Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

rac-catena-Poly[nickel(II)-di-μ-tryptophanato]

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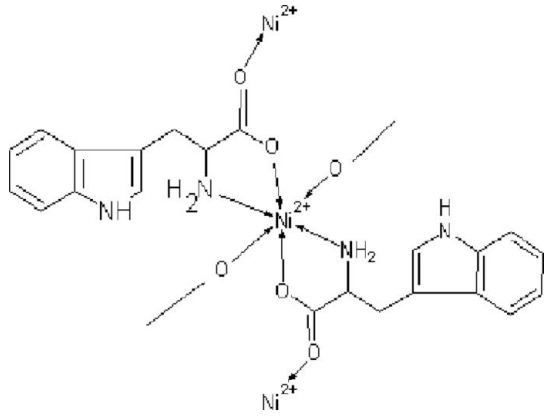
Received 18 October 2007; accepted 26 October 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; R factor = 0.053; wR factor = 0.145; data-to-parameter ratio = 12.3.

The title complex, $[Ni(C_{11}H_{11}N_2O_2)_2]_n$ or $[Ni(D\text{-trp})(L\text{-trp})]_n$ [D-trp = (*R*)-2-amino-3-(3-indolyl)propionate and L-trp = (*S*)-2-amino-3-(3-indolyl)propionate], was formed by a hydrothermal method from hexaaquanickel(II) perchlorate and L-tryptophan. The Ni^{II} atom is located on an inversion center and has an octahedral coordination geometry formed by four O atoms and two N atoms from D– and L-tryptophan ligands. Each D– and L-tryptophan ligand bridges the Ni^{II} atoms through the carboxylate group, leading to a two-dimensional structure parallel to the *bc* plane.

Related literature

For related literature, see: Cai *et al.* (2000); Cheng *et al.* (2005); Henrick *et al.* (1978); Kumita *et al.* (2001); Rodríguez *et al.* (1990); Wu *et al.* (2004); Zhang *et al.* (2005); Zhou *et al.* (2005).



Experimental

Crystal data

$[Ni(C_{11}H_{11}N_2O_2)_2]$
M_r = 465.15
Monoclinic, $P2_1/c$
a = 19.724 (3) Å
b = 5.6139 (11) Å
c = 9.0372 (18) Å
β = 97.616 (2)°
V = 991.9 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.02 mm^{-1}
T = 298 (2) K
0.23 × 0.15 × 0.12 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.800, T_{max} = 0.888
4673 measured reflections
1743 independent reflections
1268 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.145
S = 1.05
1743 reflections
142 parameters
H-atom parameters not refined
$\Delta\rho_{max}$ = 1.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	2.037 (3)	Ni1—O2^{i}	2.098 (3)
Ni1—N1	2.096 (4)		
O1—Ni1—N1	82.04 (14)	N1—Ni1—O2^{i}	85.90 (14)
O1—Ni1—N1^{ii}	97.96 (14)	O1—Ni1—O2^{iii}	89.77 (14)
O1—Ni1—O2^{i}	90.23 (14)	N1—Ni1—O2^{iii}	94.10 (14)

Symmetry codes: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x, -y+1, -z+1$; (iii) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

We acknowledge the financial support of the Foundation of Science Committee of Jiangsu Province and the Key Marine Biotechnology Laboratory of Huaihai Institute of Technology.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2224).

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supplementary materials

Acta Cryst. (2007). E**63**, m2867-m2868 [**doi:10.1107/S1600536807053421**]

rac-catena-Poly[nickel(II)-di-μ-tryptophanato]

J. Wang, X. Xu, W. Ma, L. Lu and X. Yang

Comment

Metal-organic coordination polymers have particular and special structural characteristics with some cave-holes and channels. It can be applied in selected catalysis-molecular recognition-reversible exchange of host–guest molecules(ions)-superpurity separation-biological conductor *etc*. In recent years, such polymers have been widely investigated. However, a single-crystal structure of a coordination polymer formed with nickel(II) and trp has not been reported. For this reason we prepared and characterized the title compound, $[Ni(D\text{-trp})(L\text{-trp})]_n$.

