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4-(4-Chlorophenyl)-5-(4-nitrophenyl)-3-phenyl-4*H*-1,2,4-triazole

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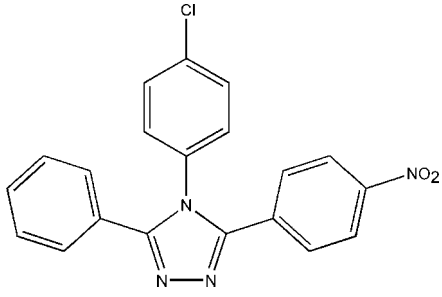
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.004 Å; R factor = 0.059; wR factor = 0.149; data-to-parameter ratio = 12.5.

The title compound, $C_{20}H_{13}ClN_4O_2$, was synthesized by the condensation of 4-nitrobenzohydrazide and *N*-(4-chlorophenyl)benzimidoyl chloride in *N*,*N*-dimethylacetamide. The asymmetric unit contains two independent molecules. In one molecule, the triazole ring is oriented at dihedral angles of 23.1 (5), 85.4 (1) and 10.5 (1)° with respect to the phenyl, chlorophenyl and nitrophenyl rings, respectively. In the other molecule, the corresponding dihedral angles are 29.8 (9), 73.4 (7) and 16.4 (3)°.

Related literature

For related literature, see: Kido *et al.* (1993); Li *et al.* (2006); Zhu *et al.* (2000, 2001).



Experimental

Crystal data

$C_{20}H_{13}ClN_4O_2$
M_r = 376.79
Monoclinic, $P2_1/c$
a = 11.4042 (7) Å
b = 7.1250 (4) Å
c = 43.506 (3) Å
β = 96.789 (4)°
V = 3510.3 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 113 (2) K
0.20 × 0.18 × 0.10 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.953, T_{max} = 0.976
19182 measured reflections
6106 independent reflections
4422 reflections with $I > 2\sigma(I)$
R_{int} = 0.063

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.149
S = 1.07
6106 reflections
489 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Rigaku/MSC, 2004); software used to prepare material for publication: *CrystalStructure*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2206).

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supplementary materials

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4-(4-Chlorophenyl)-5-(4-nitrophenyl)-3-phenyl-4*H*-1,2,4-triazole

J. Hu, H. Song, G. Chen and G. Ma

Comment

In recent years, the 1,2,4-triazole derivatives have received attention (Zhu *et al.*, 2000 and Zhu *et al.*, 2001, Kido *et al.*, 1993 and Li *et al.*, 2006). We report here the crystal structure of 4-(4-chlorophenyl)-3-pheny-5-(4-nitrophenyl)-1,2,4-triazole.

In the molecule of the title compound, (I), (Fig. 1), the asymmetric unit contains two independent molecules and the bond lengths and angles are within normal ranges. In one of the molecules, the triazole ring is oriented with dihedral angles of 9.8 (0), 23.1 (5) and 88.0 (7) ° with respect to the nitrophenyl, phenyl and chlorophenyl rings, respectively. In the other molecule the triazole ring is oriented with dihedral angles of 15.7 (1), 29.8 (7) and 73.7 (4) ° with respect to the nitrophenyl, phenyl and chlorophenyl rings, respectively.

Experimental

4-(4-chlorophenyl)-3-pheny-5-(4-nitrophenyl)-1,2,4-triazole was synthesized by the reaction of 4-nitrobenzohydrazide (2.0 g, 11.0 mmol) and *N*-(4-clorophenyl)-benzimidoyl chloride (2.75 g, 11.0 mmol) in *N*,*N*-dimethyl-acetamide (20 ml). The mixture was stirred and refluxed for 5 h. After cooling, the product crystallized from the orange reaction mixture. It was filtered off, washed with *N*,*N*-dimethyl-acetamide and dried in vacuo. The crude sample was purified on a silica-gel column using an cyclohexane-ethyl acetate (1:10 *v*/*v*) solvent mixture as eluant. The compound was crystallized by slow evaporation of the ethyl acetate solution in 15 d (yield; 57%, m.p. 507 K).

Refinement

H atoms were positioned geometrically,with C—H = 0.93 for aromatic H, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.2 for aromatic H.

