Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 1-[(2*S*)-1-Chloro-3-phenylpropan-2-yl]-2,4,5-triphenyl-1*H*-imidazole

**Yongmei Xiao, Liangru Yang, Kun He, Jinwei Yuan and Pu Mao***

School of Chemistry and Chemical Engineering, Henan University of Technology, Zhengzhou 450001, People's Republic of China
Correspondence e-mail: henangongda@yahoo.com

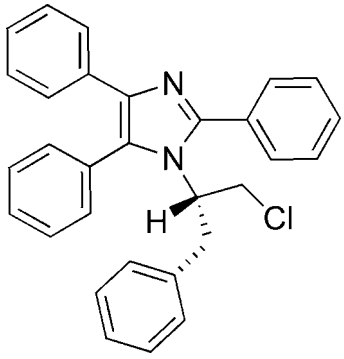
Received 20 December 2011; accepted 5 March 2012

Key indicators: single-crystal X-ray study; $T$ = 291 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.045; $wR$ factor = 0.098; data-to-parameter ratio = 14.3.

In the title compound, $C_{30}H_{25}ClN_2$, the chiral center maintains the *S* configuration of the stating L-phenylalaninol. The two phenyl groups closest to the substituted N atom adopt an almost perpendicular orientation relative to the central imidazole ring, with dihedral angles of 88.9 (4) and 84.7 (3)°. The third phenyl group is nearly coplanar with it, making a dihedral angle of 11.0 (5)°.

## Related literature

For the synthesis and applications of chiral ionic liquids, see: Ding *et al.* (2005); Bwambok *et al.* (2008); Mao *et al.* (2010).




## Experimental

### Crystal data

$C_{30}H_{25}ClN_2$
$M_r$ = 448.97
Orthorhombic, $P2_12_12_1$
$a$ = 9.6123 (4) Å
$b$ = 9.9437 (3) Å
$c$ = 24.9677 (7) Å
$V$ = 2386.47 (14) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 1.56 mm$^{-1}$
$T$ = 291 K
0.21 × 0.20 × 0.06 mm

### Data collection

Agilent Xcalibur Eos Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
$T_{min}$ = 0.657, $T_{max}$ = 1.000
9379 measured reflections
4256 independent reflections
3235 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.044

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.098
$S$ = 1.02
4256 reflections
298 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 e Å$^{-3}$
Absolute structure: Flack (1983), 1816 Friedel pairs
Flack parameter: 0.01 (2)

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

The authors thank Ms Y. Zhu for technical assistance. This research was supported by the National Natural Science Foundation of China (Nos. 20902017 and 21172055).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LD2044).

## References

Agilent (2011). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Bwambok, D. K., Marwani, H. M., Fernand, V. E., Fakayode, S. O., Lowry, M., Negulescu, I., Strongin, R. M. & Warner, I. M. (2008). *Chirality*, **20**, 151–158.
Ding, J. & Armstrong, D. W. (2005). *Chirality*, **17**, 281–292.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Mao, P., Cai, Y., Xiao, Y., Yang, L., Xue, Y. & Song, M. (2010). *Phosphorus Sulfur Silicon Relat. Elem.* **185**, 2418–2425.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supplementary materials

*Acta Cryst.* (2012). E**68**, o1153 [doi:10.1107/S1600536812009609]

## 1-[(2*S*)-1-Chloro-3-phenylpropan-2-yl]-2,4,5-triphenyl-1*H*-imidazole

**Yongmei Xiao, Liangru Yang, Kun He, Jinwei Yuan and Pu Mao**

### Comment

Current interest in the stereoselective synthesis and catalysis, chiral recognization and separation in ionic liquids has motivated the synthesis of novel chiral ionic liquids. (Ding & Armstrong, 2005; Bwambok *et al.*, 2008). Our group is interested in the preparation and application of chiral imidazolium derivatives from natural precursors (Mao *et al.*, 2010). During the study, we observed that condensation of *l*-phenylalaninol, dibenzoyl, arylaldehyde and ammonium acetate afforded multi-aryl substituted imidazole alcohol derivatives carrying a chiral functionality. The following reaction with $SOCl_2$ produced the title compound smoothly.

