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# 4-[(5-Chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)methylideneamino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one

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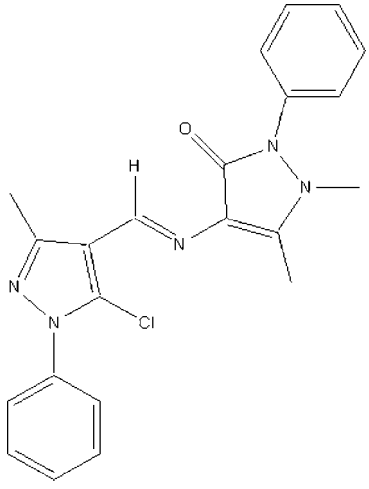
Key indicators: single-crystal X-ray study; $T$ = 113 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.044; $wR$ factor = 0.105; data-to-parameter ratio = 12.8.

In the molecule of the title compound, $C_{22}H_{20}ClN_5O$, the atoms of the two pyrazole rings and the –C═N– group which joins them are essentially coplanar, with an r.m.s. deviation of 0.054 (2) Å. The phenyl rings form dihedral angles of 41.24 (5) and 55.53 (5)° with this plane. The crystal structure is stabilized by weak intermolecular $\pi$–$\pi$ interactions, with centroid-to-centroid distances of 3.6179 (13) Å between the imidazole rings.

## Related literature

For our previous work in this area, see: Zhu *et al.* (2005, 2010*a*,*b*,*c*). For a related crystal structure, see: Shi *et al.* (2005).




## Experimental

### Crystal data

$C_{22}H_{20}ClN_5O$
$M_r$ = 405.88
Monoclinic, $P2_1/n$
$a$ = 8.3982 (17) Å
$b$ = 9.5204 (19) Å
$c$ = 24.401 (5) Å
$\beta$ = 97.24 (3)°
$V$ = 1935.4 (7) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.22 mm$^{-1}$
$T$ = 113 K
0.20 × 0.18 × 0.10 mm

### Data collection

Rigaku Saturn CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2008)
$T_{min}$ = 0.957, $T_{max}$ = 0.978
15458 measured reflections
3397 independent reflections
2871 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.046

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.105
$S$ = 1.08
3397 reflections
266 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and Mercury (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5137).

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# supporting information

*Acta Cryst.* (2010). E**66**, o2724 [https://doi.org/10.1107/S1600536810039048]

## 4-[(5-Chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)methylideneamino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one

**Hualing Zhu, Jinhua Zhu, Litong Ban, Pingping Zhang and Miao Zhang**

### S1. Comment

As part of our ongoing studies (Zhu *et al.*, 2005, 2010*a*,*b*,*c*) of pyrazolone derivatives as potential ligands (Shi *et al.*, 2005) we report the crystal structure of the title compound (I).

The molecular structure of the title compound is shown in Fig. 1. Atoms C11 and N3 and the two pyrazole rings are essentially coplplanar with the largest deviation being 0.0543 (18) Å for atom C13. The crystal structure is stabilized by weak intermolecular $\pi$–$\pi$ interactions with ring centroid to ring centroid distances of 3.6179 (13) Å between the imidazole rings (see Fig. 2).

### S2. Experimental

The title compound was synthesized by refluxing a mixture of 4-formacyl-5-methyl-3-chloro-2-phenyl-2*H*-pyrazole (15*m* mol) and 4-antipyrine (15 mmol) in ethanol (100 ml) over a steam bath for about 4 h. The solution was then cooled to room temperature. After one day, pale-yellow blocks wre obtained and they were dried in air. Recrystallization of a solution of the title compound in ethanol afforded pale-yellow crystals suitable for X-ray analysis.

### S3. Refinement

H atoms were placed in calculated positions with C—H = 0.95 and 0.98 Å and included in the refinement with $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$($C_{methyl}$).

