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Acta Cryst. (1996). **C52**, 2698–2701

**A Dinuclear Nickel(II) Compound:
 μ -{N,N,N',N'-Tetrakis[2-(3,5-dimethyl-1-pyrazolyl)ethyl]-1,2-ethylenediamine}-bis[aqua(nitrato-O,O')nickel(II)] Dinitrate Dimethanol Solvate**

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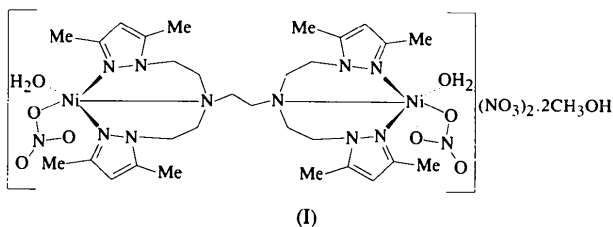
Abstract

The title compound, [Ni₂(NO₃)₂(C₃₀H₄₈N₁₀)(H₂O)₂](NO₃)₂·2CH₃OH, contains a doubly charged cation which lies across an inversion center. The hexadentate ligand *N,N,N',N'*-tetrakis[2-(3,5-dimethyl-1-pyrazolyl)ethyl]-1,2-ethylenediamine (tped) holds two Ni^{II} ions at a distance of 6.3721 (13) Å. A distorted octahedron around each Ni^{II} ion is defined by two pyrazole N atoms of tped at distances of 2.023 (4) and 2.048 (4) Å, one amine N atom of tped at a distance of 2.161 (4) Å, two O atoms of a chelating nitrate anion at distances of 2.144 (3) and 2.205 (4) Å, and a water O atom at a distance of 2.032 (4) Å. A one-dimensional hydrogen-bonding network running along the *a* axis connects the methanol molecule of crystallization to the nitrate and aqua ligands of different cations, and an aqua

ligand to the non-coordinated nitrate ion. The structure is essentially isomorphous with the previously reported Cu^{II} analog [Driessen, Haanstra & Reedijk (1992). *Acta Cryst.* **C48**, 1585–1587], the main differences being that NO₃ is involved in bidentate coordination to Ni^{II} and in a bifurcated hydrogen bond with methanol, whereas in the Cu^{II} complex, it is monodentate and only one of its O atoms hydrogen bonds to methanol.

Comment

The pyrazole group is employed as a substitute for imidazole in transition metal compounds used to model the active sites in metalloproteins (Kitajima & Morooka, 1994). Several pyrazole derivatives have been designed and synthesized for this purpose (Driessen, 1982; Bol, Driessen & Reedijk, 1995). The current X-ray study of the title compound, (I), was undertaken in order to establish the detailed coordination structure of the Ni^{II} analog of the previously reported Cu^{II} complex (Driessen, Haanstra & Reedijk, 1992), since it was thought possible that a nitrate ligand might bridge the two Ni^{II} centers.



The title compound (Figs. 1 and 2) contains a doubly charged cation residing on an inversion centre, with the asymmetric unit comprising half a cation, an NO₃⁻ anion and a methanol molecule. The Ni^{II} ion is in a distorted octahedral environment formed by two pyrazole N atoms and the amine N atom of tped, an O atom of a water molecule and two O atoms of one of the nitrate anions. The Ni—N and Ni—O bond lengths are comparable to values found in related compounds (Driessen, Haanstra & Reedijk, 1992; Claramunt, Domiano, Elguero, & Lavandera, 1989; Kleywegt, Wiesmeijer, van Driel, Driessen, Reedijk & Noordik, 1985).

The analogous hexadentate N-donor ligand *N,N,N',N'*-tetrakis(1-pyrazolylmethyl)-1,2-ethylenediamine forms coordination compounds with transition metals in which the N(pyrazole)–metal ion–N(amine) bond angles are significantly smaller than 90° due to the three-bond bite of this ligand (Hulsbergen, Driessen, Reedijk & Verschoor, 1984). With tped regular octahedral, N(pyrazole)-to-N(amine) angles can be expected since four-bond bites are involved (Driessen, Haanstra & Reedijk, 1992) and, indeed, these angles range from 90.33 (15) to 96.42 (16)°. The bidentate nitrate ion,

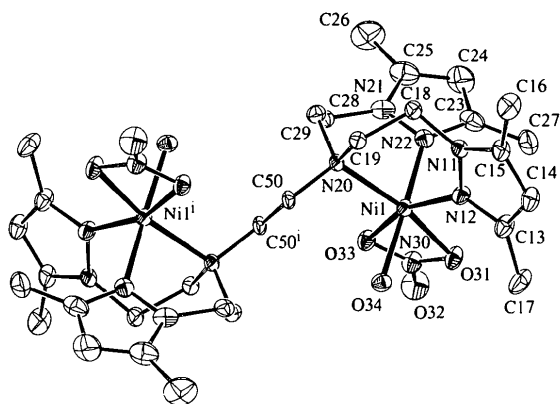


Fig. 1. Displacement ellipsoid plot (50% probability) of the title compound. H atoms, non-coordinating NO_3 ions and methanol molecules of crystallization have been omitted for clarity. [Symmetry code: (i) $1-x, 1-y, 1-z$.]

