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μ-[Bis(3,3-dimethylbut-1-ynyl)diphenylsilane]bis[(cycloocta-1,5-diene)nickel(II)](*Ni—Ni*)

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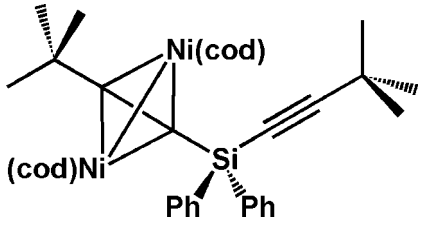
Key indicators: single-crystal X-ray study; T = 183 K; mean σ(C–C) = 0.006 Å; R factor = 0.027; wR factor = 0.070; data-to-parameter ratio = 10.8.

The title compound, $[Ni_2(C_{24}H_{28}Si)(C_8H_{12})_2]$, was obtained from the reaction of the symmetrical diyne bis(3,3-dimethylbut-1-ynyl)diphenylsilane with bis(cycloocta-1,5-diene)nickel. In the resulting molecule, two Ni(cod) (cod is cycloocta-1,5-diene) units are coordinated by one of the C≡C triple bonds, resulting in the formation of a dinickelatetrahedrane. The second triple bond remains uncoordinated even if an excess amount of the diyne is used in the reaction.

Related literature

The closely related complex [(*tert*-butyltriphenylsilylacetylene)nickel(cycloocta-1,5-diene)] was reported by Walther *et al.* (1997). For other related literature, see: Braga *et al.* (1997); Klettke *et al.* (1996); Walther *et al.* (1994, 1995); Walther, Klettke, Imhof & Görls (1996); Walther, Klettke, Schmidt *et al.* (1996).



Experimental

Crystal data

$[Ni_2(C_{24}H_{28}Si)(C_8H_{12})_2]$
M_r = 678.31
Monoclinic, $P2_1$
a = 10.167 (2) Å
b = 9.617 (2) Å
c = 18.110 (4) Å
β = 94.68 (3)°
V = 1764.8 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.13 mm^{-1}
T = 183 (2) K
0.32 × 0.28 × 0.26 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.823, T_{max} = 0.906
(expected range = 0.676–0.745)
4489 measured reflections
4246 independent reflections
3931 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
3 standard reflections
frequency: 120 min
intensity decay: 0.1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.070
S = 1.15
4246 reflections
394 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Flack (1983), with 4 Friedel pairs
Flack parameter: 0.006 (13)

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *SET4* (de Boer & Duisenberg, 1984); data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1990); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2141).

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supplementary materials

Acta Cryst. (2007). E**63**, m2567 [**doi:10.1107/S1600536807045825**]

μ-[Bis(3,3-dimethylbut-1-ynyl)diphenylsilane]bis[(cycloocta-1,5-diene)nickel(II)](*Ni-Ni*)

W. Imhof, T. Klettke and D. Walther

Comment

In the course of a study on the reactivity of alkynols and alkynylsilanes toward Ni(0) compounds such as [Ni(cdt)] (cdt = 1,5,9-cyclododecatriene) or [Ni(cod)$_2$] (cod = cycloocta-1,5-diene) it was shown that the reactions with alkynes produce organometallic compounds of the general formulae [Ni(alkyne)$_2$] or [Ni$_3$(alkyne)$_4$] which crystallize as hydrogen-bonded supramolecular structures if alkynols are used as the starting material (Braga *et al.*, 1997; Klettke *et al.*, 1996; Walther *et al.*, 1994, 1995, 1997; Walther, Klettke, Imhof & Görls, 1996; Walther, Klettke, Schmidt *et al.*, 1996). The reaction of *tert*-butyltriphenylsilylacetylene with [Ni(cod)$_2$] leads to a mononuclear complex in which one Ni(cod) unit is coordinated by the carbon-carbon triple bond (Walther *et al.*, 1997). In contrast, the reaction of the symmetrical diyne bis(3,3-dimethyl-but-1-ynyl)diphenylsilane does not lead to a dinuclear nickel complex with one Ni(cod) fragment per carbon-carbon triple bond but to the title compound 1.

Corresponding to the IR spectrum, which is indicative of one coordinated and one non-coordinated carbon-carbon triple bond, the structural analysis of the title compound shows that two Ni(cod) units are bound to one of the alkynyl subunits, thereby establishing a nickel–nickel bond and forming a dinickelatetrahedrane derivative. By coordination to the transition metal centers the C1—C2 bond is elongated by 0.152 Å compared to the uncoordinated C3—C4 bond. In addition, the bond angles Si1—C2—C1 and C2—C1—C5 are observed to be 153.8 (3) and 141.3 (3)°, respectively, whereas the corresponding bond angles Si1—C3—C4 and C3—C4—C9 are close to linearity [175.5 (3) and 178.8 (4)°].