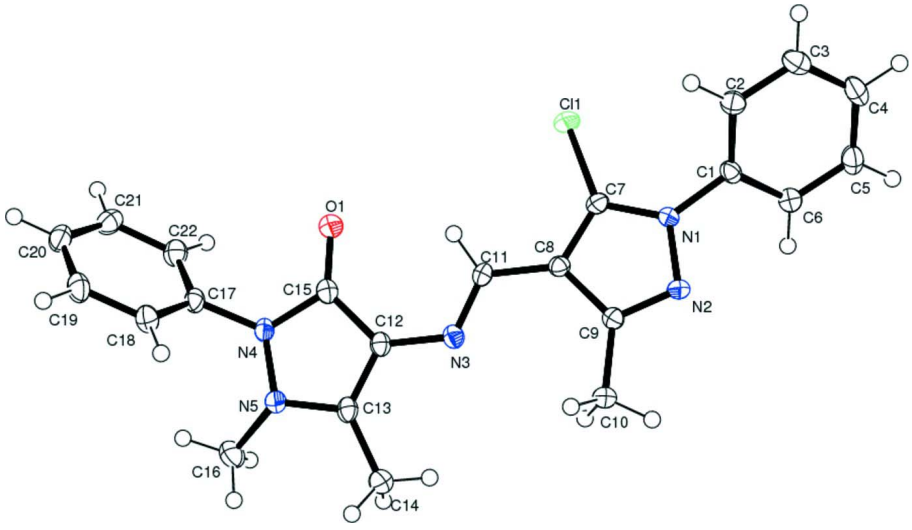


**Figure 1**

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as a small spheres of arbitrary radius.

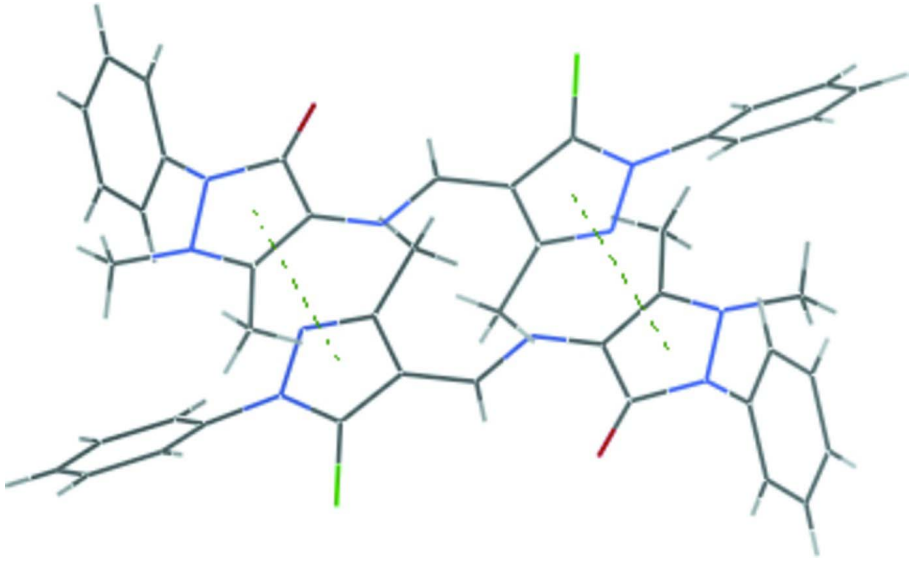

**Figure 2**

Part of the crystal structure showing intermolecular $\pi$–$\pi$ interactions as dashed lines.

**4-[(5-Chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)methylideneamino]- 1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one**

*Crystal data*

$C_{22}H_{20}ClN_5O$
$M_r$ = 405.88
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a$ = 8.3982 (17) Å
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$c$ = 24.401 (5) Å
$\beta$ = 97.24 (3)°
$V$ = 1935.4 (7) Å$^3$
$Z$ = 4
$F$(000) = 848
$D_x$ = 1.393 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 4998 reflections

$\theta$ = 1.7–27.9°
$\mu$ = 0.22 mm$^{-1}$
$T$ = 113 K

Block, pale yellow
0.20 × 0.18 × 0.10 mm

*Data collection*

Rigaku Saturn CCD diffractometer
Radiation source: rotating anode
Confocal monochromator
Detector resolution: 7.31 pixels mm$^{-1}$
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2008)
$T_{min}$ = 0.957, $T_{max}$ = 0.978

