

(2*R*,5*S*)-5-Benzyl-2,3-dimethyl-4-oxo-2-phenylimidazolidin-1-ium chloride

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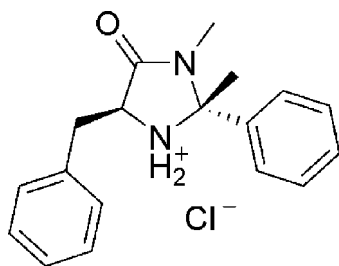
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.030; wR factor = 0.073; data-to-parameter ratio = 16.8.

The title hydrochloride salt, $\text{C}_{18}\text{H}_{21}\text{N}_2\text{O}^+\cdot\text{Cl}^-$, is an imidazolidinone catalyst, which was derived from L-phenylalanine through cyclization with acetophenone. The imidazolidinone compound has a five-membered heterocyclic ring including two chiral centres. The imidazolidinone ring displays an envelope conformation, with the flap protonated N atom lying 0.497 (3) Å above the mean plane of the remaining four atoms. In the crystal structure, one-dimensional supramolecular chains parallel to the crystallographic 2_1 screw axis are formed by $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds involving the NH_2^+ and Cl^- groups. Intramolecular $\text{N}-\text{H}\cdots\text{Cl}$ interactions are also present.

Related literature

For chiral secondary amine catalysts based on the imidazolidinone architecture, see: Ouellet *et al.* (2007). For Michael additions of aldehydes to enones with a MacMillan imidazolidinone catalyst, see: Hechavarria Fonseca & List (2004).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{21}\text{N}_2\text{O}^+\cdot\text{Cl}^-$
 $M_r = 316.83$
 Monoclinic, $P2_1$
 $a = 10.5797$ (11) Å
 $b = 7.5876$ (7) Å
 $c = 10.8741$ (12) Å
 $\beta = 105.516$ (3)°
 $V = 841.10$ (15) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.23$ mm⁻¹
 $T = 296$ K
 $0.34 \times 0.26 \times 0.11$ mm

Data collection

Rigaku R-Axis RAPID diffractometer
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.920$, $T_{\max} = 0.975$
 8064 measured reflections
 3371 independent reflections
 2933 reflections with $F^2 > 2\sigma(F^2)$
 $R_{\text{int}} = 0.024$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.073$
 $S = 1.00$
 3371 reflections
 201 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.32$ e Å⁻³
 $\Delta\rho_{\min} = -0.30$ e Å⁻³
 Absolute structure: Flack (1983), 1323 Friedel pairs
 Flack parameter: 0.03 (4)

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N2}-\text{H201}\cdots\text{Cl1}$	0.86	2.30	3.1170 (14)	160
$\text{N2}-\text{H202}\cdots\text{Cl1}^i$	0.86	2.24	3.0999 (14)	174

Symmetry code: (i) $-x + 2, y + \frac{1}{2}, -z + 1$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *CRYSTALS*.

We thank Professor Jian-Ming Gu (Zhejiang University, China), for his help.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2221).

References

- Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
- Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
- Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Hechavarria Fonseca, M. T. & List, B. (2004). *Angew. Chem. Int. Ed.* **43**, 3958–3960.
- Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
- Ouellet, S. G., Walji, A. B. & Macmillan, D. W. C. (2007). *Acc. Chem. Res.* **40**, 1327–1339.
- Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
- Rigaku/MS (2004). *CrystalStructure*. Rigaku/MS, The Woodlands, Texas, USA.

supplementary materials

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Comment

Ten years ago, MacMillan and his laboratory developed chiral secondary amine catalysts based on the imidazolidinone architecture, which has led to the development of over 30 different enantioselective transformations for asymmetric synthesis (Ouellet *et al.*, 2007). In recent years, Michael additions of aldehydes to enones with a MacMillan imidazolidinone catalyst have been reported (Hechavarria Fonseca & List, 2004). The title compound, prepared as a kind of organocatalyst for use in the asymmetric Michael addition of aldehydes to enones, was synthesized from *L*-phenylalanine. The crystal structure and absolute configuration of the title compound are reported in this article.

