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(E)-2-(4-tert-Butylphenyl)-1-(4-chloro-1ethyl-3-methyl-1H-pyrazol-5-yl)-2cyanoethenyl 2,2-dimethylpropanoate

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Key indicators: single-crystal X-ray study; T = 296 K; mean σ (C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.087; data-to-parameter ratio = 14.8.

In the title compound, $C_{24}H_{30}ClN_3O_2$, the dihedral angle between the aromatic rings is $30.78 (10)^{\circ}$.

Related literature

For further synthetic details, see: Kenzo et al. (2006); Yang et al. (2009).



Experimental

Crystal data

-	
C ₂₄ H ₃₀ ClN ₃ O ₂	
$M_r = 427.96$	
Monoclinic, $P2_1$	
a = 9.997 (2) Å	
b = 9.563 (2) Å	
c = 12.751 (3) Å	
$\beta = 95.008 \ (4)^{\circ}$	

Data collection

Bruker SMART CCD diffractometer Absorption correction: multi-scan (SADABS; Bruker, 2001) $T_{\min} = 0.951, T_{\max} = 0.965$

Refinement

$$\begin{split} R[F^2 > 2\sigma(F^2)] &= 0.033 \\ wR(F^2) &= 0.087 \end{split}$$
S = 1.044137 reflections 279 parameters 8 restraints

V = 1214.4 (5) Å³ Z = 2Mo $K\alpha$ radiation $\mu = 0.18 \text{ mm}^-$ T = 296 K $0.28 \times 0.22 \times 0.20 \text{ mm}$

6269 measured reflections 4137 independent reflections 3802 reflections with $I > 2\sigma(I)$ $R_{\rm int} = 0.016$

H-atom parameters constrained $\Delta \rho_{\rm max} = 0.11 \text{ e } \text{\AA}^ \Delta \rho_{\rm min} = -0.16 \text{ e } \text{\AA}^{-3}$ Absolute structure: Flack (1983), 1848 Friedel pairs Flack parameter: 0.08 (5)

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5743).

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(*E*)-2-(4-*tert*-Butylphenyl)-1-(4-chloro-1-ethyl-3-methyl-1*H*-pyrazol-5-yl)-2-cyanoethenyl 2,2-dimethylpropanoate

M. Xu, H. Yu and B. Li

Experimental

The title compound was synthesized by 2-(4-(*tert*-butyl) phenyl)-3-(4-chloro-1-ethyl-3-methyl-1*H*-pyrazol-5-yl) -3-hydroxyacrylonitrile (Kenzo *et al.*, 2006) with pivaloyl chloride in THF. The crude products were purified by silica-gel column chromatography and then grown from heptane to afford colorless single crystals suitable for X-ray diffraction. To the mixture of 2-(4-(*tert*-butyl)phenyl)-3-(4-chloro- 1-ethyl-3-methyl-1*H*-pyrazol-5-yl)-3-hydroxyacrylonitrile (0.69 g, 2.0 mmol) and triethyl amine (0.24 g, 2.4 mmol) in THF (10 ml), pivaloyl chloride (0.29 g, 2.4 mmol) was added dropwise at roomtemperature and reacted for 1 h (Yang *et al.*, 2009). After separation through silica gel column chromatography (fluent: ethyl acetate/petroleum ether=1/20), The title product compound was gained as a white solid (0.38 g, 44%).

Anal. Calcd for C₂₄H₃₀Cl₁N₃O₂: C, 67.35; H, 7.07; Cl, 8.28; N, 9.82; O, 7.48. Found: C, 67.33; H, 7.10; N, Cl, 8.25; N, 9.88; O, 7.44. ¹H NMR(DMSO): 1.2 (s, 9H, CO(CH₃)₃), 1.34 (s, 9H, Ph-(CH₃)₃), 1.55 (t, 3H, CH₃), 2.27 (s, 3H, CH₃), 4.21 (q, 2H, N—CH₂), 7.47 (d, 2H, Ph), 7.53 (d, 2H, Ph).

Refinement

Although all H atoms were visible in difference maps, they werefinally placed in geometrically calculated positions, with C-H distances in the range 0.93–0.97 Å, and included in the final refinement in the riding model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$ and $U_{iso}(H) = 1.5U_{eq}(C)$.

Figures



Fig. 1. The molecular structure of (I), with 30% probability displacement ellipsoids.

(E)-2-(4-tert-Butylphenyl)-1-(4-chloro-1-ethyl-3-methyl- 1H-pyrazol-5-yl)-2-cyanoethenyl 2,2-dimethylpropanoate

Crystal data

C ₂₄ H ₃₀ ClN ₃ O ₂	F(000) = 456
$M_r = 427.96$	$D_{\rm x} = 1.170 {\rm ~Mg~m}^{-3}$
Monoclinic, P2 ₁	Mo <i>K</i> α radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2yb	Cell parameters from 3335 reflections

a = 9.997 (2) Å
<i>b</i> = 9.563 (2) Å
c = 12.751 (3) Å
$\beta = 95.008 \ (4)^{\circ}$
$V = 1214.4 (5) \text{ Å}^3$
Z = 2

Data collection

Bruker SMART CCD diffractometer	4137 independent reflections
Radiation source: fine-focus sealed tube	3802 reflections with $I > 2\sigma(I)$
graphite	$R_{\rm int} = 0.016$
phi and ω scans	$\theta_{\text{max}} = 25.0^{\circ}, \ \theta_{\text{min}} = 1.6^{\circ}$
Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2001)	$h = -11 \rightarrow 5$
$T_{\min} = 0.951, T_{\max} = 0.965$	$k = -10 \rightarrow 11$
6269 measured reflections	$l = -15 \rightarrow 15$
Radiation source: fine-focus sealed tube graphite phi and ω scans Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2001) $T_{\min} = 0.951, T_{\max} = 0.965$ 6269 measured reflections	3802 reflections with $I > 2\sigma(I)$ $R_{int} = 0.016$ $\theta_{max} = 25.0^{\circ}, \ \theta_{min} = 1.6^{\circ}$ $h = -11 \rightarrow 5$ $k = -10 \rightarrow 11$ $l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.033$	H-atom parameters constrained
$wR(F^2) = 0.087$	$w = 1/[\sigma^{2}(F_{o}^{2}) + (0.0478P)^{2} + 0.1092P]$ where $P = (F_{o}^{2} + 2F_{c}^{2})/3$
<i>S</i> = 1.04	$(\Delta/\sigma)_{max} < 0.001$
4137 reflections	$\Delta \rho_{max} = 0.11 \text{ e} \text{ Å}^{-3}$
279 parameters	$\Delta \rho_{min} = -0.16 \text{ e } \text{\AA}^{-3}$
8 restraints	Absolute structure: Flack (1983), 1848 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.08 (5)

 $\theta = 2.7-25.8^{\circ}$ $\mu = 0.18 \text{ mm}^{-1}$ T = 296 KBlock, colorless

 $0.28 \times 0.22 \times 0.20 \text{ mm}$

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.

	x	у	Ζ	$U_{\rm iso}*/U_{\rm eq}$
Cl1	0.89003 (6)	1.14801 (5)	0.28949 (4)	0.06542 (17)
01	0.69009 (13)	0.98017 (15)	0.09872 (9)	0.0502 (3)
02	0.59667 (17)	0.80823 (19)	0.18582 (19)	0.0901 (6)
N1	0.92650 (17)	0.75296 (19)	0.23618 (12)	0.0542 (4)
N2	0.99429 (19)	0.7577 (2)	0.33256 (13)	0.0651 (5)
N3	1.1085 (2)	0.7957 (3)	0.01367 (16)	0.0828 (7)
C1	0.5204 (3)	1.1651 (3)	0.1878 (4)	0.1185 (13)
H1A	0.5849	1.1989	0.1423	0.178*
H1B	0.5618	1.1578	0.2584	0.178*
H1C	0.4461	1.2289	0.1863	0.178*
C2	0.4021 (3)	1.0314 (4)	0.0406 (2)	0.1012 (11)
H2A	0.4597	1.0792	-0.0040	0.152*
H2B	0.3194	1.0821	0.0420	0.152*
H2C	0.3838	0.9389	0.0138	0.152*
C3	0.3704 (3)	0.9628 (4)	0.2233 (2)	0.0981 (10)
H3A	0.2958	1.0256	0.2254	0.147*
H3B	0.4142	0.9521	0.2929	0.147*
H3C	0.3388	0.8734	0.1974	0.147*
C4	0.47022 (19)	1.0221 (2)	0.15022 (16)	0.0540 (5)
C5	0.58760 (19)	0.9229 (2)	0.15010 (15)	0.0497 (5)
C6	0.81200 (18)	0.91176 (19)	0.10034 (14)	0.0430 (4)
C7	0.88055 (17)	0.8811 (2)	0.20482 (13)	0.0440 (4)
C8	0.92091 (18)	0.9714 (2)	0.28560 (14)	0.0482 (4)
С9	0.9922 (2)	0.8913 (3)	0.36254 (15)	0.0586 (5)
C10	0.9045 (3)	0.6173 (2)	0.18532 (18)	0.0647 (6)
H10A	0.9902	0.5703	0.1831	0.078*
H10B	0.8672	0.6317	0.1133	0.078*
C11	0.8120 (3)	0.5253 (3)	0.2403 (2)	0.0935 (9)
H11A	0.8471	0.5125	0.3122	0.140*
H11B	0.8045	0.4362	0.2057	0.140*
H11C	0.7250	0.5682	0.2384	0.140*
C12	1.0620 (3)	0.9383 (4)	0.46551 (19)	0.0897 (9)
H12A	1.1091	0.8607	0.4992	0.135*
H12B	0.9968	0.9730	0.5101	0.135*
H12C	1.1247	1.0112	0.4531	0.135*
C13	0.86574 (18)	0.89023 (19)	0.00893 (13)	0.0427 (4)
C14	1.0008 (2)	0.8375 (2)	0.01452 (15)	0.0543 (5)
C15	0.80271 (17)	0.91367 (19)	-0.09958 (13)	0.0399 (4)
C16	0.71135 (19)	1.0205 (2)	-0.12567 (14)	0.0479 (4)
H16	0.6865	1.0812	-0.0738	0.058*
C17	0.6574 (2)	1.0365 (2)	-0.22854 (14)	0.0500 (4)
H17	0.5960	1.1081	-0.2443	0.060*
C18	0.69157 (18)	0.9496 (2)	-0.30907 (14)	0.0447 (4)
C19	0.78522 (18)	0.8452 (2)	-0.28222 (14)	0.0480 (4)
H19	0.8117	0.7858	-0.3344	0.058*

