H12A	119.6
C5—N1—H1B	119.0	C11—C12—H12A	119.6
C1—N1—H1B	119.0	C18—C13—C14	117.87 (15)
N1—C1—C2	119.5 (2)	C18—C13—C6	122.32 (14)
N1—C1—H1C	120.2	C14—C13—C6	119.79 (14)
C2—C1—H1C	120.2	C15—C14—C13	121.05 (16)
C3—C2—C1	118.9 (2)	C15—C14—H14A	119.5
C3—C2—H2A	120.6	C13—C14—H14A	119.5
C1—C2—H2A	120.6	C16—C15—C14	120.40 (17)
C2—C3—C4	120.3 (2)	C16—C15—H15A	119.8
C2—C3—H3A	119.9	C14—C15—H15A	119.8
C4—C3—H3A	119.9	C17—C16—C15	119.25 (17)
C5—C4—C3	119.6 (2)	C17—C16—H16A	120.4
C5—C4—H4A	120.2	C15—C16—H16A	120.4
C3—C4—H4A	120.2	C16—C17—C18	120.54 (17)
N1—C5—C4	119.7 (2)	C16—C17—H17A	119.7
N1—C5—H5A	120.2	C18—C17—H17A	119.7
C4—C5—H5A	120.2	C17—C18—C13	120.89 (16)
O1—C6—C7	104.72 (12)	C17—C18—H18A	119.6
O1—C6—C13	109.70 (12)	C13—C18—H18A	119.6
C7—C6—C13	110.56 (12)	C24—C19—C20	118.28 (14)
O1—C6—C19	109.66 (12)	C24—C19—C6	122.95 (14)
C7—C6—C19	110.93 (12)	C20—C19—C6	118.76 (14)
C13—C6—C19	111.08 (12)	C21—C20—C19	120.75 (17)
C12—C7—C8	118.24 (15)	C21—C20—H20A	119.6
C12—C7—C6	122.40 (14)	C19—C20—H20A	119.6
C8—C7—C6	119.32 (15)	C22—C21—C20	120.48 (17)
C7—C8—C9	120.60 (18)	C22—C21—H21A	119.8
C7—C8—H8A	119.7	C20—C21—H21A	119.8
C9—C8—H8A	119.7	C23—C22—C21	119.50 (16)
C10—C9—C8	120.33 (18)	C23—C22—H22A	120.3
C10—C9—H9A	119.8	C21—C22—H22A	120.3
C8—C9—H9A	119.8	C22—C23—C24	120.16 (17)
C9—C10—C11	119.80 (18)	C22—C23—H23A	119.9
C9—C10—H10A	120.1	C24—C23—H23A	119.9
C11—C10—H10A	120.1	C19—C24—C23	120.83 (16)
C10—C11—C12	120.30 (19)	C19—C24—H24A	119.6
C10—C11—H11A	119.8	C23—C24—H24A	119.6
C12—C11—H11A	119.8		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
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N1—H1B···C11	0.86	2.16	3.0077 (18)	169
O1—H1A···C11	0.85	2.32	3.1338 (12)	162
C3—H3A···C11 ⁱ	0.93	2.84	3.577 (2)	137
C15—H15A···C11 ⁱⁱ	0.93	2.84	3.7299 (19)	161
C1—H1C···C11 ⁱⁱⁱ	0.93	2.87	3.517 (2)	128

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

Fig. 1

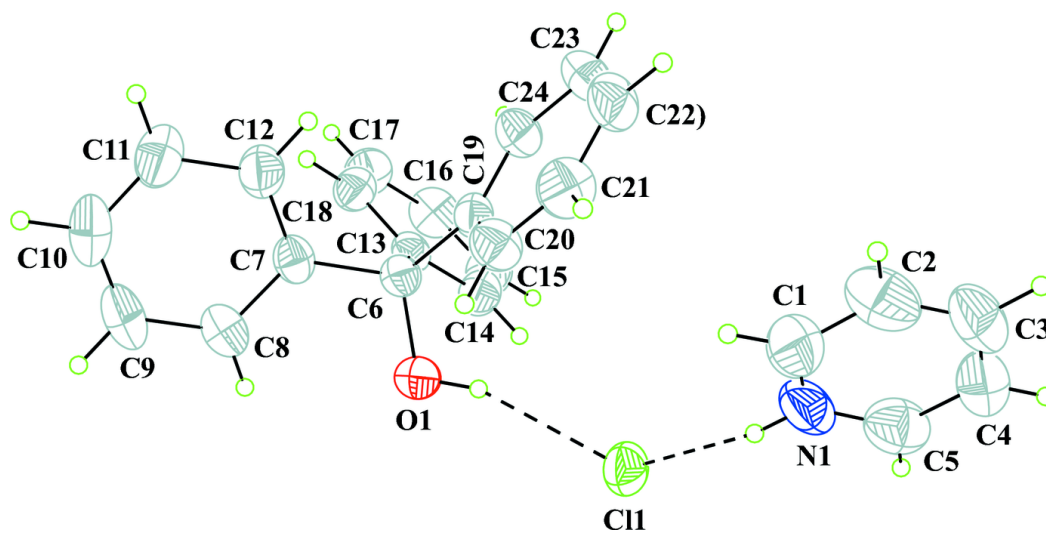


Fig. 2

