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5-Hydroxy-7-methoxy-2-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one. Corrigendum

Jeannie Bee-Jan Teh,[a] Hoong-Kun Fun,[a]* Ibrahim Abdul Razak,[a] Suchada Chantrapromma,[b]* Nawong Boonnak[b] and Chatchanok Karalai[b]

[a]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and [b]Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand

Correspondence e-mail: hkfun@usm.my, suchada.c@psu.ac.th

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In the paper by Teh, Fun, Razak, Chantrapromma, Boonnak & Karalai [*Acta Cryst.* (2005), E**61**, o3715–o3717], the data collection temperature is given incorrectly. The correct temperature is given below and in the revised '*Key indicators*'.

Crystal data

$C_{17}H_{14}O_5$
M_r = 298.28
Monoclinic, $P2_1/c$
a = 16.9406 (4) Å
b = 3.8619 (1) Å
c = 21.7968 (4) Å
β = 106.52 (1)°
V = 1367.15 (9) Å^3
Z = 4
D_x = 1.449 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3581 reflections
θ = 2.0–28.0°
μ = 0.11 mm^{-1}
T = 297 (2) K
Plate, colourless
0.54 × 0.15 × 0.08 mm

Key indicators

Single-crystal X-ray study
T = 297 K
Mean σ(C–C) = 0.002 Å
R factor = 0.046
wR factor = 0.128
Data-to-parameter ratio = 16.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

supporting information

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Crystal data

$C_{17}H_{14}O_5$
$M_r = 298.28$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 16.9406$ (4) Å
$b = 3.8619$ (1) Å
$c = 21.7968$ (4) Å
$\beta = 106.52$ (1)°
$V = 1367.15$ (9) Å^3
$Z = 4$
$F(000) = 624$
$D_x = 1.449$ Mg m^{-3}
Melting point = 447–448 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3581 reflections
$\theta = 2.0$–$28.0°$
$\mu = 0.11$ mm^{-1}
$T = 297$ K
Plate, colourless
0.54 × 0.15 × 0.08 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.33 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2005)
$T_{min} = 0.912$, $T_{max} = 0.992$
17884 measured reflections
3283 independent reflections
2207 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 28.0°$, $\theta_{min} = 2.0°$
$h = -21 \rightarrow 22$
$k = -5 \rightarrow 5$
$l = -28 \rightarrow 28$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.128$
$S = 1.05$
3283 reflections
201 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
$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2 + 0.2601P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ 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	0.15499 (6)	0.9753 (3)	0.37516 (4)	0.0409 (3)
O2	0.25586 (7)	0.5256 (3)	0.54929 (5)	0.0541 (4)
O3	0.39800 (7)	0.5554 (4)	0.52901 (5)	0.0560 (4)
H3	0.3636	0.5130	0.5479	0.084*
O4	0.40678 (7)	1.0285 (3)	0.32828 (5)	0.0538 (4)
O5	−0.22834 (7)	1.0817 (4)	0.28553 (5)	0.0533 (4)
C1	0.23874 (9)	0.9148 (4)	0.39514 (7)	0.0362 (4)
C2	0.28282 (10)	1.0058 (4)	0.35373 (7)	0.0412 (4)
H2	0.2573	1.1094	0.3146	0.049*
C3	0.36683 (10)	0.9380 (5)	0.37218 (7)	0.0414 (4)
C4	0.40646 (10)	0.7874 (5)	0.43095 (7)	0.0440 (4)
H4	0.4628	0.7452	0.4424	0.053*
C5	0.36052 (10)	0.7022 (5)	0.47179 (7)	0.0412 (4)
C6	0.27504 (9)	0.7617 (4)	0.45482 (6)	0.0362 (4)
C7	0.22512 (10)	0.6656 (4)	0.49571 (7)	0.0397 (4)
C8	0.13922 (10)	0.7345 (5)	0.47088 (7)	0.0411 (4)
H8	0.1045	0.6780	0.4956	0.049*
C9	0.10645 (9)	0.8792 (4)	0.41260 (6)	0.0362 (4)
C10	0.01916 (10)	0.9446 (4)	0.38162 (6)	0.0355 (4)
C11	−0.04119 (10)	0.8394 (5)	0.40996 (7)	0.0424 (4)
H11	−0.0249	0.7380	0.4503	0.051*
C12	−0.12400 (10)	0.8807 (5)	0.38018 (7)	0.0424 (4)
H12	−0.1628	0.8085	0.4002	0.051*
C13	−0.14880 (10)	1.0311 (4)	0.31993 (7)	0.0399 (4)
C14	−0.08988 (10)	1.1419 (5)	0.29100 (7)	0.0444 (4)
H14	−0.1064	1.2448	0.2508	0.053*
C15	−0.00750 (10)	1.1007 (5)	0.32127 (7)	0.0411 (4)
H15	0.0311	1.1775	0.3014	0.049*
C16	0.49030 (11)	0.9268 (6)	0.33992 (9)	0.0601 (5)
H16A	0.5094	0.9900	0.3040	0.090*
H16B	0.4947	0.6806	0.3460	0.090*
H16C	0.5233	1.0410	0.3777	0.090*
C17	−0.29207 (11)	0.9581 (6)	0.31075 (9)	0.0553 (5)
H17A	−0.3447	1.0069	0.2810	0.083*
H17B	−0.2882	1.0716	0.3507	0.083*

