Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-{[(2-Hydroxy-3,5-dimethylbenzyl)-(methyl)amino]methyl}-4,6-dimethylphenol

Chatchai Veranitisagul,[a] Worawat Wattanathana,[b] Attaphon Kaewvilai,[c] Tanwawan Duangthongyou,[b] Apirat Laobuthee[c] and Nattamon Koonsaeng[b]*

[a]Department of Materials and Metallurgical Engineering, Faculty of Engineering, Rajamangala University of Technology Thanyaburi, Pathumthani 12110, Thailand, [b]Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand, and [c]Department of Materials Engineering, Faculty of Engineering, Kasetsart University, Bangkok 10900, Thailand
Correspondence e-mail: fscinmk@ku.ac.th

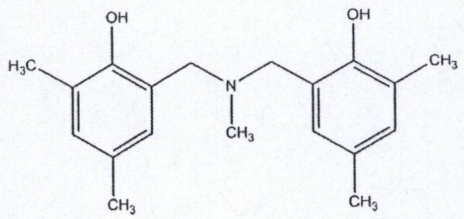
Received 11 May 2012; accepted 16 May 2012

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.050; wR factor = 0.182; data-to-parameter ratio = 13.2.

In the title compound, $C_{19}H_{25}NO_2$, the dihedral angle between the benzene rings is 53.15 (8)°. One of the –OH groups forms an intramolecular O—H···N link, generating an $S(6)$ ring. The other –OH group forms an intermolecular O—H···N hydrogen bond in the crystal, generating centrosymmetric $R_2^2(20)$ loops.

Related literature

For the synthesis, see: Chirachanchai *et al.* (2009). For metal-responsive properties of *N,N*-bis(2-hydroxybenzyl)alkylamines, see: Veranitisagul *et al.* (2011). For the use of *N,N*-bis(2-hydroxybenzyl)alkylamines in the synthesis of macrocyclic molecules, see: Rungsimanon *et al.* (2008).



Experimental

Crystal data

$C_{19}H_{25}NO_2$
M_r = 299.40
Triclinic, $P\overline{1}$
a = 5.4598 (4) Å
b = 12.3285 (12) Å
c = 13.0441 (13) Å
α = 95.412 (3)°
β = 96.482 (2)°
γ = 94.238 (2)°
V = 865.33 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 296 K
0.52 × 0.30 × 0.24 mm

Data collection

Siemens P4 diffractometer
6613 measured reflections
3944 independent reflections
2722 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.182
S = 1.06
3944 reflections
299 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H′···N	1.03 (3)	1.71 (3)	2.6895 (18)	156 (2)
O2—H″···O1^{i}	0.94 (3)	2.02 (4)	2.9114 (18)	158 (2)

Symmetry code: (i) $-x+1, -y+1, -z$.

Data collection: *XSCANS* (Siemens, 1992); cell refinement: *XSCANS*; data reduction: *XSCANS*; 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: *SHELXL97*.

This work was supported by the Thailand Research Fund (grant No. MRG5480046). The authors would like to thank the Department of Chemistry, Faculty of Science, Kasetsart University for partial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6793).

References

Chirachanchai, S., Laobuthee, A. & Phongtamrag, S. (2009). *J. Heterocycl. Chem.* **46**, 714–721.
Rungsimanon, T., Laobuthee, A., Miyata, M. & Chirachanchai, S. (2008). *J. Incl. Phenom. Macrocycl. Chem.* **62**, 333–338.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Siemens (1992). *XSCANS User's Manual*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Veranitisagul, C., Kaewvilai, A., Sangngern, S., Wattanathana, W., Suramitr, S., Koonsaeng, N. & Laobuthee, A. (2011). *Int. J. Mol. Sci.* **12**, 4365–4377.

supplementary materials

Acta Cryst. (2012). E**68**, o1826 [doi:10.1107/S1600536812022180]

2-{[(2-Hydroxy-3,5-dimethylbenzyl)(methyl)amino]methyl}-4,6-dimethylphenol

Chatchai Veranitisagul, Worawat Wattanathana, Attaphon Kaewvilai, Tanwawan Duangthongyou, Apirat Laobuthee and Nattamon Koonsaeng

Experimental

The preparation of the title compound was reported elsewhere (Chirachanchai *et al.*, 2009). Colorless blocks were recrystallized from 2-propanol solution.