Experimental

1.04 mmol (285 mg) [Ni(cod)$_2$] and 0.52 mmol (179 mg) bis-3,3-dimethylbut-1-ynyl)diphenylsilane were combined in 10 ml n-pentane and stirred at room temperature until all the starting material had dissolved. During the reaction the solution developed an intense red color. After the reaction had finished the solution was kept at 273 K. Two days later deep red crystals suitable for X-ray structural analysis could be collected (0.24 mmol, 163 mg, yield 46.4%). IR (nujol mull, 295 K): 1521 cm^{-1}, 2147 cm^{-1}; MS (EI): 676 (M^+, 1), 568 (M^+ - cod, 1), 510 (M^+– Ni(cod), 3), 460 (M^+ - Ni(cod) - C_3H_8, 5, 67 (C_5H_7, 100); elemental analysis for $C_{40}H_{52}SiNi_2$ (calcd.): C 70.72 (70.83), H 7.98 (7.73), Ni 17.42 (17.30)%.

Refinement

Hydrogen atoms were positioned geometrically and refined using a riding model with with C—H = 0.95–0.99 Å and with U_{iso}(H) = 1.5U_{eq}(C).

Figures

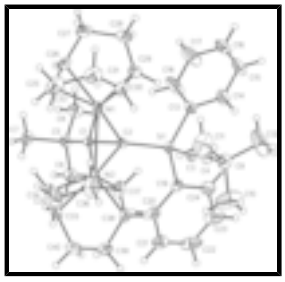


Fig. 1. The molecular structure of (I), showing the labeling scheme and 40% probability displacement ellipsoids for non-H atoms.

μ-[Bis(3,3-dimethylbut-1-ynyl)diphenylsilane]bis[(cycloocta-1,5- diene)nickel(II)](*Ni—Ni*)

Crystal data

$[Ni_2(C_{24}H_{28}Si)(C_8H_{12})_2]$	F_{000} = 724
M_r = 678.31	D_x = 1.276 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 25 reflections
a = 10.167 (2) Å	θ = 13.4–25.1º
b = 9.617 (2) Å	μ = 1.13 mm^{-1}
c = 18.110 (4) Å	T = 183 (2) K
β = 94.68 (3)º	Block, red
V = 1764.8 (6) Å^3	0.32 × 0.28 × 0.26 mm
Z = 2	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.019
Radiation source: fine-focus sealed tube	θ_{max} = 27.5º
Monochromator: graphite	θ_{min} = 3.2º
T = 183(2) K	h = −1→13
ω/2θ scans	k = −12→0
Absorption correction: ψ scan (North *et al.*, 1968)	l = −23→23
T_{min} = 0.823, T_{max} = 0.906	3 standard reflections
4489 measured reflections	every 120 min
4246 independent reflections	intensity decay: 0.1%
3931 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.027	$w = 1/[\sigma^2(F_o^2) + (0.0315P)^2 + 0.65P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.070$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.15$	$\Delta\rho_{max} = 0.38$ e Å^{-3}
4246 reflections	$\Delta\rho_{min} = -0.32$ e Å^{-3}
394 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), with 4 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.006 (13)
Secondary atom site location: difference Fourier map	

Special details

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

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.47667 (4)	0.78591 (4)	0.21857 (2)	0.02036 (9)
Ni2	0.24266 (3)	0.83291 (4)	0.14742 (2)	0.01928 (9)
Si1	0.22104 (8)	0.62681 (9)	0.29347 (4)	0.01964 (17)
C1	0.3630 (3)	0.6769 (3)	0.15160 (16)	0.0188 (6)
C2	0.3092 (3)	0.6903 (3)	0.21689 (16)	0.0191 (6)
C3	0.1678 (3)	0.7751 (4)	0.34747 (16)	0.0271 (6)
C4	0.1411 (3)	0.8711 (4)	0.38577 (18)	0.0279 (7)
C5	0.3926 (3)	0.5685 (4)	0.09442 (16)	0.0234 (6)
C6	0.2651 (4)	0.5011 (4)	0.06099 (19)	0.0314 (8)
H6A	0.2859	0.4344	0.0227	0.047*
H6B	0.2061	0.5731	0.0389	0.047*
H6C	0.2218	0.4526	0.0999	0.047*
C7	0.4639 (3)	0.6365 (4)	0.03206 (18)	0.0317 (8)
H7A	0.4717	0.5691	−0.0079	0.048*
H7B	0.5521	0.6665	0.0515	0.048*
H7C	0.4133	0.7173	0.0128	0.048*
C8	0.4802 (4)	0.4529 (4)	0.1306 (2)	0.0349 (8)
H8A	0.5083	0.3903	0.0922	0.052*
H8B	0.4302	0.4002	0.1652	0.052*
H8C	0.5581	0.4944	0.1575	0.052*
C9	0.1072 (4)	0.9914 (4)	0.4316 (2)	0.0356 (8)
C10	−0.0308 (5)	1.0402 (7)	0.4058 (4)	0.085 (2)
H10A	−0.0537	1.1209	0.4352	0.127*