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\hat{A}^2)

C20	0.83964 (18)	0.8279 (2)	-0.18000 (14)	0.0455 (4)
H20	0.9023	0.7574	-0.1646	0.055*
C21	0.6305 (2)	0.9735 (3)	-0.42226 (15)	0.0561 (5)
C22	0.6697 (3)	0.8575 (3)	-0.49666 (18)	0.0821 (8)
H22A	0.7654	0.8563	-0.4986	0.123*
H22B	0.6278	0.8746	-0.5661	0.123*
H22C	0.6402	0.7688	-0.4719	0.123*
C23	0.4769 (2)	0.9764 (4)	-0.42351 (19)	0.0783 (7)
H23A	0.4465	0.8918	-0.3927	0.117*
H23B	0.4380	0.9838	-0.4948	0.117*
H23C	0.4502	1.0553	-0.3838	0.117*
C24	0.6812 (3)	1.1146 (3)	-0.46001 (19)	0.0822 (8)
H24A	0.6507	1.1881	-0.4167	0.123*
H24B	0.6471	1.1298	-0.5318	0.123*
H24C	0.7776	1.1142	-0.4551	0.123*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0804 (4)	0.0545 (3)	0.0619 (3)	-0.0092 (3)	0.0091 (3)	-0.0059 (3)
01	0.0546 (7)	0.0564 (8)	0.0402 (6)	0.0170 (6)	0.0082 (5)	0.0091 (6)
02	0.0584 (9)	0.0596 (11)	0.1548 (18)	0.0126 (8)	0.0241 (10)	0.0312 (11)
N1	0.0626 (10)	0.0576 (11)	0.0410 (9)	0.0147 (8)	-0.0034 (7)	0.0008 (8)
N2	0.0675 (11)	0.0796 (14)	0.0456 (9)	0.0214 (10)	-0.0095 (8)	0.0045 (9)
N3	0.0511 (11)	0.1263 (19)	0.0710 (13)	0.0190 (12)	0.0066 (9)	0.0174 (13)
C1	0.0711 (17)	0.077 (2)	0.207 (4)	0.0204 (16)	0.009 (2)	-0.053 (2)
C2	0.0701 (16)	0.155 (3)	0.0763 (17)	0.0369 (19)	-0.0084 (13)	0.0102 (18)
C3	0.0764 (17)	0.121 (3)	0.102 (2)	0.0366 (17)	0.0362 (15)	0.0311 (19)
C4	0.0486 (10)	0.0575 (13)	0.0553 (11)	0.0138 (9)	0.0016 (8)	0.0002 (9)
C5	0.0475 (10)	0.0491 (12)	0.0516 (11)	0.0068 (8)	-0.0006 (8)	-0.0003 (9)
C6	0.0443 (9)	0.0452 (10)	0.0391 (9)	0.0031 (8)	0.0017 (7)	0.0025 (8)
C7	0.0426 (9)	0.0539 (11)	0.0355 (9)	0.0048 (8)	0.0042 (7)	0.0036 (8)
C8	0.0467 (10)	0.0565 (12)	0.0414 (10)	-0.0007 (9)	0.0042 (7)	-0.0012 (9)
С9	0.0513 (11)	0.0828 (16)	0.0402 (10)	0.0062 (11)	-0.0042 (8)	-0.0017 (10)
C10	0.0813 (15)	0.0554 (14)	0.0575 (12)	0.0162 (11)	0.0066 (10)	-0.0007 (10)
C11	0.125 (2)	0.075 (2)	0.0812 (17)	-0.0070 (17)	0.0135 (16)	0.0099 (14)
C12	0.0813 (17)	0.124 (3)	0.0584 (15)	0.0087 (16)	-0.0253 (12)	-0.0148 (15)
C13	0.0432 (8)	0.0458 (11)	0.0390 (9)	0.0012 (7)	0.0022 (7)	0.0026 (8)
C14	0.0452 (9)	0.0750 (14)	0.0428 (10)	0.0035 (9)	0.0043 (8)	0.0080 (9)
C15	0.0391 (9)	0.0426 (10)	0.0381 (9)	-0.0048 (7)	0.0047 (7)	0.0016 (8)
C16	0.0590 (11)	0.0455 (11)	0.0393 (9)	0.0045 (9)	0.0049 (8)	0.0006 (8)
C17	0.0603 (11)	0.0470 (11)	0.0426 (10)	0.0089 (9)	0.0039 (8)	0.0073 (8)
C18	0.0456 (9)	0.0498 (11)	0.0387 (9)	-0.0062 (8)	0.0035 (7)	0.0056 (7)
C19	0.0493 (10)	0.0575 (12)	0.0382 (10)	-0.0008 (9)	0.0090 (8)	-0.0047 (8)
C20	0.0416 (9)	0.0523 (11)	0.0431 (10)	0.0067 (8)	0.0061 (7)	0.0038 (8)
C21	0.0568 (11)	0.0720 (14)	0.0393 (10)	-0.0041 (10)	0.0024 (8)	0.0033 (10)
C22	0.0937 (18)	0.106 (2)	0.0452 (13)	0.0079 (16)	-0.0039 (12)	-0.0117 (13)
C23	0.0596 (13)	0.112 (2)	0.0608 (13)	-0.0039 (14)	-0.0105 (10)	0.0039 (14)

