Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-(1-Methylethyl)-*N*-((*E*)-4-{[1-(prop-2-en-1-yl)-1*H*-1,2,3-triazol-4-yl]methoxy}-benzylidene)aniline

Mehmet Akkurt,[a]* Aliasghar Jarrahpour,[b] Mehdi Mohammadi Chermahini,[b] Pezhman Shiri[b] and Muhammad Nawaz Tahir[c]*

[a]Department of Physics, Faculty of Sciences, Erciyes University, 38039 Kayseri, Turkey, [b]Department of Chemistry, College of Sciences, Shiraz University, 71454 Shiraz, Iran, and [c]Department of Physics, University of Sargodha, Sargodha, Pakistan
Correspondence e-mail: akkurt@erciyes.edu.tr, dmntahir_uos@yahoo.com

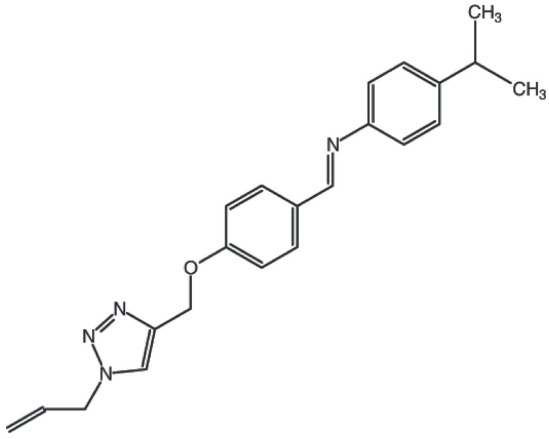
Received 3 January 2013; accepted 8 January 2013

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.068; wR factor = 0.217; data-to-parameter ratio = 13.5.

In the title compound, $C_{22}H_{24}N_4O$, the terminal and central benzene rings make dihedral angles of 52.7 (3) and 43.8 (2)°, respectively, with the triazole ring. The dihedral angle between the benzene rings is 8.9 (2)°. The crystal structure features C—H$\cdots\pi$ interactions. The atoms of the terminal propenyl group are disordered over two sets of sites, with a refined occupancy ratio of 0.714 (14):0.286 (14).

Related literature

For bond-length data, see: Allen *et al.* (1987). For general background to the properties of Schiff bases, see: Ajello & Cusmanos (1940); Dhar & Taploo (1982); Holla *et al.* (2005); Singh *et al.* (2012); Supuran *et al.* (1996).



Experimental

Crystal data

$C_{22}H_{24}N_4O$
M_r = 360.45
Monoclinic, $P2_1/c$
a = 5.5885 (11) Å
b = 8.3929 (18) Å
c = 42.069 (9) Å
β = 92.149 (10)°
V = 1971.8 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.30 × 0.20 × 0.18 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.982, T_{max} = 0.986
13866 measured reflections
3451 independent reflections
1259 reflections with $I > 2\sigma(I)$
R_{int} = 0.082

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.217
S = 0.96
3451 reflections
256 parameters
7 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 and *Cg*3 are the centroids of the N2–N4/C18/C19 1H-1,2,3-triazole and C11–C16 benzene rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C2—H2$\cdots Cg3^{i}$	0.93	2.96	3.752 (5)	144
C8—H8$A\cdots Cg1^{ii}$	0.96	2.80	3.678 (6)	153

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON*.

The authors acknowledge the provision of funds for the purchase of a diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2382).

References

Ajello, T. & Cusmanos, G. (1940). *Chim. Ital.* **70**, 770–778.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dhar, D. N. & Taploo, C. L. (1982). *J. Sci. Ind. Res.* **41**, 501–506.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Holla, B. S., Mahalinga, M., Karthikeyan, M. S., Poojary, B., Akberali, P. M. & Kumari, N. S. (2005). *Eur. J. Med. Chem.* **40**, 1173–1178.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Singh, P., Raj, R., Kumar, V., Mahajan, M. P., Bedi, P. M. S., Kaur, T. & Saxena, A. K. (2012). *Eur. J. Med. Chem.* **47**, 594–600.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Supuran, C. T., Barboiu, M., Luca, C., Pop, E., Brewster, M. E. & Dinculescu, A. (1996). *Eur. J. Med. Chem.* **31**, 597–606.

