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Crystal structure of (6,9-diacetyl-5,10,15,20-tetraphenylsecochlorinato)nickel(II)

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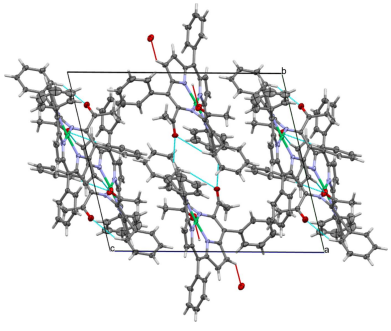
Title compound **1Ni**, [Ni($C_{46}H_{32}N_4O_2$)], a secochlorin nickel complex, was prepared by diol cleavage of a precursor *trans*-dihydroxydimethylchlorin. Two crystallographically independent molecules in the structure are related by pseudo-A lattice centering, with molecules differing mainly by a rotation of one of the acetyls and an adjacent phenyl groups. The two molecules have virtually identical conformations characterized by noticeable in-plane deformation in the A_{1g} mode and a prominent out-of-plane deformation in the B_{1u} (ruffling) mode. Directional interactions between molecules are scarce, limited to just a few C—H···O contacts, and intermolecular interactions are mostly dispersive in nature.

1. Chemical context

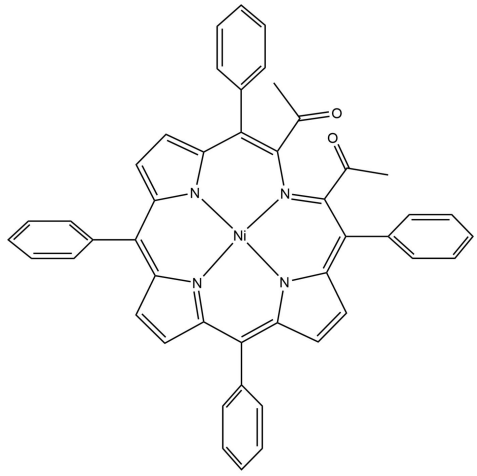
Chlorins are 7,8-dihydroporphyrins, *i.e.*, porphyrins reduced at one of the pyrrolic β,β'-double bonds (Borbas, 2016; Taniguchi & Lindsey, 2017; Lindsey, 2015). The chlorophylls, nature's light harvesting pigments, are magnesium complexes of chlorins (Taniguchi & Lindsey, 2017). In large part because of the role of this member of the 'pigments of life' (Battersby, 2000) in photosynthesis, chlorins are a broadly investigated compound class.

Secochlorins are compounds in which a pyrrolic β,β'-double bond was cleaved (Brückner *et al.*, 2014; Thuita & Brückner, 2022). These compounds have no known precedent among the natural porphyrinic pigments or their degradation products (Kräutler, 2014; Wojaczyński, 2014). The handful of examples of secochlorins prepared to date were made by oxidative modifications of functionalized porphyrin or chlorin β,β'-bonds (Brückner *et al.*, 2014; Thuita & Brückner, 2022). The first secochlorin was discovered fortuitously (Chang *et al.*, 1992). Since then, a number of rational oxidative β,β'-bond cleavage reaction sequences have been developed to prepare (metallo)secochlorins of the octaalkyl- (Adams *et al.*, 1997; Sessler *et al.*, 2001; Ryppa *et al.*, 2009) and the *meso*-tetraarylporphyrin series (Brückner *et al.*, 1998, 1999, 2005; McCarthy *et al.*, 2004; Akhigbe *et al.*, 2009; Sharma *et al.*, 2016; Lo *et al.*, 2012). Following a β,β'-bond-opening, subsequent intramolecular reactions of the secochlorins with the adjacent *meso*-aryl- or β-alkyl groups are not infrequent (Adams *et al.*, 1997; McCarthy *et al.*, 2004; Ryppa *et al.*, 2009; Banerjee *et al.*, 2012; Zhu *et al.*, 2022).

The title compound **1Ni**, a secochlorin nickel complex, was prepared by diol cleavage of *trans*-dihydroxychlorin **2Ni**, itself made in a multi-step process from *cis*-diol chlorin **3Ni** (Fig. 1). It has been used in the preparation of a number of



porphyrinoids containing non-pyrrolic heterocycles (Banerjee *et al.*, 2012; Sharma *et al.*, 2016).



1Ni

Chlorin diol **3Ni** could also be cleaved, generating bis-aldehyde **5Ni** (Brückner *et al.*, 1998, 1999, 2005). A comparison of the crystal structures of the dihydroxychlorins **2Ni/3Ni**

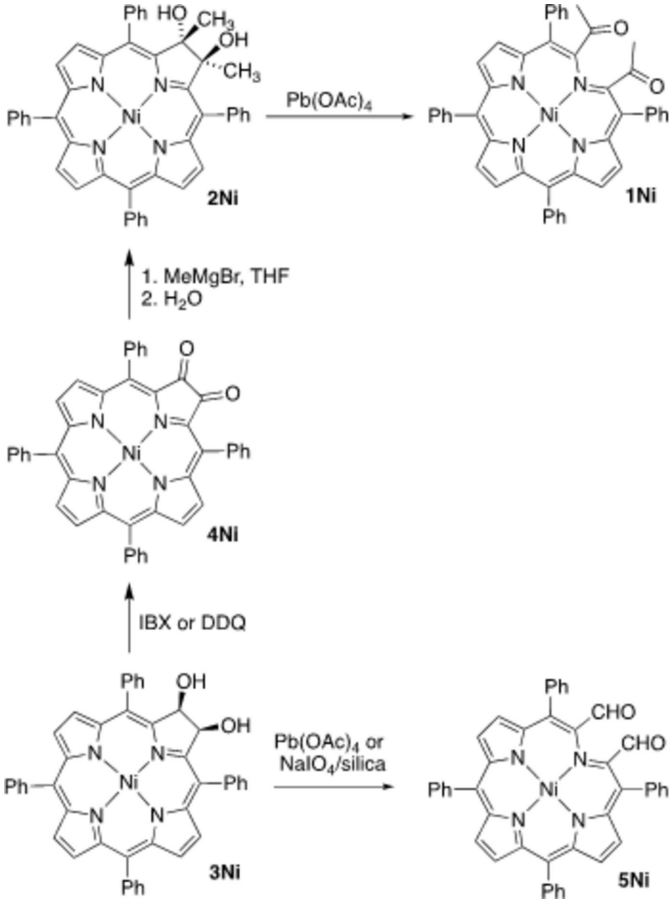


Figure 1
Synthetic pathway to secochlorin nickel(II) complexes **1Ni** and **5Ni** by oxidative diol cleavage of a precursor diol.

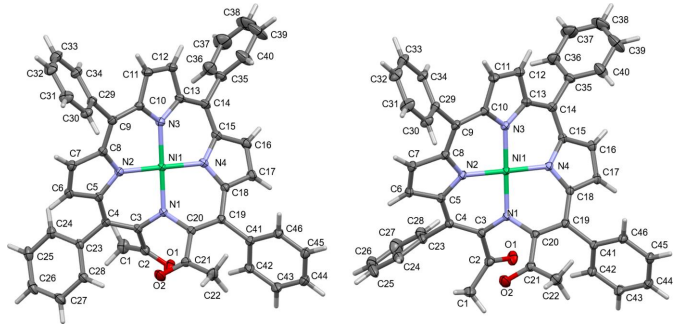


Figure 2
Displacement ellipsoid view of the two molecules of the structure of compound **1Ni** with atom-labeling scheme (50% probability ellipsoids). Left: molecule **1Ni-1**. Right: Molecule **1Ni-2**.

and the corresponding secochlorins **1Ni/5Ni** provides further insight into the conformational changes induced by breaking the structural integrity of the porphyrin framework (Brückner *et al.*, 2005) and the influence of β-alkylation.

2. Structural commentary

1Ni crystallized in a centrosymmetric triclinic setting in space group $P\overline{1}$, with two crystallographically independent molecules ($Z' = 2$) (Fig. 2). The structure of **1Ni** confirms its rare secochlorin bisketone connectivity that was previously derived spectroscopically and by means of subsequent reactions (Banerjee *et al.*, 2012; Sharma *et al.*, 2016). Bond lengths and angles are in the expected ranges. Noteworthy, however, are the C—N bonds around the cleavage site at N1, which show a clear asymmetry present in both molecules. The lengths for N1—C3 are 1.3687 (15) and 1.3661 (15) Å in the two molecules **1Ni-1** and **1Ni-2**, while the two N1—C20 bonds are substantially longer at 1.3879 (15) and 1.3997 (15) Å. For most of the other bonds of the secochlorin skeleton no such clear differentiation is observed.

The two crystallographically independent molecules of the secochlorinato nickel complex **1Ni** are related by pseudo-A lattice centering (Fig. 3). Exact translational symmetry is broken by different torsion angles for one of the acetyl groups

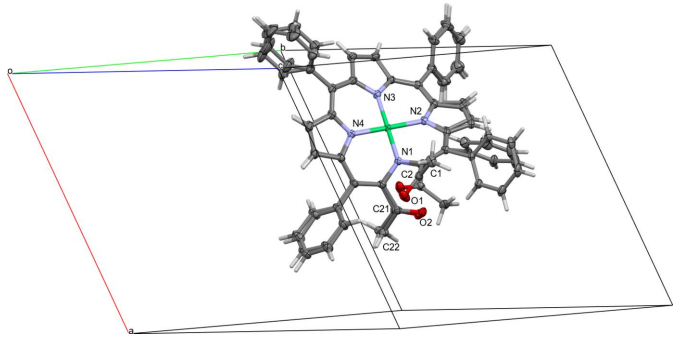


Figure 3
View down [01$\overline{1}$] (slightly offset) showing the pseudo-A lattice centering relating the two molecules with each other (front: molecule **1Ni-1**; back: molecule **1Ni-2**). For clarity only selected labels for molecule 1 are shown.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C28_1—H28_1···O2_1	0.95	2.60	3.4517 (17)	149
C42_1—H42_1···O1_1	0.95	2.55	3.3855 (17)	147
C42_2—H42_2···O1_2	0.95	2.66	3.5120 (17)	149
C6_1—H6_1···O2_1^{i}	0.95	2.49	3.3714 (16)	155
C6_2—H6_2···O2_2^{ii}	0.95	2.57	3.3569 (17)	140
C17_2—H17_2···O1_2^{iii}	0.95	2.40	3.2977 (16)	158

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $-x+1, -y+2, -z+1$; (iii) $-x+1, -y+1, -z+1$.

(O1, C1, C2). In molecule 1, the N—C—C—O torsion angle between the non-pyrrolic N atom N1 and keto-oxygen O1 is 39.90 (19)°; in molecule 2 the same torsion angle is −37.75 (17)°. The same torsion angles for the methyl C atom C1 instead of O1 are 143.45 (13)° (molecule 1) and −130.33 (13)° (molecule 2). The acetyl groups of the two molecules are thus rotated with respect to each other, by *ca* 78 and 86° for keto O and methyl C atoms, respectively. The different values for C and O atoms are caused by a slight non-planarity of the acetyl group of molecule 1, with C1 being offset from the plane of the C3, C2 and O1 by 0.230 (5) Å. This rotation results in a significantly different O1···O2 distance in the two molecules: 2.7997 (17) Å in molecule 1, and 3.2286 (16) Å in molecule 2. It also places the methyl groups in the two molecules on opposite sides of their neighboring phenyl rings of C23 to C28, which in turn induces different orientations of this ring between the two molecules [C3—C4—C23—C24 = −130.42 (14) and 115.13 (15)° for molecules 1 and 2, respectively]. The different orientation of the phenyl ring prevents an intramolecular C—H···O hydrogen bond between C28 and O2 that is present in molecule 1 to be formed in molecule 2. A second C—H···O hydrogen bond (between C42 and O1) is present for both molecules (see Table 1 for numerical details). The phenyl group on the opposite end of the molecule (C35–C40) is also slightly modulated, but much less so than the acetyl group and C23–C28 (torsion angles only differ by *ca* 29°). The remaining atoms of the two molecules are related by close to perfect translational symmetry, and the conformations of their secochlorin cores are thus qualitatively and quantitatively very similar to each other.

