

ORGANOMETALLICS

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Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic parameters ($\text{\AA}^2 \times 10^3$) for **Va**.

	x	y	z	U(eq)	SOF
Ni	8658 (1)	2765 (1)	1955 (1)	31 (1)	1
Cl	10401 (1)	3363 (1)	1743 (1)	41 (1)	1
P (1)	6679 (1)	2778 (1)	2354 (1)	31 (1)	1
C (1)	7459 (4)	3637 (4)	2587 (3)	32 (1)	1
C (11)	6429 (4)	1917 (4)	3235 (2)	30 (1)	1
C (12)	7428 (4)	1269 (4)	3741 (2)	30 (1)	1
C (121)	8880 (4)	487 (4)	3602 (2)	32 (1)	1
C (122)	9385 (5)	-577 (4)	4197 (3)	46 (1)	1
C (123)	8908 (5)	27 (4)	2974 (2)	40 (1)	1
C (124)	9884 (4)	1109 (4)	3500 (3)	40 (1)	1
C (13)	7061 (4)	1246 (4)	4422 (2)	32 (1)	1
C (14)	5746 (4)	1762 (4)	4633 (2)	33 (1)	1
C (141)	5346 (5)	1786 (4)	5377 (3)	40 (1)	1
C (142)	4582 (6)	3028 (4)	5415 (3)	49 (1)	1
C (143)	6565 (6)	1312 (5)	5839 (3)	55 (2)	1
C (144)	4431 (6)	1085 (5)	5649 (3)	56 (2)	1
C (15)	4757 (4)	2170 (4)	4141 (2)	33 (1)	1
C (16)	5046 (4)	2231 (4)	3450 (2)	31 (1)	1
C (161)	3844 (4)	2528 (4)	2975 (2)	33 (1)	1
C (162)	2627 (5)	2333 (5)	3395 (3)	50 (1)	1
C (163)	3315 (5)	3778 (4)	2551 (3)	41 (1)	1
C (164)	4243 (5)	1721 (5)	2496 (3)	46 (1)	1
P (2)	6714 (1)	5124 (1)	2327 (1)	33 (1)	1
C (211)	7663 (5)	5818 (4)	2617 (2)	35 (1)	1
C (212)	9041 (5)	5255 (4)	2742 (3)	46 (1)	1
C (213)	9739 (5)	5820 (5)	2956 (3)	53 (1)	1
C (214)	9108 (5)	6912 (5)	3040 (3)	51 (1)	1
C (215)	7742 (5)	7453 (5)	2921 (3)	52 (1)	1
C (216)	7024 (5)	6915 (4)	2708 (3)	43 (1)	1
C (221)	6503 (5)	5685 (4)	1423 (3)	37 (1)	1
C (222)	5483 (5)	5612 (4)	1086 (3)	46 (1)	1
C (223)	5318 (6)	6079 (5)	395 (3)	55 (2)	1
C (224)	6168 (6)	6605 (5)	19 (3)	64 (2)	1
C (225)	7199 (6)	6658 (5)	345 (3)	64 (2)	1
C (226)	7373 (5)	6203 (4)	1045 (3)	46 (1)	1
C (231)	5064 (4)	5647 (4)	2721 (3)	36 (1)	1
C (232)	4012 (5)	6612 (4)	2408 (3)	42 (1)	1
C (233)	2814 (5)	7013 (5)	2765 (3)	50 (1)	1
C (234)	2667 (5)	6457 (5)	3424 (3)	46 (1)	1
C (235)	3705 (5)	5482 (4)	3744 (3)	43 (1)	1
C (236)	4892 (5)	5079 (4)	3394 (2)	37 (1)	1
P (3)	9219 (1)	1755 (1)	1196 (1)	31 (1)	1
C (311)	8865 (4)	2633 (4)	318 (2)	34 (1)	1
C (312)	8482 (5)	2272 (4)	-185 (2)	43 (1)	1
C (313)	8280 (5)	2938 (5)	-846 (3)	51 (1)	1
C (314)	8475 (6)	3976 (5)	-1017 (3)	58 (2)	1
C (315)	8841 (6)	4340 (5)	-522 (3)	62 (2)	1
C (316)	9022 (5)	3683 (4)	139 (3)	50 (1)	1
C (321)	8430 (5)	704 (4)	1228 (2)	34 (1)	1
C (322)	9136 (5)	-452 (4)	1301 (2)	36 (1)	1
C (323)	8470 (5)	-1195 (4)	1331 (3)	47 (1)	1
C (324)	7086 (6)	-785 (5)	1284 (3)	55 (2)	1
C (325)	6363 (5)	367 (5)	1215 (3)	48 (1)	1
C (326)	7015 (5)	1121 (4)	1187 (2)	38 (1)	1

C(331)	11011 (4)	873 (4)	1156 (2)	34 (1)	1
C(332)	11767 (5)	473 (4)	1748 (3)	41 (1)	1
C(333)	13085 (5)	-294 (5)	1759 (3)	52 (1)	1
C(334)	13651 (5)	-658 (5)	1184 (3)	53 (2)	1
C(335)	12937 (5)	-239 (5)	591 (3)	51 (1)	1
C(336)	11620 (5)	525 (4)	579 (3)	44 (1)	1

Table 2. Bond lengths (Å) and angles (°) for Va.

Ni-C(1)	1.977 (5)	Ni-P(3)	2.1783 (14)
Ni-P(1)	2.1793 (13)	Ni-Cl	2.2338 (12)
P(1)-C(1)	1.796 (5)	P(1)-C(11)	1.892 (4)
C(1)-P(2)	1.742 (5)	C(1)-H(1)	0.86 (4)
C(11)-C(12)	1.421 (6)	C(11)-C(16)	1.432 (6)
C(12)-C(13)	1.393 (6)	C(12)-C(121)	1.550 (6)
C(121)-C(124)	1.535 (6)	C(121)-C(122)	1.535 (6)
C(121)-C(123)	1.541 (6)	C(122)-H(12A)	0.98
C(122)-H(12B)	0.98	C(122)-H(12C)	0.98
C(123)-H(12D)	0.98	C(123)-H(12E)	0.98
C(123)-H(12F)	0.98	C(124)-H(12G)	0.98
C(124)-H(12H)	0.98	C(124)-H(12I)	0.98
C(13)-C(14)	1.389 (6)	C(13)-H(13)	0.95
C(14)-C(15)	1.391 (6)	C(14)-C(141)	1.533 (7)
C(141)-C(143)	1.526 (7)	C(141)-C(142)	1.530 (7)
C(141)-C(144)	1.539 (7)	C(142)-H(14A)	0.98
C(142)-H(14B)	0.98	C(142)-H(14C)	0.98
C(143)-H(14D)	0.98	C(143)-H(14E)	0.98
C(143)-H(14F)	0.98	C(144)-H(14G)	0.98
C(144)-H(14H)	0.98	C(144)-H(14I)	0.98
C(15)-C(16)	1.394 (6)	C(15)-H(15)	0.95
C(16)-C(161)	1.563 (6)	C(161)-C(164)	1.532 (7)
C(161)-C(163)	1.539 (6)	C(161)-C(162)	1.541 (6)
C(162)-H(16A)	0.98	C(162)-H(16B)	0.98
C(162)-H(16C)	0.98	C(163)-H(16D)	0.98
C(163)-H(16E)	0.98	C(163)-H(16F)	0.98
C(164)-H(16G)	0.98	C(164)-H(16H)	0.98
C(164)-H(16I)	0.98	P(2)-C(221)	1.795 (5)
P(2)-C(211)	1.814 (5)	P(2)-C(231)	1.818 (5)
C(211)-C(216)	1.383 (7)	C(211)-C(212)	1.397 (6)
C(212)-C(213)	1.391 (7)	C(212)-H(212)	0.95
C(213)-C(214)	1.371 (7)	C(213)-H(213)	0.95
C(214)-C(215)	1.382 (7)	C(214)-H(214)	0.95
C(215)-C(216)	1.379 (7)	C(215)-H(215)	0.95
C(216)-H(216)	0.95	C(221)-C(226)	1.394 (7)
C(221)-C(222)	1.395 (7)	C(222)-C(223)	1.378 (7)
C(222)-H(222)	0.95	C(223)-C(224)	1.382 (8)
C(223)-H(223)	0.95	C(224)-C(225)	1.381 (8)
C(224)-H(224)	0.95	C(225)-C(226)	1.392 (7)
C(225)-H(225)	0.95	C(226)-H(226)	0.95
C(231)-C(232)	1.386 (6)	C(231)-C(236)	1.401 (7)
C(232)-C(233)	1.393 (7)	C(232)-H(232)	0.95
C(233)-C(234)	1.366 (7)	C(233)-H(233)	0.95
C(234)-C(235)	1.388 (7)	C(234)-H(234)	0.95
C(235)-C(236)	1.378 (7)	C(235)-H(235)	0.95
C(236)-H(236)	0.95	P(3)-C(321)	1.837 (4)
P(3)-C(331)	1.837 (5)	P(3)-C(311)	1.837 (5)
C(311)-C(316)	1.381 (7)	C(311)-C(312)	1.388 (7)
C(312)-C(313)	1.382 (7)	C(312)-H(312)	0.95
C(313)-C(314)	1.385 (8)	C(313)-H(313)	0.95
C(314)-C(315)	1.366 (8)	C(314)-H(314)	0.95
C(315)-C(316)	1.378 (7)	C(315)-H(315)	0.95
C(316)-H(316)	0.95	C(321)-C(322)	1.379 (6)
C(321)-C(326)	1.409 (6)	C(322)-C(323)	1.383 (6)
C(322)-H(322)	0.95	C(323)-C(324)	1.379 (7)
C(323)-H(323)	0.95	C(324)-C(325)	1.379 (7)
C(324)-H(324)	0.95	C(325)-C(326)	1.383 (7)
C(325)-H(325)	0.95	C(326)-H(326)	0.95
C(331)-C(336)	1.378 (7)	C(331)-C(332)	1.395 (6)