The compound consists of an ionic pair, a protonated ammonium cation and a Cl⁻ anion (Fig. 1). The chiral atom C1 has the expected *S* configuration, while the other chiral atom C3 was determined to be in a *R* configuration. The C1/C2/C3/N1 atoms of the imidazolidinone ring are almost coplanar. The distance of atom N2 to the C1/C2/C3/N1 mean plane is 0.497 (3) Å, while the distance of atom C12 of the benzyl group to the plane is 0.920 (4) Å. In the crystal structure of the title salt, one-dimensional supramolecular chains are formed, by intra- and inter-molecular N—H...Cl hydrogen bonds (Fig. 2).

Experimental

To a stirred solution of *L*-phenylalanine (3.87 g, 24 mmol) in dry methanol (50 ml) was added thionyl chloride (2.72 ml, 37.5 mmol). After refluxed for 48 h., the solution was concentrated under vacuum and *L*-phenylalanine methyl ester dichloride crystallized from methanol to give white crystals. To an ethanolic MeNH₂ solution (8 *M*, 6 ml) was added *L*-phenylalanine methyl ester dihydrochloride (2.41 g, 10 mmol). The solution was stirred at room temperature for 24 h, and then the solvent removed under reduced pressure. To this residue was added MeOH (80 ml), acetophenone (3 g, 25 mmol), and a catalytic amount of *p*-toluenesulfonic acid (30 mg, 0.16 mmol). The resulting solution was refluxed for 24 h and further stirred at room temperature for 2 h. The mixture was subsequently concentrated under reduced pressure, giving the crude product. The resolution of the racemic compounds was by means of column chromatography with methyl and petroleum ether (1:4). The residue was taken up in ethylether and a solution of HCl-dioxane (4.0 *M*) was added to the precipitate. Suitable crystals were obtained by slow evaporation of a methanol solution of the crude at room temperature.

Refinement

All H atoms were placed in calculated positions, with C—H = 0.93 (aromatic CH), 0.96 (methyl CH₃), 0.97 (methylene CH₂) or 0.98 Å (methine CH), and N—H = 0.86 Å. Displacement parameters for H atoms were calculated as $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier atom})$.

Figures

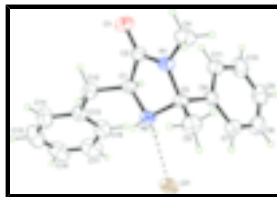


Fig. 1. The asymmetric unit of the title compound, with the atomic labelling scheme. Displacement ellipsoids are drawn at the 40% probability level.

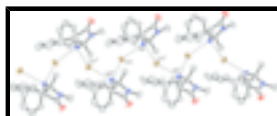


Fig. 2. A part of the crystal structure of the title salt, with hydrogen bonds represented with dashed lines.

(2*R*,5*S*)-5-Benzyl-2,3-dimethyl-4-oxo-2-phenylimidazolidin-1-ium chloride

Crystal data

$C_{18}H_{21}N_2O^+ \cdot Cl^-$

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Monoclinic, $P2_1$

Hall symbol: P 2yb

$a = 10.5797$ (11) Å

$b = 7.5876$ (7) Å

$c = 10.8741$ (12) Å

$\beta = 105.516$ (3)°

$V = 841.10$ (15) Å³

$Z = 2$

$F_{000} = 336.00$

$D_x = 1.251$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71075$ Å

Cell parameters from 5642 reflections

$\theta = 3.1$ – 27.4 °

$\mu = 0.23$ mm⁻¹

$T = 296$ K

Needle, colourless

$0.34 \times 0.26 \times 0.11$ mm

Data collection

Rigaku R-Axis RAPID
diffractometer

Detector resolution: 10.00 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(ABSCOR; Higashi, 1995)

$T_{\min} = 0.920$, $T_{\max} = 0.975$

8064 measured reflections

3371 independent reflections

2933 reflections with $F^2 > 2\sigma(F^2)$

$R_{\text{int}} = 0.024$

$\theta_{\max} = 27.4$ °

$h = -13 \rightarrow 13$

$k = -8 \rightarrow 9$

$l = -14 \rightarrow 14$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.030$