15458 measured reflections
3397 independent reflections
2871 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.046
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 1.7°
$h$ = −9→9
$k$ = −11→11
$l$ = −29→29

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.105
$S$ = 1.08
3397 reflections
266 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
$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 0.6515P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0242 (16)

*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 | 0.56582 (6) | 0.05661 (6) | 0.08916 (2) | 0.02960 (19) |
| O1 | 0.75786 (16) | 0.36105 (15) | −0.04914 (6) | 0.0251 (4) |
| N1 | 0.80398 (18) | −0.09683 (17) | 0.14372 (6) | 0.0175 (4) |
| N2 | 0.96786 (17) | −0.11576 (16) | 0.14899 (6) | 0.0172 (4) |
| N3 | 1.03166 (18) | 0.19175 (16) | 0.02437 (6) | 0.0181 (4) |
| N4 | 0.98109 (19) | 0.45266 (17) | −0.08446 (6) | 0.0196 (4) |
| N5 | 1.14617 (18) | 0.42156 (17) | −0.07913 (6) | 0.0201 (4) |
| C1 | 0.7142 (2) | −0.1746 (2) | 0.17966 (8) | 0.0181 (4) |
| C2 | 0.5695 (2) | −0.2379 (2) | 0.16005 (8) | 0.0206 (4) |
| H2 | 0.5247 | −0.2262 | 0.1226 | 0.025* |
| C3 | 0.4910 (2) | −0.3182 (2) | 0.19566 (9) | 0.0246 (5) |