C(332)-C(333)	1.388(7)	C(332)-H(332)	0.95
C(333)-C(334)	1.373(8)	C(333)-H(333)	0.95
C(334)-C(335)	1.370(8)	C(334)-H(334)	0.95
C(335)-C(336)	1.387(7)	C(335)-H(335)	0.95
C(336)-H(336)	0.95		
C(1)-Ni-P(3)	157.11(13)	C(1)-Ni-P(1)	50.92(13)
P(3)-Ni-P(1)	106.98(5)	C(1)-Ni-Cl	105.68(13)
P(3)-Ni-Cl	95.68(5)	P(1)-Ni-Cl	156.24(5)
C(1)-P(1)-C(11)	99.0(2)	C(1)-P(1)-Ni	58.7(2)
C(11)-P(1)-Ni	122.36(14)	P(2)-C(1)-P(1)	118.5(3)
P(2)-C(1)-Ni	120.1(3)	P(1)-C(1)-Ni	70.4(2)
P(2)-C(1)-H(1)	108(3)	P(1)-C(1)-H(1)	117(3)
Ni-C(1)-H(1)	120(3)	C(12)-C(11)-C(16)	117.8(4)
C(12)-C(11)-P(1)	126.8(3)	C(16)-C(11)-P(1)	113.1(3)
C(13)-C(12)-C(11)	118.5(4)	C(13)-C(12)-C(121)	116.4(4)
C(11)-C(12)-C(121)	124.9(4)	C(124)-C(121)-C(122)	107.5(4)
C(124)-C(121)-C(123)	109.9(4)	C(122)-C(121)-C(123)	105.6(4)
C(124)-C(121)-C(12)	112.2(4)	C(122)-C(121)-C(12)	111.2(4)
C(123)-C(121)-C(12)	110.2(4)	C(121)-C(122)-H(12A)	109.5(3)
C(121)-C(122)-H(12B)	109.5(2)	H(12A)-C(122)-H(12B)	109.5
C(121)-C(122)-H(12C)	109.5(3)	H(12A)-C(122)-H(12C)	109.5
H(12B)-C(122)-H(12C)	109.5	C(121)-C(123)-H(12D)	109.5(2)
C(121)-C(123)-H(12E)	109.5(2)	H(12D)-C(123)-H(12E)	109.5
C(121)-C(123)-H(12F)	109.5(2)	H(12D)-C(123)-H(12F)	109.5
H(12E)-C(123)-H(12F)	109.5	C(121)-C(124)-H(12G)	109.5(2)
C(121)-C(124)-H(12H)	109.5(3)	H(12G)-C(124)-H(12H)	109.5
C(121)-C(124)-H(12I)	109.5(2)	H(12G)-C(124)-H(12I)	109.5
H(12H)-C(124)-H(12I)	109.5	C(14)-C(13)-C(12)	123.0(4)
C(14)-C(13)-H(13)	118.5(3)	C(12)-C(13)-H(13)	118.5(2)
C(13)-C(14)-C(15)	116.4(4)	C(13)-C(14)-C(141)	123.3(4)
C(15)-C(14)-C(141)	119.9(4)	C(143)-C(141)-C(142)	107.3(4)
C(143)-C(141)-C(14)	112.5(4)	C(142)-C(141)-C(14)	109.0(4)
C(143)-C(141)-C(144)	108.8(5)	C(142)-C(141)-C(144)	109.1(4)
C(14)-C(141)-C(144)	110.2(4)	C(141)-C(142)-H(14A)	109.5(3)
C(141)-C(142)-H(14B)	109.5(3)	H(14A)-C(142)-H(14B)	109.5
C(141)-C(142)-H(14C)	109.5(3)	H(14A)-C(142)-H(14C)	109.5
H(14B)-C(142)-H(14C)	109.5	C(141)-C(143)-H(14D)	109.5(3)
C(141)-C(143)-H(14E)	109.5(3)	H(14D)-C(143)-H(14E)	109.5
C(141)-C(143)-H(14F)	109.5(3)	H(14D)-C(143)-H(14F)	109.5
H(14E)-C(143)-H(14F)	109.5	C(141)-C(144)-H(14G)	109.5(3)
C(141)-C(144)-H(14H)	109.5(3)	H(14G)-C(144)-H(14H)	109.5
C(141)-C(144)-H(14I)	109.5(3)	H(14G)-C(144)-H(14I)	109.5
H(14H)-C(144)-H(14I)	109.5	C(14)-C(15)-C(16)	123.1(4)
C(14)-C(15)-H(15)	118.4(3)	C(16)-C(15)-H(15)	118.4(3)
C(15)-C(16)-C(11)	118.1(4)	C(15)-C(16)-C(161)	117.3(4)
C(11)-C(16)-C(161)	124.4(4)	C(164)-C(161)-C(163)	109.3(4)
C(164)-C(161)-C(162)	105.9(4)	C(163)-C(161)-C(162)	105.8(4)
C(164)-C(161)-C(16)	109.9(4)	C(163)-C(161)-C(16)	114.7(3)
C(162)-C(161)-C(16)	110.8(4)	C(161)-C(162)-H(16A)	109.5(3)
C(161)-C(162)-H(16B)	109.5(3)	H(16A)-C(162)-H(16B)	109.5
C(161)-C(162)-H(16C)	109.5(3)	H(16A)-C(162)-H(16C)	109.5
H(16B)-C(162)-H(16C)	109.5	C(161)-C(163)-H(16D)	109.5(2)
C(161)-C(163)-H(16E)	109.5(3)	H(16D)-C(163)-H(16E)	109.5
C(161)-C(163)-H(16F)	109.5(3)	H(16D)-C(163)-H(16F)	109.5
H(16E)-C(163)-H(16F)	109.5	C(161)-C(164)-H(16G)	109.5(2)
C(161)-C(164)-H(16H)	109.5(3)	H(16G)-C(164)-H(16H)	109.5
C(161)-C(164)-H(16I)	109.5(2)	H(16G)-C(164)-H(16I)	109.5
H(16H)-C(164)-H(16I)	109.5	C(1)-P(2)-C(221)	114.7(2)
C(1)-P(2)-C(211)	111.2(2)	C(221)-P(2)-C(211)	108.0(2)
C(1)-P(2)-C(231)	111.7(2)	C(221)-P(2)-C(231)	107.1(2)
C(211)-P(2)-C(231)	103.5(2)	C(216)-C(211)-C(212)	119.8(4)
C(216)-C(211)-P(2)	119.8(4)	C(212)-C(211)-P(2)	120.3(4)

C(213)-C(212)-C(211)	118.7(5)	C(213)-C(212)-H(212)	120.6(3)
C(211)-C(212)-H(212)	120.6(3)	C(214)-C(213)-C(212)	121.5(5)
C(214)-C(213)-H(213)	119.3(3)	C(212)-C(213)-H(213)	119.3(3)
C(213)-C(214)-C(215)	119.1(5)	C(213)-C(214)-H(214)	120.4(3)
C(215)-C(214)-H(214)	120.4(3)	C(216)-C(215)-C(214)	120.6(5)
C(216)-C(215)-H(215)	119.7(3)	C(214)-C(215)-H(215)	119.7(3)
C(215)-C(216)-C(211)	120.2(5)	C(215)-C(216)-H(216)	119.9(3)
C(211)-C(216)-H(216)	119.9(3)	C(226)-C(221)-C(222)	118.9(5)
C(226)-C(221)-P(2)	119.8(4)	C(222)-C(221)-P(2)	121.3(4)
C(223)-C(222)-C(221)	120.2(5)	C(223)-C(222)-H(222)	119.9(3)
C(221)-C(222)-H(222)	119.9(3)	C(222)-C(223)-C(224)	121.1(5)
C(222)-C(223)-H(223)	119.4(3)	C(224)-C(223)-H(223)	119.4(3)
C(225)-C(224)-C(223)	119.1(5)	C(225)-C(224)-H(224)	120.5(4)
C(223)-C(224)-H(224)	120.5(3)	C(224)-C(225)-C(226)	120.7(6)
C(224)-C(225)-H(225)	119.7(4)	C(226)-C(225)-H(225)	119.7(4)
C(225)-C(226)-C(221)	120.0(5)	C(225)-C(226)-H(226)	120.0(4)
C(221)-C(226)-H(226)	120.0(3)	C(232)-C(231)-C(236)	118.9(4)
C(232)-C(231)-P(2)	123.6(4)	C(236)-C(231)-P(2)	117.4(3)
C(231)-C(232)-C(233)	120.1(5)	C(231)-C(232)-H(232)	120.0(3)
C(233)-C(232)-H(232)	120.0(3)	C(234)-C(233)-C(232)	120.3(5)
C(234)-C(233)-H(233)	119.9(3)	C(232)-C(233)-H(233)	119.9(3)
C(233)-C(234)-C(235)	120.5(5)	C(233)-C(234)-H(234)	119.8(3)
C(235)-C(234)-H(234)	119.8(3)	C(236)-C(235)-C(234)	119.6(5)
C(236)-C(235)-H(235)	120.2(3)	C(234)-C(235)-H(235)	120.2(3)
C(235)-C(236)-C(231)	120.6(4)	C(235)-C(236)-H(236)	119.7(3)
C(231)-C(236)-H(236)	119.7(3)	C(321)-P(3)-C(331)	101.1(2)
C(321)-P(3)-C(311)	101.6(2)	C(331)-P(3)-C(311)	103.0(2)
C(321)-P(3)-Ni	119.5(2)	C(331)-P(3)-Ni	116.0(2)
C(311)-P(3)-Ni	113.3(2)	C(316)-C(311)-C(312)	118.0(5)
C(316)-C(311)-P(3)	119.2(4)	C(312)-C(311)-P(3)	122.8(4)
C(313)-C(312)-C(311)	120.9(5)	C(313)-C(312)-H(312)	119.5(3)
C(311)-C(312)-H(312)	119.5(3)	C(312)-C(313)-C(314)	120.0(5)
C(312)-C(313)-H(313)	120.0(3)	C(314)-C(313)-H(313)	120.0(3)
C(315)-C(314)-C(313)	119.3(5)	C(315)-C(314)-H(314)	120.3(3)
C(313)-C(314)-H(314)	120.3(3)	C(314)-C(315)-C(316)	120.6(6)
C(314)-C(315)-H(315)	119.7(3)	C(316)-C(315)-H(315)	119.7(4)
C(315)-C(316)-C(311)	121.1(6)	C(315)-C(316)-H(316)	119.4(4)
C(311)-C(316)-H(316)	119.4(3)	C(322)-C(321)-C(326)	119.1(4)
C(322)-C(321)-P(3)	123.9(3)	C(326)-C(321)-P(3)	117.0(4)
C(321)-C(322)-C(323)	120.7(4)	C(321)-C(322)-H(322)	119.7(3)
C(323)-C(322)-H(322)	119.7(3)	C(324)-C(323)-C(322)	120.2(5)
C(324)-C(323)-H(323)	119.9(3)	C(322)-C(323)-H(323)	119.9(3)
C(325)-C(324)-C(323)	119.9(5)	C(325)-C(324)-H(324)	120.0(3)
C(323)-C(324)-H(324)	120.0(3)	C(324)-C(325)-C(326)	120.5(5)
C(324)-C(325)-H(325)	119.7(3)	C(326)-C(325)-H(325)	119.7(3)
C(325)-C(326)-C(321)	119.6(5)	C(325)-C(326)-H(326)	120.2(3)
C(321)-C(326)-H(326)	120.2(3)	C(336)-C(331)-C(332)	118.5(4)
C(336)-C(331)-P(3)	122.9(4)	C(332)-C(331)-P(3)	118.4(4)
C(333)-C(332)-C(331)	120.2(5)	C(333)-C(332)-H(332)	119.9(3)
C(331)-C(332)-H(332)	119.9(3)	C(334)-C(333)-C(332)	120.1(5)
C(334)-C(333)-H(333)	120.0(3)	C(332)-C(333)-H(333)	120.0(3)
C(335)-C(334)-C(333)	120.3(5)	C(335)-C(334)-H(334)	119.8(3)
C(333)-C(334)-H(334)	119.8(3)	C(334)-C(335)-C(336)	119.7(5)
C(334)-C(335)-H(335)	120.1(3)	C(336)-C(335)-H(335)	120.1(3)
C(331)-C(336)-C(335)	121.1(5)	C(331)-C(336)-H(336)	119.5(3)
C(335)-C(336)-H(336)	119.5(3)		

Symmetry transformations used to generate equivalent atoms:

Table 3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Va.

