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tert-Butyl 4-({[(*E*)-1,3-dimethyl-5-phenoxypyrazol-4-yl]methyl}aminooxymethyl)benzoate

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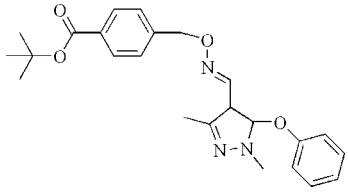
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.055; wR factor = 0.175; data-to-parameter ratio = 13.9.

The title compound, $C_{24}H_{27}N_3O_4$, also known as fenpyroximate, is a commercial acaricide. The benzene ring of the phenoxy group is approximately perpendicular to the pyrazole ring with a dihedral angle of 84.37 (11)°. The dihedral angle between the phenoxy and the benzoate benzene rings is 48.83 (8)°.

Related literature

For background to the design of bioactive molecules, see: Lewis *et al.* (1991) and for a related structure, see: Zou *et al.* (2006).



Experimental

Crystal data

$C_{24}H_{27}N_3O_4$
M_r = 421.49
Triclinic, $P\overline{1}$
a = 9.672 (3) Å
b = 9.908 (3) Å
c = 13.179 (3) Å
α = 72.487 (5)°
β = 71.614 (5)°
γ = 74.494 (4)°
V = 1122.0 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
0.32 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.972, T_{max} = 0.983
5754 measured reflections
3941 independent reflections
2284 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.175
S = 1.06
3941 reflections
284 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2396).

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Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zou, X.-M., Lin, D., Pei, J., Wang, C.-Q. & Yang, H.-Z. (2006). *Acta Cryst.* E**62**, o2471–o2472.

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supporting information

Acta Cryst. (2008). E**64**, o192 [https://doi.org/10.1107/S160053680705427X]

tert-Butyl 4-({[(*E*)-1,3-dimethyl-5-phenoxypyrazol-4-yl]methyl}amino-oxymethyl)benzoate

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S1. Comment

Since biological activities are related to the conformation of molecules, study of the relationships between chemical structure and biological activity is important in the rational design of bioactive molecules (Lewis *et al.*, 1991). The title compound, also known as Fenpyroximate, is a commercial acaricide. Details of its crystal structure may be helpful for the design of new acaricidal compounds and we report here the structure of the title compound (I), Fig. 1. In (I), the benzene ring (C1/C2/C3/C4/C5/C6) is approximately perpendicular to the pyrazole ring with a dihedral angle of 84.37 (11) ° between them. The dihedral angle between the benzoate benzene ring(C14/C15/C16/C17/C18/C19) and the pyrazole ring is 64.87 (11) °. This is different to the dihedral angle between the pyrimidine ring and the pyrazole ring in (*E*)-5(3,5-dimethylphenoxy)-1,3-dimethyl-1*H*-pyrazole-4-carbaldehyde *O*-(2-chloropyrimidin-4-yl)oxime (Zou *et al.*, 2006).

S2. Experimental

Tert-butyl-(4-bromomethyl)benzoate(2.2 mmol), anhydrous potassium carbonate (4 mmol), and 1,3-dimethyl-5-phenoxy-1*H*-pyrazole-4- carbaldehyde oxime (2 mmol) were mixed in acetonitrile (40 ml) and refluxed for 5 h. The solvent was then evaporated *in vacuo*. The residue was recrystallized from ethanol and single crystals of (I) suitable for X-ray analysis were grown from ethyl acetate and petroleum ether at room temperature.

S3. Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.93 Å, U_{iso}=1.2U_{eq} (C) for aromatic 0.97 Å, U_{iso} = 1.2U_{eq} (C) for CH_2 and 0.96 Å, U_{iso} = 1.5U_{eq} (C) for CH_3 atoms.

