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Synthesis and Characterization of Nickel(II) Tetraaza Macrocyclic Complex with 1,1-Cyclohexanediacetate Ligand

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Computing details

Data collection: Bruker APEX2; cell refinement: Bruker SAINT; data reduction: Bruker SAINT; program(s) used to solve structure: SHELXS-97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL-97 (Sheldrick, 2008); molecular graphics: Bruker SHELXTL; software used to prepare material for publication: Bruker SHELXTL.

Crystal data

$C_{30}H_{54}N_4NiO_4$	$Z = 2$
$M_r = 593.48$	$F(000) = 644$
Triclinic, $P\bar{1}$	$D_x = 1.248$ Mg m^{-3} $D_m = 0$ Mg m^{-3} D_m measured by ?
$a = 11.3918$ (7) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 12.6196$ (8) Å	Cell parameters from 3846 reflections
$c = 12.8700$ (8) Å	$\theta = 2.5$–$24.6°$
$\alpha = 69.572$ (4)°	$\mu = 0.65$ mm^{-1}
$\beta = 83.516$ (4)°	$T = 296$ K
$\gamma = 65.753$ (4)°	Block, purple
$V = 1579.88$ (17) Å^3	0.14 × 0.08 × 0.06 mm

Data collection

Bruker APEX-II CCD diffractometer	7837 independent reflections
Radiation source: fine-focus sealed tube	4651 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.0000$
ϕ and ω scans	$\theta_{max} = 28.5°$, $\theta_{min} = 1.7°$
Absorption correction: multi-scan ?	$h = -15 \rightarrow 15$
$T_{min} = 0.914$, $T_{max} = 0.962$	$k = -15 \rightarrow 16$
7837 measured reflections	$l = 0 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.074$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.276$	$w = 1/[\sigma^2(F_o^2) + (0.1639P)^2 + 0.266P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
7837 reflections	$\Delta\rangle_{max} = 1.95$ e Å^{-3}
356 parameters	$\Delta\rangle_{min} = -0.51$ e Å^{-3}
0 restraints	Extinction correction: SHELXL, $Fc^* = kFc[1+0.001\times Fc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.004 (2)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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	0.5000	0.0000	0.5000	0.0318 (2)
Ni2	0.0000	0.5000	0.0000	0.0310 (2)
O1	0.4918 (3)	0.1775 (3)	0.3785 (3)	0.0388 (7)
O2	0.5807 (4)	0.1291 (3)	0.2300 (3)	0.0702 (13)
O3	0.1073 (3)	0.4854 (3)	0.1351 (2)	0.0381 (7)
O4	0.2237 (4)	0.2838 (3)	0.2178 (3)	0.0526 (9)
N1	0.5763 (3)	-0.0880 (3)	0.3846 (3)	0.0337 (8)
HN1	0.5825	-0.0279	0.3199	0.040*
N2	0.3077 (3)	0.0700 (3)	0.4456 (3)	0.0336 (8)
HN2	0.2975	0.1417	0.3864	0.040*
N3	0.1067 (4)	0.3187 (3)	0.0142 (3)	0.0338 (8)
HN3	0.1644	0.2857	0.0741	0.041*
N4	-0.1322 (3)	0.4321 (3)	0.0941 (3)	0.0341 (8)
HN4	-0.1892	0.4453	0.0400	0.041*
C1	0.2266 (4)	0.1148 (4)	0.5323 (4)	0.0365 (10)
H1	0.2231	0.0415	0.5943	0.044*
C2	0.0883 (4)	0.2027 (5)	0.4907 (4)	0.0480 (12)
H2A	0.0897	0.2736	0.4262	0.058*
H2B	0.0479	0.1593	0.4656	0.058*
C3	0.0083 (5)	0.2496 (6)	0.5797 (5)	0.0613 (16)
H3A	-0.0029	0.1802	0.6400	0.074*
H3B	-0.0780	0.3110	0.5478	0.074*
C4	0.9271 (5)	-0.3092 (5)	0.3722 (5)	0.0608 (15)