Figures

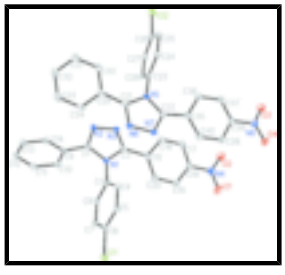


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

4-(4-Chlorophenyl)-5-(4-nitrophenyl)-3-phenyl-4*H*-1,2,4-triazole

Crystal data

$C_{20}H_{13}ClN_4O_2$	$D_x = 1.426$ Mg m^{-3}
$M_r = 376.79$	Melting point: 507 K
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71070$ Å
$a = 11.4042$ (7) Å	Cell parameters from 5260 reflections
$b = 7.1250$ (4) Å	$\theta = 1.8$–28.0º
$c = 43.506$ (3) Å	$\mu = 0.24$ mm^{-1}
$\beta = 96.789$ (4)º	$T = 113$ (2) K
$V = 3510.3$ (4) Å^3	Prism, colorless
$Z = 8$	0.20 × 0.18 × 0.10 mm
$F_{000} = 1552$	

Data collection

Rigaku Saturn diffractometer	4422 reflections with $I > 2\sigma(I)$
Radiation source: Rotating anode	$R_{int} = 0.063$
Monochromator: confocal	$\theta_{max} = 25.0$º
$T = 113$(2) K	$\theta_{min} = 1.8$º
ω scans	$h = -13\rightarrow13$
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	$k = -8\rightarrow8$
$T_{min} = 0.953$, $T_{max} = 0.976$	$l = -51\rightarrow51$
19182 measured reflections	Standard reflections: ?
6106 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.059$	$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2 + 0.6306P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.149$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.07$	$\Delta\rho_{max} = 0.41$ e Å^{-3}
6106 reflections	$\Delta\rho_{min} = -0.30$ e Å^{-3}
489 parameters	Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0049 (6)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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	1.38208 (6)	0.24773 (10)	0.171553 (16)	0.0289 (2)
Cl2	0.10925 (6)	0.74945 (11)	0.093692 (18)	0.0385 (3)
O1	0.9219 (2)	0.1877 (5)	−0.01222 (5)	0.0773 (9)
O2	0.7337 (2)	0.2379 (4)	−0.02133 (5)	0.0628 (8)
O3	0.58746 (19)	0.7653 (3)	−0.04897 (5)	0.0414 (6)
O4	0.78012 (19)	0.7469 (3)	−0.04580 (5)	0.0396 (6)
N1	0.85403 (19)	0.2199 (3)	0.15324 (5)	0.0210 (5)
N2	0.67085 (19)	0.2131 (3)	0.16657 (5)	0.0243 (6)
N3	0.66417 (19)	0.2252 (3)	0.13432 (5)	0.0223 (5)
N4	0.8253 (3)	0.2192 (4)	−0.00327 (6)	0.0430 (7)
N5	0.63553 (18)	0.7487 (3)	0.11974 (5)	0.0199 (5)
N6	0.81267 (19)	0.7365 (3)	0.14752 (5)	0.0240 (6)
N7	0.82888 (19)	0.7458 (3)	0.11606 (5)	0.0244 (6)
N8	0.6869 (2)	0.7568 (3)	−0.03384 (5)	0.0303 (6)
C1	0.7847 (2)	0.2086 (4)	0.17762 (6)	0.0216 (6)
C2	0.7737 (2)	0.2294 (4)	0.12665 (6)	0.0208 (6)
C3	0.9823 (2)	0.2244 (4)	0.15602 (6)	0.0207 (6)
C4	1.0401 (2)	0.3942 (4)	0.15194 (6)	0.0233 (7)
H4	0.9960	0.5041	0.1460	0.028*
C5	1.1634 (2)	0.4007 (4)	0.15672 (6)	0.0227 (6)
H5	1.2036	0.5152	0.1541	0.027*
C6	1.2271 (2)	0.2373 (4)	0.16536 (6)	0.0220 (6)
C7	1.1694 (2)	0.0653 (4)	0.16860 (6)	0.0267 (7)
H7	1.2137	−0.0453	0.1739	0.032*
C8	1.0458 (2)	0.0589 (4)	0.16395 (6)	0.0245 (7)
H8	1.0054	−0.0560	0.1661	0.029*
C9	0.8272 (2)	0.1976 (4)	0.21123 (6)	0.0220 (6)
C10	0.9332 (2)	0.2813 (4)	0.22481 (6)	0.0242 (7)
H10	0.9841	0.3409	0.2120	0.029*
C11	0.9638 (3)	0.2771 (4)	0.25688 (6)	0.0261 (7)
H11	1.0344	0.3361	0.2658	0.031*
C12	0.8905 (2)	0.1861 (4)	0.27591 (6)	0.0259 (7)
H12	0.9117	0.1824	0.2977	0.031*