Refinement

All H atoms were located in difference maps and freely refined.

Computing details

Data collection: *XSCANS* (Siemens, 1992); cell refinement: *XSCANS* (Siemens, 1992); data reduction: *XSCANS* (Siemens, 1992); 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: *SHELXL97* (Sheldrick, 2008).

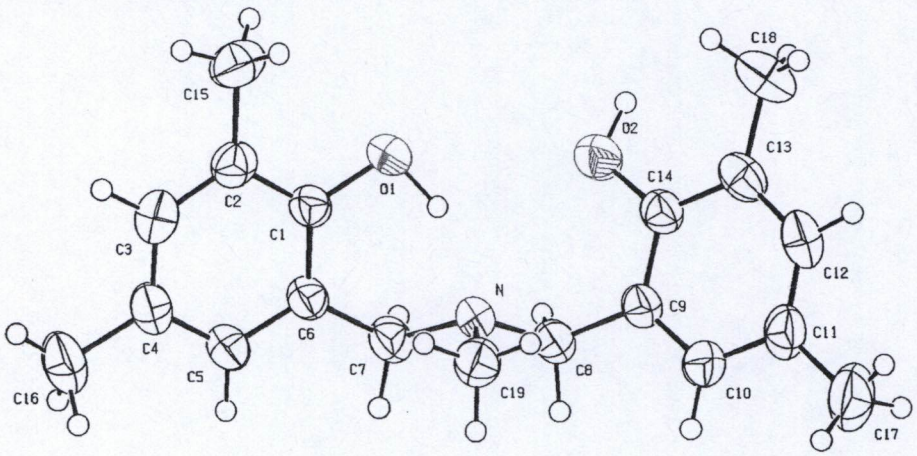


Figure 1

Molecular structure of the title compound (arbitrary spheres for the H atoms).

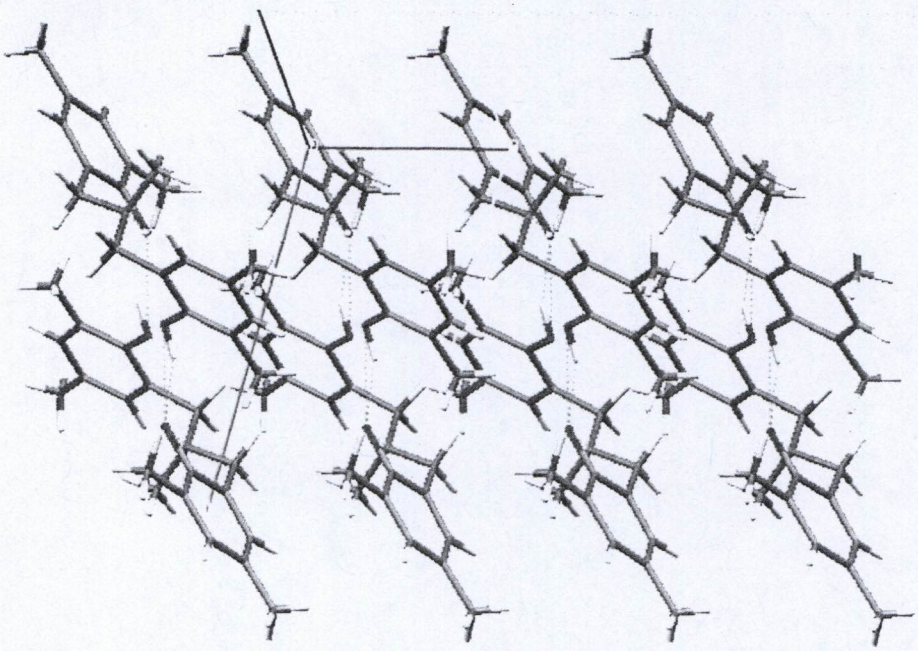


Figure 2

The packing structure of compound (Hydrogen bonds indicated by dash lines).