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

H4A	0.9778	-0.3333	0.3104	0.073*
H4B	0.9255	-0.3847	0.4303	0.073*
C5	0.7903 (5)	-0.2203 (5)	0.3303 (4)	0.0509 (13)
H5A	0.7495	-0.2618	0.3029	0.061*
H5B	0.7925	-0.1484	0.2675	0.061*
C6	0.7099 (4)	-0.1760 (4)	0.4217 (4)	0.0348 (10)
H6	0.7066	-0.2495	0.4833	0.042*
C7	0.4957 (5)	-0.1391 (4)	0.3554 (4)	0.0415 (11)
H7A	0.4877	-0.2055	0.4215	0.050*
H7B	0.5375	-0.1759	0.2974	0.050*
C8	0.3637 (5)	-0.0420 (4)	0.3137 (4)	0.0437 (11)
H8A	0.3255	-0.0727	0.2711	0.052*
H8B	0.3745	0.0319	0.2608	0.052*
C9	0.2658 (4)	-0.0007 (4)	0.3986 (4)	0.0398 (11)
H9	0.1817	0.0568	0.3576	0.048*
C10	0.2443 (6)	-0.1067 (5)	0.4864 (5)	0.0553 (14)
H10A	0.3248	-0.1638	0.5296	0.083*
H10B	0.2166	-0.1502	0.4509	0.083*
H10C	0.1776	-0.0750	0.5359	0.083*
C11	-0.0677 (4)	0.2966 (4)	0.1379 (4)	0.0357 (10)
H11	-0.0104	0.2732	0.2026	0.043*
C12	-0.1603 (5)	0.2323 (5)	0.1761 (4)	0.0488 (12)
H12A	-0.2218	0.2593	0.1143	0.059*
H12B	-0.2103	0.2570	0.2380	0.059*
C13	-0.0894 (6)	0.0918 (5)	0.2145 (5)	0.0562 (14)
H13A	-0.0340	0.0638	0.2808	0.067*
H13B	-0.1530	0.0536	0.2354	0.067*
C14	-0.0074 (6)	0.0504 (5)	0.1236 (5)	0.0576 (15)
H14A	-0.0636	0.0716	0.0598	0.069*
H14B	0.0406	-0.0403	0.1514	0.069*
C15	0.0870 (5)	0.1118 (4)	0.0859 (5)	0.0481 (12)
H15A	0.1370	0.0859	0.0245	0.058*
H15B	0.1482	0.0842	0.1480	0.058*
C16	0.0175 (4)	0.2545 (4)	0.0460 (4)	0.0369 (10)
H16	-0.0394	0.2813	-0.0200	0.044*
C17	0.1844 (5)	0.2998 (4)	-0.0822 (4)	0.0402 (11)
H17A	0.1264	0.3320	-0.1478	0.048*
H17B	0.2341	0.2104	-0.0674	0.048*
C18	-0.2763 (4)	0.6363 (4)	0.1074 (4)	0.0422 (11)
H18A	-0.3168	0.6522	0.0364	0.051*
H18B	-0.3457	0.6754	0.1525	0.051*
C19	-0.2195 (5)	0.4943 (4)	0.1694 (4)	0.0425 (11)
H19	-0.2929	0.4676	0.1841	0.051*
C20	-0.1550 (6)	0.4574 (5)	0.2787 (4)	0.0534 (14)
H20A	-0.1410	0.3717	0.3214	0.080*
H20B	-0.2098	0.5112	0.3199	0.080*
H20C	-0.0720	0.4651	0.2665	0.080*
C21	0.5168 (4)	0.2065 (4)	0.2761 (4)	0.0399 (11)
C22	0.4711 (4)	0.3394 (4)	0.2034 (4)	0.0370 (10)

