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**Key indicators**

Single-crystal X-ray study  
 T = 100 K  
 Mean  $\sigma(C-C)$  = 0.002 Å  
 R factor = 0.024  
 wR factor = 0.063  
 Data-to-parameter ratio = 20.9

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

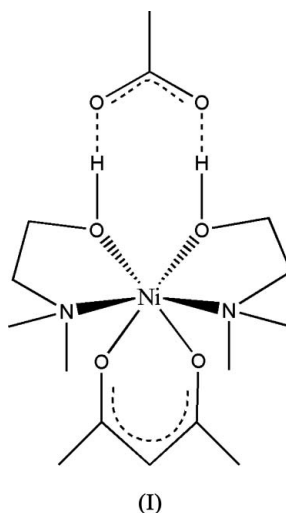
**Bis[2-(dimethylamino)ethanol- $\kappa^2N,O$ ]-  
 (2,4-pentanedionato- $\kappa^2O,O'$ )nickel(II)  
 acetate**

The Ni atom in the title complex,  $[Ni(C_5H_7O_2)(C_4H_{11}NO)_2](C_2H_3O_2)$ , has distorted octahedral coordination. The O atoms of the acetate ion are hydrogen bonded to the OH groups of the 2-(dimethylamino)ethanol ligands.

Received 1 February 2006  
 Accepted 14 March 2006

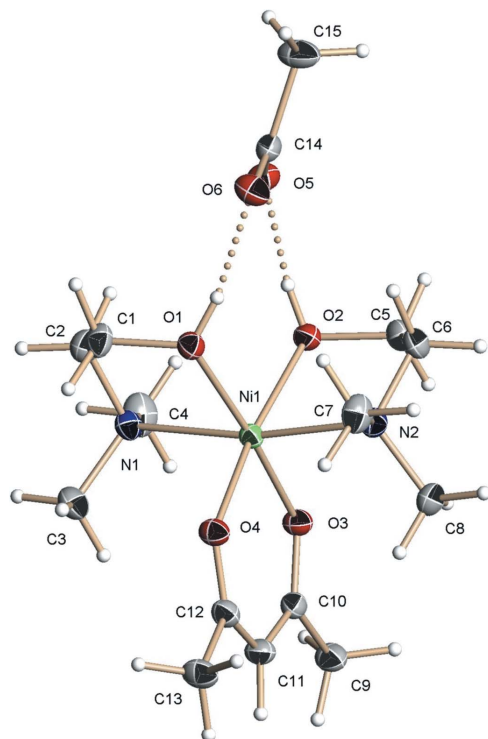
**Comment**

The title compound, (I), is a synthetic precursor for the possible deposition of nickel oxide thin films through aerosol-assisted chemical vapour deposition (AACVD). It was synthesized by the reaction of  $Ni(dmaeH)_2(OAc)_2$  with thallium acetylacetonate (dmaeH is dimethylaminoethanol), and crystals grown from toluene were analysed by single-crystal diffraction at 100 K. The compound was found to crystallize in the non-centrosymmetric orthorhombic space group  $P2_12_12_1$ ; the crystal under investigation was not racemically twinned.



The molecular structure of complex (I) is shown in Fig. 1, and selected bond lengths and angles are given in Table 1. The cationic nickel complex has a distorted octahedral coordination around the  $Ni^{II}$  atom, with two bidentate chelating dimethylaminoethanol ligands and a bidentate acetylacetonate group. The acetate anion is hydrogen bonded to the OH groups of the two 2-(dimethylamino)ethanol ligands (Fig. 1); hydrogen-bonding parameters are listed in Table 2.

The N atoms are in mutually *trans* positions, with an  $N1-N1-N2$  angle of  $170.07(5)^\circ$ . The  $Ni1-N1$  bond length of  $2.1489(13)$  Å is slightly shorter than that of  $Ni1-N2$  [ $2.1738(13)$  Å]. The  $Ni1-O1$ ,  $Ni1-O2$  and  $Ni1-O3$  bonds are very similar to the corresponding bonds in the related compounds  $[Ni(acac)_2(dmaeH)]$  (acac is acetylacetonate; Williams *et al.*, 2001) and  $[Ni(acac)(dmaeH)_2]Cl$  (Sohail *et al.*,

**Figure 1**

View of the title complex, showing the atom-labelling scheme and displacement ellipsoids drawn at the 50% probability level. Dashed lines indicate O—H...O hydrogen bonds.

2005). Not surprisingly, the Ni—O bonds of the formally neutral coordinated dmaeH groups are longer than those of the anionic acac ligand. The *cis* O—Ni—O and O—Ni—N angles in (I) are close to the ideal octahedral value of 90°, with the exception of the bite angles of the chelating dmaeH groups. Distortions of the *trans* O—Ni—O angles from the ideal value of 180° are also evident and are comparable with those of related compounds (Hubert-Pfalzgraf *et al.*, 1997; Downie *et al.*, 1971).