C13	0.7862 (2)	0.1009 (4)	0.26271 (6)	0.0263 (7)
H13	0.7372	0.0376	0.2756	0.032*
C14	0.7532 (2)	0.1079 (4)	0.23058 (6)	0.0233 (7)
H14	0.6811	0.0524	0.2219	0.028*
C15	0.7973 (2)	0.2343 (4)	0.09377 (6)	0.0217 (6)
C16	0.7004 (3)	0.2805 (4)	0.07159 (6)	0.0277 (7)
H16	0.6272	0.3145	0.0784	0.033*
C17	0.7105 (3)	0.2770 (4)	0.04030 (7)	0.0298 (7)
H17	0.6447	0.3075	0.0257	0.036*
C18	0.8175 (3)	0.2289 (4)	0.03045 (6)	0.0300 (7)
C19	0.9163 (3)	0.1831 (5)	0.05147 (7)	0.0347 (8)
H19	0.9891	0.1502	0.0443	0.042*
C20	0.9053 (3)	0.1869 (4)	0.08318 (7)	0.0318 (7)
H20	0.9715	0.1571	0.0977	0.038*
C21	0.6967 (2)	0.7373 (4)	0.14949 (6)	0.0206 (6)
C22	0.7228 (2)	0.7529 (4)	0.09990 (6)	0.0209 (6)
C23	0.5074 (2)	0.7492 (4)	0.11195 (6)	0.0204 (6)
C24	0.4473 (2)	0.9204 (4)	0.10807 (6)	0.0233 (7)
H24	0.4896	1.0355	0.1098	0.028*
C25	0.3244 (2)	0.9199 (4)	0.10167 (6)	0.0249 (7)
H25	0.2821	1.0348	0.0992	0.030*
C26	0.2640 (2)	0.7481 (4)	0.09893 (6)	0.0245 (7)
C27	0.3248 (2)	0.5776 (4)	0.10190 (6)	0.0267 (7)
H27	0.2827	0.4625	0.0993	0.032*
C28	0.4478 (2)	0.5766 (4)	0.10870 (6)	0.0231 (7)
H28	0.4901	0.4616	0.1111	0.028*
C29	0.6464 (2)	0.7224 (4)	0.17946 (6)	0.0220 (6)
C30	0.5332 (2)	0.7865 (4)	0.18415 (6)	0.0279 (7)
H30	0.4835	0.8414	0.1675	0.034*
C31	0.4937 (3)	0.7697 (4)	0.21329 (7)	0.0292 (7)
H31	0.4171	0.8134	0.2162	0.035*
C32	0.5654 (3)	0.6895 (4)	0.23807 (7)	0.0345 (8)
H32	0.5378	0.6784	0.2577	0.041*
C33	0.6789 (3)	0.6254 (4)	0.23369 (7)	0.0342 (8)
H33	0.7283	0.5705	0.2504	0.041*
C34	0.7190 (2)	0.6427 (4)	0.20469 (6)	0.0275 (7)
H34	0.7960	0.6004	0.2019	0.033*
C35	0.7066 (2)	0.7586 (4)	0.06532 (6)	0.0227 (7)
C36	0.5977 (3)	0.7906 (4)	0.04670 (7)	0.0318 (8)
H36	0.5283	0.8129	0.0562	0.038*
C37	0.5918 (3)	0.7894 (4)	0.01435 (7)	0.0323 (8)
H37	0.5186	0.8097	0.0019	0.039*
C38	0.6938 (3)	0.7585 (4)	0.00055 (6)	0.0254 (7)
C39	0.8036 (3)	0.7287 (4)	0.01803 (7)	0.0320 (8)
H39	0.8728	0.7093	0.0083	0.038*
C40	0.8080 (3)	0.7285 (4)	0.05017 (6)	0.0292 (7)
H40	0.8816	0.7074	0.0623	0.035*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0160 (4)	0.0375 (5)	0.0327 (4)	0.0006 (3)	0.0007 (3)	0.0020 (3)
Cl2	0.0158 (4)	0.0543 (6)	0.0437 (5)	−0.0011 (3)	−0.0030 (3)	0.0077 (4)
O1	0.0364 (16)	0.164 (3)	0.0327 (14)	−0.0007 (17)	0.0086 (12)	−0.0042 (16)
O2	0.0404 (15)	0.121 (3)	0.0253 (12)	0.0068 (14)	−0.0039 (11)	0.0018 (13)
O3	0.0318 (13)	0.0629 (17)	0.0273 (11)	−0.0014 (11)	−0.0063 (10)	−0.0002 (11)
O4	0.0327 (13)	0.0587 (17)	0.0281 (11)	−0.0005 (11)	0.0062 (10)	−0.0019 (10)
N1	0.0193 (12)	0.0231 (14)	0.0203 (11)	0.0015 (10)	0.0009 (9)	−0.0006 (10)
N2	0.0207 (13)	0.0278 (15)	0.0231 (12)	−0.0007 (10)	−0.0022 (10)	0.0000 (10)
N3	0.0175 (13)	0.0255 (14)	0.0235 (12)	−0.0006 (10)	0.0005 (10)	−0.0015 (10)
N4	0.0365 (17)	0.066 (2)	0.0266 (14)	−0.0034 (15)	0.0036 (13)	0.0009 (14)
N5	0.0145 (12)	0.0231 (14)	0.0214 (11)	0.0012 (9)	−0.0007 (9)	−0.0016 (10)
N6	0.0196 (13)	0.0274 (15)	0.0240 (12)	0.0024 (10)	−0.0014 (10)	−0.0020 (11)
N7	0.0187 (13)	0.0284 (15)	0.0248 (12)	0.0014 (10)	−0.0019 (10)	−0.0005 (11)
N8	0.0286 (15)	0.0354 (17)	0.0263 (13)	−0.0022 (12)	0.0011 (12)	−0.0014 (12)
C1	0.0190 (15)	0.0207 (16)	0.0253 (14)	−0.0011 (12)	0.0038 (12)	0.0020 (12)
C2	0.0209 (15)	0.0167 (16)	0.0241 (14)	−0.0005 (12)	0.0002 (12)	−0.0002 (12)
C3	0.0162 (14)	0.0282 (17)	0.0173 (13)	−0.0002 (12)	0.0005 (11)	−0.0036 (12)
C4	0.0217 (15)	0.0228 (17)	0.0252 (14)	0.0012 (12)	0.0014 (12)	0.0000 (13)
C5	0.0204 (15)	0.0241 (17)	0.0243 (14)	−0.0030 (12)	0.0058 (12)	0.0021 (12)
C6	0.0157 (14)	0.0282 (18)	0.0216 (14)	0.0014 (12)	0.0000 (11)	−0.0006 (12)
C7	0.0218 (16)	0.0227 (18)	0.0354 (16)	0.0041 (12)	0.0017 (13)	0.0038 (13)
C8	0.0227 (16)	0.0232 (17)	0.0272 (15)	−0.0024 (12)	0.0010 (12)	0.0021 (13)
C9	0.0215 (15)	0.0220 (17)	0.0223 (14)	0.0026 (12)	0.0015 (11)	−0.0020 (12)
C10	0.0229 (16)	0.0272 (18)	0.0224 (14)	−0.0021 (12)	0.0021 (12)	−0.0033 (13)
C11	0.0261 (16)	0.0236 (17)	0.0278 (15)	−0.0003 (13)	−0.0008 (12)	−0.0032 (13)
C12	0.0346 (18)	0.0220 (17)	0.0212 (14)	0.0038 (13)	0.0031 (13)	−0.0015 (12)
C13	0.0313 (17)	0.0202 (17)	0.0284 (15)	0.0022 (13)	0.0074 (13)	−0.0006 (13)
C14	0.0229 (15)	0.0220 (17)	0.0258 (14)	−0.0011 (12)	0.0060 (12)	−0.0004 (12)
C15	0.0213 (15)	0.0206 (17)	0.0226 (14)	−0.0013 (12)	−0.0001 (12)	0.0007 (12)
C16	0.0224 (16)	0.0305 (18)	0.0295 (16)	0.0048 (13)	0.0002 (12)	0.0022 (13)
C17	0.0222 (16)	0.039 (2)	0.0272 (15)	−0.0006 (14)	−0.0036 (12)	0.0019 (14)
C18	0.0316 (18)	0.034 (2)	0.0240 (15)	−0.0040 (14)	0.0037 (13)	0.0006 (14)
C19	0.0223 (16)	0.052 (2)	0.0298 (16)	0.0032 (15)	0.0029 (13)	−0.0048 (15)
C20	0.0216 (16)	0.046 (2)	0.0271 (15)	0.0009 (14)	−0.0018 (12)	−0.0026 (14)
C21	0.0170 (15)	0.0177 (16)	0.0259 (14)	−0.0004 (11)	−0.0029 (11)	−0.0030 (12)
C22	0.0150 (14)	0.0219 (17)	0.0255 (14)	0.0003 (12)	0.0015 (11)	−0.0014 (12)
C23	0.0137 (14)	0.0277 (18)	0.0196 (13)	0.0017 (12)	0.0006 (11)	0.0005 (12)
C24	0.0208 (15)	0.0222 (17)	0.0265 (15)	0.0019 (12)	0.0013 (12)	0.0015 (12)
C25	0.0205 (16)	0.0276 (18)	0.0264 (15)	0.0055 (13)	0.0022 (12)	0.0057 (13)
C26	0.0146 (14)	0.038 (2)	0.0203 (14)	0.0010 (13)	0.0007 (11)	0.0029 (13)
C27	0.0249 (16)	0.0310 (19)	0.0241 (15)	−0.0063 (13)	0.0020 (12)	−0.0025 (13)
C28	0.0213 (16)	0.0253 (17)	0.0233 (14)	0.0017 (12)	0.0054 (12)	−0.0038 (12)
C29	0.0229 (16)	0.0168 (16)	0.0256 (14)	−0.0002 (12)	−0.0004 (12)	−0.0042 (12)
C30	0.0271 (17)	0.0308 (18)	0.0251 (15)	−0.0004 (13)	0.0001 (12)	−0.0026 (13)