Importantly, the structure determination of **1Ni** also allows for a detailed analysis of the conformation of the macrocycle. For both molecules **1Ni-1** and **1Ni-2** the conformations of the chromophores deviate greatly from planarity. On account of the small central nickel(II) ion inducing strain into the macrocycle, nickel(II) porphyrin and chlorin complexes tend to be non-planar, adopting commonly a ruffled conformation (Kingsbury & Senge, 2021). This is because the ruffled deformation mode effectively shortens the Ni—N bond lengths, without distorting the near-ideal planar coordination geometry of the four nitrogen donors around the metal. This is also the case here, and the N—Ni bond lengths vary only within a small margin, with values between 1.8845 (10) and 1.9128 (10) Å, and the coordination of the nickel atoms is close to perfectly square planar. To compare **1Ni** to other

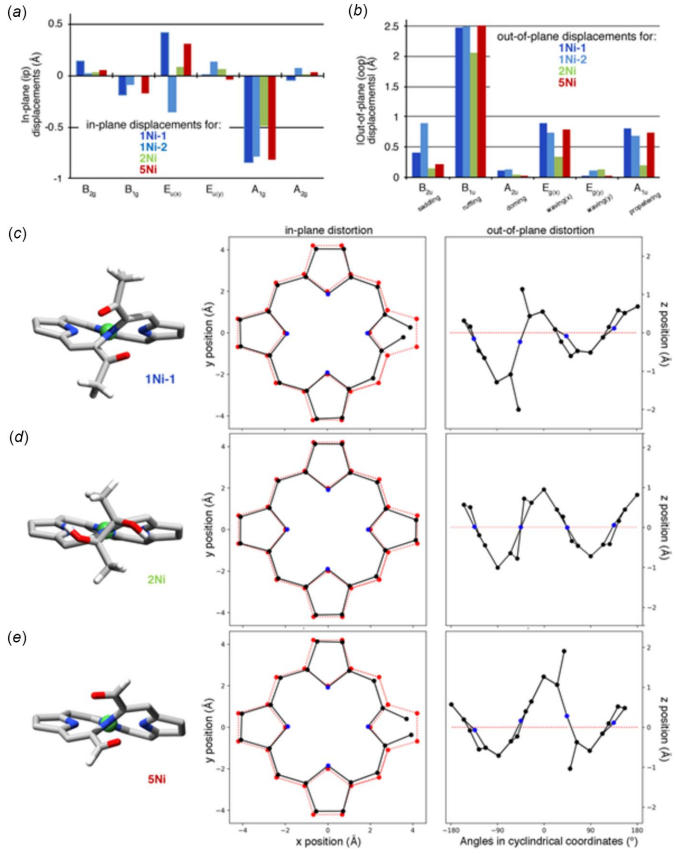


Figure 4
Bar diagrams of the in-plane (*a*) and out-of-plane (*b*) macrocycles NSD deformation analyses of the compounds **1Ni-1**, **1Ni-2**, **2Ni**, and **5Ni**; analyses by the porphyrin NSD online tool (Kingsbury & Senge, 2021), based on the method of Shelnutt (Jentzen *et al.*, 1997). Stick representations of the X-ray single-crystal structures are shown below (*c* through *e*); for **1Ni**, only **1Ni-1** is shown; all H atoms attached to sp^3-hybridized carbon atoms, all *meso*-aryl groups, as well as all disorder and solvents removed for clarity. Next to the stick structures are the in-plane skeletal plots of the porphyrin core of the compounds indicated (black trace), compared to that of a benchmark planar porphyrin [*meso*-tetraphenylporphyrinato]copper(II) (red trace), as well as their out-of-plane skeletal plots.

related compounds and obtain a qualitative and quantitative analysis of its conformation, we performed a normal-coordinate structural decomposition (NSD) analysis of the macrocycle conformation of the two molecules of **1Ni-1** and **1Ni-2**, of the starting diol nickel complex **2Ni** and of its aldehyde analogue **5Ni** (Fig. 4) (Jentzen *et al.*, 1997; Kingsbury & Senge, 2021).

Both molecules **1Ni-1** and **1Ni-2** show in-plane compressed conformations, with the most prominent in-plane deformation in the A_{1g} mode. This is combined with drastically ruffled out-of-plane deformations with significant waving and propellering contributions. These deformation modes are typical for nickel porphyrins and chlorins (Kingsbury & Senge, 2021) and their large extent was previously observed in secochlorins (Brückner *et al.*, 2005). The macrocycle conformation aligns the two ketone functionalities to be arranged antiparallel to each other. Qualitatively and quantitatively, the conformation of bisketone **1Ni** is very similar to that of bisaldehyde **5Ni**,

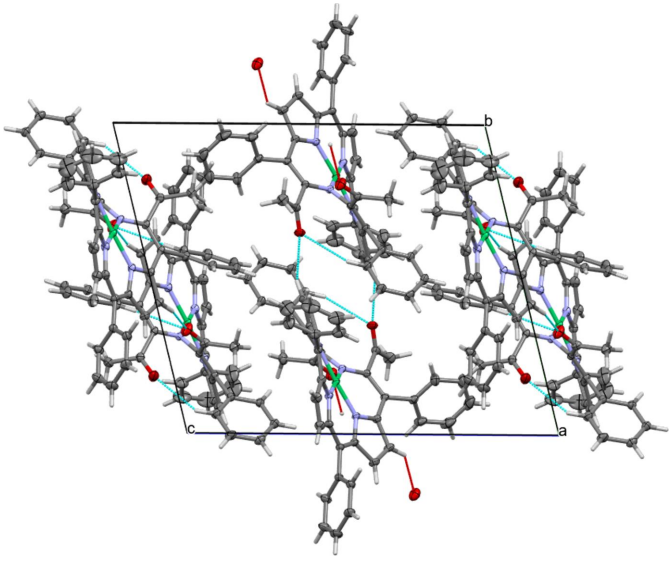


Figure 5
Packing view showing intra- and intermolecular C—H···O hydrogen bonds in **1Ni**. Molecules **1Ni-1** are to the left and right at (x, 0, z) and (x, 1, z), molecules **1Ni-2** at the center at (x, $\frac{1}{2}$, z). Note that all C—H···O hydrogen bonds are formed between molecules 1, and between molecules 2, thus forming C—H···O bonded layers, while all interactions between molecules 1 and 2 are purely van der Waals in nature.

showing that the additional alkyl substituents in **1Ni** do not have any significant steric influence. While parent chlorin diol complex **2Ni** is also ruffled, it is much less so, with much smaller waving and propellering deformations as well. Accordingly, the average N—Ni bond length in **2Ni** is longer (1.908 Å) compared to the corresponding bond lengths found in **1Ni** (1.901 Å) or **5Ni** (1.893 Å). The changes observed upon ring-opening align with what was previously observed (Brückner *et al.*, 2005).

3. Supramolecular features

In addition to the intramolecular C—H···O bonds within each molecule, there are also a small number of weak C—H···O hydrogen bond-like interactions present that connect molecules of **1Ni** with each other (Fig. 5; see Table 1 for numerical values and symmetry operators). Some weak C—H···π interactions are also present (not shown), but these are too weak to be classified as directional and they are unlikely to have any strong structure-determining effects. Instead, intermolecular interactions in the structure of **1Ni** are dominated by non-directional dispersion interactions (van der Waals interactions). This is quantitatively confirmed by analysis of the Hirshfeld surfaces of the two molecules (Spackman & Byrom, 1997; *Crystal Explorer*, Spackman *et al.*, 2021), which are dominated by C···H and H···H and reciprocal contacts, making up 23.5 and 59.2% of the Hirshfeld surface of **1Ni-1**, and 23.2 and 58.7% for **1Ni-2**. The shortest contacts are some of the H···H contacts, and the few directional C–H···O interactions (for visualization, see Fig. 6 showing the d_e *versus* d_i fingerprint plots for H···H and H···O contacts for **1Ni-1**). N···H and Ni···H contacts are also observed (5.0 and 2.0% for **1Ni-1**, 4.9% and 2.0% for **1Ni-2**), but distances are rather long and the interactions are non-directional. The deformation modes of the molecules also prevent any effective π-stacking interactions to be established in the structure, which is confirmed by the low number for C···C contacts on the Hirshfeld surface (3.6 and 3.0% for the two molecules).

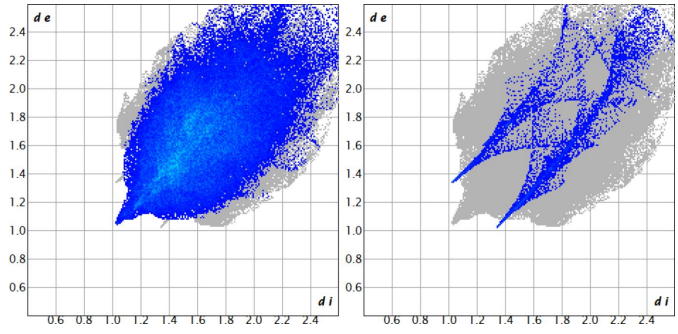


Figure 6
Selected fingerprint plots highlighting the dominance of interactions involving H atoms in the structure of **1Ni**. Shown are d_e *versus* d_i plots (*Crystal Explorer*; Spackman *et al.*, 2021) of H···H interactions (left) and O···H/H···O interactions (right) for molecule **1Ni-1** (plots for molecule **1Ni-2** are equivalent).

4. Database survey

The structures most closely related to title compound **1Ni** are its aldehyde analogue **5Ni** [CSD (Groom *et al.*, 2016) code GUBWAB; Brückner *et al.*, 1999], as well as two related bisketone derivatives in which the C atoms of the cleaved pyrrole have been annelated to the adjacent phenyl rings to form an indaphyrin (*meso*-diphenylindaporphyrinato)platinum(II) (CSD entry SUNXAB; Lau *et al.*, 2009) and its bishydroxylated indachlorin counterpart (CSD entry OJEHAO; Samankumara *et al.*, 2015).

5. Synthesis and crystallization

The title compound **1Ni** was prepared by classic lead(IV)-induced diol cleavage of *trans*-dihydroxychlorin **2Ni**. This diol was made in two steps from *cis*-diol **3Ni**: oxidation to dione **4Ni** (Daniell *et al.*, 2003), followed by double methyl-Grignard addition (Banerjee *et al.*, 2012). Crystals of **1Ni** were grown by slow evaporation of a solution of **1Ni** in $CHCl_3$/hexane to dryness. The spectroscopic data of **1Ni** have been reported previously (Banerjee *et al.*, 2012).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Two crystallographically independent molecules are present in the asymmetric unit of the structure. A common atom-naming scheme combined with residue numbers 1 and 2 were used for the two molecules, which are related by pseudo-A lattice centering. Exact translational symmetry is broken by different torsion angles of one of the acetyl groups (O1, C1, C2), of the adjacent phenyl group

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Ni(C_{46}H_{32}N_4O_2)]$
M_r	731.46
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, b, c (Å)	14.1382 (5), 15.3202 (5), 18.3835 (7)
α, β, γ (°)	72.0900 (18), 69.6031 (19), 74.6737 (18)
V (Å^3)	3495.8 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.60
Crystal size (mm)	0.24 × 0.16 × 0.14
Data collection	
Diffractometer	Bruker AXS D8 Quest
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.701, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	226909, 26754, 19735
R_{int}	0.056
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.770
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.103, 1.01
No. of reflections	26754
No. of parameters	959
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.07, −0.42

Computer programs: *APEX4* (Bruker, 2022), *SAINT* (Bruker, 2020), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*), *ShelXle* (Hübschle *et al.*, 2011), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

C23 to C28), and of the phenyl group trans across the molecule (C35 to C40).

C—H bond distances were constrained to 0.95 Å for aromatic moieties, and to 0.98 Å for CH_3 moieties. Methyl CH_3 groups were allowed to rotate but not to tip to best fit the experimental electron density. U_{iso}(H) values were set to a multiple of U_{eq}(C) with 1.5 for CH_3 and 1.2 for C—H units, respectively.

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References

Adams, K. R., Bonnett, R., Burke, P. J., Salgado, A. & Asunción Vallés, M. (1997). *J. Chem. Soc. Perkin Trans. 1*, pp. 1769–1772.
Akhigbe, J., Ryppa, C., Zeller, M. & Brückner, C. (2009). *J. Org. Chem.* **74**, 4927–4933.
Banerjee, S., Zeller, M. & Brückner, C. (2012). *J. Porphyrins Phthalocyanines*, **16**, 576–588.
Battersby, A. R. (2000). *Nat. Prod. Rep.* **17**, 507–526.
Borbas, K. E. (2016). *Handbook of Porphyrin Science*, pp. 1–149. Singapore: World Scientific Publishing Company.
Brückner, C., Akhigbe, J. & Samankumara, L. (2014). *Handbook of Porphyrin Science*, edited by K. M. Kadish, K. M. Smith & R. Guilard, pp. 1–276. River Edge, NY: World Scientific.
Brückner, C., Hyland, M. A., Sternberg, E. D., MacAlpine, J., Rettig, S. J., Patrick, B. O. & Dolphin, D. (2005). *Inorg. Chim. Acta*, **358**, 2943–2953.
Brückner, C., Rettig, S. J. & Dolphin, D. (1998). *J. Org. Chem.* **63**, 2094–2098.
Brückner, C., Sternberg, E. D., MacAlpine, J. K., Rettig, S. J. & Dolphin, D. (1999). *J. Am. Chem. Soc.* **121**, 2609–2610.
Bruker (2020). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2022). *APEX4*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chang, C. K., Wu, W., Chern, S.-S. & Peng, S.-M. (1992). *Angew. Chem. Int. Ed. Engl.* **31**, 70–72.
Daniell, H. W., Williams, S. C., Jenkins, H. A. & Brückner, C. (2003). *Tetrahedron Lett.* **44**, 4045–4049.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Hübschle, C. B., Sheldrick, G. M. & Dittrich, B. (2011). *J. Appl. Cryst.* **44**, 1281–1284.
Jentzen, W., Song, X.-Z. & Shelnutt, J. A. (1997). *J. Phys. Chem. B*, **101**, 1684–1699.
Kingsbury, C. J. & Senge, M. O. (2021). *Coord. Chem. Rev.* **431**, 213760, 23 pages.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
Kräutler, B. (2014). *Chem. Soc. Rev.* **43**, 6227–6238.
Lau, K. S. F., Zhao, S., Ryppa, C., Jockusch, S., Turro, N. J., Zeller, M., Gouterman, M., Khalil, G. E. & Brückner, C. (2009). *Inorg. Chem.* **48**, 4067–4074.
Lindsey, J. S. (2015). *Chem. Rev.* **115**, 6534–6620.
Lo, M., Lefebvre, J.-F., Marcotte, N., Tonnelé, C., Beljonne, D., Lazzaroni, R., Clément, S. & Richeter, S. (2012). *Chem. Commun.* **48**, 3460–3462.
Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.
McCarthy, J. R., Hyland, M. A. & Brückner, C. (2004). *Org. Biomol. Chem.* **2**, 1484–1491.
Ryppa, C., Niedzwiedzki, D., Morozowich, N. L., Srikanth, R., Zeller, M., Frank, H. A. & Brückner, C. (2009). *Chem. Eur. J.* **15**, 5749–5762.
Samankumara, L. P., Dorazio, S. J., Akhigbe, J., Li, R., Nimthong–Roldán, A., Zeller, M. & Brückner, C. (2015). *Chem. Eur. J.* **21**, 11118–11128.
Sessler, J. L., Shevchuk, S. V., Callaway, W. & Lynch, V. (2001). *Chem. Commun.* pp. 968–969.
Sharma, M., Banerjee, S., Zeller, M. & Brückner, C. (2016). *J. Org. Chem.* **81**, 12350–12356.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Spackman, M. A. & Byrom, P. G. (1997). *Chem. Phys. Lett.* **267**, 215–220.
Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.
Taniguchi, M. & Lindsey, J. S. (2017). *Chem. Rev.* **117**, 344–535.
Thuita, D. W. & Brückner, C. (2022). *Chem. Rev.* **122**, 7990–8052.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Wojaczyński, J. (2014). *Top. Heterocycl. Chem.* **33**, 143–202.
Zhu, M., Zhang, H., Ran, G., Yao, Y., Yang, Z.-S., Ning, Y., Yu, Y., Zhang, R., Peng, X.-X., Wu, J., Jiang, Z., Zhang, W., Wang, B.-W., Gao, S. & Zhang, J.-L. (2022). *Angew. Chem. Int. Ed.* **61**, e202204330.