The molecular structure of the title compound is shown in Figure 1. As it is expected, the imidazole core (N1, C8, C7, N2, C24) is essentially planar. featuring an average deviation of less than 0.6 (3) °. The dihedral angles formed by the three aryl substituents and the central imidazole ring are 88.9 (4) (N2—C24—C25—C26), 11.0 (5) (C5—C6—C7—C8) and 95.3 (3) ° (C7—C8—C9—C14).

Due to the presence of muti aryl groups on the imidazole ring, the basicity of the N2 of the imidazole is reduced and its quaternization by the produced chloro- substituted derivative is suppressed successfully.

### Experimental

$SOCl_2$ (40 ml) was added slowly at room temperature into a three-neck flask containing 2-(4,5-Diphenyl-2-*p*-tolyl-imidazol-1-yl)-3-phenyl-propan-1-ol (4.45 g, 0.01 mol) and $Na_2CO_3$ (1.06 g, 0.01 mol). The solids were slowly dissolved upon addition of $SOCl_2$. After complete addition, the mixture was kept at 50 °C for 5 h and then at 70 °C for 2 h. The excessive $SOCl_2$ was removed and the residue was washed with $H_2O$ and filtered to afford the crude product. Crystallization from EtOH afforded colorless crystals of the title compound.

### Refinement

A suitable crystal was selected and mounted on a Xcalibur, Eos, Gemini diffractometer.The crystal was kept at 291.15 K during data collection. Using Olex2 (Dolomanov *et al.*, 2009), the structure was solved with the *SHELXS* (Sheldrick, 2008) structure solution program using Direct Methods and refined with the *SHELXL* (Sheldrick, 2008) refinement package using Least Squares minimization.

### Computing details

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

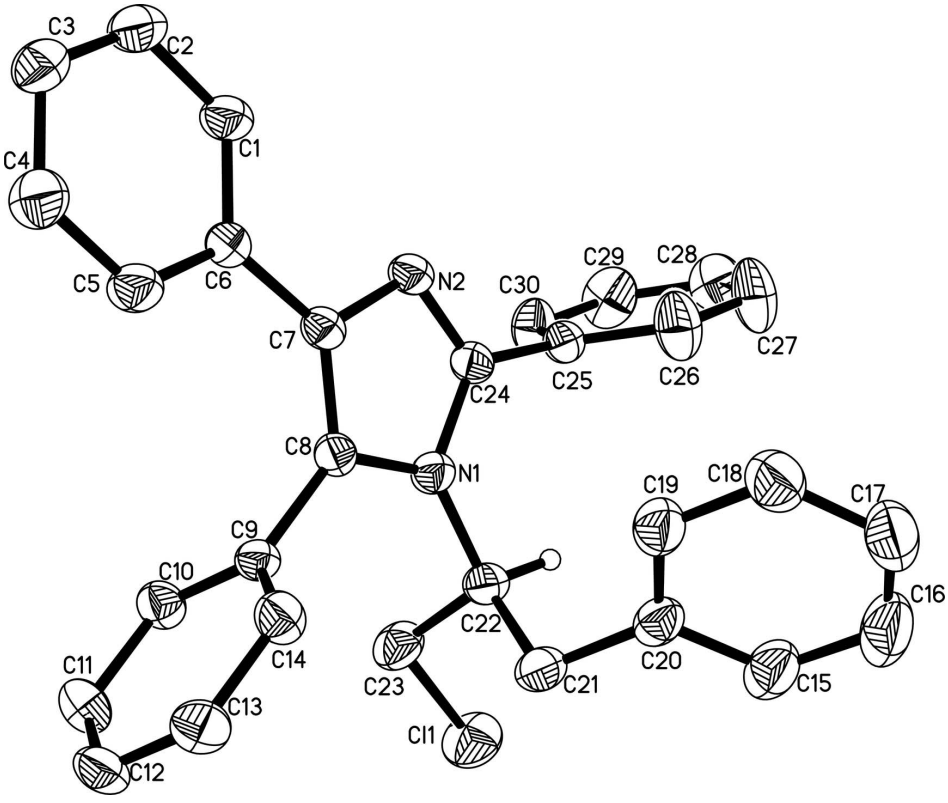



**Figure 1**

The molecular structure of the title compound showing 30% probability displacement ellipsoids. Hydrogen atoms are omitted for clarity.