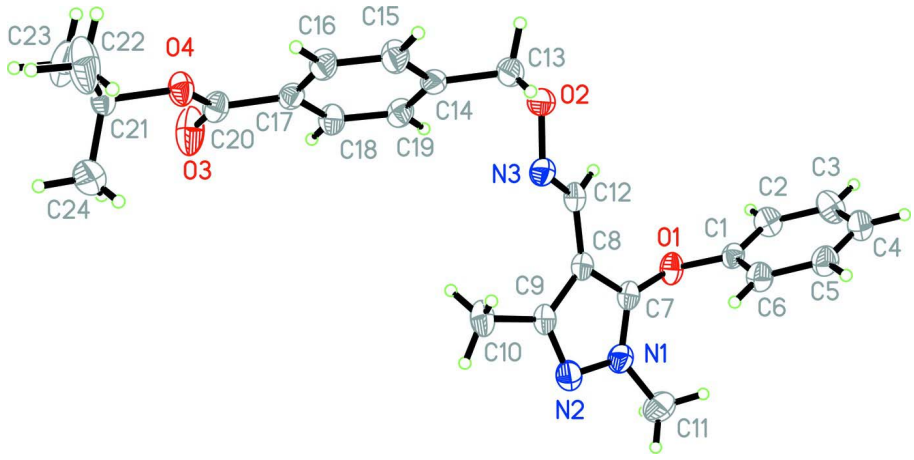

Figure 1

View of the title compound with displacement ellipsoids drawn at the 30% probability level.

tert-Butyl 4-({[(*E*)-1,3-dimethyl-5-phenoxypyrazol-4-yl]methyl}aminooxymethyl)benzoate

Crystal data

$C_{24}H_{27}N_3O_4$
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$\alpha = 72.487\ (5)°$
$\beta = 71.614\ (5)°$
$\gamma = 74.494\ (4)°$
$V = 1122.0\ (6)$ Å^3
$Z = 2$
$F(000) = 448$
$D_x = 1.248$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1585 reflections
$\theta = 2.2–22.6°$
$\mu = 0.09$ mm^{-1}
$T = 294$ K
Prism, colorless
0.32 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
$T_{min} = 0.972$, $T_{max} = 0.983$
5754 measured reflections
3941 independent reflections
2284 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.7°$
$h = -11\rightarrow11$
$k = -8\rightarrow11$
$l = -10\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.175$
$S = 1.06$
3941 reflections
284 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0841P)^2 + 0.1856P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

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}
O1	0.26628 (19)	1.1772 (2)	−0.00386 (14)	0.0554 (5)
O2	0.3962 (2)	0.6532 (2)	0.19530 (16)	0.0616 (6)
O3	1.0760 (3)	0.3688 (3)	0.34012 (19)	0.0934 (9)
O4	0.9545 (2)	0.2420 (2)	0.49895 (15)	0.0561 (5)
N1	0.3522 (3)	1.2674 (3)	0.1062 (2)	0.0559 (6)
N2	0.4285 (3)	1.2208 (3)	0.1845 (2)	0.0609 (7)
N3	0.4010 (3)	0.7806 (3)	0.2206 (2)	0.0542 (6)
C1	0.1138 (3)	1.1919 (3)	0.0179 (2)	0.0441 (7)
C2	0.0642 (3)	1.1915 (3)	−0.0686 (2)	0.0601 (8)
H2	0.1307	1.1812	−0.1356	0.072*
C3	−0.0863 (4)	1.2068 (4)	−0.0544 (3)	0.0743 (10)
H3	−0.1213	1.2064	−0.1124	0.089*
C4	−0.1839 (4)	1.2223 (3)	0.0431 (3)	0.0673 (9)
H4	−0.2850	1.2318	0.0520	0.081*
C5	−0.1329 (3)	1.2238 (3)	0.1279 (3)	0.0612 (8)
H5	−0.2000	1.2349	0.1945	0.073*
C6	0.0167 (3)	1.2090 (3)	0.1166 (2)	0.0545 (8)
H6	0.0510	1.2106	0.1746	0.065*
C7	0.3276 (3)	1.1573 (3)	0.0806 (2)	0.0479 (7)
C8	0.3863 (3)	1.0308 (3)	0.1450 (2)	0.0456 (7)
C9	0.4502 (3)	1.0776 (3)	0.2080 (2)	0.0519 (7)
C10	0.5368 (4)	0.9888 (4)	0.2888 (3)	0.0734 (10)
H10A	0.5743	1.0507	0.3132	0.110*
H10B	0.6183	0.9235	0.2545	0.110*
H10C	0.4738	0.9348	0.3507	0.110*
C11	0.3029 (4)	1.4211 (3)	0.0637 (3)	0.0784 (10)
H11A	0.3730	1.4549	−0.0036	0.118*
H11B	0.2959	1.4727	0.1168	0.118*
H11C	0.2074	1.4370	0.0499	0.118*
C12	0.3833 (3)	0.8883 (3)	0.1411 (2)	0.0493 (7)
H12	0.3681	0.8747	0.0790	0.059*
C13	0.3981 (3)	0.5385 (3)	0.2913 (3)	0.0615 (8)
H13A	0.3680	0.4583	0.2816	0.074*
H13B	0.3258	0.5706	0.3536	0.074*
C14	0.5472 (3)	0.4862 (3)	0.3174 (2)	0.0499 (7)