supporting information

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Crystal structure of (6,9-diacetyl-5,10,15,20-tetraphenyl-secochlorinato)nickel(II)

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Computing details

(6,9-Diacetyl-5,10,15,20-tetraphenylsecochlorinato)nickel(II)

Crystal data

$[Ni(C_{46}H_{32}N_4O_2)]$
M_r = 731.46
Triclinic, $P\overline{1}$
a = 14.1382 (5) Å
b = 15.3202 (5) Å
c = 18.3835 (7) Å
α = 72.0900 (18)°
β = 69.6031 (19)°
γ = 74.6737 (18)°
V = 3495.8 (2) Å^3
Z = 4
$F(000)$ = 1520
D_x = 1.390 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9410 reflections
θ = 2.2–33.1°
μ = 0.60 mm^{-1}
T = 150 K
Block, black
0.24 × 0.16 × 0.14 mm

Data collection

Bruker AXS D8 Quest diffractometer
Radiation source: fine focus sealed tube X-ray source
Triumph curved graphite crystal monochromator
Detector resolution: 7.4074 pixels mm^{-1}
ω and phi scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.701, T_{max} = 0.747
226909 measured reflections
26754 independent reflections
19735 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 33.2°, θ_{min} = 1.9°
h = −21→21
k = −23→23
l = −28→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.103
S = 1.01
26754 reflections
959 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0457P)^2 + 1.6735P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.07 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1_1	0.25969 (2)	0.35659 (2)	0.92873 (2)	0.01429 (4)
O1_1	0.50774 (9)	0.18303 (8)	1.05354 (7)	0.0319 (2)
O2_1	0.58223 (8)	0.33407 (9)	0.93406 (7)	0.0312 (2)
N1_1	0.38355 (8)	0.31234 (7)	0.95721 (6)	0.01569 (18)
N2_1	0.24377 (8)	0.46934 (7)	0.95719 (6)	0.01615 (18)
N3_1	0.13540 (8)	0.40147 (8)	0.89948 (6)	0.01684 (19)
N4_1	0.27362 (8)	0.24007 (7)	0.90697 (6)	0.01638 (18)
C1_1	0.38050 (13)	0.22630 (10)	1.16637 (9)	0.0284 (3)
H1A_1	0.309459	0.258994	1.173210	0.043*
H1B_1	0.413305	0.249917	1.193665	0.043*
H1C_1	0.381312	0.159369	1.189290	0.043*
C2_1	0.43835 (11)	0.24268 (9)	1.07820 (8)	0.0209 (2)
C3_1	0.39427 (9)	0.32810 (9)	1.02306 (7)	0.0165 (2)
C4_1	0.35152 (9)	0.41150 (9)	1.04696 (7)	0.0165 (2)
C5_1	0.29060 (9)	0.48299 (9)	1.00558 (7)	0.0164 (2)
C6_1	0.26648 (10)	0.57957 (9)	1.00854 (8)	0.0196 (2)
H6_1	0.289412	0.606624	1.038033	0.023*
C7_1	0.20478 (10)	0.62434 (9)	0.96112 (8)	0.0201 (2)
H7_1	0.177902	0.689164	0.949856	0.024*
C8_1	0.18749 (9)	0.55514 (9)	0.93090 (7)	0.0174 (2)
C9_1	0.11406 (9)	0.56829 (9)	0.89235 (7)	0.0173 (2)
C10_1	0.08651 (9)	0.49248 (9)	0.88161 (7)	0.0177 (2)
C11_1	−0.00208 (10)	0.49644 (10)	0.85849 (8)	0.0223 (2)
H11_1	−0.046378	0.551116	0.840264	0.027*
C12_1	−0.01033 (10)	0.40691 (10)	0.86772 (8)	0.0228 (2)
H12_1	−0.063470	0.387129	0.859720	0.027*
C13_1	0.07627 (10)	0.34801 (9)	0.89178 (8)	0.0189 (2)
C14_1	0.09973 (10)	0.25128 (10)	0.90294 (8)	0.0202 (2)
C15_1	0.19504 (10)	0.20055 (9)	0.90892 (8)	0.0192 (2)
C16_1	0.23266 (11)	0.10522 (9)	0.90465 (9)	0.0233 (3)
H16_1	0.193543	0.061951	0.907329	0.028*
C17_1	0.33495 (11)	0.08832 (9)	0.89605 (8)	0.0221 (2)
H17_1	0.381182	0.031590	0.890142	0.027*
C18_1	0.35961 (10)	0.17279 (9)	0.89760 (7)	0.0172 (2)
C19_1	0.45760 (9)	0.18739 (9)	0.88887 (7)	0.0166 (2)
C20_1	0.46814 (9)	0.25855 (8)	0.91549 (7)	0.0160 (2)
C21_1	0.56934 (10)	0.29057 (9)	0.89428 (8)	0.0196 (2)
C22_1	0.65030 (11)	0.27887 (11)	0.81656 (9)	0.0269 (3)
H22A_1	0.617494	0.276390	0.778420	0.040*

H22B_1	0.698974	0.220902	0.826505	0.040*
H22C_1	0.686832	0.331738	0.794441	0.040*
C23_1	0.38006 (10)	0.42935 (9)	1.11065 (7)	0.0178 (2)
C24_1	0.30557 (11)	0.45948 (10)	1.17573 (8)	0.0227 (2)
H24_1	0.235219	0.473075	1.177851	0.027*
C25_1	0.33437 (13)	0.46950 (11)	1.23718 (9)	0.0294 (3)
H25_1	0.283517	0.488885	1.281742	0.035*
C26_1	0.43730 (14)	0.45131 (11)	1.23382 (9)	0.0312 (3)
H26_1	0.456645	0.457235	1.276426	0.037*
C27_1	0.51154 (13)	0.42456 (11)	1.16830 (9)	0.0289 (3)
H27_1	0.582016	0.414031	1.165124	0.035*
C28_1	0.48303 (11)	0.41309 (10)	1.10711 (8)	0.0223 (2)
H28_1	0.534221	0.394005	1.062552	0.027*
C29_1	0.05941 (10)	0.66507 (9)	0.86838 (7)	0.0187 (2)
C30_1	0.11538 (11)	0.73360 (10)	0.81570 (8)	0.0232 (3)
H30_1	0.187249	0.717130	0.793280	0.028*
C31_1	0.06760 (12)	0.82552 (10)	0.79557 (9)	0.0292 (3)
H31_1	0.106785	0.871457	0.759764	0.035*
C32_1	−0.03757 (13)	0.85035 (11)	0.82780 (10)	0.0312 (3)
H32_1	−0.070447	0.913249	0.814379	0.037*
C33_1	−0.09416 (12)	0.78273 (11)	0.87963 (9)	0.0290 (3)
H33_1	−0.166139	0.799422	0.901361	0.035*
C34_1	−0.04645 (10)	0.69064 (10)	0.90010 (8)	0.0233 (3)
H34_1	−0.085962	0.644895	0.935791	0.028*
C35_1	0.01980 (11)	0.20077 (10)	0.90774 (9)	0.0251 (3)
C36_1	−0.04101 (13)	0.16268 (12)	0.98291 (11)	0.0350 (3)
H36_1	−0.029458	0.167244	1.029413	0.042*
C37_1	−0.11882 (16)	0.11784 (15)	0.99029 (15)	0.0520 (5)
H37_1	−0.161147	0.093025	1.041775	0.062*
C38_1	−0.13451 (18)	0.10941 (17)	0.92327 (18)	0.0633 (7)
H38_1	−0.186691	0.077627	0.928461	0.076*
C39_1	−0.0749 (2)	0.1468 (2)	0.84893 (18)	0.0702 (8)
H39_1	−0.085961	0.140904	0.802706	0.084*
C40_1	0.00205 (17)	0.19370 (17)	0.84066 (13)	0.0514 (5)
H40_1	0.042138	0.220664	0.788935	0.062*
C41_1	0.54657 (10)	0.11626 (9)	0.85978 (7)	0.0174 (2)
C42_1	0.60649 (11)	0.06204 (9)	0.90959 (8)	0.0223 (2)
H42_1	0.592115	0.072094	0.961150	0.027*
C43_1	0.68732 (11)	−0.00675 (10)	0.88368 (9)	0.0263 (3)
H43_1	0.727588	−0.043938	0.917916	0.032*
C44_1	0.70950 (11)	−0.02142 (10)	0.80829 (9)	0.0243 (3)
H44_1	0.765823	−0.067452	0.790439	0.029*
C45_1	0.64910 (10)	0.03141 (10)	0.75884 (8)	0.0223 (2)
H45_1	0.663462	0.020808	0.707480	0.027*
C46_1	0.56776 (10)	0.09969 (9)	0.78457 (8)	0.0200 (2)
H46_1	0.526294	0.135331	0.750831	0.024*
Ni1_2	0.28975 (2)	0.83249 (2)	0.43364 (2)	0.01364 (4)
O1_2	0.50805 (9)	0.64893 (7)	0.56785 (6)	0.0283 (2)

O2_2	0.62162 (8)	0.80644 (8)	0.42677 (7)	0.0302 (2)
N1_2	0.41721 (8)	0.78939 (7)	0.45871 (6)	0.01517 (18)
N2_2	0.27290 (8)	0.94258 (7)	0.46574 (6)	0.01558 (18)
N3_2	0.16423 (8)	0.87745 (7)	0.40596 (6)	0.01547 (18)
N4_2	0.30230 (8)	0.71786 (7)	0.40912 (6)	0.01522 (18)
C1_2	0.58250 (12)	0.75395 (11)	0.59279 (10)	0.0290 (3)
H1A_2	0.558184	0.739419	0.651304	0.044*
H1B_2	0.585476	0.820551	0.572148	0.044*
H1C_2	0.651045	0.717531	0.575406	0.044*
C2_2	0.50988 (10)	0.72984 (9)	0.56124 (8)	0.0198 (2)
C3_2	0.43504 (9)	0.80502 (8)	0.52168 (7)	0.0161 (2)
C4_2	0.38177 (9)	0.88045 (8)	0.55537 (7)	0.0162 (2)
C5_2	0.31356 (9)	0.95134 (8)	0.52000 (7)	0.0169 (2)
C6_2	0.27751 (10)	1.04387 (9)	0.53410 (8)	0.0215 (2)
H6_2	0.292141	1.066722	0.570835	0.026*
C7_2	0.21887 (10)	1.09181 (9)	0.48497 (8)	0.0216 (2)
H7_2	0.187965	1.155733	0.478491	0.026*
C8_2	0.21207 (9)	1.02782 (8)	0.44431 (7)	0.0169 (2)
C9_2	0.14189 (9)	1.04319 (8)	0.40260 (7)	0.0168 (2)
C10_2	0.11645 (9)	0.96877 (8)	0.38785 (7)	0.0165 (2)
C11_2	0.02957 (10)	0.97407 (9)	0.36228 (8)	0.0215 (2)
H11_2	−0.013479	1.029283	0.343245	0.026*
C12_2	0.02063 (10)	0.88518 (10)	0.37046 (9)	0.0230 (3)
H12_2	−0.031828	0.866311	0.360766	0.028*
C13_2	0.10522 (9)	0.82533 (9)	0.39647 (8)	0.0180 (2)
C14_2	0.12783 (10)	0.72855 (9)	0.40686 (7)	0.0179 (2)
C15_2	0.22293 (10)	0.67784 (8)	0.41273 (7)	0.0168 (2)
C16_2	0.26007 (10)	0.58159 (9)	0.41017 (8)	0.0188 (2)
H16_2	0.220438	0.537605	0.415128	0.023*
C17_2	0.36288 (10)	0.56561 (8)	0.39928 (7)	0.0181 (2)
H17_2	0.409213	0.508973	0.393253	0.022*
C18_2	0.38782 (9)	0.65083 (8)	0.39867 (7)	0.0157 (2)
C19_2	0.48674 (9)	0.66652 (8)	0.38682 (7)	0.0162 (2)
C20_2	0.49964 (9)	0.73750 (8)	0.41204 (7)	0.0158 (2)
C21_2	0.60192 (10)	0.76690 (9)	0.38690 (8)	0.0190 (2)
C22_2	0.67802 (11)	0.75820 (11)	0.30658 (9)	0.0270 (3)
H22A_2	0.734347	0.706390	0.314416	0.040*
H22B_2	0.705335	0.816194	0.279880	0.040*
H22C_2	0.643640	0.746389	0.273455	0.040*
C23_2	0.39074 (10)	0.88720 (9)	0.63182 (8)	0.0201 (2)
C24_2	0.43383 (13)	0.95701 (11)	0.63622 (10)	0.0304 (3)
H24_2	0.461139	1.001193	0.589070	0.037*
C25_2	0.43662 (16)	0.96161 (13)	0.70989 (13)	0.0447 (5)
H25_2	0.465790	1.009207	0.712757	0.054*
C26_2	0.39721 (17)	0.89733 (14)	0.77919 (12)	0.0465 (5)
H26_2	0.398856	0.901333	0.829278	0.056*
C27_2	0.35584 (16)	0.82798 (14)	0.77513 (10)	0.0419 (4)
H27_2	0.329646	0.783414	0.822378	0.050*

