Acta Cryst E STRUCTURE REPORTS

OPEN ACCESS

ISSN 1600-5368

Crystal structure of 2,6-bis(2,5-dimethoxyphenyl)-3,5-dimethylpiperidin-4-one

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Received 24 July 2014; accepted 7 October 2014

Edited by V. V. Chernyshev, Moscow State University, Russia

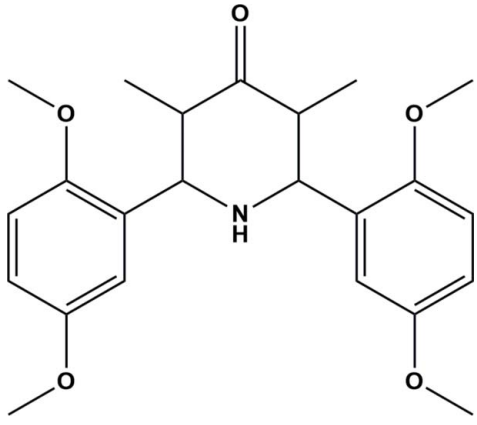
In the title molecule, $C_{23}H_{29}NO_5$, the central piperidine ring has a chair conformation. The planes of the two benzene rings are inclined each to other at 61.7 (1)°. The crystal packing exhibits no directional interactions only van der Waals contacts.

Keywords: crystal structure; chair conformation; Mannich base; piperidin-4-one.

CCDC reference: 1027842

1. Related literature

For the synthesis, stereochemistry and biological actions of piperidin-4-ones, see: Sahu *et al.* (2013); Parthiban *et al.* (2011). For a related crystal structure, see: Parthiban *et al.* (2008).



2. Experimental

2.1. Crystal data

$C_{23}H_{29}NO_5$
M_r = 399.47
Monoclinic, $P2_1/c$
a = 11.1358 (7) Å
b = 9.4756 (5) Å
c = 20.4541 (11) Å
β = 92.271 (2)°
V = 2156.6 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.25 × 0.20 × 0.15 mm

2.2. Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.979, T_{max} = 0.987
11151 measured reflections
3536 independent reflections
2262 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.116
S = 0.98
3536 reflections
272 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Acknowledgements

This research was supported by Inje University Research Grant 2013. The authors acknowledge the Department of Chemistry, IIT Madras, for the X-ray data collection.

Supporting information for this paper is available from the IUCr electronic archives (Reference: CV5470).

References

Bruker (2004). *APEXII*, *XPREP*, *SAINT-Plus* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Parthiban, P., Pallela, R., Kim, S. K., Park, D. H. & Jeong, Y. T. (2011). *Bioorg. Med. Chem. Lett.* **22**, 6004–6009.
Parthiban, P., Ramkumar, V., Kumar, N. A., Kim, J. S. & Jeong, Y. T. (2008). *Acta Cryst.* E**64**, o1631.
Sahu, S. K., Dubey, B. K., Tripathi, A. C., Koshy, M. & Saraf, S. K. (2013). *Mini Rev. Med. Chem.* **4**, 565–583.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2014). E**70**, o1160 [doi:10.1107/S1600536814022041]

Crystal structure of 2,6-bis(2,5-dimethoxyphenyl)-3,5-dimethylpiperidin-4-one

Dong Ho Park, V. Ramkumar and P. Parthiban

S1. Comment

The piperidin-4-one pharmacophore is responsible for numerous biological actions such as antibacterial, antimycobacterial, antifungal, anticancer, antioxidant, antiinflammatory, neuronal nicotinistinic, and *CNS* stimulant and depressant. Its activity is further increased by the incorporation of aryl groups on both sides of the hetero atom along with/without the introduction of functionalities on the hetero atom itself. Interestingly, the amino group of the piperidone that is flanked by aryl groups are responsible not only for the increment in activity, but also in suppressing the toxicity (Sahu *et al.* 2013; Parthiban *et al.* 2011). Generally, the piperidin-4-one moiety exists in different stereochemistries upon the modifications in their structure. Since the stereochemistry of the molecule is an important key for its biological response, it is of curious to explore the stereochemistry. Hence the present study is caried out to explore the stereochemistry of the title compound (I) (Fig. 1).