$wR(F^2) = 0.073$

$S = 1.00$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.32$ e Å⁻³

$\Delta\rho_{\min} = -0.30$ e Å⁻³

Extinction correction: CRYSTALS (Betteridge et al., 2003)

3371 reflections

Extinction coefficient: 148 (16)

201 parameters

Absolute structure: Flack (1983), 1323 Friedel pairs

H-atom parameters constrained

Flack parameter: 0.03 (4)

$$w = 1/[0.0003F_o^2 + 1.04\sigma(F_o^2)]/(4F_o^2)$$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.93865 (4)	0.37096 (8)	0.38333 (4)	0.04566 (11)
O1	0.55546 (12)	0.94486 (19)	0.53994 (12)	0.0482 (3)
N1	0.66144 (12)	0.93555 (17)	0.38197 (12)	0.0328 (3)
N2	0.80291 (11)	0.70805 (17)	0.45120 (12)	0.0282 (3)
C1	0.70374 (14)	0.7044 (2)	0.52767 (14)	0.0300 (4)
C2	0.63026 (12)	0.8761 (2)	0.48651 (13)	0.0329 (3)
C3	0.73966 (14)	0.8101 (2)	0.33039 (14)	0.0299 (3)
C4	0.6042 (2)	1.0933 (2)	0.3114 (2)	0.0506 (5)
C5	0.84477 (16)	0.9014 (2)	0.28214 (17)	0.0433 (5)
C6	0.65243 (14)	0.6841 (2)	0.23338 (14)	0.0308 (4)
C7	0.70586 (18)	0.5811 (2)	0.15399 (17)	0.0424 (5)
C8	0.6288 (2)	0.4612 (2)	0.07068 (18)	0.0539 (6)
C9	0.4987 (2)	0.4414 (2)	0.06476 (19)	0.0538 (5)
C10	0.44421 (19)	0.5420 (2)	0.14153 (19)	0.0506 (5)
C11	0.51948 (16)	0.6636 (2)	0.22594 (16)	0.0395 (4)
C12	0.76199 (17)	0.6939 (2)	0.67155 (14)	0.0353 (4)
C13	0.80340 (14)	0.5137 (2)	0.72774 (17)	0.0347 (4)
C14	0.8565 (2)	0.4999 (2)	0.8593 (2)	0.0530 (5)
C15	0.8969 (2)	0.3397 (3)	0.9158 (2)	0.0684 (7)
C16	0.8867 (2)	0.1899 (3)	0.8436 (2)	0.0618 (6)
C17	0.8346 (2)	0.2009 (2)	0.7136 (2)	0.0582 (6)
C18	0.79285 (17)	0.3619 (2)	0.65706 (18)	0.0467 (4)
H1	0.6438	0.6050	0.4996	0.036*
H7	0.7941	0.5929	0.1569	0.051*
H8	0.6658	0.3932	0.0182	0.065*
H9	0.4478	0.3602	0.0089	0.065*
H10	0.3557	0.5289	0.1373	0.061*
H11	0.4811	0.7314	0.2775	0.047*
H14	0.8647	0.6005	0.9097	0.064*
H15	0.9314	0.3332	1.0038	0.082*
H16	0.9148	0.0821	0.8819	0.074*
H17	0.8274	0.1001	0.6636	0.070*
H18	0.7568	0.3672	0.5692	0.056*
H41	0.5471	1.1496	0.3547	0.061*
H42	0.5549	1.0606	0.2269	0.061*
H43	0.6729	1.1732	0.3063	0.061*
H51	0.8041	0.9742	0.2103	0.052*
H52	0.8988	0.8145	0.2568	0.052*
H53	0.8980	0.9732	0.3489	0.052*
H121	0.6969	0.7390	0.7115	0.042*

