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# {*N*′-[(*E*)-1-(5-Bromo-2-oxidophenyl)-ethylidene]-4-chlorobenzohydrazidato}-pyridinenickel(II)

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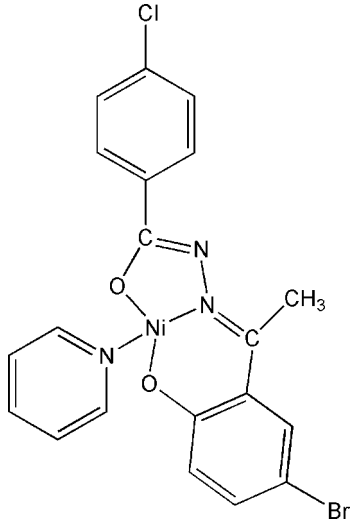
Key indicators: single-crystal X-ray study; $T$ = 278 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.032; $wR$ factor = 0.080; data-to-parameter ratio = 13.4.

The title complex, $[Ni(C_{15}H_{10}BrClN_2O_2)(C_5H_5N)]$, displays a square-planar coordination geometry around the $Ni^{II}$ ion, formed by the tridentate hydrazone and monodentate pyridine ligands, with the N atoms in a *trans* arrangement about the Ni center.

## Related literature

For the coordination properties of aroylhydrazones, see: Ali *et al.* (2004); Carcelli *et al.* (1995); Salem (1998); Singh *et al.* (1982).




## Experimental

### Crystal data

$[Ni(C_{15}H_{10}BrClN_2O_2)(C_5H_5N)]$
$M_r$ = 503.42
Monoclinic, $C2/c$
$a$ = 32.430 (4) Å
$b$ = 6.0816 (8) Å
$c$ = 22.865 (3) Å
$\beta$ = 121.422 (2)°
$V$ = 3848.3 (9) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 3.25 mm$^{-1}$
$T$ = 278 K
0.18 × 0.13 × 0.10 mm

### Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.581, $T_{max}$ = 0.723
9680 measured reflections
3401 independent reflections
2651 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.080
$S$ = 1.02
3401 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.27 e Å$^{-3}$

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: BH2230).

## References

Ali, H. M., Khamis, N. A. & Yamin, B. M. (2004). *Acta Cryst.* E**60**, m1708–m1709.
Carcelli, M., Mazza, P., Pelizzi, G. & Zani, F. (1995). *J. Inorg. Biochem.* **57**, 43–62.
Salem, A. A. (1998). *Microchem. J.* **60**, 51–66.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Singh, R. B., Jain, P. & Singh, R. P. (1982). *Talanta*, **29**, 77–84.

# supplementary materials

*Acta Cryst.* (2009). E**65**, m794 [ **doi:10.1107/S160053680902234X** ]

# {*N*'-[(*E*)-1-(5-Bromo-2-oxidophenyl)ethylidene]-4-chlorobenzohydrazidato}pyridinenickel(II)

**X.-L. Chang, B. Xie, C.-Y. Ji, Y.-G. Xiang and L.-K. Zou**

## Comment

The chemistry of aroylhydrazones continues to attract much attention due to their coordination ability to metal ions (Singh *et al.*, 1982; Salem, 1998; Ali *et al.*, 2004) and their biological activity (Singh *et al.*, 1982; Carcelli *et al.*, 1995). As an extension of work on the structural characterization of aroylhydrazone derivatives, the title compound was synthesized and its crystal structure is reported.

## Experimental

A DMF solution (5 ml) of *N*'-[(*E*)-(5-bromo-2-hydroxyphenyl)ethylidene]-4-chlorobenzo-hydrazide (0.25 mmol, 0.092 g) was mixed with a methanol solution (5 ml) of $NiCl_2.6H_2O$ (0.25 mmol, 0.059 g). The mixture was stirred at 298 K for 4 h and then filtered. A green precipitate was produced after about 10 d. A pyridine mixture (5 ml) was used to dissolve the precipitate at 330 K. Dark green block-shaped crystals were obtained after one month (yield 30%).