C15	0.5588 (3)	0.3798 (3)	0.4126 (3)	0.0631 (9)
H15	0.4754	0.3429	0.4580	0.076*
C16	0.6917 (3)	0.3281 (3)	0.4406 (2)	0.0569 (8)
H16	0.6969	0.2582	0.5055	0.068*
C17	0.8173 (3)	0.3792 (3)	0.3734 (2)	0.0457 (7)
C18	0.8060 (3)	0.4847 (3)	0.2779 (2)	0.0536 (7)
H18	0.8900	0.5200	0.2315	0.064*
C19	0.6725 (3)	0.5377 (3)	0.2510 (2)	0.0518 (7)
H19	0.6667	0.6093	0.1872	0.062*
C20	0.9636 (3)	0.3290 (3)	0.4004 (2)	0.0532 (7)
C21	1.0809 (3)	0.1863 (3)	0.5491 (2)	0.0522 (7)
C22	1.2093 (4)	0.1033 (5)	0.4795 (3)	0.1094 (16)
H22A	1.1775	0.0273	0.4668	0.164*
H22B	1.2871	0.0626	0.5167	0.164*
H22C	1.2456	0.1668	0.4103	0.164*
C23	1.0184 (5)	0.0865 (5)	0.6550 (3)	0.1151 (17)
H23A	0.9339	0.1395	0.6979	0.173*
H23B	1.0927	0.0446	0.6955	0.173*
H23C	0.9886	0.0115	0.6394	0.173*
C24	1.1218 (5)	0.3089 (4)	0.5687 (4)	0.1043 (14)
H24A	1.1617	0.3702	0.4994	0.156*
H24B	1.1949	0.2726	0.6104	0.156*
H24C	1.0352	0.3630	0.6090	0.156*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0442 (11)	0.0691 (14)	0.0429 (11)	−0.0020 (9)	−0.0124 (9)	−0.0054 (9)
O2	0.0750 (14)	0.0483 (12)	0.0716 (14)	−0.0077 (10)	−0.0418 (11)	−0.0080 (10)
O3	0.0540 (14)	0.124 (2)	0.0669 (16)	−0.0101 (14)	−0.0133 (12)	0.0198 (14)
O4	0.0515 (12)	0.0629 (13)	0.0494 (12)	−0.0120 (9)	−0.0224 (9)	0.0041 (10)
N1	0.0533 (15)	0.0509 (15)	0.0583 (15)	−0.0045 (12)	−0.0181 (12)	−0.0063 (12)
N2	0.0529 (15)	0.0655 (18)	0.0656 (17)	−0.0076 (12)	−0.0213 (13)	−0.0145 (13)
N3	0.0561 (15)	0.0490 (15)	0.0595 (16)	−0.0021 (11)	−0.0254 (12)	−0.0114 (12)
C1	0.0431 (16)	0.0375 (15)	0.0456 (16)	−0.0048 (11)	−0.0137 (13)	−0.0010 (12)
C2	0.0605 (19)	0.071 (2)	0.0476 (18)	−0.0151 (16)	−0.0105 (15)	−0.0140 (15)
C3	0.068 (2)	0.094 (3)	0.071 (2)	−0.0225 (19)	−0.0294 (19)	−0.016 (2)
C4	0.0504 (19)	0.066 (2)	0.088 (3)	−0.0082 (15)	−0.0240 (19)	−0.0171 (18)
C5	0.0486 (18)	0.065 (2)	0.065 (2)	−0.0076 (15)	−0.0050 (15)	−0.0201 (16)
C6	0.0529 (18)	0.0619 (19)	0.0471 (18)	−0.0077 (14)	−0.0146 (14)	−0.0117 (14)
C7	0.0377 (15)	0.0532 (18)	0.0447 (16)	−0.0033 (13)	−0.0087 (13)	−0.0065 (13)
C8	0.0363 (14)	0.0491 (17)	0.0457 (16)	−0.0042 (12)	−0.0104 (12)	−0.0065 (13)
C9	0.0362 (15)	0.061 (2)	0.0538 (18)	−0.0045 (13)	−0.0124 (13)	−0.0102 (14)
C10	0.0582 (19)	0.084 (2)	0.081 (2)	−0.0019 (17)	−0.0388 (17)	−0.0120 (18)
C11	0.091 (3)	0.051 (2)	0.087 (3)	−0.0066 (17)	−0.030 (2)	−0.0051 (17)
C12	0.0393 (15)	0.0579 (19)	0.0472 (17)	−0.0026 (13)	−0.0161 (13)	−0.0079 (14)
C13	0.067 (2)	0.0487 (18)	0.074 (2)	−0.0127 (15)	−0.0381 (17)	0.0007 (15)
C14	0.0603 (18)	0.0389 (15)	0.0568 (18)	−0.0069 (13)	−0.0279 (15)	−0.0091 (13)