H17C	−0.2862	0.7127	0.3175	0.083*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0397 (6)	0.0506 (7)	0.0330 (5)	0.0022 (5)	0.0113 (4)	0.0064 (5)
O2	0.0556 (7)	0.0711 (9)	0.0343 (5)	0.0069 (7)	0.0107 (5)	0.0164 (6)
O3	0.0481 (7)	0.0774 (10)	0.0384 (6)	0.0072 (7)	0.0054 (5)	0.0148 (6)
O4	0.0448 (7)	0.0732 (10)	0.0467 (6)	0.0002 (7)	0.0183 (5)	0.0100 (6)
O5	0.0428 (6)	0.0721 (9)	0.0436 (6)	0.0051 (7)	0.0102 (5)	0.0118 (6)
C1	0.0377 (8)	0.0370 (9)	0.0324 (7)	−0.0006 (7)	0.0075 (6)	−0.0016 (6)
C2	0.0455 (9)	0.0460 (11)	0.0310 (7)	−0.0009 (8)	0.0093 (6)	0.0042 (7)
C3	0.0440 (9)	0.0453 (11)	0.0363 (7)	−0.0039 (8)	0.0136 (6)	−0.0008 (7)
C4	0.0385 (8)	0.0506 (11)	0.0408 (8)	−0.0007 (8)	0.0079 (6)	−0.0003 (8)
C5	0.0453 (9)	0.0430 (10)	0.0323 (7)	0.0006 (8)	0.0060 (6)	0.0003 (7)
C6	0.0425 (8)	0.0351 (9)	0.0295 (6)	0.0002 (8)	0.0078 (6)	−0.0008 (6)
C7	0.0499 (9)	0.0383 (10)	0.0304 (7)	0.0008 (8)	0.0106 (6)	0.0004 (7)
C8	0.0458 (9)	0.0459 (10)	0.0337 (7)	0.0021 (8)	0.0150 (6)	0.0028 (7)
C9	0.0446 (9)	0.0345 (9)	0.0319 (7)	−0.0008 (8)	0.0149 (6)	−0.0026 (6)
C10	0.0432 (8)	0.0323 (9)	0.0320 (7)	0.0016 (7)	0.0125 (6)	−0.0007 (6)
C11	0.0475 (9)	0.0475 (11)	0.0328 (7)	0.0007 (9)	0.0125 (6)	0.0071 (7)
C12	0.0459 (9)	0.0463 (11)	0.0379 (7)	−0.0017 (8)	0.0165 (7)	0.0036 (7)
C13	0.0423 (9)	0.0410 (10)	0.0359 (7)	0.0044 (8)	0.0102 (6)	−0.0007 (7)
C14	0.0504 (10)	0.0499 (11)	0.0341 (7)	0.0062 (9)	0.0140 (7)	0.0075 (7)
C15	0.0473 (9)	0.0438 (10)	0.0361 (7)	0.0027 (8)	0.0183 (7)	0.0053 (7)
C16	0.0520 (11)	0.0720 (14)	0.0629 (11)	0.0021 (11)	0.0269 (9)	0.0062 (10)
C17	0.0429 (9)	0.0675 (14)	0.0551 (10)	−0.0014 (10)	0.0131 (8)	0.0029 (10)

Geometric parameters (Å, º)

O1—C9	1.3645 (17)	C8—C9	1.354 (2)
O1—C1	1.3804 (18)	C8—H8	0.93
O2—C7	1.2578 (17)	C9—C10	1.462 (2)
O3—C5	1.3526 (18)	C10—C11	1.397 (2)
O3—H3	0.82	C10—C15	1.400 (2)
O4—C3	1.3652 (19)	C11—C12	1.377 (2)
O4—C16	1.420 (2)	C11—H11	0.93
O5—C13	1.3570 (18)	C12—C13	1.387 (2)
O5—C17	1.426 (2)	C12—H12	0.93
C1—C2	1.371 (2)	C13—C14	1.391 (2)
C1—C6	1.402 (2)	C14—C15	1.373 (2)
C2—C3	1.389 (2)	C14—H14	0.93
C2—H2	0.93	C15—H15	0.93
C3—C4	1.393 (2)	C16—H16A	0.96
C4—C5	1.379 (2)	C16—H16B	0.96
C4—H4	0.93	C16—H16C	0.96
C5—C6	1.408 (2)	C17—H17A	0.96
C6—C7	1.441 (2)	C17—H17B	0.96