### 1-[(2*S*)-1-Chloro-3-phenylpropan-2-yl]-2,4,5-triphenyl- 1*H*-imidazole

*Crystal data*

$C_{30}H_{25}ClN_2$
$M_r = 448.97$
Orthorhombic, $P2_12_12_1$
$a = 9.6123$ (4) Å
$b = 9.9437$ (3) Å
$c = 24.9677$ (7) Å
$V = 2386.47$ (14) Å$^3$
$Z = 4$
$F(000) = 944$
$D_x = 1.250$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.5418$ Å
Cell parameters from 2343 reflections
$\theta = 3.5$–66.9°
$\mu = 1.56$ mm$^{-1}$
$T = 291$ K
Prismatic, colorless
0.21 × 0.20 × 0.06 mm

*Data collection*

Agilent Xcalibur Eos Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.2312 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
$T_{min} = 0.657$, $T_{max} = 1.000$
9379 measured reflections
4256 independent reflections
3235 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 67.0°$, $\theta_{min} = 3.5°$
$h = -8 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -29 \rightarrow 29$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.098$
$S = 1.02$
4256 reflections
298 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0291P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.14$ e Å$^{-3}$
$\Delta\rho_{min} = -0.15$ e Å$^{-3}$
Absolute structure: Flack (1983), 1816 Friedel pairs
Flack parameter: 0.01 (2)

*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 $F^2 > \sigma(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.02166 (10) | 0.49291 (10) | 0.54575 (3) | 0.0805 (3) |
| N1 | 0.2271 (2) | 0.64694 (19) | 0.67166 (8) | 0.0430 (5) |
| N2 | 0.2501 (3) | 0.80764 (18) | 0.73267 (8) | 0.0433 (5) |
| C1 | 0.2662 (3) | 0.7993 (3) | 0.84491 (10) | 0.0525 (7) |
| H1 | 0.2457 | 0.8782 | 0.8266 | 0.063* |
| C2 | 0.2834 (4) | 0.8033 (3) | 0.90011 (11) | 0.0619 (8) |
| H2 | 0.2755 | 0.8844 | 0.9184 | 0.074* |
| C3 | 0.3121 (4) | 0.6867 (3) | 0.92756 (10) | 0.0617 (8) |
| H3 | 0.3223 | 0.6884 | 0.9646 | 0.074* |
| C4 | 0.3255 (4) | 0.5675 (3) | 0.90000 (11) | 0.0626 (8) |
| H4 | 0.3461 | 0.4887 | 0.9185 | 0.075* |
| C5 | 0.3085 (3) | 0.5641 (3) | 0.84478 (11) | 0.0545 (8) |
| H5 | 0.3171 | 0.4830 | 0.8266 | 0.065* |
| C6 | 0.2790 (3) | 0.6806 (2) | 0.81663 (9) | 0.0415 (5) |
| C7 | 0.2604 (3) | 0.6838 (2) | 0.75749 (9) | 0.0395 (5) |
| C8 | 0.2469 (3) | 0.5829 (2) | 0.72076 (9) | 0.0382 (5) |
| C9 | 0.2431 (3) | 0.4337 (2) | 0.72724 (9) | 0.0394 (6) |
| C10 | 0.1175 (3) | 0.3689 (3) | 0.73505 (11) | 0.0477 (6) |
| H10 | 0.0357 | 0.4187 | 0.7364 | 0.057* |
| C11 | 0.1120 (3) | 0.2302 (3) | 0.74093 (12) | 0.0564 (8) |
| H11 | 0.0269 | 0.1877 | 0.7461 | 0.068* |
| C12 | 0.2317 (4) | 0.1558 (2) | 0.73909 (12) | 0.0574 (8) |
| H12 | 0.2280 | 0.0628 | 0.7425 | 0.069* |
| C13 | 0.3575 (3) | 0.2192 (3) | 0.73211 (12) | 0.0556 (7) |

