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# *catena*-Poly[[diaquanickel(II)]-bis[$\mu$-(4-pyridylsulfanyl)acetato-$\kappa^2N$:$O$;$\kappa^2O$:$N$]]

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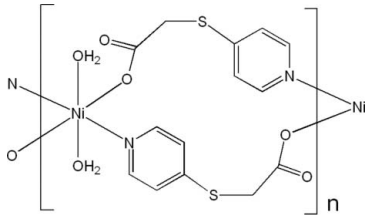
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.012 Å; $R$ factor = 0.084; $wR$ factor = 0.191; data-to-parameter ratio = 12.1.

The Ni atom in the title compound, $[Ni(C_7H_6NO_2S)_2(H_2O)_2]_n$, occupies a special position on an inversion centre and has an octahedral coordination formed by two water molecules and two pyridyl N and two carboxylate O atoms belonging to four different anionic ligands. Each ligand has a bidentate bridging function, so that each Ni atom is connected to each of its two Ni neighbours by two ligand bridges, thus producing infinite chains running along the $a$ axis in the crystal structure. O—H···O bonds link the chains into a three-dimensional framework.

## Related literature

For related literature, see: Huang *et al.* (2004*a*,*b*); Zhang *et al.* (2004).




## Experimental

*Crystal data*

$[Ni(C_7H_6NO_2S)_2(H_2O)_2]$
$M_r$ = 431.12
Monoclinic, $P2_1/c$
$a$ = 8.9232 (9) Å
$b$ = 10.6901 (10) Å
$c$ = 8.8887 (9) Å
$\beta$ = 90.378 (3)°
$V$ = 847.87 (14) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.42 mm$^{-1}$
$T$ = 298 (2) K
0.32 × 0.24 × 0.16 mm

*Data collection*

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.658, $T_{max}$ = 0.804
2425 measured reflections
1489 independent reflections
1198 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.050

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.084
$wR(F^2)$ = 0.191
$S$ = 1.14
1489 reflections
123 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.96 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.91 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Ni1—O1$^{i}$ | 2.081 (6) | Ni1—N1 | 2.125 (7) |
| Ni1—O3 | 2.060 (6) | | |
| O3—Ni1—O1$^{i}$ | 91.5 (3) | O1$^{i}$—Ni1—N1$^{ii}$ | 91.7 (3) |
| O3—Ni1—N1$^{ii}$ | 88.0 (3) | | |

Symmetry codes: (i) $-x+1, -y, -z$; (ii) $-x, -y, -z$.

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H3···O2$^{i}$ | 0.85 (2) | 1.81 (3) | 2.631 (9) | 161 (8) |
| O3—H6···O2$^{iii}$ | 0.85 (2) | 1.97 (4) | 2.792 (8) | 163 (12) |

Symmetry codes: (i) $-x+1, -y, -z$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*b*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*b*); molecular graphics: *SHELXTL* (Sheldrick, 1997*a*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: YA2052).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, m1745 [ **doi:10.1107/S1600536807023550** ]

# *catena*-Poly[[diaquanickel(II)]-bis[$\mu$-(4-pyridylsulfanyl)acetato-$\kappa^2N$:$O$;$\kappa^2O$:$N$]]

**X.-P. Luo and L. Han**

## Comment

Three compounds obtained by the reaction of pyridin-4-ylthioacetic acid with nickel(II) salts have been recently crystallographically characterized, namely one zwitterionic complex $[Ni(C_7H_6NO_2S)_2(H_2O)_4]$ (Zhang *et al.*, 2004) and two coordination polymers, $[Ni(C_7H_6NO_2S)_2(H_2O)]_n$ (Huang *et al.*, 2004*a*) and $[Ni_2(C_7H_6NO_2S)_4(H_2O)_2]_n$ (Huang *et al.*, 2004*b*). Herein we report the structure of a new Ni(II) complex (**I**) with pyridin-4-ylthioacetato ligand.

In the crystal structure of the title compound, the Ni1 atom occupies a special position in the inversion centre and has an octahedral coordination formed by two water molecules, as well as two pyridyl N and two carboxylate O atoms belonging to four different anionic ligands. Each ligand has a bidentate bridging function, so that each Ni atom is connected to each of its two Ni neighbours by two ligand bridges, thus producing infinite chains running along the *a*-axis in the crystal structure (Fig. 1). The O—H···O bonds link the chains into a three-dimensional framework (Table 2, Fig. 2).