H10B	−0.0939	0.9650	0.4122	0.127*
H10C	−0.0339	1.0663	0.3534	0.127*
C11	0.2042 (6)	1.1091 (6)	0.4213 (3)	0.0704 (16)
H11A	0.1797	1.1904	0.4498	0.106*
H11B	0.2018	1.1336	0.3687	0.106*
H11C	0.2935	1.0791	0.4387	0.106*
C12	0.1168 (7)	0.9489 (7)	0.5128 (3)	0.087 (2)
H12A	0.0858	1.0253	0.5426	0.130*
H12B	0.2089	0.9275	0.5292	0.130*
H12C	0.0621	0.8664	0.5188	0.130*
C13	0.3236 (3)	0.5201 (4)	0.36372 (17)	0.0266 (7)
C14	0.3126 (4)	0.5377 (5)	0.4386 (2)	0.0442 (10)
H14	0.2504	0.6027	0.4545	0.066*
C15	0.3905 (5)	0.4625 (6)	0.4915 (2)	0.0506 (11)
H15	0.3805	0.4765	0.5427	0.076*
C16	0.4795 (5)	0.3707 (5)	0.4706 (2)	0.0491 (11)
H16	0.5317	0.3188	0.5068	0.074*
C17	0.4948 (6)	0.3521 (7)	0.3972 (2)	0.082 (2)
H17	0.5583	0.2877	0.3822	0.123*
C18	0.4180 (6)	0.4269 (6)	0.3444 (2)	0.0665 (17)
H18	0.4308	0.4137	0.2935	0.100*
C19	0.0709 (3)	0.5251 (3)	0.25825 (17)	0.0226 (6)
C20	0.0106 (3)	0.5454 (4)	0.18705 (19)	0.0318 (8)
H20	0.0484	0.6098	0.1551	0.048*
C21	−0.1031 (4)	0.4744 (5)	0.1614 (2)	0.0403 (9)
H21	−0.1423	0.4899	0.1127	0.061*
C22	−0.1582 (4)	0.3807 (5)	0.2079 (3)	0.0550 (12)
H22	−0.2363	0.3319	0.1914	0.082*
C23	−0.1006 (4)	0.3587 (6)	0.2772 (3)	0.0642 (15)
H23	−0.1388	0.2940	0.3089	0.096*
C24	0.0122 (4)	0.4286 (5)	0.3022 (2)	0.0442 (10)
H24	0.0510	0.4105	0.3508	0.066*
C25	0.6186 (3)	0.8906 (4)	0.1628 (2)	0.0326 (8)
H25	0.5692	0.8752	0.1167	0.049*
C26	0.6765 (3)	0.7778 (5)	0.19708 (18)	0.0321 (7)
H26	0.6623	0.6903	0.1735	0.048*
C27	0.7616 (3)	0.7799 (6)	0.2694 (2)	0.0427 (9)
H27A	0.8041	0.8722	0.2759	0.064*
H27B	0.8322	0.7094	0.2676	0.064*
C28	0.6818 (4)	0.7499 (5)	0.3366 (2)	0.0438 (10)
H28A	0.6726	0.6481	0.3421	0.066*
H28B	0.7313	0.7857	0.3820	0.066*
C29	0.5460 (3)	0.8150 (5)	0.32953 (17)	0.0361 (9)
H29	0.4766	0.7608	0.3466	0.054*
C30	0.5120 (4)	0.9419 (5)	0.3016 (2)	0.0361 (9)
H30	0.4211	0.9658	0.2987	0.054*
C31	0.6064 (4)	1.0495 (5)	0.2746 (2)	0.0478 (10)
H31A	0.6932	1.0393	0.3030	0.072*
H31B	0.5725	1.1435	0.2845	0.072*