## Refinement

H atoms were placed in calculated positions, with C—H bond lengths fixed to 0.93 (aromatic CH) or 0.96 Å (methyl $CH_3$). Isotropic displacement parameters for H atoms were computed as $U_{iso}$(H) =$xU_{eq}$(carrier C) with $x$ = 1.2 (aromatic CH) or 1.5 (methyl $CH_3$).

## Figures

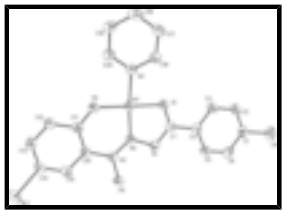


Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted.

### {*N*'-[(*E*)-1-(5-Bromo-2-oxidophenyl)ethylidene]-4- chlorobenzohydrazidato}pyridinenickel(II)

*Crystal data*

| | |
|---|---|
| $[Ni(C_{15}H_{10}BrClNO_2)(C_5H_5N)]$ | $F_{000}$ = 2016 |
| $M_r$ = 503.42 | $D_x$ = 1.738 Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Melting point: 330 K |
| Hall symbol: -C 2yc | Mo *K*α radiation, λ = 0.71073 Å |
| *a* = 32.430 (4) Å | Cell parameters from 2958 reflections |

| | |
|---|---|
| $b$ = 6.0816 (8) Å | θ = 2.6–25.0º |
| $c$ = 22.865 (3) Å | μ = 3.25 mm$^{-1}$ |
| β = 121.422 (2)º | $T$ = 278 K |
| $V$ = 3848.3 (9) Å$^3$ | Block, green |
| $Z$ = 8 | 0.18 × 0.13 × 0.10 mm |

*Data collection*

| | |
|---|---|
| Siemens SMART CCD area-detector diffractometer | 3401 independent reflections |
| Radiation source: fine-focus sealed tube | 2651 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.028 |
| $T$ = 278 K | $\theta_{max}$ = 25.1º |
| φ and ω scans | $\theta_{min}$ = 1.5º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h$ = −37→38 |
| $T_{min}$ = 0.581, $T_{max}$ = 0.723 | $k$ = −7→7 |
| 9680 measured reflections | $l$ = −24→27 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.032 | H-atom parameters constrained |
| $wR(F^2)$ = 0.080 | $w = 1/[\sigma^2(F_o^2) + (0.0383P)^2 + 2.3403P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.02 | $(\Delta/\sigma)_{max} < 0.001$ |
| 3401 reflections | $\Delta\rho_{max}$ = 0.48 e Å$^{-3}$ |
| 253 parameters | $\Delta\rho_{min}$ = −0.27 e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Ni1 | 0.041268 (13) | 0.23786 (6) | 0.156018 (18) | 0.04192 (13) |
| Br1 | −0.211124 (13) | −0.09987 (7) | −0.01369 (2) | 0.07519 (15) |
| Cl1 | 0.26998 (4) | −0.39055 (19) | 0.14682 (6) | 0.0893 (3) |
| O1 | 0.09933 (7) | 0.1537 (3) | 0.16792 (10) | 0.0483 (5) |
| O2 | −0.01644 (7) | 0.3235 (3) | 0.14192 (11) | 0.0532 (5) |
| N1 | 0.05323 (9) | −0.1250 (4) | 0.09609 (12) | 0.0460 (6) |
| N2 | 0.01755 (9) | −0.0048 (4) | 0.09955 (11) | 0.0418 (6) |
| N3 | 0.07253 (9) | 0.4809 (4) | 0.22016 (12) | 0.0449 (6) |
| C1 | 0.21951 (12) | −0.2894 (6) | 0.14580 (16) | 0.0572 (9) |
| C2 | 0.22207 (12) | −0.0906 (6) | 0.17554 (17) | 0.0647 (9) |
| H2 | 0.2510 | −0.0129 | 0.1980 | 0.078* |
| C3 | 0.18122 (12) | −0.0071 (6) | 0.17171 (16) | 0.0578 (8) |