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

H22A	0.4316	0.3460	0.1356	0.044*
H22B	0.5493	0.3564	0.1802	0.044*
C23	0.1904 (4)	0.3957 (4)	0.2056 (4)	0.0339 (9)
C24	0.2531 (4)	0.4255 (4)	0.2824 (4)	0.0358 (10)
H24A	0.2734	0.3577	0.3545	0.043*
H24B	0.1902	0.5012	0.2957	0.043*
C25	0.3781 (4)	0.4452 (4)	0.2406 (4)	0.0345 (10)
C26	0.3477 (5)	0.5651 (4)	0.1416 (4)	0.0467 (12)
H26A	0.4297	0.5696	0.1105	0.056*
H26B	0.3001	0.5626	0.0833	0.056*
C27	0.2680 (6)	0.6817 (5)	0.1708 (5)	0.0621 (16)
H27A	0.2573	0.7552	0.1047	0.075*
H27B	0.1813	0.6832	0.1928	0.075*
C28	0.3328 (7)	0.6866 (5)	0.2655 (6)	0.0749 (19)
H28A	0.4142	0.6964	0.2400	0.090*
H28B	0.2759	0.7591	0.2867	0.090*
C29	0.3614 (6)	0.5711 (5)	0.3655 (5)	0.0641 (16)
H29A	0.2794	0.5664	0.3967	0.077*
H29B	0.4089	0.5746	0.4233	0.077*
C30	0.4424 (5)	0.4550 (5)	0.3339 (5)	0.0470 (12)
H30A	0.5275	0.4564	0.3098	0.056*
H30B	0.4568	0.3809	0.4003	0.056*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0287 (4)	0.0311 (4)	0.0357 (5)	-0.0073 (3)	-0.0020 (3)	-0.0160 (3)
Ni2	0.0286 (4)	0.0316 (4)	0.0318 (4)	-0.0103 (3)	0.0000 (3)	-0.0110 (3)
O1	0.0386 (18)	0.0320 (16)	0.0433 (18)	-0.0119 (14)	-0.0040 (14)	-0.0109 (14)
O2	0.089 (3)	0.039 (2)	0.061 (3)	-0.013 (2)	0.029 (2)	-0.0156 (18)
O3	0.0363 (17)	0.0349 (16)	0.0367 (17)	-0.0092 (14)	-0.0103 (14)	-0.0069 (14)
O4	0.062 (2)	0.0366 (17)	0.057 (2)	-0.0164 (16)	-0.0256 (19)	-0.0087 (16)
N1	0.035 (2)	0.0311 (18)	0.035 (2)	-0.0089 (16)	-0.0046 (16)	-0.0145 (16)
N2	0.0325 (19)	0.0350 (19)	0.0334 (19)	-0.0113 (16)	-0.0014 (16)	-0.0133 (16)
N3	0.0341 (19)	0.0346 (19)	0.0314 (19)	-0.0122 (16)	-0.0023 (15)	-0.0101 (16)
N4	0.0308 (19)	0.0352 (19)	0.035 (2)	-0.0123 (16)	0.0005 (16)	-0.0115 (16)
C1	0.032 (2)	0.039 (2)	0.039 (2)	-0.0109 (19)	0.0034 (19)	-0.017 (2)
C2	0.032 (2)	0.056 (3)	0.050 (3)	-0.006 (2)	0.001 (2)	-0.024 (3)
C3	0.029 (3)	0.066 (4)	0.070 (4)	0.000 (2)	0.005 (3)	-0.024 (3)
C4	0.048 (3)	0.051 (3)	0.070 (4)	0.003 (3)	0.003 (3)	-0.033 (3)
C5	0.048 (3)	0.052 (3)	0.050 (3)	-0.010 (2)	0.003 (2)	-0.027 (3)
C6	0.033 (2)	0.032 (2)	0.033 (2)	-0.0058 (18)	0.0011 (19)	-0.0126 (19)
C7	0.043 (3)	0.038 (2)	0.048 (3)	-0.011 (2)	-0.006 (2)	-0.024 (2)
C8	0.047 (3)	0.043 (3)	0.047 (3)	-0.015 (2)	-0.006 (2)	-0.024 (2)
C9	0.035 (2)	0.043 (3)	0.042 (3)	-0.015 (2)	-0.008 (2)	-0.014 (2)
C10	0.058 (3)	0.053 (3)	0.071 (4)	-0.030 (3)	0.006 (3)	-0.030 (3)
C11	0.034 (2)	0.035 (2)	0.035 (2)	-0.0128 (19)	-0.0005 (19)	-0.0085 (19)
C12	0.050 (3)	0.045 (3)	0.049 (3)	-0.023 (2)	0.005 (2)	-0.008 (2)
C13	0.062 (4)	0.043 (3)	0.062 (3)	-0.027 (3)	0.002 (3)	-0.008 (3)

Atomic displacement parameters ($Å^2$)