| | | | | |
|---|---|---|---|---|
| H3 | 0.3912 | −0.3610 | 0.1826 | 0.030* |
| C4 | 0.5566 (2) | −0.3368 (2) | 0.25005 (9) | 0.0263 (5) |
| H4 | 0.5026 | −0.3927 | 0.2742 | 0.032* |
| C5 | 0.7015 (2) | −0.2736 (2) | 0.26924 (8) | 0.0254 (5) |
| H5 | 0.7469 | −0.2867 | 0.3066 | 0.031* |
| C6 | 0.7808 (2) | −0.1913 (2) | 0.23432 (8) | 0.0213 (5) |
| H6 | 0.8794 | −0.1468 | 0.2477 | 0.026* |
| C7 | 0.7592 (2) | 0.0000 (2) | 0.10393 (8) | 0.0186 (4) |
| C8 | 0.8934 (2) | 0.04644 (19) | 0.08215 (8) | 0.0164 (4) |
| C9 | 1.0207 (2) | −0.0306 (2) | 0.11224 (7) | 0.0163 (4) |
| C10 | 1.1952 (2) | −0.0254 (2) | 0.10710 (8) | 0.0209 (4) |
| H10A | 1.2521 | −0.0946 | 0.1321 | 0.031* |
| H10B | 1.2366 | 0.0688 | 0.1168 | 0.031* |
| H10C | 1.2119 | −0.0470 | 0.0690 | 0.031* |
| C11 | 0.8978 (2) | 0.14939 (19) | 0.03858 (8) | 0.0174 (4) |
| H11 | 0.8001 | 0.1860 | 0.0203 | 0.021* |
| C12 | 1.0353 (2) | 0.2915 (2) | −0.01714 (8) | 0.0178 (4) |
| C13 | 1.1767 (2) | 0.3331 (2) | −0.03503 (7) | 0.0189 (4) |
| C14 | 1.3431 (2) | 0.2994 (2) | −0.01061 (8) | 0.0265 (5) |
| H14A | 1.4097 | 0.2833 | −0.0402 | 0.040* |
| H14B | 1.3425 | 0.2145 | 0.0121 | 0.040* |
| H14C | 1.3871 | 0.3779 | 0.0124 | 0.040* |
| C15 | 0.9051 (2) | 0.3662 (2) | −0.04929 (8) | 0.0191 (4) |
| C16 | 1.2558 (2) | 0.5346 (2) | −0.09045 (9) | 0.0277 (5) |
| H16A | 1.2703 | 0.5994 | −0.0590 | 0.042* |
| H16B | 1.2106 | 0.5856 | −0.1237 | 0.042* |
| H16C | 1.3598 | 0.4944 | −0.0962 | 0.042* |
| C17 | 0.9040 (2) | 0.5093 (2) | −0.13518 (8) | 0.0194 (4) |
| C18 | 0.9457 (2) | 0.4650 (2) | −0.18560 (8) | 0.0231 (5) |
| H18 | 1.0276 | 0.3968 | −0.1870 | 0.028* |
| C19 | 0.8665 (2) | 0.5215 (2) | −0.23385 (8) | 0.0257 (5) |
| H19 | 0.8960 | 0.4932 | −0.2685 | 0.031* |
| C20 | 0.7448 (2) | 0.6188 (2) | −0.23199 (8) | 0.0250 (5) |
| H20 | 0.6897 | 0.6560 | −0.2652 | 0.030* |
| C21 | 0.7038 (2) | 0.6615 (2) | −0.18128 (9) | 0.0256 (5) |
| H21 | 0.6198 | 0.7278 | −0.1799 | 0.031* |
| C22 | 0.7844 (2) | 0.6082 (2) | −0.13259 (8) | 0.0235 (5) |
| H22 | 0.7578 | 0.6393 | −0.0979 | 0.028* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0146 (3) | 0.0348 (3) | 0.0391 (3) | 0.0050 (2) | 0.0026 (2) | 0.0133 (2) |
| O1 | 0.0202 (8) | 0.0284 (8) | 0.0269 (8) | 0.0014 (6) | 0.0035 (6) | 0.0068 (6) |
| N1 | 0.0137 (8) | 0.0208 (9) | 0.0185 (8) | −0.0001 (7) | 0.0033 (6) | 0.0039 (7) |
| N2 | 0.0132 (8) | 0.0197 (9) | 0.0187 (8) | 0.0005 (7) | 0.0021 (6) | 0.0010 (7) |
| N3 | 0.0204 (9) | 0.0170 (9) | 0.0169 (8) | −0.0018 (7) | 0.0024 (7) | 0.0003 (6) |
| N4 | 0.0204 (8) | 0.0215 (9) | 0.0171 (8) | 0.0023 (7) | 0.0031 (7) | 0.0051 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N5 | 0.0189 (9) | 0.0227 (9) | 0.0185 (8) | −0.0020 (7) | 0.0012 (7) | 0.0040 (7) |
| C1 | 0.0181 (10) | 0.0162 (10) | 0.0213 (10) | 0.0016 (8) | 0.0073 (8) | 0.0021 (8) |