2-{[(2-Hydroxy-3,5-dimethylbenzyl)(methyl)amino]methyl}-4,6-dimethylphenol

Crystal data

$C_{19}H_{25}NO_2$
$M_r = 299.40$
Triclinic, $P\overline{1}$
$a = 5.4598$ (4) Å
$b = 12.3285$ (12) Å
$c = 13.0441$ (13) Å
$\alpha = 95.412$ (3)°
$\beta = 96.482$ (2)°
$\gamma = 94.238$ (2)°
$V = 865.33$ (14) Å^3
$Z = 2$
$F(000) = 324$
$D_x = 1.149$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2370 reflections
$\theta = 3.2$–$27.2°$
$\mu = 0.07$ mm^{-1}
$T = 296$ K
Block, colorless
0.52 × 0.30 × 0.24 mm

Data collection

Siemens P4
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
6613 measured reflections
3944 independent reflections
2722 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 27.6°$, $\theta_{min} = 1.6°$
$h = -6 \rightarrow 7$
$k = -16 \rightarrow 15$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.182$
$S = 1.06$
3944 reflections
299 parameters
0 restraints
Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.1149P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} < 0.001$
All H-atom parameters refined	$\Delta\rho_{max} = 0.27$ e Å^{-3}
	$\Delta\rho_{min} = -0.26$ 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	0.5039 (2)	0.38818 (10)	0.16018 (10)	0.0517 (3)
N	0.2371 (2)	0.21998 (11)	0.04228 (10)	0.0404 (3)
C1	0.4085 (3)	0.34523 (12)	0.24228 (13)	0.0427 (4)
C14	0.4502 (3)	0.30149 (13)	−0.15535 (12)	0.0428 (4)
C10	0.3116 (4)	0.11247 (15)	−0.20468 (13)	0.0532 (4)
C2	0.5258 (3)	0.37697 (14)	0.34231 (14)	0.0479 (4)
C6	0.1937 (3)	0.27292 (13)	0.22555 (12)	0.0423 (4)
C9	0.2935 (3)	0.20900 (14)	−0.14369 (12)	0.0435 (4)
C3	0.4254 (3)	0.33434 (15)	0.42452 (14)	0.0529 (4)
C7	0.0629 (3)	0.24498 (16)	0.11772 (13)	0.0487 (4)
C5	0.1029 (3)	0.23192 (15)	0.31059 (14)	0.0496 (4)
C13	0.6237 (3)	0.29546 (15)	−0.22569 (14)	0.0490 (4)
C8	0.1141 (3)	0.21588 (16)	−0.06464 (13)	0.0472 (4)
C11	0.4815 (4)	0.10371 (16)	−0.27587 (14)	0.0571 (5)
C4	0.2141 (3)	0.26180 (15)	0.41101 (14)	0.0529 (4)
C12	0.6338 (4)	0.19581 (17)	−0.28429 (14)	0.0556 (5)
C19	0.3486 (4)	0.11876 (15)	0.06030 (16)	0.0532 (4)
C16	0.1053 (6)	0.2193 (3)	0.50252 (19)	0.0796 (7)
C15	0.7506 (4)	0.45821 (19)	0.3588 (2)	0.0640 (5)
C18	0.7977 (4)	0.3916 (2)	−0.2386 (2)	0.0651 (6)
C17	0.4954 (9)	−0.0025 (2)	−0.3427 (2)	0.0933 (9)
O2	0.4257 (2)	0.39465 (10)	−0.09216 (10)	0.0585 (4)
H5	−0.048 (3)	0.1827 (16)	0.2992 (14)	0.052 (5)*
H12	0.751 (4)	0.1965 (19)	−0.3286 (19)	0.079 (7)*
H7B	−0.068 (4)	0.1831 (17)	0.1203 (15)	0.061 (5)*
H10	0.205 (4)	0.0478 (19)	−0.1977 (17)	0.067 (6)*
H3	0.510 (4)	0.353 (2)	0.497 (2)	0.083 (7)*
H19C	0.222 (4)	0.0535 (19)	0.0524 (17)	0.073 (6)*
H8B	−0.017 (4)	0.1503 (18)	−0.0811 (16)	0.066 (6)*
H8A	0.020 (3)	0.2867 (16)	−0.0664 (15)	0.056 (5)*
H19B	0.430 (4)	0.1259 (18)	0.1319 (19)	0.069 (6)*
H16A	−0.068 (8)	0.216 (4)	0.490 (3)	0.167 (16)*