C31	0.0253 (16)	0.0288 (18)	0.0336 (16)	−0.0045 (13)	0.0044 (13)	−0.0042 (14)
C32	0.046 (2)	0.0313 (19)	0.0279 (16)	−0.0069 (15)	0.0093 (14)	0.0019 (14)
C33	0.047 (2)	0.0252 (19)	0.0285 (16)	0.0007 (15)	−0.0031 (15)	0.0046 (14)
C34	0.0271 (16)	0.0233 (17)	0.0310 (16)	0.0023 (13)	−0.0015 (13)	0.0001 (13)
C35	0.0189 (15)	0.0212 (17)	0.0273 (15)	0.0000 (12)	−0.0007 (12)	0.0001 (12)
C36	0.0238 (17)	0.042 (2)	0.0303 (16)	0.0052 (14)	0.0042 (13)	−0.0020 (14)
C37	0.0214 (16)	0.045 (2)	0.0287 (16)	0.0048 (14)	−0.0044 (13)	−0.0036 (14)
C38	0.0311 (17)	0.0252 (18)	0.0192 (14)	−0.0040 (13)	−0.0003 (12)	0.0009 (12)
C39	0.0212 (16)	0.045 (2)	0.0299 (16)	−0.0010 (14)	0.0027 (13)	−0.0002 (15)
C40	0.0198 (16)	0.039 (2)	0.0276 (16)	−0.0023 (13)	−0.0016 (12)	−0.0014 (14)