supporting information

Acta Cryst. (2013). E**69**, o247 [doi:10.1107/S1600536813000755]

4-(1-Methylethyl)-*N*-((*E*)-4-{[1-(prop-2-en-1-yl)-1*H*-1,2,3-triazol-4-yl]methoxy}-benzylidene)aniline

Mehmet Akkurt, Aliasghar Jarrahpour, Mehdi Mohammadi Chermahini, Pezhman Shiri and Muhammad Nawaz Tahir

S1. Comment

Compounds containing an azomethine group (–CH=N–), known as Schiff bases are formed by the condensation of a primary amine with a carbonyl compound. Schiff bases are some of the most widely used organic compounds. They are used as pigments and dyes, catalysts, intermediates in organic synthesis, and as polymer stabilisers (Dhar & Taploo, 1982). In azomethine derivatives, the C=N linkage is essential for biological activity, several azomethines were reported to possess remarkable antibacterial, antifungal, anticancer and diuretic activities (Supuran *et al.*, 1996). Triazoles are also important class of heterocycles because of their varied biological activities (Singh *et al.*, 2012). 1,2,3-triazoles, are five-membered, doubly unsaturated heterocycles, the ring consisting of three sequentially linked nitrogen atoms and two carbon atoms (Ajello & Cusmanos, 1940). The 1,2,3-triazole moiety has several good properties: high chemical stability (hydrolytic, oxidant, and reducing conditions), aromatic character, good hydrogen-bond-accepting ability and this moiety is relatively resistant to metabolic degradation (Holla *et al.*, 2005). Therefore, compound (I), was synthesized and its X-ray studies is reported here.

The C1–C6 and C11–C16 benzene rings of the title compound (I), (Fig. 1), make a dihedral angle of 8.9 (2)° with each other. They form dihedral angles of 52.7 (3) and 43.8 (2) ° with the N2–N4/C18/C19 propenyl ring. The C1—N1—C10—C11, C14—O1—C17—C18 and N4—C20A—C21A—C22A torsion angles are 179.7 (4), -174.2 (3) and 151.9 (14)°, respectively. The values of the bond lengths and bond angles in (I) are normal (Allen *et al.*, 1987).

In the crystal, the molecular packing of (I) is stabilized by C—H···π interactions (Table 1).

S2. Experimental

Reaction of 4-((1-allyl-1*H*-1,2,3-triazol-4-yl)methoxy)benzaldehyde (1.00 mmol) with 4-isopropylbenzenamine (1.00 mmol) in refluxing ethanol gave the title compound. Recrystallization from ethanol gave colourless crystals in 70% yield. Mp: 119–121 0 C. IR (KBr, cm-1):1620 (C=N). 1*H*-NMR(250 MHz, CDCl3) δ (p.p.m.): 1.11 (2CH3, d, 6H, J=7.5), 2.75 (CH, m, 1H), 4.87 (d, 2H, J=5), 5.05 (s, 2H), 5.25 (d, 2H, J=10), 5.92 (m, 1H), 6.71–7.07 (aromatic protons, m, 8H), 7.50 (H triazole, s, 1H), 8.13 (HC═N, s, 1H). 13CNMR δ (p.p.m): 23.9 (2CH3), 33.6 (CH), 52.8 (CH2—N), 61.6 (CH2—O), 114.6–145.3 (aromatic carbons and C=C triazole), 158.5 (C=N).

S3. Refinement

H atoms were placed in calculated positions with C—H = 0.93 - 0.98 Å and refined by using a riding model, with U_{iso}(H) = 1.2Ueq(C) or 1.5Ueq(methyl C). The atoms of the terminal propenyl group, C20, C21 and C22, are disordered over two sites with refined occupancies of 0.714 (14) and 0.286 (14).