| C2 | 0.0198 (10) | 0.0218 (11) | 0.0209 (10) | 0.0011 (8) | 0.0049 (8) | −0.0013 (8) |
| C3 | 0.0223 (11) | 0.0198 (11) | 0.0330 (12) | −0.0023 (8) | 0.0087 (9) | −0.0020 (9) |
| C4 | 0.0305 (12) | 0.0190 (11) | 0.0324 (12) | 0.0012 (9) | 0.0155 (10) | 0.0055 (9) |
| C5 | 0.0308 (12) | 0.0253 (12) | 0.0213 (10) | 0.0037 (9) | 0.0075 (9) | 0.0055 (9) |
| C6 | 0.0211 (10) | 0.0213 (11) | 0.0215 (10) | −0.0002 (8) | 0.0028 (8) | 0.0018 (8) |
| C7 | 0.0152 (10) | 0.0192 (11) | 0.0208 (10) | 0.0022 (8) | 0.0006 (8) | 0.0016 (8) |
| C8 | 0.0154 (9) | 0.0168 (10) | 0.0166 (9) | −0.0007 (8) | 0.0010 (8) | −0.0004 (8) |
| C9 | 0.0170 (9) | 0.0172 (10) | 0.0148 (9) | −0.0010 (8) | 0.0024 (8) | −0.0014 (8) |
| C10 | 0.0158 (10) | 0.0248 (11) | 0.0220 (10) | 0.0005 (8) | 0.0030 (8) | 0.0026 (8) |
| C11 | 0.0192 (10) | 0.0160 (10) | 0.0166 (10) | 0.0021 (8) | 0.0001 (8) | 0.0021 (8) |
| C12 | 0.0218 (10) | 0.0162 (10) | 0.0154 (9) | −0.0008 (8) | 0.0021 (8) | 0.0000 (8) |
| C13 | 0.0239 (10) | 0.0199 (11) | 0.0127 (9) | −0.0014 (8) | 0.0012 (8) | −0.0008 (8) |
| C14 | 0.0213 (11) | 0.0367 (13) | 0.0217 (11) | −0.0007 (9) | 0.0035 (9) | 0.0048 (9) |
| C15 | 0.0231 (11) | 0.0174 (11) | 0.0169 (10) | −0.0015 (8) | 0.0028 (8) | −0.0001 (8) |
| C16 | 0.0283 (12) | 0.0251 (12) | 0.0305 (12) | −0.0043 (9) | 0.0072 (9) | 0.0051 (9) |
| C17 | 0.0233 (10) | 0.0162 (10) | 0.0182 (10) | −0.0040 (8) | 0.0001 (8) | 0.0033 (8) |
| C18 | 0.0275 (11) | 0.0207 (11) | 0.0215 (10) | 0.0009 (9) | 0.0054 (9) | 0.0028 (8) |
| C19 | 0.0334 (12) | 0.0276 (12) | 0.0160 (10) | −0.0055 (10) | 0.0030 (9) | 0.0006 (9) |
| C20 | 0.0279 (11) | 0.0231 (12) | 0.0219 (10) | −0.0055 (9) | −0.0048 (9) | 0.0046 (9) |
| C21 | 0.0239 (11) | 0.0221 (11) | 0.0293 (12) | 0.0015 (9) | −0.0025 (9) | 0.0016 (9) |
| C22 | 0.0277 (11) | 0.0228 (11) | 0.0198 (10) | −0.0011 (9) | 0.0019 (9) | −0.0013 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C7 | 1.7064 (19) | C8—C11 | 1.450 (3) |
| O1—C15 | 1.238 (2) | C9—C10 | 1.487 (3) |
| N1—C7 | 1.357 (2) | C10—H10A | 0.9800 |
| N1—N2 | 1.378 (2) | C10—H10B | 0.9800 |
| N1—C1 | 1.433 (2) | C10—H10C | 0.9800 |
| N2—C9 | 1.326 (2) | C11—H11 | 0.9500 |
| N3—C11 | 1.282 (2) | C12—C13 | 1.374 (3) |
| N3—C12 | 1.392 (2) | C12—C15 | 1.449 (3) |
| N4—C15 | 1.400 (2) | C13—C14 | 1.484 (3) |
| N4—N5 | 1.408 (2) | C14—H14A | 0.9800 |
| N4—C17 | 1.428 (2) | C14—H14B | 0.9800 |
| N5—C13 | 1.365 (2) | C14—H14C | 0.9800 |
| N5—C16 | 1.465 (3) | C16—H16A | 0.9800 |
| C1—C2 | 1.386 (3) | C16—H16B | 0.9800 |
| C1—C6 | 1.389 (3) | C16—H16C | 0.9800 |
| C2—C3 | 1.385 (3) | C17—C22 | 1.384 (3) |
| C2—H2 | 0.9500 | C17—C18 | 1.387 (3) |
| C3—C4 | 1.383 (3) | C18—C19 | 1.385 (3) |
| C3—H3 | 0.9500 | C18—H18 | 0.9500 |
| C4—C5 | 1.385 (3) | C19—C20 | 1.385 (3) |
| C4—H4 | 0.9500 | C19—H19 | 0.9500 |
| C5—C6 | 1.388 (3) | C20—C21 | 1.387 (3) |

