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5-[(Benzo[*d*][1,3]dioxol-5-yl)methyl]-3-[4-(pyridin-2-yl)phenyl]-4,5-dihydroisoxazole

Nasseem El-Khatatneh,[a] A. C. Vinayaka,[b] Chandra,[a] M. P. Sadashiva,[b] S. Jeyaseelan[c] and M. Mahendra[a]*

[a]Department of Studies in Physics, Manasagangotri, University of Mysore, Mysore 570 006, India, [b]Department of Studies in Chemistry, Manasagangotri, University of Mysore, Mysore 570 006, India, and [c]Department of Physics, St Philomena's College, Mysore, India. *Correspondence e-mail: mahendra@physics.uni-mysore.ac.in

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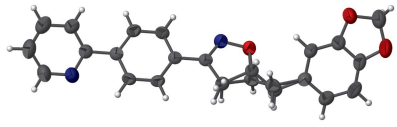
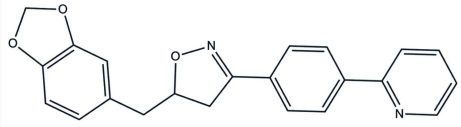
In the molecule of the title compound $C_{22}H_{18}N_2O_3$, the benzodioxole and dihydroisoxazole rings are bridged *via* a methylene (CH_2) group. The linkage is disordered over two positions with a occupancy factors of 0.887 (5) and 0.113 (5). The dihydroisoxazole and pyridine rings exhibit *syn-clinal* and *anti-periplanar* conformations with respect to the benzodioxole and benzene ring groups, as quantified by the torsion angle values of 70.7 (3) and 157.00 (17)°. Aside from van der Waals contacts, there are no significant intermolecular interactions.

3D view



Chemical scheme



Structure description

Isoxazolines are heterocyclic compounds bearing nitrogen and oxygen at adjacent positions of five-membered rings. Substituted isoxazolines have demonstrated diverse properties, including their use as anti-bacterial (Shah & Desai, 2007), anti-cancer (Kamal *et al.*, 2010), anti-inflammatory (Habeeb *et al.*, 2001) and antifungal agents (Dighade *et al.*, 2003). In addition, isoxazolines produced from cycloaddition reactions of nitrile oxide and alkenes have been used as masked β-amino alcohols and β-hydroxy carbonyl aldolates. With this background and as a part of our continuing study of isoxazole derivatives (Chandra *et al.*, 2013), the title compound was synthesized and its crystal structure determined.

In the title compound (Fig. 1), there is a small amount of disorder of the methylene linkage between the benzodioxazole and isoxazoline rings, involving atoms C10 and C11, with refined occupancies of 0.887 (5) and 0.113 (5), respectively, for the major and minor components. The dihydroisoxazole and pyridine rings exhibit *syn-clinal* and *anti-periplanar* orientations with respect to the benzodioxole and phenyl rings, as indicated by the

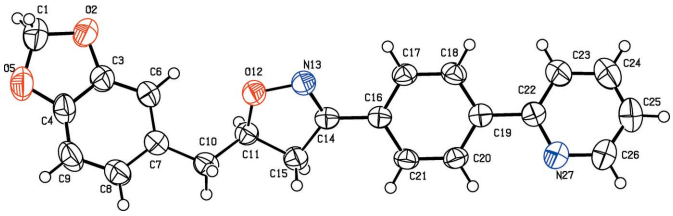


Figure 1
A view of the molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at 50° probability. Atoms C10 and C11 are shown for the major disorder component [occupancy = 0.887 (5)]. The minor component atoms have been omitted to enhance clarity.

torsion angles of 70.7 (3)° (O12—C11—C10—C7) and 157.00 (17)° (C18—C19—C22—N27), respectively. In addition, the benzene ring makes dihedral angles of 17.54 (11) and 24.82 (9)° with the mean planes of the dihydroisoxazole and pyridine rings, respectively.

Aside from van der Waals contacts, there are no significant intermolecular interactions. The packing of the molecules viewed down the *a* axis is shown in Fig. 2.

Synthesis and crystallization

A solution of 4-(pyridin-2-yl)benzaldehyde (0.002 mol), hydroxylamine hydrochloride (0.002 mol) and triethylamine (0.0025 mol) in DMF was stirred at room temperature for 6 h.