Geometric parameters (Å, °)

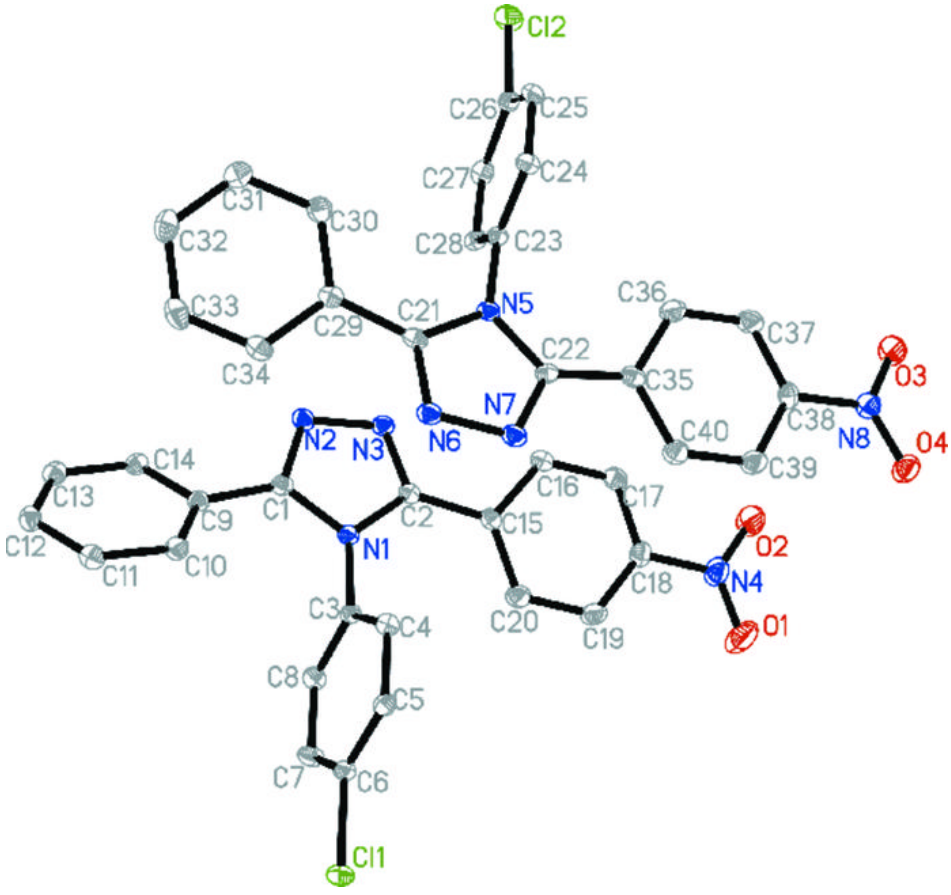
Cl1—C6	1.757 (3)	C15—C20	1.406 (4)
Cl2—C26	1.752 (3)	C15—C16	1.417 (4)
O1—N4	1.231 (3)	C16—C17	1.380 (4)
O2—N4	1.238 (3)	C16—H16	0.9500
O3—N8	1.244 (3)	C17—C18	1.383 (4)
O4—N8	1.240 (3)	C17—H17	0.9500
N1—C2	1.390 (3)	C18—C19	1.403 (4)
N1—C1	1.398 (3)	C19—C20	1.400 (4)
N1—C3	1.454 (3)	C19—H19	0.9500
N2—C1	1.330 (3)	C20—H20	0.9500
N2—N3	1.399 (3)	C21—C29	1.490 (4)
N3—C2	1.330 (3)	C22—C35	1.494 (4)
N4—C18	1.482 (4)	C23—C24	1.400 (4)
N5—C22	1.392 (3)	C23—C28	1.404 (4)
N5—C21	1.398 (3)	C24—C25	1.396 (3)
N5—C23	1.460 (3)	C24—H24	0.9500
N6—C21	1.335 (3)	C25—C26	1.403 (4)
N6—N7	1.404 (3)	C25—H25	0.9500
N7—C22	1.327 (3)	C26—C27	1.397 (4)
N8—C38	1.489 (3)	C27—C28	1.399 (4)
C1—C9	1.487 (4)	C27—H27	0.9500
C2—C15	1.487 (4)	C28—H28	0.9500
C3—C4	1.399 (4)	C29—C30	1.406 (4)
C3—C8	1.405 (4)	C29—C34	1.413 (4)
C4—C5	1.397 (3)	C30—C31	1.400 (4)
C4—H4	0.9500	C30—H30	0.9500
C5—C6	1.400 (4)	C31—C32	1.396 (4)
C5—H5	0.9500	C31—H31	0.9500
C6—C7	1.406 (4)	C32—C33	1.407 (4)
C7—C8	1.401 (4)	C32—H32	0.9500
C7—H7	0.9500	C33—C34	1.397 (4)
C8—H8	0.9500	C33—H33	0.9500
C9—C10	1.413 (4)	C34—H34	0.9500
C9—C14	1.414 (4)	C35—C40	1.413 (4)
C10—C11	1.398 (4)	C35—C36	1.419 (4)
C10—H10	0.9500	C36—C37	1.401 (4)

