Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Pseudokobusine. Erratum

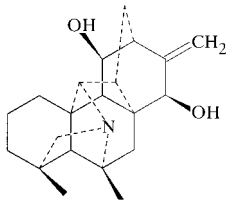
Mehmet Akkurt

Department of Physics, Faculty of Arts and Sciences, Erciyes University, 38039 Kayseri, Turkey
Correspondence e-mail: akkurt@erciyes.edu.tr

In the paper by Bhattacharyya *et al.* [*Acta Cryst*. (2001), C**57**, 68–69], the chemical diagram of the title compound, $C_{20}H_{27}NO_3$, is incorrect.

Comment

When comparing the revised diagram of pseudokobusine, (I), with the *ORTEP* drawing (Fig. 1), the N1 atom is connected to



(I)

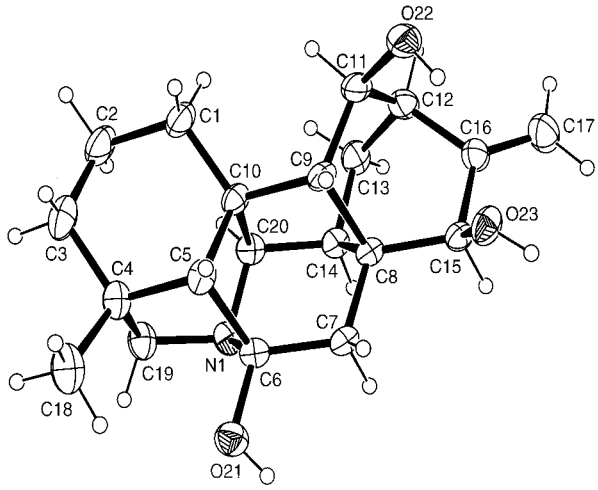


Figure 1
The structure of (I) showing 30% probability displacement ellipsoids and the atom-numbering scheme.

the C6 atom of the hydroxyl group, but in the diagram published originally, the N1 atom is not connected to a C atom bearing a hydroxyl group. The molecular formula of the erroneous structure would be $C_{21}H_{29}NO_3$ and not $C_{20}H_{27}NO_3$, as it should be.

References

Bhattacharyya, K., Kar, T., Bocelli, G., Righi, L. & Joshi, B. S. (2001). *Acta Cryst.* C**57**, 68–69.

supporting information

Acta Cryst. (2001). C**57**, 500 [https://doi.org/10.1107/S0108270101003948]

Pseudokobusine. Erratum

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Computing details

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: SHELXTLNT (Bruker, 1999); program(s) used to solve structure: *SIR97* (Cascarano *et al.*, 1996); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ZORTEP* (Zsolnai & Huttner, 1994); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1983).

Hetisan-6, 11(*β*), 15(*β*)-triol

Crystal data

$C_{20}H_{27}NO_3$
$M_r = 329.43$
Monoclinic, $P2_1$
$a = 8.0746$ (8) Å
$b = 11.4613$ (11) Å
$c = 9.1121$ (9) Å
$\beta = 90.338$ (2)°
$V = 843.27$ (14) Å^3
$Z = 2$
$F(000) = 356$
$D_x = 1.297$ Mg m^{-3}
Melting point: 271° K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from >10σ reflections
$\theta = 3.0$–30.6°
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Plate, colourless
0.38 × 0.26 × 0.19 mm

Data collection

Bruker 1000 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: empirical (using intensity measurements) (SADABS; Bruker, 1998)
$T_{min} = 0.97$, $T_{max} = 0.98$
6766 measured reflections
2455 independent reflections
1335 reflections with $I > 2\sigma(I)$
$R_{int} = 0.05$
$\theta_{max} = 30.6°$, $\theta_{min} = 2.2°$
$h = -11 \rightarrow 7$
$k = -16 \rightarrow 16$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.094$
$S = 0.81$
2455 reflections
222 parameters
1 restraint
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 0.0279P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}
Extinction correction: SHELXL97 (Sheldrick, 1997)
Extinction coefficient: 0.006 (2)
Absolute structure: Flack (1983)
Absolute structure parameter: −0.5 (16)