| | | | | |
|---|---|---|---|---|
| H3 | 0.1827 | 0.1285 | 0.1915 | 0.069* |
| C4 | 0.13809 (11) | −0.1220 (5) | 0.13888 (14) | 0.0454 (7) |
| C5 | 0.13736 (13) | −0.3249 (5) | 0.11103 (18) | 0.0595 (9) |
| H5 | 0.1089 | −0.4065 | 0.0899 | 0.071* |
| C6 | 0.17748 (13) | −0.4080 (6) | 0.11382 (18) | 0.0646 (9) |
| H6 | 0.1763 | −0.5437 | 0.0942 | 0.077* |
| C7 | 0.09448 (11) | −0.0276 (5) | 0.13425 (14) | 0.0437 (7) |
| C8 | −0.02649 (11) | −0.0808 (5) | 0.06426 (13) | 0.0417 (7) |
| C9 | −0.03642 (12) | −0.2861 (5) | 0.02193 (16) | 0.0539 (8) |
| H9A | −0.0094 | −0.3164 | 0.0169 | 0.081* |
| H9B | −0.0649 | −0.2649 | −0.0225 | 0.081* |
| H9C | −0.0413 | −0.4077 | 0.0444 | 0.081* |
| C10 | −0.06526 (10) | 0.0294 (5) | 0.06629 (13) | 0.0415 (7) |
| C11 | −0.05843 (11) | 0.2266 (5) | 0.10261 (15) | 0.0456 (7) |
| C12 | −0.09895 (12) | 0.3312 (5) | 0.09768 (16) | 0.0545 (8) |
| H12 | −0.0947 | 0.4649 | 0.1198 | 0.065* |
| C13 | −0.14427 (12) | 0.2416 (6) | 0.06125 (17) | 0.0564 (8) |
| H13 | −0.1706 | 0.3138 | 0.0582 | 0.068* |
| C14 | −0.15003 (11) | 0.0428 (6) | 0.02932 (15) | 0.0516 (8) |
| C15 | −0.11213 (11) | −0.0603 (5) | 0.03060 (14) | 0.0487 (7) |
| H15 | −0.1174 | −0.1926 | 0.0074 | 0.058* |
| C16 | 0.12054 (12) | 0.4904 (6) | 0.25973 (16) | 0.0600 (9) |
| H16 | 0.1387 | 0.3768 | 0.2571 | 0.072* |
| C17 | 0.14431 (14) | 0.6615 (6) | 0.30425 (19) | 0.0701 (10) |
| H17 | 0.1779 | 0.6628 | 0.3311 | 0.084* |
| C18 | 0.11809 (15) | 0.8293 (6) | 0.30861 (17) | 0.0655 (10) |
| H18 | 0.1335 | 0.9482 | 0.3375 | 0.079* |
| C19 | 0.06898 (14) | 0.8192 (5) | 0.26974 (17) | 0.0589 (9) |
| H19 | 0.0503 | 0.9294 | 0.2727 | 0.071* |
| C20 | 0.04720 (12) | 0.6437 (5) | 0.22580 (15) | 0.0525 (8) |
| H20 | 0.0136 | 0.6388 | 0.1992 | 0.063* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ni1 | 0.0420 (2) | 0.0397 (2) | 0.0444 (2) | −0.00392 (17) | 0.02273 (18) | −0.00596 (17) |
| Br1 | 0.0486 (2) | 0.0968 (3) | 0.0797 (3) | −0.0210 (2) | 0.0332 (2) | −0.0084 (2) |
| Cl1 | 0.0596 (6) | 0.1029 (8) | 0.1085 (8) | 0.0179 (6) | 0.0461 (6) | −0.0134 (6) |
| O1 | 0.0456 (12) | 0.0462 (12) | 0.0522 (12) | −0.0061 (9) | 0.0248 (10) | −0.0130 (10) |