C11—C12	1.403 (4)	C36—H36	0.9500
C11—H11	0.9500	C37—C38	1.388 (4)
C12—C13	1.397 (4)	C37—H37	0.9500
C12—H12	0.9500	C38—C39	1.401 (4)
C13—C14	1.405 (4)	C39—C40	1.393 (4)
C13—H13	0.9500	C39—H39	0.9500
C14—H14	0.9500	C40—H40	0.9500
C2—N1—C1	104.9 (2)	C17—C18—N4	118.5 (3)
C2—N1—C3	128.8 (2)	C19—C18—N4	119.8 (3)
C1—N1—C3	126.3 (2)	C20—C19—C18	118.6 (3)
C1—N2—N3	107.4 (2)	C20—C19—H19	120.7
C2—N3—N2	108.1 (2)	C18—C19—H19	120.7
O1—N4—O2	122.6 (3)	C19—C20—C15	120.8 (3)
O1—N4—C18	118.9 (3)	C19—C20—H20	119.6
O2—N4—C18	118.6 (3)	C15—C20—H20	119.6
C22—N5—C21	105.1 (2)	N6—C21—N5	109.3 (2)
C22—N5—C23	128.7 (2)	N6—C21—C29	122.9 (2)
C21—N5—C23	126.2 (2)	N5—C21—C29	127.8 (2)
C21—N6—N7	107.9 (2)	N7—C22—N5	110.2 (2)
C22—N7—N6	107.5 (2)	N7—C22—C35	122.0 (2)
O4—N8—O3	123.6 (2)	N5—C22—C35	127.8 (2)
O4—N8—C38	118.4 (2)	C24—C23—C28	121.8 (2)
O3—N8—C38	118.0 (2)	C24—C23—N5	119.5 (2)
N2—C1—N1	109.9 (2)	C28—C23—N5	118.7 (2)
N2—C1—C9	123.2 (2)	C25—C24—C23	119.2 (3)
N1—C1—C9	126.9 (2)	C25—C24—H24	120.4
N3—C2—N1	109.7 (2)	C23—C24—H24	120.4
N3—C2—C15	121.6 (2)	C24—C25—C26	119.4 (3)
N1—C2—C15	128.7 (2)	C24—C25—H25	120.3
C4—C3—C8	121.3 (2)	C26—C25—H25	120.3
C4—C3—N1	119.5 (2)	C27—C26—C25	121.2 (2)
C8—C3—N1	119.1 (2)	C27—C26—Cl2	119.9 (2)
C5—C4—C3	119.4 (2)	C25—C26—Cl2	118.9 (2)
C5—C4—H4	120.3	C26—C27—C28	119.9 (3)
C3—C4—H4	120.3	C26—C27—H27	120.1
C4—C5—C6	119.6 (3)	C28—C27—H27	120.1
C4—C5—H5	120.2	C27—C28—C23	118.6 (3)
C6—C5—H5	120.2	C27—C28—H28	120.7
C5—C6—C7	121.1 (2)	C23—C28—H28	120.7
C5—C6—Cl1	119.2 (2)	C30—C29—C34	118.8 (3)
C7—C6—Cl1	119.7 (2)	C30—C29—C21	124.0 (2)
C8—C7—C6	119.3 (3)	C34—C29—C21	117.2 (2)
C8—C7—H7	120.4	C31—C30—C29	120.2 (3)
C6—C7—H7	120.4	C31—C30—H30	119.9
C7—C8—C3	119.3 (3)	C29—C30—H30	119.9
C7—C8—H8	120.4	C32—C31—C30	120.8 (3)
C3—C8—H8	120.4	C32—C31—H31	119.6
C10—C9—C14	118.9 (2)	C30—C31—H31	119.6
C10—C9—C1	123.6 (2)	C31—C32—C33	119.5 (3)

