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

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Key indicators

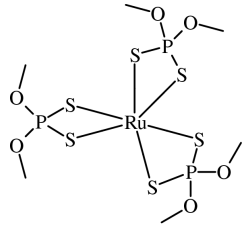
Single-crystal X-ray study
T = 298 K
Mean σ(O–C) = 0.004 Å
R factor = 0.023
wR factor = 0.065
Data-to-parameter ratio = 17.8

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)ruthenium(III), $[Ru(C_2H6O_2PS_2)_3]$, originally reported as *Cc*, is revised to *C*2/*c*.

Comment

The crystal structure of tris(dimethyldithiophosphato)-ruthenium(III), (I), was originally described in the *Cc* space group (Jain *et al.*, 2000). 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 ruthenium atom and one of the P atoms, P2, lie on a twofold axis.



(I)

Experimental

Crystal data

$[Ru(C_2H_6O_2PS_2)_3]$
M_r = 572.54
Monoclinic, *C*2/*c*
a = 14.1212 (6) Å
b = 11.1919 (8) Å
c = 12.9788 (7) Å
β = 97.121 (4)°
V = 2035.4 (2) Å^3
Z = 4
D_x = 1.868 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10.3–17.1°
μ = 1.64 mm^{-1}
T = 298 (2) K
Red, block
0.30 × 0.25 × 0.20 mm

Data collection

Nonius MACH3 four-circle diffractometer
ω scans
Absorption correction: empirical *via* ψ scan (North *et al.*, 1968)
T_{min} = 0.474, T_{max} = 0.554
3583 measured reflections
1796 independent reflections
1700 reflections with $I > 2\sigma(I)$
R_{int} = 0.001
θ_{max} = 25.0°
$h = -16 \rightarrow 5$
$k = -13 \rightarrow 1$
$l = -15 \rightarrow 15$
3 standard reflections
frequency: 60 min
intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.065
S = 1.17
1796 reflections
101 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 2.6319P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.72 e Å^{-3}

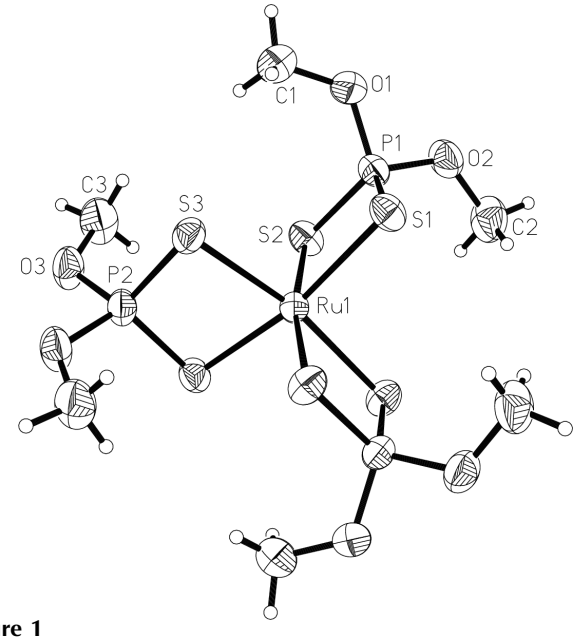


Figure 1
*ORTEP*II (Johnson, 1976) plot of the title compound with ellipsoids at the 50% probability level.

Data collection: *ARGUS-MACH*3 (Nonius, 1997); cell refinement: *ARGUS-MACH*3; data reduction: XCAD4 (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.

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