C28_2	0.35222 (12)	0.82288 (12)	0.70191 (9)	0.0289 (3)
H28_2	0.323090	0.774892	0.699672	0.035*
C29_2	0.08651 (10)	1.14013 (9)	0.38022 (7)	0.0179 (2)
C30_2	0.14249 (11)	1.21040 (10)	0.33178 (9)	0.0248 (3)
H30_2	0.215163	1.195838	0.313527	0.030*
C31_2	0.09302 (13)	1.30144 (10)	0.30996 (10)	0.0315 (3)
H31_2	0.131933	1.348605	0.276725	0.038*
C32_2	−0.01331 (13)	1.32372 (10)	0.33665 (10)	0.0311 (3)
H32_2	−0.047186	1.385792	0.321171	0.037*
C33_2	−0.06940 (11)	1.25501 (10)	0.38582 (9)	0.0259 (3)
H33_2	−0.141950	1.270177	0.404883	0.031*
C34_2	−0.02000 (10)	1.16353 (9)	0.40760 (8)	0.0205 (2)
H34_2	−0.059200	1.116750	0.441346	0.025*
C35_2	0.04848 (10)	0.67982 (9)	0.40823 (9)	0.0227 (2)
C36_2	−0.03873 (12)	0.67244 (12)	0.47409 (11)	0.0331 (3)
H36_2	−0.047012	0.698605	0.517019	0.040*
C37_2	−0.11354 (14)	0.62693 (14)	0.47709 (14)	0.0470 (5)
H37_2	−0.172623	0.621842	0.522162	0.056*
C38_2	−0.10216 (17)	0.58903 (15)	0.41462 (15)	0.0515 (5)
H38_2	−0.153674	0.558473	0.416581	0.062*
C39_2	−0.01596 (19)	0.59565 (16)	0.34947 (14)	0.0533 (6)
H39_2	−0.008131	0.569213	0.306810	0.064*
C40_2	0.05973 (15)	0.64087 (14)	0.34582 (11)	0.0388 (4)
H40_2	0.118940	0.645131	0.300818	0.047*
C41_2	0.57430 (9)	0.59449 (8)	0.35779 (7)	0.0165 (2)
C42_2	0.63499 (10)	0.54212 (9)	0.40731 (8)	0.0210 (2)
H42_2	0.623945	0.556485	0.456686	0.025*
C43_2	0.71183 (11)	0.46877 (10)	0.38480 (9)	0.0248 (3)
H43_2	0.752475	0.432818	0.419087	0.030*
C44_2	0.72899 (11)	0.44820 (10)	0.31237 (9)	0.0243 (3)
H44_2	0.781599	0.398362	0.296955	0.029*
C45_2	0.66938 (10)	0.50038 (10)	0.26241 (8)	0.0220 (2)
H45_2	0.681787	0.486610	0.212556	0.026*
C46_2	0.59137 (10)	0.57292 (9)	0.28510 (8)	0.0201 (2)
H46_2	0.549798	0.607702	0.251235	0.024*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1_1	0.01363 (7)	0.01572 (7)	0.01559 (7)	−0.00219 (5)	−0.00567 (5)	−0.00531 (5)
O1_1	0.0388 (6)	0.0289 (5)	0.0262 (5)	0.0111 (5)	−0.0166 (5)	−0.0106 (4)
O2_1	0.0250 (5)	0.0426 (6)	0.0359 (6)	−0.0121 (5)	−0.0064 (4)	−0.0206 (5)
N1_1	0.0157 (4)	0.0169 (5)	0.0168 (4)	−0.0017 (4)	−0.0061 (4)	−0.0067 (4)
N2_1	0.0156 (4)	0.0177 (5)	0.0165 (4)	−0.0019 (4)	−0.0058 (4)	−0.0055 (4)
N3_1	0.0154 (4)	0.0189 (5)	0.0178 (5)	−0.0026 (4)	−0.0064 (4)	−0.0051 (4)
N4_1	0.0165 (4)	0.0180 (5)	0.0172 (4)	−0.0045 (4)	−0.0065 (4)	−0.0047 (4)
C1_1	0.0365 (8)	0.0232 (6)	0.0215 (6)	−0.0060 (6)	−0.0057 (6)	−0.0022 (5)
C2_1	0.0246 (6)	0.0209 (6)	0.0211 (6)	−0.0032 (5)	−0.0109 (5)	−0.0062 (5)

C3_1	0.0165 (5)	0.0189 (5)	0.0170 (5)	−0.0025 (4)	−0.0070 (4)	−0.0063 (4)
C4_1	0.0161 (5)	0.0187 (5)	0.0170 (5)	−0.0030 (4)	−0.0056 (4)	−0.0066 (4)
C5_1	0.0152 (5)	0.0182 (5)	0.0174 (5)	−0.0028 (4)	−0.0047 (4)	−0.0069 (4)
C6_1	0.0194 (6)	0.0192 (5)	0.0230 (6)	−0.0040 (4)	−0.0057 (5)	−0.0089 (5)
C7_1	0.0201 (6)	0.0175 (5)	0.0233 (6)	−0.0017 (4)	−0.0064 (5)	−0.0067 (5)
C8_1	0.0166 (5)	0.0178 (5)	0.0180 (5)	−0.0016 (4)	−0.0052 (4)	−0.0055 (4)
C9_1	0.0152 (5)	0.0193 (5)	0.0161 (5)	−0.0011 (4)	−0.0043 (4)	−0.0043 (4)
C10_1	0.0151 (5)	0.0214 (6)	0.0170 (5)	−0.0019 (4)	−0.0058 (4)	−0.0049 (4)
C11_1	0.0174 (5)	0.0270 (6)	0.0244 (6)	−0.0007 (5)	−0.0106 (5)	−0.0065 (5)
C12_1	0.0174 (6)	0.0284 (7)	0.0263 (6)	−0.0039 (5)	−0.0094 (5)	−0.0083 (5)
C13_1	0.0161 (5)	0.0234 (6)	0.0191 (5)	−0.0055 (4)	−0.0058 (4)	−0.0054 (5)
C14_1	0.0194 (6)	0.0238 (6)	0.0209 (6)	−0.0084 (5)	−0.0065 (5)	−0.0054 (5)
C15_1	0.0198 (6)	0.0205 (6)	0.0198 (5)	−0.0058 (5)	−0.0072 (4)	−0.0047 (4)
C16_1	0.0274 (7)	0.0187 (6)	0.0283 (6)	−0.0081 (5)	−0.0111 (5)	−0.0051 (5)
C17_1	0.0255 (6)	0.0175 (6)	0.0268 (6)	−0.0040 (5)	−0.0100 (5)	−0.0071 (5)
C18_1	0.0194 (5)	0.0166 (5)	0.0177 (5)	−0.0025 (4)	−0.0076 (4)	−0.0051 (4)
C19_1	0.0178 (5)	0.0170 (5)	0.0166 (5)	−0.0009 (4)	−0.0070 (4)	−0.0058 (4)
C20_1	0.0158 (5)	0.0176 (5)	0.0161 (5)	−0.0010 (4)	−0.0061 (4)	−0.0059 (4)
C21_1	0.0166 (5)	0.0194 (6)	0.0241 (6)	−0.0018 (4)	−0.0075 (5)	−0.0064 (5)
C22_1	0.0227 (6)	0.0265 (7)	0.0291 (7)	−0.0075 (5)	0.0000 (5)	−0.0096 (5)
C23_1	0.0223 (6)	0.0178 (5)	0.0167 (5)	−0.0037 (4)	−0.0074 (4)	−0.0066 (4)
C24_1	0.0266 (6)	0.0232 (6)	0.0198 (6)	−0.0042 (5)	−0.0051 (5)	−0.0089 (5)
C25_1	0.0403 (8)	0.0306 (7)	0.0204 (6)	−0.0066 (6)	−0.0069 (6)	−0.0124 (5)
C26_1	0.0472 (9)	0.0314 (7)	0.0254 (7)	−0.0092 (7)	−0.0189 (6)	−0.0098 (6)
C27_1	0.0329 (7)	0.0338 (8)	0.0298 (7)	−0.0079 (6)	−0.0166 (6)	−0.0108 (6)
C28_1	0.0230 (6)	0.0264 (6)	0.0222 (6)	−0.0061 (5)	−0.0085 (5)	−0.0088 (5)
C29_1	0.0177 (5)	0.0197 (5)	0.0176 (5)	0.0008 (4)	−0.0065 (4)	−0.0047 (4)
C30_1	0.0211 (6)	0.0218 (6)	0.0237 (6)	−0.0021 (5)	−0.0067 (5)	−0.0024 (5)
C31_1	0.0314 (7)	0.0227 (6)	0.0295 (7)	−0.0041 (6)	−0.0119 (6)	0.0024 (5)
C32_1	0.0325 (8)	0.0223 (7)	0.0348 (8)	0.0043 (6)	−0.0155 (6)	−0.0024 (6)
C33_1	0.0226 (6)	0.0293 (7)	0.0299 (7)	0.0058 (5)	−0.0086 (5)	−0.0074 (6)
C34_1	0.0198 (6)	0.0252 (6)	0.0208 (6)	0.0008 (5)	−0.0057 (5)	−0.0043 (5)
C35_1	0.0214 (6)	0.0253 (6)	0.0341 (7)	−0.0075 (5)	−0.0114 (5)	−0.0078 (5)
C36_1	0.0337 (8)	0.0299 (8)	0.0424 (9)	−0.0146 (6)	−0.0076 (7)	−0.0063 (7)
C37_1	0.0419 (10)	0.0411 (10)	0.0732 (15)	−0.0254 (9)	−0.0101 (10)	−0.0063 (10)
C38_1	0.0483 (12)	0.0566 (13)	0.103 (2)	−0.0304 (11)	−0.0321 (13)	−0.0149 (13)
C39_1	0.0726 (17)	0.092 (2)	0.0810 (18)	−0.0400 (15)	−0.0403 (15)	−0.0267 (15)
C40_1	0.0539 (12)	0.0751 (15)	0.0450 (11)	−0.0336 (11)	−0.0198 (9)	−0.0167 (10)
C41_1	0.0179 (5)	0.0162 (5)	0.0190 (5)	−0.0013 (4)	−0.0066 (4)	−0.0055 (4)
C42_1	0.0258 (6)	0.0217 (6)	0.0228 (6)	0.0020 (5)	−0.0131 (5)	−0.0085 (5)
C43_1	0.0265 (7)	0.0230 (6)	0.0333 (7)	0.0052 (5)	−0.0168 (6)	−0.0108 (5)
C44_1	0.0203 (6)	0.0223 (6)	0.0307 (7)	0.0014 (5)	−0.0073 (5)	−0.0116 (5)
C45_1	0.0220 (6)	0.0227 (6)	0.0210 (6)	−0.0013 (5)	−0.0040 (5)	−0.0084 (5)
C46_1	0.0214 (6)	0.0199 (6)	0.0189 (5)	−0.0004 (5)	−0.0072 (5)	−0.0058 (4)
Ni1_2	0.01412 (7)	0.01168 (7)	0.01588 (7)	0.00009 (5)	−0.00590 (5)	−0.00456 (5)
O1_2	0.0418 (6)	0.0154 (4)	0.0287 (5)	0.0027 (4)	−0.0177 (5)	−0.0046 (4)
O2_2	0.0261 (5)	0.0371 (6)	0.0332 (6)	−0.0126 (4)	−0.0036 (4)	−0.0162 (5)
N1_2	0.0159 (4)	0.0135 (4)	0.0170 (4)	−0.0003 (3)	−0.0063 (4)	−0.0051 (3)