C14—C9—C1	117.4 (2)	C31—C32—H32	120.2
C11—C10—C9	120.6 (3)	C33—C32—H32	120.2
C11—C10—H10	119.7	C34—C33—C32	119.9 (3)
C9—C10—H10	119.7	C34—C33—H33	120.1
C10—C11—C12	120.2 (3)	C32—C33—H33	120.1
C10—C11—H11	119.9	C33—C34—C29	120.9 (3)
C12—C11—H11	119.9	C33—C34—H34	119.6
C13—C12—C11	119.7 (2)	C29—C34—H34	119.6
C13—C12—H12	120.1	C40—C35—C36	117.8 (3)
C11—C12—H12	120.1	C40—C35—C22	117.1 (2)
C12—C13—C14	120.6 (3)	C36—C35—C22	125.1 (3)
C12—C13—H13	119.7	C37—C36—C35	120.5 (3)
C14—C13—H13	119.7	C37—C36—H36	119.7
C13—C14—C9	120.0 (3)	C35—C36—H36	119.7
C13—C14—H14	120.0	C38—C37—C36	119.5 (3)
C9—C14—H14	120.0	C38—C37—H37	120.3
C20—C15—C16	118.4 (3)	C36—C37—H37	120.3
C20—C15—C2	125.1 (2)	C37—C38—C39	122.0 (3)
C16—C15—C2	116.4 (2)	C37—C38—N8	119.2 (2)
C17—C16—C15	121.2 (3)	C39—C38—N8	118.8 (3)
C17—C16—H16	119.4	C40—C39—C38	117.9 (3)
C15—C16—H16	119.4	C40—C39—H39	121.0
C16—C17—C18	119.3 (3)	C38—C39—H39	121.0
C16—C17—H17	120.3	C39—C40—C35	122.3 (3)
C18—C17—H17	120.3	C39—C40—H40	118.9
C17—C18—C19	121.7 (3)	C35—C40—H40	118.9
C1—N2—N3—C2	−0.5 (3)	C2—C15—C20—C19	175.4 (3)
C21—N6—N7—C22	0.3 (3)	N7—N6—C21—N5	−0.5 (3)
N3—N2—C1—N1	0.7 (3)	N7—N6—C21—C29	177.9 (2)
N3—N2—C1—C9	179.4 (2)	C22—N5—C21—N6	0.5 (3)
C2—N1—C1—N2	−0.7 (3)	C23—N5—C21—N6	178.6 (2)
C3—N1—C1—N2	178.2 (2)	C22—N5—C21—C29	−177.8 (2)
C2—N1—C1—C9	−179.3 (3)	C23—N5—C21—C29	0.3 (4)
C3—N1—C1—C9	−0.4 (4)	N6—N7—C22—N5	0.1 (3)
N2—N3—C2—N1	0.1 (3)	N6—N7—C22—C35	−178.3 (2)
N2—N3—C2—C15	177.5 (2)	C21—N5—C22—N7	−0.3 (3)
C1—N1—C2—N3	0.3 (3)	C23—N5—C22—N7	−178.4 (2)
C3—N1—C2—N3	−178.5 (2)	C21—N5—C22—C35	177.9 (2)
C1—N1—C2—C15	−176.8 (3)	C23—N5—C22—C35	−0.1 (4)
C3—N1—C2—C15	4.3 (4)	C22—N5—C23—C24	−87.9 (3)
C2—N1—C3—C4	74.4 (3)	C21—N5—C23—C24	94.5 (3)
C1—N1—C3—C4	−104.2 (3)	C22—N5—C23—C28	92.4 (3)
C2—N1—C3—C8	−108.0 (3)	C21—N5—C23—C28	−85.2 (3)
C1—N1—C3—C8	73.4 (3)	C28—C23—C24—C25	1.9 (4)
C8—C3—C4—C5	−1.9 (4)	N5—C23—C24—C25	−177.8 (2)
N1—C3—C4—C5	175.6 (2)	C23—C24—C25—C26	−0.7 (4)
C3—C4—C5—C6	0.3 (4)	C24—C25—C26—C27	−1.3 (4)
C4—C5—C6—C7	1.6 (4)	C24—C25—C26—Cl2	175.4 (2)
C4—C5—C6—Cl1	−179.57 (19)	C25—C26—C27—C28	2.1 (4)