	U11	U22	U33	U23	U13	U12
Ni	26 (1)	31 (1)	37 (1)	-7 (1)	-2 (1)	-12 (1)
Cl	35 (1)	45 (1)	49 (1)	-10 (1)	0 (1)	-23 (1)
P (1)	26 (1)	30 (1)	36 (1)	-6 (1)	-3 (1)	-10 (1)
C (1)	28 (2)	36 (3)	33 (3)	-5 (2)	-6 (2)	-14 (2)
C (11)	30 (2)	28 (2)	34 (3)	-10 (2)	0 (2)	-11 (2)
C (12)	29 (2)	28 (2)	33 (3)	-2 (2)	-3 (2)	-13 (2)
C (121)	24 (2)	35 (3)	40 (3)	-9 (2)	-1 (2)	-13 (2)
C (122)	31 (3)	40 (3)	53 (3)	-2 (2)	-8 (2)	-2 (2)
C (123)	37 (3)	34 (3)	44 (3)	-13 (2)	-4 (2)	-3 (2)
C (124)	25 (2)	42 (3)	49 (3)	-10 (2)	-4 (2)	-8 (2)
C (13)	25 (2)	36 (3)	34 (3)	-5 (2)	-7 (2)	-11 (2)
C (14)	34 (3)	36 (3)	34 (3)	-8 (2)	2 (2)	-18 (2)
C (141)	31 (3)	46 (3)	44 (3)	-15 (2)	3 (2)	-13 (2)
C (142)	49 (3)	53 (3)	46 (3)	-16 (3)	5 (3)	-18 (3)
C (143)	50 (3)	70 (4)	40 (3)	-13 (3)	-8 (3)	-14 (3)
C (144)	59 (4)	67 (4)	44 (4)	-9 (3)	9 (3)	-31 (3)
C (15)	24 (2)	38 (3)	41 (3)	-9 (2)	1 (2)	-16 (2)
C (16)	30 (2)	22 (2)	39 (3)	-6 (2)	-6 (2)	-7 (2)
C (161)	27 (2)	38 (3)	37 (3)	-5 (2)	-5 (2)	-18 (2)
C (162)	30 (3)	68 (4)	53 (3)	-10 (3)	-4 (2)	-23 (3)
C (163)	28 (3)	40 (3)	55 (3)	-6 (2)	-15 (2)	-12 (2)
C (164)	34 (3)	52 (3)	57 (3)	-14 (3)	-12 (3)	-17 (2)
P (2)	28 (1)	30 (1)	42 (1)	-9 (1)	-2 (1)	-10 (1)
C (211)	37 (3)	30 (3)	42 (3)	-8 (2)	2 (2)	-18 (2)
C (212)	32 (3)	37 (3)	73 (4)	-21 (3)	-10 (3)	-9 (2)
C (213)	36 (3)	57 (4)	77 (4)	-28 (3)	-7 (3)	-19 (3)
C (214)	44 (3)	55 (4)	71 (4)	-25 (3)	2 (3)	-30 (3)
C (215)	42 (3)	44 (3)	82 (4)	-32 (3)	11 (3)	-23 (3)
C (216)	38 (3)	41 (3)	53 (3)	-14 (2)	1 (2)	-17 (2)
C (221)	33 (3)	24 (2)	51 (3)	-8 (2)	-5 (2)	-5 (2)
C (222)	44 (3)	43 (3)	49 (3)	-10 (2)	-2 (3)	-14 (2)
C (223)	44 (3)	60 (4)	52 (4)	-7 (3)	-11 (3)	-10 (3)
C (224)	61 (4)	68 (4)	39 (3)	1 (3)	-10 (3)	-4 (3)
C (225)	66 (4)	60 (4)	51 (4)	3 (3)	6 (3)	-21 (3)
C (226)	43 (3)	41 (3)	49 (3)	-5 (2)	-5 (3)	-11 (2)
C (231)	24 (2)	36 (3)	52 (3)	-15 (2)	-6 (2)	-12 (2)
C (232)	36 (3)	37 (3)	43 (3)	-3 (2)	-3 (2)	-7 (2)
C (233)	34 (3)	42 (3)	66 (4)	-13 (3)	-4 (3)	-5 (2)
C (234)	34 (3)	52 (3)	59 (4)	-24 (3)	2 (3)	-18 (2)
C (235)	35 (3)	52 (3)	42 (3)	-15 (2)	2 (2)	-16 (2)
C (236)	34 (3)	30 (3)	43 (3)	-6 (2)	-3 (2)	-7 (2)
P (3)	26 (1)	33 (1)	35 (1)	-6 (1)	-1 (1)	-13 (1)
C (311)	23 (2)	35 (3)	40 (3)	-7 (2)	0 (2)	-9 (2)
C (312)	35 (3)	47 (3)	40 (3)	-2 (2)	-3 (2)	-12 (2)
C (313)	37 (3)	69 (4)	38 (3)	-13 (3)	-6 (2)	-7 (3)
C (314)	49 (3)	59 (4)	40 (3)	7 (3)	-3 (3)	-4 (3)
C (315)	73 (4)	53 (4)	52 (4)	2 (3)	2 (3)	-23 (3)
C (316)	56 (3)	48 (3)	49 (3)	-8 (3)	1 (3)	-25 (3)
C (321)	36 (3)	44 (3)	26 (2)	-6 (2)	0 (2)	-22 (2)
C (322)	30 (3)	35 (3)	44 (3)	-9 (2)	-3 (2)	-13 (2)
C (323)	39 (3)	33 (3)	68 (4)	-13 (2)	2 (3)	-14 (2)
C (324)	50 (3)	55 (4)	74 (4)	-18 (3)	1 (3)	-33 (3)
C (325)	33 (3)	55 (4)	64 (4)	-23 (3)	4 (2)	-22 (3)
C (326)	35 (3)	35 (3)	47 (3)	-13 (2)	2 (2)	-14 (2)

C(331)	30(2)	32(3)	42(3)	-6(2)	-3(2)	-14(2)
C(332)	37(3)	42(3)	42(3)	-7(2)	0(2)	-15(2)
C(333)	36(3)	48(3)	70(4)	-9(3)	-19(3)	-13(3)
C(334)	29(3)	46(3)	83(5)	-18(3)	-2(3)	-13(2)
C(335)	36(3)	55(3)	65(4)	-26(3)	8(3)	-14(3)
C(336)	32(3)	57(3)	41(3)	-16(3)	-3(2)	-11(2)

Table 4. Torsion angles (°) for Va.

C(1)-Ni-P(1)-C(1)	0.0	P(3)-Ni-P(1)-C(1)	-173.2(2)
Cl-Ni-P(1)-C(1)	-11.3(2)	C(1)-Ni-P(1)-C(11)	-80.4(2)
P(3)-Ni-P(1)-C(11)	106.4(2)	Cl-Ni-P(1)-C(11)	-91.7(2)
C(11)-P(1)-C(1)-P(2)	-123.1(3)	Ni-P(1)-C(1)-P(2)	114.3(3)
C(11)-P(1)-C(1)-Ni	122.5(2)	Ni-P(1)-C(1)-Ni	0.0
P(3)-Ni-C(1)-P(2)	-95.4(4)	P(1)-Ni-C(1)-P(2)	-112.3(3)
Cl-Ni-C(1)-P(2)	63.0(3)	P(3)-Ni-C(1)-P(1)	17.0(4)
P(1)-Ni-C(1)-P(1)	0.0	Cl-Ni-C(1)-P(1)	175.28(9)
C(1)-P(1)-C(11)-C(12)	-52.9(4)	Ni-P(1)-C(11)-C(12)	5.6(5)
C(1)-P(1)-C(11)-C(16)	108.9(3)	Ni-P(1)-C(11)-C(16)	167.5(3)
C(16)-C(11)-C(12)-C(13)	-17.7(6)	P(1)-C(11)-C(12)-C(13)	143.4(4)
C(16)-C(11)-C(12)-C(121)	156.5(4)	P(1)-C(11)-C(12)-C(121)	-42.4(6)
C(13)-C(12)-C(121)-C(124)	-91.0(5)	C(11)-C(12)-C(121)-C(124)	94.7(5)
C(13)-C(12)-C(121)-C(122)	29.4(5)	C(11)-C(12)-C(121)-C(122)	-144.9(4)
C(13)-C(12)-C(121)-C(123)	146.1(4)	C(11)-C(12)-C(121)-C(123)	-28.2(6)
C(11)-C(12)-C(13)-C(14)	4.5(6)	C(121)-C(12)-C(13)-C(14)	-170.2(4)
C(12)-C(13)-C(14)-C(15)	9.1(7)	C(12)-C(13)-C(14)-C(141)	-177.3(4)
C(13)-C(14)-C(141)-C(143)	7.0(7)	C(15)-C(14)-C(141)-C(143)	-179.6(4)
C(13)-C(14)-C(141)-C(142)	125.8(5)	C(15)-C(14)-C(141)-C(142)	-60.8(5)
C(13)-C(14)-C(141)-C(144)	-114.5(5)	C(15)-C(14)-C(141)-C(144)	58.9(6)
C(13)-C(14)-C(15)-C(16)	-9.6(6)	C(141)-C(14)-C(15)-C(16)	176.6(4)
C(14)-C(15)-C(16)-C(11)	-3.6(6)	C(14)-C(15)-C(16)-C(161)	170.8(4)
C(12)-C(11)-C(16)-C(15)	17.3(6)	P(1)-C(11)-C(16)-C(15)	-146.3(3)
C(12)-C(11)-C(16)-C(161)	-156.7(4)	P(1)-C(11)-C(16)-C(161)	39.7(5)
C(15)-C(16)-C(161)-C(164)	-134.5(4)	C(11)-C(16)-C(161)-C(164)	39.5(6)
C(15)-C(16)-C(161)-C(163)	101.9(5)	C(11)-C(16)-C(161)-C(163)	-84.1(5)
C(15)-C(16)-C(161)-C(162)	-17.8(6)	C(11)-C(16)-C(161)-C(162)	156.2(4)
P(1)-C(1)-P(2)-C(221)	-57.2(4)	Ni-C(1)-P(2)-C(221)	25.5(3)
P(1)-C(1)-P(2)-C(211)	179.9(3)	Ni-C(1)-P(2)-C(211)	-97.3(3)
P(1)-C(1)-P(2)-C(231)	64.9(4)	Ni-C(1)-P(2)-C(231)	147.6(2)
C(1)-P(2)-C(211)-C(216)	-154.7(4)	C(221)-P(2)-C(211)-C(216)	78.7(4)
C(231)-P(2)-C(211)-C(216)	-34.6(4)	C(1)-P(2)-C(211)-C(212)	26.2(5)
C(221)-P(2)-C(211)-C(212)	-100.4(4)	C(231)-P(2)-C(211)-C(212)	146.2(4)
C(216)-C(211)-C(212)-C(213)	0.1(8)	P(2)-C(211)-C(212)-C(213)	179.3(4)
C(211)-C(212)-C(213)-C(214)	-0.7(9)	C(212)-C(211)-C(213)-C(214)	1.3(9)
C(213)-C(214)-C(215)-C(216)	-1.3(9)	C(214)-C(215)-C(216)-C(211)	0.8(8)
C(212)-C(211)-C(216)-C(215)	-0.2(8)	P(2)-C(211)-C(216)-C(215)	-179.3(4)
C(1)-P(2)-C(221)-C(226)	-103.6(4)	C(211)-P(2)-C(221)-C(226)	21.0(5)
C(231)-P(2)-C(221)-C(226)	131.9(4)	C(1)-P(2)-C(221)-C(222)	76.2(4)
C(211)-P(2)-C(221)-C(222)	-159.2(4)	C(231)-P(2)-C(221)-C(222)	-48.3(4)
C(226)-C(221)-C(222)-C(223)	-2.1(7)	P(2)-C(221)-C(222)-C(223)	178.1(4)
C(221)-C(222)-C(223)-C(224)	1.4(8)	C(222)-C(223)-C(224)-C(225)	0.1(9)
C(223)-C(224)-C(225)-C(226)	-0.9(9)	C(224)-C(225)-C(226)-C(221)	0.1(9)
C(222)-C(221)-C(226)-C(225)	1.3(7)	P(2)-C(221)-C(226)-C(225)	-178.9(4)
C(1)-P(2)-C(231)-C(232)	-148.3(4)	C(221)-P(2)-C(231)-C(232)	-22.0(5)
C(211)-P(2)-C(231)-C(232)	92.1(4)	C(1)-P(2)-C(231)-C(236)	36.1(4)
C(221)-P(2)-C(231)-C(236)	162.4(4)	C(211)-P(2)-C(231)-C(236)	-83.6(4)
C(236)-C(231)-C(232)-C(233)	0.9(7)	P(2)-C(231)-C(232)-C(233)	-174.7(4)
C(231)-C(232)-C(233)-C(234)	-0.1(8)	C(232)-C(233)-C(234)-C(235)	-0.5(8)
C(233)-C(234)-C(235)-C(236)	0.4(8)	C(234)-C(235)-C(236)-C(231)	0.4(7)
C(232)-C(231)-C(236)-C(235)	-1.0(7)	P(2)-C(231)-C(236)-C(235)	174.9(4)
C(1)-Ni-P(3)-C(321)	-36.1(4)	P(1)-Ni-P(3)-C(321)	-22.4(2)
Cl-Ni-P(3)-C(321)	164.8(2)	C(1)-Ni-P(3)-C(331)	-157.6(4)
P(1)-Ni-P(3)-C(331)	-143.9(2)	Cl-Ni-P(3)-C(331)	43.4(2)
C(1)-Ni-P(3)-C(311)	83.6(4)	P(1)-Ni-P(3)-C(311)	97.3(2)
Cl-Ni-P(3)-C(311)	-75.5(2)	C(321)-P(3)-C(311)-C(316)	165.1(4)
C(331)-P(3)-C(311)-C(316)	-90.5(4)	Ni-P(3)-C(311)-C(316)	35.5(4)
C(321)-P(3)-C(311)-C(312)	-17.0(4)	C(331)-P(3)-C(311)-C(312)	87.4(4)
Ni-P(3)-C(311)-C(312)	-146.6(4)	C(316)-C(311)-C(312)-C(313)	0.7(7)