| | | | | |
|---|---|---|---|---|
| H13 | 0.4388 | 0.1686 | 0.7312 | 0.067* |
| C14 | 0.3644 (3) | 0.3580 (3) | 0.72642 (11) | 0.0494 (7) |
| H14 | 0.4501 | 0.4000 | 0.7221 | 0.059* |
| C15 | 0.5054 (4) | 0.6007 (3) | 0.53636 (12) | 0.0726 (10) |
| H15 | 0.4501 | 0.5715 | 0.5081 | 0.087* |
| C16 | 0.6292 (5) | 0.6662 (4) | 0.52570 (16) | 0.0907 (13) |
| H16 | 0.6567 | 0.6799 | 0.4904 | 0.109* |
| C17 | 0.7110 (4) | 0.7106 (3) | 0.56644 (17) | 0.0845 (12) |
| H17 | 0.7943 | 0.7544 | 0.5590 | 0.101* |
| C18 | 0.6708 (4) | 0.6909 (3) | 0.61861 (16) | 0.0719 (9) |
| H18 | 0.7260 | 0.7218 | 0.6466 | 0.086* |
| C19 | 0.5479 (3) | 0.6250 (3) | 0.62902 (12) | 0.0611 (8) |
| H19 | 0.5210 | 0.6114 | 0.6644 | 0.073* |
| C20 | 0.4629 (3) | 0.5783 (3) | 0.58816 (10) | 0.0521 (7) |
| C21 | 0.3307 (3) | 0.5022 (3) | 0.59933 (10) | 0.0539 (7) |
| H21A | 0.3494 | 0.4355 | 0.6267 | 0.065* |
| H21B | 0.3036 | 0.4546 | 0.5671 | 0.065* |
| C22 | 0.2082 (3) | 0.5894 (3) | 0.61769 (10) | 0.0482 (7) |
| H22 | 0.2023 | 0.6653 | 0.5927 | 0.058* |
| C23 | 0.0692 (3) | 0.5147 (3) | 0.61442 (10) | 0.0612 (8) |
| H23A | −0.0023 | 0.5657 | 0.6329 | 0.073* |
| H23B | 0.0773 | 0.4277 | 0.6317 | 0.073* |
| C24 | 0.2292 (3) | 0.7824 (2) | 0.68147 (10) | 0.0414 (5) |
| C25 | 0.2084 (3) | 0.8899 (2) | 0.64130 (10) | 0.0449 (6) |
| C26 | 0.3191 (4) | 0.9466 (3) | 0.61519 (14) | 0.0750 (10) |
| H26 | 0.4076 | 0.9104 | 0.6197 | 0.090* |
| C27 | 0.3010 (5) | 1.0571 (4) | 0.58219 (16) | 0.0921 (13) |
| H27 | 0.3770 | 1.0946 | 0.5646 | 0.111* |
| C28 | 0.1709 (4) | 1.1112 (3) | 0.57538 (13) | 0.0762 (11) |
| H28 | 0.1585 | 1.1856 | 0.5533 | 0.091* |
| C29 | 0.0601 (4) | 1.0555 (4) | 0.60104 (14) | 0.0781 (11) |
| H29 | −0.0283 | 1.0919 | 0.5965 | 0.094* |
| C30 | 0.0785 (3) | 0.9450 (3) | 0.63390 (12) | 0.0640 (8) |
| H30 | 0.0021 | 0.9074 | 0.6512 | 0.077* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0822 (6) | 0.1023 (6) | 0.0571 (3) | −0.0076 (6) | −0.0157 (4) | −0.0137 (5) |