C15	0.0567 (19)	0.0589 (19)	0.067 (2)	−0.0178 (15)	−0.0245 (16)	0.0097 (15)
C16	0.0611 (19)	0.0506 (18)	0.0541 (18)	−0.0128 (14)	−0.0244 (15)	0.0067 (14)
C17	0.0513 (17)	0.0414 (15)	0.0439 (16)	−0.0029 (12)	−0.0165 (13)	−0.0102 (12)
C18	0.0520 (17)	0.0590 (19)	0.0445 (17)	−0.0078 (14)	−0.0138 (14)	−0.0055 (14)
C19	0.0616 (19)	0.0490 (17)	0.0413 (16)	−0.0051 (14)	−0.0195 (14)	−0.0034 (13)
C20	0.0542 (19)	0.0549 (18)	0.0452 (18)	−0.0018 (14)	−0.0160 (15)	−0.0083 (14)
C21	0.0502 (16)	0.0573 (18)	0.0492 (17)	−0.0058 (14)	−0.0231 (14)	−0.0055 (14)
C22	0.105 (3)	0.112 (3)	0.106 (3)	0.049 (3)	−0.059 (3)	−0.046 (3)
C23	0.089 (3)	0.156 (4)	0.080 (3)	−0.039 (3)	−0.048 (2)	0.042 (3)
C24	0.122 (3)	0.080 (3)	0.140 (4)	−0.012 (2)	−0.085 (3)	−0.021 (3)

Geometric parameters (Å, º)