C5—C6—C7—C8	−1.8 (4)	Cl2—C26—C27—C28	−174.6 (2)
Cl1—C6—C7—C8	179.3 (2)	C26—C27—C28—C23	−0.9 (4)
C6—C7—C8—C3	0.3 (4)	C24—C23—C28—C27	−1.1 (4)
C4—C3—C8—C7	1.6 (4)	N5—C23—C28—C27	178.6 (2)
N1—C3—C8—C7	−175.9 (2)	N6—C21—C29—C30	156.8 (3)
N2—C1—C9—C10	−147.5 (3)	N5—C21—C29—C30	−25.1 (4)
N1—C1—C9—C10	30.9 (4)	N6—C21—C29—C34	−21.6 (4)
N2—C1—C9—C14	28.5 (4)	N5—C21—C29—C34	156.5 (3)
N1—C1—C9—C14	−153.0 (3)	C34—C29—C30—C31	−0.5 (4)
C14—C9—C10—C11	−0.6 (4)	C21—C29—C30—C31	−178.9 (2)
C1—C9—C10—C11	175.4 (2)	C29—C30—C31—C32	0.0 (4)
C9—C10—C11—C12	1.3 (4)	C30—C31—C32—C33	0.2 (4)
C10—C11—C12—C13	−0.6 (4)	C31—C32—C33—C34	0.1 (5)
C11—C12—C13—C14	−0.9 (4)	C32—C33—C34—C29	−0.6 (4)
C12—C13—C14—C9	1.6 (4)	C30—C29—C34—C33	0.8 (4)
C10—C9—C14—C13	−0.9 (4)	C21—C29—C34—C33	179.3 (3)
C1—C9—C14—C13	−177.1 (2)	N7—C22—C35—C40	9.0 (4)
N3—C2—C15—C20	−161.3 (3)	N5—C22—C35—C40	−169.0 (2)
N1—C2—C15—C20	15.6 (4)	N7—C22—C35—C36	−171.4 (3)
N3—C2—C15—C16	15.0 (4)	N5—C22—C35—C36	10.5 (4)
N1—C2—C15—C16	−168.1 (3)	C40—C35—C36—C37	0.8 (4)
C20—C15—C16—C17	0.8 (4)	C22—C35—C36—C37	−178.7 (3)
C2—C15—C16—C17	−175.7 (3)	C35—C36—C37—C38	−0.6 (5)
C15—C16—C17—C18	−0.5 (4)	C36—C37—C38—C39	−0.2 (4)
C16—C17—C18—C19	0.0 (5)	C36—C37—C38—N8	179.8 (3)
C16—C17—C18—N4	177.8 (3)	O4—N8—C38—C37	173.2 (2)
O1—N4—C18—C17	175.6 (3)	O3—N8—C38—C37	−6.8 (4)
O2—N4—C18—C17	−6.4 (4)	O4—N8—C38—C39	−6.8 (4)
O1—N4—C18—C19	−6.6 (5)	O3—N8—C38—C39	173.2 (2)
O2—N4—C18—C19	171.4 (3)	C37—C38—C39—C40	0.8 (4)
C17—C18—C19—C20	0.0 (5)	N8—C38—C39—C40	−179.2 (2)
N4—C18—C19—C20	−177.7 (3)	C38—C39—C40—C35	−0.6 (4)
C18—C19—C20—C15	0.4 (5)	C36—C35—C40—C39	−0.2 (4)
C16—C15—C20—C19	−0.8 (4)	C22—C35—C40—C39	179.3 (3)

Fig. 1


Cl2
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