N2_2	0.0166 (4)	0.0133 (4)	0.0173 (4)	0.0000 (3)	−0.0062 (4)	−0.0050 (4)
N3_2	0.0151 (4)	0.0143 (4)	0.0173 (4)	−0.0007 (3)	−0.0056 (4)	−0.0045 (4)
N4_2	0.0157 (4)	0.0131 (4)	0.0171 (4)	−0.0002 (3)	−0.0057 (4)	−0.0049 (3)
C1_2	0.0254 (7)	0.0317 (7)	0.0349 (8)	0.0023 (6)	−0.0180 (6)	−0.0104 (6)
C2_2	0.0214 (6)	0.0185 (5)	0.0187 (5)	0.0013 (4)	−0.0083 (5)	−0.0046 (4)
C3_2	0.0176 (5)	0.0138 (5)	0.0174 (5)	−0.0017 (4)	−0.0063 (4)	−0.0038 (4)
C4_2	0.0180 (5)	0.0151 (5)	0.0177 (5)	−0.0024 (4)	−0.0072 (4)	−0.0052 (4)
C5_2	0.0176 (5)	0.0148 (5)	0.0197 (5)	−0.0009 (4)	−0.0069 (4)	−0.0061 (4)
C6_2	0.0228 (6)	0.0177 (6)	0.0290 (6)	0.0015 (5)	−0.0112 (5)	−0.0123 (5)
C7_2	0.0223 (6)	0.0152 (5)	0.0291 (6)	0.0011 (4)	−0.0100 (5)	−0.0089 (5)
C8_2	0.0164 (5)	0.0134 (5)	0.0194 (5)	0.0006 (4)	−0.0053 (4)	−0.0046 (4)
C9_2	0.0164 (5)	0.0149 (5)	0.0163 (5)	0.0002 (4)	−0.0041 (4)	−0.0032 (4)
C10_2	0.0160 (5)	0.0157 (5)	0.0164 (5)	0.0000 (4)	−0.0055 (4)	−0.0033 (4)
C11_2	0.0198 (6)	0.0208 (6)	0.0248 (6)	0.0022 (5)	−0.0116 (5)	−0.0060 (5)
C12_2	0.0191 (6)	0.0245 (6)	0.0290 (7)	0.0000 (5)	−0.0124 (5)	−0.0085 (5)
C13_2	0.0166 (5)	0.0185 (5)	0.0200 (5)	−0.0020 (4)	−0.0066 (4)	−0.0059 (4)
C14_2	0.0175 (5)	0.0185 (5)	0.0191 (5)	−0.0030 (4)	−0.0060 (4)	−0.0057 (4)
C15_2	0.0190 (5)	0.0154 (5)	0.0171 (5)	−0.0037 (4)	−0.0054 (4)	−0.0048 (4)
C16_2	0.0233 (6)	0.0151 (5)	0.0193 (5)	−0.0040 (4)	−0.0068 (5)	−0.0046 (4)
C17_2	0.0239 (6)	0.0140 (5)	0.0174 (5)	−0.0015 (4)	−0.0072 (4)	−0.0055 (4)
C18_2	0.0188 (5)	0.0136 (5)	0.0159 (5)	−0.0001 (4)	−0.0067 (4)	−0.0053 (4)
C19_2	0.0175 (5)	0.0153 (5)	0.0154 (5)	0.0013 (4)	−0.0063 (4)	−0.0052 (4)
C20_2	0.0156 (5)	0.0148 (5)	0.0170 (5)	0.0006 (4)	−0.0065 (4)	−0.0046 (4)
C21_2	0.0181 (5)	0.0162 (5)	0.0215 (6)	−0.0010 (4)	−0.0060 (4)	−0.0041 (4)
C22_2	0.0233 (6)	0.0320 (7)	0.0228 (6)	−0.0079 (6)	−0.0012 (5)	−0.0064 (5)
C23_2	0.0214 (6)	0.0198 (6)	0.0231 (6)	0.0018 (4)	−0.0112 (5)	−0.0099 (5)
C24_2	0.0387 (8)	0.0216 (6)	0.0416 (8)	−0.0015 (6)	−0.0247 (7)	−0.0105 (6)
C25_2	0.0596 (12)	0.0327 (9)	0.0645 (12)	0.0075 (8)	−0.0443 (11)	−0.0262 (9)
C26_2	0.0631 (13)	0.0490 (11)	0.0394 (9)	0.0152 (9)	−0.0348 (9)	−0.0254 (8)
C27_2	0.0516 (11)	0.0508 (11)	0.0225 (7)	0.0007 (9)	−0.0145 (7)	−0.0114 (7)
C28_2	0.0321 (7)	0.0357 (8)	0.0205 (6)	−0.0070 (6)	−0.0076 (5)	−0.0078 (6)
C29_2	0.0191 (5)	0.0152 (5)	0.0162 (5)	0.0012 (4)	−0.0051 (4)	−0.0030 (4)
C30_2	0.0208 (6)	0.0200 (6)	0.0263 (6)	−0.0017 (5)	−0.0039 (5)	−0.0003 (5)
C31_2	0.0318 (8)	0.0179 (6)	0.0344 (8)	−0.0028 (5)	−0.0073 (6)	0.0041 (5)
C32_2	0.0331 (8)	0.0181 (6)	0.0351 (8)	0.0052 (5)	−0.0138 (6)	−0.0007 (6)
C33_2	0.0222 (6)	0.0210 (6)	0.0293 (7)	0.0059 (5)	−0.0081 (5)	−0.0061 (5)
C34_2	0.0188 (6)	0.0189 (6)	0.0190 (5)	0.0007 (4)	−0.0042 (4)	−0.0027 (4)
C35_2	0.0208 (6)	0.0199 (6)	0.0310 (7)	−0.0051 (5)	−0.0114 (5)	−0.0053 (5)
C36_2	0.0245 (7)	0.0303 (8)	0.0442 (9)	−0.0082 (6)	−0.0039 (6)	−0.0126 (7)
C37_2	0.0272 (8)	0.0414 (10)	0.0714 (14)	−0.0150 (7)	−0.0060 (8)	−0.0138 (9)
C38_2	0.0454 (11)	0.0474 (11)	0.0769 (15)	−0.0252 (9)	−0.0286 (11)	−0.0092 (10)
C39_2	0.0707 (15)	0.0594 (13)	0.0539 (12)	−0.0339 (12)	−0.0297 (11)	−0.0144 (10)
C40_2	0.0469 (10)	0.0483 (10)	0.0332 (8)	−0.0235 (8)	−0.0128 (7)	−0.0122 (7)
C41_2	0.0169 (5)	0.0164 (5)	0.0165 (5)	0.0011 (4)	−0.0062 (4)	−0.0063 (4)
C42_2	0.0234 (6)	0.0205 (6)	0.0201 (6)	0.0032 (5)	−0.0098 (5)	−0.0084 (5)
C43_2	0.0239 (6)	0.0244 (6)	0.0268 (6)	0.0074 (5)	−0.0136 (5)	−0.0098 (5)
C44_2	0.0204 (6)	0.0242 (6)	0.0289 (7)	0.0049 (5)	−0.0077 (5)	−0.0139 (5)
C45_2	0.0203 (6)	0.0269 (6)	0.0198 (6)	0.0001 (5)	−0.0043 (5)	−0.0122 (5)

C46_2	0.0197 (6)	0.0225 (6)	0.0183 (5)	0.0019 (5)	−0.0069 (4)	−0.0085 (5)

Geometric parameters (Å, º)

Ni1_1—N2_1	1.8911 (11)	Ni1_2—N2_2	1.8845 (10)
Ni1_1—N4_1	1.8930 (11)	Ni1_2—N4_2	1.8934 (10)
Ni1_1—N1_1	1.8957 (10)	Ni1_2—N3_2	1.9106 (10)
Ni1_1—N3_1	1.9084 (11)	Ni1_2—N1_2	1.9128 (10)
O1_1—C2_1	1.2141 (17)	O1_2—C2_2	1.2141 (16)
O2_1—C21_1	1.2122 (16)	O2_2—C21_2	1.2192 (16)
N1_1—C3_1	1.3687 (15)	N1_2—C3_2	1.3661 (15)
N1_1—C20_1	1.3879 (15)	N1_2—C20_2	1.3997 (15)
N2_1—C5_1	1.3680 (15)	N2_2—C5_2	1.3661 (16)
N2_1—C8_1	1.3853 (16)	N2_2—C8_2	1.3880 (15)
N3_1—C10_1	1.3772 (16)	N3_2—C10_2	1.3766 (15)
N3_1—C13_1	1.3804 (16)	N3_2—C13_2	1.3796 (16)
N4_1—C18_1	1.3678 (16)	N4_2—C18_2	1.3626 (15)
N4_1—C15_1	1.3844 (16)	N4_2—C15_2	1.3879 (16)
C1_1—C2_1	1.514 (2)	C1_2—C2_2	1.508 (2)
C1_1—H1A_1	0.9800	C1_2—H1A_2	0.9800
C1_1—H1B_1	0.9800	C1_2—H1B_2	0.9800
C1_1—H1C_1	0.9800	C1_2—H1C_2	0.9800
C2_1—C3_1	1.5239 (18)	C2_2—C3_2	1.5336 (17)
C3_1—C4_1	1.3938 (17)	C3_2—C4_2	1.3934 (17)
C4_1—C5_1	1.4022 (17)	C4_2—C5_2	1.4075 (17)
C4_1—C23_1	1.4808 (16)	C4_2—C23_2	1.4908 (17)
C5_1—C6_1	1.4417 (17)	C5_2—C6_2	1.4452 (17)
C6_1—C7_1	1.3556 (19)	C6_2—C7_2	1.3544 (19)
C6_1—H6_1	0.9500	C6_2—H6_2	0.9500
C7_1—C8_1	1.4442 (18)	C7_2—C8_2	1.4420 (18)
C7_1—H7_1	0.9500	C7_2—H7_2	0.9500
C8_1—C9_1	1.3912 (17)	C8_2—C9_2	1.3870 (17)
C9_1—C10_1	1.4048 (18)	C9_2—C10_2	1.4063 (17)
C9_1—C29_1	1.4898 (18)	C9_2—C29_2	1.4906 (17)
C10_1—C11_1	1.4381 (17)	C10_2—C11_2	1.4362 (18)
C11_1—C12_1	1.361 (2)	C11_2—C12_2	1.3583 (19)
C11_1—H11_1	0.9500	C11_2—H11_2	0.9500
C12_1—C13_1	1.4342 (19)	C12_2—C13_2	1.4315 (18)
C12_1—H12_1	0.9500	C12_2—H12_2	0.9500
C13_1—C14_1	1.3960 (19)	C13_2—C14_2	1.3981 (18)
C14_1—C15_1	1.3889 (19)	C14_2—C15_2	1.3858 (18)
C14_1—C35_1	1.4948 (18)	C14_2—C35_2	1.4927 (18)
C15_1—C16_1	1.4328 (19)	C15_2—C16_2	1.4383 (17)
C16_1—C17_1	1.361 (2)	C16_2—C17_2	1.3609 (18)
C16_1—H16_1	0.9500	C16_2—H16_2	0.9500
C17_1—C18_1	1.4371 (17)	C17_2—C18_2	1.4355 (17)
C17_1—H17_1	0.9500	C17_2—H17_2	0.9500
C18_1—C19_1	1.4078 (17)	C18_2—C19_2	1.4121 (17)

C19_1—C20_1	1.3839 (17)	C19_2—C20_2	1.3801 (17)
C19_1—C41_1	1.4902 (17)	C19_2—C41_2	1.4881 (16)
C20_1—C21_1	1.5179 (17)	C20_2—C21_2	1.5027 (18)
C21_1—C22_1	1.5142 (19)	C21_2—C22_2	1.5145 (19)
C22_1—H22A_1	0.9800	C22_2—H22A_2	0.9800
C22_1—H22B_1	0.9800	C22_2—H22B_2	0.9800
C22_1—H22C_1	0.9800	C22_2—H22C_2	0.9800
C23_1—C28_1	1.3922 (18)	C23_2—C28_2	1.393 (2)
C23_1—C24_1	1.3992 (18)	C23_2—C24_2	1.3977 (19)
C24_1—C25_1	1.3878 (19)	C24_2—C25_2	1.392 (2)
C24_1—H24_1	0.9500	C24_2—H24_2	0.9500
C25_1—C26_1	1.390 (2)	C25_2—C26_2	1.388 (3)
C25_1—H25_1	0.9500	C25_2—H25_2	0.9500
C26_1—C27_1	1.384 (2)	C26_2—C27_2	1.373 (3)
C26_1—H26_1	0.9500	C26_2—H26_2	0.9500
C27_1—C28_1	1.3906 (19)	C27_2—C28_2	1.391 (2)
C27_1—H27_1	0.9500	C27_2—H27_2	0.9500
C28_1—H28_1	0.9500	C28_2—H28_2	0.9500
C29_1—C30_1	1.3950 (19)	C29_2—C34_2	1.3952 (18)
C29_1—C34_1	1.3985 (18)	C29_2—C30_2	1.3957 (18)
C30_1—C31_1	1.388 (2)	C30_2—C31_2	1.390 (2)
C30_1—H30_1	0.9500	C30_2—H30_2	0.9500
C31_1—C32_1	1.390 (2)	C31_2—C32_2	1.391 (2)
C31_1—H31_1	0.9500	C31_2—H31_2	0.9500
C32_1—C33_1	1.386 (2)	C32_2—C33_2	1.382 (2)
C32_1—H32_1	0.9500	C32_2—H32_2	0.9500
C33_1—C34_1	1.391 (2)	C33_2—C34_2	1.3944 (18)
C33_1—H33_1	0.9500	C33_2—H33_2	0.9500
C34_1—H34_1	0.9500	C34_2—H34_2	0.9500
C35_1—C40_1	1.381 (2)	C35_2—C40_2	1.393 (2)
C35_1—C36_1	1.389 (2)	C35_2—C36_2	1.396 (2)
C36_1—C37_1	1.392 (2)	C36_2—C37_2	1.390 (2)
C36_1—H36_1	0.9500	C36_2—H36_2	0.9500
C37_1—C38_1	1.374 (4)	C37_2—C38_2	1.383 (3)
C37_1—H37_1	0.9500	C37_2—H37_2	0.9500
C38_1—C39_1	1.370 (4)	C38_2—C39_2	1.380 (3)
C38_1—H38_1	0.9500	C38_2—H38_2	0.9500
C39_1—C40_1	1.397 (3)	C39_2—C40_2	1.394 (2)
C39_1—H39_1	0.9500	C39_2—H39_2	0.9500
C40_1—H40_1	0.9500	C40_2—H40_2	0.9500
C41_1—C42_1	1.3953 (18)	C41_2—C42_2	1.3928 (17)
C41_1—C46_1	1.3975 (17)	C41_2—C46_2	1.3993 (17)
C42_1—C43_1	1.3915 (19)	C42_2—C43_2	1.3934 (18)
C42_1—H42_1	0.9500	C42_2—H42_2	0.9500
C43_1—C44_1	1.386 (2)	C43_2—C44_2	1.3869 (19)
C43_1—H43_1	0.9500	C43_2—H43_2	0.9500
C44_1—C45_1	1.391 (2)	C44_2—C45_2	1.387 (2)
C44_1—H44_1	0.9500	C44_2—H44_2	0.9500