P(3)-C(311)-C(312)-C(313)	-177.3(4)	C(311)-C(312)-C(313)-C(314)	0.8(8)
C(312)-C(313)-C(314)-C(315)	-1.4(8)	C(313)-C(314)-C(315)-C(316)	0.4(9)
C(314)-C(315)-C(316)-C(311)	1.1(9)	C(312)-C(311)-C(316)-C(315)	-1.7(8)
P(3)-C(311)-C(316)-C(315)	176.3(4)	C(331)-P(3)-C(321)-C(322)	8.1(4)
C(311)-P(3)-C(321)-C(322)	114.0(4)	Ni-P(3)-C(321)-C(322)	-120.5(4)
C(331)-P(3)-C(321)-C(326)	-173.2(4)	C(311)-P(3)-C(321)-C(326)	-67.3(4)
Ni-P(3)-C(321)-C(326)	58.2(4)	C(326)-C(321)-C(322)-C(323)	0.3(7)
P(3)-C(321)-C(322)-C(323)	179.0(4)	C(321)-C(322)-C(323)-C(324)	0.3(8)
C(322)-C(323)-C(324)-C(325)	-0.8(9)	C(323)-C(324)-C(325)-C(326)	0.6(9)
C(324)-C(325)-C(326)-C(321)	0.1(8)	C(322)-C(321)-C(326)-C(325)	-0.5(7)
P(3)-C(321)-C(326)-C(325)	-179.3(4)	C(321)-P(3)-C(331)-C(336)	73.3(4)
C(311)-P(3)-C(331)-C(336)	-31.5(5)	Ni-P(3)-C(331)-C(336)	-155.8(4)
C(321)-P(3)-C(331)-C(332)	-102.2(4)	C(311)-P(3)-C(331)-C(332)	153.0(4)
Ni-P(3)-C(331)-C(332)	28.6(4)	C(336)-C(331)-C(332)-C(333)	-2.6(7)
P(3)-C(331)-C(332)-C(333)	173.1(4)	C(331)-C(332)-C(333)-C(334)	0.4(8)
C(332)-C(333)-C(334)-C(335)	2.0(8)	C(333)-C(334)-C(335)-C(336)	-2.2(8)
C(332)-C(331)-C(336)-C(335)	2.5(7)	P(3)-C(331)-C(336)-C(335)	-173.1(4)
C(334)-C(335)-C(336)-C(331)	-0.1(8)		

Symmetry transformations used to generate equivalent atoms:

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **Va**.

	x	y	z	U(eq)	SOF
H(1)	7685 (39)	3467 (32)	3005 (21)	16 (11)	1
H(12A)	10250 (17)	-1104 (14)	4071 (7)	77 (19)	1
H(12B)	8727 (17)	-961 (17)	4299 (12)	65 (17)	1
H(12C)	9500 (33)	-345 (5)	4600 (6)	66 (18)	1
H(12D)	9816 (9)	-510 (21)	2912 (10)	50 (15)	1
H(12E)	8661 (31)	667 (5)	2568 (4)	65 (17)	1
H(12F)	8265 (23)	-369 (23)	3043 (7)	60 (16)	1
H(12G)	10798 (6)	567 (7)	3455 (14)	39 (13)	1
H(12H)	9838 (20)	1422 (20)	3894 (7)	40 (14)	1
H(12I)	9658 (17)	1734 (15)	3086 (8)	56 (16)	1
H(13)	7742 (4)	859 (4)	4757 (2)	11 (9)	1
H(14A)	5148 (13)	3484 (8)	5227 (16)	47 (14)	1
H(14B)	4356 (30)	3053 (5)	5892 (3)	99 (24)	1
H(14C)	3753 (17)	3341 (10)	5151 (14)	66 (18)	1
H(14D)	7152 (17)	1755 (18)	5672 (10)	57 (16)	1
H(14E)	7064 (19)	507 (9)	5838 (13)	73 (20)	1
H(14F)	6261 (6)	1369 (26)	6305 (4)	67 (18)	1
H(14G)	4907 (14)	292 (9)	5614 (17)	104 (26)	1
H(14H)	3608 (17)	1422 (19)	5379 (12)	66 (18)	1
H(1IC)	4196 (30)	1093 (26)	6127 (6)	72 (19)	1
H(15)	3839 (4)	2420 (4)	4283 (2)	48 (14)	1
H(16A)	1943 (14)	2401 (26)	3086 (3)	55 (15)	1
H(16B)	2243 (19)	2908 (16)	3662 (12)	59 (17)	1
H(16C)	2920 (8)	1565 (11)	3703 (11)	51 (15)	1
H(16D)	2476 (15)	3927 (8)	2328 (11)	38 (13)	1
H(16E)	3988 (12)	3905 (7)	2204 (9)	46 (14)	1
H(16F)	3143 (25)	4296 (4)	2851 (3)	34 (13)	1
H(16G)	3481 (11)	1903 (17)	2205 (10)	55 (15)	1
H(16H)	4493 (28)	926 (5)	2766 (3)	37 (13)	1
H(16I)	5012 (19)	1816 (18)	2211 (10)	59 (16)	1
H(212)	9493 (5)	4502 (4)	2681 (3)	45 (14)	1
H(213)	10674 (5)	5440 (5)	3047 (3)	94 (23)	1
H(214)	9603 (5)	7291 (5)	3178 (3)	74 (19)	1
H(215)	7293 (5)	8204 (5)	2987 (3)	53 (15)	1
H(216)	6087 (5)	7300 (4)	2622 (3)	44 (14)	1
H(222)	4901 (5)	5238 (4)	1334 (3)	51 (15)	1
H(223)	4608 (6)	6038 (5)	172 (3)	66 (18)	1
H(224)	6045 (6)	6926 (5)	-458 (3)	59 (16)	1
H(225)	7796 (6)	7009 (5)	90 (3)	70 (19)	1
H(226)	8084 (5)	6246 (4)	1265 (3)	47 (15)	1
H(232)	4108 (5)	7001 (4)	1949 (3)	46 (14)	1
H(233)	2096 (5)	7676 (5)	2549 (3)	57 (16)	1
H(234)	1850 (5)	6739 (5)	3665 (3)	61 (17)	1
H(235)	3596 (5)	5095 (4)	4201 (3)	39 (13)	1
H(236)	5601 (5)	4410 (4)	3612 (2)	38 (13)	1
H(312)	8358 (5)	1557 (4)	-73 (2)	31 (12)	1
H(313)	8007 (5)	2685 (5)	-1184 (3)	72 (19)	1
H(314)	8357 (6)	4429 (5)	-1473 (3)	59 (16)	1
H(315)	8971 (6)	5053 (5)	-636 (3)	56 (16)	1
H(316)	9261 (5)	3957 (4)	478 (3)	48 (15)	1
H(322)	10090 (5)	-741 (4)	1332 (2)	35 (12)	1
H(323)	8967 (5)	-1990 (4)	1384 (3)	43 (14)	1
H(324)	6632 (6)	-1296 (5)	1298 (3)	59 (16)	1

H(325)	5409 (5)	646 (5)	1187 (3)	58 (16)	1
H(326)	6512 (5)	1914 (4)	1140 (2)	39 (13)	1
H(332)	11380 (5)	728 (4)	2146 (3)	41 (14)	1
H(333)	13594 (5)	-568 (5)	2164 (3)	58 (16)	1
H(334)	14543 (5)	-1202 (5)	1197 (3)	55 (16)	1
H(335)	13343 (5)	-472 (5)	189 (3)	67 (18)	1
H(336)	11128 (5)	813 (4)	167 (3)	32 (12)	1

Figure 1. Fully labeled thermal ellipsoid drawing of Va.

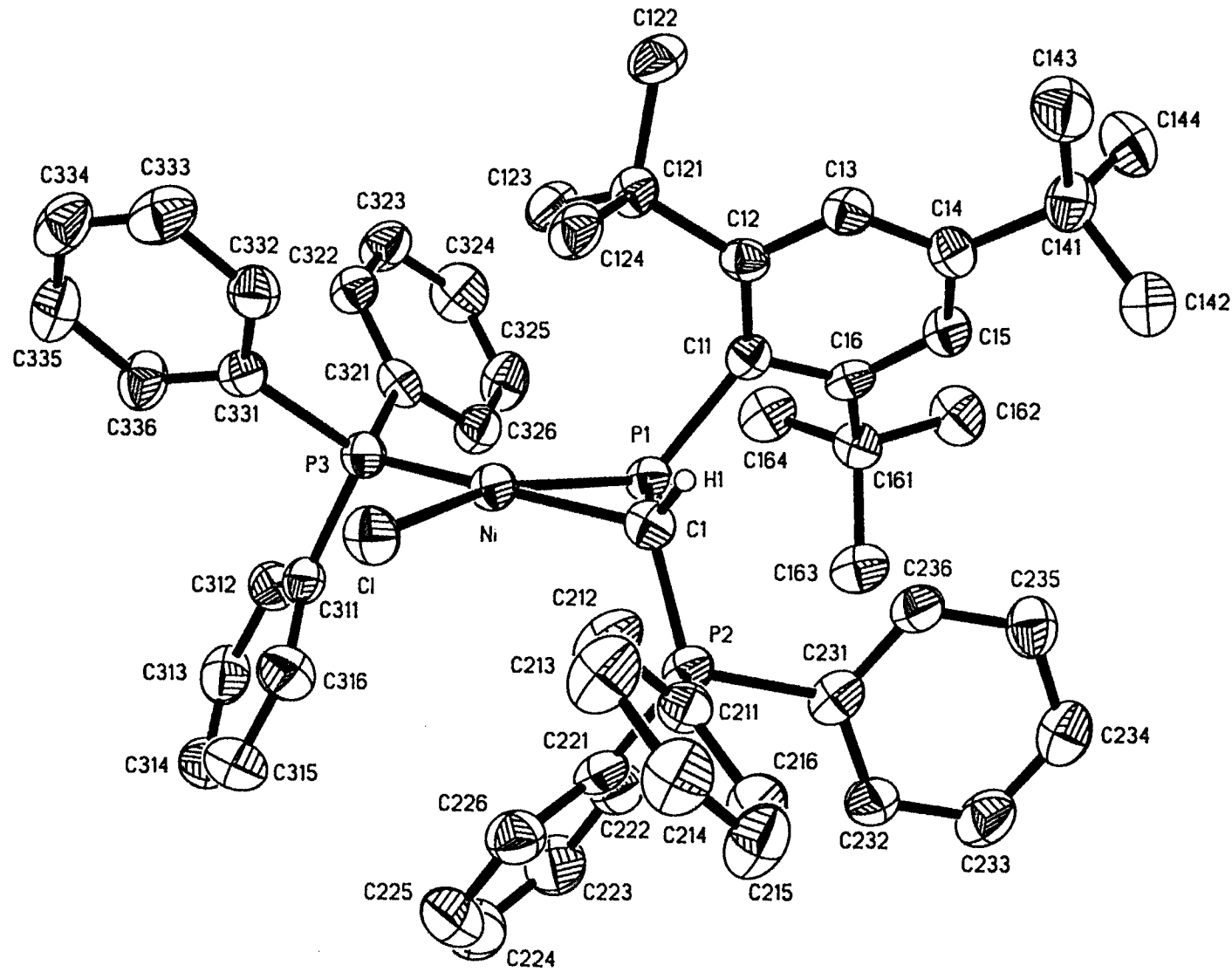


Figure 2. Unit cell and packing diagram for **Va**.