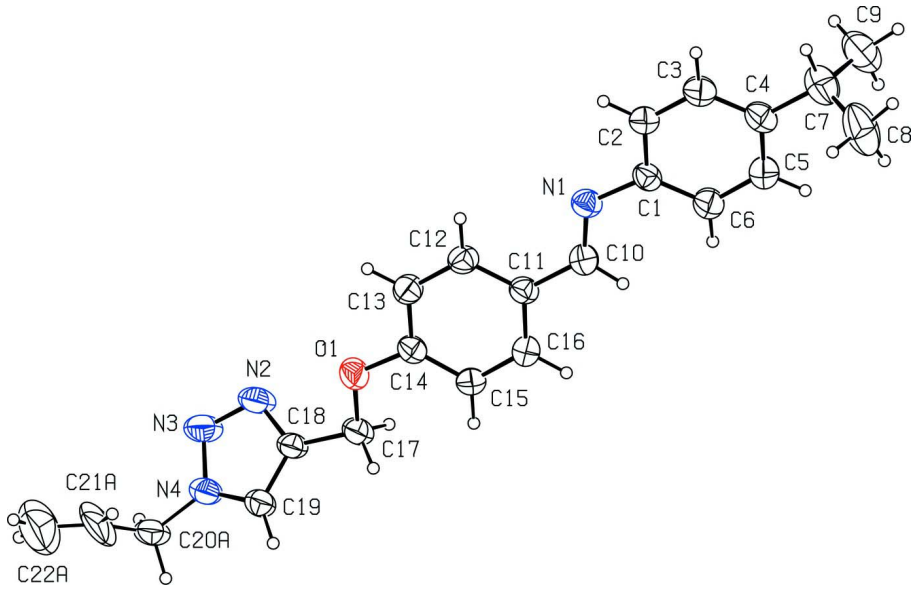


Figure 1

ORTEP drawing of the title compound with atomic numbering scheme and thermal ellipsoids at 30% probability level. The minor disorder component is not shown.

4-(1-Methylethyl)-*N*-((*E*)-4-{[1-(prop-2-en-1-yl)-1*H*- 1,2,3-triazol-4-yl]methoxy}benzylidene)aniline

Crystal data

$C_{22}H_{24}N_4O$
$M_r = 360.45$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.5885$ (11) Å
$b = 8.3929$ (18) Å
$c = 42.069$ (9) Å
$\beta = 92.149$ (10)°
$V = 1971.8$ (7) Å^3
$Z = 4$
$F(000) = 768$
$D_x = 1.214$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 219 reflections
$\theta = 3.5$–21.5°
$\mu = 0.08$ mm^{-1}
$T = 296$ K
Prism, colorless
0.30 × 0.20 × 0.18 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.982$, $T_{max} = 0.986$
13866 measured reflections
3451 independent reflections
1259 reflections with $I > 2\sigma(I)$
$R_{int} = 0.082$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
$h = -6 \rightarrow 4$
$k = -9 \rightarrow 9$
$l = -49 \rightarrow 49$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.217$
$S = 0.96$
3451 reflections
256 parameters
7 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