The crystallographic parameters *viz*., torsion angles, asymmetry parameters and ring puckering parameters calculated for (I) show that the piperidone ring adopts a chair conformation. According to Cremer & Pople and Nardelli, the total puckering amplitude, Q_T is 0.5875 (8) Å, the phase angle θ is 0.94 (8)° and phi is 34 (4)°. The smallest displacement asymmetry parameters q_2 and q_3 are 0.0114 (8) and -0.5874 Å, respectively.

The benzene rings of anisyl groups are oriented at an angle of 61.7 (1)°, respect to each other. The torsion angles of C6—C1—C2—C3 and C3—C4—C5—C16 are 174.94 (18) and -174.42 (18)°, respectively. Similarly, the torsion angles of C2—C3—C4—C15 and C14—C2—C3—C4 are -177.8 (2) and 177.1 (2)%, respectively. The torsion angle values also clearly confirm the equatorial orientation of aryl and alkyl groups on the piperidin-4-one moiety.

On the whole, the complete crystallographic analysis of the title compound, $C_{23}H_{29}NO_5$, exhibits a chair conformation with equatorial orientations of all the aryl and alkyl substituents.

S2. Experimental

The 2,6-*bis*(2,5-dimethoxyphenyl)-3,5-dimethylpiperidin-4-one was synthesized by a modified and an optimized Mannich condensation in one-pot, using 2,5-dimethoxybenzaldehyde (0.1 mol, 16.618 g), 2-pentanone (0.05 mol) and ammonium acetate (0.075 mol, 5.78 g) in a 50 ml of absolute ethanol (Parthiban *et al.*, 2011). The mixture was gently warmed on a hot plate at 303–308 K (30–35° C) with moderate stirring till the complete consumption of the starting materials, which was monitored by TLC. At the end, the crude azabicyclic ketone was separated by filtration and gently washed with 1:5 cold ethanol-ether mixture. X-ray diffraction quality crystals of the title compound were obtained by slow evaporation from ethanol.

S3. Refinement

All hydrogen atoms were fixed geometrically and allowed to ride on the parent carbon atoms with aromatic C—H = 0.93 Å, aliphatic C—H = 0.98 Å, methylene C—H = 0.97 Å. The displacement parameters were set for phenyl, methylene and

aliphatic H atoms at U_{iso}(H) = 1.2U_{eq}(C), methyl H atoms at U_{iso}(H) = 1.5U_{eq}(C) and the hydrogen atoms were fixed geometrically and allowed to ride on the parent nitrogen atom with N—H = 0.86 Å and the displacement parameter was set at U_{iso}(H)= 1.2U_{eq}(N).