## Experimental

Nickel(II) acetate (50 mg, 0.2 mmol), pyridin-4-ylthioacetic acid (39 mg, 0.2 mmol) and NaOH (8 mg, 0.2 mmol) were dissolved in 10 ml of water. The solution was placed in a Teflon-lined stainless-steel bomb (23 ml) and heated at 423 K for 48 h. After cooling to room temperature, green crystals of (**I**) precipitated from the solution in about 60% yield.

## Refinement

The water H atoms were located and refined, subject to an O—H = 0.85±0.02 Å restraint. The aromatic and aliphatic H atoms were placed at calculated positions (C—H 0.93 Å and 0.97 Å respectively) and refined using the riding-model approximation with $U_{iso}(H) = 1.2U_{eq}(C)$.

## Figures

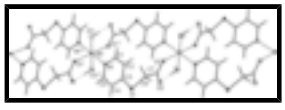

Fig. 1. **Figure 1** Infinite chains in the crystal structure of (**I**) with atom-labelling scheme, showing the coordination sphere of metal and coordination mode of the ligand. Displacement ellipsoids are drawn at the 30% probability level and H atoms are depicted as small spheres of arbitrary radius. Hydrogen bonds are shown as dashed lines [Symmetry codes: (i): $x-1, y, z$; (ii): $1-x, -y, -z$; (iii): $-x, -y, -z$].

Fig. 2. **Figure 2** The packing diagram of the title compound viewed down the *a*-axis. Hydrogen bonds are shown as dashed lines.

**_catena_-Poly[[diaquanickel(II)]-bis[μ-(4-pyridylsulfanyl)acetato- κ<sup>2</sup>N:_O_;κ<sup>2</sup>O:_N_]]**

*Crystal data*

| | |
|---|---|
| $[Ni(C_7H_6NO_2S)_2(H_2O)_2]$ | $F_{000}$ = 444 |
| $M_r$ = 431.12 | $D_x$ = 1.689 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 2522 reflections |
| $a$ = 8.9232 (9) Å | θ = 2.3–25.0º |
| $b$ = 10.6901 (10) Å | μ = 1.42 mm$^{-1}$ |
| $c$ = 8.8887 (9) Å | $T$ = 298 (2) K |
| β = 90.378 (3)º | Prism, green |
| $V$ = 847.87 (14) Å$^3$ | 0.32 × 0.24 × 0.16 mm |
| $Z$ = 2 | |

