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Key indicators

Single-crystal X-ray study
 $T = 150$ K
Mean $\sigma(\text{O}-\text{N}) = 0.002$ Å
 R factor = 0.021
 wR factor = 0.057
Data-to-parameter ratio = 21.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Hexakis(dimethyl sulfoxide)nickel(II) dinitrate
dimethyl sulfoxide disolvate

The title compound, $[\text{Ni}(\text{C}_2\text{H}_6\text{OS})_6](\text{NO}_3)_2 \cdot 2\text{C}_2\text{H}_6\text{OS}$, comprises centrosymmetric $[\text{Ni}(\text{dmsO})_6]^{2+}$ cations, nitrate anions and non-coordinated dimethyl sulfoxide solvent molecules. The octahedral geometry of the cation is very regular, with Ni—O interatomic distances and O—Ni—O interatomic angles falling within narrow ranges 2.0485 (9)–2.0665 (9) Å and 89.12 (4)–93.27 (4)°, respectively. Two weak C—H···O hydrogen-bonding contacts link cations and anions to form a chain which lies along the [111] direction.

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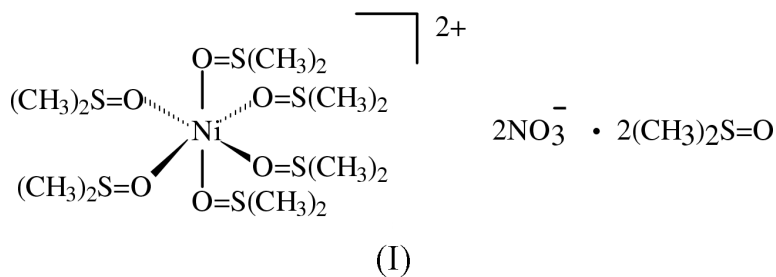
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Comment

The title structure, (I), comprises crystallographically centrosymmetric $[\text{Ni}(\text{dmsO})_6]^{2+}$ cations, nitrate anions and non-coordinated dimethyl sulfoxide molecules. The octahedral geometry of the cation (Fig. 1) is very regular, with Ni—O interatomic distances and O—Ni—O angles falling within narrow ranges.

Although the long-range structure is dominated by electrostatic and dipole–dipole interactions, two weak C—H···O hydrogen-bonding contacts [C22—H22C···O11: C—H 0.96, H···O 2.60, C···O 3.403 (2) Å and C—H···O 142°; C32—H32B···O12: C—H 0.96, H···O 2.49, C···O 3.439 (2) Å and C—H···O 171°] link cations and anions to form a chain which lies along the [111] direction (Fig. 2). The non-coordinated dimethyl sulfoxide molecules lie in the space between the centrosymmetrically related nitrate anions.



A search of the Cambridge Structural Database (Allen & Kennard, 1993) revealed 14 reports of compounds containing transition metal hexakis(dimethyl sulfoxide) cations, of which two described the structure of the $[\text{Ni}(\text{dmsO})_6]^{2+}$ cation in $[\text{Ni}(\text{dmsO})_6][\text{I}_4]$ (Reibenspies & Kim, 1996; Long *et al.*, 1999): the reports differ in their interpretation of the nature of the iodine-containing moiety. The $[\text{Ni}(\text{dmsO})_6]^{2+}$ cation in these structures is similar to, but more symmetrical than, that in the title compound. The nickel(II) centre is located on a $\bar{3}$ site, giving a single Ni—O interatomic distance of 2.077 (2) Å and a single O—Ni—O valence angle of 87.63 (7)°.

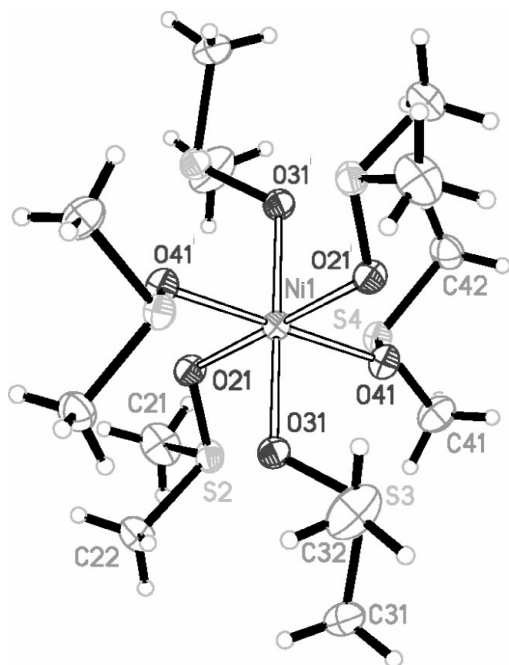


Figure 1

A view of the title cation which occupies a crystallographic inversion centre, showing the atom-numbering scheme. The nitrate anions and uncoordinated solvent molecules have been omitted for clarity. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) $2 - x, -y, -z$.]