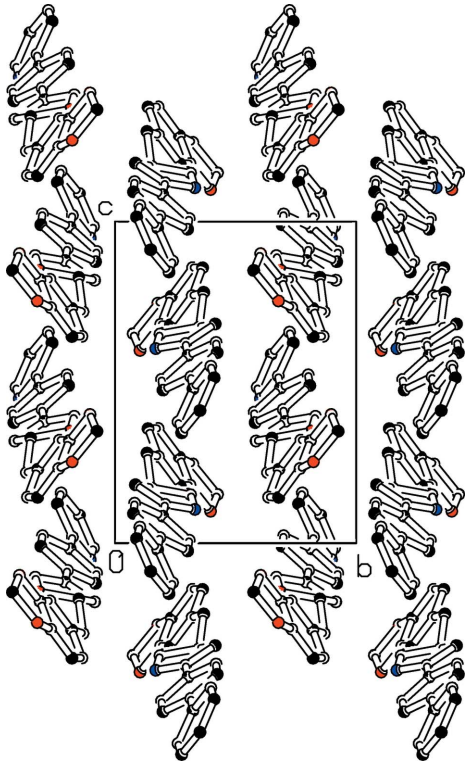


Figure 2
A packing diagram viewed parallel to the *a* axis. H atoms have been omitted for the sake of clarity.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{18}N_2O_3$
M_r	358.38
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	17.548 (5), 8.719 (3), 12.237 (4)
β (°)	108.380 (9)
V (Å^3)	1776.8 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.30 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker MicroStar microfocus rotating anode
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12236, 3242, 2353
R_{int}	0.067
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.127, 1.05
No. of reflections	3242
No. of parameters	263
No. of restraints	60
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.15, −0.16

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS* (Sheldrick, 2008), *SHELXL2016/6* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008).

After completion of the reaction (monitored by TLC), crushed ice was added to the reaction mixture and the precipitated solid product (an oxime) was filtered, washed with hexane and dried. *N*-chlorosuccinimide (0.0015 mol) and triethylamine (0.0015 mol) were added to a solution of the oxime (0.001 mol) and safrole (0.0012 mol) in DMF at 0°C. This reaction mixture was stirred at room temperature for 12 h. After completion of reaction, water was added and the product was extracted with ethyl acetate. The combined organic layers were dried and concentrated under reduced pressure. The crude product was purified using silica gel column chromatography. Recrystallization from absolute ethanol solution by slow evaporation yielded block-shaped single crystals after five days.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The disordered positions of the atoms C10 and C11, located between the benzodioxole and dihydroisoxazole rings, were refined with an occupancy ratio of 0.887 (5):0.113 (5).