H19A	0.466 (4)	0.1081 (18)	0.0130 (17)	0.069 (6)*
H18B	0.855 (4)	0.4335 (17)	−0.1729 (18)	0.059 (6)*
H7A	−0.030 (4)	0.3078 (17)	0.0938 (15)	0.060 (5)*
H17A	0.644 (8)	−0.001 (4)	−0.363 (4)	0.155 (17)*
H18A	0.944 (5)	0.369 (2)	−0.257 (2)	0.091 (8)*
H15B	0.827 (5)	0.459 (2)	0.433 (3)	0.110 (9)*
H15C	0.718 (4)	0.535 (2)	0.335 (2)	0.088 (7)*
H′	0.426 (5)	0.331 (2)	0.100 (2)	0.097 (8)*
H16C	0.188 (6)	0.241 (3)	0.565 (3)	0.142 (13)*
H18C	0.729 (4)	0.443 (2)	−0.276 (2)	0.086 (7)*
H″	0.483 (5)	0.457 (3)	−0.122 (2)	0.104 (9)*
H16B	0.079 (7)	0.133 (4)	0.490 (3)	0.139 (12)*
H17C	0.424 (9)	0.000 (4)	−0.409 (5)	0.184 (18)*
H15A	0.879 (5)	0.432 (2)	0.327 (2)	0.086 (8)*
H17B	0.490 (6)	−0.064 (3)	−0.304 (3)	0.136 (12)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0599 (7)	0.0452 (7)	0.0506 (7)	−0.0098 (5)	0.0196 (6)	0.0038 (5)
N	0.0436 (7)	0.0421 (7)	0.0366 (7)	0.0005 (5)	0.0092 (5)	0.0067 (5)
C1	0.0477 (8)	0.0374 (8)	0.0446 (9)	0.0025 (6)	0.0148 (7)	0.0026 (6)
C14	0.0455 (8)	0.0447 (9)	0.0392 (8)	0.0025 (6)	0.0059 (6)	0.0098 (7)
C10	0.0697 (11)	0.0510 (10)	0.0369 (9)	−0.0053 (9)	0.0038 (8)	0.0053 (7)
C2	0.0483 (8)	0.0428 (9)	0.0521 (10)	0.0064 (7)	0.0093 (7)	−0.0029 (7)
C6	0.0434 (8)	0.0437 (9)	0.0415 (9)	0.0027 (6)	0.0124 (6)	0.0056 (7)
C9	0.0477 (8)	0.0474 (9)	0.0355 (8)	−0.0013 (7)	0.0050 (6)	0.0089 (6)
C3	0.0585 (10)	0.0568 (11)	0.0435 (10)	0.0127 (8)	0.0054 (8)	0.0006 (8)
C7	0.0412 (8)	0.0608 (11)	0.0445 (9)	−0.0020 (8)	0.0112 (7)	0.0062 (8)
C5	0.0514 (9)	0.0518 (10)	0.0479 (10)	−0.0001 (7)	0.0159 (8)	0.0083 (8)
C13	0.0454 (8)	0.0567 (10)	0.0489 (9)	0.0067 (7)	0.0072 (7)	0.0216 (8)
C8	0.0453 (8)	0.0563 (10)	0.0392 (9)	−0.0056 (8)	0.0053 (7)	0.0081 (7)
C11	0.0812 (12)	0.0549 (11)	0.0375 (9)	0.0118 (9)	0.0101 (8)	0.0082 (8)
C4	0.0618 (10)	0.0563 (10)	0.0444 (10)	0.0097 (8)	0.0168 (8)	0.0096 (8)
C12	0.0653 (11)	0.0656 (12)	0.0429 (10)	0.0187 (9)	0.0186 (8)	0.0174 (8)
C19	0.0667 (11)	0.0461 (10)	0.0479 (10)	0.0079 (8)	0.0072 (9)	0.0075 (8)
C16	0.0953 (18)	0.100 (2)	0.0474 (12)	−0.0027 (15)	0.0207 (12)	0.0215 (12)
C15	0.0553 (11)	0.0583 (13)	0.0727 (14)	−0.0043 (9)	0.0034 (10)	−0.0104 (10)
C18	0.0531 (11)	0.0650 (13)	0.0848 (17)	0.0039 (10)	0.0231 (11)	0.0303 (13)
C17	0.160 (3)	0.0665 (16)	0.0577 (15)	0.0170 (17)	0.0367 (17)	−0.0026 (12)
O2	0.0753 (8)	0.0424 (7)	0.0598 (8)	−0.0029 (6)	0.0221 (6)	0.0052 (6)