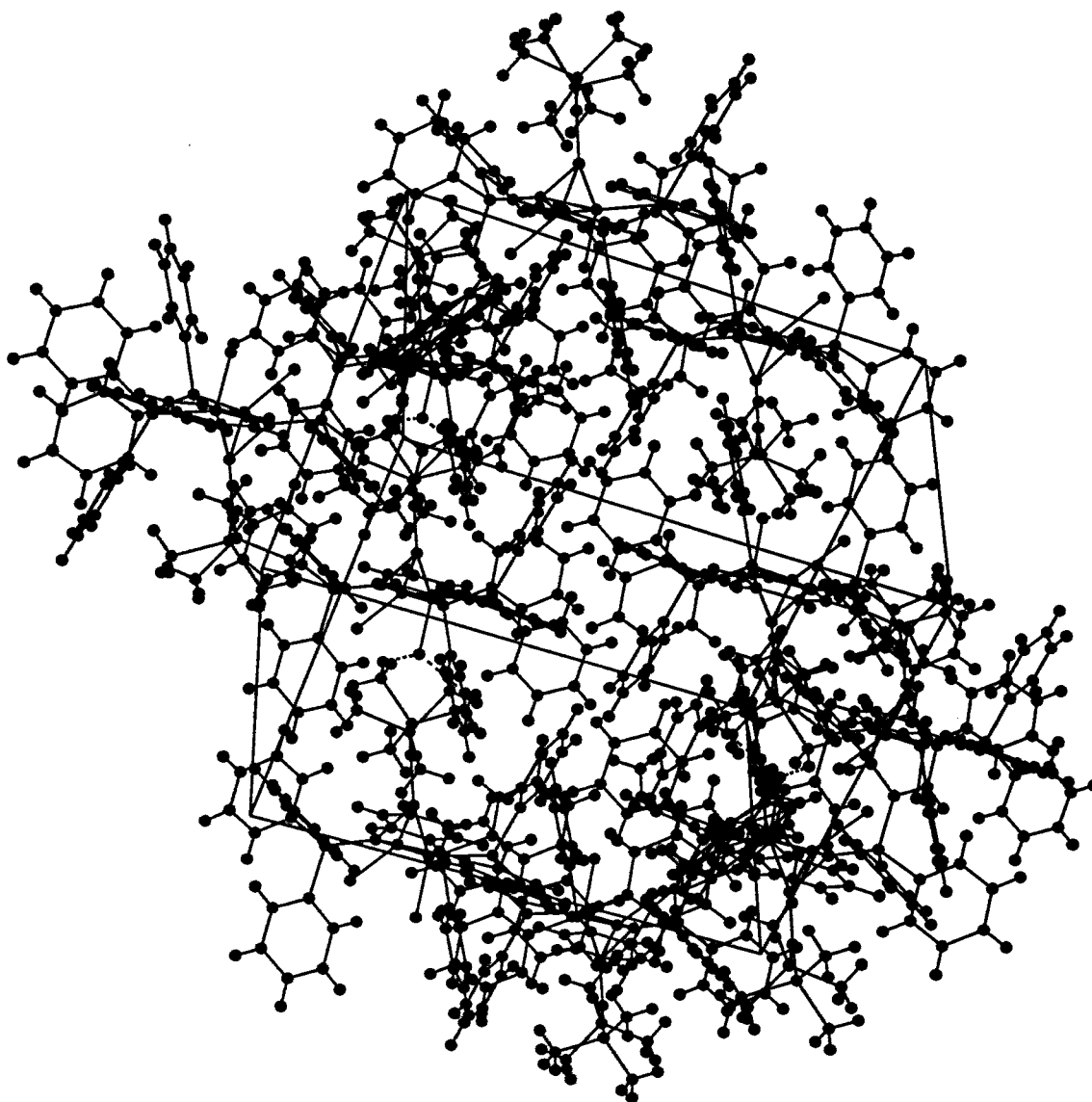


Table 6. Atomic coordinates ($\times 10^4$) and equivalent isotropic parameters ($\text{\AA}^2 \times 10^3$) for **IIIa**.

	x	y	z	U(eq)	SOF
Ni (1)	1722 (1)	8530 (1)	2386 (1)	26 (1)	1
Ni (2)	3816 (1)	7166 (1)	2587 (1)	23 (1)	1
Cl (1)	1866 (2)	9704 (1)	1832 (1)	42 (1)	1
Cl (2)	5674 (2)	7505 (1)	2458 (1)	33 (1)	1
C (1)	2855 (6)	7780 (4)	1775 (4)	22 (2)	1
P (1)	1944 (2)	7268 (1)	2322 (1)	22 (1)	1
N (1)	1009 (5)	6657 (3)	2085 (3)	26 (1)	1
Si (1)	1626 (2)	5694 (1)	1782 (1)	29 (1)	1
C (11)	1402 (7)	5676 (5)	816 (4)	40 (2)	1
C (12)	858 (8)	4925 (5)	2291 (5)	46 (2)	1
C (13)	3325 (7)	5407 (5)	1907 (4)	38 (2)	1
Si (2)	-655 (2)	6966 (1)	2183 (1)	29 (1)	1
C (21)	-1421 (7)	6547 (5)	1479 (4)	44 (2)	1
C (22)	-1212 (7)	6597 (5)	3064 (4)	37 (2)	1
C (23)	-1135 (7)	8070 (5)	2092 (5)	42 (2)	1
P (2)	3304 (2)	7971 (1)	910 (1)	26 (1)	1
C (211)	4505 (7)	8574 (5)	799 (4)	38 (2)	1
C (212)	5174 (8)	8585 (5)	154 (5)	60 (3)	1
C (213)	6184 (9)	8979 (7)	77 (7)	92 (5)	1
C (214)	6535 (9)	9323 (7)	649 (8)	98 (6)	1
C (215)	5866 (9)	9327 (5)	1278 (7)	74 (4)	1
C (216)	4812 (7)	8966 (5)	1356 (5)	53 (3)	1
C (221)	1995 (6)	8390 (4)	379 (4)	29 (2)	1
C (222)	2047 (8)	8994 (5)	-126 (5)	48 (2)	1
C (223)	1032 (9)	9283 (5)	-540 (5)	61 (3)	1
C (224)	-20 (8)	8954 (5)	-455 (5)	54 (3)	1
C (225)	-88 (7)	8343 (5)	58 (5)	51 (2)	1
C (226)	923 (7)	8063 (5)	473 (4)	39 (2)	1
C (231)	4090 (6)	7082 (4)	483 (4)	27 (2)	1
C (232)	5221 (7)	6693 (5)	747 (4)	40 (2)	1
C (233)	5913 (7)	6052 (5)	393 (5)	49 (2)	1
C (234)	5511 (8)	5800 (5)	-202 (5)	54 (3)	1
C (235)	4376 (8)	6179 (5)	-462 (5)	54 (3)	1
C (236)	3676 (7)	6817 (5)	-119 (4)	38 (2)	1
P (3)	872 (2)	9064 (1)	3370 (1)	28 (1)	1
C (311)	-620 (6)	9783 (4)	3357 (4)	31 (2)	1
C (312)	-1323 (7)	10014 (5)	3955 (4)	39 (2)	1
C (313)	-2472 (7)	10527 (5)	3918 (5)	51 (2)	1
C (314)	-2907 (8)	10795 (5)	3253 (5)	57 (3)	1
C (315)	-2225 (8)	10557 (6)	2656 (4)	56 (3)	1
C (316)	-1068 (7)	10049 (5)	2683 (4)	38 (2)	1
C (321)	2024 (6)	9601 (4)	3689 (4)	29 (2)	1
C (322)	3280 (7)	9293 (5)	3534 (4)	42 (2)	1
C (323)	4207 (7)	9640 (5)	3785 (5)	45 (2)	1
C (324)	3886 (7)	10314 (5)	4175 (5)	48 (2)	1
C (325)	2648 (8)	10628 (5)	4312 (5)	49 (2)	1
C (326)	1715 (7)	10283 (5)	4068 (4)	41 (2)	1

C(331)	558 (6)	8425 (4)	4153 (4)	32 (2)	1
C(332)	1347 (7)	8265 (5)	4712 (4)	44 (2)	1
C(333)	1087 (8)	7779 (6)	5292 (5)	55 (3)	1
C(334)	43 (9)	7431 (5)	5320 (4)	58 (3)	1
C(335)	-739 (8)	7575 (5)	4757 (4)	47 (2)	1
C(336)	-479 (7)	8070 (5)	4180 (4)	40 (2)	1
P(4)	4315 (2)	6367 (1)	3522 (1)	23 (1)	1
C(411)	5782 (6)	5650 (4)	3399 (3)	24 (2)	1
C(412)	6477 (6)	5313 (5)	3979 (4)	38 (2)	1
C(413)	7541 (7)	4732 (5)	3858 (4)	43 (2)	1
C(414)	7902 (7)	4486 (5)	3199 (4)	43 (2)	1
C(415)	7238 (7)	4831 (5)	2621 (4)	43 (2)	1
C(416)	6168 (6)	5422 (4)	2730 (4)	30 (2)	1
C(421)	4544 (6)	6858 (4)	4332 (4)	28 (2)	1
C(422)	5224 (8)	7474 (5)	4271 (4)	42 (2)	1
C(423)	5438 (9)	7842 (5)	4870 (4)	53 (2)	1
C(424)	5001 (8)	7611 (5)	5531 (4)	47 (2)	1
C(425)	4327 (8)	7004 (5)	5590 (4)	44 (2)	1
C(426)	4108 (7)	6629 (5)	4989 (4)	38 (2)	1
C(431)	3218 (6)	5719 (4)	3840 (4)	23 (2)	1
C(432)	3555 (6)	4894 (4)	3959 (4)	33 (2)	1
C(433)	2701 (7)	4432 (4)	4205 (5)	41 (2)	1
C(434)	1474 (7)	4775 (5)	4343 (4)	43 (2)	1
C(435)	1110 (7)	5598 (4)	4221 (4)	37 (2)	1
C(436)	1969 (5)	6057 (3)	3972 (3)	32 (2)	1
C(31)	3330 (5)	2362 (3)	2760 (3)	84 (3)	1
C(32)	4054 (5)	2949 (3)	2604 (3)	121 (5)	1
C(33)	5075 (13)	2781 (11)	2145 (8)	201 (9)	1
C(34)	5364 (16)	2066 (12)	1820 (10)	238 (13)	1
C(35)	4648 (18)	1470 (10)	1984 (9)	211 (10)	1
C(36)	3643 (11)	1637 (7)	2466 (6)	125 (5)	1
C(37)	2223 (13)	2547 (7)	3238 (7)	125 (5)	1
C(41)	-94 (22)	2576 (11)	1719 (10)	96 (9)	0.55 (2)
C(42)	1127 (21)	2518 (15)	1463 (16)	112 (11)	0.55 (2)
C(43)	1480 (25)	3072 (19)	960 (20)	119 (11)	0.55 (2)
C(44)	579 (30)	3670 (15)	692 (14)	126 (12)	0.55 (2)
C(45)	-635 (27)	3745 (15)	967 (16)	111 (12)	0.55 (2)
C(46)	-967 (24)	3208 (19)	1486 (20)	96 (9)	0.55 (2)
C(47)	-418 (36)	2016 (21)	2284 (23)	234 (27)	0.55 (2)
C(41')	799 (19)	2907 (14)	1213 (16)	75 (8)	0.45 (2)
C(42')	-342 (24)	3426 (19)	1143 (22)	131 (18)	0.45 (2)
C(43')	-1391 (23)	3237 (28)	1509 (29)	214 (29)	0.45 (2)
C(44')	-1340 (27)	2555 (26)	1929 (24)	203 (30)	0.45 (2)
C(45')	-208 (32)	2039 (24)	2003 (21)	148 (18)	0.45 (2)
C(46')	834 (22)	2213 (15)	1611 (19)	75 (9)	0.45 (2)
C(47')	1894 (32)	3076 (28)	792 (30)	145 (19)	0.45 (2)