Acknowledgements

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full crystallographic data

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Crystal data

$C_{22}H_{18}N_2O_3$
M_r = 358.38
Monoclinic, $P2_1/c$
a = 17.548 (5) Å
b = 8.719 (3) Å
c = 12.237 (4) Å
β = 108.380 (9)°
V = 1776.8 (9) Å^3
Z = 4
$F(000)$ = 752
D_x = 1.340 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3242 reflections
θ = 2.5–25.4°
μ = 0.09 mm^{-1}
T = 293 K
Block, colourless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker MicroStar microfocus rotating anode diffractometer
φ and ω scans
12236 measured reflections
3242 independent reflections
2353 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 25.4°, θ_{min} = 2.5°
h = −21→19
k = −10→10
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.127
S = 1.05
3242 reflections
263 parameters
60 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
$w = 1/[\sigma^2(F_o^2) + (0.0725P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.47963 (13)	0.9248 (3)	0.34808 (19)	0.0910 (7)	
H1A	0.476464	1.030174	0.321532	0.109*	
H1B	0.532351	0.908313	0.403500	0.109*	
O2	0.41886 (8)	0.89620 (18)	0.40031 (11)	0.0904 (5)	
C3	0.36100 (10)	0.8108 (2)	0.31934 (14)	0.0573 (5)	
C4	0.39006 (10)	0.7669 (2)	0.23254 (15)	0.0590 (5)	
O5	0.46718 (7)	0.82244 (18)	0.25346 (12)	0.0840 (5)	
C6	0.28619 (10)	0.7700 (2)	0.32070 (14)	0.0599 (5)	
H6	0.267161	0.801304	0.379978	0.072*	
C8	0.26959 (11)	0.6370 (2)	0.14350 (15)	0.0639 (5)	
H8	0.237722	0.577815	0.083071	0.077*	
C9	0.34576 (11)	0.6787 (2)	0.14300 (15)	0.0705 (6)	
H9	0.365640	0.647985	0.084423	0.085*	
C7	0.23922 (10)	0.67991 (18)	0.23030 (14)	0.0516 (4)	0.887 (5)
C10	0.15409 (14)	0.6325 (3)	0.2197 (2)	0.0547 (6)	0.887 (5)
H10A	0.117542	0.692128	0.158454	0.066*	0.887 (5)
H10B	0.147334	0.525643	0.196520	0.066*	0.887 (5)
C11	0.12945 (13)	0.6508 (2)	0.3270 (2)	0.0424 (6)	0.887 (5)
H11	0.170276	0.604578	0.392771	0.051*	0.887 (5)
O12	0.12162 (6)	0.81353 (11)	0.34924 (10)	0.0531 (3)	0.887 (5)
C15	0.04667 (9)	0.58461 (17)	0.31803 (14)	0.0499 (4)	0.887 (5)
H15A	0.013153	0.573540	0.238529	0.060*	0.887 (5)
H15B	0.051054	0.486500	0.356906	0.060*	0.887 (5)
C7′	0.23922 (10)	0.67991 (18)	0.23030 (14)	0.0516 (4)	0.113 (5)
C10′	0.1723 (11)	0.582 (2)	0.276 (2)	0.054 (3)	0.113 (5)
H10C	0.157134	0.487997	0.232027	0.065*	0.113 (5)
H10D	0.196003	0.554748	0.356613	0.065*	0.113 (5)
C11′	0.1014 (11)	0.6773 (18)	0.2615 (18)	0.047 (3)	0.113 (5)
H11′	0.074237	0.708414	0.181713	0.057*	0.113 (5)
O12′	0.12162 (6)	0.81353 (11)	0.34924 (10)	0.0531 (3)	0.113 (5)
C15′	0.04667 (9)	0.58461 (17)	0.31803 (14)	0.0499 (4)	0.113 (5)
H15C	0.003058	0.534073	0.260051	0.060*	0.113 (5)
H15D	0.077513	0.508525	0.371765	0.060*	0.113 (5)
N13	0.05736 (8)	0.83097 (14)	0.39460 (12)	0.0506 (4)	
C14	0.01581 (9)	0.70717 (15)	0.37897 (12)	0.0398 (4)	
C16	−0.05616 (8)	0.69760 (15)	0.41597 (12)	0.0393 (4)	
C17	−0.07063 (9)	0.80733 (16)	0.49036 (13)	0.0455 (4)	
H17	−0.033776	0.886052	0.517743	0.055*	
C18	−0.13835 (9)	0.80089 (16)	0.52372 (13)	0.0473 (4)	
H18	−0.146039	0.874131	0.574493	0.057*	
C19	−0.19610 (9)	0.68566 (16)	0.48246 (12)	0.0426 (4)	
C20	−0.18195 (9)	0.57667 (17)	0.40750 (12)	0.0465 (4)	
H20	−0.219542	0.499587	0.378580	0.056*	
C21	−0.11317 (9)	0.58109 (16)	0.37545 (12)	0.0447 (4)	
H21	−0.104622	0.506083	0.326543	0.054*	