The Ni^{II} atom is coordinated by two N atoms and two O atoms from a *L*-trp ligand and a D-trp ligand, and two O atoms from another two carboxyl groups of adjacent *L*-trp and D-trp (Fig. 1). The angles at the Ni^{II} atom (Table 1) show the Ni^{II} atom exists in a distorted octahedral geometry. The Ni—N bond distances is 2.096 (4) Å and the Ni—O bond distances are 2.037 (3) and 2.096 (4) Å. Furthermore, from Fig. 2, it can be seen that the complex shows a two-dimensional network structure assembled by double chains of ···-O—C—O—Ni—O—C—O—Ni.

Experimental

To an aqueous solution (5 ml) of *L*-trp (1.00 mmol), KOH (1.0 mmol) was added and stirred for 0.5 h at room temperature. Then an aqueous solution of nickel perchlorate (0.5 mmol) was dropped. The reaction mixture was airproofed with autoclave and keeped at 423 K for 72 h. The Cambridge blue rhomboidal column crystals were obtained after cooling to room temperature.

Refinement

H atoms were located in a difference map and refined as riding, with C—H = 0.93 − 0.98 and N—H = 0.86 − 0.90 Å, and with $U_{iso}(H) = 1.2U_{eq}(N,C)$. The highest peak in a difference Fourier map is located 1.17 Å from atom H2A.

Figures

Fig. 1. A part of the polymeric structure of the title complex. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted.

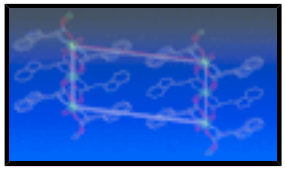

Fig. 2. A packing diagram of the title complex, viewed along the *b* axis. H atoms have been omitted.

rac-catena-Poly[nickel(II)-μ-[(_R_)-2-amino-3-(3-indolyl)propionato]- μ-[(_S_)-2-amino-3-(3-indolyl)propionato]]

Crystal data

$[Ni(C_{11}H_{11}N_2O_2)_2]$	F_{000} = 484
M_r = 465.15	D_x = 1.557 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point > 573 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 19.724 (3) Å	Cell parameters from 1329 reflections
b = 5.6139 (11) Å	θ = 3.1–25.3º
c = 9.0372 (18) Å	μ = 1.02 mm^{-1}
β = 97.616 (2)º	T = 298 (2) K
V = 991.9 (3) Å^3	Column, blue
Z = 2	0.23 × 0.15 × 0.12 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	1743 independent reflections
Radiation source: fine-focus sealed tube	1268 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.056
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	h = −23→23
T_{min} = 0.800, T_{max} = 0.888	k = −6→4
4673 measured reflections	l = −10→10