C32	0.6256 (5)	1.0369 (5)	0.1912 (3)	0.0471 (10)
H32A	0.5569	1.0929	0.1630	0.071*
H32B	0.7125	1.0767	0.1819	0.071*
C33	0.1711 (3)	0.8718 (4)	0.03922 (18)	0.0334 (8)
H33	0.2032	0.7850	0.0232	0.050*
C34	0.2636 (4)	0.9702 (4)	0.0607 (2)	0.0334 (8)
H34	0.3537	0.9437	0.0615	0.050*
C35	0.2341 (5)	1.1186 (5)	0.0832 (3)	0.0488 (11)
H35A	0.1511	1.1494	0.0557	0.073*
H35B	0.3058	1.1800	0.0688	0.073*
C36	0.2208 (6)	1.1350 (5)	0.1664 (3)	0.0556 (12)
H36A	0.3086	1.1568	0.1914	0.083*
H36B	0.1621	1.2150	0.1741	0.083*
C37	0.1669 (4)	1.0092 (4)	0.2022 (2)	0.0367 (8)
H37	0.2110	0.9816	0.2481	0.055*
C38	0.0622 (3)	0.9299 (5)	0.1766 (2)	0.0353 (8)
H38	0.0418	0.8504	0.2046	0.053*
C39	−0.0238 (4)	0.9600 (7)	0.1062 (2)	0.0571 (14)
H39A	−0.0254	1.0616	0.0974	0.086*
H39B	−0.1151	0.9298	0.1128	0.086*
C40	0.0242 (4)	0.8871 (7)	0.0385 (2)	0.0540 (13)
H40A	−0.0162	0.7934	0.0345	0.081*
H40B	−0.0078	0.9399	−0.0064	0.081*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01796 (17)	0.02247 (19)	0.02058 (18)	−0.00277 (16)	0.00111 (13)	−0.00417 (16)
Ni2	0.01797 (17)	0.01904 (18)	0.02100 (18)	0.00099 (15)	0.00264 (13)	0.00367 (15)
Si1	0.0218 (4)	0.0197 (4)	0.0176 (4)	−0.0009 (3)	0.0027 (3)	0.0016 (3)
C1	0.0178 (13)	0.0168 (14)	0.0211 (13)	−0.0009 (12)	−0.0017 (10)	−0.0001 (12)
C2	0.0183 (13)	0.0197 (15)	0.0193 (13)	−0.0005 (12)	0.0010 (11)	0.0036 (12)
C3	0.0313 (15)	0.0281 (16)	0.0224 (13)	−0.0017 (15)	0.0056 (12)	0.0016 (14)
C4	0.0317 (17)	0.0283 (18)	0.0243 (15)	0.0001 (14)	0.0058 (13)	−0.0008 (13)
C5	0.0274 (15)	0.0217 (16)	0.0208 (14)	0.0022 (13)	0.0000 (12)	−0.0042 (12)
C6	0.0336 (18)	0.0288 (19)	0.0313 (18)	−0.0054 (15)	−0.0009 (14)	−0.0086 (15)
C7	0.0330 (17)	0.034 (2)	0.0287 (16)	0.0009 (16)	0.0095 (14)	−0.0079 (15)
C8	0.0389 (19)	0.0273 (19)	0.0375 (18)	0.0113 (16)	−0.0037 (15)	−0.0073 (16)
C9	0.041 (2)	0.0310 (19)	0.0358 (18)	0.0017 (17)	0.0059 (15)	−0.0112 (16)
C10	0.053 (3)	0.067 (4)	0.133 (5)	0.019 (3)	−0.005 (3)	−0.047 (4)
C11	0.085 (4)	0.037 (3)	0.092 (4)	−0.016 (3)	0.029 (3)	−0.026 (3)
C12	0.165 (7)	0.062 (4)	0.035 (2)	0.019 (4)	0.019 (3)	−0.012 (2)
C13	0.0324 (17)	0.0248 (17)	0.0220 (14)	−0.0032 (14)	−0.0020 (12)	0.0042 (13)
C14	0.053 (2)	0.051 (3)	0.0297 (18)	0.014 (2)	0.0068 (17)	0.0096 (18)
C15	0.071 (3)	0.057 (3)	0.0232 (17)	0.010 (2)	−0.0018 (18)	0.0112 (19)
C16	0.063 (3)	0.049 (3)	0.0328 (19)	0.011 (2)	−0.0110 (18)	0.0103 (18)
C17	0.112 (4)	0.094 (5)	0.038 (2)	0.075 (4)	−0.004 (3)	0.000 (3)
C18	0.095 (4)	0.080 (4)	0.0233 (18)	0.052 (3)	−0.007 (2)	−0.005 (2)