Geometric parameters (Å, º)

O1—C1	1.3750 (19)	C13—C12	1.393 (3)
O1—H′	1.04 (3)	C13—C18	1.498 (3)
N—C19	1.456 (2)	C8—H8B	1.03 (2)
N—C7	1.472 (2)	C8—H8A	1.05 (2)
N—C8	1.473 (2)	C11—C12	1.378 (3)
C1—C2	1.394 (2)	C11—C17	1.515 (3)

C1—C6	1.403 (2)	C4—C16	1.511 (3)
C14—O2	1.373 (2)	C12—H12	0.91 (2)
C14—C13	1.392 (2)	C19—H19C	1.01 (2)
C14—C9	1.405 (2)	C19—H19B	0.98 (2)
C10—C9	1.384 (2)	C19—H19A	0.94 (2)
C10—C11	1.387 (3)	C16—H16A	0.94 (4)
C10—H10	0.97 (2)	C16—H16C	0.89 (4)
C2—C3	1.387 (3)	C16—H16B	1.05 (4)
C2—C15	1.508 (3)	C15—H15B	1.01 (3)
C6—C5	1.387 (2)	C15—H15C	1.05 (3)
C6—C7	1.501 (2)	C15—H15A	0.92 (3)
C9—C8	1.501 (2)	C18—H18B	0.96 (2)
C3—C4	1.391 (3)	C18—H18A	0.92 (3)
C3—H3	1.00 (3)	C18—H18C	0.91 (3)
C7—H7B	1.01 (2)	C17—H17A	0.88 (4)
C7—H7A	1.01 (2)	C17—H17C	0.91 (6)
C5—C4	1.384 (3)	C17—H17B	0.96 (4)
C5—H5	0.973 (18)	O2—H″	0.95 (3)