Table 7. Bond lengths (Å) and angles (°) for **IIIa**.

Ni (1) -C (1)	1.983 (7)	Ni (1) -P (1)	2.133 (2)
Ni (1) -P (3)	2.202 (2)	Ni (1) -Cl (1)	2.231 (2)
Ni (2) -C (1)	2.036 (7)	Ni (2) -P (1)	2.103 (2)
Ni (2) -P (4)	2.195 (2)	Ni (2) -Cl (2)	2.205 (2)
C (1) -P (1)	1.707 (7)	C (1) -P (2)	1.709 (7)
P (1) -N (1)	1.684 (6)	N (1) -Si (1)	1.773 (6)
N (1) -Si (2)	1.795 (6)	Si (1) -C (13)	1.852 (8)
Si (1) -C (11)	1.862 (8)	Si (1) -C (12)	1.873 (9)
Si (2) -C (22)	1.856 (8)	Si (2) -C (23)	1.859 (8)
Si (2) -C (21)	1.861 (8)	P (2) -C (211)	1.806 (8)
P (2) -C (221)	1.806 (6)	P (2) -C (231)	1.811 (7)
C (211) -C (216)	1.374 (10)	C (211) -C (212)	1.385 (10)
C (212) -C (213)	1.391 (12)	C (213) -C (214)	1.370 (14)
C (214) -C (215)	1.358 (13)	C (215) -C (216)	1.399 (11)
C (221) -C (222)	1.368 (9)	C (221) -C (226)	1.385 (9)
C (222) -C (223)	1.390 (10)	C (223) -C (224)	1.365 (11)
C (224) -C (225)	1.389 (10)	C (225) -C (226)	1.386 (9)
C (231) -C (236)	1.383 (9)	C (231) -C (232)	1.393 (9)
C (232) -C (233)	1.393 (10)	C (233) -C (234)	1.355 (10)
C (234) -C (235)	1.388 (10)	C (235) -C (236)	1.381 (10)
P (3) -C (321)	1.836 (7)	P (3) -C (331)	1.839 (8)
P (3) -C (311)	1.847 (6)	C (311) -C (312)	1.366 (9)
C (311) -C (316)	1.410 (9)	C (312) -C (313)	1.391 (9)
C (313) -C (314)	1.391 (10)	C (314) -C (315)	1.357 (10)
C (315) -C (316)	1.393 (10)	C (321) -C (326)	1.384 (9)
C (321) -C (322)	1.394 (9)	C (322) -C (323)	1.382 (10)
C (323) -C (324)	1.385 (10)	C (324) -C (325)	1.372 (10)
C (325) -C (326)	1.381 (10)	C (331) -C (336)	1.376 (10)
C (331) -C (332)	1.385 (9)	C (332) -C (333)	1.382 (10)
C (333) -C (334)	1.376 (11)	C (334) -C (335)	1.387 (11)
C (335) -C (336)	1.387 (10)	P (4) -C (431)	1.828 (7)
P (4) -C (411)	1.836 (6)	P (4) -C (421)	1.844 (7)
C (411) -C (416)	1.369 (9)	C (411) -C (412)	1.402 (9)
C (412) -C (413)	1.396 (9)	C (413) -C (414)	1.353 (10)
C (414) -C (415)	1.387 (10)	C (415) -C (416)	1.407 (9)
C (421) -C (426)	1.366 (9)	C (421) -C (422)	1.391 (9)
C (422) -C (423)	1.382 (10)	C (423) -C (424)	1.373 (10)
C (424) -C (425)	1.375 (10)	C (425) -C (426)	1.393 (10)
C (431) -C (436)	1.391 (8)	C (431) -C (432)	1.397 (9)
C (432) -C (433)	1.371 (9)	C (433) -C (434)	1.374 (10)
C (434) -C (435)	1.396 (10)	C (435) -C (436)	1.374 (8)
C (31) -C (36)	1.364 (10)	C (31) -C (32)	1.40
C (31) -C (37)	1.463 (13)	C (32) -C (33)	1.370 (13)
C (33) -C (34)	1.38 (2)	C (34) -C (35)	1.40 (2)
C (35) -C (36)	1.383 (14)	C (41) -C (46)	1.37 (2)
C (41) -C (42)	1.38 (2)	C (41) -C (47)	1.46 (2)
C (42) -C (43)	1.39 (2)	C (43) -C (44)	1.37 (2)
C (44) -C (45)	1.38 (2)	C (45) -C (46)	1.38 (2)
C (41') -C (46')	1.36 (2)	C (41') -C (42')	1.39 (2)
C (41') -C (47')	1.46 (2)	C (42') -C (43')	1.38 (2)
C (43') -C (44')	1.36 (2)	C (44') -C (45')	1.39 (2)
C (45') -C (46')	1.39 (2)		
C (1) -Ni (1) -P (1)	48.8 (2)	C (1) -Ni (1) -P (3)	158.1 (2)

P(1)-Ni(1)-P(3)	118.28(9)	C(1)-Ni(1)-Cl(1)	101.5(2)
P(1)-Ni(1)-Cl(1)	147.54(10)	P(3)-Ni(1)-Cl(1)	94.01(9)
C(1)-Ni(2)-P(1)	48.7(2)	C(1)-Ni(2)-P(4)	162.4(2)
P(1)-Ni(2)-P(4)	113.85(9)	C(1)-Ni(2)-Cl(2)	104.2(2)
P(1)-Ni(2)-Cl(2)	152.57(9)	P(4)-Ni(2)-Cl(2)	93.41(8)
P(1)-C(1)-P(2)	144.4(4)	P(1)-C(1)-Ni(1)	70.2(3)
P(2)-C(1)-Ni(1)	126.1(4)	P(1)-C(1)-Ni(2)	67.7(2)
P(2)-C(1)-Ni(2)	131.3(4)	Ni(1)-C(1)-Ni(2)	95.0(3)
N(1)-P(1)-C(1)	127.2(3)	N(1)-P(1)-Ni(2)	137.2(2)
C(1)-P(1)-Ni(2)	63.6(2)	N(1)-P(1)-Ni(1)	133.8(2)
C(1)-P(1)-Ni(1)	61.0(2)	Ni(2)-P(1)-Ni(1)	88.80(8)
P(1)-N(1)-Si(1)	121.7(3)	P(1)-N(1)-Si(2)	119.3(3)
Si(1)-N(1)-Si(2)	118.9(3)	N(1)-Si(1)-C(13)	111.9(3)
N(1)-Si(1)-C(11)	110.1(3)	C(13)-Si(1)-C(11)	107.0(4)
N(1)-Si(1)-C(12)	110.3(3)	C(13)-Si(1)-C(12)	106.9(4)
C(11)-Si(1)-C(12)	110.6(4)	N(1)-Si(2)-C(22)	109.1(3)
N(1)-Si(2)-C(23)	112.0(3)	C(22)-Si(2)-C(23)	109.5(4)
N(1)-Si(2)-C(21)	109.9(3)	C(22)-Si(2)-C(21)	109.3(4)
C(23)-Si(2)-C(21)	106.9(4)	C(1)-P(2)-C(211)	114.0(4)
C(1)-P(2)-C(221)	112.4(3)	C(211)-P(2)-C(221)	110.7(3)
C(1)-P(2)-C(231)	112.7(3)	C(211)-P(2)-C(231)	100.3(3)
C(221)-P(2)-C(231)	105.9(3)	C(216)-C(211)-C(212)	120.5(7)
C(216)-C(211)-P(2)	120.8(6)	C(212)-C(211)-P(2)	118.5(7)
C(211)-C(212)-C(213)	119.7(9)	C(214)-C(213)-C(212)	119.3(10)
C(215)-C(214)-C(213)	121.1(9)	C(214)-C(215)-C(216)	120.3(9)
C(211)-C(216)-C(215)	118.8(9)	C(222)-C(221)-C(226)	119.4(6)
C(222)-C(221)-P(2)	122.4(6)	C(226)-C(221)-P(2)	118.2(5)
C(221)-C(222)-C(223)	120.6(7)	C(224)-C(223)-C(222)	120.1(8)
C(223)-C(224)-C(225)	120.0(7)	C(226)-C(225)-C(224)	119.6(7)
C(221)-C(226)-C(225)	120.3(7)	C(236)-C(231)-C(232)	119.2(6)
C(236)-C(231)-P(2)	123.3(5)	C(232)-C(231)-P(2)	117.3(5)
C(231)-C(232)-C(233)	119.1(7)	C(234)-C(233)-C(232)	121.5(7)
C(233)-C(234)-C(235)	119.6(7)	C(236)-C(235)-C(234)	119.9(7)
C(235)-C(236)-C(231)	120.8(7)	C(321)-P(3)-C(331)	102.1(3)
C(321)-P(3)-C(311)	106.0(3)	C(331)-P(3)-C(311)	100.1(3)
C(321)-P(3)-Ni(1)	105.8(2)	C(331)-P(3)-Ni(1)	120.5(2)
C(311)-P(3)-Ni(1)	120.3(2)	C(312)-C(311)-C(316)	120.1(6)
C(312)-C(311)-P(3)	123.3(5)	C(316)-C(311)-P(3)	116.4(5)
C(311)-C(312)-C(313)	121.4(7)	C(314)-C(313)-C(312)	118.4(7)
C(315)-C(314)-C(313)	120.6(7)	C(314)-C(315)-C(316)	121.7(7)
C(315)-C(316)-C(311)	117.8(7)	C(326)-C(321)-C(322)	118.9(7)
C(326)-C(321)-P(3)	124.0(5)	C(322)-C(321)-P(3)	117.0(5)
C(323)-C(322)-C(321)	120.6(7)	C(322)-C(323)-C(324)	119.8(7)
C(325)-C(324)-C(323)	119.5(7)	C(324)-C(325)-C(326)	121.2(7)
C(325)-C(326)-C(321)	119.9(7)	C(336)-C(331)-C(332)	118.2(7)
C(336)-C(331)-P(3)	119.2(5)	C(332)-C(331)-P(3)	122.6(6)
C(333)-C(332)-C(331)	121.1(8)	C(334)-C(333)-C(332)	120.5(8)
C(333)-C(334)-C(335)	118.8(8)	C(334)-C(335)-C(336)	120.4(8)
C(331)-C(336)-C(335)	120.9(7)	C(431)-P(4)-C(411)	102.2(3)
C(431)-P(4)-C(421)	102.2(3)	C(411)-P(4)-C(421)	103.2(3)
C(431)-P(4)-Ni(2)	117.2(2)	C(411)-P(4)-Ni(2)	114.1(2)
C(421)-P(4)-Ni(2)	115.9(2)	C(416)-C(411)-C(412)	120.0(6)
C(416)-C(411)-P(4)	118.7(5)	C(412)-C(411)-P(4)	121.3(5)
C(413)-C(412)-C(411)	118.7(7)	C(414)-C(413)-C(412)	121.5(7)
C(413)-C(414)-C(415)	120.1(7)	C(414)-C(415)-C(416)	119.3(7)
C(411)-C(416)-C(415)	120.3(6)	C(426)-C(421)-C(422)	118.7(7)
C(426)-C(421)-P(4)	123.0(6)	C(422)-C(421)-P(4)	118.3(5)
C(423)-C(422)-C(421)	119.7(7)	C(424)-C(423)-C(422)	121.7(8)
C(423)-C(424)-C(425)	118.5(7)	C(424)-C(425)-C(426)	120.2(7)