C14	0.068 (4)	0.034 (3)	0.069 (4)	-0.023 (3)	0.004 (3)	-0.013 (3)
C15	0.049 (3)	0.040 (3)	0.051 (3)	-0.016 (2)	0.004 (2)	-0.014 (2)
C16	0.040 (2)	0.034 (2)	0.034 (2)	-0.015 (2)	-0.002 (2)	-0.0070 (19)
C17	0.045 (3)	0.037 (2)	0.037 (2)	-0.013 (2)	0.005 (2)	-0.015 (2)
C18	0.033 (2)	0.041 (3)	0.046 (3)	-0.008 (2)	0.009 (2)	-0.017 (2)
C19	0.042 (3)	0.047 (3)	0.042 (3)	-0.020 (2)	0.012 (2)	-0.018 (2)
C20	0.066 (4)	0.053 (3)	0.039 (3)	-0.020 (3)	0.008 (3)	-0.021 (2)
C21	0.037 (2)	0.036 (2)	0.042 (3)	-0.012 (2)	0.009 (2)	-0.013 (2)
C22	0.035 (2)	0.037 (2)	0.037 (2)	-0.0147 (19)	0.0039 (19)	-0.009 (2)
C23	0.031 (2)	0.035 (2)	0.033 (2)	-0.0124 (18)	-0.0024 (18)	-0.0081 (19)
C24	0.035 (2)	0.040 (2)	0.035 (2)	-0.0146 (19)	-0.0005 (19)	-0.015 (2)
C25	0.032 (2)	0.029 (2)	0.040 (2)	-0.0092 (18)	-0.0044 (19)	-0.0115 (19)
C26	0.046 (3)	0.038 (3)	0.053 (3)	-0.018 (2)	-0.004 (2)	-0.008 (2)
C27	0.065 (4)	0.034 (3)	0.077 (4)	-0.015 (3)	-0.005 (3)	-0.010 (3)
C28	0.082 (5)	0.051 (3)	0.105 (5)	-0.025 (3)	-0.013 (4)	-0.040 (4)
C29	0.071 (4)	0.057 (3)	0.076 (4)	-0.020 (3)	-0.019 (3)	-0.036 (3)
C30	0.039 (3)	0.042 (3)	0.058 (3)	-0.011 (2)	-0.015 (2)	-0.015 (2)

Geometric parameters (Å, º)

Ni1—Ni2	8.0051 (6)	C10—H10A	0.9800
Ni1—N1^{i}	2.064 (3)	C10—H10B	0.9800
Ni1—N1	2.064 (3)	C10—H10C	0.9800
Ni1—N2^{i}	2.097 (4)	C11—C12	1.523 (6)
Ni1—N2	2.097 (4)	C11—C16	1.542 (6)
Ni1—O1^{i}	2.211 (3)	C11—H11	1.0000
Ni1—O1	2.211 (3)	C12—C13	1.531 (7)
Ni2—N3^{ii}	2.054 (4)	C12—H12A	0.9900
Ni2—N3	2.054 (4)	C12—H12B	0.9900
Ni2—N4^{ii}	2.096 (3)	C13—C14	1.514 (8)
Ni2—N4	2.096 (3)	C13—H13A	0.9900
Ni2—O3	2.150 (3)	C13—H13B	0.9900
Ni2—O3^{ii}	2.150 (3)	C14—C15	1.515 (7)
O1—C21	1.271 (5)	C14—H14A	0.9900
O2—C21	1.248 (6)	C14—H14B	0.9900
O3—C23	1.264 (5)	C15—C16	1.552 (6)
O4—C23	1.257 (5)	C15—H15A	0.9900
N1—C7	1.460 (6)	C15—H15B	0.9900
N1—C6	1.478 (6)	C16—H16	1.0000
N1—HN1	0.9300	C17—C18^{ii}	1.512 (7)
N2—C9	1.476 (6)	C17—H17A	0.9900
N2—C1	1.483 (5)	C17—H17B	0.9900
N2—HN2	0.9300	C18—C17^{ii}	1.512 (7)
N3—C17	1.471 (6)	C18—C19	1.559 (6)
N3—C16	1.486 (6)	C18—H18A	0.9900
N3—HN3	0.9300	C18—H18B	0.9900
N4—C11	1.473 (5)	C19—C20	1.493 (7)
N4—C19	1.489 (6)	C19—H19	1.0000
N4—HN4	0.9300	C20—H20A	0.9800

Geometric parameters (Å, º)