C19	0.0216 (14)	0.0198 (15)	0.0270 (15)	−0.0011 (12)	0.0051 (12)	−0.0010 (12)
C20	0.0294 (17)	0.036 (2)	0.0299 (17)	−0.0027 (16)	0.0044 (14)	−0.0026 (15)
C21	0.0326 (18)	0.042 (2)	0.045 (2)	0.0022 (18)	−0.0055 (16)	−0.0128 (18)
C22	0.032 (2)	0.035 (2)	0.094 (4)	−0.0092 (18)	−0.015 (2)	0.002 (2)
C23	0.039 (2)	0.055 (3)	0.097 (4)	−0.017 (2)	−0.006 (2)	0.038 (3)
C24	0.0343 (19)	0.046 (2)	0.051 (2)	−0.0139 (18)	−0.0038 (17)	0.021 (2)
C25	0.0291 (17)	0.0346 (19)	0.0350 (18)	−0.0114 (15)	0.0082 (14)	−0.0045 (16)
C26	0.0199 (14)	0.0391 (19)	0.0378 (17)	−0.0057 (16)	0.0061 (12)	−0.0104 (18)
C27	0.0255 (16)	0.055 (2)	0.047 (2)	0.0020 (19)	−0.0045 (14)	−0.011 (2)
C28	0.0377 (19)	0.057 (3)	0.0341 (18)	−0.003 (2)	−0.0123 (15)	−0.0043 (19)
C29	0.0315 (16)	0.052 (3)	0.0238 (14)	−0.0107 (18)	−0.0033 (12)	−0.0116 (16)
C30	0.0316 (18)	0.042 (2)	0.0341 (18)	−0.0038 (17)	0.0011 (15)	−0.0203 (17)
C31	0.047 (2)	0.037 (2)	0.059 (3)	−0.008 (2)	0.002 (2)	−0.019 (2)
C32	0.049 (2)	0.031 (2)	0.063 (3)	−0.0119 (19)	0.010 (2)	−0.005 (2)
C33	0.0330 (17)	0.040 (2)	0.0266 (16)	0.0051 (16)	−0.0020 (13)	0.0090 (15)
C34	0.0343 (18)	0.033 (2)	0.0346 (18)	0.0073 (16)	0.0111 (15)	0.0150 (15)
C35	0.063 (3)	0.030 (2)	0.056 (3)	0.005 (2)	0.024 (2)	0.015 (2)
C36	0.083 (3)	0.024 (2)	0.065 (3)	0.004 (2)	0.031 (3)	0.004 (2)
C37	0.045 (2)	0.0276 (19)	0.0398 (19)	0.0096 (17)	0.0172 (16)	0.0038 (16)
C38	0.0290 (17)	0.045 (2)	0.0334 (18)	0.0102 (17)	0.0110 (14)	0.0100 (17)
C39	0.0280 (19)	0.095 (4)	0.048 (2)	0.021 (2)	0.0048 (17)	0.013 (3)
C40	0.032 (2)	0.088 (4)	0.040 (2)	0.010 (2)	−0.0097 (17)	0.003 (2)

Geometric parameters (Å, °)

Ni1—C1	1.917 (3)	C17—H17	0.950
Ni1—C2	1.933 (3)	C18—H18	0.950
Ni1—C25	2.086 (3)	C19—C24	1.389 (5)
Ni1—C29	2.093 (3)	C19—C20	1.396 (5)
Ni1—C26	2.101 (3)	C20—C21	1.389 (5)
Ni1—C30	2.134 (4)	C20—H20	0.950
Ni1—Ni2	2.6505 (9)	C21—C22	1.382 (7)
Ni2—C1	1.933 (3)	C21—H21	0.950
Ni2—C2	1.945 (3)	C22—C23	1.358 (7)
Ni2—C33	2.068 (3)	C22—H22	0.950
Ni2—C34	2.077 (3)	C23—C24	1.374 (6)
Ni2—C37	2.139 (4)	C23—H23	0.950
Ni2—C38	2.161 (4)	C24—H24	0.950
Si1—C2	1.817 (3)	C25—C26	1.360 (6)
Si1—C3	1.836 (4)	C25—C32	1.498 (6)
Si1—C19	1.880 (3)	C25—H25	0.950
Si1—C13	1.882 (3)	C26—C27	1.510 (5)
C1—C2	1.349 (4)	C26—H26	0.950
C1—C5	1.517 (4)	C27—C28	1.542 (5)
C3—C4	1.199 (5)	C27—H27A	0.990
C4—C9	1.480 (5)	C27—H27B	0.990
C5—C6	1.529 (4)	C28—C29	1.512 (5)
C5—C8	1.538 (5)	C28—H28A	0.990
C5—C7	1.537 (5)	C28—H28B	0.990