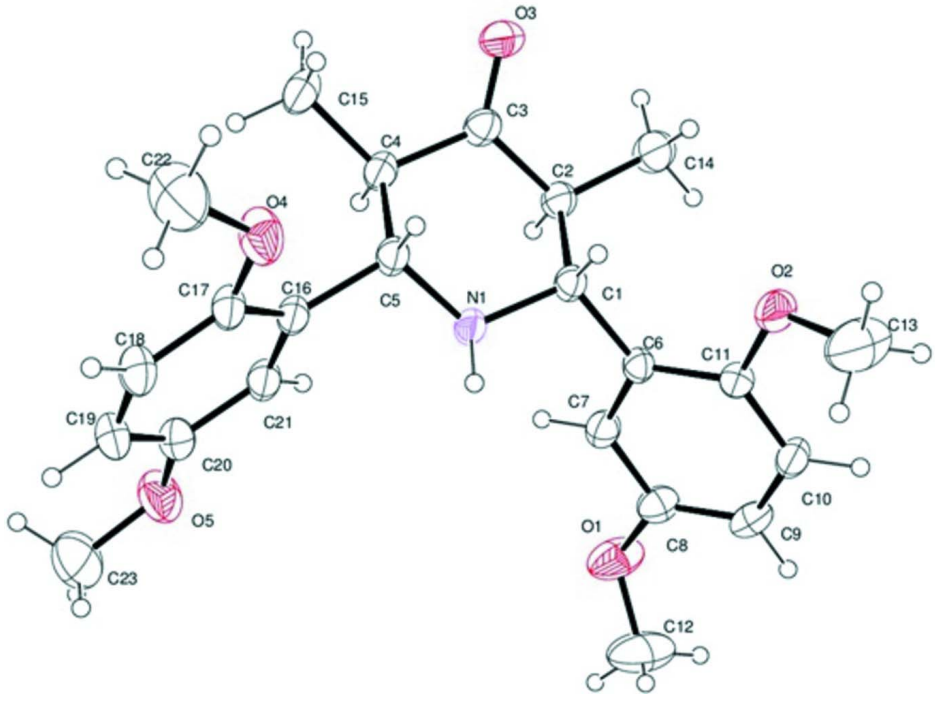


Figure 1

View of (I) showing the atomic numbering and 30% probability displacement ellipsoids.

2,6-Bis(2,5-dimethoxyphenyl)-3,5-dimethylpiperidin-4-one

Crystal data

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M_r = 399.47
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V = 2156.6 (2) Å^3
Z = 4
F(000) = 856
D_x = 1.230 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
μ = 0.09 mm^{-1}
T = 298 K
Block, yellow
0.25 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.979, T_{max} = 0.987
11151 measured reflections
3536 independent reflections
2262 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 25.0°, θ_{min} = 2.4°
h = −12→12
k = −11→10
l = −20→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.116$
$S = 0.98$
3536 reflections
272 parameters
0 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0405P)^2 + 0.9547P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.54320 (17)	0.4952 (2)	0.14728 (9)	0.0380 (5)
H1	0.5445	0.3918	0.1468	0.046*
C2	0.59048 (18)	0.5485 (2)	0.21515 (10)	0.0439 (5)
H2	0.5876	0.6519	0.2147	0.053*
C3	0.50346 (19)	0.4971 (2)	0.26472 (10)	0.0447 (6)
C4	0.37508 (18)	0.5434 (3)	0.25295 (10)	0.0465 (6)
H4	0.3737	0.6469	0.2526	0.056*
C5	0.33417 (17)	0.4916 (2)	0.18398 (9)	0.0413 (5)
H5	0.3343	0.3882	0.1834	0.050*
C6	0.61644 (17)	0.5504 (2)	0.09201 (9)	0.0369 (5)
C7	0.6022 (2)	0.6895 (2)	0.07205 (10)	0.0461 (6)
H7	0.5514	0.7484	0.0946	0.055*
C8	0.6620 (2)	0.7426 (2)	0.01924 (11)	0.0510 (6)
C9	0.7397 (2)	0.6581 (3)	−0.01319 (10)	0.0520 (6)
H9	0.7807	0.6936	−0.0484	0.062*
C10	0.7570 (2)	0.5200 (3)	0.00665 (10)	0.0495 (6)
H10	0.8106	0.4631	−0.0150	0.059*
C11	0.69529 (18)	0.4653 (2)	0.05833 (9)	0.0404 (5)
C12	0.6457 (4)	0.9225 (3)	−0.06178 (14)	0.1112 (13)
H12A	0.7285	0.9324	−0.0725	0.167*
H12B	0.6053	1.0112	−0.0681	0.167*
H12C	0.6080	0.8525	−0.0896	0.167*
C13	0.7419 (4)	0.2273 (3)	0.03408 (15)	0.1146 (14)
H13A	0.6913	0.2362	−0.0048	0.172*
H13B	0.7329	0.1347	0.0523	0.172*
H13C	0.8242	0.2416	0.0233	0.172*
C14	0.7187 (2)	0.5047 (3)	0.23158 (12)	0.0684 (8)
H14A	0.7390	0.5282	0.2763	0.103*
H14B	0.7718	0.5533	0.2034	0.103*
H14C	0.7266	0.4047	0.2255	0.103*

