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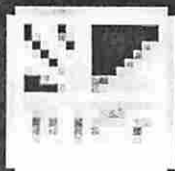
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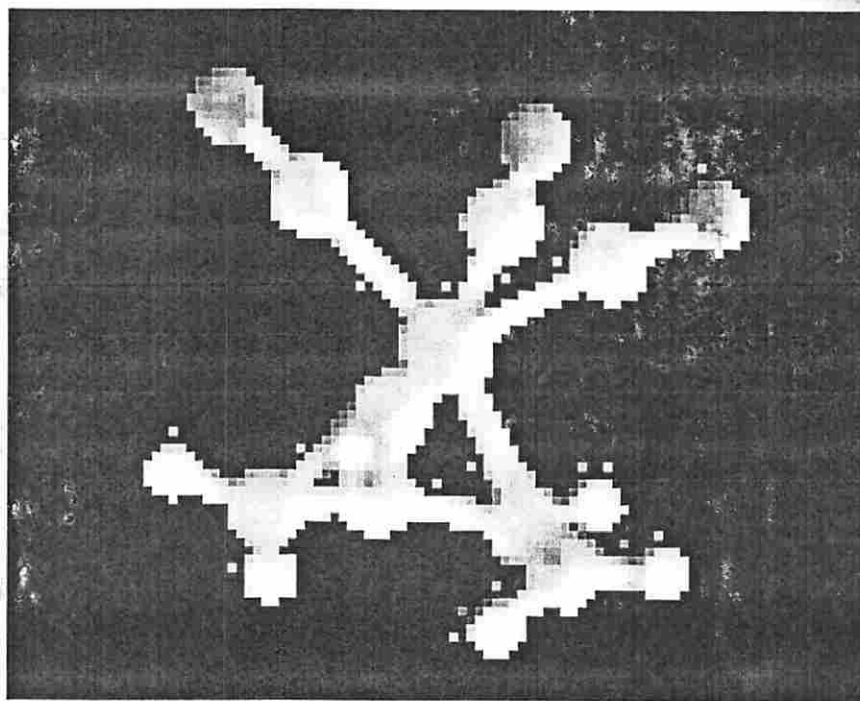
Section E

Structure Reports



Acta Crystallographica Section E Structure Reports Online

Editors: W. L. A. Harrison, J. Simpson and
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**Editors and co-editors of *Acta Crystallographica Section E*
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Editor-in-chief

G. Kostorz, ETH Zurich, Wolfgang-Pauli-Str. 16, CH-8093 Zurich, Switzerland (fax: +41-446331105; E-mail: gk-iucr@ethz.ch)

Section editors

W. T. A. Harrison, Department of Chemistry, University of Aberdeen, Aberdeen AB24 3UE, Scotland (e-mail: w.harrison@abdn.ac.uk)

J. Simpson, Department of Chemistry, University of Otago, PO Box 56, Dunedin, New Zealand (e-mail: jsimpson@alkali.otago.ac.nz)

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D. G. Billing, School of Chemistry, University of the Witwatersrand, Private Bag 3, PO Wits, Johannesburg 2050, South Africa (e-mail: dave.billing@wits.ac.za)

O. Blacque, Department of Inorganic Chemistry (ACI), University of Zürich, Winterthurerstrasse 190, 8057 Zürich, Switzerland (e-mail: oblacque@aci.uzh.ch)

M. Bolte, Institut für Inorganische Chemie der Goethe-Universität Frankfurt, Max-von-Laue-Str. 7, D-60438 Frankfurt/M., Germany (e-mail: bolte@chemie.uni-frankfurt.de)

A. Bond, Department of Chemistry, University of Southern Denmark, Campusvej 55, 5230 Odense M, Denmark (e-mail: adb@chem.sdu.dk)

I. Brito, Department of Chemistry, Faculty of Basic Science, University of Antofagasta, PO Box 170, Antofagasta, Chile (e-mail: ivanbritob@yahoo.com)

I. D. Brown, Institute for Materials Research, McMaster University, Hamilton, Ontario, Canada L8S 4M1 (e-mail: idbrown@mcmaster.ca)

R. J. Butcher, Chemistry Department, Howard University, Washington, DC 20059, USA (e-mail: raymond.butcher@nrl.navy.mil)

O. Büyükgüngör, Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, TR-55139 Samsun, Turkey (e-mail: orhanb@omu.edu.tr)