$w = 1/[\sigma^2(F_o^2) + (0.0893P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.6921 (5)	0.1556 (4)	0.35472 (7)	0.0741 (14)	
N1	0.0796 (6)	0.1766 (4)	0.22415 (8)	0.0634 (14)	
N2	0.7693 (6)	0.0586 (5)	0.41985 (9)	0.0879 (18)	
N3	0.8731 (6)	0.0688 (6)	0.44832 (9)	0.0939 (18)	
N4	1.1055 (6)	0.0885 (5)	0.44413 (9)	0.0762 (16)	
C1	−0.0186 (7)	0.1560 (5)	0.19307 (10)	0.0581 (17)	
C2	−0.2092 (7)	0.2503 (6)	0.18440 (11)	0.0708 (19)	
C3	−0.3158 (8)	0.2422 (6)	0.15464 (12)	0.084 (2)	
C4	−0.2360 (8)	0.1385 (6)	0.13217 (11)	0.0717 (19)	
C5	−0.0502 (9)	0.0411 (6)	0.14117 (11)	0.0805 (19)	
C6	0.0617 (7)	0.0478 (6)	0.17103 (11)	0.0763 (19)	
C7	−0.3528 (10)	0.1319 (8)	0.09917 (12)	0.106 (3)	
C8	−0.1850 (11)	0.1621 (7)	0.07339 (12)	0.137 (3)	
C9	−0.4985 (10)	−0.0154 (8)	0.09435 (12)	0.132 (3)	
C10	0.2749 (8)	0.1146 (5)	0.23238 (10)	0.0681 (19)	
C11	0.3876 (7)	0.1292 (5)	0.26388 (10)	0.0577 (17)	
C12	0.2894 (7)	0.2200 (5)	0.28752 (10)	0.0633 (17)	
C13	0.3977 (7)	0.2279 (5)	0.31714 (10)	0.0653 (19)	
C14	0.6026 (7)	0.1427 (5)	0.32409 (10)	0.0578 (17)	
C15	0.7072 (7)	0.0562 (5)	0.30096 (10)	0.0638 (17)	
C16	0.5967 (8)	0.0500 (5)	0.27125 (10)	0.0683 (19)	
C17	0.8850 (7)	0.0529 (6)	0.36388 (9)	0.0683 (19)	
C18	0.9390 (7)	0.0723 (5)	0.39809 (10)	0.0618 (18)	
C19	1.1516 (7)	0.0906 (5)	0.41344 (10)	0.0684 (19)	
C20A	1.2557 (18)	0.0919 (15)	0.4733 (2)	0.083 (3)	0.714 (14)
C21A	1.251 (2)	0.254 (2)	0.4850 (4)	0.138 (7)	0.714 (14)
C22A	1.272 (2)	0.3163 (18)	0.5105 (3)	0.203 (8)	0.714 (14)
C21B	1.341 (6)	0.263 (6)	0.4899 (12)	0.138 (7)	0.286 (14)
C22B	1.120 (5)	0.342 (4)	0.4916 (8)	0.203 (8)	0.286 (14)
C20B	1.318 (4)	0.118 (5)	0.4674 (6)	0.083 (3)	0.286 (14)

H2	−0.26800	0.32180	0.19910	0.0850*	
H3	−0.44500	0.30850	0.14950	0.1010*	
H8A	−0.08690	0.25270	0.07880	0.2060*	
H8B	−0.27430	0.18290	0.05390	0.2060*	
H8C	−0.08510	0.07040	0.07080	0.2060*	
H9A	−0.39530	−0.10690	0.09540	0.1980*	
H5	0.00360	−0.03290	0.12660	0.0970*	
H6	0.18930	−0.01960	0.17620	0.0910*	
H7	−0.46740	0.22030	0.09820	0.1270*	
H12	0.14840	0.27620	0.28320	0.0760*	
H13	0.33210	0.29140	0.33270	0.0790*	
H15	0.85030	0.00240	0.30520	0.0760*	
H16	0.66660	−0.01020	0.25550	0.0820*	
H17A	1.02500	0.07910	0.35200	0.0820*	
H17B	0.84150	−0.05690	0.35930	0.0820*	
H19	1.30020	0.10220	0.40450	0.0820*	
H20A	1.19370	0.01930	0.48890	0.1000*	0.714 (14)
H20B	1.41820	0.06050	0.46890	0.1000*	0.714 (14)
H21A	1.22690	0.32730	0.46860	0.1660*	0.714 (14)
H22A	1.29690	0.25460	0.52870	0.2430*	0.714 (14)
H22B	1.26220	0.42660	0.51220	0.2430*	0.714 (14)
H9B	−0.58050	−0.01150	0.07390	0.1980*	
H9C	−0.61350	−0.02290	0.11070	0.1980*	
H10	0.35350	0.05510	0.21730	0.0820*	
H20C	1.45990	0.11910	0.45480	0.1000*	0.286 (14)
H20D	1.33110	0.02440	0.48090	0.1000*	0.286 (14)
H21B	1.48080	0.29430	0.50080	0.1660*	0.286 (14)
H22C	0.98690	0.30480	0.48000	0.2430*	0.286 (14)
H22D	1.10720	0.43250	0.50430	0.2430*	0.286 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.077 (2)	0.081 (3)	0.063 (2)	0.0161 (18)	−0.0145 (16)	−0.0069 (16)
N1	0.057 (2)	0.072 (3)	0.061 (2)	0.001 (2)	−0.0013 (19)	0.0060 (19)
N2	0.047 (2)	0.146 (4)	0.070 (3)	0.000 (2)	−0.005 (2)	0.016 (3)
N3	0.052 (2)	0.159 (4)	0.071 (3)	0.003 (3)	0.005 (2)	0.020 (3)
N4	0.049 (2)	0.111 (3)	0.068 (3)	0.002 (2)	−0.007 (2)	0.001 (2)
C1	0.054 (3)	0.066 (3)	0.054 (3)	−0.010 (3)	−0.001 (2)	0.004 (2)
C2	0.056 (3)	0.081 (4)	0.075 (3)	0.009 (3)	−0.004 (2)	−0.013 (3)
C3	0.071 (3)	0.096 (4)	0.084 (4)	0.023 (3)	−0.014 (3)	−0.009 (3)
C4	0.068 (3)	0.080 (4)	0.066 (3)	−0.004 (3)	−0.011 (3)	0.008 (3)
C5	0.078 (3)	0.092 (4)	0.071 (3)	0.008 (3)	−0.002 (3)	−0.014 (3)
C6	0.073 (3)	0.085 (4)	0.070 (3)	0.015 (3)	−0.009 (3)	−0.006 (3)
C7	0.112 (4)	0.122 (6)	0.082 (4)	−0.003 (4)	−0.022 (4)	−0.004 (3)
C8	0.184 (6)	0.154 (6)	0.073 (4)	−0.071 (5)	−0.010 (4)	0.010 (4)
C9	0.112 (4)	0.187 (7)	0.096 (4)	−0.044 (5)	−0.020 (3)	−0.008 (4)
C10	0.069 (3)	0.076 (4)	0.059 (3)	0.001 (3)	0.000 (2)	−0.003 (2)

