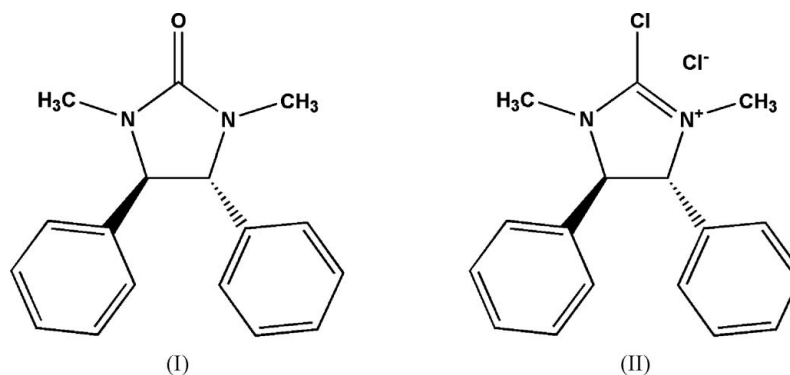


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Key indicators

Single-crystal X-ray study
 $T = 150$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.032
 wR factor = 0.083
Data-to-parameter ratio = 10.5For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.(4*R*,5*R*)-1,3-Dimethyl-4,5-diphenylimidazolidin-2-oneThe title compound, $\text{C}_{17}\text{H}_{18}\text{N}_2\text{O}$, was obtained by methylation of (4*R*,5*R*)-4,5-diphenylimidazolidin-2-one. The C—O bond exhibits double-bond character, and both C—N bonds in the urea group are intermediate between single and double bonds.Received 10 July 2006
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Comment

We have been developing guanidine chemistry (Ishikawa *et al.*, 2006), focusing on the potential abilities of the guanidyl functions, such as for chiral auxiliaries (Kitani *et al.*, 2005). The title compound, (I), is an important key intermediate and can be chlorinated with oxalyl chloride to afford the corresponding chloroamidinium chloride, (II). Recently, (II) was found to be a good source for a carbene ligand (Kremzow *et al.*, 2005).

The molecular structure and atom-numbering scheme of (I) are shown in Fig. 1. Selected geometric parameters are presented in Table 1. The urea group is found to be almost planar, with the sum of angles (N1—C1—N2, N1—C1—O1 and N2—C1—O1) being almost 360° . In calculating the mean plane through the urea group, the largest deviation from planarity is for C1 [0.0021 (13) Å]. The shortness of the C1—O1 bond indicates obvious double-bond character, while the N1—C1 and N2—C1 bonds are intermediate between single and double bonds due to resonance.

Experimental

(4*R*,5*R*)-1,3-Dimethyl-4,5-diphenylimidazolidin-2-one was prepared by methylation of (4*R*,5*R*)-4,5-diphenylimidazolidin-2-one according to the literature method of Isobe *et al.* (1998). To a suspension of NaH (60% in mineral oil, 1.64 g, 41.10 mmol) in DMF was added a solution of (4*R*,5*R*)-4,5-diphenylimidazolidin-2-one (4.42 g, 18.56 mmol, 1.0 equivalent) in DMF (4 ml) under argon and the mixture was stirred at room temperature for 1 h. After addition of iodomethane (2.6 ml, 40.93 mmol, 2.2 equivalents), the mixture was stirred at room

temperature for 1 h, poured into 5% aqueous HCl (100 ml), and then extracted with AcOEt (100 ml, 50 ml \times 2). The organic solutions were combined, successively washed with 20% aqueous Na₂S₂O₃ (40 ml), water and brine, dried over Mg₂SO₄, and then evaporated to dryness under reduced pressure. Purification of the residue by recrystallization from AcOEt gave (4*R*,5*R*)-1,3-dimethyl-4,5-diphenylimidazolidin-2-one as colourless prisms (4.26 g, 86%; m.p. 432–434 K). IR (ATR, cm⁻¹): 1702 (C=O).

Crystal data

C ₁₇ H ₁₈ N ₂ O	Z = 4
M _r = 266.33	D _x = 1.210 Mg m ⁻³
Orthorhombic, P ₂ ₁ 2 ₁ 2 ₁	Mo K α radiation
a = 10.0509 (14) Å	μ = 0.08 mm ⁻¹
b = 10.3340 (15) Å	T = 150 K
c = 14.075 (2) Å	Prism, colourless
V = 1461.9 (4) Å ³	0.40 \times 0.20 \times 0.20 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	1928 independent reflections
φ and ω scans	1738 reflections with $I > 2\sigma(I)$
Absorption correction: none	R _{int} = 0.038
8831 measured reflections	θ_{\max} = 27.5°

Refinement

Refinement on F ²	$w = 1/[\sigma^2(F_o^2) + (0.0407P)^2 + 0.0934P]$
R[F ² > 2 σ (F ²)] = 0.032	where $P = (F_o^2 + 2F_c^2)/3$
wR(F ²) = 0.083	(Δ/σ) _{max} < 0.001
S = 1.18	$\Delta\rho_{\max} = 0.15 \text{ e } \text{Å}^{-3}$
1928 reflections	$\Delta\rho_{\min} = -0.17 \text{ e } \text{Å}^{-3}$
183 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

N1–C1	1.382 (2)	O1–C1	1.222 (2)
N2–C1	1.371 (2)		
N1–C1–N2	107.98 (13)	N2–C1–O1	126.67 (15)
N1–C1–O1	125.35 (15)		

H atoms were placed in calculated positions (C–H = 0.95–1.00 Å) and treated as riding atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The absolute configuration was assumed from that of the starting material, which

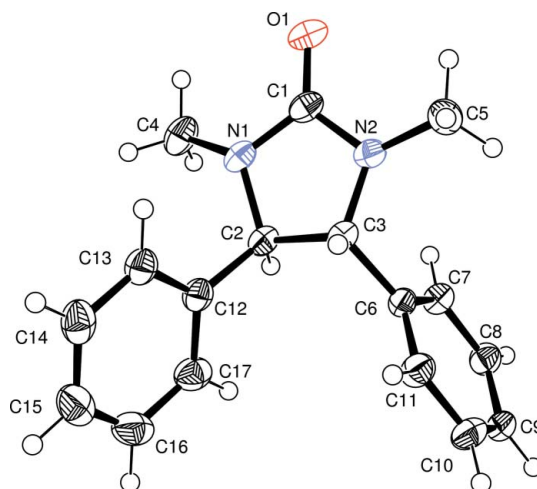


Figure 1

The molecular structure of (I), showing atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

reacts with retention of the configuration; in the absence of significant anomalous scattering effects, Friedel pairs were averaged.

Data collection: SMART (Bruker, 1998); cell refinement: SMART; data reduction: SAINT (Bruker, 1998); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: SHELXL97.

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