C15	0.2921 (2)	0.4933 (3)	0.30574 (12)	0.0722 (8)
H15A	0.2847	0.3924	0.3037	0.108*
H15B	0.2143	0.5355	0.2988	0.108*
H15C	0.3251	0.5203	0.3480	0.108*
C16	0.20999 (18)	0.5443 (2)	0.16386 (10)	0.0425 (5)
C17	0.10969 (19)	0.4552 (3)	0.16077 (11)	0.0487 (6)
C18	0.0001 (2)	0.5069 (3)	0.13831 (12)	0.0595 (7)
H18	−0.0658	0.4466	0.1353	0.071*
C19	−0.0138 (2)	0.6459 (3)	0.12020 (12)	0.0610 (7)
H19	−0.0886	0.6794	0.1055	0.073*
C20	0.0835 (2)	0.7349 (3)	0.12398 (11)	0.0534 (6)
C21	0.1949 (2)	0.6839 (3)	0.14593 (10)	0.0480 (6)
H21	0.2604	0.7448	0.1486	0.058*
C22	0.0276 (3)	0.2382 (4)	0.19599 (19)	0.1093 (13)
H22A	−0.0150	0.2881	0.2287	0.164*
H22B	0.0536	0.1484	0.2131	0.164*
H22C	−0.0244	0.2240	0.1580	0.164*
C23	−0.0296 (3)	0.9292 (4)	0.08139 (18)	0.1084 (12)
H23A	−0.0539	0.8772	0.0428	0.163*
H23B	−0.0200	1.0270	0.0704	0.163*
H23C	−0.0897	0.9201	0.1135	0.163*
N1	0.41929 (15)	0.5441 (2)	0.13674 (9)	0.0418 (5)
O1	0.6391 (2)	0.88138 (18)	0.00307 (9)	0.0849 (6)
O2	0.70918 (15)	0.32842 (17)	0.07975 (7)	0.0610 (5)
O3	0.53408 (14)	0.4179 (2)	0.30899 (8)	0.0667 (5)
O4	0.12791 (14)	0.31712 (18)	0.17881 (9)	0.0684 (5)
O5	0.08013 (16)	0.8756 (2)	0.10695 (10)	0.0790 (6)
H1N	0.3918 (19)	0.522 (2)	0.0956 (11)	0.054 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0316 (12)	0.0430 (13)	0.0398 (12)	−0.0014 (10)	0.0056 (9)	−0.0003 (9)
C2	0.0343 (13)	0.0565 (14)	0.0410 (12)	−0.0045 (11)	0.0012 (9)	0.0011 (10)
C3	0.0425 (14)	0.0560 (15)	0.0355 (12)	−0.0051 (11)	0.0007 (10)	−0.0054 (11)
C4	0.0396 (14)	0.0601 (15)	0.0405 (12)	0.0024 (11)	0.0086 (10)	−0.0017 (11)
C5	0.0325 (13)	0.0491 (14)	0.0428 (12)	−0.0005 (10)	0.0065 (9)	−0.0020 (10)
C6	0.0293 (12)	0.0436 (13)	0.0378 (11)	−0.0002 (10)	0.0020 (9)	−0.0019 (9)
C7	0.0478 (14)	0.0469 (15)	0.0442 (13)	0.0044 (11)	0.0081 (10)	−0.0026 (10)
C8	0.0621 (16)	0.0460 (15)	0.0452 (13)	−0.0051 (13)	0.0062 (12)	0.0016 (11)
C9	0.0586 (16)	0.0618 (17)	0.0364 (12)	−0.0123 (13)	0.0106 (11)	0.0012 (11)
C10	0.0435 (14)	0.0636 (17)	0.0422 (13)	0.0039 (12)	0.0122 (10)	−0.0060 (11)
C11	0.0377 (13)	0.0461 (14)	0.0374 (11)	0.0030 (11)	0.0028 (10)	−0.0005 (10)
C12	0.191 (4)	0.077 (2)	0.065 (2)	0.003 (2)	0.001 (2)	0.0232 (16)
C13	0.212 (4)	0.059 (2)	0.075 (2)	0.041 (2)	0.034 (2)	−0.0018 (16)
C14	0.0398 (15)	0.111 (2)	0.0547 (15)	−0.0071 (15)	−0.0020 (11)	0.0093 (15)
C15	0.0505 (16)	0.117 (2)	0.0500 (15)	0.0073 (16)	0.0181 (12)	0.0062 (15)
C16	0.0325 (13)	0.0549 (15)	0.0407 (12)	0.0019 (11)	0.0079 (9)	−0.0023 (10)