| | | | |
|---|---|---|---|
| C5—H5 | 0.9500 | C20—H20 | 0.9500 |
| C6—H6 | 0.9500 | C21—C22 | 1.387 (3) |
| C7—C8 | 1.378 (3) | C21—H21 | 0.9500 |
| C8—C9 | 1.422 (3) | C22—H22 | 0.9500 |

| | | | |
|---|---|---|---|
| C7—N1—N2 | 109.82 (14) | H10B—C10—H10C | 109.5 |
| C7—N1—C1 | 132.03 (16) | N3—C11—C8 | 121.01 (17) |
| N2—N1—C1 | 118.13 (15) | N3—C11—H11 | 119.5 |
| C9—N2—N1 | 105.80 (15) | C8—C11—H11 | 119.5 |
| C11—N3—C12 | 120.78 (16) | C13—C12—N3 | 121.80 (17) |
| C15—N4—N5 | 109.84 (15) | C13—C12—C15 | 108.06 (17) |
| C15—N4—C17 | 124.14 (16) | N3—C12—C15 | 130.13 (17) |
| N5—N4—C17 | 119.57 (15) | N5—C13—C12 | 110.13 (17) |
| C13—N5—N4 | 106.72 (14) | N5—C13—C14 | 121.60 (17) |
| C13—N5—C16 | 122.81 (16) | C12—C13—C14 | 128.17 (18) |
| N4—N5—C16 | 117.58 (15) | C13—C14—H14A | 109.5 |
| C2—C1—C6 | 120.76 (18) | C13—C14—H14B | 109.5 |
| C2—C1—N1 | 121.27 (17) | H14A—C14—H14B | 109.5 |
| C6—C1—N1 | 117.88 (17) | C13—C14—H14C | 109.5 |
| C3—C2—C1 | 119.28 (19) | H14A—C14—H14C | 109.5 |
| C3—C2—H2 | 120.4 | H14B—C14—H14C | 109.5 |
| C1—C2—H2 | 120.4 | O1—C15—N4 | 123.90 (17) |
| C4—C3—C2 | 120.61 (19) | O1—C15—C12 | 131.67 (18) |
| C4—C3—H3 | 119.7 | N4—C15—C12 | 104.43 (16) |
| C2—C3—H3 | 119.7 | N5—C16—H16A | 109.5 |
| C3—C4—C5 | 119.72 (19) | N5—C16—H16B | 109.5 |
| C3—C4—H4 | 120.1 | H16A—C16—H16B | 109.5 |
| C5—C4—H4 | 120.1 | N5—C16—H16C | 109.5 |
| C4—C5—C6 | 120.45 (19) | H16A—C16—H16C | 109.5 |
| C4—C5—H5 | 119.8 | H16B—C16—H16C | 109.5 |
| C6—C5—H5 | 119.8 | C22—C17—C18 | 120.90 (18) |
| C5—C6—C1 | 119.18 (18) | C22—C17—N4 | 118.02 (17) |
| C5—C6—H6 | 120.4 | C18—C17—N4 | 121.07 (18) |
| C1—C6—H6 | 120.4 | C19—C18—C17 | 119.21 (19) |
| N1—C7—C8 | 109.14 (16) | C19—C18—H18 | 120.4 |
| N1—C7—Cl1 | 122.43 (14) | C17—C18—H18 | 120.4 |
| C8—C7—Cl1 | 128.31 (15) | C20—C19—C18 | 120.59 (19) |
| C7—C8—C9 | 103.49 (16) | C20—C19—H19 | 119.7 |
| C7—C8—C11 | 126.70 (17) | C18—C19—H19 | 119.7 |
| C9—C8—C11 | 129.81 (17) | C19—C20—C21 | 119.54 (19) |
| N2—C9—C8 | 111.75 (16) | C19—C20—H20 | 120.2 |
| N2—C9—C10 | 119.64 (17) | C21—C20—H20 | 120.2 |
| C8—C9—C10 | 128.61 (17) | C20—C21—C22 | 120.50 (19) |
| C9—C10—H10A | 109.5 | C20—C21—H21 | 119.8 |
| C9—C10—H10B | 109.5 | C22—C21—H21 | 119.8 |
| H10A—C10—H10B | 109.5 | C17—C22—C21 | 119.24 (19) |
| C9—C10—H10C | 109.5 | C17—C22—H22 | 120.4 |
| H10A—C10—H10C | 109.5 | C21—C22—H22 | 120.4 |