*Data collection*

| | |
|---|---|
| BRUKER SMART CCD Apex II diffractometer | 1489 independent reflections |
| Radiation source: fine-focus sealed tube | 1198 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.050 |
| Detector resolution: 8.40 pixels mm$^{-1}$ | $\theta_{max}$ = 25.0º |
| $T$ = 298(2) K | $\theta_{min}$ = 2.3º |
| ω scans | $h$ = −10→7 |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $k$ = −11→12 |
| $T_{min}$ = 0.658, $T_{max}$ = 0.804 | $l$ = −10→10 |
| 2425 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.084 | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2)$ = 0.191 | $w = 1/[\sigma^2(F_o^2) + 14.8565P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.14 | $(\Delta/\sigma)_{max} < 0.001$ |
| 1489 reflections | $\Delta\rho_{max}$ = 0.96 e Å$^{-3}$ |
| 123 parameters | $\Delta\rho_{min}$ = −0.91 e Å$^{-3}$ |
| 2 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Ni1 | 0.0000 | 0.0000 | 0.0000 | 0.0233 (4) |
| S1 | 0.5686 (2) | −0.1649 (2) | 0.4472 (2) | 0.0294 (6) |
| O1 | 0.8661 (6) | −0.0028 (6) | 0.1907 (7) | 0.0311 (14) |
| O2 | 0.8051 (7) | −0.2052 (6) | 0.2088 (7) | 0.0315 (15) |
| O3 | 0.0489 (7) | 0.1845 (6) | 0.0462 (7) | 0.0287 (14) |
| N1 | 0.1893 (8) | −0.0633 (7) | 0.1246 (8) | 0.0298 (18) |
| C1 | 0.3188 (9) | 0.0012 (9) | 0.1215 (9) | 0.0271 (19) |
| H1 | 0.3263 | 0.0683 | 0.0555 | 0.033* |
| C2 | 0.4433 (10) | −0.0276 (9) | 0.2126 (11) | 0.033 (2) |
| H2 | 0.5317 | 0.0179 | 0.2049 | 0.040* |
| C3 | 0.4312 (9) | −0.1255 (8) | 0.3141 (10) | 0.0246 (19) |
| C4 | 0.3014 (10) | −0.1952 (9) | 0.3123 (10) | 0.031 (2) |
| H4 | 0.2924 | −0.2647 | 0.3745 | 0.037* |
| C5 | 0.1847 (10) | −0.1616 (9) | 0.2178 (10) | 0.031 (2) |
| H5 | 0.0980 | −0.2100 | 0.2189 | 0.037* |
| C6 | 0.7218 (10) | −0.0638 (9) | 0.4016 (10) | 0.030 (2) |
| H6A | 0.6842 | 0.0212 | 0.3952 | 0.036* |
| H6B | 0.7939 | −0.0665 | 0.4838 | 0.036* |
| C7 | 0.8041 (9) | −0.0940 (8) | 0.2550 (9) | 0.0243 (19) |
| H3 | 0.110 (7) | 0.201 (8) | −0.025 (6) | 0.02 (2)* |
| H6 | 0.100 (11) | 0.202 (11) | 0.124 (8) | 0.07 (4)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ni1 | 0.0199 (8) | 0.0251 (8) | 0.0249 (8) | −0.0015 (7) | −0.0033 (6) | −0.0003 (7) |
| S1 | 0.0232 (11) | 0.0395 (13) | 0.0255 (11) | 0.0049 (10) | −0.0031 (9) | 0.0067 (10) |
| O1 | 0.029 (3) | 0.032 (3) | 0.032 (3) | 0.000 (3) | 0.000 (3) | 0.001 (3) |
| O2 | 0.037 (4) | 0.030 (4) | 0.028 (3) | −0.001 (3) | 0.003 (3) | −0.003 (3) |
| O3 | 0.031 (4) | 0.031 (4) | 0.025 (3) | −0.004 (3) | −0.003 (3) | −0.009 (3) |
| N1 | 0.021 (4) | 0.033 (4) | 0.035 (4) | 0.002 (3) | 0.000 (3) | 0.000 (3) |
| C1 | 0.021 (4) | 0.031 (4) | 0.029 (5) | −0.004 (4) | −0.005 (3) | 0.004 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | 0.022 (4) | 0.035 (6) | 0.043 (5) | 0.000 (4) | −0.001 (4) | 0.003 (4) |
| C3 | 0.017 (4) | 0.026 (5) | 0.030 (5) | 0.006 (3) | −0.002 (3) | −0.007 (4) |
| C4 | 0.033 (5) | 0.027 (5) | 0.032 (5) | −0.004 (4) | 0.005 (4) | 0.007 (4) |
| C5 | 0.020 (4) | 0.034 (5) | 0.037 (5) | −0.005 (4) | 0.001 (4) | 0.015 (4) |
| C6 | 0.023 (5) | 0.034 (5) | 0.031 (5) | 0.004 (4) | 0.000 (4) | 0.002 (4) |
| C7 | 0.015 (4) | 0.033 (5) | 0.024 (4) | 0.002 (4) | −0.009 (3) | 0.006 (4) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Ni1—O3$^{i}$ | 2.060 (6) | O3—H6 | 0.85 (2) |
| Ni1—O1$^{ii}$ | 2.081 (6) | N1—C5 | 1.339 (11) |
| Ni1—O3 | 2.060 (6) | N1—C1 | 1.346 (11) |
| Ni1—O1$^{iii}$ | 2.081 (6) | C1—C2 | 1.404 (12) |
| Ni1—N1$^{i}$ | 2.125 (7) | C1—H1 | 0.9300 |
| Ni1—N1 | 2.125 (7) | C2—C3 | 1.386 (12) |
| S1—C3 | 1.749 (8) | C2—H2 | 0.9300 |
| S1—C6 | 1.792 (9) | C3—C4 | 1.378 (12) |
| O1—C7 | 1.260 (10) | C4—C5 | 1.382 (12) |
| O1—Ni1$^{iv}$ | 2.081 (6) | C4—H4 | 0.9300 |
| O2—C7 | 1.258 (11) | C5—H5 | 0.9300 |
| O3—O2$^{ii}$ | 2.631 (9) | C6—C7 | 1.535 (12) |
| O3—O2$^{v}$ | 2.792 (8) | C6—H6A | 0.9700 |
| O3—H3 | 0.85 (2) | C6—H6B | 0.9700 |
| O3—Ni1—O3$^{i}$ | 180.0 (3) | C5—N1—C1 | 116.4 (7) |
| O3—Ni1—O1$^{ii}$ | 91.5 (3) | C5—N1—Ni1 | 123.0 (6) |
| O3$^{i}$—Ni1—O1$^{ii}$ | 88.5 (3) | C1—N1—Ni1 | 120.4 (6) |
| O3—Ni1—O1$^{iii}$ | 88.5 (3) | N1—C1—C2 | 123.5 (8) |
| O3$^{i}$—Ni1—O1$^{iii}$ | 91.5 (3) | N1—C1—H1 | 118.2 |
| O1$^{ii}$—Ni1—O1$^{iii}$ | 180.0 (3) | C2—C1—H1 | 118.2 |
| O3—Ni1—N1$^{i}$ | 88.0 (3) | C3—C2—C1 | 118.4 (8) |
| O3$^{i}$—Ni1—N1$^{i}$ | 92.0 (3) | C3—C2—H2 | 120.8 |
| O1$^{ii}$—Ni1—N1$^{i}$ | 91.7 (3) | C1—C2—H2 | 120.8 |
| O1$^{iii}$—Ni1—N1$^{i}$ | 88.3 (3) | C4—C3—C2 | 118.0 (8) |
| O3—Ni1—N1 | 92.0 (3) | C4—C3—S1 | 117.6 (7) |
| O3$^{i}$—Ni1—N1 | 88.0 (3) | C2—C3—S1 | 124.4 (7) |
| O1$^{ii}$—Ni1—N1 | 88.3 (3) | C3—C4—C5 | 119.8 (8) |
| O1$^{iii}$—Ni1—N1 | 91.7 (3) | C3—C4—H4 | 120.1 |
| N1$^{i}$—Ni1—N1 | 180.0 (6) | C5—C4—H4 | 120.1 |
| C3—S1—C6 | 103.5 (4) | N1—C5—C4 | 123.6 (8) |
| C7—O1—Ni1$^{iv}$ | 129.6 (6) | N1—C5—H5 | 118.2 |
| Ni1—O3—O2$^{ii}$ | 90.8 (3) | C4—C5—H5 | 118.2 |
| Ni1—O3—O2$^{v}$ | 131.1 (3) | C7—C6—S1 | 115.8 (7) |
| O2$^{ii}$—O3—O2$^{v}$ | 113.9 (3) | C7—C6—H6A | 108.3 |
| Ni1—O3—H3 | 101 (6) | S1—C6—H6A | 108.3 |