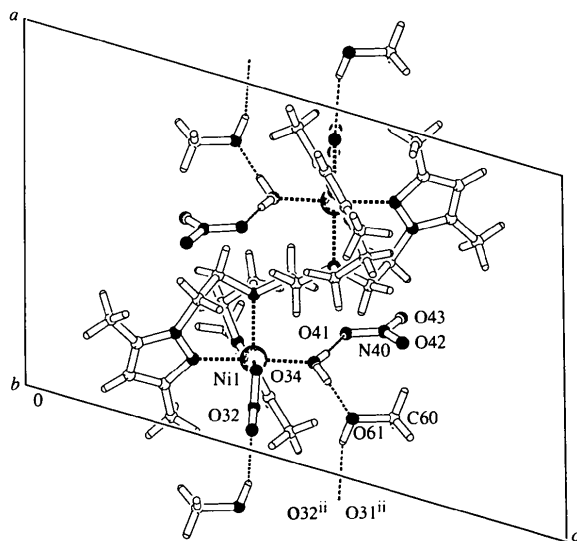


Fig. 2. Projection of part of the structure down the b axis illustrating the infinite hydrogen-bonded chain running along the a axis. The hydrogen bond coming from O61 bifurcates to O32ⁱⁱ and O31ⁱⁱ of the coordinating NO_3 ion [symmetry code: (ii) $-x, 1-y, 1-z$].

however, forms an O—Ni—O angle of $59.46(11)^\circ$, thereby causing the Ni^{II} coordination geometry to deviate markedly from regular octahedral. The coordination around Cu^{II} in its tped compound (Driessen, Haanstra & Reedijk, 1992) is square pyramidal, with less regular metal–ligand bond distances than in the Ni^{II} compound, which can be ascribed to the Jahn–Teller effect and the fluxional behaviour of coordinated Cu^{II} (Hathaway, 1984). The second nitrate ligand is at a distance of $2.629(3)$ Å in the Cu^{II} complex as opposed to 2.205 Å in the Ni^{II} analog.

The tped ligand sets the two Ni ions at a distance of $6.3721(13)$ Å, so that the two NiN_3O_3 chromophores

are well separated. The crystal structure features a one-dimensional hydrogen-bonding network running along the a axis (Fig. 2 and Table 3). The water O34 atom takes part in this network by donating to the methanol O61 atom and to the O41 atom of the non-coordinating nitrate anion. In addition, the methanol H61 atom forms a bifurcated hydrogen bond to O31ⁱⁱ and O32ⁱⁱ of the coordinating nitrate anion [symmetry code: (ii) $-x, 1-y, 1-z$]. The present structure is essentially isomorphous with the Cu^{II} analog. The main differences are that in the latter the copper-bonded NO_3 group is rotated in such a way that it is monodentate and that it is involved only in a two-centre hydrogen bond from methanol. The pyrazole rings are planar, with deviations from the least-squares planes of <0.001 Å and no stacking interactions between the rings. The crystal packing is therefore determined by van der Waals contacts and hydrogen bonding.

Experimental

The tped ligand was synthesized according to the method of Haanstra, Driessen, de Graaff, Sebregts, Suriano, Reedijk, Turpeinen, Hämäläinen & Wood (1991). Pale-blue crystals of the title compound were prepared by addition of 0.091 mmol of solid tped to a methanol solution of 0.182 mmol of $\text{Ni}(\text{H}_2\text{O})_6(\text{NO}_3)_2$ and 27 mmol of trimethylorthoformate, followed by slow diffusion of diethyl ether into the mixture.