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.053	H-atom parameters not refined
$wR(F^2)$ = 0.145	$w = 1/[\sigma^2(F_o^2) + (0.068P)^2 + 1.7837P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
1743 reflections	$\Delta\rho_{max}$ = 1.12 e Å^{-3}
142 parameters	$\Delta\rho_{min}$ = −0.37 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	0.5000	0.5000	0.0247 (3)
N1	0.08527 (18)	0.3482 (8)	0.4204 (4)	0.0319 (9)
H1A	0.1170	0.3089	0.4975	0.038*
H1B	0.0728	0.2150	0.3683	0.038*
N2	0.3207 (2)	0.2013 (10)	0.3808 (5)	0.0553 (13)
H2	0.3397	0.0766	0.3494	0.066*
O1	0.01149 (15)	0.7461 (6)	0.3396 (3)	0.0326 (8)
O2	0.07096 (15)	0.8160 (7)	0.1518 (3)	0.0419 (9)
C1	0.0607 (2)	0.7074 (9)	0.2681 (5)	0.0311 (11)
C2	0.1135 (2)	0.5215 (11)	0.3245 (5)	0.0402 (13)
H2A	0.1249	0.4346	0.2370	0.048*
C3	0.1768 (3)	0.6344 (12)	0.3952 (6)	0.0511 (15)
H3A	0.1694	0.6884	0.4938	0.061*
H3B	0.1853	0.7743	0.3375	0.061*
C4	0.2533 (3)	0.2782 (14)	0.3365 (6)	0.0578 (18)
H4	0.2220	0.2016	0.2663	0.069*
C5	0.2400 (3)	0.4820 (11)	0.4112 (7)	0.0469 (13)
C6	0.3012 (2)	0.5362 (11)	0.5021 (6)	0.0449 (14)
C7	0.3498 (2)	0.3595 (11)	0.4816 (6)	0.0426 (13)
C8	0.4167 (3)	0.3702 (15)	0.5587 (7)	0.0641 (18)
H8	0.4483	0.2513	0.5463	0.077*
C9	0.4342 (3)	0.5554 (14)	0.6507 (8)	0.070 (2)
H9	0.4789	0.5669	0.6982	0.084*
C10	0.3882 (3)	0.7258 (15)	0.6757 (8)	0.073 (2)
H10	0.4018	0.8477	0.7428	0.087*
C11	0.3217 (3)	0.7233 (12)	0.6041 (8)	0.0614 (17)
H11	0.2909	0.8419	0.6225	0.074*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0225 (4)	0.0370 (5)	0.0160 (4)	0.0001 (4)	0.0077 (3)	−0.0006 (4)

N1	0.0244 (19)	0.046 (3)	0.0254 (19)	0.0039 (19)	0.0044 (15)	0.0032 (18)
N2	0.046 (3)	0.061 (3)	0.059 (3)	0.011 (3)	0.008 (2)	−0.005 (3)
O1	0.0296 (16)	0.046 (2)	0.0250 (16)	0.0046 (15)	0.0126 (13)	0.0082 (15)
O2	0.0276 (16)	0.066 (3)	0.0341 (18)	0.0095 (18)	0.0122 (14)	0.0230 (17)
C1	0.024 (2)	0.049 (3)	0.021 (2)	0.002 (2)	0.0064 (18)	0.006 (2)
C2	0.027 (2)	0.055 (4)	0.041 (3)	0.008 (3)	0.016 (2)	0.023 (3)
C3	0.044 (3)	0.059 (4)	0.050 (3)	0.003 (3)	0.005 (3)	−0.003 (3)
C4	0.038 (3)	0.088 (5)	0.045 (3)	−0.018 (3)	−0.006 (2)	0.014 (3)
C5	0.036 (3)	0.049 (3)	0.058 (3)	0.003 (3)	0.012 (2)	0.015 (3)
C6	0.028 (3)	0.054 (4)	0.054 (3)	0.004 (3)	0.014 (2)	0.012 (3)
C7	0.033 (3)	0.050 (4)	0.046 (3)	0.006 (3)	0.005 (2)	0.004 (3)
C8	0.039 (3)	0.083 (5)	0.069 (4)	0.016 (4)	0.000 (3)	0.013 (4)
C9	0.049 (4)	0.086 (6)	0.071 (5)	−0.003 (4)	−0.007 (3)	0.005 (4)
C10	0.062 (4)	0.085 (6)	0.070 (4)	−0.022 (4)	0.002 (3)	−0.005 (4)
C11	0.068 (4)	0.047 (4)	0.077 (4)	0.010 (3)	0.038 (3)	0.007 (3)

Geometric parameters (Å, °)