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H122	0.8388	0.7692	0.6932	0.042*
H201	0.8213	0.6026	0.4327	0.034*
H202	0.8734	0.7600	0.4934	0.034*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0397 (2)	0.0372 (2)	0.0553 (2)	0.0126 (2)	0.00437 (17)	-0.0024 (2)
O1	0.0443 (6)	0.0550 (8)	0.0494 (7)	0.0169 (5)	0.0195 (5)	-0.0050 (5)
N1	0.0349 (6)	0.0262 (6)	0.0368 (7)	0.0080 (5)	0.0084 (5)	0.0012 (5)
N2	0.0240 (5)	0.0249 (7)	0.0344 (6)	0.0015 (5)	0.0056 (5)	-0.0035 (5)
C1	0.0271 (7)	0.0279 (8)	0.0354 (8)	-0.0013 (6)	0.0091 (6)	-0.0020 (6)
C2	0.0269 (6)	0.0344 (8)	0.0357 (8)	0.0021 (8)	0.0056 (5)	-0.0057 (8)
C3	0.0289 (7)	0.0261 (8)	0.0340 (8)	0.0033 (6)	0.0074 (6)	0.0013 (6)
C4	0.0570 (11)	0.0356 (10)	0.0565 (12)	0.0167 (9)	0.0107 (9)	0.0075 (8)
C5	0.0408 (8)	0.0405 (11)	0.0521 (10)	-0.0058 (8)	0.0188 (8)	0.0026 (8)
C6	0.0337 (7)	0.0297 (8)	0.0276 (7)	0.0034 (7)	0.0058 (6)	0.0025 (6)
C7	0.0430 (9)	0.0445 (10)	0.0392 (9)	0.0087 (8)	0.0100 (8)	-0.0045 (8)
C8	0.0678 (12)	0.0526 (12)	0.0392 (10)	0.0090 (11)	0.0109 (9)	-0.0113 (9)
C9	0.0638 (12)	0.0493 (11)	0.0408 (10)	-0.0109 (10)	0.0009 (9)	-0.0103 (8)
C10	0.0413 (9)	0.0615 (13)	0.0448 (11)	-0.0121 (9)	0.0042 (8)	-0.0023 (9)
C11	0.0337 (8)	0.0477 (11)	0.0376 (9)	-0.0032 (8)	0.0103 (7)	-0.0031 (8)
C12	0.0388 (8)	0.0333 (9)	0.0342 (8)	-0.0027 (7)	0.0104 (7)	-0.0009 (7)
C13	0.0311 (8)	0.0350 (9)	0.0384 (9)	-0.0029 (7)	0.0100 (7)	0.0036 (7)
C14	0.0629 (12)	0.0495 (12)	0.0408 (10)	-0.0015 (10)	0.0037 (9)	0.0017 (9)
C15	0.0731 (13)	0.0708 (19)	0.0514 (12)	0.0022 (13)	-0.0005 (10)	0.0230 (12)
C16	0.0491 (11)	0.0464 (13)	0.0818 (17)	-0.0030 (10)	0.0035 (11)	0.0232 (12)
C17	0.0566 (11)	0.0342 (11)	0.0807 (15)	-0.0043 (9)	0.0129 (11)	0.0047 (10)
C18	0.0484 (9)	0.0387 (9)	0.0496 (10)	-0.0024 (10)	0.0072 (7)	0.0003 (10)

Geometric parameters (\AA , $^\circ$)

O1—C2	1.218 (2)	C17—C18	1.385 (2)
N1—C2	1.344 (2)	N2—H201	0.860
N1—C3	1.467 (2)	N2—H202	0.860
N1—C4	1.463 (2)	C1—H1	0.980
N2—C1	1.503 (2)	C4—H41	0.960
N2—C3	1.5176 (19)	C4—H42	0.960
C1—C2	1.521 (2)	C4—H43	0.960
C1—C12	1.523 (2)	C5—H51	0.960
C3—C5	1.518 (2)	C5—H52	0.960
C3—C6	1.536 (2)	C5—H53	0.960
C6—C7	1.392 (2)	C7—H7	0.930
C6—C11	1.396 (2)	C8—H8	0.930
C7—C8	1.385 (2)	C9—H9	0.930
C8—C9	1.368 (3)	C10—H10	0.930
C9—C10	1.367 (3)	C11—H11	0.930
C10—C11	1.392 (2)	C12—H121	0.970
C12—C13	1.514 (2)	C12—H122	0.970