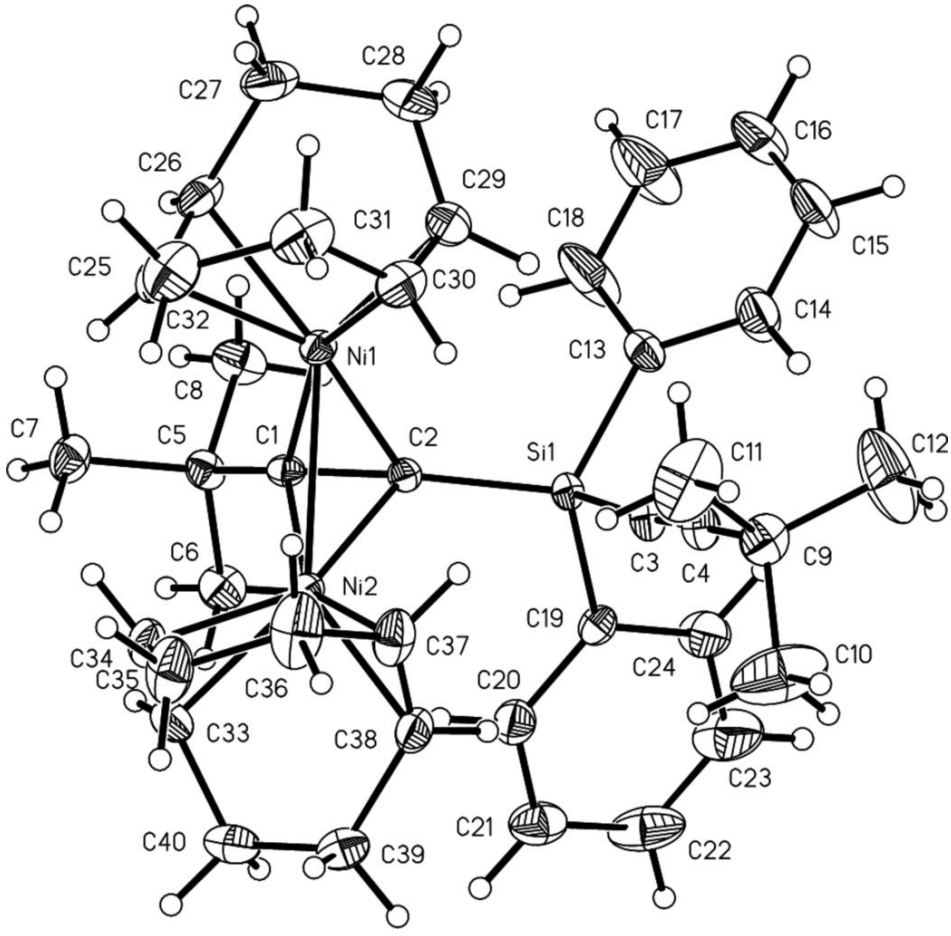
C6—H6A	0.980	C29—C30	1.355 (6)
C6—H6B	0.980	C29—H29	0.950
C6—H6C	0.980	C30—C31	1.519 (6)
C7—H7A	0.980	C30—H30	0.950
C7—H7B	0.980	C31—C32	1.543 (6)
C7—H7C	0.980	C31—H31A	0.990
C8—H8A	0.980	C31—H31B	0.990
C8—H8B	0.980	C32—H32A	0.990
C8—H8C	0.980	C32—H32B	0.990
C9—C10	1.516 (6)	C33—C34	1.368 (5)
C9—C11	1.523 (6)	C33—C40	1.500 (5)
C9—C12	1.522 (6)	C33—H33	0.950
C10—H10A	0.980	C34—C35	1.520 (6)
C10—H10B	0.980	C34—H34	0.950
C10—H10C	0.980	C35—C36	1.532 (6)
C11—H11A	0.980	C35—H35A	0.990
C11—H11B	0.980	C35—H35B	0.990
C11—H11C	0.980	C36—C37	1.497 (6)
C12—H12A	0.980	C36—H36A	0.990
C12—H12B	0.980	C36—H36B	0.990
C12—H12C	0.980	C37—C38	1.360 (6)
C13—C18	1.379 (6)	C37—H37	0.950
C13—C14	1.380 (5)	C38—C39	1.513 (5)
C14—C15	1.395 (6)	C38—H38	0.950
C14—H14	0.950	C39—C40	1.527 (7)
C15—C16	1.341 (7)	C39—H39A	0.990
C15—H15	0.950	C39—H39B	0.990
C16—C17	1.363 (6)	C40—H40A	0.990
C16—H16	0.950	C40—H40B	0.990
C17—C18	1.385 (6)		
C1—Ni1—C2	41.02 (12)	C17—C16—H16	120.2
C1—Ni1—C25	111.24 (13)	C16—C17—C18	120.1 (4)
C2—Ni1—C25	149.87 (13)	C16—C17—H17	119.9
C1—Ni1—C29	144.97 (15)	C18—C17—H17	119.9
C2—Ni1—C29	107.81 (13)	C13—C18—C17	121.9 (4)
C25—Ni1—C29	102.01 (15)	C13—C18—H18	119.1
C1—Ni1—C26	113.86 (13)	C17—C18—H18	119.1
C2—Ni1—C26	147.49 (15)	C24—C19—C20	116.5 (3)
C25—Ni1—C26	37.89 (16)	C24—C19—Si1	121.9 (3)
C29—Ni1—C26	85.86 (14)	C20—C19—Si1	121.6 (3)
C1—Ni1—C30	152.67 (14)	C21—C20—C19	122.1 (4)
C2—Ni1—C30	116.29 (14)	C21—C20—H20	119.0
C25—Ni1—C30	85.32 (15)	C19—C20—H20	119.0
C29—Ni1—C30	37.37 (17)	C22—C21—C20	118.9 (4)
C26—Ni1—C30	92.68 (14)	C22—C21—H21	120.5
C1—Ni1—Ni2	46.76 (9)	C20—C21—H21	120.5
C2—Ni1—Ni2	47.07 (9)	C23—C22—C21	120.0 (4)
C25—Ni1—Ni2	108.13 (11)	C23—C22—H22	120.0
C29—Ni1—Ni2	131.49 (10)	C21—C22—H22	120.0