C45_1—C46_1	1.3891 (18)	C45_2—C46_2	1.3935 (18)
C45_1—H45_1	0.9500	C45_2—H45_2	0.9500
C46_1—H46_1	0.9500	C46_2—H46_2	0.9500
N2_1—Ni1_1—N4_1	176.50 (5)	N2_2—Ni1_2—N4_2	175.90 (5)
N2_1—Ni1_1—N1_1	90.06 (4)	N2_2—Ni1_2—N3_2	90.19 (4)
N4_1—Ni1_1—N1_1	88.86 (4)	N4_2—Ni1_2—N3_2	90.20 (4)
N2_1—Ni1_1—N3_1	89.92 (5)	N2_2—Ni1_2—N1_2	89.59 (4)
N4_1—Ni1_1—N3_1	91.19 (5)	N4_2—Ni1_2—N1_2	90.12 (4)
N1_1—Ni1_1—N3_1	179.68 (5)	N3_2—Ni1_2—N1_2	178.50 (5)
C3_1—N1_1—C20_1	114.99 (10)	C3_2—N1_2—C20_2	115.41 (10)
C3_1—N1_1—Ni1_1	121.95 (8)	C3_2—N1_2—Ni1_2	124.13 (8)
C20_1—N1_1—Ni1_1	123.00 (8)	C20_2—N1_2—Ni1_2	120.46 (8)
C5_1—N2_1—C8_1	106.09 (10)	C5_2—N2_2—C8_2	106.48 (10)
C5_1—N2_1—Ni1_1	126.12 (9)	C5_2—N2_2—Ni1_2	125.72 (8)
C8_1—N2_1—Ni1_1	127.72 (8)	C8_2—N2_2—Ni1_2	127.65 (8)
C10_1—N3_1—C13_1	106.00 (10)	C10_2—N3_2—C13_2	105.79 (10)
C10_1—N3_1—Ni1_1	127.71 (9)	C10_2—N3_2—Ni1_2	127.17 (8)
C13_1—N3_1—Ni1_1	126.29 (9)	C13_2—N3_2—Ni1_2	126.99 (8)
C18_1—N4_1—C15_1	106.00 (10)	C18_2—N4_2—C15_2	105.74 (10)
C18_1—N4_1—Ni1_1	127.08 (8)	C18_2—N4_2—Ni1_2	126.63 (8)
C15_1—N4_1—Ni1_1	126.32 (9)	C15_2—N4_2—Ni1_2	126.67 (8)
C2_1—C1_1—H1A_1	109.5	C2_2—C1_2—H1A_2	109.5
C2_1—C1_1—H1B_1	109.5	C2_2—C1_2—H1B_2	109.5
H1A_1—C1_1—H1B_1	109.5	H1A_2—C1_2—H1B_2	109.5
C2_1—C1_1—H1C_1	109.5	C2_2—C1_2—H1C_2	109.5
H1A_1—C1_1—H1C_1	109.5	H1A_2—C1_2—H1C_2	109.5
H1B_1—C1_1—H1C_1	109.5	H1B_2—C1_2—H1C_2	109.5
O1_1—C2_1—C1_1	119.75 (13)	O1_2—C2_2—C1_2	120.23 (12)
O1_1—C2_1—C3_1	122.85 (12)	O1_2—C2_2—C3_2	117.78 (12)
C1_1—C2_1—C3_1	116.68 (12)	C1_2—C2_2—C3_2	121.98 (12)
N1_1—C3_1—C4_1	122.96 (11)	N1_2—C3_2—C4_2	123.14 (11)
N1_1—C3_1—C2_1	115.49 (11)	N1_2—C3_2—C2_2	117.19 (10)
C4_1—C3_1—C2_1	120.56 (11)	C4_2—C3_2—C2_2	119.38 (11)
C3_1—C4_1—C5_1	120.68 (11)	C3_2—C4_2—C5_2	120.86 (11)
C3_1—C4_1—C23_1	119.78 (11)	C3_2—C4_2—C23_2	121.66 (11)
C5_1—C4_1—C23_1	119.17 (11)	C5_2—C4_2—C23_2	117.42 (11)
N2_1—C5_1—C4_1	123.75 (11)	N2_2—C5_2—C4_2	124.37 (11)
N2_1—C5_1—C6_1	110.40 (11)	N2_2—C5_2—C6_2	109.94 (11)
C4_1—C5_1—C6_1	125.84 (11)	C4_2—C5_2—C6_2	125.68 (11)
C7_1—C6_1—C5_1	106.76 (11)	C7_2—C6_2—C5_2	106.94 (11)
C7_1—C6_1—H6_1	126.6	C7_2—C6_2—H6_2	126.5
C5_1—C6_1—H6_1	126.6	C5_2—C6_2—H6_2	126.5
C6_1—C7_1—C8_1	107.26 (11)	C6_2—C7_2—C8_2	107.30 (11)
C6_1—C7_1—H7_1	126.4	C6_2—C7_2—H7_2	126.4
C8_1—C7_1—H7_1	126.4	C8_2—C7_2—H7_2	126.4
N2_1—C8_1—C9_1	124.27 (11)	C9_2—C8_2—N2_2	124.72 (11)
N2_1—C8_1—C7_1	109.40 (11)	C9_2—C8_2—C7_2	125.10 (11)

C9_1—C8_1—C7_1	125.61 (12)	N2_2—C8_2—C7_2	109.18 (11)
C8_1—C9_1—C10_1	121.36 (12)	C8_2—C9_2—C10_2	121.26 (11)
C8_1—C9_1—C29_1	117.74 (11)	C8_2—C9_2—C29_2	118.14 (11)
C10_1—C9_1—C29_1	120.73 (11)	C10_2—C9_2—C29_2	120.36 (11)
N3_1—C10_1—C9_1	124.35 (11)	N3_2—C10_2—C9_2	124.11 (11)
N3_1—C10_1—C11_1	109.92 (11)	N3_2—C10_2—C11_2	109.93 (11)
C9_1—C10_1—C11_1	125.44 (12)	C9_2—C10_2—C11_2	125.47 (11)
C12_1—C11_1—C10_1	106.90 (12)	C12_2—C11_2—C10_2	107.00 (11)
C12_1—C11_1—H11_1	126.6	C12_2—C11_2—H11_2	126.5
C10_1—C11_1—H11_1	126.6	C10_2—C11_2—H11_2	126.5
C11_1—C12_1—C13_1	107.12 (12)	C11_2—C12_2—C13_2	107.00 (12)
C11_1—C12_1—H12_1	126.4	C11_2—C12_2—H12_2	126.5
C13_1—C12_1—H12_1	126.4	C13_2—C12_2—H12_2	126.5
N3_1—C13_1—C14_1	124.80 (12)	N3_2—C13_2—C14_2	124.81 (11)
N3_1—C13_1—C12_1	109.91 (11)	N3_2—C13_2—C12_2	110.12 (11)
C14_1—C13_1—C12_1	125.25 (12)	C14_2—C13_2—C12_2	125.00 (12)
C15_1—C14_1—C13_1	122.27 (12)	C15_2—C14_2—C13_2	121.64 (11)
C15_1—C14_1—C35_1	118.93 (12)	C15_2—C14_2—C35_2	119.60 (11)
C13_1—C14_1—C35_1	118.80 (12)	C13_2—C14_2—C35_2	118.71 (11)
N4_1—C15_1—C14_1	123.63 (12)	C14_2—C15_2—N4_2	123.45 (11)
N4_1—C15_1—C16_1	109.74 (11)	C14_2—C15_2—C16_2	126.11 (11)
C14_1—C15_1—C16_1	125.89 (12)	N4_2—C15_2—C16_2	109.72 (11)
C17_1—C16_1—C15_1	107.11 (11)	C17_2—C16_2—C15_2	106.83 (11)
C17_1—C16_1—H16_1	126.4	C17_2—C16_2—H16_2	126.6
C15_1—C16_1—H16_1	126.4	C15_2—C16_2—H16_2	126.6
C16_1—C17_1—C18_1	106.80 (12)	C16_2—C17_2—C18_2	106.79 (11)
C16_1—C17_1—H17_1	126.6	C16_2—C17_2—H17_2	126.6
C18_1—C17_1—H17_1	126.6	C18_2—C17_2—H17_2	126.6
N4_1—C18_1—C19_1	123.53 (11)	N4_2—C18_2—C19_2	123.16 (11)
N4_1—C18_1—C17_1	110.26 (11)	N4_2—C18_2—C17_2	110.73 (11)
C19_1—C18_1—C17_1	126.19 (12)	C19_2—C18_2—C17_2	126.08 (11)
C20_1—C19_1—C18_1	120.46 (11)	C20_2—C19_2—C18_2	120.95 (11)
C20_1—C19_1—C41_1	122.21 (11)	C20_2—C19_2—C41_2	122.01 (11)
C18_1—C19_1—C41_1	116.89 (11)	C18_2—C19_2—C41_2	116.37 (11)
C19_1—C20_1—N1_1	121.39 (11)	C19_2—C20_2—N1_2	121.86 (11)
C19_1—C20_1—C21_1	123.37 (11)	C19_2—C20_2—C21_2	121.72 (11)
N1_1—C20_1—C21_1	114.92 (10)	N1_2—C20_2—C21_2	116.33 (10)
O2_1—C21_1—C22_1	119.18 (12)	O2_2—C21_2—C20_2	120.92 (12)
O2_1—C21_1—C20_1	121.03 (12)	O2_2—C21_2—C22_2	118.27 (12)
C22_1—C21_1—C20_1	119.32 (11)	C20_2—C21_2—C22_2	120.43 (11)
C21_1—C22_1—H22A_1	109.5	C21_2—C22_2—H22A_2	109.5
C21_1—C22_1—H22B_1	109.5	C21_2—C22_2—H22B_2	109.5
H22A_1—C22_1—H22B_1	109.5	H22A_2—C22_2—H22B_2	109.5
C21_1—C22_1—H22C_1	109.5	C21_2—C22_2—H22C_2	109.5
H22A_1—C22_1—H22C_1	109.5	H22A_2—C22_2—H22C_2	109.5
H22B_1—C22_1—H22C_1	109.5	H22B_2—C22_2—H22C_2	109.5
C28_1—C23_1—C24_1	119.16 (12)	C28_2—C23_2—C24_2	118.74 (13)
C28_1—C23_1—C4_1	119.38 (11)	C28_2—C23_2—C4_2	118.70 (12)