C13—C14	1.394 (2)	C14—H14	0.930
C13—C18	1.373 (2)	C15—H15	0.930
C14—C15	1.378 (3)	C16—H16	0.930
C15—C16	1.369 (3)	C17—H17	0.930
C16—C17	1.375 (3)	C18—H18	0.930
C2—N1—C3	113.37 (13)	C2—C1—H1	109.3
C2—N1—C4	123.90 (16)	C12—C1—H1	109.3
C3—N1—C4	121.80 (15)	N1—C4—H41	109.5
C1—N2—C3	106.07 (11)	N1—C4—H42	109.5
N2—C1—C2	101.48 (12)	N1—C4—H43	109.5
N2—C1—C12	114.76 (12)	H41—C4—H42	109.5
C2—C1—C12	112.44 (13)	H41—C4—H43	109.5
O1—C2—N1	126.71 (16)	H42—C4—H43	109.5
O1—C2—C1	124.95 (15)	C3—C5—H51	109.5
N1—C2—C1	108.34 (14)	C3—C5—H52	109.5
N1—C3—N2	99.40 (12)	C3—C5—H53	109.5
N1—C3—C5	112.12 (13)	H51—C5—H52	109.5
N1—C3—C6	111.70 (12)	H51—C5—H53	109.5
N2—C3—C5	109.75 (11)	H52—C5—H53	109.5
N2—C3—C6	108.76 (12)	C6—C7—H7	119.7
C5—C3—C6	114.07 (14)	C8—C7—H7	119.7
C3—C6—C7	120.44 (14)	C7—C8—H8	119.6
C3—C6—C11	121.35 (15)	C9—C8—H8	119.6
C7—C6—C11	118.15 (14)	C8—C9—H9	120.2
C6—C7—C8	120.59 (18)	C10—C9—H9	120.2
C7—C8—C9	120.8 (2)	C9—C10—H10	119.6
C8—C9—C10	119.57 (18)	C11—C10—H10	119.6
C9—C10—C11	120.81 (18)	C6—C11—H11	119.9
C6—C11—C10	120.13 (17)	C10—C11—H11	119.9
C1—C12—C13	117.13 (14)	C1—C12—H121	107.5
C12—C13—C14	118.38 (16)	C1—C12—H122	107.5
C12—C13—C18	124.10 (15)	C13—C12—H121	107.5
C14—C13—C18	117.52 (17)	C13—C12—H122	107.5
C13—C14—C15	121.02 (19)	H121—C12—H122	109.5
C14—C15—C16	120.6 (2)	C13—C14—H14	119.5
C15—C16—C17	119.2 (2)	C15—C14—H14	119.5
C16—C17—C18	120.2 (2)	C14—C15—H15	119.7
C13—C18—C17	121.50 (17)	C16—C15—H15	119.7
C1—N2—H201	110.3	C15—C16—H16	120.4
C1—N2—H202	110.3	C17—C16—H16	120.4
C3—N2—H201	110.3	C16—C17—H17	119.9
C3—N2—H202	110.3	C18—C17—H17	119.9
H201—N2—H202	109.5	C13—C18—H18	119.2
N2—C1—H1	109.3	C17—C18—H18	119.2
C2—N1—C3—N2	-25.51 (14)	N2—C3—C6—C7	-85.03 (19)
C2—N1—C3—C5	-141.42 (12)	N2—C3—C6—C11	92.14 (17)
C2—N1—C3—C6	89.12 (15)	C5—C3—C6—C7	37.8 (2)
C3—N1—C2—O1	-171.77 (14)	C5—C3—C6—C11	-145.00 (16)