C1—C2	1.529 (6)	C20—H20B	0.9800
C1—C6^{i}	1.531 (6)	C20—H20C	0.9800
C1—H1	1.0000	C21—C22	1.503 (6)
C2—C3	1.513 (7)	C22—C25	1.518 (6)
C2—H2A	0.9900	C22—H22A	0.9900
C2—H2B	0.9900	C22—H22B	0.9900
C3—C4^{i}	1.541 (8)	C23—C24	1.507 (6)
C3—H3A	0.9900	C24—C25	1.549 (6)
C3—H3B	0.9900	C24—H24A	0.9900
C4—C5	1.519 (7)	C24—H24B	0.9900
C4—C3^{i}	1.541 (8)	C25—C26	1.535 (6)
C4—H4A	0.9900	C25—C30	1.539 (6)
C4—H4B	0.9900	C26—C27	1.531 (7)
C5—C6	1.526 (6)	C26—H26A	0.9900
C5—H5A	0.9900	C26—H26B	0.9900
C5—H5B	0.9900	C27—C28	1.526 (9)
C6—C1^{i}	1.531 (6)	C27—H27A	0.9900
C6—H6	1.0000	C27—H27B	0.9900
C7—C8	1.503 (6)	C28—C29	1.510 (9)
C7—H7A	0.9900	C28—H28A	0.9900
C7—H7B	0.9900	C28—H28B	0.9900
C8—C9	1.535 (7)	C29—C30	1.544 (7)
C8—H8A	0.9900	C29—H29A	0.9900
C8—H8B	0.9900	C29—H29B	0.9900
C9—C10	1.509 (7)	C30—H30A	0.9900
C9—H9	1.0000	C30—H30B	0.9900
N1^{i}—Ni1—N1	180.00 (11)	H10B—C10—H10C	109.5
N1^{i}—Ni1—N2^{i}	95.53 (14)	N4—C11—C12	113.8 (4)
N1—Ni1—N2^{i}	84.47 (14)	N4—C11—C16	107.4 (3)
N1^{i}—Ni1—N2	84.47 (14)	C12—C11—C16	110.7 (4)
N1—Ni1—N2	95.53 (14)	N4—C11—H11	108.3
N2^{i}—Ni1—N2	180.0	C12—C11—H11	108.3
N1^{i}—Ni1—O1^{i}	91.22 (13)	C16—C11—H11	108.3
N1—Ni1—O1^{i}	88.78 (13)	C11—C12—C13	111.9 (4)
N2^{i}—Ni1—O1^{i}	82.63 (13)	C11—C12—H12A	109.2
N2—Ni1—O1^{i}	97.37 (13)	C13—C12—H12A	109.2
N1^{i}—Ni1—O1	88.78 (13)	C11—C12—H12B	109.2
N1—Ni1—O1	91.22 (13)	C13—C12—H12B	109.2
N2^{i}—Ni1—O1	97.37 (13)	H12A—C12—H12B	107.9
N2—Ni1—O1	82.63 (13)	C14—C13—C12	111.0 (4)
O1^{i}—Ni1—O1	180.0	C14—C13—H13A	109.4
N3^{ii}—Ni2—N3	180.0 (2)	C12—C13—H13A	109.4
N3^{ii}—Ni2—N4^{ii}	83.97 (14)	C14—C13—H13B	109.4
N3—Ni2—N4^{ii}	96.03 (14)	C12—C13—H13B	109.4
N3^{ii}—Ni2—N4	96.03 (14)	H13A—C13—H13B	108.0
N3—Ni2—N4	83.97 (14)	C13—C14—C15	110.8 (5)
N4^{ii}—Ni2—N4	180.0	C13—C14—H14A	109.5
N3^{ii}—Ni2—O3	88.03 (13)	C15—C14—H14A	109.5

Geometric parameters (Å, º)