C24_1—C23_1—C4_1	121.43 (12)	C24_2—C23_2—C4_2	122.54 (13)
C25_1—C24_1—C23_1	120.05 (14)	C25_2—C24_2—C23_2	119.80 (16)
C25_1—C24_1—H24_1	120.0	C25_2—C24_2—H24_2	120.1
C23_1—C24_1—H24_1	120.0	C23_2—C24_2—H24_2	120.1
C24_1—C25_1—C26_1	120.31 (14)	C26_2—C25_2—C24_2	120.66 (17)
C24_1—C25_1—H25_1	119.8	C26_2—C25_2—H25_2	119.7
C26_1—C25_1—H25_1	119.8	C24_2—C25_2—H25_2	119.7
C27_1—C26_1—C25_1	119.88 (13)	C27_2—C26_2—C25_2	119.79 (16)
C27_1—C26_1—H26_1	120.1	C27_2—C26_2—H26_2	120.1
C25_1—C26_1—H26_1	120.1	C25_2—C26_2—H26_2	120.1
C26_1—C27_1—C28_1	120.04 (14)	C26_2—C27_2—C28_2	120.08 (18)
C26_1—C27_1—H27_1	120.0	C26_2—C27_2—H27_2	120.0
C28_1—C27_1—H27_1	120.0	C28_2—C27_2—H27_2	120.0
C27_1—C28_1—C23_1	120.51 (13)	C27_2—C28_2—C23_2	120.91 (16)
C27_1—C28_1—H28_1	119.7	C27_2—C28_2—H28_2	119.5
C23_1—C28_1—H28_1	119.7	C23_2—C28_2—H28_2	119.5
C30_1—C29_1—C34_1	118.59 (12)	C34_2—C29_2—C30_2	118.63 (12)
C30_1—C29_1—C9_1	119.49 (11)	C34_2—C29_2—C9_2	122.00 (11)
C34_1—C29_1—C9_1	121.85 (12)	C30_2—C29_2—C9_2	119.35 (11)
C31_1—C30_1—C29_1	120.97 (13)	C31_2—C30_2—C29_2	120.67 (13)
C31_1—C30_1—H30_1	119.5	C31_2—C30_2—H30_2	119.7
C29_1—C30_1—H30_1	119.5	C29_2—C30_2—H30_2	119.7
C30_1—C31_1—C32_1	120.01 (14)	C30_2—C31_2—C32_2	120.20 (14)
C30_1—C31_1—H31_1	120.0	C30_2—C31_2—H31_2	119.9
C32_1—C31_1—H31_1	120.0	C32_2—C31_2—H31_2	119.9
C33_1—C32_1—C31_1	119.56 (14)	C33_2—C32_2—C31_2	119.61 (13)
C33_1—C32_1—H32_1	120.2	C33_2—C32_2—H32_2	120.2
C31_1—C32_1—H32_1	120.2	C31_2—C32_2—H32_2	120.2
C32_1—C33_1—C34_1	120.55 (14)	C32_2—C33_2—C34_2	120.32 (13)
C32_1—C33_1—H33_1	119.7	C32_2—C33_2—H33_2	119.8
C34_1—C33_1—H33_1	119.7	C34_2—C33_2—H33_2	119.8
C33_1—C34_1—C29_1	120.32 (13)	C33_2—C34_2—C29_2	120.55 (13)
C33_1—C34_1—H34_1	119.8	C33_2—C34_2—H34_2	119.7
C29_1—C34_1—H34_1	119.8	C29_2—C34_2—H34_2	119.7
C40_1—C35_1—C36_1	119.26 (15)	C40_2—C35_2—C36_2	119.25 (14)
C40_1—C35_1—C14_1	122.55 (15)	C40_2—C35_2—C14_2	121.69 (13)
C36_1—C35_1—C14_1	118.15 (13)	C36_2—C35_2—C14_2	119.06 (13)
C35_1—C36_1—C37_1	120.20 (18)	C37_2—C36_2—C35_2	120.23 (17)
C35_1—C36_1—H36_1	119.9	C37_2—C36_2—H36_2	119.9
C37_1—C36_1—H36_1	119.9	C35_2—C36_2—H36_2	119.9
C38_1—C37_1—C36_1	120.1 (2)	C38_2—C37_2—C36_2	120.17 (19)
C38_1—C37_1—H37_1	119.9	C38_2—C37_2—H37_2	119.9
C36_1—C37_1—H37_1	119.9	C36_2—C37_2—H37_2	119.9
C39_1—C38_1—C37_1	119.99 (18)	C39_2—C38_2—C37_2	119.96 (17)
C39_1—C38_1—H38_1	120.0	C39_2—C38_2—H38_2	120.0
C37_1—C38_1—H38_1	120.0	C37_2—C38_2—H38_2	120.0
C38_1—C39_1—C40_1	120.4 (2)	C38_2—C39_2—C40_2	120.44 (19)
C38_1—C39_1—H39_1	119.8	C38_2—C39_2—H39_2	119.8

C40_1—C39_1—H39_1	119.8	C40_2—C39_2—H39_2	119.8
C35_1—C40_1—C39_1	119.9 (2)	C35_2—C40_2—C39_2	119.95 (18)
C35_1—C40_1—H40_1	120.0	C35_2—C40_2—H40_2	120.0
C39_1—C40_1—H40_1	120.0	C39_2—C40_2—H40_2	120.0
C42_1—C41_1—C46_1	119.32 (12)	C42_2—C41_2—C46_2	119.39 (11)
C42_1—C41_1—C19_1	119.83 (11)	C42_2—C41_2—C19_2	119.00 (11)
C46_1—C41_1—C19_1	120.77 (11)	C46_2—C41_2—C19_2	121.38 (11)
C43_1—C42_1—C41_1	119.96 (12)	C41_2—C42_2—C43_2	120.33 (12)
C43_1—C42_1—H42_1	120.0	C41_2—C42_2—H42_2	119.8
C41_1—C42_1—H42_1	120.0	C43_2—C42_2—H42_2	119.8
C44_1—C43_1—C42_1	120.47 (13)	C44_2—C43_2—C42_2	120.04 (12)
C44_1—C43_1—H43_1	119.8	C44_2—C43_2—H43_2	120.0
C42_1—C43_1—H43_1	119.8	C42_2—C43_2—H43_2	120.0
C43_1—C44_1—C45_1	119.84 (13)	C43_2—C44_2—C45_2	120.04 (12)
C43_1—C44_1—H44_1	120.1	C43_2—C44_2—H44_2	120.0
C45_1—C44_1—H44_1	120.1	C45_2—C44_2—H44_2	120.0
C46_1—C45_1—C44_1	119.99 (12)	C44_2—C45_2—C46_2	120.23 (12)
C46_1—C45_1—H45_1	120.0	C44_2—C45_2—H45_2	119.9
C44_1—C45_1—H45_1	120.0	C46_2—C45_2—H45_2	119.9
C45_1—C46_1—C41_1	120.39 (12)	C45_2—C46_2—C41_2	119.97 (12)
C45_1—C46_1—H46_1	119.8	C45_2—C46_2—H46_2	120.0
C41_1—C46_1—H46_1	119.8	C41_2—C46_2—H46_2	120.0

N2_1—Ni1_1—N1_1—C3_1	39.81 (10)	C42_1—C41_1—C46_1—C45_1	−1.5 (2)
N4_1—Ni1_1—N1_1—C3_1	−136.86 (10)	C19_1—C41_1—C46_1—C45_1	−178.15 (12)
N2_1—Ni1_1—N1_1—C20_1	−143.06 (10)	N3_2—Ni1_2—N2_2—C5_2	154.78 (11)
N4_1—Ni1_1—N1_1—C20_1	40.28 (10)	N1_2—Ni1_2—N2_2—C5_2	−26.71 (11)
N1_1—Ni1_1—N2_1—C5_1	−19.48 (10)	N3_2—Ni1_2—N2_2—C8_2	−20.15 (11)
N3_1—Ni1_1—N2_1—C5_1	160.83 (10)	N1_2—Ni1_2—N2_2—C8_2	158.36 (11)
N1_1—Ni1_1—N2_1—C8_1	157.04 (11)	N3_2—Ni1_2—N4_2—C18_2	165.64 (10)
N3_1—Ni1_1—N2_1—C8_1	−22.64 (11)	N1_2—Ni1_2—N4_2—C18_2	−12.89 (11)
N1_1—Ni1_1—N4_1—C18_1	−14.98 (11)	N3_2—Ni1_2—N4_2—C15_2	−27.18 (10)
N3_1—Ni1_1—N4_1—C18_1	164.71 (11)	N1_2—Ni1_2—N4_2—C15_2	154.29 (10)
N1_1—Ni1_1—N4_1—C15_1	154.90 (11)	C20_2—N1_2—C3_2—C4_2	154.90 (12)
N3_1—Ni1_1—N4_1—C15_1	−25.42 (11)	Ni1_2—N1_2—C3_2—C4_2	−25.72 (17)
C20_1—N1_1—C3_1—C4_1	144.70 (12)	C20_2—N1_2—C3_2—C2_2	−31.32 (15)
Ni1_1—N1_1—C3_1—C4_1	−37.95 (16)	Ni1_2—N1_2—C3_2—C2_2	148.07 (9)
C20_1—N1_1—C3_1—C2_1	−46.59 (15)	O1_2—C2_2—C3_2—N1_2	−37.75 (17)
Ni1_1—N1_1—C3_1—C2_1	130.76 (10)	C1_2—C2_2—C3_2—N1_2	143.45 (13)
O1_1—C2_1—C3_1—N1_1	39.90 (19)	O1_2—C2_2—C3_2—C4_2	136.28 (13)
C1_1—C2_1—C3_1—N1_1	−130.33 (13)	C1_2—C2_2—C3_2—C4_2	−42.52 (18)
O1_1—C2_1—C3_1—C4_1	−151.09 (14)	N1_2—C3_2—C4_2—C5_2	−7.22 (19)
C1_1—C2_1—C3_1—C4_1	38.67 (17)	C2_2—C3_2—C4_2—C5_2	179.12 (11)
N1_1—C3_1—C4_1—C5_1	2.82 (19)	N1_2—C3_2—C4_2—C23_2	169.86 (12)
C2_1—C3_1—C4_1—C5_1	−165.34 (12)	C2_2—C3_2—C4_2—C23_2	−3.80 (18)
N1_1—C3_1—C4_1—C23_1	−170.12 (11)	C8_2—N2_2—C5_2—C4_2	−178.62 (12)
C2_1—C3_1—C4_1—C23_1	21.71 (18)	Ni1_2—N2_2—C5_2—C4_2	5.57 (18)
C8_1—N2_1—C5_1—C4_1	177.17 (12)	C8_2—N2_2—C5_2—C6_2	0.42 (14)

Ni1_1—N2_1—C5_1—C4_1	−5.69 (18)	Ni1_2—N2_2—C5_2—C6_2	−175.40 (9)
C8_1—N2_1—C5_1—C6_1	−1.73 (14)	C3_2—C4_2—C5_2—N2_2	18.0 (2)
Ni1_1—N2_1—C5_1—C6_1	175.41 (8)	C23_2—C4_2—C5_2—N2_2	−159.19 (12)
C3_1—C4_1—C5_1—N2_1	20.07 (19)	C3_2—C4_2—C5_2—C6_2	−160.86 (13)
C23_1—C4_1—C5_1—N2_1	−166.94 (11)	C23_2—C4_2—C5_2—C6_2	21.93 (19)
C3_1—C4_1—C5_1—C6_1	−161.20 (12)	N2_2—C5_2—C6_2—C7_2	−2.88 (16)
C23_1—C4_1—C5_1—C6_1	11.78 (19)	C4_2—C5_2—C6_2—C7_2	176.14 (13)
N2_1—C5_1—C6_1—C7_1	−0.22 (15)	C5_2—C6_2—C7_2—C8_2	4.00 (15)
C4_1—C5_1—C6_1—C7_1	−179.09 (12)	C5_2—N2_2—C8_2—C9_2	−166.97 (12)
C5_1—C6_1—C7_1—C8_1	2.00 (15)	Ni1_2—N2_2—C8_2—C9_2	8.74 (18)
C5_1—N2_1—C8_1—C9_1	−167.75 (12)	C5_2—N2_2—C8_2—C7_2	2.07 (14)
Ni1_1—N2_1—C8_1—C9_1	15.17 (18)	Ni1_2—N2_2—C8_2—C7_2	177.78 (9)
C5_1—N2_1—C8_1—C7_1	2.96 (14)	C6_2—C7_2—C8_2—C9_2	165.08 (13)
Ni1_1—N2_1—C8_1—C7_1	−174.12 (9)	C6_2—C7_2—C8_2—N2_2	−3.91 (15)
C6_1—C7_1—C8_1—N2_1	−3.17 (15)	N2_2—C8_2—C9_2—C10_2	8.94 (19)
C6_1—C7_1—C8_1—C9_1	167.39 (13)	C7_2—C8_2—C9_2—C10_2	−158.39 (13)
N2_1—C8_1—C9_1—C10_1	4.21 (19)	N2_2—C8_2—C9_2—C29_2	−176.68 (11)
C7_1—C8_1—C9_1—C10_1	−164.99 (12)	C7_2—C8_2—C9_2—C29_2	15.99 (19)
N2_1—C8_1—C9_1—C29_1	179.48 (11)	C13_2—N3_2—C10_2—C9_2	169.02 (12)
C7_1—C8_1—C9_1—C29_1	10.28 (19)	Ni1_2—N3_2—C10_2—C9_2	−13.63 (17)
C13_1—N3_1—C10_1—C9_1	171.29 (12)	C13_2—N3_2—C10_2—C11_2	−3.32 (14)
Ni1_1—N3_1—C10_1—C9_1	−8.88 (18)	Ni1_2—N3_2—C10_2—C11_2	174.03 (9)
C13_1—N3_1—C10_1—C11_1	−2.88 (14)	C8_2—C9_2—C10_2—N3_2	−6.32 (19)
Ni1_1—N3_1—C10_1—C11_1	176.95 (9)	C29_2—C9_2—C10_2—N3_2	179.42 (11)
C8_1—C9_1—C10_1—N3_1	−7.29 (19)	C8_2—C9_2—C10_2—C11_2	164.83 (12)
C29_1—C9_1—C10_1—N3_1	177.58 (11)	C29_2—C9_2—C10_2—C11_2	−9.42 (19)
C8_1—C9_1—C10_1—C11_1	165.98 (12)	N3_2—C10_2—C11_2—C12_2	4.29 (15)
C29_1—C9_1—C10_1—C11_1	−9.14 (19)	C9_2—C10_2—C11_2—C12_2	−167.93 (12)
N3_1—C10_1—C11_1—C12_1	4.04 (15)	C10_2—C11_2—C12_2—C13_2	−3.36 (15)
C9_1—C10_1—C11_1—C12_1	−170.06 (13)	C10_2—N3_2—C13_2—C14_2	178.23 (12)
C10_1—C11_1—C12_1—C13_1	−3.42 (15)	Ni1_2—N3_2—C13_2—C14_2	0.87 (18)
C10_1—N3_1—C13_1—C14_1	178.53 (12)	C10_2—N3_2—C13_2—C12_2	1.21 (14)
Ni1_1—N3_1—C13_1—C14_1	−1.30 (19)	Ni1_2—N3_2—C13_2—C12_2	−176.14 (9)
C10_1—N3_1—C13_1—C12_1	0.73 (14)	C11_2—C12_2—C13_2—N3_2	1.43 (16)
Ni1_1—N3_1—C13_1—C12_1	−179.10 (9)	C11_2—C12_2—C13_2—C14_2	−175.58 (13)
C11_1—C12_1—C13_1—N3_1	1.77 (16)	N3_2—C13_2—C14_2—C15_2	−12.8 (2)
C11_1—C12_1—C13_1—C14_1	−176.01 (13)	C12_2—C13_2—C14_2—C15_2	163.74 (13)
N3_1—C13_1—C14_1—C15_1	−12.0 (2)	N3_2—C13_2—C14_2—C35_2	169.71 (12)
C12_1—C13_1—C14_1—C15_1	165.47 (13)	C12_2—C13_2—C14_2—C35_2	−13.7 (2)
N3_1—C13_1—C14_1—C35_1	168.68 (12)	C13_2—C14_2—C15_2—N4_2	0.21 (19)
C12_1—C13_1—C14_1—C35_1	−13.9 (2)	C35_2—C14_2—C15_2—N4_2	177.64 (12)
C18_1—N4_1—C15_1—C14_1	−167.68 (12)	C13_2—C14_2—C15_2—C16_2	−169.01 (12)
Ni1_1—N4_1—C15_1—C14_1	20.71 (18)	C35_2—C14_2—C15_2—C16_2	8.4 (2)
C18_1—N4_1—C15_1—C16_1	2.93 (14)	C18_2—N4_2—C15_2—C14_2	−166.51 (12)
Ni1_1—N4_1—C15_1—C16_1	−168.68 (9)	Ni1_2—N4_2—C15_2—C14_2	24.16 (17)
C13_1—C14_1—C15_1—N4_1	2.1 (2)	C18_2—N4_2—C15_2—C16_2	4.26 (13)
C35_1—C14_1—C15_1—N4_1	−178.56 (12)	Ni1_2—N4_2—C15_2—C16_2	−165.08 (8)
C13_1—C14_1—C15_1—C16_1	−166.96 (13)	C14_2—C15_2—C16_2—C17_2	166.20 (12)