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}
C1	0.1656 (4)	0.1295 (3)	0.3742 (3)	0.0534 (9)
H1A	0.1036	0.1852	0.4323	0.064*
H1B	0.0884	0.0909	0.3083	0.064*
C2	0.2429 (5)	0.0398 (3)	0.4751 (4)	0.0639 (10)
H2A	0.1585	0.0079	0.5389	0.077*
H2B	0.2877	−0.0236	0.4171	0.077*
C3	0.3784 (5)	0.0925 (3)	0.5667 (4)	0.0597 (9)
H3A	0.4325	0.0306	0.6215	0.072*
H3B	0.3288	0.1452	0.6372	0.072*
C4	0.5109 (4)	0.1598 (3)	0.4808 (3)	0.0456 (7)
C5	0.4346 (4)	0.2504 (2)	0.3757 (3)	0.0393 (7)
H5	0.4032	0.3237	0.4235	0.047*
C6	0.5675 (3)	0.2651 (2)	0.2554 (3)	0.0371 (7)
C7	0.5155 (3)	0.3358 (2)	0.1237 (3)	0.0364 (7)
H7A	0.6006	0.3302	0.0494	0.044*
H7B	0.5064	0.4171	0.1522	0.044*
C8	0.3522 (3)	0.2963 (2)	0.0585 (3)	0.0332 (6)
C9	0.2203 (3)	0.2903 (2)	0.1809 (3)	0.0376 (7)
H9	0.2168	0.3650	0.2331	0.045*
C10	0.2944 (3)	0.1949 (2)	0.2838 (3)	0.0380 (7)
C11	0.0504 (4)	0.2661 (3)	0.1100 (4)	0.0505 (8)
H11	−0.0059	0.2068	0.1690	0.061*
C12	0.0718 (4)	0.2175 (3)	−0.0445 (4)	0.0509 (8)
H12	−0.0342	0.1896	−0.0839	0.061*
C13	0.1968 (4)	0.1183 (3)	−0.0356 (3)	0.0492 (8)
H13A	0.2123	0.0849	−0.1324	0.059*
H13B	0.1551	0.0576	0.0285	0.059*
C14	0.3648 (4)	0.1638 (2)	0.0244 (3)	0.0385 (7)
H14	0.4552	0.1473	−0.0438	0.046*
C15	0.2939 (3)	0.3693 (2)	−0.0724 (3)	0.0364 (6)
H15	0.3828	0.3754	−0.1448	0.044*
C16	0.1429 (4)	0.3117 (3)	−0.1415 (3)	0.0461 (7)
C17	0.0814 (5)	0.3421 (3)	−0.2683 (4)	0.0689 (10)
H17A	−0.0127	0.3050	−0.3047	0.083*
H17B	0.1315	0.4010	−0.3225	0.083*

