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Bis[*O*-methyl (4-ethoxyphenyl)dithiophosphonato-κ^2S,S']nickel(II)

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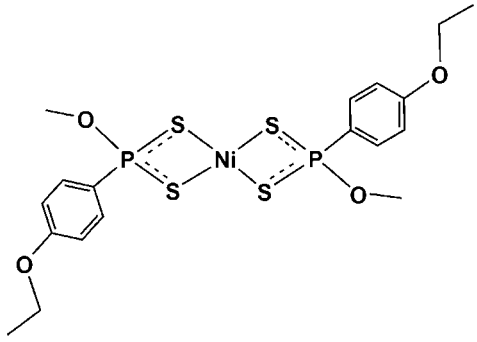
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.023; wR factor = 0.062; data-to-parameter ratio = 21.1.

In the title compound, $[Ni(C_9H_{12}O_2PS_2)_2]$, the Ni^{II} atom resides on an inversion center and is coordinated by four S atoms [Ni—S = 2.2328 (4) and 2.2455 (3) Å] in a distorted square-planar geometry [S—Ni—S = 88.443 (13) and 91.557 (13)°]. In the crystal, molecules related by translation in [110] are linked into chains *via* weak C—H···O interactions. The crystal packing exhibits short intermolecular S···S contacts of 3.3366 (5) Å.

Related literature

For information on dithiophosphonate compounds, see: Van Zyl & Fackler (2000); Van Zyl (2010); Van Zyl & Woollins (2012). For related structures of nickel(II) dithiophosphonate complexes, see: Hartung (1967); Liu *et al.* (2004); Gray *et al.* (2004); Aragoni *et al.* (2007); Arca *et al.* (1997); Özcan *et al.* (2002).



Experimental

Crystal data

$[Ni(C_9H_{12}O_2PS_2)_2]$ M_r = 553.26
Monoclinic, $P2_1/c$
a = 13.5866 (5) Å
b = 6.4212 (2) Å
c = 14.1047 (5) Å
β = 109.389 (2)°
V = 1160.74 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.36 mm^{-1}
T = 173 K
0.43 × 0.31 × 0.24 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.593, T_{max} = 0.737
19824 measured reflections
2850 independent reflections
2609 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.062
S = 1.07
2850 reflections
135 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O1^{i}	0.95	2.57	3.5123 (18)	171

Symmetry code: (i) $-x+1, -y+1, -z+2$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT-Plus* (Bruker, 2008); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5358).

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