O1—C7	1.360 (3)	C11—H11A	0.9600
O1—C1	1.386 (3)	C11—H11B	0.9600
O2—N3	1.414 (3)	C11—H11C	0.9600
O2—C13	1.425 (3)	C12—H12	0.9300
O3—C20	1.210 (3)	C13—C14	1.507 (4)
O4—C20	1.316 (3)	C13—H13A	0.9700
O4—C21	1.471 (3)	C13—H13B	0.9700
N1—C7	1.332 (4)	C14—C19	1.373 (4)
N1—N2	1.355 (3)	C14—C15	1.388 (4)
N1—C11	1.458 (4)	C15—C16	1.373 (4)
N2—C9	1.331 (4)	C15—H15	0.9300
N3—C12	1.268 (3)	C16—C17	1.377 (4)
C1—C2	1.370 (4)	C16—H16	0.9300
C1—C6	1.371 (4)	C17—C18	1.386 (4)
C2—C3	1.380 (4)	C17—C20	1.487 (4)
C2—H2	0.9300	C18—C19	1.373 (4)
C3—C4	1.358 (4)	C18—H18	0.9300
C3—H3	0.9300	C19—H19	0.9300
C4—C5	1.361 (4)	C21—C24	1.487 (5)
C4—H4	0.9300	C21—C23	1.499 (4)
C5—C6	1.379 (4)	C21—C22	1.500 (5)
C5—H5	0.9300	C22—H22A	0.9600
C6—H6	0.9300	C22—H22B	0.9600
C7—C8	1.377 (4)	C22—H22C	0.9600
C8—C9	1.413 (4)	C23—H23A	0.9600
C8—C12	1.436 (4)	C23—H23B	0.9600
C9—C10	1.489 (4)	C23—H23C	0.9600
C10—H10A	0.9600	C24—H24A	0.9600
C10—H10B	0.9600	C24—H24B	0.9600
C10—H10C	0.9600	C24—H24C	0.9600
C7—O1—C1	119.0 (2)	O2—C13—H13A	108.8
N3—O2—C13	108.3 (2)	C14—C13—H13A	108.8
C20—O4—C21	122.9 (2)	O2—C13—H13B	108.8
C7—N1—N2	111.3 (2)	C14—C13—H13B	108.8

C7—N1—C11	128.0 (3)	H13A—C13—H13B	107.7
N2—N1—C11	120.7 (3)	C19—C14—C15	118.4 (3)
C9—N2—N1	105.4 (2)	C19—C14—C13	123.2 (3)
C12—N3—O2	110.3 (2)	C15—C14—C13	118.4 (3)
C2—C1—C6	121.1 (3)	C16—C15—C14	121.0 (3)
C2—C1—O1	114.9 (2)	C16—C15—H15	119.5
C6—C1—O1	123.9 (2)	C14—C15—H15	119.5
C1—C2—C3	118.8 (3)	C15—C16—C17	120.4 (3)
C1—C2—H2	120.6	C15—C16—H16	119.8
C3—C2—H2	120.6	C17—C16—H16	119.8
C4—C3—C2	120.8 (3)	C16—C17—C18	118.6 (3)
C4—C3—H3	119.6	C16—C17—C20	122.8 (3)
C2—C3—H3	119.6	C18—C17—C20	118.6 (3)
C3—C4—C5	119.7 (3)	C19—C18—C17	120.8 (3)
C3—C4—H4	120.2	C19—C18—H18	119.6
C5—C4—H4	120.2	C17—C18—H18	119.6
C4—C5—C6	121.0 (3)	C18—C19—C14	120.8 (3)
C4—C5—H5	119.5	C18—C19—H19	119.6
C6—C5—H5	119.5	C14—C19—H19	119.6
C1—C6—C5	118.5 (3)	O3—C20—O4	124.4 (3)
C1—C6—H6	120.7	O3—C20—C17	123.4 (3)
C5—C6—H6	120.7	O4—C20—C17	112.1 (3)
N1—C7—O1	121.8 (2)	O4—C21—C24	108.7 (2)
N1—C7—C8	108.6 (3)	O4—C21—C23	102.6 (2)
O1—C7—C8	129.4 (3)	C24—C21—C23	111.6 (3)
C7—C8—C9	103.6 (3)	O4—C21—C22	111.5 (2)
C7—C8—C12	125.5 (3)	C24—C21—C22	112.2 (3)
C9—C8—C12	130.9 (2)	C23—C21—C22	109.9 (3)
N2—C9—C8	111.1 (2)	C21—C22—H22A	109.5
N2—C9—C10	120.4 (3)	C21—C22—H22B	109.5
C8—C9—C10	128.5 (3)	H22A—C22—H22B	109.5
C9—C10—H10A	109.5	C21—C22—H22C	109.5
C9—C10—H10B	109.5	H22A—C22—H22C	109.5
H10A—C10—H10B	109.5	H22B—C22—H22C	109.5
C9—C10—H10C	109.5	C21—C23—H23A	109.5
H10A—C10—H10C	109.5	C21—C23—H23B	109.5
H10B—C10—H10C	109.5	H23A—C23—H23B	109.5
N1—C11—H11A	109.5	C21—C23—H23C	109.5
N1—C11—H11B	109.5	H23A—C23—H23C	109.5
H11A—C11—H11B	109.5	H23B—C23—H23C	109.5
N1—C11—H11C	109.5	C21—C24—H24A	109.5
H11A—C11—H11C	109.5	C21—C24—H24B	109.5
H11B—C11—H11C	109.5	H24A—C24—H24B	109.5
N3—C12—C8	121.5 (3)	C21—C24—H24C	109.5
N3—C12—H12	119.3	H24A—C24—H24C	109.5
C8—C12—H12	119.3	H24B—C24—H24C	109.5
O2—C13—C14	114.0 (2)		

