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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

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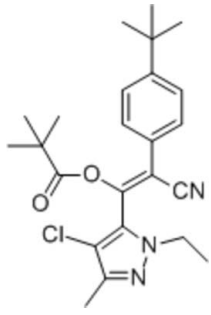
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.087; data-to-parameter ratio = 14.8.

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

Related literature

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



Experimental

Crystal data

$C_{24}H_{30}ClN_3O_2$
M_r = 427.96
Monoclinic, $P2_1$
a = 9.997 (2) Å
b = 9.563 (2) Å
c = 12.751 (3) Å
β = 95.008 (4)°
V = 1214.4 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 296 K
0.28 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.951, T_{max} = 0.965
6269 measured reflections
4137 independent reflections
3802 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.087
S = 1.04
4137 reflections
279 parameters
8 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-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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Yang, P., Shen, D. L., Tan, C. X., Weng, J. Q., Lu, Q., Wei, Y. C. & Kong, X. L. (2009). *Zhejiang Daxue Xuebao*, **36**, 183–185.

supporting information

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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

Man Xu, Haibo Yu and Bin Li

S1. 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 $C_{24}H_{30}Cl_1N_3O_2$: 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. ^{1}H NMR(DMSO): 1.2 (s, 9H, $CO(CH_3)_3$), 1.34 (s, 9H, Ph-$(CH_3)_3$), 1.55 (t, 3H, CH_3), 2.27 (s, 3H, CH_3), 4.21 (q, 2H, N—CH_2), 7.47 (d, 2H, Ph), 7.53 (d, 2H, Ph).

S2. Refinement

Although all H atoms were visible in difference maps, they werefinally placed in geometrically calculated positions, with C-Hdistances in the range 0.93–0.97 Å, andincluded 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).

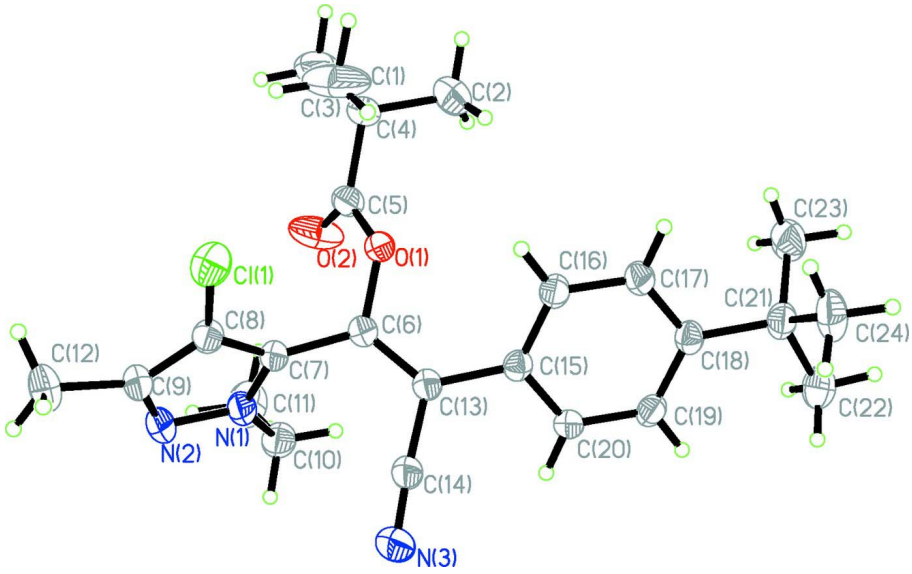

Figure 1

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

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

Crystal data

$C_{24}H_{30}ClN_3O_2$
$M_r = 427.96$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 9.997$ (2) Å
$b = 9.563$ (2) Å
$c = 12.751$ (3) Å
$\beta = 95.008$ (4)°
$V = 1214.4$ (5) Å^3
$Z = 2$
$F(000) = 456$
$D_x = 1.170$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3335 reflections
$\theta = 2.7$–25.8°
$\mu = 0.18$ mm^{-1}
$T = 296$ K
Block, colorless
0.28 × 0.22 × 0.20 mm

Data collection

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

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.087$
$S = 1.04$
4137 reflections
279 parameters
8 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
$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 0.1092P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.11$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Absolute structure: Flack (1983), 1848 Friedel pairs
Absolute structure parameter: 0.08 (5)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.89003 (6)	1.14801 (5)	0.28949 (4)	0.06542 (17)
O1	0.69009 (13)	0.98017 (15)	0.09872 (9)	0.0502 (3)
O2	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)
C9	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*
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 (Å²)

	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)
O1	0.0546 (7)	0.0564 (8)	0.0402 (6)	0.0170 (6)	0.0082 (5)	0.0091 (6)
O2	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)
C9	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)
C24	0.0965 (18)	0.096 (2)	0.0527 (13)	−0.0131 (15)	−0.0027 (12)	0.0278 (13)

Geometric parameters (Å, º)

Cl1—C8	1.718 (2)	C11—H11B	0.9600
O1—C5	1.377 (2)	C11—H11C	0.9600
O1—C6	1.382 (2)	C12—H12A	0.9600
O2—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—C20	1.388 (3)
N3—C14	1.149 (3)	C15—C16	1.391 (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	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—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		

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
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)
H1A—C1—H1C	109.5	C6—C13—C15	128.05 (16)
H1B—C1—H1C	109.5	C14—C13—C15	114.78 (15)
C4—C2—H2A	109.5	N3—C14—C13	176.6 (2)
C4—C2—H2B	109.5	C20—C15—C16	117.94 (16)
H2A—C2—H2B	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	C17—C16—H16	119.9
C4—C3—H3A	109.5	C15—C16—H16	119.9
C4—C3—H3B	109.5	C16—C17—C18	122.38 (17)
H3A—C3—H3B	109.5	C16—C17—H17	118.8
C4—C3—H3C	109.5	C18—C17—H17	118.8
H3A—C3—H3C	109.5	C17—C18—C19	116.85 (16)
H3B—C3—H3C	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)	C20—C19—H19	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)	C19—C20—H20	119.4
O2—C5—O1	120.98 (18)	C15—C20—H20	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
C7—C8—C9	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)
C13—C6—C7—C8	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—Cl1	−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)