| O2 | 0.0433 (13) | 0.0501 (12) | 0.0657 (13) | −0.0055 (10) | 0.0281 (11) | −0.0161 (11) |
| N1 | 0.0454 (15) | 0.0431 (15) | 0.0514 (15) | 0.0007 (12) | 0.0265 (13) | −0.0048 (12) |
| N2 | 0.0445 (15) | 0.0388 (13) | 0.0440 (13) | −0.0011 (11) | 0.0245 (12) | −0.0025 (11) |
| N3 | 0.0486 (16) | 0.0436 (14) | 0.0464 (14) | −0.0058 (12) | 0.0275 (12) | −0.0051 (11) |
| C1 | 0.047 (2) | 0.067 (2) | 0.058 (2) | 0.0122 (17) | 0.0272 (17) | 0.0007 (17) |
| C2 | 0.044 (2) | 0.074 (3) | 0.074 (2) | −0.0059 (17) | 0.0297 (18) | −0.0151 (19) |
| C3 | 0.054 (2) | 0.057 (2) | 0.067 (2) | −0.0062 (17) | 0.0347 (18) | −0.0163 (17) |
| C4 | 0.0454 (18) | 0.0493 (19) | 0.0432 (16) | 0.0000 (14) | 0.0242 (15) | −0.0001 (14) |
| C5 | 0.050 (2) | 0.054 (2) | 0.072 (2) | −0.0075 (16) | 0.0299 (18) | −0.0163 (17) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C6 | 0.065 (2) | 0.056 (2) | 0.078 (2) | 0.0055 (18) | 0.040 (2) | −0.0129 (18) |
| C7 | 0.0457 (18) | 0.0448 (17) | 0.0423 (16) | 0.0001 (14) | 0.0241 (15) | 0.0003 (14) |
| C8 | 0.0465 (18) | 0.0381 (16) | 0.0388 (15) | −0.0049 (13) | 0.0210 (14) | 0.0000 (13) |
| C9 | 0.055 (2) | 0.0444 (19) | 0.0595 (19) | −0.0082 (15) | 0.0274 (17) | −0.0105 (15) |
| C10 | 0.0414 (17) | 0.0421 (17) | 0.0425 (15) | −0.0046 (13) | 0.0229 (14) | 0.0012 (13) |
| C11 | 0.0441 (18) | 0.0476 (18) | 0.0494 (17) | −0.0047 (14) | 0.0274 (15) | 0.0001 (14) |
| C12 | 0.053 (2) | 0.0525 (19) | 0.064 (2) | −0.0029 (16) | 0.0350 (17) | −0.0048 (16) |
| C13 | 0.047 (2) | 0.066 (2) | 0.066 (2) | 0.0010 (17) | 0.0358 (17) | 0.0043 (18) |
| C14 | 0.0421 (18) | 0.063 (2) | 0.0496 (18) | −0.0102 (16) | 0.0239 (15) | 0.0023 (16) |
| C15 | 0.0504 (19) | 0.0510 (18) | 0.0465 (17) | −0.0095 (15) | 0.0266 (15) | −0.0020 (14) |
| C16 | 0.048 (2) | 0.064 (2) | 0.070 (2) | −0.0108 (17) | 0.0320 (18) | −0.0193 (18) |
| C17 | 0.059 (2) | 0.075 (2) | 0.074 (2) | −0.025 (2) | 0.033 (2) | −0.028 (2) |
| C18 | 0.085 (3) | 0.059 (2) | 0.062 (2) | −0.028 (2) | 0.045 (2) | −0.0210 (18) |
| C19 | 0.079 (3) | 0.0463 (19) | 0.059 (2) | −0.0047 (18) | 0.042 (2) | −0.0088 (16) |
| C20 | 0.056 (2) | 0.0511 (19) | 0.0510 (18) | −0.0009 (16) | 0.0288 (17) | −0.0042 (15) |