## Experimental

Ni(dmaeH)<sub>2</sub>(OAc)<sub>2</sub> (0.12 g, 0.32 mmol), prepared according to a literature procedure (Williams *et al.*, 2001), was reacted with Tl(acac) (0.1 g, 0.32 mmol) in dry toluene under inert conditions using Schlenk tube techniques. The resulting product was recrystallized from toluene at 263 K, giving crystals of (I) suitable for single-crystal X-ray analysis.

### Crystal data

[Ni(C<sub>5</sub>H<sub>7</sub>O<sub>2</sub>)(C<sub>4</sub>H<sub>11</sub>NO)<sub>2</sub>](C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>)  
*M<sub>r</sub>* = 395.14  
 Orthorhombic, *P*2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>  
*a* = 8.5456 (10) Å  
*b* = 12.5165 (15) Å  
*c* = 18.109 (2) Å  
*V* = 1937.0 (4) Å<sup>3</sup>  
*Z* = 4  
*D<sub>x</sub>* = 1.355 Mg m<sup>-3</sup>

Mo *K*α radiation  
 Cell parameters from 8795 reflections  
 $\theta$  = 2.6–30.6°  
 $\mu$  = 1.03 mm<sup>-1</sup>  
*T* = 100 (2) K  
 Block, blue  
 0.52 × 0.52 × 0.34 mm

### Data collection

Bruker SMART APEX CCD diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS in S<sub>AINT-Plus</sub>; Bruker, 2003)  
 $T_{\min}$  = 0.571,  $T_{\max}$  = 0.704  
 19915 measured reflections

4812 independent reflections  
 4717 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}}$  = 0.027  
 $\theta_{\max}$  = 28.3°  
 $h$  = -11 → 11  
 $k$  = -16 → 16  
 $l$  = -23 → 24

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)]$  = 0.024  
 $wR(F^2)$  = 0.063  
 $S$  = 1.07  
 4812 reflections  
 230 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0383P)^2 + 0.3423P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max}$  = 0.002  
 $\Delta\rho_{\max}$  = 0.66 e Å<sup>-3</sup>  
 $\Delta\rho_{\min}$  = -0.26 e Å<sup>-3</sup>  
 Absolute structure: (Flack, 1983),  
 with 2077 Friedel pairs  
 Flack parameter: -0.008 (8)

**Table 1**

Selected geometric parameters (Å, °).

N1—Ni1	2.1489 (13)	Ni1—O3	2.0102 (11)
N2—Ni1	2.1738 (13)	Ni1—O1	2.0962 (11)
Ni1—O4	2.0080 (10)	Ni1—O2	2.0961 (11)
O4—Ni1—O3	91.68 (4)	O1—Ni1—N1	81.78 (5)
O4—Ni1—O1	88.95 (4)	O2—Ni1—N1	91.92 (5)
O3—Ni1—O1	174.06 (5)	O4—Ni1—N2	90.11 (5)
O4—Ni1—O2	171.97 (4)	O3—Ni1—N2	95.28 (5)
O3—Ni1—O2	87.67 (4)	O1—Ni1—N2	90.63 (5)
O1—Ni1—O2	92.53 (4)	O2—Ni1—N2	81.98 (5)
O4—Ni1—N1	96.11 (5)	N1—Ni1—N2	170.07 (5)
O3—Ni1—N1	92.28 (5)		

**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H1...O6	0.84 (2)	1.73 (2)	2.5634 (16)	169 (2)
O2—H2...O5	0.87 (2)	1.70 (2)	2.5627 (15)	172 (2)

The hydroxyl H atoms were located in a difference density Fourier map, restrained to have equal O—H distances within a standard deviation of 0.02 Å and refined with an isotropic displacement parameter 1.5 times  $U_{\text{eq}}$  of the parent O atom. All other H atoms were placed in calculated positions (C—H = 0.98 and 0.99 Å) and were refined with  $U_{\text{iso}}(\text{H})$  values of 1.5 (methyl) or 1.2 (methylene) times  $U_{\text{eq}}$  of the parent C atom. Methyl H atoms were allowed to rotate to best fit the experimental electron density. The s.u. values of the cell parameters are taken from the software, recognizing that the values are unreasonably small (Herbstein, 2000).

Data collection: SMART (Bruker, 2002); cell refinement: S<sub>AINT-Plus</sub> (Bruker, 2003); data reduction: S<sub>AINT-Plus</sub>; program(s) used to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

The role of the Higher Education Commission of Pakistan is acknowledged for funding through grant No. 20-91/Acad-(R)-419. The diffractometer was funded by NSF grant No. 0087210 and by Ohio Board of Regents grant No. CAP-491.

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