Ni1—O1^{i}	2.037 (3)	C2—H2A	0.9800
Ni1—O1	2.037 (3)	C3—C5	1.504 (8)
Ni1—N1	2.096 (4)	C3—H3A	0.9700
Ni1—N1^{i}	2.096 (4)	C3—H3B	0.9700
Ni1—O2^{ii}	2.098 (3)	C4—C5	1.371 (9)
Ni1—O2^{iii}	2.098 (3)	C4—H4	0.9300
N1—C2	1.462 (6)	C5—C6	1.400 (8)
N1—H1A	0.9000	C6—C7	1.408 (8)
N1—H1B	0.9000	C6—C11	1.420 (9)
N2—C7	1.346 (7)	C7—C8	1.410 (7)
N2—C4	1.405 (7)	C8—C9	1.347 (10)
N2—H2	0.8600	C8—H8	0.9300
O1—C1	1.254 (5)	C9—C10	1.358 (10)
O2—C1	1.254 (5)	C9—H9	0.9300
O2—Ni1^{iv}	2.098 (3)	C10—C11	1.384 (9)
C1—C2	1.514 (7)	C10—H10	0.9300
C2—C3	1.468 (7)	C11—H11	0.9300
O1^{i}—Ni1—O1	180.0	C3—C2—H2A	107.0
O1^{i}—Ni1—N1	97.96 (14)	C1—C2—H2A	107.0
O1—Ni1—N1	82.04 (14)	C2—C3—C5	116.3 (5)
O1^{i}—Ni1—N1^{i}	82.04 (14)	C2—C3—H3A	108.2
O1—Ni1—N1^{i}	97.96 (14)	C5—C3—H3A	108.2
N1—Ni1—N1^{i}	180.00 (10)	C2—C3—H3B	108.2
O1^{i}—Ni1—O2^{ii}	89.77 (14)	C5—C3—H3B	108.2
O1—Ni1—O2^{ii}	90.23 (14)	H3A—C3—H3B	107.4
N1—Ni1—O2^{ii}	85.90 (14)	C5—C4—N2	110.6 (5)
N1^{i}—Ni1—O2^{ii}	94.10 (14)	C5—C4—H4	124.7
O1^{i}—Ni1—O2^{iii}	90.23 (14)	N2—C4—H4	124.7