N3—Ni2—O3	91.97 (13)	C13—C14—H14B	109.5
N4^{ii}—Ni2—O3	82.06 (13)	C15—C14—H14B	109.5
N4—Ni2—O3	97.94 (13)	H14A—C14—H14B	108.1
N3^{ii}—Ni2—O3^{ii}	91.97 (13)	C14—C15—C16	111.8 (4)
N3—Ni2—O3^{ii}	88.03 (13)	C14—C15—H15A	109.3
N4^{ii}—Ni2—O3^{ii}	97.94 (13)	C16—C15—H15A	109.3
N4—Ni2—O3^{ii}	82.06 (13)	C14—C15—H15B	109.3
O3—Ni2—O3^{ii}	180.0	C16—C15—H15B	109.3
C21—O1—Ni1	130.8 (3)	H15A—C15—H15B	107.9
C23—O3—Ni2	133.4 (3)	N3—C16—C11	107.9 (4)
C7—N1—C6	115.3 (3)	N3—C16—C15	113.7 (4)
C7—N1—Ni1	114.8 (3)	C11—C16—C15	110.2 (4)
C6—N1—Ni1	107.9 (3)	N3—C16—H16	108.3
C7—N1—HN1	106.0	C11—C16—H16	108.3
C6—N1—HN1	106.0	C15—C16—H16	108.3
Ni1—N1—HN1	106.0	N3—C17—C18^{ii}	111.8 (4)
C9—N2—C1	116.4 (3)	N3—C17—H17A	109.3
C9—N2—Ni1	119.6 (3)	C18^{ii}—C17—H17A	109.3
C1—N2—Ni1	106.8 (3)	N3—C17—H17B	109.3
C9—N2—HN2	104.0	C18^{ii}—C17—H17B	109.3
C1—N2—HN2	104.0	H17A—C17—H17B	107.9
Ni1—N2—HN2	104.0	C17^{ii}—C18—C19	117.4 (4)
C17—N3—C16	114.6 (3)	C17^{ii}—C18—H18A	108.0
C17—N3—Ni2	114.8 (3)	C19—C18—H18A	108.0
C16—N3—Ni2	107.1 (3)	C17^{ii}—C18—H18B	108.0
C17—N3—HN3	106.6	C19—C18—H18B	108.0
C16—N3—HN3	106.6	H18A—C18—H18B	107.2
Ni2—N3—HN3	106.6	N4—C19—C20	112.3 (4)
C11—N4—C19	117.1 (3)	N4—C19—C18	108.7 (4)
C11—N4—Ni2	108.0 (3)	C20—C19—C18	113.4 (4)
C19—N4—Ni2	120.9 (3)	N4—C19—H19	107.4
C11—N4—HN4	102.6	C20—C19—H19	107.4
C19—N4—HN4	102.6	C18—C19—H19	107.4
Ni2—N4—HN4	102.6	C19—C20—H20A	109.5
N2—C1—C2	112.9 (4)	C19—C20—H20B	109.5
N2—C1—C6^{i}	109.3 (3)	H20A—C20—H20B	109.5
C2—C1—C6^{i}	110.9 (4)	C19—C20—H20C	109.5
N2—C1—H1	107.9	H20A—C20—H20C	109.5
C2—C1—H1	107.9	H20B—C20—H20C	109.5
C6^{i}—C1—H1	107.9	O2—C21—O1	123.4 (4)
C3—C2—C1	111.9 (4)	O2—C21—C22	116.0 (4)
C3—C2—H2A	109.2	O1—C21—C22	120.6 (4)
C1—C2—H2A	109.2	C21—C22—C25	123.4 (4)
C3—C2—H2B	109.2	C21—C22—H22A	106.5
C1—C2—H2B	109.2	C25—C22—H22A	106.5
H2A—C2—H2B	107.9	C21—C22—H22B	106.5
C2—C3—C4^{i}	111.2 (5)	C25—C22—H22B	106.5
C2—C3—H3A	109.4	H22A—C22—H22B	106.5
C4^{i}—C3—H3A	109.4	O4—C23—O3	125.5 (4)

Geometric parameters (Å, º)