C7—C8	1.426 (2)	C17—H17C	0.96
C9—O1—C1	120.35 (11)	C11—C10—C15	117.37 (15)
C5—O3—H3	109.5	C11—C10—C9	121.11 (13)
C3—O4—C16	118.12 (14)	C15—C10—C9	121.46 (14)
C13—O5—C17	118.72 (13)	C12—C11—C10	122.24 (14)
C2—C1—O1	116.89 (13)	C12—C11—H11	118.9
C2—C1—C6	122.80 (14)	C10—C11—H11	118.9
O1—C1—C6	120.31 (13)	C11—C12—C13	119.23 (14)
C1—C2—C3	117.78 (14)	C11—C12—H12	120.4
C1—C2—H2	121.1	C13—C12—H12	120.4
C3—C2—H2	121.1	O5—C13—C12	124.69 (14)
O4—C3—C2	114.83 (14)	O5—C13—C14	115.66 (13)
O4—C3—C4	123.09 (15)	C12—C13—C14	119.65 (15)
C2—C3—C4	122.08 (14)	C15—C14—C13	120.59 (14)
C5—C4—C3	118.71 (15)	C15—C14—H14	119.7
C5—C4—H4	120.6	C13—C14—H14	119.7
C3—C4—H4	120.6	C14—C15—C10	120.92 (14)
O3—C5—C4	119.48 (14)	C14—C15—H15	119.5
O3—C5—C6	119.26 (14)	C10—C15—H15	119.5
C4—C5—C6	121.25 (14)	O4—C16—H16A	109.5
C1—C6—C5	117.37 (14)	O4—C16—H16B	109.5
C1—C6—C7	120.18 (14)	H16A—C16—H16B	109.5
C5—C6—C7	122.44 (13)	O4—C16—H16C	109.5
O2—C7—C8	122.75 (14)	H16A—C16—H16C	109.5
O2—C7—C6	121.62 (15)	H16B—C16—H16C	109.5
C8—C7—C6	115.63 (13)	O5—C17—H17A	109.5
C9—C8—C7	122.34 (14)	O5—C17—H17B	109.5
C9—C8—H8	118.8	H17A—C17—H17B	109.5
C7—C8—H8	118.8	O5—C17—H17C	109.5
C8—C9—O1	121.16 (14)	H17A—C17—H17C	109.5
C8—C9—C10	126.55 (14)	H17B—C17—H17C	109.5
O1—C9—C10	112.28 (12)		
C9—O1—C1—C2	177.38 (14)	C5—C6—C7—C8	−178.31 (15)
C9—O1—C1—C6	−1.6 (2)	O2—C7—C8—C9	−178.69 (16)
O1—C1—C2—C3	−178.23 (14)	C6—C7—C8—C9	0.3 (2)
C6—C1—C2—C3	0.7 (3)	C7—C8—C9—O1	−1.7 (3)
C16—O4—C3—C2	−171.93 (16)	C7—C8—C9—C10	176.83 (16)
C16—O4—C3—C4	7.7 (3)	C1—O1—C9—C8	2.4 (2)
C1—C2—C3—O4	178.75 (15)	C1—O1—C9—C10	−176.37 (13)
C1—C2—C3—C4	−0.9 (3)	C8—C9—C10—C11	−3.7 (3)
O4—C3—C4—C5	−179.36 (16)	O1—C9—C10—C11	174.93 (14)
C2—C3—C4—C5	0.3 (3)	C8—C9—C10—C15	179.17 (16)
C3—C4—C5—O3	179.93 (16)	O1—C9—C10—C15	−2.2 (2)
C3—C4—C5—C6	0.6 (3)	C15—C10—C11—C12	0.9 (3)
C2—C1—C6—C5	0.1 (2)	C9—C10—C11—C12	−176.32 (15)
O1—C1—C6—C5	179.00 (14)	C10—C11—C12—C13	0.1 (3)

C2—C1—C6—C7	−178.76 (16)	C17—O5—C13—C12	−3.3 (3)
O1—C1—C6—C7	0.1 (2)	C17—O5—C13—C14	176.77 (16)
O3—C5—C6—C1	179.90 (15)	C11—C12—C13—O5	179.16 (16)
C4—C5—C6—C1	−0.8 (3)	C11—C12—C13—C14	−0.9 (3)
O3—C5—C6—C7	−1.3 (3)	O5—C13—C14—C15	−179.42 (15)
C4—C5—C6—C7	178.07 (15)	C12—C13—C14—C15	0.6 (3)
C1—C6—C7—O2	179.49 (15)	C13—C14—C15—C10	0.4 (3)
C5—C6—C7—O2	0.7 (3)	C11—C10—C15—C14	−1.1 (2)
C1—C6—C7—C8	0.5 (2)	C9—C10—C15—C14	176.05 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2	0.82	1.83	2.571 (2)	149
C4—H4···O3^{i}	0.93	2.54	3.441 (2)	163
C12—H12···O2^{ii}	0.93	2.52	3.430 (2)	167

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*, −*y*+1, −*z*+1.