Geometric parameters (Å, °) Cl1—C8 1.718 (2) Cl1—H11B 0.9600 Ol—C5 1.377 (2) Cl1—H11C 0.9600 Ol—C6 1.382 (2) Cl2—H12A 0.9600 Ol—C6 1.382 (2) Cl2—H12C 0.9600 NI—N2 1.351 (2) Cl2—H12C 0.9600 NI—C7 1.356 (3) Cl3—C14 1.437 (3) N1—C10 1.499 (3) Cl5—C20 1.388 (3) N3—C14 1.149 (3) Cl5—C16 1.391 (3) Cl—H1A 0.9600 Cl7—H17 0.9300 Cl—H1A 0.9600 Cl7—H17 0.9300 Cl—H1B 0.9600 Cl8—C19 1.391 (3) C2—C4 1.503 (3) Cl8—C19 1.391 (3) C2—H2A 0.9600 Cl9—C20 1.338 (3) C2—H2A 0.9600 Cl9—C20 1.338 (3) C2—H2A 0.9600 Cl1—C22 1.534 (4) C2—H2A 0.9600 Cl1—C24 1.534 (3) C2—H2A 0.9600 Cl1—C24	C24	0.0965 (18)	0.096 (2)	0.0527 (13)	-0.0131 (15)	-0.0027 (12)	0.0278 (13)
Generating parameters (n. f) Clinetics (n. f) Clinetics (n. f) Clinetics (n. f) OII-C5 1.377 (2) Cli-H11E 0.9600 OI-C6 1.382 (2) Cl2-H12A 0.9600 OI-C7 1.351 (2) Cl2-H12C 0.9600 NI-N2 1.351 (2) Cl2-H12C 0.9600 NI-C7 1.356 (3) Cl3-C14 1.437 (3) N2-C9 1.334 (3) Cl5-C20 1.388 (3) N3-C14 1.149 (3) Cl5-C16 1.391 (3) Cl-H1A 0.9600 Cl6-H16 0.9300 Cl-H1B 0.9600 Cl7-H17 0.9300 C2-H2A 0.9600 Cl8-C19 1.391 (3) C2-H2A 0.9600 Cl8-C19 1.391 (3) C2-H2A 0.9600 Cl9-L19 0.9300 C3-H3A 0.9600 Cl9-C20 1.378 (3) C2-H2A 0.9600 Cl1-C22 1.531 (4) C3-H3A 0.9600 C21-C24 1.534 (3) C3-H3A 0.9600 C21-C24 <td< td=""><td>Geometric par</td><td>ameters (Å °)</td><td></td><td></td><td></td><td></td><td></td></td<>	Geometric par	ameters (Å °)					
Cl1—C8 1.718 (2) Cl1—H11B 0.9600 OI—C5 1.377 (2) Cl1—H11C 0.9600 OI—C6 1.382 (2) Cl2—H12A 0.9600 OI—C6 1.382 (2) Cl2—H12A 0.9600 NI—N2 1.351 (2) Cl2—H12C 0.9600 NI—C7 1.356 (3) Cl3—Cl4 1.437 (3) NI—C10 1.459 (3) Cl5—Cl6 1.391 (3) Cl—C4 1.519 (4) Cl6—Cl7 1.382 (2) Cl—H1A 0.9600 Cl7—H17 0.9300 Cl—H1B 0.9600 Cl7—H17 0.9300 C2—H2A 0.9600 Cl8—Cl1 1.537 (3) C2—H2A 0.9600 Cl9—Cl2 1.538 (3) C2—H2A 0.9600 Cl9—Cl2 1.538 (3) C2—H2A 0.9600 Cl9—Cl2 1.538 (3) C2—H2A 0.9600 Cl9—Cl2 1.534 (3) C2—H2A 0.9600 Cl9—Cl2 1.534 (3) C3—H3A 0.9600 C21—C22 1.534 (3) <	Geometric pure	umeters (A,)					
OI-C5 1377 (2) $C11-H11C$ 0.9600 $OI-C6$ 1.382 (2) $C12-H12A$ 0.9600 $OI-C5$ 1.187 (3) $C12-H12B$ 0.9600 $NI-N2$ 1.351 (2) $C12-H12C$ 0.9600 $NI-C10$ 1.459 (3) $C13-C14$ 1.437 (3) $NI-C10$ 1.459 (3) $C15-C15$ 1.486 (2) $N2-C9$ 1.334 (3) $C15-C16$ 1.391 (3) $CI-C4$ 1.519 (4) $C16-C17$ 1.332 (2) $CI-H1A$ 0.9600 $C17-C18$ 1.337 (3) $CI-H1B$ 0.9600 $C17-H17$ 0.9300 $C1-H2A$ 0.9600 $C19-C20$ 1.378 (3) $C2-H2A$ 0.9600 $C19-C20$ 1.378 (3) $C2-H2A$ 0.9600 $C1-C22$ 1.333 (4) $C2-H2A$ 0.9600 $C21-C22$ 1.334 (3) $C2-H2A$ 0.9600 $C21-C23$ 1.334 (3) $C3-H3A$ 0.9600 $C21-C23$ 1.534 (3) <t< td=""><td>Cl1—C8</td><td></td><td>1.718 (2)</td><td>C11—</td><td>H11B</td><td>0.96</td><td>00</td></t<>	Cl1—C8		1.718 (2)	C11—	H11B	0.96	00
OI-C6 1.382 (2) $C12-H12A$ 0.9600 $O2-C5$ 1.187 (3) $C12-H12B$ 0.9600 $NI-N2$ 1.351 (2) $C12-H12C$ 0.9600 $NI-C7$ 1.356 (3) $C13-C15$ 1.486 (2) $N2-C9$ 1.334 (3) $C15-C20$ 1.388 (3) $N3-C14$ 1.149 (3) $C15-C16$ 1.391 (3) $C1-H1A$ 0.9600 $C1-H16$ 0.9300 $C1-H1B$ 0.9600 $C17-C18$ 1.387 (3) $C1-H1B$ 0.9600 $C17-H17$ 0.9300 $C2-C4$ 1.503 (3) $C18-C19$ 1.391 (3) $C2-H2A$ 0.9600 $C19-H19$ 0.9300 $C2-H2A$ 0.9600 $C19-H19$ 0.9300 $C3-H3A$ 0.9600 $C1-C22$ 1.533 (4) $C3-H3A$ 0.9600 $C21-C22$ 1.533 (4) $C3-H3A$ 0.9600 $C21-C23$ 1.534 (3) $C3-H3A$ 0.9600 $C21-C23$ 1.534 (3) $C3-H3A$ 0.9600 $C21-H22A$	O1—C5		1.377 (2)	C11—	H11C	0.96	00
02-c5 1,187 (3) $C12-H12B$ 0.9600 N1-N2 1,351 (2) $C12-H12C$ 0.9600 N1-C7 1,356 (3) $C13-C14$ 1,437 (3) N1-C10 1,459 (3) $C13-C15$ 1,486 (2) N2-C9 1,334 (3) $C15-C16$ 1,391 (3) C1-C4 1,519 (4) $C16-C17$ 1,382 (2) C1-H1A 0.9600 $C17-C18$ 1,387 (3) C1-H1B 0.9600 $C17-H17$ 0.9300 C2-C4 1,503 (3) $C18-C19$ 1,391 (3) C2-H2A 0.9600 $C19-C20$ 1,378 (3) C2-H2A 0.9600 $C19-C20$ 0.9300 C3-C4 1,532 (3) $C20-H20$ 0.9300 C3-H3A 0.9600 $C1-C23$ 1,534 (3) C3-H3B 0.9600 $C12-C23$ 1,534 (3) C3-H3B 0.9600 $C21-C23$ 1,534 (3) C3-H3B 0.9600 $C21-C23$ 0.9600 C4-C5 1,509 (3) $C22-H$	O1—C6		1.382 (2)	C12—	-H12A	0.96	00
N1-N21.351 (2) $C12-H12C$ 0.9600N1-C71.356 (3)C13-C141.437 (3)N1-C101.459 (3)C13-C151.486 (2)N2-C91.334 (3)C15-C201.388 (3)N3-C141.149 (3)C16-C161.391 (3)C1-C41.519 (4)C16-C171.382 (2)C1-H1A0.9600C17-H170.9300C1-H1B0.9600C17-H170.9300C2-C41.503 (3)C18-C191.391 (3)C2-H2A0.9600C19-C201.378 (3)C2-H2B0.9600C19-C201.378 (3)C3-H2C0.9600C1-C221.533 (4)C3-H3A0.9600C21-C241.534 (3)C3-H3A0.9600C21-C241.534 (3)C3-H3B0.9600C21-C231.534 (3)C4-C51.509 (3)C22-H22A0.9600C6-C131.341 (3)C22-H22A0.9600C6-C71.473 (2)C22-H22A0.9600C6-C71.473 (2)C22-H22A0.9600C7-C81.378 (3)C23-H23A0.9600C9-C121.501 (3)C23-H23A0.9600C10-H10A0.9700C24-H24A0.9600C10-H10B0.9700C24-H24A0.9600C10-H10A0.9700C24-H24A0.9600C10-H10A0.9700C24-H24A0.9600C10-H10A0.9700C24-H24A0.9600C10-H10A0.9700C24-H24A0.9600C10-H10B0.9500C2-H12B <td< td=""><td>O2—C5</td><td></td><td>1.187 (3)</td><td>C12—</td><td>-H12B</td><td>0.96</td><td>00</td></td<>	O2—C5		1.187 (3)	C12—	-H12B	0.96	00
NI-C71.356 (3)C13-C141.437 (3)N1-C101.459 (3)C13-C151.486 (2)N2-C91.334 (3)C15-C201.388 (3)N3-C141.149 (3)C15-C161.391 (3)C1-C41.519 (4)C16-C171.382 (2)C1-HIB0.9600C17-C181.387 (3)C1-HIB0.9600C17-C181.387 (3)C2-H2A0.9600C18-C191.391 (3)C2-H2A0.9600C18-C191.391 (3)C2-H2B0.9600C19-C191.378 (3)C2-H2B0.9600C19-C190.9300C3-H3A0.9600C1-C221.533 (4)C3-H3A0.9600C1-C221.533 (4)C3-H3A0.9600C1-C221.534 (3)C3-H3A0.9600C1-C221.534 (3)C4-C51.509 (3)C2-H22A0.9600C4-C51.509 (3)C22-H22A0.9600C6-C71.473 (2)C22-H22A0.9600C6-C71.473 (2)C23-H23A0.9600C6-C71.391 (3)C23-H23A0.9600C7-C81.391 (3)C23-H23A0.9600C10-C111.495 (4)C24-H24A0.9600C10-C111.495 (1)C14-C1-H11C109.5C10-C111.495 (1)C24-H24A0.9600C10-H10A0.9700C24-H24B0.9600C10-H10A0.9700C24-H24B0.9600C10-H10A0.9700C24-H24B0.9500C10-H10B1.976 (15)H11A-C11-H	N1—N2		1.351 (2)	C12—	-H12C	0.96	00
N1-C101.459 (3)C13-C151.486 (2)N2-C91.334 (3)C15-C201.388 (3)N3-C141.149 (3)C15-C161.391 (3)C1-C41.519 (4)C16-C171.382 (2)C1-HIA0.9600C16-H160.9300C1-HIB0.9600C17-C181.387 (3)C2-C41.503 (3)C18-C191.391 (3)C2-H2A0.9600C19-C201.378 (3)C2-H2B0.9600C19-H190.9300C3-C41.532 (3)C20-H200.9300C3-C41.532 (3)C20-H200.9300C3-C41.532 (3)C20-H200.9300C3-H3A0.9600C21-C221.533 (4)C3-H3B0.9600C21-C231.534 (3)C4-C51.509 (3)C22-H22A0.9600C4-C51.509 (3)C22-H22A0.9600C6-C131.341 (3)C22-H22A0.9600C6-C71.473 (2)C23-H23A0.9600C6-C71.391 (3)C23-H23A0.9600C6-C71.391 (3)C23-H23A0.9600C7-C81.391 (3)C23-H23A0.9600C10-H10A0.9700C24-H24A0.9600C10-H10A0.9700C24-H24A0.9600C10-H10B0.9700C24-H24A0.9600C10-H10B0.9700C24-H24A0.9600C10-H10B0.9700C24-H24A0.9600C10-H10B0.9700C24-H24A0.9600C10-H10B0.9700C24-H24A0.960	N1—C7		1.356 (3)	C13—	-C14	1.43	7 (3)