C11	0.052 (3)	0.067 (3)	0.054 (3)	−0.002 (2)	−0.001 (2)	0.006 (2)
C12	0.059 (3)	0.072 (3)	0.059 (3)	0.010 (2)	0.002 (2)	0.008 (3)
C13	0.066 (3)	0.070 (4)	0.060 (3)	0.008 (3)	0.002 (2)	0.002 (2)
C14	0.056 (3)	0.061 (3)	0.056 (3)	−0.003 (2)	−0.004 (2)	0.005 (2)
C15	0.054 (3)	0.069 (3)	0.068 (3)	0.009 (2)	−0.002 (2)	−0.005 (3)
C16	0.068 (3)	0.075 (4)	0.062 (3)	0.004 (3)	0.003 (2)	−0.011 (3)
C17	0.053 (3)	0.077 (4)	0.074 (3)	0.001 (3)	−0.011 (2)	−0.002 (3)
C18	0.045 (2)	0.080 (4)	0.060 (3)	0.001 (2)	−0.005 (2)	0.005 (3)
C19	0.051 (3)	0.091 (4)	0.063 (3)	−0.009 (3)	−0.001 (2)	0.000 (3)
C20A	0.044 (5)	0.140 (7)	0.065 (5)	−0.006 (5)	0.002 (4)	0.014 (5)
C21A	0.142 (16)	0.172 (9)	0.094 (10)	0.010 (11)	−0.082 (8)	−0.019 (7)
C22A	0.227 (14)	0.216 (13)	0.158 (13)	0.046 (10)	−0.088 (10)	−0.053 (10)
C21B	0.142 (16)	0.172 (9)	0.094 (10)	0.010 (11)	−0.082 (8)	−0.019 (7)
C22B	0.227 (14)	0.216 (13)	0.158 (13)	0.046 (10)	−0.088 (10)	−0.053 (10)
C20B	0.044 (5)	0.140 (7)	0.065 (5)	−0.006 (5)	0.002 (4)	0.014 (5)

Geometric parameters (Å, º)