C18	0.6292 (5)	0.2123 (3)	0.5956 (3)	0.0666 (10)
H18A	0.7163	0.2538	0.5468	0.100*
H18B	0.6760	0.1509	0.6543	0.100*
H18C	0.5693	0.2651	0.6575	0.100*
C19	0.6057 (4)	0.0843 (3)	0.3667 (3)	0.0490 (8)
H19A	0.7231	0.0835	0.3897	0.059*
H19B	0.5653	0.0046	0.3686	0.059*
C20	0.4017 (4)	0.1159 (2)	0.1768 (3)	0.0403 (7)
H20	0.3717	0.0333	0.1848	0.048*
O21	0.7181 (3)	0.30584 (19)	0.3133 (2)	0.0520 (6)
H21	0.7772	0.3287	0.2464	0.078*
O22	−0.0502 (3)	0.3697 (2)	0.1095 (3)	0.0650 (7)
H22	0.0034	0.4245	0.0766	0.098*
O23	0.2510 (3)	0.48421 (16)	−0.0186 (2)	0.0494 (6)
H23	0.2844	0.5338	−0.0761	0.074*
N1	0.5773 (3)	0.13643 (19)	0.2191 (3)	0.0419 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0526 (19)	0.0507 (19)	0.0572 (19)	−0.0001 (16)	0.0152 (17)	0.0183 (16)
C2	0.072 (2)	0.0528 (19)	0.067 (2)	−0.0072 (19)	0.014 (2)	0.0259 (19)
C3	0.081 (2)	0.0485 (19)	0.0500 (18)	0.0078 (18)	0.0123 (19)	0.0157 (16)
C4	0.0573 (19)	0.0412 (15)	0.0385 (16)	0.0056 (15)	−0.0002 (15)	0.0000 (14)
C5	0.0502 (17)	0.0302 (14)	0.0375 (15)	0.0056 (13)	0.0091 (14)	−0.0015 (12)
C6	0.0360 (16)	0.0346 (15)	0.0408 (16)	−0.0009 (13)	0.0026 (13)	−0.0054 (13)
C7	0.0359 (15)	0.0331 (14)	0.0404 (16)	−0.0024 (12)	0.0092 (13)	−0.0007 (12)
C8	0.0347 (15)	0.0263 (12)	0.0385 (15)	0.0004 (12)	0.0075 (13)	−0.0031 (12)
C9	0.0353 (15)	0.0290 (14)	0.0485 (17)	0.0012 (12)	0.0122 (14)	0.0059 (13)
C10	0.0416 (16)	0.0294 (13)	0.0430 (15)	0.0018 (12)	0.0096 (14)	0.0038 (13)
C11	0.0349 (16)	0.0394 (17)	0.077 (2)	0.0027 (14)	0.0077 (16)	0.0203 (16)
C12	0.0378 (17)	0.0457 (18)	0.069 (2)	−0.0125 (15)	−0.0094 (16)	0.0100 (17)
C13	0.0558 (19)	0.0352 (15)	0.0567 (19)	−0.0077 (15)	−0.0061 (17)	0.0034 (14)
C14	0.0419 (16)	0.0319 (13)	0.0419 (15)	−0.0002 (12)	0.0027 (14)	−0.0028 (13)
C15	0.0367 (15)	0.0321 (14)	0.0405 (15)	−0.0014 (12)	0.0053 (13)	0.0004 (13)
C16	0.0444 (18)	0.0403 (16)	0.0536 (19)	−0.0003 (13)	−0.0048 (15)	0.0064 (14)
C17	0.065 (2)	0.062 (2)	0.079 (2)	−0.0146 (19)	−0.024 (2)	0.018 (2)
C18	0.092 (3)	0.059 (2)	0.0488 (19)	0.009 (2)	−0.005 (2)	−0.0011 (18)
C19	0.058 (2)	0.0428 (17)	0.0458 (17)	0.0118 (15)	−0.0002 (16)	0.0013 (14)
C20	0.0442 (17)	0.0256 (13)	0.0513 (17)	0.0015 (13)	0.0016 (15)	−0.0026 (13)
O21	0.0461 (13)	0.0595 (14)	0.0505 (13)	−0.0068 (11)	−0.0031 (11)	−0.0026 (12)
O22	0.0430 (13)	0.0596 (14)	0.0926 (18)	0.0134 (12)	0.0126 (13)	0.0258 (14)
O23	0.0603 (14)	0.0328 (10)	0.0551 (13)	0.0023 (10)	0.0119 (11)	0.0071 (10)
N1	0.0446 (15)	0.0368 (13)	0.0441 (14)	0.0094 (12)	−0.0021 (12)	−0.0035 (11)

Geometric parameters (Å, º)