Experimental

Vapour-phase diffusion of diethyl ether into the mixture formed by combination of a dimethyl sulfoxide solution containing both nickel nitrate hexahydrate (0.146 g, 0.5 mmol) and pyrazine (0.040 g, 0.5 mmol) with a methanol solution of dipicolinic acid gave, after a period of 14 days, large crystals of the title compound.

Crystal data

$[\text{Ni}(\text{C}_2\text{H}_6\text{OS})_6](\text{NO}_3)_2 \cdot 2\text{C}_2\text{H}_6\text{OS}$	$Z = 1$
$M_r = 807.75$	$D_x = 1.421 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 9.6907(9) \text{ \AA}$	Cell parameters from 3076 reflections
$b = 10.3119(10) \text{ \AA}$	$\theta = 2.9\text{--}28.4^\circ$
$c = 11.2549(11) \text{ \AA}$	$\mu = 1.01 \text{ mm}^{-1}$
$\alpha = 63.954(1)^\circ$	$T = 150(2) \text{ K}$
$\beta = 70.282(1)^\circ$	Irregular block, pale green
$\gamma = 87.414(2)^\circ$	$0.46 \times 0.38 \times 0.26 \text{ mm}$
$V = 944.1(3) \text{ \AA}^3$	

Data collection

Bruker SMART1000 CCD area-detector diffractometer	4251 independent reflections
ω scans	3931 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (Bruker, 2001)	$R_{\text{int}} = 0.010$
$T_{\text{min}} = 0.703$, $T_{\text{max}} = 0.769$	$\theta_{\text{max}} = 28.7^\circ$
8316 measured reflections	$h = -12 \rightarrow 12$
	$k = -13 \rightarrow 13$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.030P)^2 + 0.318P]$
$R[F^2 > 2\sigma(F^2)] = 0.021$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.057$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.46 \text{ e \AA}^{-3}$
4251 reflections	$\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$
195 parameters	
H atoms: see below	

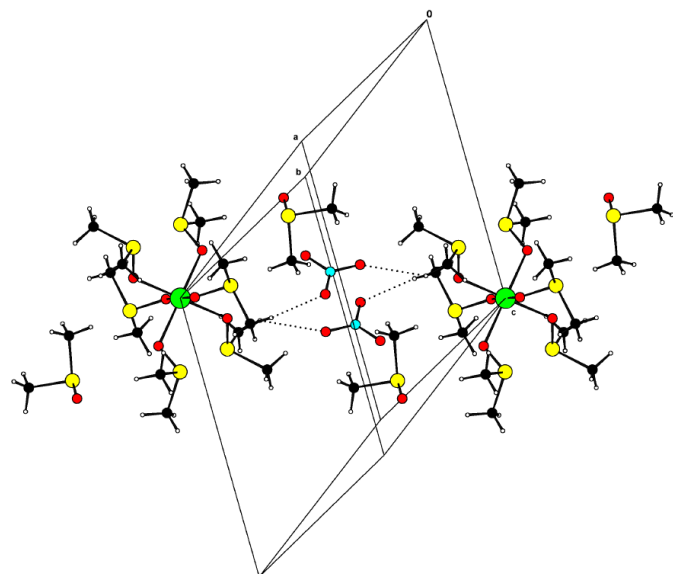


Figure 2

A view of the structure showing the weak C—H...O hydrogen-bonding contacts which link cations and anions into a chain running in the [111] direction.

H atoms were located from circular difference Fourier syntheses and refined as part of rigid groups allowed to rotate about the local C—S vectors but not to tip or distort. The C—H distance was constrained to 0.96 \AA and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* and *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CAMERON* (Watkin *et al.*, 1996) and *SHELXTL*; software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2001).

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