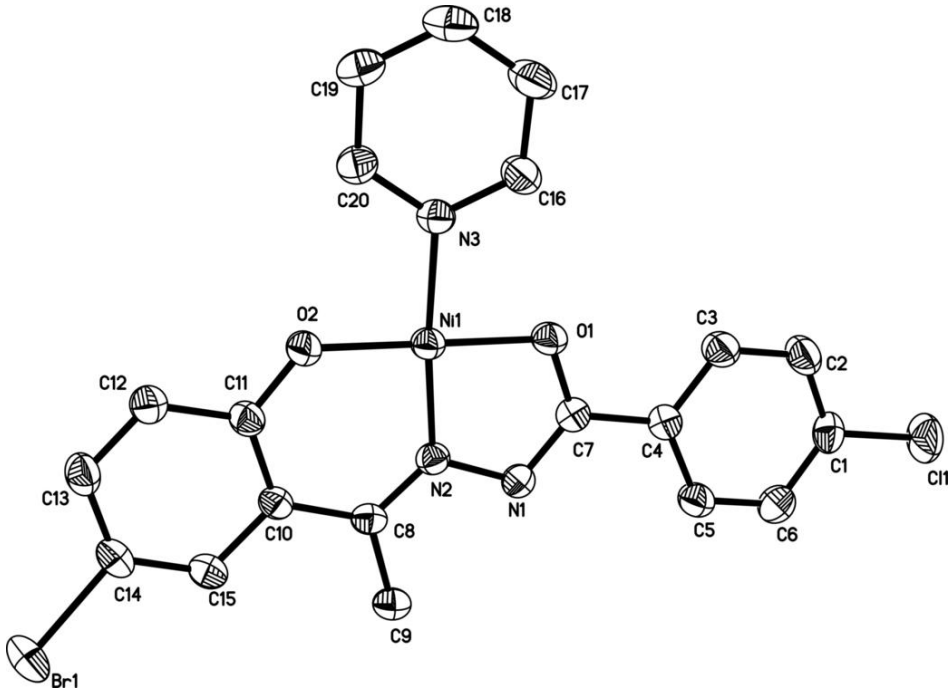
*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Ni1—O2 | 1.802 (2) | C8—C10 | 1.447 (4) |
| Ni1—O1 | 1.830 (2) | C8—C9 | 1.508 (4) |
| Ni1—N2 | 1.844 (2) | C9—H9A | 0.9600 |
| Ni1—N3 | 1.953 (2) | C9—H9B | 0.9600 |
| Br1—C14 | 1.901 (3) | C9—H9C | 0.9600 |
| Cl1—C1 | 1.737 (3) | C10—C15 | 1.407 (4) |
| O1—C7 | 1.306 (3) | C10—C11 | 1.409 (4) |
| O2—C11 | 1.317 (3) | C11—C12 | 1.410 (4) |
| N1—C7 | 1.298 (4) | C12—C13 | 1.369 (4) |
| N1—N2 | 1.405 (3) | C12—H12 | 0.9300 |
| N2—C8 | 1.305 (4) | C13—C14 | 1.374 (4) |
| N3—C16 | 1.333 (4) | C13—H13 | 0.9300 |
| N3—C20 | 1.335 (4) | C14—C15 | 1.366 (4) |
| C1—C2 | 1.368 (5) | C15—H15 | 0.9300 |
| C1—C6 | 1.369 (5) | C16—C17 | 1.377 (4) |
| C2—C3 | 1.378 (4) | C16—H16 | 0.9300 |
| C2—H2 | 0.9300 | C17—C18 | 1.364 (5) |
| C3—C4 | 1.383 (4) | C17—H17 | 0.9300 |
| C3—H3 | 0.9300 | C18—C19 | 1.362 (5) |
| C4—C5 | 1.383 (4) | C18—H18 | 0.9300 |
| C4—C7 | 1.478 (4) | C19—C20 | 1.381 (4) |
| C5—C6 | 1.366 (5) | C19—H19 | 0.9300 |
| C5—H5 | 0.9300 | C20—H20 | 0.9300 |
| C6—H6 | 0.9300 | | |
| O2—Ni1—O1 | 178.39 (9) | C8—C9—H9A | 109.5 |
| O2—Ni1—N2 | 95.20 (10) | C8—C9—H9B | 109.5 |
| O1—Ni1—N2 | 84.35 (9) | H9A—C9—H9B | 109.5 |
| O2—Ni1—N3 | 89.99 (10) | C8—C9—H9C | 109.5 |
| O1—Ni1—N3 | 90.52 (9) | H9A—C9—H9C | 109.5 |
| N2—Ni1—N3 | 174.43 (11) | H9B—C9—H9C | 109.5 |
| C7—O1—Ni1 | 110.50 (18) | C15—C10—C11 | 117.5 (3) |