| | | | |
|---|---|---|---|
| O2$^{ii}$—O3—H3 | 13 (6) | C7—C6—H6B | 108.3 |
| O2$^{v}$—O3—H3 | 101 (6) | S1—C6—H6B | 108.3 |
| Ni1—O3—H6 | 119 (9) | H6A—C6—H6B | 107.4 |
| O2$^{ii}$—O3—H6 | 115 (8) | O2—C7—O1 | 125.4 (8) |
| O2$^{v}$—O3—H6 | 12 (8) | O2—C7—C6 | 118.7 (8) |
| H3—O3—H6 | 102 (10) | O1—C7—C6 | 115.9 (8) |
| O3$^{i}$—Ni1—O3—O2$^{ii}$ | 72 (100) | N1$^{i}$—Ni1—N1—C1 | 94 (100) |
| O1$^{ii}$—Ni1—O3—O2$^{ii}$ | 6.2 (3) | C5—N1—C1—C2 | −2.0 (13) |
| O1$^{iii}$—Ni1—O3—O2$^{ii}$ | −173.8 (3) | Ni1—N1—C1—C2 | 173.2 (7) |
| N1$^{i}$—Ni1—O3—O2$^{ii}$ | −85.5 (3) | N1—C1—C2—C3 | −1.8 (14) |
| N1—Ni1—O3—O2$^{ii}$ | 94.5 (3) | C1—C2—C3—C4 | 4.8 (13) |
| O3$^{i}$—Ni1—O3—O2$^{v}$ | −52 (100) | C1—C2—C3—S1 | −174.0 (7) |
| O1$^{ii}$—Ni1—O3—O2$^{v}$ | −117.2 (4) | C6—S1—C3—C4 | 175.0 (7) |
| O1$^{iii}$—Ni1—O3—O2$^{v}$ | 62.8 (4) | C6—S1—C3—C2 | −6.2 (9) |
| N1$^{i}$—Ni1—O3—O2$^{v}$ | 151.2 (4) | C2—C3—C4—C5 | −4.1 (13) |
| N1—Ni1—O3—O2$^{v}$ | −28.8 (4) | S1—C3—C4—C5 | 174.8 (7) |
| O3—Ni1—N1—C5 | 137.4 (7) | C1—N1—C5—C4 | 2.7 (14) |
| O3$^{i}$—Ni1—N1—C5 | −42.6 (7) | Ni1—N1—C5—C4 | −172.3 (7) |
| O1$^{ii}$—Ni1—N1—C5 | −131.1 (7) | C3—C4—C5—N1 | 0.3 (15) |
| O1$^{iii}$—Ni1—N1—C5 | 48.9 (7) | C3—S1—C6—C7 | −70.8 (7) |
| N1$^{i}$—Ni1—N1—C5 | −91 (100) | Ni1$^{iv}$—O1—C7—O2 | −4.3 (12) |
| O3—Ni1—N1—C1 | −37.5 (7) | Ni1$^{iv}$—O1—C7—C6 | 175.6 (5) |
| O3$^{i}$—Ni1—N1—C1 | 142.5 (7) | S1—C6—C7—O2 | −27.7 (10) |
| O1$^{ii}$—Ni1—N1—C1 | 54.0 (7) | S1—C6—C7—O1 | 152.4 (6) |
| O1$^{iii}$—Ni1—N1—C1 | −126.0 (7) | | |