C2—C3—H3B	109.4	O4—C23—C24	117.4 (4)
C4^{i}—C3—H3B	109.4	O3—C23—C24	117.1 (4)
H3A—C3—H3B	108.0	C23—C24—C25	115.5 (4)
C5—C4—C3^{i}	110.8 (4)	C23—C24—H24A	108.4
C5—C4—H4A	109.5	C25—C24—H24A	108.4
C3^{i}—C4—H4A	109.5	C23—C24—H24B	108.4
C5—C4—H4B	109.5	C25—C24—H24B	108.4
C3^{i}—C4—H4B	109.5	H24A—C24—H24B	107.5
H4A—C4—H4B	108.1	C22—C25—C26	108.0 (4)
C4—C5—C6	111.4 (4)	C22—C25—C30	109.7 (4)
C4—C5—H5A	109.4	C26—C25—C30	108.0 (4)
C6—C5—H5A	109.4	C22—C25—C24	110.7 (3)
C4—C5—H5B	109.4	C26—C25—C24	110.6 (4)
C6—C5—H5B	109.4	C30—C25—C24	109.7 (4)
H5A—C5—H5B	108.0	C27—C26—C25	113.8 (5)
N1—C6—C5	113.4 (4)	C27—C26—H26A	108.8
N1—C6—C1^{i}	108.5 (3)	C25—C26—H26A	108.8
C5—C6—C1^{i}	110.3 (4)	C27—C26—H26B	108.8
N1—C6—H6	108.2	C25—C26—H26B	108.8
C5—C6—H6	108.2	H26A—C26—H26B	107.7
C1^{i}—C6—H6	108.2	C28—C27—C26	111.2 (5)
N1—C7—C8	111.5 (4)	C28—C27—H27A	109.4
N1—C7—H7A	109.3	C26—C27—H27A	109.4
C8—C7—H7A	109.3	C28—C27—H27B	109.4
N1—C7—H7B	109.3	C26—C27—H27B	109.4
C8—C7—H7B	109.3	H27A—C27—H27B	108.0
H7A—C7—H7B	108.0	C29—C28—C27	111.5 (5)
C7—C8—C9	118.4 (4)	C29—C28—H28A	109.3
C7—C8—H8A	107.7	C27—C28—H28A	109.3
C9—C8—H8A	107.7	C29—C28—H28B	109.3
C7—C8—H8B	107.7	C27—C28—H28B	109.3
C9—C8—H8B	107.7	H28A—C28—H28B	108.0
H8A—C8—H8B	107.1	C28—C29—C30	110.9 (5)
N2—C9—C10	112.9 (4)	C28—C29—H29A	109.5
N2—C9—C8	108.5 (4)	C30—C29—H29A	109.5
C10—C9—C8	112.7 (4)	C28—C29—H29B	109.5
N2—C9—H9	107.5	C30—C29—H29B	109.5
C10—C9—H9	107.5	H29A—C29—H29B	108.1
C8—C9—H9	107.5	C25—C30—C29	113.0 (4)
C9—C10—H10A	109.5	C25—C30—H30A	109.0
C9—C10—H10B	109.5	C29—C30—H30A	109.0
H10A—C10—H10B	109.5	C25—C30—H30B	109.0
C9—C10—H10C	109.5	C29—C30—H30B	109.0
H10A—C10—H10C	109.5	H30A—C30—H30B	107.8
N1^{i}—Ni1—O1—C21	-175.1 (4)	C4—C5—C6—N1	179.3 (4)
N1—Ni1—O1—C21	4.9 (4)	C4—C5—C6—C1^{i}	57.4 (6)
N2^{i}—Ni1—O1—C21	89.5 (4)	C6—N1—C7—C8	-177.3 (4)
N2—Ni1—O1—C21	-90.5 (4)	Ni1—N1—C7—C8	56.3 (5)

Geometric parameters (Å, º)