C17	0.0326 (14)	0.0611 (17)	0.0530 (14)	0.0022 (12)	0.0087 (10)	−0.0008 (12)
C18	0.0338 (15)	0.0736 (19)	0.0712 (17)	−0.0039 (13)	0.0049 (12)	0.0005 (14)
C19	0.0351 (15)	0.083 (2)	0.0648 (17)	0.0121 (15)	0.0022 (12)	0.0024 (14)
C20	0.0474 (16)	0.0579 (17)	0.0556 (15)	0.0122 (14)	0.0087 (12)	0.0018 (12)
C21	0.0368 (14)	0.0584 (16)	0.0494 (13)	0.0013 (12)	0.0085 (10)	−0.0027 (11)
C22	0.065 (2)	0.098 (3)	0.165 (3)	−0.0243 (19)	0.002 (2)	0.051 (2)
C23	0.096 (3)	0.102 (3)	0.128 (3)	0.043 (2)	0.012 (2)	0.030 (2)
N1	0.0293 (10)	0.0615 (13)	0.0347 (10)	0.0010 (9)	0.0031 (8)	−0.0022 (9)
O1	0.1432 (19)	0.0502 (12)	0.0627 (12)	0.0013 (11)	0.0232 (11)	0.0144 (9)
O2	0.0819 (12)	0.0503 (10)	0.0522 (10)	0.0217 (9)	0.0209 (8)	0.0043 (8)
O3	0.0544 (11)	0.0958 (14)	0.0499 (10)	0.0008 (10)	0.0020 (8)	0.0231 (9)
O4	0.0420 (10)	0.0605 (12)	0.1031 (14)	−0.0078 (9)	0.0086 (9)	0.0132 (10)
O5	0.0660 (13)	0.0680 (13)	0.1032 (15)	0.0206 (10)	0.0044 (10)	0.0128 (11)

Geometric parameters (Å, º)

C1—N1	1.463 (2)	C13—O2	1.396 (3)
C1—C6	1.513 (3)	C13—H13A	0.9600
C1—C2	1.550 (3)	C13—H13B	0.9600
C1—H1	0.9800	C13—H13C	0.9600
C2—C14	1.511 (3)	C14—H14A	0.9600
C2—C3	1.511 (3)	C14—H14B	0.9600
C2—H2	0.9800	C14—H14C	0.9600
C3—O3	1.215 (2)	C15—H15A	0.9600
C3—C4	1.506 (3)	C15—H15B	0.9600
C4—C15	1.525 (3)	C15—H15C	0.9600
C4—C5	1.545 (3)	C16—C21	1.381 (3)
C4—H4	0.9800	C16—C17	1.399 (3)
C5—N1	1.467 (2)	C17—O4	1.373 (3)
C5—C16	1.512 (3)	C17—C18	1.377 (3)
C5—H5	0.9800	C18—C19	1.376 (3)
C6—C7	1.388 (3)	C18—H18	0.9300
C6—C11	1.394 (3)	C19—C20	1.372 (3)
C7—C8	1.386 (3)	C19—H19	0.9300
C7—H7	0.9300	C20—O5	1.378 (3)
C8—C9	1.369 (3)	C20—C21	1.389 (3)
C8—O1	1.378 (3)	C21—H21	0.9300
C9—C10	1.381 (3)	C22—O4	1.400 (3)
C9—H9	0.9300	C22—H22A	0.9600
C10—C11	1.384 (3)	C22—H22B	0.9600
C10—H10	0.9300	C22—H22C	0.9600
C11—O2	1.376 (2)	C23—O5	1.405 (3)
C12—O1	1.387 (3)	C23—H23A	0.9600
C12—H12A	0.9600	C23—H23B	0.9600
C12—H12B	0.9600	C23—H23C	0.9600
C12—H12C	0.9600	N1—H1N	0.91 (2)
N1—C1—C6	108.28 (16)	H13A—C13—H13B	109.5