| N1 | 0.0504 (13) | 0.0381 (10) | 0.0404 (10) | 0.0030 (10) | 0.0030 (10) | −0.0012 (9) |
| N2 | 0.0537 (13) | 0.0320 (9) | 0.0441 (10) | −0.0012 (11) | −0.0006 (11) | −0.0012 (9) |
| C1 | 0.0667 (19) | 0.0384 (12) | 0.0524 (13) | −0.0001 (16) | −0.0016 (15) | −0.0048 (12) |
| C2 | 0.081 (2) | 0.0531 (15) | 0.0520 (14) | −0.0010 (18) | −0.0013 (16) | −0.0120 (13) |
| C3 | 0.077 (2) | 0.0647 (18) | 0.0431 (13) | −0.0035 (18) | −0.0066 (14) | −0.0035 (14) |
| C4 | 0.082 (2) | 0.0540 (15) | 0.0517 (14) | 0.0087 (17) | −0.0078 (15) | 0.0070 (14) |
| C5 | 0.074 (2) | 0.0402 (13) | 0.0491 (13) | 0.0059 (15) | −0.0017 (14) | −0.0030 (12) |
| C6 | 0.0432 (13) | 0.0391 (12) | 0.0422 (11) | −0.0024 (12) | −0.0001 (11) | 0.0001 (10) |
| C7 | 0.0406 (14) | 0.0329 (10) | 0.0449 (12) | 0.0006 (12) | −0.0001 (12) | 0.0004 (10) |
| C8 | 0.0367 (13) | 0.0345 (11) | 0.0435 (12) | 0.0020 (11) | 0.0045 (12) | 0.0006 (10) |
| C9 | 0.0466 (15) | 0.0331 (10) | 0.0384 (11) | 0.0026 (12) | 0.0011 (12) | −0.0022 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C10 | 0.0459 (15) | 0.0394 (14) | 0.0579 (14) | 0.0057 (13) | 0.0043 (14) | 0.0019 (13) |
| C11 | 0.0532 (17) | 0.0477 (16) | 0.0683 (18) | −0.0100 (14) | −0.0030 (16) | 0.0052 (15) |
| C12 | 0.079 (2) | 0.0311 (11) | 0.0618 (15) | −0.0025 (15) | −0.0026 (18) | 0.0010 (12) |
| C13 | 0.0596 (18) | 0.0421 (16) | 0.0650 (17) | 0.0192 (15) | 0.0023 (16) | 0.0022 (14) |
| C14 | 0.0441 (15) | 0.0445 (15) | 0.0596 (15) | 0.0011 (13) | 0.0062 (14) | 0.0021 (13) |
| C15 | 0.092 (3) | 0.073 (2) | 0.0528 (16) | 0.011 (2) | 0.0135 (18) | 0.0050 (15) |
| C16 | 0.108 (3) | 0.092 (3) | 0.072 (2) | 0.008 (3) | 0.034 (2) | 0.023 (2) |
| C17 | 0.079 (3) | 0.0602 (19) | 0.114 (3) | 0.001 (2) | 0.036 (3) | 0.014 (2) |
| C18 | 0.070 (2) | 0.0579 (17) | 0.087 (2) | −0.0023 (18) | 0.0098 (19) | 0.0003 (18) |
| C19 | 0.070 (2) | 0.0577 (16) | 0.0555 (15) | 0.0019 (17) | 0.0098 (16) | 0.0060 (15) |
| C20 | 0.0629 (19) | 0.0471 (15) | 0.0464 (13) | 0.0125 (15) | 0.0084 (14) | 0.0004 (12) |