N2—C91.334 (3)C15—C201.388 (3)N3—C141.149 (3)C15—C161.391 (3)C1—C41.519 (4)C16—C171.382 (2)C1—H1A0.9600C16—H160.9300C1—H1B0.9600C17—C181.387 (3)C1—H1C0.9600C17—H170.9300C2—C41.503 (3)C18—C211.534 (3)C2—H2A0.9600C19—C201.378 (3)C2—H2B0.9600C19—C100.9300C3—C41.532 (3)C20—H200.9300C3—H3A0.9600C21—C221.533 (4)C3—H3A0.9600C21—C231.534 (3)C3—H3A0.9600C21—C231.534 (3)C4—C51.509 (3)C22—H22A0.9600C6—C71.473 (2)C22—H22A0.9600C6—C71.473 (2)C22—H22A0.9600C6—C71.473 (2)C22—H22A0.9600C7—C81.378 (3)C23—H23A0.9600C9—C121.501 (3)C23—H23A0.9600C10—C111.495 (4)C24—H24A0.9600C10—H10A0.9700C24—H24B0.9600C10—H10A0.9700C24—H24B0.9600C10—H10A0.9700C24—H24B0.9600C10—H10A0.9700C24—H24B0.9600C10—H10A0.9700C24—H24B0.9600C10—H10A0.9700C24—H24B0.9600C10—H10A0.9700C24—H24B0.9600C10—H10A0.950C14—C1-H11C10.95	N1-C10		1.459 (3)	C13—	-C15	1.48	5 (2)
N3—C141.149 (3)C15—C161.391 (3)C1—C41.519 (4)C16—C171.382 (2)C1—H1A0.9600C16—H160.9300C1—H1B0.9600C17—C181.387 (3)C1—H1C0.9600C17—H170.9300C2—C41.503 (3)C18—C191.391 (3)C2—H2A0.9600C19—C101.378 (3)C2—H2B0.9600C19—H190.9300C3—C41.532 (3)C20—H200.9300C3—C41.532 (3)C20—H200.9300C3—H3A0.9600C21—C241.534 (3)C3—H3B0.9600C21—C231.534 (3)C3—H3B0.9600C21—C231.534 (3)C4—C51.509 (3)C22—H22A0.9600C6—C71.473 (2)C22—H22A0.9600C6—C71.378 (3)C23—H23A0.9600C6—C71.378 (3)C23—H23A0.9600C7—C81.378 (3)C23—H23A0.9600C9—C121.501 (3)C23—H23A0.9600C10—C111.495 (4)C24—H24A0.9600C10—H10A0.9700C24—H24A0.9600C10—H10A0.9700C24—H24B0.9600C10—H10A0.9600C24—H24B0.9600C10—H10A0.9600C24—H24B0.9600C10—H10A0.9600C24—H24A0.9600C10—H10A0.9600C24—H24B0.9600C10—H10A0.9600C24—H24B0.9600C10—H10A0.9600C24—H24B0.9600 <td>N2—C9</td> <td></td> <td>1.334 (3)</td> <td>C15—</td> <td>-C20</td> <td>1.38</td> <td>8 (3)</td>	N2—C9		1.334 (3)	C15—	-C20	1.38	8 (3)
C1-C4 1.519 (4) $C16-C17$ 1.382 (2) $C1-H1A$ 0.9600 $C16-H16$ 0.9300 $C1-H1B$ 0.9600 $C17-C18$ 1.387 (3) $C1-H1C$ 0.9600 $C17-H17$ 0.9300 $C2-C4$ 1.503 (3) $C18-C19$ 1.391 (3) $C2-H2A$ 0.9600 $C19-C20$ 1.378 (3) $C2-H2B$ 0.9600 $C19-H19$ 0.9300 $C3-C4$ 1.532 (3) $C20-H20$ 0.9300 $C3-C4$ 1.532 (3) $C20-H20$ 0.9300 $C3-H3A$ 0.9600 $C21-C22$ 1.533 (4) $C3-H3B$ 0.9600 $C21-C24$ 1.534 (3) $C3-H3B$ 0.9600 $C21-C23$ 1.534 (3) $C4-C5$ 1.599 (3) $C22-H22A$ 0.9600 $C6-C13$ 1.341 (3) $C22-H22B$ 0.9600 $C6-C7$ 1.473 (2) $C22-H22A$ 0.9600 $C7-C8$ 1.378 (3) $C23-H23A$ 0.9600 $C9-C12$ 1.501 (3) $C23-H23C$ 0.9600 $C10-C11$ 1.495 (4) $C24-H24A$ 0.9600 $C10-H10A$ 0.9700 $C24-H24A$ 0.9600 $C10-H10A$ 0.9700 $C24-H24C$ 0.9500 $C1-H10$	N3—C14		1.149 (3)	C15—	-C16	1.39	1 (3)
C1—H1A0.9600C16—H160.9300C1—H1B0.9600C17—C181.387 (3)C1—H1C0.9600C17—H170.9300C2—C41.503 (3)C18—C191.391 (3)C2—H2A0.9600C18—C211.534 (3)C2—H2B0.9600C19—C201.378 (3)C3—C41.532 (3)C20—H200.9300C3—C41.532 (3)C20—H200.9300C3—H3A0.9600C21—C221.533 (4)C3—H3B0.9600C21—C241.534 (3)C3—H3C0.9600C21—C231.534 (3)C4—C51.509 (3)C22—H22A0.9600C6—C131.341 (3)C22—H22B0.9600C6—C71.473 (2)C22—H22C0.9600C6—C71.391 (3)C23—H23A0.9600C8—C91.391 (3)C23—H23A0.9600C9—C121.501 (3)C23—H23A0.9600C10—C111.495 (4)C24—H24A0.9600C10—H10A0.9700C24—H24A0.9600C10—H10B0.9700C24—H24A0.9600C10—H10A0.9700C24—H24C0.9600C10—H10B0.9700C24—H24A0.9600C10—H10B0.9700C24—H24B0.9600C10—H10B0.9700C24—H24C0.9600C10—H10B0.9700C24—H24C0.9600C10—H10B0.9700C24—H24C0.9600C10—H10B0.9700C24—H24B0.9500C4—C1-H10B10.956H11A—C11—H11C109.	C1—C4		1.519 (4)	C16—	-C17	1.38	2 (2)
C1—H1B0.9600C17—C181.387 (3)C1—H1C0.9600C17—H170.9300C2—C41.503 (3)C18—C191.391 (3)C2—H2A0.9600C19—C201.534 (3)C2—H2B0.9600C19—C201.578 (3)C2—H2C0.9600C19—H190.9300C3—C41.532 (3)C20—H200.9300C3—H3A0.9600C21—C221.534 (3)C3—H3B0.9600C21—C231.534 (3)C3—H3A0.9600C21—C231.534 (3)C3—H3C0.9600C21—C231.534 (3)C4—C51.509 (3)C22—H22A0.9600C6—C131.341 (3)C22—H22B0.9600C6—C71.473 (2)C22—H22B0.9600C6—C71.473 (2)C23—H23A0.9600C7—C81.378 (3)C23—H23B0.9600C8—C91.391 (3)C23—H23B0.9600C10—C111.495 (4)C24—H24A0.9600C10—H10A0.9700C24—H24B0.9600C10—H10A0.9700C24—H24B0.9600C10—H10A0.9700C24—H24B0.9600C5—O1—C6119.76 (15)H11A—C11—H11C109.5N2—N1—C7111.58 (17)H11B—C11—H11C109.5N2—N1—C10118.59 (18)C9—C12—H12B109.5C4—C1—H1A109.5C9—C12—H12B109.5C4—C1—H1A109.5C12—H12C109.5C4—C1—H1B109.5H12A—C12—H12C109.5H1A—C1—H1B109.5	C1—H1A		0.9600	C16—	-H16	0.93	00
C1-H1C $0,9600$ C17-H17 $0,9300$ C2-C4 $1,503$ (3)C18-C19 $1,391$ (3)C2-H2A $0,9600$ C18-C21 1.534 (3)C2-H2B $0,9600$ C19-C20 1.378 (3)C2-H2C $0,9600$ C19-H19 $0,9300$ C3-C4 1.532 (3)C20-H20 $0,9300$ C3-H3A $0,9600$ C21-C22 1.533 (4)C3-H3B $0,9600$ C21-C24 1.534 (3)C3-H3C $0,9600$ C21-C23 1.534 (3)C4-C5 1.509 (3)C22-H12A $0,9600$ C6-C13 1.341 (3)C22-H12A $0,9600$ C6-C7 1.473 (2)C2-H12C $0,9600$ C6-C7 1.473 (2)C2-H12A $0,9600$ C7-C8 1.378 (3)C23-H23A $0,9600$ C9-C12 1.501 (3)C23-H23A $0,9600$ C10-C11 1.495 (4)C24-H24A $0,9600$ C10-H10A 0.9700 C24-H24B $0,9600$ C10-H10B 0.9700 C24-H24C $0,9600$ C10-H10B 0.9700 C24-H24C $0,9600$ C11-H11A 0.9600 0.9600 0.9600 C1-H1A 0.9600 $0.9-C12-H12A$ 109.5 N2-N1-C7 11.58 (17) $H11A-C11-H11C$ 109.5 N2-N1-C10 12.966 (16) $C9-C12-H12A$ 109.5 C4-C1-H1A 109.5 $0.9-C12-H12A$ 109.5 C4-C1-H1B 109.5 $112A-C12-H12C$ 109.5 H1A-C1-H1B 109.5 $112A-C12-H12C$ 109.5 </td <td>C1—H1B</td> <td></td> <td>0.9600</td> <td>C17—</td> <td>-C18</td> <td>1.38</td> <td>7 (3)</td>	C1—H1B		0.9600	C17—	-C18	1.38	7 (3)
C2-C41.503 (3) $C18-C19$ $1.391 (3)$ $C2-H2A$ 0.9600 $C18-C21$ $1.534 (3)$ $C2-H2B$ 0.9600 $C19-C20$ $1.378 (3)$ $C2-H2C$ 0.9600 $C19-H19$ 0.9300 $C3-C4$ 1.532 (3) $C20-H2O$ 0.9300 $C3-H3A$ 0.9600 $C21-C22$ 1.533 (4) $C3-H3B$ 0.9600 $C21-C24$ 1.534 (3) $C3-H3C$ 0.9600 $C21-C23$ 1.534 (3) $C3-H3C$ 0.9600 $C22-H22A$ 0.9600 $C6-C13$ 1.341 (3) $C22-H22B$ 0.9600 $C6-C7$ 1.473 (2) $C22-H22C$ 0.9600 $C6-C7$ 1.473 (2) $C23-H23A$ 0.9600 $C8-C9$ 1.391 (3) $C23-H23A$ 0.9600 $C9-C12$ 1.501 (3) $C23-H23B$ 0.9600 $C10-C11$ 1.495 (4) $C24-H24A$ 0.9600 $C10-H10A$ 0.9700 $C24-H24B$ 0.9600 $C1-H10A$ 0.9700 $C24-H24C$ 0.9600 $C1-H10B$ 0.9700 $C24-H24C$ 0.9600 $C1-H10A$ 0.9600 $C2-H12A$ 0.950 $C1-H10A$ 0.9600 $C2-H12A$ 0.950 $C4-C1-H10$ 119.56 (15)H11A-C11-H11C109.5 $N2-N1-C7$ 111.58 (17)H11B-C11-H11C109.5 $N2-N1-C10$ 118.59 (18) $C9-C12-H12A$ 109.5 $C4-C1-H1A$ 109.5 $C9-C12-H12C$ 109.5 $C4-C1-H1B$ 109.5H12A-C12-H12C109.5 $H1A-C1-H1B$ 109.5H12A-C12-H12C109.5 <td< td=""><td>C1—H1C</td><td></td><td>0.9600</td><td>C17—</td><td>-H17</td><td>0.93</td><td>00</td></td<>	C1—H1C		0.9600	C17—	-H17	0.93	00
C2-H2A0.9600 $C18-C21$ 1.534 (3) $C2-H2B$ 0.9600 $C19-C20$ 1.378 (3) $C2-H2C$ 0.9600 $C19-H19$ 0.9300 $C3-C4$ 1.532 (3) $C20-H20$ 0.9300 $C3-H3A$ 0.9600 $C21-C22$ 1.533 (4) $C3-H3B$ 0.9600 $C21-C23$ 1.534 (3) $C3-H3C$ 0.9600 $C21-C23$ 1.534 (3) $C4-C5$ 1.509 (3) $C22-H22A$ 0.9600 $C6-C13$ 1.341 (3) $C22-H22B$ 0.9600 $C6-C7$ 1.473 (2) $C22-H22C$ 0.9600 $C6-C7$ 1.578 (3) $C23-H23A$ 0.9600 $C8-C9$ 1.391 (3) $C23-H23B$ 0.9600 $C9-C12$ 1.501 (3) $C23-H23C$ 0.9600 $C10-C11$ 1.495 (4) $C24-H24A$ 0.9600 $C10-H10A$ 0.9700 $C24-H24A$ 0.9600 $C10-H10B$ 0.9700 $C24-H24B$ 0.9600 $C10-H10B$ 0.9700 $C24-H24A$ 0.9600 $C1-H11A$ 0.9600 $C2-H12A$ <td>C2—C4</td> <td></td> <td>1.503 (3)</td> <td>C18—</td> <td>-C19</td> <td>1.39</td> <td>1 (3)</td>	C2—C4		1.503 (3)	C18—	-C19	1.39	1 (3)