Crystal data

$[\text{Ni}_2(\text{NO}_3)_2(\text{C}_{30}\text{H}_{48}\text{N}_{10})\cdot(\text{H}_2\text{O})_2](\text{NO}_3)_2\cdot 2\text{CH}_4\text{O}$
 $M_r = 1014.30$
 Monoclinic
 $P2_1/c$
 $a = 12.2450(12)$ Å
 $b = 10.3134(12)$ Å
 $c = 18.770(3)$ Å
 $\beta = 106.530(12)^\circ$
 $V = 2272.5(5)$ Å³
 $Z = 2$
 $D_x = 1.482$ Mg m⁻³
 D_m not measured

Mo $K\alpha$ radiation
 $\lambda = 0.71073$ Å
 Cell parameters from 22 reflections
 $\theta = 11.7\text{--}13.7^\circ$
 $\mu = 0.91$ mm⁻¹
 $T = 150$ K
 Block
 $0.50 \times 0.25 \times 0.25$ mm
 Blue

Data collection

CAD-4T rotating-anode diffractometer
 ω scans
 Absorption correction: none
 9579 measured reflections
 4917 independent reflections
 3197 observed reflections
 $[I > 2\sigma(I)]$

$R_{\text{int}} = 0.1098$
 $\theta_{\text{max}} = 27.48^\circ$
 $h = -15 \rightarrow 15$
 $k = -12 \rightarrow 0$
 $l = -24 \rightarrow 23$
 3 standard reflections
 frequency: 60 min
 intensity decay: none

Refinement

Refinement on F^2
 $R(F) = 0.0637$
 $wR(F^2) = 0.1647$

$\Delta\rho_{\text{max}} = 0.98$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.65$ e Å⁻³
 Extinction correction: none

$S = 1.02$
 4917 reflections
 297 parameters
 $w = 1/[\sigma^2(F_o^2) + (0.066P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$

Atomic scattering factors
 from *International Tables*
 for *Crystallography* (1992),
 Vol. C, Tables 4.2.6.8 and
 6.1.1.4)

N12—N11—C15 110.8 (4) N20—C29—C28 115.1 (4)
 N12—N11—C18 119.8 (3) N20—C50—C50¹ 113.3 (3)
 C15—N11—C18 128.8 (4)

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

Table 3. *Hydrogen-bonding geometry* (Å, °)

D—H...A	D—H	H...A	D...A	D—H...A
O61—H61...O31 ⁱⁱ	0.84 (3)	2.18 (2)	2.941 (5)	151 (5)
O61—H61...O32 ⁱⁱ	0.84 (3)	2.54 (5)	3.247 (6)	143 (6)
O34—H341...O41	0.91 (2)	1.78 (2)	2.683 (5)	176 (2)
O34—H342...O61	0.93 (2)	1.76 (2)	2.690 (6)	180 (1)

Symmetry code: (ii) $-x, 1 - y, 1 - z$.

The unit cell was checked for higher metric symmetry with the program *LEPAGE* (Le Page, 1987; Spek, 1988). H atoms were included at calculated positions, riding on their carrier atoms, except for those involved in hydrogen bonding, whose positions were initially obtained from a difference Fourier map and subsequently refined. The two H atoms bonded to the water O34 atom were refined with individual isotropic displacement parameters. For all other H atoms, the isotropic displacement parameters were derived from the U_{eq} values of their carrier atoms. The structure was shown not to contain voids accessible to solvent molecules using the *SOLV* option in *PLATON* (Spek, 1990).

Data collection: locally modified *CAD-4 Software* (Enraf-Nonius, 1989). Cell refinement: *SET4* (de Boer & Duisenberg, 1984). Data reduction: *HELENA* (Spek, 1993). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *PLUTON* (Spek, 1996) and *PLATON*. Software used to prepare material for publication: *PLATON*.

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Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å²)