supplementary materials

C3—N1—C2—C1	7.66 (16)	C3—C6—C7—C8	176.89 (16)
C4—N1—C2—O1	-2.7 (2)	C3—C6—C11—C10	-176.77 (16)
C4—N1—C2—C1	176.74 (13)	C7—C6—C11—C10	0.5 (2)
C4—N1—C3—N2	165.15 (13)	C11—C6—C7—C8	-0.4 (2)
C4—N1—C3—C5	49.24 (18)	C6—C7—C8—C9	-0.0 (2)
C4—N1—C3—C6	-80.22 (18)	C7—C8—C9—C10	0.3 (3)
C1—N2—C3—N1	33.21 (13)	C8—C9—C10—C11	-0.2 (3)
C1—N2—C3—C5	150.92 (13)	C9—C10—C11—C6	-0.2 (2)
C1—N2—C3—C6	-83.66 (14)	C1—C12—C13—C14	-179.68 (17)
C3—N2—C1—C2	-29.59 (13)	C1—C12—C13—C18	0.8 (2)
C3—N2—C1—C12	-151.10 (12)	C12—C13—C14—C15	-179.5 (2)
N2—C1—C2—O1	-166.51 (14)	C12—C13—C18—C17	178.83 (18)
N2—C1—C2—N1	14.06 (14)	C14—C13—C18—C17	-0.7 (2)
N2—C1—C12—C13	-81.41 (18)	C18—C13—C14—C15	0.1 (2)
C2—C1—C12—C13	163.27 (14)	C13—C14—C15—C16	0.5 (3)
C12—C1—C2—O1	-43.4 (2)	C14—C15—C16—C17	-0.5 (3)
C12—C1—C2—N1	137.17 (14)	C15—C16—C17—C18	-0.1 (2)
N1—C3—C6—C7	166.27 (15)	C16—C17—C18—C13	0.7 (3)
N1—C3—C6—C11	-16.6 (2)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N2—H201...C11	0.86	2.30	3.1170 (14)	160
N2—H202...C11 ⁱ	0.86	2.24	3.0999 (14)	174

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

Fig. 1

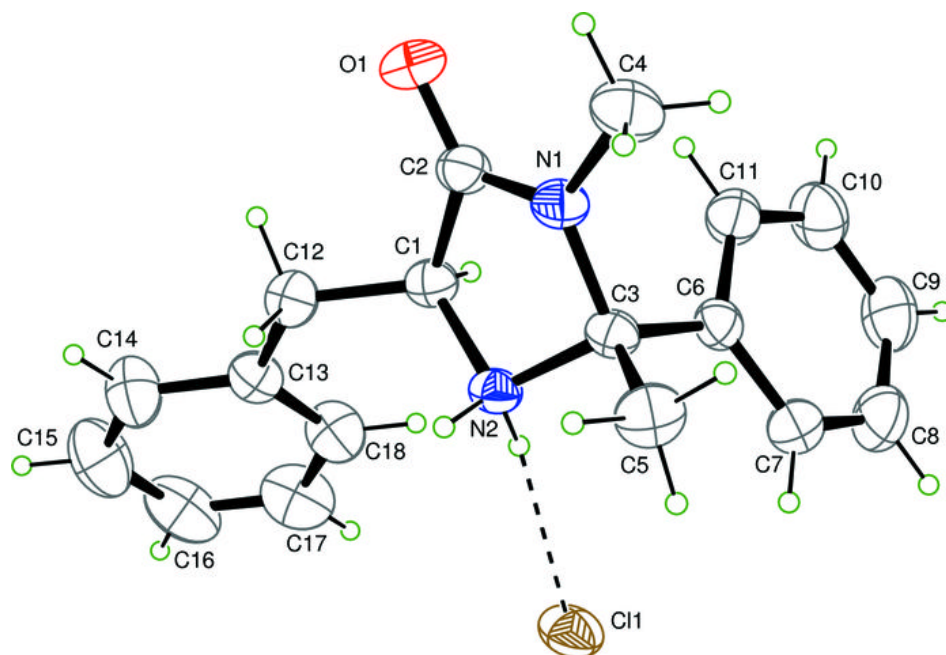


Fig. 2