C(421)-C(426)-C(425)	121.2(7)	C(436)-C(431)-C(432)	117.1(6)
C(436)-C(431)-P(4)	119.0(5)	C(432)-C(431)-P(4)	123.9(5)
C(433)-C(432)-C(431)	121.8(6)	C(432)-C(433)-C(434)	120.5(7)
C(433)-C(434)-C(435)	118.8(7)	C(436)-C(435)-C(434)	120.4(6)
C(435)-C(436)-C(431)	121.3(6)	C(36)-C(31)-C(32)	120.6(6)
C(36)-C(31)-C(37)	121.1(6)	C(32)-C(31)-C(37)	118.3(5)
C(33)-C(32)-C(31)	118.3(8)	C(32)-C(33)-C(34)	121.5(12)
C(33)-C(34)-C(35)	120.2(12)	C(36)-C(35)-C(34)	117.7(13)
C(31)-C(36)-C(35)	121.6(12)	C(46)-C(41)-C(42)	119.0(11)
C(46)-C(41)-C(47)	120.6(12)	C(42)-C(41)-C(47)	120.0(12)
C(41)-C(42)-C(43)	121.5(14)	C(44)-C(43)-C(42)	119(2)
C(43)-C(44)-C(45)	119.4(14)	C(44)-C(45)-C(46)	121.0(14)
C(41)-C(46)-C(45)	119.8(14)	C(46')-C(41')-C(42')	119.1(11)
C(46')-C(41')-C(47')	121.5(12)	C(42')-C(41')-C(47')	119.1(12)
C(43')-C(42')-C(41')	119(2)	C(44')-C(43')-C(42')	122(2)
C(43')-C(44')-C(45')	120(2)	C(44')-C(45')-C(46')	118(2)
C(41')-C(46')-C(45')	122(2)		

Symmetry transformations used to generate equivalent atoms:

Table 8. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for IIIa.

	U11	U22	U33	U23	U13	U12
Ni (1)	18 (1)	25 (1)	31 (1)	-3 (1)	-5 (1)	5 (1)
Ni (2)	11 (1)	26 (1)	29 (1)	0 (1)	-5 (1)	2 (1)
Cl (1)	40 (1)	31 (1)	50 (1)	6 (1)	-5 (1)	6 (1)
Cl (2)	14 (1)	42 (1)	43 (1)	7 (1)	-7 (1)	-4 (1)
C (1)	11 (3)	23 (4)	32 (4)	1 (3)	-9 (3)	1 (3)
P (1)	13 (1)	26 (1)	25 (1)	-1 (1)	-4 (1)	1 (1)
N (1)	13 (3)	32 (4)	34 (4)	-4 (3)	-2 (3)	-1 (3)
Si (1)	20 (1)	31 (1)	37 (1)	-6 (1)	-3 (1)	-3 (1)
C (11)	33 (5)	44 (5)	42 (5)	-12 (4)	6 (4)	-7 (4)
C (12)	58 (6)	30 (5)	47 (5)	-11 (4)	-12 (5)	4 (4)
C (13)	29 (4)	40 (5)	44 (5)	-7 (4)	-2 (4)	-1 (4)
Si (2)	14 (1)	39 (1)	34 (1)	-3 (1)	-4 (1)	0 (1)
C (21)	17 (4)	66 (6)	47 (5)	-11 (5)	3 (4)	-3 (4)
C (22)	27 (4)	40 (5)	39 (5)	6 (4)	-9 (4)	3 (4)
C (23)	25 (4)	37 (5)	58 (6)	4 (4)	-11 (4)	7 (4)
P (2)	18 (1)	27 (1)	30 (1)	3 (1)	-3 (1)	2 (1)
C (211)	19 (4)	37 (5)	54 (6)	14 (4)	-3 (4)	-1 (4)
C (212)	38 (5)	50 (6)	84 (8)	20 (5)	16 (5)	1 (5)
C (213)	33 (6)	73 (9)	151 (14)	54 (9)	34 (7)	3 (6)
C (214)	28 (6)	60 (8)	201 (18)	63 (10)	-18 (9)	-14 (6)
C (215)	39 (6)	36 (6)	148 (12)	21 (7)	-46 (7)	-8 (5)
C (216)	33 (5)	23 (5)	102 (8)	6 (5)	-29 (5)	-1 (4)
C (221)	20 (4)	33 (4)	29 (4)	0 (4)	-4 (3)	6 (3)
C (222)	44 (5)	45 (5)	59 (6)	13 (5)	-24 (5)	-14 (4)
C (223)	75 (8)	47 (6)	58 (7)	18 (5)	-31 (6)	0 (5)
C (224)	42 (6)	64 (6)	50 (6)	1 (5)	-28 (5)	10 (5)
C (225)	30 (5)	67 (6)	53 (6)	12 (5)	-22 (4)	2 (4)
C (226)	27 (5)	50 (5)	37 (5)	9 (4)	-8 (4)	2 (4)
C (231)	22 (4)	31 (4)	25 (4)	-2 (3)	5 (3)	-1 (3)
C (232)	29 (5)	39 (5)	46 (5)	-4 (4)	-6 (4)	9 (4)
C (233)	35 (5)	45 (5)	61 (6)	-7 (5)	-5 (5)	10 (4)
C (234)	47 (6)	58 (6)	52 (6)	-29 (5)	9 (5)	8 (5)
C (235)	52 (6)	62 (6)	45 (6)	-16 (5)	-1 (5)	-1 (5)
C (236)	32 (5)	46 (5)	32 (5)	1 (4)	-4 (4)	6 (4)
P (3)	22 (1)	27 (1)	31 (1)	-4 (1)	-5 (1)	6 (1)
C (311)	19 (4)	30 (4)	39 (5)	-5 (4)	-4 (4)	12 (3)
C (312)	26 (4)	41 (5)	46 (5)	-8 (4)	-4 (4)	6 (4)
C (313)	33 (5)	56 (6)	57 (6)	-13 (5)	-4 (4)	14 (4)
C (314)	29 (5)	59 (6)	72 (7)	-10 (5)	-14 (5)	26 (4)
C (315)	42 (6)	71 (7)	45 (6)	-6 (5)	-6 (5)	15 (5)
C (316)	33 (5)	39 (5)	36 (5)	0 (4)	-7 (4)	15 (4)
C (321)	26 (4)	24 (4)	33 (4)	-3 (3)	-5 (3)	5 (3)
C (322)	39 (5)	35 (5)	53 (6)	-16 (4)	-8 (4)	1 (4)
C (323)	32 (5)	37 (5)	65 (6)	-6 (4)	-11 (4)	4 (4)
C (324)	36 (5)	53 (6)	59 (6)	-10 (5)	-9 (4)	-14 (4)
C (325)	52 (6)	37 (5)	63 (6)	-23 (5)	-6 (5)	-12 (4)
C (326)	30 (5)	45 (5)	48 (5)	-14 (4)	4 (4)	-1 (4)

C(331)	24(4)	28(4)	39(5)	-13(4)	-2(4)	12(3)
C(332)	38(5)	54(6)	37(5)	3(4)	-9(4)	4(4)
C(333)	50(6)	62(6)	45(6)	10(5)	-11(5)	6(5)
C(334)	77(8)	45(6)	40(6)	8(4)	5(5)	11(5)
C(335)	47(5)	45(5)	44(6)	3(4)	9(4)	-4(4)
C(336)	42(5)	41(5)	36(5)	-8(4)	-2(4)	-2(4)
P(4)	16(1)	25(1)	27(1)	-1(1)	-5(1)	2(1)
C(411)	11(3)	32(4)	26(4)	8(3)	-5(3)	3(3)
C(412)	17(4)	51(5)	43(5)	6(4)	2(4)	3(4)
C(413)	27(5)	44(5)	51(6)	12(4)	-3(4)	10(4)
C(414)	22(4)	31(5)	66(6)	13(4)	-2(4)	11(4)
C(415)	32(5)	38(5)	55(6)	-9(4)	8(4)	1(4)
C(416)	19(4)	36(4)	36(5)	-6(4)	-2(3)	-2(3)
C(421)	24(4)	22(4)	33(5)	-1(3)	-12(3)	9(3)
C(422)	50(5)	47(5)	34(5)	-5(4)	-7(4)	-16(4)
C(423)	65(7)	48(6)	48(6)	-5(5)	-14(5)	-10(5)
C(424)	51(6)	43(5)	44(6)	-17(4)	-20(5)	12(5)
C(425)	51(6)	47(5)	27(5)	-7(4)	-3(4)	9(5)
C(426)	39(5)	42(5)	30(5)	-2(4)	-8(4)	1(4)
C(431)	22(4)	26(4)	22(4)	0(3)	-1(3)	-4(3)
C(432)	24(4)	35(5)	38(5)	-1(4)	-1(4)	3(4)
C(433)	33(5)	31(5)	57(6)	7(4)	-8(4)	-2(4)
C(434)	31(5)	48(6)	50(6)	8(4)	-4(4)	-13(4)
C(435)	22(4)	50(5)	36(5)	4(4)	4(4)	-5(4)
C(436)	16(4)	34(4)	43(5)	0(4)	-2(3)	5(3)
C(31)	72(7)	113(9)	58(7)	12(6)	-20(5)	3(6)
C(32)	100(10)	178(12)	84(10)	48(9)	-27(7)	-34(9)
C(33)	87(12)	366(25)	117(17)	139(16)	-7(9)	-3(15)
C(34)	110(14)	434(32)	79(13)	93(16)	5(11)	145(15)
C(35)	200(22)	286(20)	68(12)	4(14)	-42(11)	168(15)
C(36)	112(10)	133(9)	104(11)	-19(8)	-71(8)	64(8)
C(37)	130(12)	142(14)	95(11)	-13(9)	20(8)	-16(10)
C(41)	159(21)	51(13)	82(18)	-16(10)	-58(16)	-11(13)
C(42)	120(18)	58(24)	161(36)	-11(14)	-100(19)	6(17)
C(43)	154(26)	114(29)	102(36)	-58(16)	-33(22)	-34(21)
C(44)	233(35)	71(18)	94(23)	-6(15)	-60(22)	-64(21)
C(45)	195(29)	51(17)	88(21)	-30(11)	-94(21)	10(17)
C(46)	118(19)	72(20)	98(25)	-48(13)	-50(17)	13(15)
C(47)	367(58)	86(29)	232(59)	44(28)	30(46)	-31(36)
C(41')	92(17)	57(18)	82(26)	-13(13)	-34(16)	-16(13)
C(42')	157(27)	66(33)	168(70)	-39(23)	-120(32)	29(26)
C(43')	80(19)	198(55)	378(91)	-191(50)	-67(28)	14(25)
C(44')	118(21)	264(61)	274(68)	-212(48)	97(36)	-122(29)
C(45')	179(31)	191(45)	120(33)	-28(27)	-12(26)	-148(31)
C(46')	71(15)	54(20)	109(25)	-4(15)	-46(15)	-19(13)
C(47')	208(35)	181(49)	76(28)	-31(30)	22(31)	-113(34)

Table 9. Torsion angles (°) for **IIIa**.