N1—C1—C2	108.30 (16)	O2—C13—H13C	109.5
C6—C1—C2	112.50 (16)	H13A—C13—H13C	109.5
N1—C1—H1	109.2	H13B—C13—H13C	109.5
C6—C1—H1	109.2	C2—C14—H14A	109.5
C2—C1—H1	109.2	C2—C14—H14B	109.5
C14—C2—C3	112.79 (18)	H14A—C14—H14B	109.5
C14—C2—C1	113.20 (18)	C2—C14—H14C	109.5
C3—C2—C1	106.98 (16)	H14A—C14—H14C	109.5
C14—C2—H2	107.9	H14B—C14—H14C	109.5
C3—C2—H2	107.9	C4—C15—H15A	109.5
C1—C2—H2	107.9	C4—C15—H15B	109.5
O3—C3—C4	122.4 (2)	H15A—C15—H15B	109.5
O3—C3—C2	122.1 (2)	C4—C15—H15C	109.5
C4—C3—C2	115.40 (18)	H15A—C15—H15C	109.5
C3—C4—C15	113.20 (19)	H15B—C15—H15C	109.5
C3—C4—C5	107.28 (16)	C21—C16—C17	118.5 (2)
C15—C4—C5	112.49 (19)	C21—C16—C5	119.26 (19)
C3—C4—H4	107.9	C17—C16—C5	122.2 (2)
C15—C4—H4	107.9	O4—C17—C18	123.2 (2)
C5—C4—H4	107.9	O4—C17—C16	117.0 (2)
N1—C5—C16	108.48 (17)	C18—C17—C16	119.8 (2)
N1—C5—C4	108.59 (17)	C17—C18—C19	121.3 (2)
C16—C5—C4	112.15 (17)	C17—C18—H18	119.4
N1—C5—H5	109.2	C19—C18—H18	119.4
C16—C5—H5	109.2	C20—C19—C18	119.5 (2)
C4—C5—H5	109.2	C20—C19—H19	120.2
C7—C6—C11	118.11 (19)	C18—C19—H19	120.2
C7—C6—C1	119.29 (18)	C19—C20—O5	124.5 (2)
C11—C6—C1	122.56 (19)	C19—C20—C21	119.8 (2)
C8—C7—C6	121.4 (2)	O5—C20—C21	115.7 (2)
C8—C7—H7	119.3	C16—C21—C20	121.1 (2)
C6—C7—H7	119.3	C16—C21—H21	119.4
C9—C8—O1	123.8 (2)	C20—C21—H21	119.4
C9—C8—C7	119.9 (2)	O4—C22—H22A	109.5
O1—C8—C7	116.3 (2)	O4—C22—H22B	109.5
C8—C9—C10	119.6 (2)	H22A—C22—H22B	109.5
C8—C9—H9	120.2	O4—C22—H22C	109.5
C10—C9—H9	120.2	H22A—C22—H22C	109.5
C11—C10—C9	120.8 (2)	H22B—C22—H22C	109.5
C11—C10—H10	119.6	O5—C23—H23A	109.5
C9—C10—H10	119.6	O5—C23—H23B	109.5
O2—C11—C10	122.92 (19)	H23A—C23—H23B	109.5
O2—C11—C6	116.93 (18)	O5—C23—H23C	109.5
C10—C11—C6	120.1 (2)	H23A—C23—H23C	109.5
O1—C12—H12A	109.5	H23B—C23—H23C	109.5
O1—C12—H12B	109.5	C1—N1—C5	115.22 (16)
H12A—C12—H12B	109.5	C1—N1—H1N	110.3 (13)
O1—C12—H12C	109.5	C5—N1—H1N	109.3 (13)

