Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tris(*O,O′*-dimethyldithiophosphato)chromium(III)

Tetsuzo Ito

Department of Applied Chemistry, Kanagawa Institute of Technology, Atsugi, Kanagawa 243-0292, Japan

Correspondence e-mail: ito@chem.kanagawa-it.ac.jp

Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(O–C) = 0.006 Å
R factor = 0.037
wR factor = 0.021
Data-to-parameter ratio = 15.8

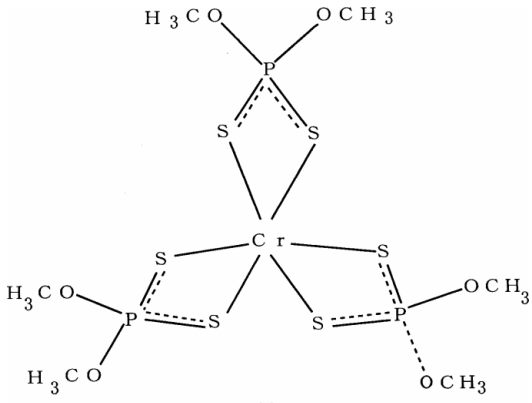
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 17 July 2002
Accepted 22 July 2002
Online 25 July 2002

The title complex molecule, $[Cr(C_2H_6O_2PS_2)_3]$, has a twofold rotation axis passing through the Cr atom and a P atom. The Cr atom is coordinated by six S atoms in a distorted octahedral arrangement. The Cr—S bond distances are in the range 2.420 (2)–2.441 (5) Å, with an average of 2.429 (7) Å.

Comment

As part of the study of metal dialkyl dithiophosphates (Ito & Otake, 1996), the crystal and molecular structure of the title compound, (I), have been determined. As shown in Fig. 1, (I) has approximate threefold rotation symmetry around the Cr atom, as well as a crystallographic twofold rotation axis passing through atoms Cr and P1. The structures of the two independent dimethyldithiophophate ligands are very similar, and are also similar to that in bis(*O,O′*-dimethyldithiophosphato)cadmium(II) (Ito & Otake, 1996).



(I)

Experimental

Diphosphorus pentasulfide (11.5 g) was slowly added to methanol (70 ml) at 323 K. After the generation of hydrogen sulfide had ceased, hexaaquachromium(III) chloride (7.9 g) was added to precipitate a powder of (I). Recrystallization from a chloroform solution at 278 K gave dark-violet plate-shaped crystals of (I).

Crystal data

$[Cr(C_2H_6O_2PS_2)_3]$
M_r = 523.53
Monoclinic, *C*2/*c*
a = 14.28 (2) Å
b = 11.17 (2) Å
c = 12.98 (1) Å
β = 97.67 (9)°
V = 2052 (5) Å^3
Z = 4
D_x = 1.695 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 25 reflections
θ = 15.3–16.5°
μ = 1.42 mm^{-1}
T = 296 K
Plate, dark violet
0.70 × 0.50 × 0.20 mm

Data collection

Rigaku AFC-5*S* diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.431, T_{max} = 0.753
2591 measured reflections
2372 independent reflections
1597 reflections with $I > 3\sigma(I)$
R_{int} = 0.016
θ_{max} = 27.5°
$h = 0 \rightarrow 18$
$k = 0 \rightarrow 14$
$l = -16 \rightarrow 16$
3 standard reflections
every 150 reflections
intensity decay: 0.5%

Refinement

Refinement on F
R = 0.037
wR = 0.021
S = 2.20
1597 reflections
101 parameters
H-atom parameters constrained
$w = 1/\sigma^2(F_o)$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cr—S1	2.420 (2)	P1—O1	1.574 (3)
Cr—S2	2.425 (3)	P2—O2	1.568 (3)
Cr—S3	2.441 (5)	P2—O3	1.569 (3)
S1—P1	1.986 (2)	O1—C1	1.435 (5)
S2—P2	1.985 (2)	O2—C2	1.446 (4)
S3—P2	1.984 (3)	O3—C3	1.453 (4)
S1—Cr—S2	90.1 (1)	S2—Cr—S3	81.7 (1)
S1—Cr—S3	168.3 (1)	S2—Cr—S2^{i}	169.9 (1)
S1—Cr—S1^{i}	81.9 (1)	S2—Cr—S3^{i}	91.6 (1)
S1—Cr—S2^{i}	97.6 (1)	S3—Cr—S3^{i}	97.8 (1)
S1—Cr—S3^{i}	90.8 (1)		

Symmetry code: (i) $1-x, y, \frac{1}{2}-z$.

H atoms were placed in geometrically calculated positions and allowed to ride on their parent atoms, with U_{iso} parameters equal to 1.2 times the U_{eq} parameters of their parent atoms.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *CrystalStructure* (Molecular Structure Corporation and Rigaku, 2001); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *CrystalStructure*; molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *CrystalStructure*.

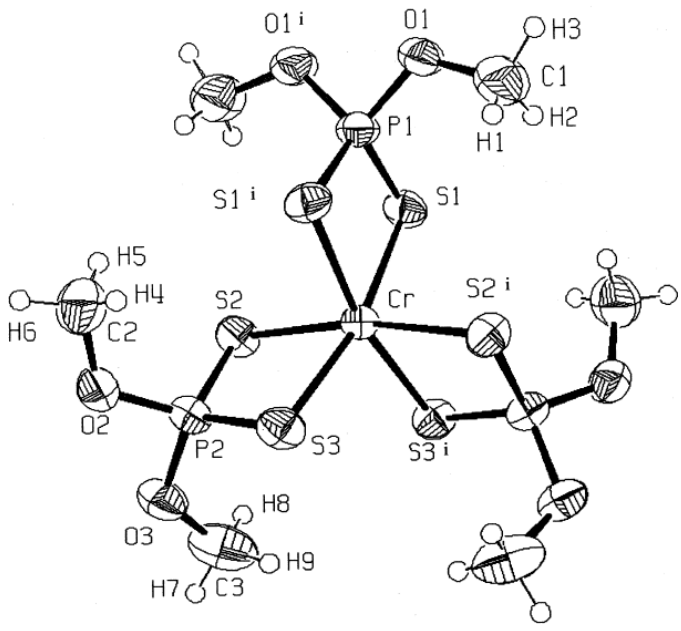


Figure 1
*ORTEP*III (Burnett & Johnson, 1996) drawing of the title chromium dimethyldithiophosphate complex. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) $1-x, y, \frac{1}{2}-z$.]

References

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Burnett, M. N. & Johnson, C. K. (1996). *ORTEP*III. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Ito, T. & Otake, M. (1996). *Acta Cryst.* C**52**, 3024–3025.
Molecular Structure Corporation (1988). *MSC/AFC Diffractometer Control Software*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Molecular Structure Corporation & Rigaku (2001). *CrystalStructure*. Version 2.00. MSC, 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA, and Rigaku Corporation, Akishima, Tokyo 196-8666, Japan.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.