C35_1—C14_1—C15_1—C16_1	12.4 (2)
N4_1—C15_1—C16_1—C17_1	−3.01 (16)
C14_1—C15_1—C16_1—C17_1	167.33 (13)
C15_1—C16_1—C17_1—C18_1	1.81 (16)
C15_1—N4_1—C18_1—C19_1	176.72 (12)
Ni1_1—N4_1—C18_1—C19_1	−11.76 (18)
C15_1—N4_1—C18_1—C17_1	−1.80 (14)
Ni1_1—N4_1—C18_1—C17_1	169.73 (9)
C16_1—C17_1—C18_1—N4_1	−0.04 (15)
C16_1—C17_1—C18_1—C19_1	−178.51 (13)
N4_1—C18_1—C19_1—C20_1	21.94 (19)
C17_1—C18_1—C19_1—C20_1	−159.78 (13)
N4_1—C18_1—C19_1—C41_1	−165.57 (11)
C17_1—C18_1—C19_1—C41_1	12.70 (19)
C18_1—C19_1—C20_1—N1_1	5.43 (18)
C41_1—C19_1—C20_1—N1_1	−166.64 (11)
C18_1—C19_1—C20_1—C21_1	−167.78 (12)
C41_1—C19_1—C20_1—C21_1	20.15 (19)
C3_1—N1_1—C20_1—C19_1	135.50 (12)
Ni1_1—N1_1—C20_1—C19_1	−41.81 (16)
C3_1—N1_1—C20_1—C21_1	−50.75 (15)
Ni1_1—N1_1—C20_1—C21_1	131.93 (10)
C19_1—C20_1—C21_1—O2_1	−160.19 (13)
N1_1—C20_1—C21_1—O2_1	26.20 (18)
C19_1—C20_1—C21_1—C22_1	27.72 (19)
N1_1—C20_1—C21_1—C22_1	−145.89 (12)
C3_1—C4_1—C23_1—C28_1	47.55 (18)
C5_1—C4_1—C23_1—C28_1	−125.51 (14)
C3_1—C4_1—C23_1—C24_1	−130.42 (14)
C5_1—C4_1—C23_1—C24_1	56.53 (17)
C28_1—C23_1—C24_1—C25_1	−2.4 (2)
C4_1—C23_1—C24_1—C25_1	175.60 (13)
C23_1—C24_1—C25_1—C26_1	1.1 (2)
C24_1—C25_1—C26_1—C27_1	1.1 (2)
C25_1—C26_1—C27_1—C28_1	−2.0 (2)
C26_1—C27_1—C28_1—C23_1	0.7 (2)
C24_1—C23_1—C28_1—C27_1	1.4 (2)
C4_1—C23_1—C28_1—C27_1	−176.57 (13)
C8_1—C9_1—C29_1—C30_1	59.97 (17)
C10_1—C9_1—C29_1—C30_1	−124.73 (14)
C8_1—C9_1—C29_1—C34_1	−116.99 (14)
C10_1—C9_1—C29_1—C34_1	58.30 (18)
C34_1—C29_1—C30_1—C31_1	0.6 (2)
C9_1—C29_1—C30_1—C31_1	−176.44 (13)
C29_1—C30_1—C31_1—C32_1	−0.2 (2)
C30_1—C31_1—C32_1—C33_1	−0.4 (2)
C31_1—C32_1—C33_1—C34_1	0.6 (2)
C32_1—C33_1—C34_1—C29_1	−0.2 (2)
N4_2—C15_2—C16_2—C17_2	−4.26 (14)
C15_2—C16_2—C17_2—C18_2	2.45 (14)
C15_2—N4_2—C18_2—C19_2	175.66 (11)
Ni1_2—N4_2—C18_2—C19_2	−14.99 (17)
C15_2—N4_2—C18_2—C17_2	−2.73 (13)
Ni1_2—N4_2—C18_2—C17_2	166.61 (8)
C16_2—C17_2—C18_2—N4_2	0.13 (14)
C16_2—C17_2—C18_2—C19_2	−178.21 (12)
N4_2—C18_2—C19_2—C20_2	22.87 (18)
C17_2—C18_2—C19_2—C20_2	−158.98 (12)
N4_2—C18_2—C19_2—C41_2	−166.25 (11)
C17_2—C18_2—C19_2—C41_2	11.90 (18)
C18_2—C19_2—C20_2—N1_2	7.98 (18)
C41_2—C19_2—C20_2—N1_2	−162.37 (11)
C18_2—C19_2—C20_2—C21_2	−168.41 (11)
C41_2—C19_2—C20_2—C21_2	21.23 (18)
C3_2—N1_2—C20_2—C19_2	135.71 (12)
Ni1_2—N1_2—C20_2—C19_2	−43.69 (15)
C3_2—N1_2—C20_2—C21_2	−47.71 (15)
Ni1_2—N1_2—C20_2—C21_2	132.89 (9)
C19_2—C20_2—C21_2—O2_2	−156.63 (13)
N1_2—C20_2—C21_2—O2_2	26.78 (18)
C19_2—C20_2—C21_2—C22_2	30.58 (18)
N1_2—C20_2—C21_2—C22_2	−146.01 (12)
C3_2—C4_2—C23_2—C28_2	−66.61 (18)
C5_2—C4_2—C23_2—C28_2	110.57 (15)
C3_2—C4_2—C23_2—C24_2	115.13 (15)
C5_2—C4_2—C23_2—C24_2	−67.69 (17)
C28_2—C23_2—C24_2—C25_2	−0.6 (2)
C4_2—C23_2—C24_2—C25_2	177.65 (14)
C23_2—C24_2—C25_2—C26_2	0.2 (3)
C24_2—C25_2—C26_2—C27_2	0.6 (3)
C25_2—C26_2—C27_2—C28_2	−0.8 (3)
C26_2—C27_2—C28_2—C23_2	0.4 (3)
C24_2—C23_2—C28_2—C27_2	0.4 (2)
C4_2—C23_2—C28_2—C27_2	−177.98 (15)
C8_2—C9_2—C29_2—C34_2	−119.00 (14)
C10_2—C9_2—C29_2—C34_2	55.43 (17)
C8_2—C9_2—C29_2—C30_2	59.66 (17)
C10_2—C9_2—C29_2—C30_2	−125.91 (14)
C34_2—C29_2—C30_2—C31_2	−1.3 (2)
C9_2—C29_2—C30_2—C31_2	−179.96 (14)
C29_2—C30_2—C31_2—C32_2	0.3 (3)
C30_2—C31_2—C32_2—C33_2	0.8 (3)
C31_2—C32_2—C33_2—C34_2	−1.0 (2)
C32_2—C33_2—C34_2—C29_2	0.1 (2)
C30_2—C29_2—C34_2—C33_2	1.0 (2)
C9_2—C29_2—C34_2—C33_2	179.70 (12)

C30_1—C29_1—C34_1—C33_1	−0.4 (2)	C15_2—C14_2—C35_2—C40_2	−68.11 (19)
C9_1—C29_1—C34_1—C33_1	176.56 (13)	C13_2—C14_2—C35_2—C40_2	109.40 (17)
C15_1—C14_1—C35_1—C40_1	−97.1 (2)	C15_2—C14_2—C35_2—C36_2	111.32 (16)
C13_1—C14_1—C35_1—C40_1	82.3 (2)	C13_2—C14_2—C35_2—C36_2	−71.18 (18)
C15_1—C14_1—C35_1—C36_1	85.30 (18)	C40_2—C35_2—C36_2—C37_2	−0.2 (3)
C13_1—C14_1—C35_1—C36_1	−95.35 (17)	C14_2—C35_2—C36_2—C37_2	−179.63 (16)
C40_1—C35_1—C36_1—C37_1	0.1 (3)	C35_2—C36_2—C37_2—C38_2	−0.3 (3)
C14_1—C35_1—C36_1—C37_1	177.75 (17)	C36_2—C37_2—C38_2—C39_2	0.6 (3)
C35_1—C36_1—C37_1—C38_1	1.3 (3)	C37_2—C38_2—C39_2—C40_2	−0.4 (4)
C36_1—C37_1—C38_1—C39_1	−1.3 (4)	C36_2—C35_2—C40_2—C39_2	0.4 (3)
C37_1—C38_1—C39_1—C40_1	0.0 (4)	C14_2—C35_2—C40_2—C39_2	179.78 (18)
C36_1—C35_1—C40_1—C39_1	−1.4 (3)	C38_2—C39_2—C40_2—C35_2	−0.1 (3)
C14_1—C35_1—C40_1—C39_1	−179.0 (2)	C20_2—C19_2—C41_2—C42_2	56.12 (17)
C38_1—C39_1—C40_1—C35_1	1.4 (4)	C18_2—C19_2—C41_2—C42_2	−114.65 (14)
C20_1—C19_1—C41_1—C42_1	57.29 (18)	C20_2—C19_2—C41_2—C46_2	−129.46 (14)
C18_1—C19_1—C41_1—C42_1	−115.05 (14)	C18_2—C19_2—C41_2—C46_2	59.77 (16)
C20_1—C19_1—C41_1—C46_1	−126.06 (14)	C46_2—C41_2—C42_2—C43_2	−0.2 (2)
C18_1—C19_1—C41_1—C46_1	61.60 (16)	C19_2—C41_2—C42_2—C43_2	174.36 (13)
C46_1—C41_1—C42_1—C43_1	0.9 (2)	C41_2—C42_2—C43_2—C44_2	0.7 (2)
C19_1—C41_1—C42_1—C43_1	177.64 (13)	C42_2—C43_2—C44_2—C45_2	−0.3 (2)
C41_1—C42_1—C43_1—C44_1	0.6 (2)	C43_2—C44_2—C45_2—C46_2	−0.7 (2)
C42_1—C43_1—C44_1—C45_1	−1.6 (2)	C44_2—C45_2—C46_2—C41_2	1.3 (2)
C43_1—C44_1—C45_1—C46_1	1.0 (2)	C42_2—C41_2—C46_2—C45_2	−0.8 (2)
C44_1—C45_1—C46_1—C41_1	0.5 (2)	C19_2—C41_2—C46_2—C45_2	−175.22 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C28_1—H28_1···O2_1	0.95	2.60	3.4517 (17)	149
C42_1—H42_1···O1_1	0.95	2.55	3.3855 (17)	147
C42_2—H42_2···O1_2	0.95	2.66	3.5120 (17)	149
C6_1—H6_1···O2_1^{i}	0.95	2.49	3.3714 (16)	155
C6_2—H6_2···O2_2^{ii}	0.95	2.57	3.3569 (17)	140
C17_2—H17_2···O1_2^{iii}	0.95	2.40	3.2977 (16)	158

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