C2-H2B0.9600 $C19-C20$ 1.378 (3) $C2-H2C$ 0.9600 $C19-H19$ 0.9300 $C3-C4$ 1.532 (3) $C20-H20$ 0.9300 $C3-H3A$ 0.9600 $C21-C22$ 1.533 (4) $C3-H3B$ 0.9600 $C21-C24$ 1.534 (3) $C3-H3C$ 0.9600 $C21-C23$ 1.534 (3) $C4-C5$ 1.509 (3) $C22-H22A$ 0.9600 $C6-C13$ 1.341 (3) $C22-H22B$ 0.9600 $C6-C7$ 1.473 (2) $C22-H22C$ 0.9600 $C6-C7$ 1.473 (2) $C23-H23A$ 0.9600 $C8-C9$ 1.391 (3) $C23-H23B$ 0.9600 $C9-C12$ 1.501 (3) $C23-H23B$ 0.9600 $C10-C11$ 1.495 (4) $C24-H24A$ 0.9600 $C10-H10A$ 0.9700 $C24-H24B$ 0.9600 $C10-H10A$ 0.9700 $C24-H24B$ 0.9600 $C1-H1A$ 0.9600 $C1-H1A$ 0.950 $C2-N1-C7$ 11.58 (17)H11A-C11-H11C109.5 $N2-N1-C7$ 11.58 (17)H11B-C11-H11C109.5 $N2-N1-C7$ 11.58 (17)H11B-C11-H11C109.5 $N2-N1-C10$ 129.66 (16) $C9-C12-H12B$ 109.5 $C4-C1-H1A$ 109.5 $C9-C12-H12B$ 109.5 $C4-C1-H1B$ 109.5 $C9-C12-H12C$ 109.5 $C4-C1-H1B$ 109.5 $C9-C12-H12C$ 109.5 $C4-C1-H1B$ 109.5 $C12-H12C$ 109.5 $C4-C1-H1B$ 109.5 $C12-H12C$ 109.5 $C4-C1-H1B$ 109.5 $C12-H12C$ 109.5 $C4$	C2—H2A		0.9600	C18—	-C21	1.53	4 (3)
C2-H2C 0.9600 $C19-H19$ 0.9300 $C3-C4$ $1.532 (3)$ $C20-H20$ 0.9300 $C3-H3A$ 0.9600 $C21-C22$ $1.533 (4)$ $C3-H3B$ 0.9600 $C21-C23$ $1.534 (3)$ $C3-H3C$ 0.9600 $C21-C23$ $1.534 (3)$ $C4-C5$ $1.509 (3)$ $C22-H22A$ 0.9600 $C6-C13$ $1.341 (3)$ $C22-H22B$ 0.9600 $C6-C7$ $1.473 (2)$ $C22-H22C$ 0.9600 $C7-C8$ $1.378 (3)$ $C23-H23A$ 0.9600 $C8-C9$ $1.391 (3)$ $C23-H23C$ 0.9600 $C9-C12$ $1.501 (3)$ $C23-H23C$ 0.9600 $C10-C11$ $1.495 (4)$ $C24-H24A$ 0.9600 $C10-H10A$ 0.9700 $C24-H24B$ 0.9600 $C10-H10B$ 0.9700 $C24-H24B$ 0.9600 $C1-H11A$ 0.9600 $C24-H24C$ 0.9600 $C1-H11A$ 0.9600 $C24-H24C$ 0.9600 $C1-H10B$ 0.9700 $C24-H24B$ 0.9600 $C1-H10B$ 0.9700 $C24-H24C$ 0.9600 $C1-H10B$ 0.9700 $C24-H24C$ 0.9600 $C5-O1-C6$ $119.76 (15)$ $H11A-C11-H11C$ 109.5 $N2-N1-C10$ $118.59 (18)$ $C9-C12-H12B$ 109.5 $C7-N1-C10$ $129.66 (16)$ $C9-C12-H12B$ 109.5 $C4-C1-H1A$ 109.5 $C9-C12-H12C$ 109.5 $C4-C1-H1B$ 109.5 $C9-C12-H12C$ 109.5 $C4-C1-H1B$ 109.5 $C12-H12C$ 109.5	C2—H2B		0.9600	C19—	-C20	1.37	8 (3)
C3C4 $1.532 (3)$ C20H20 0.9300 C3H3A 0.9600 C21C22 $1.533 (4)$ C3H3B 0.9600 C21C24 $1.534 (3)$ C3H3C 0.9600 C21C23 $1.534 (3)$ C4C5 $1.509 (3)$ C22H22A 0.9600 C6C13 $1.341 (3)$ C22H22B 0.9600 C6C7 $1.473 (2)$ C22H22C 0.9600 C7C8 $1.378 (3)$ C23H23B 0.9600 C9C12 $1.501 (3)$ C23H23B 0.9600 C9C12 $1.501 (3)$ C23H23B 0.9600 C10C11 $1.495 (4)$ C24H24A 0.9600 C10C11 $1.495 (4)$ C24H24B 0.9600 C10H10B 0.9700 C24H24B 0.9600 C10H10B 0.9600 C24H24C 0.9600 C11H11A 0.9600 C24H24C 0.9600 C1H10B 0.9600 C24H24C 0.9600 C1H10B 0.9600 C24H24B 0.9500 C5O1C6 $119.76 (15)$ $H11AC11-H11C$ 109.5 N2N1C7 $111.58 (17)$ $H11BC11-H11C$ 109.5 N2N1C10 $129.66 (16)$ $C9C12H12B$ 109.5 C4C1H1A 109.5 $C9C12H12C$ 109.5 C4C1H1B 109.5 $H12AC12H12C$ 109.5 H1AC1H1B 109.5 $H12BC12H12C$ 109.5 C4C1H1B 109.5 $H12BC12H12C$ 109.5 C4C1H1B 109.5 $H12BC12H12C$	C2—H2C		0.9600	C19—	-H19	0.93	00
C3—H3A0.9600C21—C221.533 (4)C3—H3B0.9600C21—C241.534 (3)C3—H3C0.9600C21—C231.534 (3)C4—C51.509 (3)C22—H22A0.9600C6—C131.341 (3)C22—H22B0.9600C6—C71.473 (2)C22—H22C0.9600C7—C81.391 (3)C23—H23A0.9600C8—C91.391 (3)C23—H23B0.9600C10—C111.495 (4)C24—H24A0.9600C10—C111.495 (4)C24—H24A0.9600C10—H10A0.9700C24—H24C0.9600C10—H10B0.9700C24—H24C0.9600C11—H11A0.9600UUC5—O1—C6119.76 (15)H11A—C11—H11C109.5N2—N1—C7111.58 (17)H11B—C11—H11C109.5N2—N1—C10129.66 (16)C9—C12—H12B109.5C7—N1—C10129.66 (16)C9—C12—H12B109.5C4—C1—H1A109.5C9—C12—H12C109.5C4—C1—H1B109.5H12A—C12—H12C109.5H1A—C1—H1B109.5H12B—C12—H12C109.5H1A—C1—H1B109.5H12B—C12—H12C109.5C4—C1—H1B109.5H12B—C12—H12C109.5C4—C1—H1B109.5H12B—C12—H12C109.5C4—C1—H1B109.5H12B—C12—H12C109.5C4—C1—H1B109.5H12B—C12—H12C109.5C4—C1—H1B109.5H12B—C12—H12C109.5C4—C1—H1B109.5H12B—C12—H12C109.5 <td>C3—C4</td> <td></td> <td>1.532 (3)</td> <td>C20—</td> <td>-H20</td> <td>0.93</td> <td>00</td>	C3—C4		1.532 (3)	C20—	-H20	0.93	00
C3-H3B0.9600C21C241.534 (3)C3-H3C0.9600C21C231.534 (3)C4-C51.509 (3)C22-H22A0.9600C6-C131.341 (3)C22-H22B0.9600C6-C71.473 (2)C22-H22C0.9600C7-C81.378 (3)C23-H23A0.9600C8-C91.391 (3)C23-H23B0.9600C9-C121.501 (3)C23-H23C0.9600C10-C111.495 (4)C24-H24A0.9600C10-H10A0.9700C24-H24B0.9600C10-H10B0.9700C24-H24C0.9600C1-H11A0.9600VVC5-O1-C6119.76 (15)H11A-C11-H11C109.5N2-N1-C7111.58 (17)H11B-C11-H11C109.5N2-N1-C10129.66 (16)C9-C12-H12B109.5C7-N1-C10129.66 (16)C9-C12-H12B109.5C4-C1-H1A109.5C9-C12-H12C109.5C4-C1-H1B109.5C9-C12-H12C109.5H1A-C1-H1B109.5C9-C12-H12C109.5C4-C1-H1B109.5C9-C12-H12C109.5C4-C1-H1B109.5C9-C12-H12C109.5C4-C1-H1B109.5C12-H12C109.5C4-C1-H1B109.5C12-H12C109.5C4-C1-H1B109.5C12-H12C109.5C4-C1-H1B109.5C12-H12C109.5C4-C1-H1B109.5C12-H12C109.5C4-C1-H1B109.5C12-H12C109.5C4-C1-H1B109.5 <td>С3—НЗА</td> <td></td> <td>0.9600</td> <td>C21—</td> <td>-C22</td> <td>1.53</td> <td>3 (4)</td>	С3—НЗА		0.9600	C21—	-C22	1.53	3 (4)
C3-H3C 0.9600 C21C23 $1.534 (3)$ C4-C5 $1.509 (3)$ C22-H22A 0.9600 C6-C13 $1.341 (3)$ C22-H22B 0.9600 C6-C7 $1.473 (2)$ C22-H22C 0.9600 C7-C8 $1.378 (3)$ C23-H23A 0.9600 C8-C9 $1.391 (3)$ C23-H23B 0.9600 C9-C12 $1.501 (3)$ C23-H23C 0.9600 C10-C11 $1.495 (4)$ C24-H24A 0.9600 C10-H10A 0.9700 C24-H24B 0.9600 C10-H10B 0.9700 C24-H24C 0.9600 C11-H11A 0.9600 $C24$ -H24C 0.9600 C1-H10A 0.9700 C24-H24C 0.9600 C1-H11A 0.9600 $C24$ -H24C 0.9600 C1-H11A 0.9600 $C1$ -H12A 109.5 C7-N1-C10 $118.59 (18)$ $C9$ -C12-H12A 109.5 C9-N2-N1 $105.88 (17)$ $H12A$ -C12-H12B 109.5 C4-C1-H1A 109.5 $C9$ -C12-H12C 109.5 C4-C1-H1B 109.5 $H12A$ -C12-H12C 109.5 H1A-C1-H1B 109.5 $H12A$ -C12-H12C 109.5 C4-C1-H1B 109.5 $H12A$ -C12-H12C 109.5 C4-C1-H1B 109.5 $H12A$ -C12-H12C	С3—Н3В		0.9600	C21—	-C24	1.53	4 (3)
C4—C5 1.509 (3) C22—H22A 0.9600 C6—C13 1.341 (3) C22—H22B 0.9600 C6—C7 1.473 (2) C22—H22C 0.9600 C7—C8 1.378 (3) C23—H23A 0.9600 C8—C9 1.391 (3) C23—H23B 0.9600 C9—C12 1.501 (3) C23—H23C 0.9600 C10—C11 1.495 (4) C24—H24A 0.9600 C10—H10A 0.9700 C24—H24B 0.9600 C10—H10B 0.9700 C24—H24C 0.9600 C11—H11A 0.9600 C11—H11C 109.5 C2—N1—C7 111.58 (17) H11A—C11—H11C 109.5 C7—N1—C10 129.66 (16) C9—C12—H12A 109.5 C9—N2—N1 105.88 (17) H12A—C12—H12B 109.5 C4—C1—H1A 109.5 C9—C12—H12C 109.5 C4—C1—H1B 109.5 H12A—C12—H12C 109.5 C4—C1—H1B 109.5 H12B—C12—H12C 109.5 C4—C1—H1B 109.5 C9—C12—H12C 109.5	С3—НЗС		0.9600	C21—	-C23	1.53	4 (3)