$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* a_i a_j.$$

	x	y	z	U_{eq}
Ni1	0.25317 (4)	0.38403 (5)	0.42383 (3)	0.0164 (2)
O31	0.0834 (3)	0.4579 (3)	0.4219 (2)	0.0248 (12)
O32	0.0547 (3)	0.6664 (3)	0.4199 (2)	0.0406 (14)
O33	0.2239 (2)	0.5883 (3)	0.4292 (2)	0.0219 (12)
O34	0.2923 (3)	0.3897 (3)	0.5365 (2)	0.0218 (10)
N11	0.2878 (3)	0.1059 (3)	0.3939 (2)	0.0189 (12)
N12	0.2282 (3)	0.1902 (4)	0.4242 (2)	0.0210 (12)
N20	0.4302 (3)	0.3739 (3)	0.4256 (2)	0.0161 (12)
N21	0.2624 (3)	0.4915 (4)	0.2788 (2)	0.0250 (12)
N22	0.2062 (3)	0.4054 (4)	0.3107 (2)	0.0210 (12)
N30	0.1189 (3)	0.5740 (4)	0.4241 (2)	0.0242 (12)
C13	0.1595 (4)	0.1177 (4)	0.4521 (3)	0.0253 (14)
C14	0.1758 (4)	-0.0134 (4)	0.4393 (3)	0.0256 (14)
C15	0.2575 (4)	-0.0175 (4)	0.4025 (3)	0.0221 (12)
C16	0.3104 (5)	-0.1310 (4)	0.3763 (3)	0.0339 (16)
C17	0.0796 (5)	0.1753 (5)	0.4907 (3)	0.0383 (19)
C18	0.3803 (4)	0.1530 (4)	0.3669 (2)	0.0207 (12)
C19	0.4621 (4)	0.2343 (4)	0.4252 (2)	0.0186 (12)
C23	0.1119 (4)	0.3728 (5)	0.2577 (3)	0.0313 (14)
C24	0.1093 (5)	0.4394 (7)	0.1927 (3)	0.0449 (19)
C25	0.2048 (5)	0.5132 (6)	0.2075 (3)	0.0376 (17)
C26	0.2472 (5)	0.6055 (7)	0.1591 (3)	0.053 (2)
C27	0.0274 (4)	0.2782 (6)	0.2706 (3)	0.0401 (19)
C28	0.3726 (4)	0.5426 (4)	0.3224 (2)	0.0212 (12)
C29	0.4543 (4)	0.4343 (4)	0.3594 (2)	0.0206 (12)
C50	0.5082 (3)	0.4281 (4)	0.4953 (2)	0.0162 (12)
O61	0.1650 (3)	0.5232 (5)	0.6068 (2)	0.0497 (14)
C60	0.1999 (6)	0.4778 (9)	0.6829 (4)	0.074 (3)
O41	0.3957 (3)	0.1699 (4)	0.5965 (2)	0.0414 (12)
O42	0.4156 (4)	0.2676 (4)	0.7009 (2)	0.0487 (14)
O43	0.4826 (3)	0.0748 (4)	0.6991 (2)	0.0383 (12)
N40	0.4309 (3)	0.1705 (4)	0.6663 (2)	0.0261 (12)

Table 2. *Selected geometric parameters* (Å, °)

Ni1—O31	2.205 (4)	N12—C13	1.339 (6)
Ni1—O33	2.144 (3)	N20—C19	1.492 (5)
Ni1—O34	2.032 (4)	N20—C29	1.493 (5)
Ni1—N12	2.023 (4)	N20—C50	1.492 (5)
Ni1—N20	2.161 (4)	N21—N22	1.362 (6)
Ni1—N22	2.048 (4)	N21—C25	1.342 (7)
O31—N30	1.271 (5)	N21—C28	1.463 (6)
O32—N30	1.224 (5)	N22—C23	1.335 (6)
O33—N30	1.270 (5)	O61—C60	1.447 (8)
N11—N12	1.359 (5)	O41—N40	1.257 (5)
N11—C15	1.348 (5)	O42—N40	1.237 (6)
N11—C18	1.450 (6)	O43—N40	1.238 (6)
O31—Ni1—O33	59.46 (11)	C19—N20—C29	106.5 (3)
O31—Ni1—O34	87.09 (14)	C19—N20—C50	105.2 (3)
O31—Ni1—N12	101.47 (14)	C29—N20—C50	110.2 (3)
O31—Ni1—N20	162.55 (12)	N22—N21—C25	111.0 (4)
O31—Ni1—N22	87.73 (14)	C25—N21—C28	129.6 (4)
O33—Ni1—O34	85.17 (13)	N21—N22—C23	105.9 (4)
O33—Ni1—N20	103.13 (11)	O31—N30—O33	116.2 (4)
O33—Ni1—N22	86.65 (15)	O32—N30—O33	122.4 (4)
O34—Ni1—N12	90.92 (14)	N12—C13—C14	109.7 (4)
O34—Ni1—N20	92.69 (15)	N11—C15—C14	107.3 (4)
O34—Ni1—N22	171.74 (15)	N11—C18—C19	110.8 (3)
O34—Ni1—N30	86.40 (13)	N20—C19—C18	114.8 (4)
N12—Ni1—N20	95.98 (14)	N22—C23—C24	109.1 (5)
N12—Ni1—N22	96.42 (16)	N21—C25—C24	106.8 (5)
N20—Ni1—N22	90.33 (15)	N21—C28—C29	111.8 (4)

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: MU1285). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Photochemical Reactions of Transition Metal Organyl Complexes with Olefins.