O1—C14	1.369 (5)	C21B—C22B	1.41 (5)
O1—C17	1.422 (5)	C2—H2	0.9300
N1—C1	1.410 (5)	C3—H3	0.9300
N1—C10	1.246 (6)	C5—H5	0.9300
N2—N3	1.314 (5)	C6—H6	0.9300
N2—C18	1.348 (5)	C7—H7	0.9800
N3—N4	1.328 (5)	C8—H8A	0.9600
N4—C19	1.326 (6)	C8—H8B	0.9600
N4—C20A	1.461 (10)	C8—H8C	0.9600
N4—C20B	1.53 (2)	C9—H9A	0.9600
C1—C2	1.366 (6)	C9—H9B	0.9600
C1—C6	1.385 (6)	C9—H9C	0.9600
C2—C3	1.368 (7)	C10—H10	0.9300
C3—C4	1.372 (7)	C12—H12	0.9300
C4—C5	1.364 (7)	C13—H13	0.9300
C4—C7	1.513 (7)	C15—H15	0.9300
C5—C6	1.383 (7)	C16—H16	0.9300
C7—C8	1.482 (8)	C17—H17A	0.9700
C7—C9	1.490 (9)	C17—H17B	0.9700
C10—C11	1.451 (6)	C19—H19	0.9300
C11—C12	1.383 (6)	C20A—H20A	0.9700
C11—C16	1.370 (6)	C20A—H20B	0.9700
C12—C13	1.366 (6)	C20B—H20C	0.9700
C13—C14	1.372 (6)	C20B—H20D	0.9700
C14—C15	1.363 (6)	C21A—H21A	0.9300
C15—C16	1.374 (6)	C21B—H21B	0.9300
C17—C18	1.468 (6)	C22A—H22A	0.9300
C18—C19	1.340 (6)	C22A—H22B	0.9300
C20A—C21A	1.45 (2)	C22B—H22C	0.9300
C20B—C21B	1.54 (6)	C22B—H22D	0.9300

C21A—C22A	1.20 (2)		
C14—O1—C17	117.0 (3)	C8—C7—H7	106.00
C1—N1—C10	120.9 (4)	C9—C7—H7	106.00
N3—N2—C18	108.4 (3)	C7—C8—H8A	109.00
N2—N3—N4	106.7 (3)	C7—C8—H8B	109.00
N3—N4—C19	111.0 (3)	C7—C8—H8C	109.00
N3—N4—C20A	115.2 (5)	H8A—C8—H8B	109.00
N3—N4—C20B	132.4 (9)	H8A—C8—H8C	109.00
C19—N4—C20A	133.7 (5)	H8B—C8—H8C	110.00
C19—N4—C20B	116.5 (9)	C7—C9—H9A	109.00
N1—C1—C2	116.7 (4)	C7—C9—H9B	109.00
N1—C1—C6	125.2 (4)	C7—C9—H9C	109.00
C2—C1—C6	118.1 (4)	H9A—C9—H9B	110.00
C1—C2—C3	121.6 (4)	H9A—C9—H9C	109.00
C2—C3—C4	121.4 (4)	H9B—C9—H9C	110.00
C3—C4—C5	116.9 (4)	N1—C10—H10	118.00
C3—C4—C7	121.0 (4)	C11—C10—H10	118.00
C5—C4—C7	122.1 (5)	C11—C12—H12	120.00
C4—C5—C6	122.8 (4)	C13—C12—H12	120.00
C1—C6—C5	119.2 (4)	C12—C13—H13	120.00
C4—C7—C8	113.7 (5)	C14—C13—H13	120.00
C4—C7—C9	111.7 (5)	C14—C15—H15	121.00
C8—C7—C9	113.6 (5)	C16—C15—H15	121.00
N1—C10—C11	124.3 (4)	C11—C16—H16	119.00
C10—C11—C12	122.2 (4)	C15—C16—H16	119.00
C10—C11—C16	120.2 (4)	O1—C17—H17A	110.00
C12—C11—C16	117.6 (4)	O1—C17—H17B	110.00
C11—C12—C13	120.6 (4)	C18—C17—H17A	110.00
C12—C13—C14	120.4 (4)	C18—C17—H17B	110.00
O1—C14—C13	115.6 (4)	H17A—C17—H17B	108.00
O1—C14—C15	124.2 (4)	N4—C19—H19	127.00
C13—C14—C15	120.2 (4)	C18—C19—H19	127.00
C14—C15—C16	118.6 (4)	N4—C20A—H20A	110.00
C11—C16—C15	122.5 (4)	N4—C20A—H20B	110.00
O1—C17—C18	108.9 (3)	C21A—C20A—H20A	110.00
N2—C18—C17	122.2 (4)	C21A—C20A—H20B	110.00
N2—C18—C19	108.4 (4)	H20A—C20A—H20B	109.00
C17—C18—C19	129.1 (4)	C21B—C20B—H20C	106.00
N4—C19—C18	105.5 (4)	C21B—C20B—H20D	106.00
N4—C20A—C21A	106.7 (10)	H20C—C20B—H20D	106.00
N4—C20B—C21B	124 (3)	N4—C20B—H20D	106.00
C20A—C21A—C22A	135.6 (16)	N4—C20B—H20C	106.00
C20B—C21B—C22B	111 (3)	C20A—C21A—H21A	112.00
C1—C2—H2	119.00	C22A—C21A—H21A	113.00
C3—C2—H2	119.00	C20B—C21B—H21B	125.00
C2—C3—H3	119.00	C22B—C21B—H21B	124.00
C4—C3—H3	119.00	C21A—C22A—H22A	120.00