C6—C13 1.341 (3) C22—H22B 0.9600 C6—C7 1.473 (2) C22—H22C 0.9600 C7—C8 1.378 (3) C23—H23A 0.9600 C8—C9 1.391 (3) C23—H23B 0.9600 C9—C12 1.501 (3) C23—H23C 0.9600 C10—C11 1.495 (4) C24—H24A 0.9600 C10—H10A 0.9700 C24—H24B 0.9600 C11—H11A 0.9600 C11—H11C 109.5 N2—N1—C7 111.58 (17) H11A—C11—H11C 109.5 N2—N1—C10 118.59 (18) C9—C12—H12B 109.5 C7—N1—C10 129.66 (16) C9—C12—H12B 109.5 C4—C1—H1A 109.5 C9—C12—H12B 109.5 C4—C1—H1B 109.5 C9—C12—H12C 109.5 C4—C1—H1B 109.5 H12A—C12—H12C 109.5 C4—C1—H1B 109.5 H12A—C12—H12C 109.5 H1A—C1—H1B 109.5 C9—C12—H12C 109.5 C4—C1—H1B 109.5 C9—C12—H12C 109.5 C4—C1—H1B 109.5 H12A—C12—H12C 109.5 <td>C4—C5</td> <td></td> <td>1.509 (3)</td> <td>C22—</td> <td>-H22A</td> <td>0.96</td> <td>00</td>	C4—C5		1.509 (3)	C22—	-H22A	0.96	00
C6—C7 1.473 (2) C22—H22C 0.9600 C7—C8 1.378 (3) C23—H23A 0.9600 C8—C9 1.391 (3) C23—H23B 0.9600 C9—C12 1.501 (3) C23—H23C 0.9600 C10—C11 1.495 (4) C24—H24A 0.9600 C10—H10A 0.9700 C24—H24B 0.9600 C10—H10B 0.9700 C24—H24C 0.9600 C11—H11A 0.9600 C1 1.158 (17) H11A—C11—H11C 109.5 N2—N1—C7 111.58 (17) H11B—C11—H11C 109.5 109.5 N2—N1—C10 129.66 (16) C9—C12—H12A 109.5 C7—N1—C10 129.66 (16) C9—C12—H12B 109.5 C4—C1—H1A 109.5 C9—C12—H12C 109.5 C4—C1—H1B 109.5 H12A—C12—H12C 109.5 H1A—C1—H1B 109.5 H12B—C12—H12C 109.5 C4—C1—H1B 109.5 H12B—C12—H12C 109.5 C4—C1—H1B 109.5 H12B—C12—H12C 109.5 C4—C1—H1B 109.5 H12B—C12—H12C 109.5 C4—C1—H1	C6—C13		1.341 (3)	C22—	-H22B	0.96	00
C7—C8 1.378 (3) C23—H23A 0.9600 C8—C9 1.391 (3) C23—H23B 0.9600 C9—C12 1.501 (3) C23—H23C 0.9600 C10—C11 1.495 (4) C24—H24A 0.9600 C10—H10A 0.9700 C24—H24B 0.9600 C10—H10B 0.9700 C24—H24C 0.9600 C11—H11A 0.9600 C24—H24C 0.9600 C5—O1—C6 119.76 (15) H11A—C11—H11C 109.5 N2—N1—C7 111.58 (17) H11B—C11—H11C 109.5 N2—N1—C10 129.66 (16) C9—C12—H12A 109.5 C7—N1—C10 129.66 (16) C9—C12—H12B 109.5 C9—N2—N1 105.88 (17) H12A—C12—H12B 109.5 C4—C1—H1A 109.5 C9—C12—H12C 109.5 C4—C1—H1B 109.5 H12A—C12—H12C 109.5 H1A—C1—H1B 109.5 H12A—C12—H12C 109.5 C4—C1—H1B 109.5 H12A—C12—H12C 109.5 C4—C1—H1B 109.5 H12A—C12—H12C 109.5 C4—C1—H1B 109.5 C6—C13—C14	C6—C7		1.473 (2)	C22—	-H22C	0.96	00
C8—C9 1.391 (3)C23—H23B 0.9600 C9—C12 1.501 (3)C23—H23C 0.9600 C10—C11 1.495 (4)C24—H24A 0.9600 C10—H10A 0.9700 C24—H24B 0.9600 C10—H10B 0.9700 C24—H24C 0.9600 C11—H11A 0.9600 C11—H11C 109.5 C5—O1—C6 119.76 (15) $H11A$ —C11—H11C 109.5 N2—N1—C7 111.58 (17) $H11B$ —C11—H11C 109.5 N2—N1—C10 129.66 (16)C9—C12—H12A 109.5 C9—N2—N1 105.88 (17) $H12A$ —C12—H12B 109.5 C4—C1—H1A 109.5 C9—C12—H12C 109.5 H1A—C1—H1B 109.5 $H12A$ —C12—H12C 109.5 H1A—C1—H1B 109.5 $H12B$ —C12—H12C 109.5	С7—С8		1.378 (3)	C23—	-H23A	0.96	00
C9—C12 1.501 (3) C23—H23C 0.9600 C10—C11 1.495 (4) C24—H24A 0.9600 C10—H10A 0.9700 C24—H24B 0.9600 C10—H10B 0.9700 C24—H24C 0.9600 C11—H11A 0.9600 C11—H11C 109.5 C5—O1—C6 119.76 (15) H11A—C11—H11C 109.5 N2—N1—C7 111.58 (17) H11B—C11—H11C 109.5 N2—N1—C10 118.59 (18) C9—C12—H12A 109.5 C7—N1—C10 129.66 (16) C9—C12—H12B 109.5 C4—C1—H1A 109.5 C9—C12—H12B 109.5 C4—C1—H1A 109.5 C9—C12—H12B 109.5 C4—C1—H1B 109.5 H12A—C12—H12C 109.5 H1A—C1—H1B 109.5 H12A—C12—H12C 109.5 C4—C1—H1B 109.5 H12B—C12—H12C 109.5 C4—C1—H1B 109.5 H12B—C12—H12C 109.5 C4—C1—H1B 109.5 C6—C13—C14 117.17 (16)	C8—C9		1.391 (3)	C23—	-H23B	0.96	00
C10—C111.495 (4)C24—H24A0.9600C10—H10A0.9700C24—H24B0.9600C10—H10B0.9700C24—H24C0.9600C11—H11A0.9600C24—H24C0.9600C5—O1—C6119.76 (15)H11A—C11—H11C109.5N2—N1—C7111.58 (17)H11B—C11—H11C109.5N2—N1—C10118.59 (18)C9—C12—H12A109.5C7—N1—C10129.66 (16)C9—C12—H12B109.5C9—N2—N1105.88 (17)H12A—C12—H12B109.5C4—C1—H1A109.5C9—C12—H12C109.5H1A—C1—H1B109.5H12A—C12—H12C109.5H1A—C1—H1B109.5H12B—C12—H12C109.5C4—C1—H1B109.5C6—C13—C14117.17 (16)	C9—C12		1.501 (3)	C23—	-H23C	0.96	00
C10—H10A0.9700C24—H24B0.9600C10—H10B0.9700C24—H24C0.9600C11—H11A0.9600	C10-C11		1.495 (4)	C24—	H24A	0.96	00
C10—H10B0.9700C24—H24C0.9600C11—H11A0.9600	C10—H10A		0.9700	C24—	-H24B	0.96	00
C11—H11A0.9600C5—O1—C6119.76 (15)H11A—C11—H11C109.5N2—N1—C7111.58 (17)H11B—C11—H11C109.5N2—N1—C10118.59 (18)C9—C12—H12A109.5C7—N1—C10129.66 (16)C9—C12—H12B109.5C9—N2—N1105.88 (17)H12A—C12—H12B109.5C4—C1—H1A109.5C9—C12—H12C109.5C4—C1—H1B109.5H12A—C12—H12C109.5H1A—C1—H1B109.5H12B—C12—H12C109.5C4—C1—H1B109.5H12B—C12—H12C109.5H1A—C1—H1B109.5C6—C13—C14117.17 (16)	C10—H10B		0.9700	C24—	H24C	0.96	00
C501C6119.76 (15)H11AC11H11C109.5N2N1C7111.58 (17)H11BC11H11C109.5N2N1C10118.59 (18)C9C12H12A109.5C7N1C10129.66 (16)C9C12H12B109.5C9N2N1105.88 (17)H12AC12H12B109.5C4C1H1A109.5C9C12H12C109.5H1AC1H1B109.5H12AC12H12C109.5C4C1H1B109.5H12BC12H12C109.5C4C1H1B109.5C6C13C14117.17 (16)	C11—H11A		0.9600				
N2-N1-C7 111.58 (17) H11B-C11-H11C 109.5 N2-N1-C10 118.59 (18) C9-C12-H12A 109.5 C7-N1-C10 129.66 (16) C9-C12-H12B 109.5 C9-N2-N1 105.88 (17) H12A-C12-H12B 109.5 C4-C1-H1A 109.5 C9-C12-H12C 109.5 C4-C1-H1B 109.5 H12A-C12-H12C 109.5 H1A-C1-H1B 109.5 H12B-C12-H12C 109.5 C4-C1-H1B 109.5 H12B-C12-H12C 109.5 V4-C1-H1B 109.5 H12B-C12-H12C 109.5 V4-C1-H1B 109.5 H12B-C12-H12C 109.5 V4-C1-H1B 109.5 K12B-C12-K12C 109.5 V4-C1-H1B 109.5 K12B-C12-K12C 109.5	C5—O1—C6		119.76 (15)	H11A-		109.	5
N2—N1—C10 118.59 (18) C9—C12—H12A 109.5 C7—N1—C10 129.66 (16) C9—C12—H12B 109.5 C9—N2—N1 105.88 (17) H12A—C12—H12B 109.5 C4—C1—H1A 109.5 C9—C12—H12C 109.5 C4—C1—H1B 109.5 H12A—C12—H12C 109.5 H1A—C1—H1B 109.5 H12B—C12—H12C 109.5 C4—C1—H1C 109.5 C6—C13—C14 117.17 (16)	N2—N1—C7		111.58 (17)	H11B-		109.	5
C7—N1—C10129.66 (16)C9—C12—H12B109.5C9—N2—N1105.88 (17)H12A—C12—H12B109.5C4—C1—H1A109.5C9—C12—H12C109.5C4—C1—H1B109.5H12A—C12—H12C109.5H1A—C1—H1B109.5H12B—C12—H12C109.5C4—C1—H1B109.5C6—C13—C14117.17 (16)	N2—N1—C10		118.59 (18)	С9—С	C12—H12A	109.	5
C9—N2—N1 105.88 (17) H12A—C12—H12B 109.5 C4—C1—H1A 109.5 C9—C12—H12C 109.5 C4—C1—H1B 109.5 H12A—C12—H12C 109.5 H1A—C1—H1B 109.5 H12B—C12—H12C 109.5 C4—C1—H1B 109.5 H12B—C12—H12C 109.5 C4—C1—H1B 109.5 C6—C13—C14 117.17 (16)	C7—N1—C10		129.66 (16)	С9—С	С12—Н12В	109.	5
C4—C1—H1A 109.5 C9—C12—H12C 109.5 C4—C1—H1B 109.5 H12A—C12—H12C 109.5 H1A—C1—H1B 109.5 H12B—C12—H12C 109.5 C4—C1—H1C 109.5 C6—C13—C14 117.17 (16)	C9—N2—N1		105.88 (17)	H12A-	—C12—H12B	109.	5
C4—C1—H1B 109.5 H12A—C12—H12C 109.5 H1A—C1—H1B 109.5 H12B—C12—H12C 109.5 C4—C1—H1C 109.5 C6—C13—C14 117.17 (16)	C4—C1—H1A		109.5	С9—С	С12—Н12С	109.	5
H1A—C1—H1B 109.5 H12B—C12—H12C 109.5 C4—C1—H1C 109.5 C6—C13—C14 117.17 (16)	C4—C1—H1B		109.5	H12A-	—С12—Н12С	109.	5
C4—C1—H1C 109.5 C6—C13—C14 117.17 (16)	H1A—C1—H11	В	109.5	H12B-		109.	5
	C4—C1—H1C		109.5	C6—0	C13—C14	117.	17 (16)
H1A-C1-H1C 109.5 C6-C13-C15 128.05 (16)	H1A-C1-H10	С	109.5	C6—0	C13—C15	128.	05 (16)
H1B-C1-H1C 109.5 C14-C13-C15 114 78 (15)	H1B-C1-H10	С	109.5	C14—	C13—C15	114	78 (15)
C4—C2—H2A 109.5 N3—C14—C13 176.6 (2)	C4—C2—H2A		109.5	N3—0	C14—C13	176.	6 (2)
C4—C2—H2B 109.5 C20—C15—C16 117.94 (16)	C4—C2—H2B		109.5	C20—	C15—C16	117	94 (16)
H2A—C2—H2B 109.5 C20—C15—C13 118.69 (16)	H2A—C2—H2I	В	109.5	C20—	C15—C13	118.	69 (16)