C1—O1—H′	100.4 (15)	H8B—C8—H8A	107.3 (15)
C19—N—C7	111.00 (14)	C12—C11—C10	117.31 (17)
C19—N—C8	111.41 (14)	C12—C11—C17	121.5 (2)
C7—N—C8	110.75 (12)	C10—C11—C17	121.2 (2)
O1—C1—C2	118.74 (14)	C5—C4—C3	117.52 (16)
O1—C1—C6	120.42 (15)	C5—C4—C16	121.06 (19)
C2—C1—C6	120.82 (14)	C3—C4—C16	121.40 (19)
O2—C14—C13	123.18 (14)	C11—C12—C13	123.26 (16)
O2—C14—C9	116.30 (14)	C11—C12—H12	122.7 (15)
C13—C14—C9	120.50 (16)	C13—C12—H12	114.1 (15)
C9—C10—C11	122.18 (17)	N—C19—H19C	112.4 (12)
C9—C10—H10	120.0 (13)	N—C19—H19B	108.3 (13)
C11—C10—H10	117.8 (13)	H19C—C19—H19B	107.1 (18)
C3—C2—C1	118.13 (15)	N—C19—H19A	108.2 (13)
C3—C2—C15	121.91 (17)	H19C—C19—H19A	110.3 (18)
C1—C2—C15	119.93 (17)	H19B—C19—H19A	110.5 (18)
C5—C6—C1	118.57 (15)	C4—C16—H16A	109 (3)
C5—C6—C7	121.62 (14)	C4—C16—H16C	116 (2)
C1—C6—C7	119.77 (14)	H16A—C16—H16C	123 (3)
C10—C9—C14	118.83 (15)	C4—C16—H16B	109 (2)
C10—C9—C8	121.39 (15)	H16A—C16—H16B	84 (3)
C14—C9—C8	119.77 (15)	H16C—C16—H16B	111 (3)
C2—C3—C4	122.74 (17)	C2—C15—H15B	107.5 (17)
C2—C3—H3	119.9 (13)	C2—C15—H15C	114.4 (13)
C4—C3—H3	117.3 (13)	H15B—C15—H15C	116 (2)
N—C7—C6	111.73 (13)	C2—C15—H15A	111.8 (16)
N—C7—H7B	113.6 (11)	H15B—C15—H15A	98 (2)
C6—C7—H7B	107.5 (12)	H15C—C15—H15A	109 (2)
N—C7—H7A	107.2 (11)	C13—C18—H18B	111.5 (12)
C6—C7—H7A	111.3 (11)	C13—C18—H18A	110.3 (17)

H7B—C7—H7A	105.5 (16)	H18B—C18—H18A	101 (2)
C4—C5—C6	122.20 (16)	C13—C18—H18C	114.8 (15)
C4—C5—H5	119.1 (11)	H18B—C18—H18C	102 (2)
C6—C5—H5	118.7 (11)	H18A—C18—H18C	116 (2)
C14—C13—C12	117.91 (15)	C11—C17—H17A	107 (3)
C14—C13—C18	122.03 (18)	C11—C17—H17C	111 (3)
C12—C13—C18	120.06 (17)	H17A—C17—H17C	91 (3)
N—C8—C9	112.46 (12)	C11—C17—H17B	112 (2)
N—C8—H8B	110.9 (11)	H17A—C17—H17B	104 (4)
C9—C8—H8B	108.7 (11)	H17C—C17—H17B	127 (4)
N—C8—H8A	105.3 (11)	C14—O2—H″	110.3 (18)
C9—C8—H8A	112.1 (10)		

O1—C1—C2—C3	179.02 (15)	C1—C6—C5—C4	1.4 (3)
C6—C1—C2—C3	0.6 (2)	C7—C6—C5—C4	−176.34 (16)
O1—C1—C2—C15	0.9 (2)	O2—C14—C13—C12	178.87 (15)
C6—C1—C2—C15	−177.59 (17)	C9—C14—C13—C12	0.8 (2)
O1—C1—C6—C5	−179.66 (14)	O2—C14—C13—C18	−0.5 (3)
C2—C1—C6—C5	−1.2 (2)	C9—C14—C13—C18	−178.61 (17)
O1—C1—C6—C7	−1.9 (2)	C19—N—C8—C9	−65.34 (18)
C2—C1—C6—C7	176.55 (15)	C7—N—C8—C9	170.58 (14)
C11—C10—C9—C14	0.9 (3)	C10—C9—C8—N	105.66 (17)
C11—C10—C9—C8	−177.98 (17)	C14—C9—C8—N	−73.2 (2)
O2—C14—C9—C10	−179.40 (15)	C9—C10—C11—C12	−0.2 (3)
C13—C14—C9—C10	−1.2 (2)	C9—C10—C11—C17	−179.2 (2)
O2—C14—C9—C8	−0.5 (2)	C6—C5—C4—C3	−0.9 (3)
C13—C14—C9—C8	177.70 (14)	C6—C5—C4—C16	177.5 (2)
C1—C2—C3—C4	0.0 (3)	C2—C3—C4—C5	0.2 (3)
C15—C2—C3—C4	178.09 (18)	C2—C3—C4—C16	−178.2 (2)
C19—N—C7—C6	67.71 (18)	C10—C11—C12—C13	−0.3 (3)
C8—N—C7—C6	−167.98 (14)	C17—C11—C12—C13	178.8 (2)
C5—C6—C7—N	−136.72 (16)	C14—C13—C12—C11	0.0 (3)
C1—C6—C7—N	45.6 (2)	C18—C13—C12—C11	179.35 (19)