C4—C5—H5	119.00	C21A—C22A—H22B	120.00
C6—C5—H5	119.00	H22A—C22A—H22B	120.00
C1—C6—H6	120.00	C21B—C22B—H22C	120.00
C5—C6—H6	120.00	C21B—C22B—H22D	120.00
C4—C7—H7	106.00	H22C—C22B—H22D	120.00

C17—O1—C14—C15	−10.0 (6)	C5—C4—C7—C9	71.5 (6)
C17—O1—C14—C13	171.9 (4)	C3—C4—C7—C9	−107.5 (6)
C14—O1—C17—C18	−174.2 (3)	C7—C4—C5—C6	178.7 (5)
C1—N1—C10—C11	−179.7 (4)	C5—C4—C7—C8	−58.6 (7)
C10—N1—C1—C6	11.9 (6)	C3—C4—C7—C8	122.3 (6)
C10—N1—C1—C2	−168.6 (4)	C4—C5—C6—C1	0.9 (7)
N3—N2—C18—C19	0.3 (5)	N1—C10—C11—C16	176.6 (4)
C18—N2—N3—N4	−0.1 (5)	N1—C10—C11—C12	−2.5 (7)
N3—N2—C18—C17	174.9 (4)	C10—C11—C16—C15	−178.2 (4)
N2—N3—N4—C20A	−176.1 (6)	C10—C11—C12—C13	178.4 (4)
N2—N3—N4—C19	−0.2 (6)	C12—C11—C16—C15	1.0 (6)
N3—N4—C20A—C21A	−84.7 (9)	C16—C11—C12—C13	−0.7 (6)
N3—N4—C19—C18	0.3 (5)	C11—C12—C13—C14	−1.6 (6)
C20A—N4—C19—C18	175.2 (8)	C12—C13—C14—C15	3.6 (6)
C19—N4—C20A—C21A	100.6 (9)	C12—C13—C14—O1	−178.1 (4)
N1—C1—C6—C5	−179.4 (4)	C13—C14—C15—C16	−3.3 (6)
C2—C1—C6—C5	1.1 (7)	O1—C14—C15—C16	178.6 (4)
N1—C1—C2—C3	178.9 (4)	C14—C15—C16—C11	1.0 (6)
C6—C1—C2—C3	−1.6 (7)	O1—C17—C18—N2	53.0 (6)
C1—C2—C3—C4	0.1 (7)	O1—C17—C18—C19	−133.6 (5)
C2—C3—C4—C7	−179.2 (5)	N2—C18—C19—N4	−0.4 (5)
C2—C3—C4—C5	1.8 (7)	C17—C18—C19—N4	−174.5 (4)
C3—C4—C5—C6	−2.3 (7)	N4—C20A—C21A—C22A	151.9 (14)

Hydrogen-bond geometry (Å, º)

Cg1 and Cg3 are the centroids of the N2–N4/C18/C19 1H-1,2,3-triazole and C11–C16 benzene rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···*Cg*3^{i}	0.93	2.96	3.752 (5)	144
C8—H8*A*···*Cg*1^{ii}	0.96	2.80	3.678 (6)	153

Symmetry codes: (i) −*x*, *y*+1/2, −*z*+1/2; (ii) −*x*+1, *y*+1/2, −*z*+1/2.