C26—Ni1—Ni2	139.42 (10)	C22—C23—C24	120.9 (4)
C30—Ni1—Ni2	108.40 (11)	C22—C23—H23	119.5
C1—Ni2—C2	40.71 (12)	C24—C23—H23	119.5
C1—Ni2—C33	110.49 (14)	C23—C24—C19	121.6 (4)
C2—Ni2—C33	144.84 (15)	C23—C24—H24	119.2
C1—Ni2—C34	114.79 (14)	C19—C24—H24	119.2
C2—Ni2—C34	152.39 (13)	C26—C25—C32	125.9 (4)
C33—Ni2—C34	38.54 (15)	C26—C25—Ni1	71.7 (2)
C1—Ni2—C37	147.93 (14)	C32—C25—Ni1	107.6 (3)
C2—Ni2—C37	112.22 (14)	C26—C25—H25	117.1
C33—Ni2—C37	100.60 (16)	C32—C25—H25	117.1
C34—Ni2—C37	84.82 (15)	Ni1—C25—H25	90.8
C1—Ni2—C38	150.73 (14)	C25—C26—C27	125.6 (4)
C2—Ni2—C38	113.81 (14)	C25—C26—Ni1	70.46 (19)
C33—Ni2—C38	85.03 (14)	C27—C26—Ni1	109.4 (2)
C34—Ni2—C38	92.97 (14)	C25—C26—H26	117.2
C37—Ni2—C38	36.87 (16)	C27—C26—H26	117.2
C1—Ni2—Ni1	46.25 (8)	Ni1—C26—H26	90.1
C2—Ni2—Ni1	46.69 (9)	C26—C27—C28	112.4 (3)
C33—Ni2—Ni1	136.38 (10)	C26—C27—H27A	109.1
C34—Ni2—Ni1	109.45 (11)	C28—C27—H27A	109.1
C37—Ni2—Ni1	104.63 (12)	C26—C27—H27B	109.1
C38—Ni2—Ni1	134.50 (10)	C28—C27—H27B	109.1
C2—Si1—C3	109.30 (15)	H27A—C27—H27B	107.9
C2—Si1—C19	110.69 (14)	C29—C28—C27	113.0 (3)
C3—Si1—C19	108.57 (14)	C29—C28—H28A	109.0
C2—Si1—C13	114.74 (14)	C27—C28—H28A	109.0
C3—Si1—C13	103.58 (15)	C29—C28—H28B	109.0
C19—Si1—C13	109.59 (15)	C27—C28—H28B	109.0
C2—C1—C5	141.4 (3)	H28A—C28—H28B	107.8
C2—C1—Ni1	70.11 (18)	C30—C29—C28	127.4 (4)
C5—C1—Ni1	131.7 (2)	C30—C29—Ni1	72.9 (2)
C2—C1—Ni2	70.10 (18)	C28—C29—Ni1	105.0 (2)
C5—C1—Ni2	131.8 (2)	C30—C29—H29	116.3
Ni1—C1—Ni2	87.00 (13)	C28—C29—H29	116.3
C1—C2—Si1	153.8 (3)	Ni1—C29—H29	92.2
C1—C2—Ni1	68.86 (17)	C29—C30—C31	125.8 (4)
Si1—C2—Ni1	129.53 (16)	C29—C30—Ni1	69.7 (2)
C1—C2—Ni2	69.19 (18)	C31—C30—Ni1	109.0 (2)
Si1—C2—Ni2	124.29 (16)	C29—C30—H30	117.1
Ni1—C2—Ni2	86.24 (13)	C31—C30—H30	117.1
C4—C3—Si1	175.5 (3)	Ni1—C30—H30	91.3
C3—C4—C9	178.8 (4)	C30—C31—C32	113.3 (3)
C1—C5—C6	110.7 (3)	C30—C31—H31A	108.9
C1—C5—C8	110.3 (2)	C32—C31—H31A	108.9
C6—C5—C8	107.8 (3)	C30—C31—H31B	108.9
C1—C5—C7	109.9 (3)	C32—C31—H31B	108.9
C6—C5—C7	108.9 (3)	H31A—C31—H31B	107.7
C8—C5—C7	109.2 (3)	C25—C32—C31	113.8 (4)