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| C7—N1—N2—C9 | −0.2 (2) | C7—C8—C11—N3 | 175.01 (19) |
| C1—N1—N2—C9 | −178.74 (16) | C9—C8—C11—N3 | −5.4 (3) |
| C15—N4—N5—C13 | −9.4 (2) | C11—N3—C12—C13 | −176.57 (18) |
| C17—N4—N5—C13 | −162.32 (16) | C11—N3—C12—C15 | 2.0 (3) |
| C15—N4—N5—C16 | −152.04 (17) | N4—N5—C13—C12 | 8.4 (2) |
| C17—N4—N5—C16 | 55.0 (2) | C16—N5—C13—C12 | 148.65 (18) |
| C7—N1—C1—C2 | 44.7 (3) | N4—N5—C13—C14 | −168.34 (17) |
| N2—N1—C1—C2 | −137.15 (18) | C16—N5—C13—C14 | −28.1 (3) |
| C7—N1—C1—C6 | −138.7 (2) | N3—C12—C13—N5 | 174.47 (16) |
| N2—N1—C1—C6 | 39.5 (2) | C15—C12—C13—N5 | −4.4 (2) |
| C6—C1—C2—C3 | 0.1 (3) | N3—C12—C13—C14 | −9.1 (3) |
| N1—C1—C2—C3 | 176.61 (17) | C15—C12—C13—C14 | 172.05 (19) |
| C1—C2—C3—C4 | −0.7 (3) | N5—N4—C15—O1 | −172.85 (17) |
| C2—C3—C4—C5 | 0.5 (3) | C17—N4—C15—O1 | −21.4 (3) |
| C3—C4—C5—C6 | 0.3 (3) | N5—N4—C15—C12 | 6.6 (2) |
| C4—C5—C6—C1 | −0.9 (3) | C17—N4—C15—C12 | 158.02 (17) |
| C2—C1—C6—C5 | 0.7 (3) | C13—C12—C15—O1 | 177.9 (2) |
| N1—C1—C6—C5 | −175.93 (17) | N3—C12—C15—O1 | −0.8 (4) |
| N2—N1—C7—C8 | 0.1 (2) | C13—C12—C15—N4 | −1.4 (2) |
| C1—N1—C7—C8 | 178.39 (18) | N3—C12—C15—N4 | 179.85 (18) |
| N2—N1—C7—Cl1 | −176.18 (13) | C15—N4—C17—C22 | 67.4 (3) |
| C1—N1—C7—Cl1 | 2.1 (3) | N5—N4—C17—C22 | −143.73 (18) |
| N1—C7—C8—C9 | 0.0 (2) | C15—N4—C17—C18 | −111.6 (2) |
| Cl1—C7—C8—C9 | 176.01 (15) | N5—N4—C17—C18 | 37.3 (3) |
| N1—C7—C8—C11 | 179.71 (17) | C22—C17—C18—C19 | 0.3 (3) |
| Cl1—C7—C8—C11 | −4.3 (3) | N4—C17—C18—C19 | 179.23 (18) |
| N1—N2—C9—C8 | 0.2 (2) | C17—C18—C19—C20 | −1.4 (3) |
| N1—N2—C9—C10 | −179.94 (16) | C18—C19—C20—C21 | 1.0 (3) |
| C7—C8—C9—N2 | −0.1 (2) | C19—C20—C21—C22 | 0.4 (3) |
| C11—C8—C9—N2 | −179.82 (18) | C18—C17—C22—C21 | 1.1 (3) |
| C7—C8—C9—C10 | −179.97 (19) | N4—C17—C22—C21 | −177.85 (17) |
| C11—C8—C9—C10 | 0.3 (3) | C20—C21—C22—C17 | −1.5 (3) |
| C12—N3—C11—C8 | −179.42 (16) | | |