Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

The space group of tris(dimethyldithiophosphato)-osmium(III)

Seik Weng Ng

Institute of Postgraduate Studies, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: h1nswen@umcsd.um.edu.my

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(O–C) = 0.005 Å
R factor = 0.017
wR factor = 0.043
Data-to-parameter ratio = 17.9

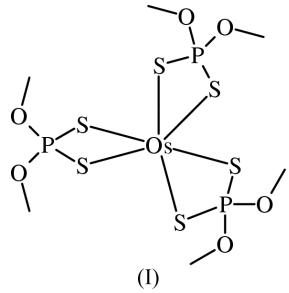
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The space group of tris(dimethyldithiophosphato)-osmium(III), $[Os(C_2H_6O_2PS_2)_3]$, originally reported as *Cc*, is revised to *C*2/*c*.

Received 13 November 2001
Accepted 5 December 2001
Online 14 December 2001

Comment

The crystal structure of tris(dimethyldithiophosphato)-osmium(III), (I), was originally described in the *Cc* space group (Jain *et al.*, 2001). A check for additional symmetry using the program *PLATON* (Spek, 1990) indicated that the correct space group for this structure is *C*2/*c*. When the structure is refined in *C*2/*c*, the osmium atom and one of the P atoms, P2, lie on a twofold axis.



(I)

Experimental

Crystal data

$[Os(C_2H_6O_2PS_2)_3]$
M_r = 661.67
Monoclinic, *C*2/*c*
a = 14.138 (1) Å
b = 11.228 (4) Å
c = 12.970 (1) Å
β = 96.99 (1)°
V = 2043.6 (8) Å^3
Z = 4
D_x = 2.151 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 11.4–14.2°
μ = 7.11 mm^{-1}
T = 298 (2) K
Plate, violet
0.35 × 0.20 × 0.10 mm

Data collection

Nonius MACH-3 four-circle diffractometer
ω scans
Absorption correction: empirical *via* ψ scan (North *et al.*, 1968)
T_{min} = 0.119, T_{max} = 0.180
3741 measured reflections
1805 independent reflections
1691 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 25.0°
$h = -16 \rightarrow 10$
$k = -13 \rightarrow 10$
$l = -15 \rightarrow 15$
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.043
S = 1.09
1805 reflections
101 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0282P)^2]$ where P $F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.80 e Å^{-3}

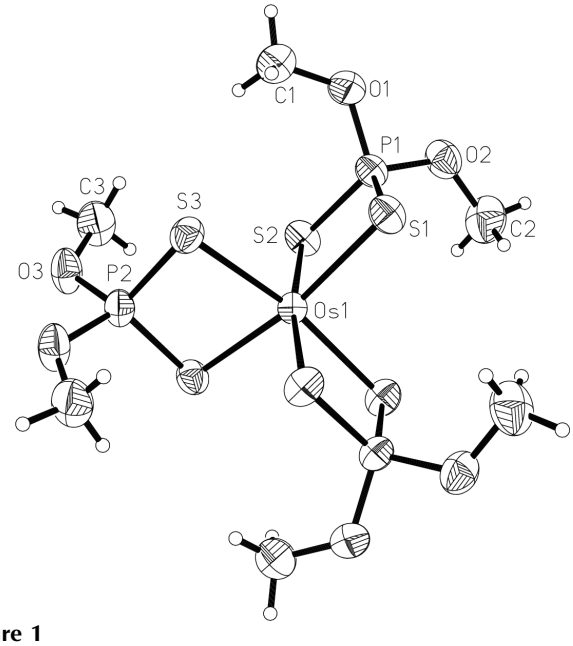


Figure 1
*ORTEP*II (Johnson, 1976) plot of the title compound with ellipsoids at the 50% probability level.

Data collection: *ARGUS-MACH*3 (Nonius, 1997); cell refinement: *ARGUS-MACH*3; data reduction: *XCAD*4 (Harms, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

The author thanks Professor Goutam K. Lahiri of the Indidan Institute of Technology, Mumbai, for the diffraction data, and the University of Malaya (F0758/2001A) for supporting this work.

References

Harms, K. (1997). *XCAD*4. University of Marburg, Germany.
Jain, P. U., Paul, H., Munshi, P., Walawalkar, M. G. & Lahiri, G. K. (2001). *Polyhedron*, **20**, 245–252.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Nonius (1997). *ARGUS-MACH*3. Nonius BV, Delft, The Netherlands.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (1990). *Acta Cryst.* A**46**, C-34.