C22	−0.26850 (10)	0.67674 (18)	0.52005 (14)	0.0498 (4)
C23	−0.27040 (12)	0.7388 (2)	0.62257 (17)	0.0738 (6)
H23	−0.225885	0.791438	0.669142	0.089*
C24	−0.33721 (13)	0.7237 (3)	0.6566 (2)	0.0890 (7)
H24	−0.338453	0.765019	0.726104	0.107*
C25	−0.40116 (14)	0.6478 (3)	0.5874 (2)	0.0954 (8)
H25	−0.447397	0.635161	0.608123	0.114*
C26	−0.39649 (14)	0.5894 (3)	0.4855 (2)	0.1125 (10)
H26	−0.440903	0.537175	0.438327	0.135*
N27	−0.33213 (10)	0.6029 (2)	0.44961 (15)	0.0849 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0725 (13)	0.1224 (19)	0.0919 (15)	−0.0282 (13)	0.0456 (12)	−0.0187 (14)
O2	0.0684 (8)	0.1366 (13)	0.0756 (9)	−0.0439 (9)	0.0362 (7)	−0.0360 (9)
C3	0.0549 (10)	0.0713 (12)	0.0488 (10)	−0.0075 (9)	0.0207 (8)	−0.0040 (8)
C4	0.0497 (10)	0.0810 (12)	0.0518 (10)	0.0025 (9)	0.0240 (8)	0.0077 (9)
O5	0.0583 (8)	0.1301 (13)	0.0742 (9)	−0.0154 (8)	0.0360 (7)	−0.0085 (9)
C6	0.0603 (11)	0.0757 (12)	0.0526 (10)	−0.0100 (9)	0.0306 (8)	−0.0120 (9)
C8	0.0614 (11)	0.0793 (13)	0.0529 (10)	−0.0003 (9)	0.0208 (8)	−0.0142 (9)
C9	0.0661 (12)	0.1025 (16)	0.0512 (11)	0.0064 (11)	0.0302 (9)	−0.0079 (10)
C7	0.0536 (10)	0.0527 (10)	0.0513 (9)	−0.0013 (8)	0.0205 (8)	−0.0056 (8)
C10	0.0606 (14)	0.0617 (15)	0.0455 (14)	−0.0097 (11)	0.0218 (11)	−0.0101 (11)
C11	0.0484 (12)	0.0368 (9)	0.0434 (14)	−0.0023 (8)	0.0162 (10)	0.0014 (8)
O12	0.0586 (7)	0.0405 (6)	0.0691 (8)	−0.0076 (5)	0.0328 (6)	−0.0050 (5)
C15	0.0565 (10)	0.0413 (9)	0.0570 (10)	−0.0056 (7)	0.0253 (8)	−0.0051 (7)
C7′	0.0536 (10)	0.0527 (10)	0.0513 (9)	−0.0013 (8)	0.0205 (8)	−0.0056 (8)
C10′	0.059 (6)	0.050 (7)	0.053 (8)	−0.010 (5)	0.016 (6)	0.000 (6)
C11′	0.056 (6)	0.043 (6)	0.039 (7)	−0.016 (5)	0.011 (6)	−0.001 (5)
O12′	0.0586 (7)	0.0405 (6)	0.0691 (8)	−0.0076 (5)	0.0328 (6)	−0.0050 (5)
C15′	0.0565 (10)	0.0413 (9)	0.0570 (10)	−0.0056 (7)	0.0253 (8)	−0.0051 (7)
N13	0.0569 (8)	0.0387 (7)	0.0624 (9)	−0.0057 (6)	0.0277 (7)	−0.0041 (6)
C14	0.0465 (8)	0.0329 (8)	0.0381 (8)	0.0003 (7)	0.0104 (6)	0.0028 (6)
C16	0.0448 (9)	0.0329 (8)	0.0390 (8)	0.0012 (6)	0.0115 (6)	0.0028 (6)
C17	0.0516 (9)	0.0338 (8)	0.0511 (9)	−0.0049 (7)	0.0162 (7)	−0.0038 (7)
C18	0.0572 (10)	0.0365 (8)	0.0505 (9)	0.0013 (7)	0.0203 (8)	−0.0060 (7)
C19	0.0454 (9)	0.0402 (8)	0.0412 (8)	0.0008 (7)	0.0121 (7)	0.0031 (6)
C20	0.0506 (9)	0.0427 (9)	0.0454 (8)	−0.0109 (7)	0.0142 (7)	−0.0064 (7)
C21	0.0546 (9)	0.0372 (8)	0.0435 (8)	−0.0044 (7)	0.0173 (7)	−0.0079 (7)
C22	0.0502 (9)	0.0494 (9)	0.0510 (9)	−0.0015 (8)	0.0177 (8)	−0.0018 (7)
C23	0.0637 (12)	0.0994 (15)	0.0632 (12)	−0.0121 (10)	0.0270 (9)	−0.0261 (11)
C24	0.0831 (15)	0.1189 (19)	0.0782 (14)	−0.0061 (14)	0.0442 (12)	−0.0245 (13)
C25	0.0810 (15)	0.1163 (19)	0.1119 (19)	−0.0210 (14)	0.0634 (15)	−0.0224 (15)
C26	0.0797 (15)	0.151 (2)	0.128 (2)	−0.0545 (15)	0.0627 (15)	−0.0619 (18)
N27	0.0682 (11)	0.1091 (14)	0.0893 (12)	−0.0340 (10)	0.0419 (9)	−0.0387 (11)