O1—Ni1—O2^{iii}	89.77 (14)	C4—C5—C6	105.3 (5)
N1—Ni1—O2^{iii}	94.10 (14)	C4—C5—C3	129.6 (5)
N1^{i}—Ni1—O2^{iii}	85.90 (14)	C6—C5—C3	124.9 (6)
O2^{ii}—Ni1—O2^{iii}	180.0	C5—C6—C7	108.6 (5)
C2—N1—Ni1	108.6 (3)	C5—C6—C11	133.6 (6)
C2—N1—H1A	110.0	C7—C6—C11	117.8 (5)
Ni1—N1—H1A	110.0	N2—C7—C6	108.5 (5)
C2—N1—H1B	110.0	N2—C7—C8	130.5 (6)
Ni1—N1—H1B	110.0	C6—C7—C8	120.9 (6)
H1A—N1—H1B	108.4	C9—C8—C7	118.9 (6)
C7—N2—C4	107.0 (5)	C9—C8—H8	120.6
C7—N2—H2	126.5	C7—C8—H8	120.6
C4—N2—H2	126.5	C8—C9—C10	121.7 (6)
C1—O1—Ni1	114.6 (3)	C8—C9—H9	119.2
C1—O2—Ni1^{iv}	128.3 (3)	C10—C9—H9	119.2
O2—C1—O1	124.7 (4)	C9—C10—C11	121.9 (7)
O2—C1—C2	115.9 (4)	C9—C10—H10	119.1
O1—C1—C2	119.4 (4)	C11—C10—H10	119.1
N1—C2—C3	113.4 (4)	C10—C11—C6	118.8 (6)
N1—C2—C1	111.0 (3)	C10—C11—H11	120.6
C3—C2—C1	110.9 (5)	C6—C11—H11	120.6
N1—C2—H2A	107.0		
O1^{i}—Ni1—N1—C2	−167.6 (3)	N2—C4—C5—C6	1.3 (6)
O1—Ni1—N1—C2	12.4 (3)	N2—C4—C5—C3	176.6 (6)
O2^{ii}—Ni1—N1—C2	−78.4 (3)	C2—C3—C5—C4	19.8 (9)
O2^{iii}—Ni1—N1—C2	101.6 (3)	C2—C3—C5—C6	−165.7 (5)
N1—Ni1—O1—C1	−0.5 (3)	C4—C5—C6—C7	−1.1 (6)
N1^{i}—Ni1—O1—C1	179.5 (3)	C3—C5—C6—C7	−176.7 (5)
O2^{ii}—Ni1—O1—C1	85.3 (3)	C4—C5—C6—C11	179.1 (6)
O2^{iii}—Ni1—O1—C1	−94.7 (3)	C3—C5—C6—C11	3.5 (10)
Ni1^{iv}—O2—C1—O1	−22.6 (8)	C4—N2—C7—C6	0.2 (6)
Ni1^{iv}—O2—C1—C2	158.9 (3)	C4—N2—C7—C8	−178.5 (6)
Ni1—O1—C1—O2	169.3 (4)	C5—C6—C7—N2	0.6 (6)
Ni1—O1—C1—C2	−12.1 (6)	C11—C6—C7—N2	−179.6 (5)
Ni1—N1—C2—C3	104.8 (4)	C5—C6—C7—C8	179.4 (5)
Ni1—N1—C2—C1	−20.8 (5)	C11—C6—C7—C8	−0.8 (8)
O2—C1—C2—N1	−158.3 (4)	N2—C7—C8—C9	177.2 (6)
O1—C1—C2—N1	23.0 (7)	C6—C7—C8—C9	−1.3 (9)
O2—C1—C2—C3	74.6 (6)	C7—C8—C9—C10	2.9 (11)
O1—C1—C2—C3	−104.0 (5)	C8—C9—C10—C11	−2.4 (11)
N1—C2—C3—C5	73.4 (6)	C9—C10—C11—C6	0.2 (10)
C1—C2—C3—C5	−160.9 (5)	C5—C6—C11—C10	−178.9 (6)
C7—N2—C4—C5	−0.9 (7)	C7—C6—C11—C10	1.3 (8)

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) *x*, −*y*+3/2, *z*+1/2; (iii) −*x*, *y*−1/2, −*z*+1/2; (iv) −*x*, *y*+1/2, −*z*+1/2.

Fig. 1

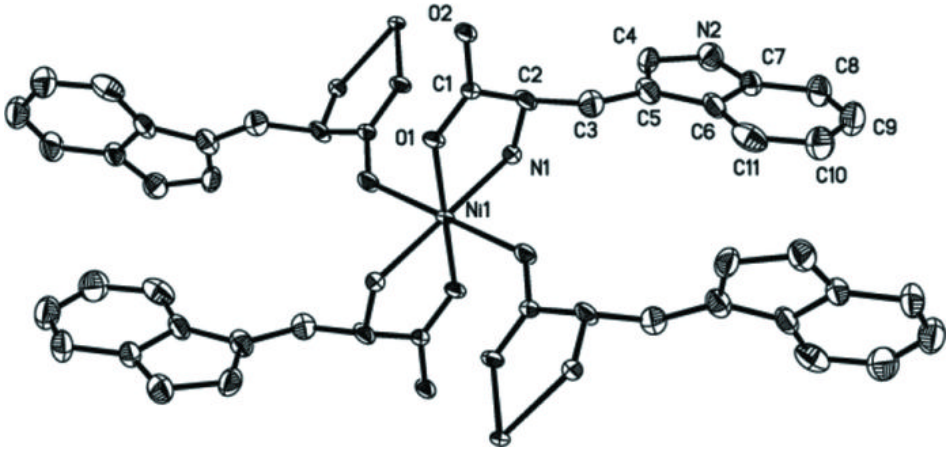

Fig. 2