C7—N1—N2—C9	−0.4 (3)	C7—C8—C9—C10	−176.7 (3)
C11—N1—N2—C9	177.3 (3)	C12—C8—C9—C10	1.2 (5)
C13—O2—N3—C12	−172.9 (2)	O2—N3—C12—C8	−178.9 (2)
C7—O1—C1—C2	−171.4 (2)	C7—C8—C12—N3	−160.1 (3)
C7—O1—C1—C6	10.0 (4)	C9—C8—C12—N3	22.4 (4)
C6—C1—C2—C3	−0.9 (4)	N3—O2—C13—C14	−73.9 (3)
O1—C1—C2—C3	−179.5 (3)	O2—C13—C14—C19	−3.9 (4)
C1—C2—C3—C4	0.2 (5)	O2—C13—C14—C15	176.7 (3)
C2—C3—C4—C5	0.4 (5)	C19—C14—C15—C16	0.7 (5)
C3—C4—C5—C6	−0.3 (5)	C13—C14—C15—C16	−179.9 (3)
C2—C1—C6—C5	0.9 (4)	C14—C15—C16—C17	−1.3 (5)
O1—C1—C6—C5	179.5 (2)	C15—C16—C17—C18	0.8 (4)
C4—C5—C6—C1	−0.3 (4)	C15—C16—C17—C20	179.0 (3)
N2—N1—C7—O1	−173.2 (2)	C16—C17—C18—C19	0.3 (4)
C11—N1—C7—O1	9.3 (4)	C20—C17—C18—C19	−178.0 (3)
N2—N1—C7—C8	1.2 (3)	C17—C18—C19—C14	−0.8 (4)
C11—N1—C7—C8	−176.3 (3)	C15—C14—C19—C18	0.4 (4)
C1—O1—C7—N1	−93.0 (3)	C13—C14—C19—C18	−179.1 (3)
C1—O1—C7—C8	93.9 (3)	C21—O4—C20—O3	2.1 (5)
N1—C7—C8—C9	−1.4 (3)	C21—O4—C20—C17	−175.1 (2)
O1—C7—C8—C9	172.5 (3)	C16—C17—C20—O3	177.0 (3)
N1—C7—C8—C12	−179.4 (2)	C18—C17—C20—O3	−4.8 (4)
O1—C7—C8—C12	−5.6 (4)	C16—C17—C20—O4	−5.7 (4)
N1—N2—C9—C8	−0.5 (3)	C18—C17—C20—O4	172.4 (2)
N1—N2—C9—C10	177.6 (2)	C20—O4—C21—C24	65.5 (4)
C7—C8—C9—N2	1.2 (3)	C20—O4—C21—C23	−176.2 (3)
C12—C8—C9—N2	179.0 (3)	C20—O4—C21—C22	−58.7 (4)