V. V. Chernyshev, Laboratory of Structural Chemistry, General Chemistry Faculty, Chemistry Department, Moscow State University, Moscow 119899, Russia (e-mail: vladimir@struct.chem.msu.ru)

K. Chinnakali, Department of Physics, Anna University, Chennai 600025, India (e-mail: kali@annauniv.edu)

M. Czugler, Department of X-ray Diffraction, Institute of Structural Chemistry, Chemical Research Center, Hungarian Academy of Sciences, Pusztaszeri ut. 59-67, 1025 Budapest, Hungary (e-mail: mcz@chemres.hu)

J.-C. Daran, Laboratoire de Chimie de Coordination, UPR-CNRS 8241, 205 Route de Narbonne, F-31077 Toulouse CEDEX, France (e-mail: daran@lcc-toulouse.fr)

P. Dastidar, Department of Organic Chemistry, Indian Association for the Cultivation of Science (IACS), 2A & 2B Raja S.C. Mullick Road, Jadavpur, India (e-mail: parthod123@rediffmail.com)

L. Eriksson, Division of Structural Chemistry, Stockholm University, S-106 91 Stockholm, Sweden (e-mail: lerik@struc.su.se)

C. Esterhuysen, Department of Chemistry and Polymer Science, University of Stellenbosch, Private Bag X1, Matieland, Stellenbosch, 7602, South Africa (e-mail: ce@sun.ac.za)

J. Fabry, Department of Dielectrics, Institute of Physics, Academy of Science of the Czech Republic, Na Slovance 2, 182 21 Praha 8, Czech Republic (e-mail: fabry@fzu.cz)

L. Farrugia, Department of Chemistry, The University, Glasgow G12 8QQ, Scotland (e-mail: louis@chem.gla.ac.uk)

A. Fischer, Inorganic Chemistry, Royal Institute of Technology, Teknikringen 36, 100 44 Stockholm, Sweden (e-mail: andif@inorg.kth.se)

J. Flippen-Anderson, 3521 Launcelot Way, Annandale, VA 22003-1359, USA (e-mail: flippen@rcsb.rutgers.edu)

U. Flörke, Inorganic and Analytical Chemistry, University of Paderborn, Warburgerstrasse 100, Paderborn, D-33098 Germany (e-mail: ulrich.floerke@upb.de)

M. Gdaniec, Department of Chemistry, Adam Mickiewicz University, Grunwaldzka 6, 60-780 Poznan, Poland (e-mail: magdan@amu.edu.pl)

T. N. Guru Row, Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560012, India (e-mail: ssctng@sscu.iisc.ernet.in)

P. C. Healy, School of Science, Griffith University, Nathan, Brisbane 4111, Australia (e-mail: p.healy@griffith.edu.au)

N.-H. Hu, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, People's Republic of China (e-mail: hunh@ciac.jl.cn)

W. Imhof, Institute of Inorganic and Analytical Chemistry, Friedrich Schiller University, August-Bebel-Str. 2, 07743 Jena, Germany (e-mail: Wolfgang.Imhof@uni-jena.de)

H. Ishida, Department of Chemistry, Faculty of Science, Okayama University, 700-8530 Okayama, Japan (e-mail: ishidah@cc.okayama-u.ac.jp)

J.P. Jasinski, Department of Chemistry, Keene State College, 229 Main Street, Keene, NH 03435-2001, USA (e-mail: jjasinski@keene.edu)

O. Johnson, Kirkside, Station Road, Waterbeach, Cambridgeshire CB25 9HT, England (e-mail: ClFreview@googlemail.com)

B. Kojic-Prodic, Rudjer Boskovic Institute, POB 180, HR-10002 Zagreb, Croatia (e-mail: kojic@rudjer.irb.hr)

H. Kooijman, Shell Global Solutions International BV, Analytical Technology Amsterdam, PO Box 38000, 1030 BN Amsterdam, The Netherlands (e-mail: [Huub.Kooijman@shell.com](mailto:Huib.Kooijman@shell.com))

U. Lee, Department of Chemistry, Pukyong National University, 599-1 Daeyeon 3-dong Nam-ku, Busan 608-737, Republic of Korea (e-mail: uklee@pknu.ac.kr)

A. J. Lough, Department of Chemistry, University of Toronto, 80 St George Street, Toronto, Ontario, Canada M5S 3H6 (e-mail: alough@chem.utoronto.ca)