Geometric parameters (Å, º)

C1—O5	1.423 (2)	C11′—O12′	1.565 (15)
C1—O2	1.427 (2)	C11′—C15′	1.573 (15)
O2—C3	1.390 (2)	O12′—N13	1.4134 (15)
C3—C6	1.365 (2)	C15′—C14	1.499 (2)
C3—C4	1.370 (2)	N13—C14	1.2827 (18)
C4—C9	1.364 (3)	C14—C16	1.4723 (19)
C4—O5	1.383 (2)	C16—C17	1.398 (2)
C6—C7′	1.395 (2)	C16—C21	1.402 (2)
C6—C7	1.395 (2)	C17—C18	1.374 (2)
C8—C7′	1.382 (2)	C18—C19	1.403 (2)
C8—C7	1.382 (2)	C19—C20	1.396 (2)
C8—C9	1.387 (2)	C19—C22	1.483 (2)
C7—C10	1.516 (2)	C20—C21	1.382 (2)
C10—C11	1.514 (4)	C22—N27	1.341 (2)
C11—O12	1.459 (2)	C22—C23	1.376 (2)
C11—C15	1.535 (2)	C23—C24	1.369 (3)
O12—N13	1.4134 (15)	C24—C25	1.348 (3)
C15—C14	1.499 (2)	C25—C26	1.372 (3)
C7′—C10′	1.686 (18)	C26—N27	1.340 (2)
C10′—C11′	1.46 (3)		
O5—C1—O2	108.04 (15)	O12′—C11′—C15′	97.2 (9)
C3—O2—C1	104.80 (13)	N13—O12′—C11′	108.3 (6)
C6—C3—C4	122.10 (17)	C14—C15′—C11′	102.6 (6)
C6—C3—O2	128.30 (15)	C14—N13—O12	109.71 (11)
C4—C3—O2	109.59 (15)	C14—N13—O12′	109.71 (11)
C9—C4—C3	121.55 (16)	N13—C14—C16	120.28 (12)
C9—C4—O5	128.53 (16)	N13—C14—C15′	113.37 (13)
C3—C4—O5	109.91 (17)	C16—C14—C15′	126.32 (12)
C4—O5—C1	105.10 (14)	N13—C14—C15	113.37 (13)
C3—C6—C7′	117.84 (15)	C16—C14—C15	126.32 (12)
C3—C6—C7	117.84 (15)	C17—C16—C21	118.06 (13)
C7′—C8—C9	122.56 (17)	C17—C16—C14	120.73 (12)
C7—C8—C9	122.56 (17)	C21—C16—C14	121.19 (13)
C4—C9—C8	116.77 (16)	C18—C17—C16	121.14 (13)
C8—C7—C6	119.18 (15)	C17—C18—C19	121.10 (14)
C8—C7—C10	117.97 (16)	C20—C19—C18	117.77 (14)
C6—C7—C10	122.78 (15)	C20—C19—C22	121.00 (13)
C11—C10—C7	116.1 (2)	C18—C19—C22	121.20 (13)
O12—C11—C10	109.52 (19)	C21—C20—C19	121.29 (13)
O12—C11—C15	103.67 (13)	C20—C21—C16	120.62 (13)
C10—C11—C15	114.90 (19)	N27—C22—C23	121.34 (16)
N13—O12—C11	108.16 (10)	N27—C22—C19	116.55 (14)
C14—C15—C11	100.29 (13)	C23—C22—C19	122.10 (15)
C8—C7′—C6	119.18 (15)	C24—C23—C22	120.60 (18)
C8—C7′—C10′	126.6 (6)	C25—C24—C23	118.6 (2)

C6—C7′—C10′	108.8 (7)	C24—C25—C26	118.5 (2)
C11′—C10′—C7′	109.0 (16)	N27—C26—C25	124.3 (2)
C10′—C11′—O12′	110.4 (16)	C26—N27—C22	116.64 (17)
C10′—C11′—C15′	105.5 (16)		