C6—O21	1.403 (3)	C8—C14	1.553 (3)
C11—O22	1.440 (3)	C8—C9	1.548 (3)
C15—O23	1.448 (3)	C9—C11	1.538 (4)
C6—N1	1.513 (3)	C9—C10	1.557 (4)
C14—C20	1.522 (4)	C9—H9	0.9800
C16—C17	1.303 (4)	C10—C20	1.590 (4)
C19—N1	1.488 (4)	C11—C12	1.525 (5)
C20—N1	1.486 (4)	C11—H11	0.9800
C1—C2	1.512 (4)	C12—C16	1.511 (4)
C1—C10	1.527 (4)	C12—C13	1.521 (4)
C1—H1A	0.9700	C12—H12	0.9800
C1—H1B	0.9700	C13—C14	1.550 (4)
C2—C3	1.499 (5)	C13—H13A	0.9700
C2—H2A	0.9700	C13—H13B	0.9700
C2—H2B	0.9700	C14—H14	0.9800
C3—C4	1.536 (4)	C15—C16	1.520 (4)
C3—H3A	0.9700	C15—H15	0.9800
C3—H3B	0.9700	C17—H17A	0.9300
C4—C5	1.540 (4)	C17—H17B	0.9300
C4—C18	1.535 (5)	C18—H18A	0.9600
C4—C19	1.558 (4)	C18—H18B	0.9600
C5—C6	1.547 (4)	C18—H18C	0.9600
C5—C10	1.542 (4)	C19—H19A	0.9700
C5—H5	0.9800	C19—H19B	0.9700
C6—C7	1.506 (4)	C20—H20	0.9800
C7—C8	1.513 (4)	O21—H21	0.8200
C7—H7A	0.9700	O22—H22	0.8200
C7—H7B	0.9700	O23—H23	0.8200
C8—C15	1.529 (4)		
O21—C6—C5	111.9 (2)	C1—C10—C9	114.1 (2)
O21—C6—C7	110.9 (2)	C5—C10—C9	108.4 (2)
N1—C6—C7	111.4 (2)	C1—C10—C20	115.3 (2)
C17—C16—C12	124.5 (3)	C5—C10—C20	99.6 (2)
C17—C16—C15	123.5 (3)	C9—C10—C20	103.8 (2)
C19—N1—C20	108.2 (2)	O22—C11—C12	111.5 (3)
C19—N1—C6	101.6 (2)	O22—C11—C9	110.8 (2)
C20—N1—C6	99.2 (2)	C12—C11—C9	110.4 (2)
C2—C1—C10	112.4 (3)	O22—C11—H11	108.0
C2—C1—H1A	109.1	C12—C11—H11	108.0
C10—C1—H1A	109.1	C9—C11—H11	108.0
C2—C1—H1B	109.1	C16—C12—C13	108.1 (3)
C10—C1—H1B	109.1	C16—C12—C11	108.9 (3)
H1A—C1—H1B	107.8	C13—C12—C11	107.6 (3)
C3—C2—C1	111.2 (3)	C16—C12—H12	110.7
C3—C2—H2A	109.4	C13—C12—H12	110.7