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) −*x*+1, −*y*, −*z*; (iii) *x*−1, *y*, *z*; (iv) *x*+1, *y*, *z*; (v) −*x*+1, *y*+1/2, −*z*+1/2.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O3—H3···O2$^{ii}$ | 0.85 (2) | 1.81 (3) | 2.631 (9) | 161 (8) |
| O3—H6···O2$^{v}$ | 0.85 (2) | 1.97 (4) | 2.792 (8) | 163 (12) |

Symmetry codes: (ii) −*x*+1, −*y*, −*z*; (v) −*x*+1, *y*+1/2, −*z*+1/2.

**Fig. 1**

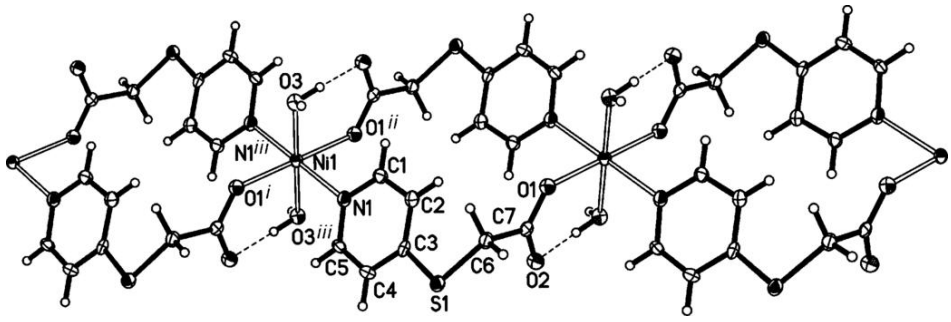

**Fig. 2**