C4—C2—H2C	109.5	C16—C15—C13	123.34 (16)
H2A—C2—H2C	109.5	C17—C16—C15	120.12 (17)
H2B—C2—H2C	109.5	С17—С16—Н16	119.9
С4—С3—НЗА	109.5	C15—C16—H16	119.9
С4—С3—Н3В	109.5	C16—C17—C18	122.38 (17)
НЗА—СЗ—НЗВ	109.5	C16—C17—H17	118.8
С4—С3—Н3С	109.5	С18—С17—Н17	118.8
НЗА—СЗ—НЗС	109.5	C17—C18—C19	116.85 (16)
НЗВ—СЗ—НЗС	109.5	C17—C18—C21	120.26 (18)
C2—C4—C5	108.99 (18)	C19—C18—C21	122.86 (17)
C2—C4—C1	110.5 (3)	C20-C19-C18	121.39 (17)
C5—C4—C1	109.33 (18)	С20—С19—Н19	119.3
C2—C4—C3	108.8 (2)	C18—C19—H19	119.3
C5—C4—C3	108.39 (19)	C19—C20—C15	121.29 (17)
C1—C4—C3	110.9 (2)	С19—С20—Н20	119.4
O2—C5—O1	120.98 (18)	С15—С20—Н20	119.4
O2—C5—C4	127.8 (2)	C22—C21—C24	109.5 (2)
O1—C5—C4	111.17 (17)	C22—C21—C18	111.85 (19)
C13—C6—O1	118.64 (15)	C24—C21—C18	108.12 (17)
C13—C6—C7	124.41 (16)	C22—C21—C23	108.4 (2)
O1—C6—C7	116.61 (15)	C24—C21—C23	109.8 (2)
N1—C7—C8	106.06 (16)	C18—C21—C23	109.15 (16)
N1—C7—C6	124.43 (17)	C21—C22—H22A	109.5
C8—C7—C6	129.32 (18)	C21—C22—H22B	109.5
С7—С8—С9	106.28 (19)	H22A—C22—H22B	109.5
C7—C8—Cl1	126.62 (15)	C21—C22—H22C	109.5
C9—C8—Cl1	127.10 (16)	H22A—C22—H22C	109.5
N2—C9—C8	110.19 (17)	H22B—C22—H22C	109.5
N2—C9—C12	121.3 (2)	C21—C23—H23A	109.5
C8—C9—C12	128.5 (2)	C21—C23—H23B	109.5
N1-C10-C11	113.0 (2)	H23A—C23—H23B	109.5
N1-C10-H10A	109.0	C21—C23—H23C	109.5
C11—C10—H10A	109.0	H23A—C23—H23C	109.5
N1—C10—H10B	109.0	H23B—C23—H23C	109.5
C11-C10-H10B	109.0	C21—C24—H24A	109.5
H10A-C10-H10B	107.8	C21—C24—H24B	109.5
C10-C11-H11A	109.5	H24A—C24—H24B	109.5
C10-C11-H11B	109.5	C21—C24—H24C	109.5
H11A—C11—H11B	109.5	H24A—C24—H24C	109.5
C10—C11—H11C	109.5	H24B—C24—H24C	109.5
C7—N1—N2—C9	-0.5 (2)	Cl1—C8—C9—C12	-1.7 (3)
C10—N1—N2—C9	-176.2 (2)	N2-N1-C10-C11	67.3 (3)
C6—O1—C5—O2	-8.6 (3)	C7—N1—C10—C11	-107.5 (3)
C6—O1—C5—C4	172.86 (15)	O1—C6—C13—C14	171.17 (17)
C2—C4—C5—O2	-107.5 (3)	C7—C6—C13—C14	-1.9 (3)
C1—C4—C5—O2	131.6 (3)	O1—C6—C13—C15	-9.1 (3)
C3—C4—C5—O2	10.7 (3)	C7—C6—C13—C15	177.85 (18)
C2—C4—C5—O1	70.9 (2)	C6—C13—C14—N3	-178 (100)
C1-C4-C5-O1	-49.9 (3)	C15—C13—C14—N3	2(4)