C1—C2—H2A	109.4	C11—C12—H12	110.7
C3—C2—H2B	109.4	C12—C13—C14	110.3 (2)
C1—C2—H2B	109.4	C12—C13—H13A	109.6
H2A—C2—H2B	108.0	C14—C13—H13A	109.6
C2—C3—C4	115.3 (3)	C12—C13—H13B	109.6
C2—C3—H3A	108.5	C14—C13—H13B	109.6
C4—C3—H3A	108.5	H13A—C13—H13B	108.1
C2—C3—H3B	108.5	C20—C14—C8	100.5 (2)
C4—C3—H3B	108.5	C20—C14—C13	111.5 (2)
H3A—C3—H3B	107.5	C8—C14—C13	110.0 (2)
C3—C4—C5	112.2 (3)	C20—C14—H14	111.5
C3—C4—C18	106.4 (2)	C8—C14—H14	111.5
C5—C4—C18	113.8 (3)	C13—C14—H14	111.5
C3—C4—C19	114.1 (2)	O23—C15—C16	110.0 (2)
C5—C4—C19	99.0 (2)	O23—C15—C8	107.9 (2)
C18—C4—C19	111.5 (3)	C16—C15—C8	109.1 (2)
C4—C5—C6	103.7 (2)	O23—C15—H15	109.9
C4—C5—C10	110.4 (2)	C16—C15—H15	109.9
C6—C5—C10	99.8 (2)	C8—C15—H15	109.9
C4—C5—H5	113.9	C12—C16—C15	112.0 (3)
C6—C5—H5	113.9	C16—C17—H17A	120.0
C10—C5—H5	113.9	C16—C17—H17B	120.0
O21—C6—N1	111.1 (2)	H17A—C17—H17B	120.0
N1—C6—C5	95.0 (2)	C4—C18—H18A	109.5
C7—C6—C5	115.6 (2)	C4—C18—H18B	109.5
C6—C7—C8	112.9 (2)	H18A—C18—H18B	109.5
C6—C7—H7A	109.0	C4—C18—H18C	109.5
C8—C7—H7A	109.0	H18A—C18—H18C	109.5
C6—C7—H7B	109.0	H18B—C18—H18C	109.5
C8—C7—H7B	109.0	N1—C19—C4	107.9 (2)
H7A—C7—H7B	107.8	N1—C19—H19A	110.1
C7—C8—C15	113.9 (2)	C4—C19—H19A	110.1
C7—C8—C14	108.3 (2)	N1—C19—H19B	110.1
C15—C8—C14	113.5 (2)	C4—C19—H19B	110.1
C7—C8—C9	109.4 (2)	H19A—C19—H19B	108.4
C15—C8—C9	112.1 (2)	N1—C20—C14	111.2 (2)
C14—C8—C9	98.5 (2)	N1—C20—C10	105.9 (2)
C11—C9—C8	108.7 (2)	C14—C20—C10	104.5 (2)
C11—C9—C10	117.7 (2)	N1—C20—H20	111.7
C8—C9—C10	101.6 (2)	C14—C20—H20	111.7
C11—C9—H9	109.5	C10—C20—H20	111.7
C8—C9—H9	109.5	C6—O21—H21	109.5
C10—C9—H9	109.5	C11—O22—H22	109.5
C1—C10—C5	114.2 (2)	C15—O23—H23	109.5

C10—C5—C6—O21	−174.7 (2)	C8—C9—C11—C12	18.3 (3)
O21—C6—C7—C8	−179.2 (2)	C10—C9—C11—C12	−96.4 (3)
C8—C9—C11—O22	−105.6 (3)	C9—C11—C12—C16	−67.6 (3)