H12A—C12—H12C	109.5	C8—O1—C12	118.8 (2)
H12B—C12—H12C	109.5	C11—O2—C13	117.55 (19)
O2—C13—H13A	109.5	C17—O4—C22	117.8 (2)
O2—C13—H13B	109.5	C20—O5—C23	117.3 (2)
N1—C1—C2—C14	−179.85 (19)	C7—C6—C11—C10	0.1 (3)
C6—C1—C2—C14	−60.2 (2)	C1—C6—C11—C10	177.74 (19)
N1—C1—C2—C3	55.3 (2)	N1—C5—C16—C21	−45.6 (3)
C6—C1—C2—C3	174.94 (18)	C4—C5—C16—C21	74.4 (2)
C14—C2—C3—O3	−6.6 (3)	N1—C5—C16—C17	132.4 (2)
C1—C2—C3—O3	118.5 (2)	C4—C5—C16—C17	−107.7 (2)
C14—C2—C3—C4	177.1 (2)	C21—C16—C17—O4	179.87 (19)
C1—C2—C3—C4	−57.8 (2)	C5—C16—C17—O4	1.9 (3)
O3—C3—C4—C15	5.9 (3)	C21—C16—C17—C18	1.9 (3)
C2—C3—C4—C15	−177.8 (2)	C5—C16—C17—C18	−176.0 (2)
O3—C3—C4—C5	−118.8 (2)	O4—C17—C18—C19	−179.4 (2)
C2—C3—C4—C5	57.5 (2)	C16—C17—C18—C19	−1.6 (4)
C3—C4—C5—N1	−54.6 (2)	C17—C18—C19—C20	0.6 (4)
C15—C4—C5—N1	−179.68 (19)	C18—C19—C20—O5	179.7 (2)
C3—C4—C5—C16	−174.42 (18)	C18—C19—C20—C21	0.1 (4)
C15—C4—C5—C16	60.5 (3)	C17—C16—C21—C20	−1.3 (3)
N1—C1—C6—C7	44.2 (2)	C5—C16—C21—C20	176.73 (19)
C2—C1—C6—C7	−75.5 (2)	C19—C20—C21—C16	0.3 (3)
N1—C1—C6—C11	−133.4 (2)	O5—C20—C21—C16	−179.4 (2)
C2—C1—C6—C11	106.9 (2)	C6—C1—N1—C5	176.09 (17)
C11—C6—C7—C8	1.5 (3)	C2—C1—N1—C5	−61.6 (2)
C1—C6—C7—C8	−176.22 (19)	C16—C5—N1—C1	−176.60 (17)
C6—C7—C8—C9	−1.9 (3)	C4—C5—N1—C1	61.3 (2)
C6—C7—C8—O1	178.8 (2)	C9—C8—O1—C12	30.9 (4)
O1—C8—C9—C10	179.9 (2)	C7—C8—O1—C12	−149.8 (3)
C7—C8—C9—C10	0.7 (3)	C10—C11—O2—C13	−28.2 (3)
C8—C9—C10—C11	0.9 (3)	C6—C11—O2—C13	153.0 (3)
C9—C10—C11—O2	179.8 (2)	C18—C17—O4—C22	−21.9 (4)
C9—C10—C11—C6	−1.3 (3)	C16—C17—O4—C22	160.3 (2)
C7—C6—C11—O2	179.04 (18)	C19—C20—O5—C23	−2.8 (4)
C1—C6—C11—O2	−3.3 (3)	C21—C20—O5—C23	176.8 (2)