A. Mar, Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada T6G 2G2 (e-mail: arthur.mar@ualberta.ca)

C. Näther, Institute of Inorganic Chemistry, Universität Kiel, Olshausenstraße 40, Kiel 24098, Germany (e-mail: cnaether@ac.uni-kiel.de)

S. W. Ng, Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia (e-mail: seikweng@um.edu.my)

G.S. Nichol, Department of Chemistry and Biochemistry, The University of Arizona, 1306 E University Boulevard, Tucson, Arizona, USA (e-mail: gsnichol@email.arizona.edu)

M. M. Olmstead, Department of Chemistry, University of California, Davis CA 95616, USA (e-mail: olmstead@chem.ucdavis.edu)

S. Parkin, Department of Chemistry, CP-135, Chemistry-Physics Building, University of Kentucky, Lexington, KY 40506-0055, USA (e-mail: s.parkin@uky.edu)

D. Parrish, Naval Research Laboratory Code 6030, 4555 Overlook Avenue, Washington, DC 20375, USA (e-mail: damon.parrish@nrl.navy.mil)

M. Parvez, Department of Chemistry, University of Calgary, 2500 University Drive N.W., Calgary, Alberta, Canada (e-mail: parvez@ucalgary.ca)

V.R. Pedireddi, School of Basic Sciences, Indian Institute of Technology, Bhubaneswar 751 013, India (e-mail: vr.pedireddi@iitbbs.ac.in, vr.pedireddi@gmail.com)

C. Rizzoli, Dipartimento di Chimica Generale ed Inorganica, Chimica Analitica, Chimica Fisica, Università degli Studi di Parma, Viale delle Scienze 17/A, I-43100 Parma, Italy (e-mail: corrado.rizzoli@unipr.it)

G. M. Rosair, William Perkin Building, Department of Chemistry, Heriot-Watt University, Edinburgh EH14 4AS, Scotland (e-mail: g.m.rosair@hw.ac.uk)

V. Rybakov, Laboratory of Structural Chemistry, General Chemistry Faculty, Chemistry Department, Moscow State University, Moscow 119992, Russia (e-mail: rybakov20021@yandex.ru)

H. W. Schmalle, Wiesliacher 11, CH-8053 Zurich, Switzerland (e-mail: hws@bluewin.ch)

G. Smith, Faculty of Science and Technology, Queensland University of Technology, GPO Box 2434, Brisbane, 40001, Australia (e-mail: g.smith@qut.edu.au)

H. Stoeckli-Evans, Institute of Physics, Université de Neuchâtel, Avenue de Bellevaux 51, CP2, CH-2007 Neuchâtel, Switzerland (e-mail: helen.stoeckli-evans@unine.ch)

E. R. T. Tiekink, Department of Chemistry, University of Malaya, Kuala Lumpur 50603, Malaysia (e-mail: edward.tiekink@gmail.com)

L. Van Meervelt, Biomolecular Architecture, Departement Chemie, Katholieke Universiteit Leuven, Celestijnenlaan 200F - box 2404, B-3001 Leuven (Heverlee), Belgium (e-mail: Luc.VanMeervelt@chem.kuleuven.be)

D. G. Watson, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, England (e-mail: watson@ccdc.cam.ac.uk)

W.-T. Wong, Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong, People's Republic of China (e-mail: wt Wong@hkucc.hku.hk)

D.-J. Xu, Chemistry Department, Zhejiang University (Yuquan Campus), 38 Zheda Road, Hangzhou, People's Republic of China (e-mail: xudj@mail.hz.zj.cn)

A. I. Yanovsky, Institute of Organoelement Compounds, 28 Vavilov St., Moscow 117813, Russia (e-mail: yan@xray.ineos.ac.ru)

M. Zeller, Department of Chemistry, Youngstown State University, Youngstown, Ohio 44555-3663, USA (e-mail: mzeller@ysu.edu)

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The Executive Secretary of the IUCr (Mr M. H. Dacombe) may be contacted at:

International Union of Crystallography
2 Abbey Square CHESTER CH1 2HU
England

Telephone: *International dialing prefix* + 44 (1244) 345431
Fax: *International dialing prefix* + 44 (1244) 344843
E-mail: execsec@iucr.org