| C21 | 0.0678 (19) | 0.0488 (14) | 0.0451 (12) | 0.0048 (17) | 0.0049 (13) | −0.0073 (13) |
| C22 | 0.0606 (18) | 0.0424 (13) | 0.0417 (12) | −0.0012 (14) | 0.0010 (13) | −0.0041 (11) |
| C23 | 0.0660 (19) | 0.076 (2) | 0.0416 (12) | −0.0059 (19) | −0.0029 (13) | −0.0096 (15) |
| C24 | 0.0453 (14) | 0.0342 (11) | 0.0448 (12) | 0.0020 (13) | 0.0022 (12) | 0.0003 (10) |
| C25 | 0.0547 (16) | 0.0388 (12) | 0.0412 (12) | −0.0009 (13) | 0.0015 (12) | 0.0020 (11) |
| C26 | 0.063 (2) | 0.073 (2) | 0.089 (2) | 0.0052 (18) | 0.0099 (19) | 0.0319 (19) |
| C27 | 0.090 (3) | 0.088 (3) | 0.098 (3) | −0.010 (2) | 0.015 (2) | 0.048 (2) |
| C28 | 0.107 (3) | 0.0606 (19) | 0.0615 (18) | 0.012 (2) | −0.003 (2) | 0.0232 (16) |
| C29 | 0.084 (3) | 0.079 (2) | 0.0713 (19) | 0.030 (2) | −0.004 (2) | 0.0219 (18) |
| C30 | 0.0601 (19) | 0.0696 (19) | 0.0623 (16) | 0.0061 (16) | 0.0063 (16) | 0.0164 (16) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C23 | 1.788 (2) | C15—H15 | 0.9300 |
| N1—C8 | 1.395 (3) | C15—C16 | 1.383 (6) |
| N1—C22 | 1.475 (3) | C15—C20 | 1.374 (4) |
| N1—C24 | 1.370 (3) | C16—H16 | 0.9300 |
| N2—C7 | 1.382 (3) | C16—C17 | 1.360 (6) |
| N2—C24 | 1.318 (3) | C17—H17 | 0.9300 |
| C1—H1 | 0.9300 | C17—C18 | 1.373 (5) |
| C1—C2 | 1.389 (4) | C18—H18 | 0.9300 |
| C1—C6 | 1.380 (3) | C18—C19 | 1.376 (5) |
| C2—H2 | 0.9300 | C19—H19 | 0.9300 |
| C2—C3 | 1.374 (4) | C19—C20 | 1.387 (4) |
| C3—H3 | 0.9300 | C20—C21 | 1.506 (4) |
| C3—C4 | 1.377 (4) | C21—H21A | 0.9700 |
| C4—H4 | 0.9300 | C21—H21B | 0.9700 |
| C4—C5 | 1.389 (4) | C21—C22 | 1.532 (4) |
| C5—H5 | 0.9300 | C22—H22 | 0.9800 |
| C5—C6 | 1.384 (3) | C22—C23 | 1.531 (4) |
| C6—C7 | 1.488 (3) | C23—H23A | 0.9700 |
| C7—C8 | 1.366 (3) | C23—H23B | 0.9700 |
| C8—C9 | 1.492 (3) | C24—C25 | 1.479 (3) |
| C9—C10 | 1.383 (4) | C25—C26 | 1.370 (4) |
| C9—C14 | 1.388 (4) | C25—C30 | 1.376 (4) |
| C10—H10 | 0.9300 | C26—H26 | 0.9300 |
| C10—C11 | 1.388 (4) | C26—C27 | 1.384 (4) |
| C11—H11 | 0.9300 | C27—H27 | 0.9300 |
| C11—C12 | 1.369 (4) | C27—C28 | 1.372 (5) |