| | | | |
|---|---|---|---|
| C11—O2—Ni1 | 126.92 (19) | C15—C10—C8 | 119.7 (3) |
| C7—N1—N2 | 108.4 (2) | C11—C10—C8 | 122.7 (3) |
| C8—N2—N1 | 116.7 (2) | O2—C11—C10 | 124.9 (3) |
| C8—N2—Ni1 | 129.7 (2) | O2—C11—C12 | 116.2 (3) |
| N1—N2—Ni1 | 113.61 (18) | C10—C11—C12 | 118.9 (3) |
| C16—N3—C20 | 117.5 (3) | C13—C12—C11 | 122.0 (3) |
| C16—N3—Ni1 | 120.5 (2) | C13—C12—H12 | 119.0 |
| C20—N3—Ni1 | 122.0 (2) | C11—C12—H12 | 119.0 |
| C2—C1—C6 | 121.1 (3) | C12—C13—C14 | 118.6 (3) |
| C2—C1—Cl1 | 119.6 (3) | C12—C13—H13 | 120.7 |
| C6—C1—Cl1 | 119.3 (3) | C14—C13—H13 | 120.7 |
| C1—C2—C3 | 119.1 (3) | C15—C14—C13 | 121.4 (3) |
| C1—C2—H2 | 120.4 | C15—C14—Br1 | 119.0 (3) |
| C3—C2—H2 | 120.4 | C13—C14—Br1 | 119.5 (2) |
| C2—C3—C4 | 121.0 (3) | C14—C15—C10 | 121.5 (3) |
| C2—C3—H3 | 119.5 | C14—C15—H15 | 119.3 |
| C4—C3—H3 | 119.5 | C10—C15—H15 | 119.3 |
| C3—C4—C5 | 118.1 (3) | N3—C16—C17 | 122.7 (3) |
| C3—C4—C7 | 120.1 (3) | N3—C16—H16 | 118.6 |
| C5—C4—C7 | 121.8 (3) | C17—C16—H16 | 118.6 |
| C6—C5—C4 | 121.4 (3) | C18—C17—C16 | 119.3 (4) |
| C6—C5—H5 | 119.3 | C18—C17—H17 | 120.4 |
| C4—C5—H5 | 119.3 | C16—C17—H17 | 120.4 |
| C5—C6—C1 | 119.2 (3) | C19—C18—C17 | 118.7 (3) |
| C5—C6—H6 | 120.4 | C19—C18—H18 | 120.7 |
| C1—C6—H6 | 120.4 | C17—C18—H18 | 120.7 |
| N1—C7—O1 | 123.1 (3) | C18—C19—C20 | 119.4 (3) |
| N1—C7—C4 | 118.9 (3) | C18—C19—H19 | 120.3 |
| O1—C7—C4 | 118.0 (3) | C20—C19—H19 | 120.3 |
| N2—C8—C10 | 120.4 (3) | N3—C20—C19 | 122.4 (3) |
| N2—C8—C9 | 119.3 (3) | N3—C20—H20 | 118.8 |
| C10—C8—C9 | 120.4 (3) | C19—C20—H20 | 118.8 |
| N2—Ni1—O1—C7 | −2.06 (18) | N1—N2—C8—C10 | 178.4 (2) |
| N3—Ni1—O1—C7 | 175.76 (18) | Ni1—N2—C8—C10 | −0.2 (4) |
| N2—Ni1—O2—C11 | 0.0 (2) | N1—N2—C8—C9 | −1.0 (4) |
| N3—Ni1—O2—C11 | −178.0 (2) | Ni1—N2—C8—C9 | −179.5 (2) |
| C7—N1—N2—C8 | −179.6 (2) | N2—C8—C10—C15 | −177.0 (2) |
| C7—N1—N2—Ni1 | −0.8 (3) | C9—C8—C10—C15 | 2.4 (4) |
| O2—Ni1—N2—C8 | −1.3 (3) | N2—C8—C10—C11 | 3.4 (4) |
| O1—Ni1—N2—C8 | −179.8 (3) | C9—C8—C10—C11 | −177.3 (3) |
| O2—Ni1—N2—N1 | −179.92 (18) | Ni1—O2—C11—C10 | 2.9 (4) |
| O1—Ni1—N2—N1 | 1.62 (17) | Ni1—O2—C11—C12 | −177.3 (2) |
| O2—Ni1—N3—C16 | 168.9 (2) | C15—C10—C11—O2 | 175.5 (3) |
| O1—Ni1—N3—C16 | −12.6 (2) | C8—C10—C11—O2 | −4.9 (4) |
| O2—Ni1—N3—C20 | −11.7 (2) | C15—C10—C11—C12 | −4.3 (4) |
| O1—Ni1—N3—C20 | 166.7 (2) | C8—C10—C11—C12 | 175.4 (3) |
| C6—C1—C2—C3 | −1.5 (5) | O2—C11—C12—C13 | −176.7 (3) |
| Cl1—C1—C2—C3 | 177.0 (3) | C10—C11—C12—C13 | 3.1 (5) |
| C1—C2—C3—C4 | 0.5 (5) | C11—C12—C13—C14 | 0.7 (5) |