C3—C4—C5—O1	-170.9 (2)	C6—C13—C15—C20	-148.6 (2)
C5—O1—C6—C13	129.59 (19)	C14—C13—C15—C20	31.2 (2)
C5—O1—C6—C7	-56.8 (2)	C6-C13-C15-C16	33.6 (3)
N2—N1—C7—C8	-0.2 (2)	C14—C13—C15—C16	-146.64 (19)
C10—N1—C7—C8	174.9 (2)	C20-C15-C16-C17	1.7 (3)
N2—N1—C7—C6	175.15 (17)	C13-C15-C16-C17	179.58 (17)
C10—N1—C7—C6	-9.7 (3)	C15-C16-C17-C18	-0.5 (3)
C13—C6—C7—N1	-58.8 (3)	C16-C17-C18-C19	-0.9 (3)
O1—C6—C7—N1	128.03 (19)	C16-C17-C18-C21	-178.96 (18)
С13—С6—С7—С8	115.5 (2)	C17—C18—C19—C20	1.0 (3)
O1—C6—C7—C8	-57.7 (3)	C21—C18—C19—C20	178.99 (17)
N1—C7—C8—C9	0.8 (2)	C18—C19—C20—C15	0.3 (3)
C6—C7—C8—C9	-174.29 (17)	C16-C15-C20-C19	-1.7 (3)
N1—C7—C8—C11	-179.68 (14)	C13—C15—C20—C19	-179.61 (17)
C6—C7—C8—Cl1	5.3 (3)	C17—C18—C21—C22	-174.0 (2)
N1—N2—C9—C8	1.0 (2)	C19—C18—C21—C22	8.1 (3)
N1—N2—C9—C12	-178.1 (2)	C17—C18—C21—C24	65.4 (2)
C7—C8—C9—N2	-1.1 (2)	C19—C18—C21—C24	-112.5 (2)
Cl1—C8—C9—N2	179.36 (16)	C17—C18—C21—C23	-54.0 (3)
C7—C8—C9—C12	177.9 (2)	C19—C18—C21—C23	128.0 (2)