15.† Tricarbonyl(η^4 -1,3-butadiene)- μ -hydrido-(μ - $\eta^{1:5}$ -indene-1,1-diyl)(η^5 -indenyl)dimolybdenum(Mo—Mo)

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Abstract

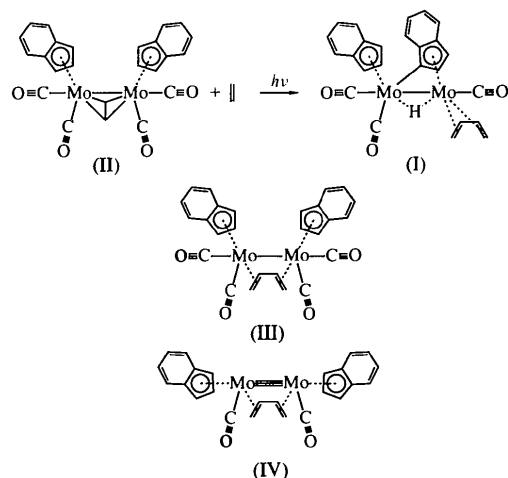
The Mo centres of the dinuclear title complex, [1(η^4 -1,3-butadiene)tricarbonyl-1 κ C,2 κ^2 C- μ -hydrido-[2(1,2,3,3a,7a- η)-indenyl][μ -1(1,2,3,3a,7a- η):2 κ^1 -indenylidene]dimolybdenum(Mo—Mo), [Mo₂(H)(C₉H₆)(C₉H₇)(C₄H₆)(CO)₃], are bridged by a μ - $\eta^{1:5}$ -indene-1,1-diyl and a hydrido ligand. The Mo—Mo distance of 3.2024 (7) Å is normal for an Mo—Mo single bond.

Comment

When tetracarbonylbis(η^5 -cyclopentadienyl)(μ - $\eta^{2:2}$ -ethyne)dimolybdenum, (III), is UV irradiated in the presence of ethene, the stable products (η^4 -butadiene)tricarbonylbis(η^5 -cyclopentadienyl)dimolybdenum, (η^4 -butadiene)tetracarbonylbis(η^5 -cyclopentadienyl)dimolybdenum and (μ - $\eta^{1:3}$ -2-buten-1-ylidene)tetracarbonylbis(η^5 -

cyclopentadienyl)dimolybdenum (Kern, 1992; Kreiter & Kern, 1993) are formed. The butadiene and 2-buten-1-ylidene ligands are formed by insertion of ethene into an Mo—C bond of the tetrahedral Mo₂C₂ core of compound (III) and successive metal-mediated hydride shifts.

η^5 -Indenyl complexes often show a different reaction behaviour from the corresponding η^5 -cyclopentadienyl compounds because of the ability of the indenyl ligand to change its hapticity. In order to study the differences caused by indenyl ligands, tetracarbonyl(μ - $\eta^{2:2}$ -ethyne)-bis(η^5 -indenyl)dimolybdenum, (II), was reacted photochemically with simple mono-olefins (Meuser, 1993). Compound (II) when reacted with ethene forms three butadiene complexes, namely, the title compound, (η^4 -1,3-butadiene)tricarbonyl- μ -hydrido-(μ - $\eta^{1:5}$ -indene-1,1-diyl)(η^5 -indenyl)dimolybdenum, (I), (μ - $\eta^{2:2}$ -1,3-butadiene)tetracarbonylbis(η^5 -indenyl)dimolybdenum, (IV), and (μ - $\eta^{2:2}$ -1,3-butadiene)dicarbonylbis(η^5 -indenyl)dimolybdenum, (V). The variability of the products reflects the different possibilities of coordination for the butadiene ligand at complex fragments with metal–metal single or triple bonds. In contrast to (η^4 -butadiene)tricarbonylbis(η^5 -cyclopentadienyl)dimolybdenum, where the electron deficiency of the binuclear 32-electron complex is compensated for by a μ - $\eta^{2:1}$ -CO ligand, the comparable indenyl complex (I) is stabilized by the oxidative addition of a C—H bond of one indenyl ligand to the Mo1 atom.



Compound (I) (Fig. 1) contains three terminal carbonyl, an *S-cis*- η^4 -1,3-butadiene, a η^5 -indenyl, a bridging μ - $\eta^{5:1}$ -indene-1,1-diyl and a bridging hydrido ligand. The Mo—Mo distance of 3.2024 (7) Å is in agreement with the Mo—Mo single-bond distance found in hexacarbonyldi(η^5 -cyclopentadienyl)dimolybdenum (Adams, Collins & Cotton, 1974). In order to fulfil the 18-electron rule for both metal centres, the hydrido ligand could be bonded terminally to the Mo1 atom. In fact,

† Part 14: Kreiter, Eckert, Frank & Reiß (1996).