| | | | |
|---|---|---|---|
| C12—H12 | 0.9300 | C28—H28 | 0.9300 |
| C12—C13 | 1.374 (5) | C28—C29 | 1.361 (5) |
| C13—H13 | 0.9300 | C29—H29 | 0.9300 |
| C13—C14 | 1.389 (4) | C29—C30 | 1.383 (4) |
| C14—H14 | 0.9300 | C30—H30 | 0.9300 |
| | | | |
| C8—N1—C22 | 130.0 (2) | C16—C17—H17 | 120.0 |
| C24—N1—C8 | 106.9 (2) | C16—C17—C18 | 120.0 (4) |
| C24—N1—C22 | 123.1 (2) | C18—C17—H17 | 120.0 |
| C24—N2—C7 | 106.05 (19) | C17—C18—H18 | 120.3 |
| C2—C1—H1 | 119.3 | C17—C18—C19 | 119.3 (4) |
| C6—C1—H1 | 119.3 | C19—C18—H18 | 120.3 |
| C6—C1—C2 | 121.4 (3) | C18—C19—H19 | 119.1 |
| C1—C2—H2 | 120.2 | C18—C19—C20 | 121.7 (3) |
| C3—C2—C1 | 119.6 (3) | C20—C19—H19 | 119.1 |
| C3—C2—H2 | 120.2 | C15—C20—C19 | 117.6 (3) |
| C2—C3—H3 | 120.1 | C15—C20—C21 | 120.4 (3) |
| C2—C3—C4 | 119.7 (3) | C19—C20—C21 | 121.9 (2) |
| C4—C3—H3 | 120.1 | C20—C21—H21A | 108.6 |
| C3—C4—H4 | 119.8 | C20—C21—H21B | 108.6 |
| C3—C4—C5 | 120.4 (3) | C20—C21—C22 | 114.8 (2) |
| C5—C4—H4 | 119.8 | H21A—C21—H21B | 107.5 |
| C4—C5—H5 | 119.7 | C22—C21—H21A | 108.6 |
| C6—C5—C4 | 120.6 (3) | C22—C21—H21B | 108.6 |
| C6—C5—H5 | 119.7 | N1—C22—C21 | 113.4 (2) |
| C1—C6—C5 | 118.3 (2) | N1—C22—H22 | 106.8 |
| C1—C6—C7 | 118.6 (2) | N1—C22—C23 | 110.2 (2) |
| C5—C6—C7 | 123.1 (2) | C21—C22—H22 | 106.8 |
| N2—C7—C6 | 118.23 (19) | C23—C22—C21 | 112.3 (2) |
| C8—C7—N2 | 110.3 (2) | C23—C22—H22 | 106.8 |
| C8—C7—C6 | 131.4 (2) | Cl1—C23—H23A | 109.8 |
| N1—C8—C9 | 123.1 (2) | Cl1—C23—H23B | 109.8 |
| C7—C8—N1 | 105.5 (2) | C22—C23—Cl1 | 109.44 (19) |
| C7—C8—C9 | 131.3 (2) | C22—C23—H23A | 109.8 |
| C10—C9—C8 | 120.0 (3) | C22—C23—H23B | 109.8 |
| C10—C9—C14 | 118.8 (2) | H23A—C23—H23B | 108.2 |
| C14—C9—C8 | 121.2 (3) | N1—C24—C25 | 126.0 (2) |
| C9—C10—H10 | 119.6 | N2—C24—N1 | 111.3 (2) |
| C9—C10—C11 | 120.8 (3) | N2—C24—C25 | 122.8 (2) |
| C11—C10—H10 | 119.6 | C26—C25—C24 | 121.0 (3) |
| C10—C11—H11 | 120.0 | C26—C25—C30 | 118.5 (3) |
| C12—C11—C10 | 120.1 (3) | C30—C25—C24 | 120.1 (3) |
| C12—C11—H11 | 120.0 | C25—C26—H26 | 119.6 |
| C11—C12—H12 | 120.1 | C25—C26—C27 | 120.8 (3) |
| C11—C12—C13 | 119.8 (2) | C27—C26—H26 | 119.6 |
| C13—C12—H12 | 120.1 | C26—C27—H27 | 120.0 |
| C12—C13—H13 | 119.6 | C28—C27—C26 | 120.0 (4) |
| C12—C13—C14 | 120.7 (3) | C28—C27—H27 | 120.0 |
| C14—C13—H13 | 119.6 | C27—C28—H28 | 120.2 |