(20*S*)-Dammar-24-ene-3 β ,20-diol mono-
hydrate from the bark of *Aglaia exima*
(Meliaceae)Agus Safariari,^a Asep Supriadin,^a Unang Supratman,^a
Khalijah Awang^b and Seik Weng Ng^{b,c,*}^aDepartment of Chemistry, Faculty of Mathematics and Natural Sciences, Padjadjaran University, Jatinangor 45363, West Java, Indonesia, ^bDepartment of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, and ^cChemistry Department, Faculty of Science, King Abdulaziz University, PO Box 80203 Jeddah, Saudi Arabia
Correspondence e-mail: seikweng@um.edu.my

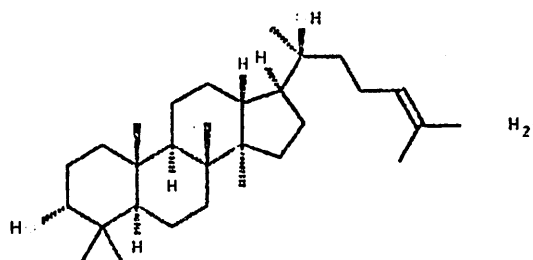
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; disorder in main residue; R factor = 0.077; wR factor = 0.266; data-to-parameter ratio = 44.4.

In the title compound [systematic name: (1*R*,2*R*,5*R*,7*R*,10*R*,11*R*,14*S*,15*R*)-14-[(2*S*)-2-hydroxy-6-methylhept-5-en-2-yl]-2,6,6,10,11-pentamethyltetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadecan-5-ol monohydrate], $\text{C}_{30}\text{H}_{52}\text{O}_2 \cdot \text{H}_2\text{O}$, the three fused cyclohexane rings adopt chair conformations and the hydroxy substituent of one of these occupies an axial position. The fused cyclopentane ring adopts an envelope conformation (with the flap atom being the C atom bearing the methyl group) and the 3-methylbut-2-enyl portion of its substituent is disordered over three sets of sites in a 0.413 (7):0.250 (7):0.337 (7) ratio. The O atoms of both water molecules occupy special positions of 2 site symmetry. In the crystal, $\text{O}_s-\text{H}\cdots\text{O}_w$ and $\text{O}_w-\text{H}\cdots\text{O}_s$ (s = steroid and w = water) hydrogen bonds link hydroxy groups and water molecules, forming a three-dimensional network. The crystal studied was found to be a non-merohedral twin with a 0.518 (1):0.482 (1) component ratio.

Related literature

For the isolation of 20*S*-dammar-24-ene-3 β ,20-diol from other plants, see: Anjaneyulu *et al.* (1985); Bianchini *et al.* (1988); Huang *et al.* (2010); Leonti *et al.* (2004); Pakhathirathien *et al.* (2005); Ukiya *et al.* (2010).



Experimental

Crystal data

$\text{C}_{30}\text{H}_{52}\text{O}_2 \cdot \text{H}_2\text{O}$
 $M_r = 462.73$
Tetragonal, $P4_1$
 $a = 19.9229$ (1) Å
 $c = 7.3302$ (1) Å
 $V = 2909.52$ (4) Å³

$Z = 4$
Cu $K\alpha$ radiation
 $\mu = 0.50$ mm⁻¹
 $T = 100$ K
0.30 × 0.10 × 0.05 mm

Data collection

Agilent SuperNova Dual
diffractometer with an Atlas
detector
Absorption correction: multi-scan
(*CrysAlis PRO*; Agilent, 2012)
 $T_{\min} = 0.864$, $T_{\max} = 0.975$

11893 measured reflections
15153 independent reflections
14049 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.068$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.077$
 $wR(F^2) = 0.266$
 $S = 1.15$
15153 reflections
341 parameters
45 restraints

H-atom parameters constrained
 $\Delta\rho_{\max} = 1.15$ e Å⁻³
 $\Delta\rho_{\min} = -0.37$ e Å⁻³
Absolute structure: Flack (1983),
2575 Friedel pairs
Flack parameter: 0.1 (3)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1}\cdots\text{O1}^w$	0.84	1.96	2.745 (2)	154
$\text{O2}-\text{H2}\cdots\text{O2}^w$	0.84	2.03	2.809 (2)	154
$\text{O1}^w-\text{H1}^w\cdots\text{O2}^i$	0.84	1.88	2.712 (2)	171
$\text{O2}^w-\text{H2}^w\cdots\text{O1}^{ii}$	0.84	1.95	2.786 (2)	171

Symmetry codes: (i) $-y + 1, x + 1, z - \frac{1}{2}$; (ii) $-y + 1, x, z - \frac{1}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6931).