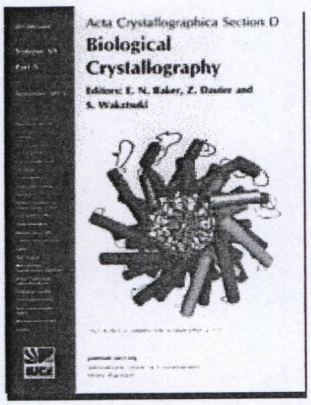
Hydrogen-bond geometry (Å, º)

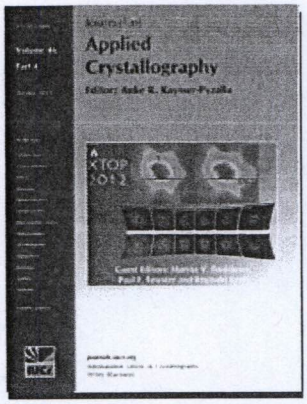
D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H′···N	1.03 (3)	1.71 (3)	2.6895 (18)	156 (2)
O2—H″···O1^{i}	0.94 (3)	2.02 (4)	2.9114 (18)	158 (2)

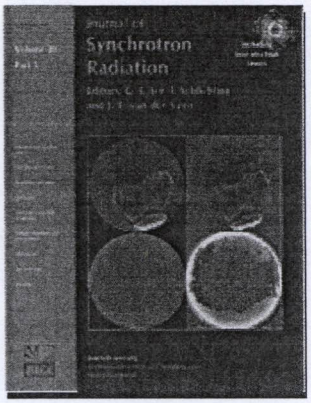
Symmetry code: (i) −*x*+1, −*y*+1, −*z*.

impact factors for IUCr journals

Thomson Reuters have released their 2012 Journal Citation Reports and these are summarised below. *Acta Crystallographica Section D* leads the crystallography rankings with its highest ever impact factor of 14.1.







	2012	2011	2010	2009	2008	2007	2006	2005	2004	2003	2002	2001	2000	1999	1998	1997
Acta Crystallographica Section A	2.244	2.076	54.33	49.93	2.051	2.385	1.676	1.791	1.829	1.558	1.417	1.749	1.491	1.601	2.146	1.806
Acta Crystallographica Section B	2.175	2.286	1.829	1.801	2.341	2.163	2.172	1.910	5.418	3.643	2.026	1.955	1.734	1.700	1.612	1.463
Acta Crystallographica Section C	0.492	0.518	0.745	0.782	0.561	0.719	0.896	0.777	0.728	0.828	0.659	0.570	0.543	0.581	0.577	0.459
Acta Crystallographica Section D	14.103	12.619	6.326	2.257	2.943	2.620	1.687	1.401	1.693	2.208	1.760	2.124	3.067	2.935	2.244	2.118
Acta Crystallographica Section E		0.347	0.413	0.411	0.367	0.508	0.567	0.581	0.491	0.453						
Acta Crystallographica Section F	0.552	0.506	0.563	0.551	0.606	0.645										
Journal of Applied Crystallography	3.343	5.152	3.794	3.018	3.212	3.629	2.495	5.248	3.534	2.324	1.871	2.583	1.752	1.901	1.569	1.988
Journal of Synchrotron Radiation	2.186	2.726	2.335	1.994	2.333	2.978	2.38	2.392	1.919	1.144	0.885	1.519	0.924	1.114	1.874	1.688

Impact factors are generally calculated based on a three-year period. For example, the 2012 impact factor for a journal would be calculated as follows:

2012 Impact Factor = *A*/*B*

where *A* = number of times articles published in 2010-2011 were cited in tracked journals during 2012 and *B* = number of articles published in 2010-2011.