| | | | |
|---|---|---|---|
| C9—C14—C13 | 119.8 (3) | C29—C28—C27 | 119.7 (3) |
| C9—C14—H14 | 120.1 | C29—C28—H28 | 120.2 |
| C13—C14—H14 | 120.1 | C28—C29—H29 | 119.9 |
| C16—C15—H15 | 119.6 | C28—C29—C30 | 120.2 (3) |
| C20—C15—H15 | 119.6 | C30—C29—H29 | 119.9 |
| C20—C15—C16 | 120.9 (4) | C25—C30—C29 | 120.8 (3) |
| C15—C16—H16 | 119.8 | C25—C30—H30 | 119.6 |
| C17—C16—C15 | 120.5 (3) | C29—C30—H30 | 119.6 |
| C17—C16—H16 | 119.8 | | |

| | | | |
|---|---|---|---|
| N1—C8—C9—C10 | −85.7 (3) | C10—C11—C12—C13 | 0.9 (5) |
| N1—C8—C9—C14 | 95.3 (3) | C11—C12—C13—C14 | −0.6 (5) |
| N1—C22—C23—Cl1 | 161.61 (19) | C12—C13—C14—C9 | −0.6 (4) |
| N1—C24—C25—C26 | −92.4 (4) | C14—C9—C10—C11 | −1.2 (4) |
| N1—C24—C25—C30 | 94.9 (4) | C15—C16—C17—C18 | −0.2 (6) |
| N2—C7—C8—N1 | −0.2 (3) | C15—C20—C21—C22 | −105.2 (3) |
| N2—C7—C8—C9 | −176.5 (3) | C16—C15—C20—C19 | 0.7 (5) |
| N2—C24—C25—C26 | 88.9 (4) | C16—C15—C20—C21 | −177.6 (3) |
| N2—C24—C25—C30 | −83.8 (4) | C16—C17—C18—C19 | 0.6 (5) |
| C1—C2—C3—C4 | 1.0 (5) | C17—C18—C19—C20 | −0.3 (5) |
| C1—C6—C7—N2 | 8.6 (4) | C18—C19—C20—C15 | −0.3 (5) |
| C1—C6—C7—C8 | −169.1 (3) | C18—C19—C20—C21 | 178.0 (3) |
| C2—C1—C6—C5 | 0.5 (5) | C19—C20—C21—C22 | 76.5 (3) |
| C2—C1—C6—C7 | −179.5 (3) | C20—C15—C16—C17 | −0.5 (6) |
| C2—C3—C4—C5 | −0.8 (6) | C20—C21—C22—N1 | −69.1 (3) |
| C3—C4—C5—C6 | 0.5 (5) | C20—C21—C22—C23 | 165.1 (2) |
| C4—C5—C6—C1 | −0.3 (5) | C21—C22—C23—Cl1 | −70.9 (3) |
| C4—C5—C6—C7 | 179.6 (3) | C22—N1—C8—C7 | 179.2 (3) |
| C5—C6—C7—N2 | −171.3 (3) | C22—N1—C8—C9 | −4.1 (5) |
| C5—C6—C7—C8 | 11.0 (5) | C22—N1—C24—N2 | −178.8 (2) |
| C6—C1—C2—C3 | −0.8 (5) | C22—N1—C24—C25 | 2.4 (5) |
| C6—C7—C8—N1 | 177.7 (3) | C24—N1—C8—C7 | −0.3 (3) |
| C6—C7—C8—C9 | 1.3 (5) | C24—N1—C8—C9 | 176.5 (3) |
| C7—N2—C24—N1 | −0.7 (3) | C24—N1—C22—C21 | 119.7 (3) |
| C7—N2—C24—C25 | 178.1 (3) | C24—N1—C22—C23 | −113.4 (3) |
| C7—C8—C9—C10 | 90.2 (4) | C24—N2—C7—C6 | −177.7 (2) |
| C7—C8—C9—C14 | −88.8 (4) | C24—N2—C7—C8 | 0.5 (3) |
| C8—N1—C22—C21 | −59.6 (4) | C24—C25—C26—C27 | −172.7 (3) |
| C8—N1—C22—C23 | 67.3 (4) | C24—C25—C30—C29 | 172.6 (3) |
| C8—N1—C24—N2 | 0.6 (3) | C25—C26—C27—C28 | 0.1 (6) |
| C8—N1—C24—C25 | −178.2 (3) | C26—C25—C30—C29 | −0.3 (5) |
| C8—C9—C10—C11 | 179.7 (3) | C26—C27—C28—C29 | −0.2 (6) |
| C8—C9—C14—C13 | −179.5 (2) | C27—C28—C29—C30 | 0.1 (6) |
| C9—C10—C11—C12 | 0.0 (5) | C28—C29—C30—C25 | 0.2 (5) |
| C10—C9—C14—C13 | 1.5 (4) | C30—C25—C26—C27 | 0.1 (5) |