C5—C6—H6A	109.5	C25—C32—H32A	108.8
C5—C6—H6B	109.5	C31—C32—H32A	108.8
H6A—C6—H6B	109.5	C25—C32—H32B	108.8
C5—C6—H6C	109.5	C31—C32—H32B	108.8
H6A—C6—H6C	109.5	H32A—C32—H32B	107.7
H6B—C6—H6C	109.5	C34—C33—C40	126.5 (4)
C5—C7—H7A	109.5	C34—C33—Ni2	71.1 (2)
C5—C7—H7B	109.5	C40—C33—Ni2	107.4 (2)
H7A—C7—H7B	109.5	C34—C33—H33	116.7
C5—C7—H7C	109.5	C40—C33—H33	116.7
H7A—C7—H7C	109.5	Ni2—C33—H33	91.6
H7B—C7—H7C	109.5	C33—C34—C35	125.4 (4)
C5—C8—H8A	109.5	C33—C34—Ni2	70.4 (2)
C5—C8—H8B	109.5	C35—C34—Ni2	111.0 (3)
H8A—C8—H8B	109.5	C33—C34—H34	117.3
C5—C8—H8C	109.5	C35—C34—H34	117.3
H8A—C8—H8C	109.5	Ni2—C34—H34	88.5
H8B—C8—H8C	109.5	C34—C35—C36	113.3 (3)
C4—C9—C10	108.7 (3)	C34—C35—H35A	108.9
C4—C9—C11	109.2 (3)	C36—C35—H35A	108.9
C10—C9—C11	108.9 (5)	C34—C35—H35B	108.9
C4—C9—C12	109.4 (4)	C36—C35—H35B	108.9
C10—C9—C12	111.5 (5)	H35A—C35—H35B	107.7
C11—C9—C12	109.1 (4)	C37—C36—C35	114.0 (4)
C9—C10—H10A	109.5	C37—C36—H36A	108.7
C9—C10—H10B	109.5	C35—C36—H36A	108.7
H10A—C10—H10B	109.5	C37—C36—H36B	108.7
C9—C10—H10C	109.5	C35—C36—H36B	108.7
H10A—C10—H10C	109.5	H36A—C36—H36B	107.6
H10B—C10—H10C	109.5	C38—C37—C36	127.5 (4)
C9—C11—H11A	109.5	C38—C37—Ni2	72.4 (2)
C9—C11—H11B	109.5	C36—C37—Ni2	106.4 (2)
H11A—C11—H11B	109.5	C38—C37—H37	116.2
C9—C11—H11C	109.5	C36—C37—H37	116.2
H11A—C11—H11C	109.5	Ni2—C37—H37	91.3
H11B—C11—H11C	109.5	C37—C38—C39	124.2 (4)
C9—C12—H12A	109.5	C37—C38—Ni2	70.7 (2)
C9—C12—H12B	109.5	C39—C38—Ni2	108.7 (3)
H12A—C12—H12B	109.5	C37—C38—H38	117.9
C9—C12—H12C	109.5	C39—C38—H38	117.9
H12A—C12—H12C	109.5	Ni2—C38—H38	90.6
H12B—C12—H12C	109.5	C38—C39—C40	112.8 (4)
C18—C13—C14	116.3 (3)	C38—C39—H39A	109.0
C18—C13—Si1	122.8 (3)	C40—C39—H39A	109.0
C14—C13—Si1	120.8 (3)	C38—C39—H39B	109.0
C13—C14—C15	121.6 (4)	C40—C39—H39B	109.0
C13—C14—H14	119.2	H39A—C39—H39B	107.8
C15—C14—H14	119.2	C33—C40—C39	114.9 (3)
C16—C15—C14	120.4 (4)	C33—C40—H40A	108.5

C16—C15—H15	119.8	C39—C40—H40A	108.5
C14—C15—H15	119.8	C33—C40—H40B	108.5
C15—C16—C17	119.7 (4)	C39—C40—H40B	108.5
C15—C16—H16	120.2	H40A—C40—H40B	107.5

Fig. 1


C28
C27
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C7
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C2
Si1
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