| | | | |
|---|---|---|---|
| C2—C3—C4—C5 | 1.1 (5) | C12—C13—C14—C15 | −3.2 (5) |
| C2—C3—C4—C7 | −178.9 (3) | C12—C13—C14—Br1 | 173.6 (2) |
| C3—C4—C5—C6 | −1.9 (5) | C13—C14—C15—C10 | 1.9 (5) |
| C7—C4—C5—C6 | 178.1 (3) | Br1—C14—C15—C10 | −175.0 (2) |
| C4—C5—C6—C1 | 1.0 (5) | C11—C10—C15—C14 | 2.0 (4) |
| C2—C1—C6—C5 | 0.7 (5) | C8—C10—C15—C14 | −177.7 (3) |
| Cl1—C1—C6—C5 | −177.8 (3) | C20—N3—C16—C17 | −1.3 (5) |
| N2—N1—C7—O1 | −1.1 (4) | Ni1—N3—C16—C17 | 178.0 (3) |
| N2—N1—C7—C4 | −179.6 (2) | N3—C16—C17—C18 | 0.0 (5) |
| Ni1—O1—C7—N1 | 2.4 (3) | C16—C17—C18—C19 | 1.5 (5) |
| Ni1—O1—C7—C4 | −179.08 (19) | C17—C18—C19—C20 | −1.8 (5) |
| C3—C4—C7—N1 | 171.6 (3) | C16—N3—C20—C19 | 1.0 (4) |
| C5—C4—C7—N1 | −8.4 (4) | Ni1—N3—C20—C19 | −178.3 (2) |
| C3—C4—C7—O1 | −7.0 (4) | C18—C19—C20—N3 | 0.5 (5) |
| C5—C4—C7—O1 | 173.0 (3) | | |

**Fig. 1**


C18
C19
C17
C20
C16
N3
O2
Ni1
O1
C3
C2
C12
C11
C7
C4
C1
Cl1
C13
N2
N1
C10
C8
C5
C6
C14
C15
C9
Br1