O22—C11—C12—C16	55.9 (3)	O22—C11—C12—C13	172.9 (2)
C9—C8—C15—O23	56.6 (3)	C9—C11—C12—C13	49.3 (3)
C11—C12—C16—C17	−129.2 (3)	C16—C12—C13—C14	57.7 (3)
O23—C15—C16—C12	−105.4 (3)	C11—C12—C13—C14	−59.8 (3)
C8—C15—C16—C17	−168.4 (3)	C7—C8—C14—C20	59.6 (3)
C10—C1—C2—C3	51.8 (4)	C15—C8—C14—C20	−172.9 (2)
C1—C2—C3—C4	−52.0 (4)	C9—C8—C14—C20	−54.2 (3)
C2—C3—C4—C5	51.2 (4)	C7—C8—C14—C13	177.2 (2)
C2—C3—C4—C18	176.4 (3)	C15—C8—C14—C13	−55.2 (3)
C2—C3—C4—C19	−60.3 (4)	C9—C8—C14—C13	63.4 (3)
C3—C4—C5—C6	−154.7 (2)	C12—C13—C14—C20	111.3 (3)
C18—C4—C5—C6	84.4 (3)	C12—C13—C14—C8	0.7 (3)
C19—C4—C5—C6	−34.0 (3)	C7—C8—C15—O23	−68.4 (3)
C3—C4—C5—C10	−48.6 (3)	C14—C8—C15—O23	167.0 (2)
C18—C4—C5—C10	−169.5 (2)	C7—C8—C15—C16	172.1 (2)
C19—C4—C5—C10	72.1 (3)	C14—C8—C15—C16	47.5 (3)
C4—C5—C6—O21	−60.7 (3)	C9—C8—C15—C16	−63.0 (3)
C4—C5—C6—N1	54.4 (3)	C13—C12—C16—C17	114.2 (4)
C10—C5—C6—N1	−59.6 (2)	C13—C12—C16—C15	−67.0 (3)
C4—C5—C6—C7	171.0 (2)	C11—C12—C16—C15	49.6 (3)
C10—C5—C6—C7	57.0 (3)	O23—C15—C16—C17	73.5 (4)
N1—C6—C7—C8	56.5 (3)	C8—C15—C16—C12	12.8 (3)
C5—C6—C7—C8	−50.4 (3)	C3—C4—C19—N1	119.9 (3)
C6—C7—C8—C15	178.1 (2)	C5—C4—C19—N1	0.5 (3)
C6—C7—C8—C14	−54.5 (3)	C18—C4—C19—N1	−119.6 (3)
C6—C7—C8—C9	51.8 (3)	C8—C14—C20—N1	−76.8 (3)
C7—C8—C9—C11	172.5 (2)	C13—C14—C20—N1	166.7 (2)
C15—C8—C9—C11	45.1 (3)	C8—C14—C20—C10	36.9 (3)
C14—C8—C9—C11	−74.6 (3)	C13—C14—C20—C10	−79.6 (3)
C7—C8—C9—C10	−62.7 (2)	C1—C10—C20—N1	−122.9 (3)
C15—C8—C9—C10	169.9 (2)	C5—C10—C20—N1	−0.3 (2)
C14—C8—C9—C10	50.2 (2)	C9—C10—C20—N1	111.5 (2)
C2—C1—C10—C5	−53.2 (3)	C1—C10—C20—C14	119.6 (3)
C2—C1—C10—C9	−178.6 (3)	C5—C10—C20—C14	−117.7 (2)
C2—C1—C10—C20	61.3 (4)	C9—C10—C20—C14	−6.0 (3)
C4—C5—C10—C1	51.0 (3)	C4—C19—N1—C20	−70.2 (3)
C6—C5—C10—C1	159.7 (2)	C4—C19—N1—C6	33.7 (3)
C4—C5—C10—C9	179.4 (2)	C14—C20—N1—C19	−178.2 (2)
C6—C5—C10—C9	−71.9 (2)	C10—C20—N1—C19	68.9 (2)
C4—C5—C10—C20	−72.4 (2)	C14—C20—N1—C6	76.2 (2)
C6—C5—C10—C20	36.3 (2)	C10—C20—N1—C6	−36.7 (2)
C11—C9—C10—C1	−35.2 (3)	O21—C6—N1—C19	63.5 (3)
C8—C9—C10—C1	−153.8 (2)	C7—C6—N1—C19	−172.2 (2)
C11—C9—C10—C5	−163.6 (2)	C5—C6—N1—C19	−52.3 (2)
C8—C9—C10—C5	77.8 (2)	O21—C6—N1—C20	174.4 (2)
C11—C9—C10—C20	91.1 (3)	C7—C6—N1—C20	−61.4 (2)
C8—C9—C10—C20	−27.5 (2)	C5—C6—N1—C20	58.6 (2)
C10—C9—C11—O22	139.7 (2)		