O1^{i}—Ni1—O1—C21	0 (100)	N1—C7—C8—C9	-77.5 (6)
N3^{ii}—Ni2—O3—C23	170.9 (4)	C1—N2—C9—C10	-52.6 (5)
N3—Ni2—O3—C23	-9.1 (4)	Ni1—N2—C9—C10	78.3 (4)
N4^{ii}—Ni2—O3—C23	-104.9 (4)	C1—N2—C9—C8	-178.2 (4)
N4—Ni2—O3—C23	75.1 (4)	Ni1—N2—C9—C8	-47.4 (4)
O3^{ii}—Ni2—O3—C23	-157.5 (4)	C7—C8—C9—N2	70.0 (5)
N1^{i}—Ni1—N1—C7	-172 (100)	C7—C8—C9—C10	-55.8 (6)
N2^{i}—Ni1—N1—C7	145.6 (3)	C19—N4—C11—C12	57.7 (5)
N2—Ni1—N1—C7	-34.4 (3)	Ni2—N4—C11—C12	-161.7 (3)
O1^{i}—Ni1—N1—C7	62.8 (3)	C19—N4—C11—C16	-179.4 (4)
O1—Ni1—N1—C7	-117.2 (3)	Ni2—N4—C11—C16	-38.8 (4)
N1^{i}—Ni1—N1—C6	58 (100)	N4—C11—C12—C13	176.6 (4)
N2^{i}—Ni1—N1—C6	15.5 (3)	C16—C11—C12—C13	55.6 (6)
N2—Ni1—N1—C6	-164.5 (3)	C11—C12—C13—C14	-56.6 (6)
O1^{i}—Ni1—N1—C6	-67.2 (3)	C12—C13—C14—C15	56.6 (7)
O1—Ni1—N1—C6	112.8 (3)	C13—C14—C15—C16	-56.7 (6)
N1^{i}—Ni1—N2—C9	-148.0 (3)	C17—N3—C16—C11	-173.1 (4)
N1—Ni1—N2—C9	32.0 (3)	Ni2—N3—C16—C11	-44.5 (4)
N2^{i}—Ni1—N2—C9	169 (100)	C17—N3—C16—C15	64.4 (5)
O1^{i}—Ni1—N2—C9	-57.4 (3)	Ni2—N3—C16—C15	-167.0 (3)
O1—Ni1—N2—C9	122.6 (3)	N4—C11—C16—N3	56.3 (5)
N1^{i}—Ni1—N2—C1	-13.0 (3)	C12—C11—C16—N3	-179.0 (4)
N1—Ni1—N2—C1	167.0 (3)	N4—C11—C16—C15	-179.1 (4)
N2^{i}—Ni1—N2—C1	-56 (100)	C12—C11—C16—C15	-54.3 (5)
O1^{i}—Ni1—N2—C1	77.5 (3)	C14—C15—C16—N3	176.7 (4)
O1—Ni1—N2—C1	-102.5 (3)	C14—C15—C16—C11	55.5 (6)
N3^{ii}—Ni2—N3—C17	-73 (100)	C16—N3—C17—C18^{ii}	-177.9 (4)
N4^{ii}—Ni2—N3—C17	-33.2 (3)	Ni2—N3—C17—C18^{ii}	57.4 (5)
N4—Ni2—N3—C17	146.8 (3)	C11—N4—C19—C20	53.2 (5)
O3—Ni2—N3—C17	-115.5 (3)	Ni2—N4—C19—C20	-82.1 (4)
O3^{ii}—Ni2—N3—C17	64.5 (3)	C11—N4—C19—C18	179.5 (4)
N3^{ii}—Ni2—N3—C16	159 (100)	Ni2—N4—C19—C18	44.3 (5)
N4^{ii}—Ni2—N3—C16	-161.7 (3)	C17^{ii}—C18—C19—N4	-68.0 (5)
N4—Ni2—N3—C16	18.3 (3)	C17^{ii}—C18—C19—C20	57.8 (6)
O3—Ni2—N3—C16	116.1 (3)	Ni1—O1—C21—O2	-17.5 (7)
O3^{ii}—Ni2—N3—C16	-63.9 (3)	Ni1—O1—C21—C22	163.6 (3)
N3^{ii}—Ni2—N4—C11	-168.0 (3)	O2—C21—C22—C25	171.8 (5)
N3—Ni2—N4—C11	12.0 (3)	O1—C21—C22—C25	-9.2 (7)
N4^{ii}—Ni2—N4—C11	0 (100)	Ni2—O3—C23—O4	-6.3 (7)
O3—Ni2—N4—C11	-79.1 (3)	Ni2—O3—C23—C24	174.6 (3)
O3^{ii}—Ni2—N4—C11	100.9 (3)	O4—C23—C24—C25	90.5 (5)
N3^{ii}—Ni2—N4—C19	-29.2 (3)	O3—C23—C24—C25	-90.3 (5)
N3—Ni2—N4—C19	150.8 (3)	C21—C22—C25—C26	-176.2 (4)
N4^{ii}—Ni2—N4—C19	0 (100)	C21—C22—C25—C30	66.3 (6)
O3—Ni2—N4—C19	59.7 (3)	C21—C22—C25—C24	-54.9 (6)
O3^{ii}—Ni2—N4—C19	-120.3 (3)	C23—C24—C25—C22	-50.2 (5)
C9—N2—C1—C2	-60.9 (5)	C23—C24—C25—C26	69.5 (5)
Ni1—N2—C1—C2	162.4 (3)	C23—C24—C25—C30	-171.4 (4)
C9—N2—C1—C6^{i}	175.2 (4)	C22—C25—C26—C27	-172.7 (4)

Geometric parameters (Å, º)

Ni1—N2—C1—C6^{i}	38.6 (4)	C30—C25—C26—C27	-54.1 (6)
N2—C1—C2—C3	-178.6 (4)	C24—C25—C26—C27	66.0 (6)
C6^{i}—C1—C2—C3	-55.6 (6)	C25—C26—C27—C28	55.1 (6)
C1—C2—C3—C4^{i}	54.6 (6)	C26—C27—C28—C29	-54.3 (7)
C3^{i}—C4—C5—C6	-56.5 (6)	C27—C28—C29—C30	55.1 (7)
C7—N1—C6—C5	66.7 (5)	C22—C25—C30—C29	172.1 (5)
Ni1—N1—C6—C5	-163.5 (3)	C26—C25—C30—C29	54.6 (6)
C7—N1—C6—C1^{i}	-170.4 (4)	C24—C25—C30—C29	-66.1 (6)
Ni1—N1—C6—C1^{i}	-40.6 (4)	C28—C29—C30—C25	-56.6 (7)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···O2	0.93	1.91	2.785 (5)	157
N2—H*N*2···O4	0.93	2.26	3.127 (5)	156
N3—H*N*3···O4	0.93	2.03	2.888 (5)	153