O5—C1—O2—C3	−15.6 (2)	C10′—C11′—C15′—C14	139.5 (13)
C1—O2—C3—C6	−171.1 (2)	O12′—C11′—C15′—C14	25.9 (11)
C1—O2—C3—C4	9.9 (2)	C11—O12—N13—C14	−13.84 (18)
C6—C3—C4—C9	−0.6 (3)	C11′—O12′—N13—C14	19.5 (9)
O2—C3—C4—C9	178.55 (18)	O12—N13—C14—C16	−178.32 (11)
C6—C3—C4—O5	−179.39 (16)	O12′—N13—C14—C16	−178.32 (11)
O2—C3—C4—O5	−0.3 (2)	O12′—N13—C14—C15′	−0.43 (17)
C9—C4—O5—C1	171.8 (2)	O12—N13—C14—C15	−0.43 (17)
C3—C4—O5—C1	−9.4 (2)	C11′—C15′—C14—N13	−18.2 (9)
O2—C1—O5—C4	15.5 (2)	C11′—C15′—C14—C16	159.6 (8)
C4—C3—C6—C7′	0.5 (3)	C11—C15—C14—N13	13.34 (18)
O2—C3—C6—C7′	−178.47 (18)	C11—C15—C14—C16	−168.92 (15)
C4—C3—C6—C7	0.5 (3)	N13—C14—C16—C17	−14.3 (2)
O2—C3—C6—C7	−178.47 (18)	C15′—C14—C16—C17	168.09 (14)
C3—C4—C9—C8	0.7 (3)	C15—C14—C16—C17	168.09 (14)
O5—C4—C9—C8	179.26 (18)	N13—C14—C16—C21	163.95 (14)
C7′—C8—C9—C4	−0.7 (3)	C15′—C14—C16—C21	−13.6 (2)
C7—C8—C9—C4	−0.7 (3)	C15—C14—C16—C21	−13.6 (2)
C9—C8—C7—C6	0.7 (3)	C21—C16—C17—C18	0.5 (2)
C9—C8—C7—C10	177.9 (2)	C14—C16—C17—C18	178.82 (12)
C3—C6—C7—C8	−0.5 (3)	C16—C17—C18—C19	−1.3 (2)
C3—C6—C7—C10	−177.6 (2)	C17—C18—C19—C20	0.8 (2)
C8—C7—C10—C11	167.2 (2)	C17—C18—C19—C22	178.84 (13)
C6—C7—C10—C11	−15.8 (3)	C18—C19—C20—C21	0.4 (2)
C7—C10—C11—O12	70.7 (3)	C22—C19—C20—C21	−177.61 (13)
C7—C10—C11—C15	−173.16 (15)	C19—C20—C21—C16	−1.2 (2)
C10—C11—O12—N13	144.47 (18)	C17—C16—C21—C20	0.7 (2)
C15—C11—O12—N13	21.4 (2)	C14—C16—C21—C20	−177.59 (13)
O12—C11—C15—C14	−19.99 (19)	C20—C19—C22—N27	−25.0 (2)
C10—C11—C15—C14	−139.5 (2)	C18—C19—C22—N27	157.00 (17)
C9—C8—C7′—C6	0.7 (3)	C20—C19—C22—C23	154.08 (17)
C9—C8—C7′—C10′	−150.2 (10)	C18—C19—C22—C23	−23.9 (2)
C3—C6—C7′—C8	−0.5 (3)	N27—C22—C23—C24	1.4 (3)
C3—C6—C7′—C10′	155.2 (8)	C19—C22—C23—C24	−177.63 (18)
C8—C7′—C10′—C11′	−120.6 (13)	C22—C23—C24—C25	−0.4 (4)
C6—C7′—C10′—C11′	86.1 (16)	C23—C24—C25—C26	−0.3 (4)
C7′—C10′—C11′—O12′	−70 (2)	C24—C25—C26—N27	0.0 (4)
C7′—C10′—C11′—C15′	−174.2 (9)	C25—C26—N27—C22	1.0 (4)
C10′—C11′—O12′—N13	−137.7 (14)	C23—C22—N27—C26	−1.6 (3)
C15′—C11′—O12′—N13	−28.1 (12)	C19—C22—N27—C26	177.46 (18)