P(1)-Ni(1)-C(1)-P(1)	0.0	P(3)-Ni(1)-C(1)-P(1)	60.7(6)
Cl(1)-Ni(1)-C(1)-P(1)	-165.0(2)	P(1)-Ni(1)-C(1)-P(2)	143.8(5)
P(3)-Ni(1)-C(1)-P(2)	-155.5(3)	Cl(1)-Ni(1)-C(1)-P(2)	-21.2(4)
P(1)-Ni(1)-C(1)-Ni(2)	-64.1(2)	P(3)-Ni(1)-C(1)-Ni(2)	-3.4(7)
Cl(1)-Ni(1)-C(1)-Ni(2)	130.9(2)	P(1)-Ni(2)-C(1)-P(1)	0.0
P(4)-Ni(2)-C(1)-P(1)	6.4(8)	Cl(2)-Ni(2)-C(1)-P(1)	-175.8(2)
P(1)-Ni(2)-C(1)-P(2)	-144.1(6)	P(4)-Ni(2)-C(1)-P(2)	-137.7(5)
Cl(2)-Ni(2)-C(1)-P(2)	40.1(5)	P(1)-Ni(2)-C(1)-Ni(1)	66.2(2)
P(4)-Ni(2)-C(1)-Ni(1)	72.5(7)	Cl(2)-Ni(2)-C(1)-Ni(1)	-109.6(2)
P(2)-C(1)-P(1)-N(1)	0.1(9)	Ni(1)-C(1)-P(1)-N(1)	124.9(3)
Ni(2)-C(1)-P(1)-N(1)	-130.7(3)	P(2)-C(1)-P(1)-Ni(2)	130.8(7)
Ni(1)-C(1)-P(1)-Ni(2)	-104.4(2)	Ni(2)-C(1)-P(1)-Ni(2)	0.0
P(2)-C(1)-P(1)-Ni(1)	-124.8(7)	Ni(1)-C(1)-P(1)-Ni(1)	0.0
Ni(2)-C(1)-P(1)-Ni(1)	104.4(2)	C(1)-Ni(2)-P(1)-N(1)	117.3(4)
P(4)-Ni(2)-P(1)-N(1)	-60.6(3)	Cl(2)-Ni(2)-P(1)-N(1)	126.1(4)
C(1)-Ni(2)-P(1)-C(1)	0.0	P(4)-Ni(2)-P(1)-C(1)	-177.9(3)
Cl(2)-Ni(2)-P(1)-C(1)	8.9(3)	C(1)-Ni(2)-P(1)-Ni(1)	-57.9(3)
P(4)-Ni(2)-P(1)-Ni(1)	124.18(9)	Cl(2)-Ni(2)-P(1)-Ni(1)	-49.0(2)
C(1)-Ni(1)-P(1)-N(1)	-115.2(4)	P(3)-Ni(1)-P(1)-N(1)	86.4(3)
Cl(1)-Ni(1)-P(1)-N(1)	-87.1(4)	C(1)-Ni(1)-P(1)-C(1)	0.0
P(3)-Ni(1)-P(1)-C(1)	-158.3(3)	Cl(1)-Ni(1)-P(1)-C(1)	28.2(3)
C(1)-Ni(1)-P(1)-Ni(2)	60.2(2)	P(3)-Ni(1)-P(1)-Ni(2)	-98.12(10)
Cl(1)-Ni(1)-P(1)-Ni(2)	88.4(2)	C(1)-P(1)-N(1)-Si(1)	73.2(5)
Ni(2)-P(1)-N(1)-Si(1)	-16.7(6)	Ni(1)-P(1)-N(1)-Si(1)	156.6(2)
C(1)-P(1)-N(1)-Si(2)	-109.9(4)	Ni(2)-P(1)-N(1)-Si(2)	160.2(2)
Ni(1)-P(1)-N(1)-Si(2)	-26.5(5)	P(1)-N(1)-Si(1)-C(13)	9.6(5)
Si(2)-N(1)-Si(1)-C(13)	-167.3(4)	P(1)-N(1)-Si(1)-C(11)	-109.2(4)
Si(2)-N(1)-Si(1)-C(11)	73.9(5)	P(1)-N(1)-Si(1)-C(12)	128.5(4)
Si(2)-N(1)-Si(1)-C(12)	-48.4(5)	P(1)-N(1)-Si(2)-C(22)	-92.0(5)
Si(1)-N(1)-Si(2)-C(22)	85.0(4)	P(1)-N(1)-Si(2)-C(23)	29.5(5)
Si(1)-N(1)-Si(2)-C(23)	-153.5(4)	P(1)-N(1)-Si(2)-C(21)	148.1(4)
Si(1)-N(1)-Si(2)-C(21)	-34.9(5)	P(1)-C(1)-P(2)-C(211)	-174.8(6)
Ni(1)-C(1)-P(2)-C(211)	78.0(5)	Ni(2)-C(1)-P(2)-C(211)	-63.7(6)
P(1)-C(1)-P(2)-C(221)	58.2(8)	Ni(1)-C(1)-P(2)-C(221)	-49.1(5)
Ni(2)-C(1)-P(2)-C(221)	169.3(4)	P(1)-C(1)-P(2)-C(231)	-61.4(7)

Ni (1) -C (1) -P (2) -C (231)	-168.6 (4)	Ni (2) -C (1) -P (2) -C (231)	49.7 (6)
C (1) -P (2) -C (211) -C (216)	-12.6 (8)	C (221) -P (2) -C (211) -C (216)	115.3 (7)
C (231) -P (2) -C (211) -C (216)	-133.2 (6)	C (1) -P (2) -C (211) -C (212)	162.6 (6)
C (221) -P (2) -C (211) -C (212)	-69.5 (7)	C (231) -P (2) -C (211) -C (212)	42.0 (7)
C (216) -C (211) -C (212) -C (213)	1.6 (13)	P (2) -C (211) -C (212) -C (213)	-173.6 (7)
C (211) -C (212) -C (213) -C (214)	3 (2)	C (212) -C (213) -C (214) -C (215)	-4 (2)
C (213) -C (214) -C (215) -C (216)	1 (2)	C (212) -C (211) -C (216) -C (215)	-4.5 (12)
P (2) -C (211) -C (216) -C (215)	170.6 (6)	C (214) -C (215) -C (216) -C (211)	3.2 (13)
C (1) -P (2) -C (221) -C (222)	139.6 (7)	C (211) -P (2) -C (221) -C (222)	10.8 (8)
C (231) -P (2) -C (221) -C (222)	-97.0 (7)	C (1) -P (2) -C (221) -C (226)	-42.8 (7)
C (211) -P (2) -C (221) -C (226)	-171.5 (6)	C (231) -P (2) -C (221) -C (226)	80.7 (7)
C (226) -C (221) -C (222) -C (223)	0.3 (13)	P (2) -C (221) -C (222) -C (223)	177.9 (7)
C (221) -C (222) -C (223) -C (224)	-1 (2)	C (222) -C (223) -C (224) -C (225)	2 (2)
C (223) -C (224) -C (225) -C (226)	-1 (2)	C (222) -C (221) -C (226) -C (225)	0.3 (13)
P (2) -C (221) -C (226) -C (225)	-177.4 (7)	C (224) -C (225) -C (226) -C (221)	0.0 (14)
C (1) -P (2) -C (231) -C (236)	121.8 (7)	C (211) -P (2) -C (231) -C (236)	-116.6 (7)
C (221) -P (2) -C (231) -C (236)	-1.4 (8)	C (1) -P (2) -C (231) -C (232)	-63.8 (7)
C (211) -P (2) -C (231) -C (232)	57.8 (7)	C (221) -P (2) -C (231) -C (232)	173.0 (6)
C (236) -C (231) -C (232) -C (233)	0.6 (12)	P (2) -C (231) -C (232) -C (233)	-174.0 (7)
C (231) -C (232) -C (233) -C (234)	0.1 (14)	C (232) -C (233) -C (234) -C (235)	-1 (2)
C (233) -C (234) -C (235) -C (236)	1 (2)	C (234) -C (235) -C (236) -C (231)	-0.3 (14)
C (232) -C (231) -C (236) -C (235)	-0.5 (12)	P (2) -C (231) -C (236) -C (235)	173.8 (7)
C (1) -Ni (1) -P (3) -C (321)	74.5 (6)	P (1) -Ni (1) -P (3) -C (321)	122.7 (2)
Cl (1) -Ni (1) -P (3) -C (321)	-60.7 (2)	C (1) -Ni (1) -P (3) -C (331)	-40.3 (6)
P (1) -Ni (1) -P (3) -C (331)	7.9 (3)	Cl (1) -Ni (1) -P (3) -C (331)	-175.6 (3)
C (1) -Ni (1) -P (3) -C (311)	-165.6 (6)	P (1) -Ni (1) -P (3) -C (311)	-117.4 (3)
Cl (1) -Ni (1) -P (3) -C (311)	59.1 (3)	C (321) -P (3) -C (311) -C (312)	-73.8 (8)
C (331) -P (3) -C (311) -C (312)	32.0 (8)	Ni (1) -P (3) -C (311) -C (312)	166.5 (6)
C (321) -P (3) -C (311) -C (316)	110.8 (7)	C (331) -P (3) -C (311) -C (316)	-143.3 (6)
Ni (1) -P (3) -C (311) -C (316)	-8.9 (8)	C (316) -C (311) -C (312) -C (313)	-1.6 (13)
P (3) -C (311) -C (312) -C (313)	-176.8 (7)	C (311) -C (312) -C (313) -C (314)	1.0 (14)
C (312) -C (313) -C (314) -C (315)	0 (2)	C (313) -C (314) -C (315) -C (316)	-1 (2)
C (314) -C (315) -C (316) -C (311)	0 (2)	C (312) -C (311) -C (316) -C (315)	1.0 (13)
P (3) -C (311) -C (316) -C (315)	176.5 (7)	C (331) -P (3) -C (321) -C (326)	-83.9 (7)
C (311) -P (3) -C (321) -C (326)	20.5 (8)	Ni (1) -P (3) -C (321) -C (326)	149.3 (6)
C (331) -P (3) -C (321) -C (322)	96.0 (7)	C (311) -P (3) -C (321) -C (322)	-159.7 (6)
Ni (1) -P (3) -C (321) -C (322)	-30.9 (7)	C (326) -C (321) -C (322) -C (323)	3.1 (12)
P (3) -C (321) -C (322) -C (323)	-176.8 (7)	C (321) -C (322) -C (323) -C (324)	-1.9 (13)
C (322) -C (323) -C (324) -C (325)	0.3 (14)	C (323) -C (324) -C (325) -C (326)	0.1 (14)

C(324)-C(325)-C(326)-C(321)	1.1(14)	C(322)-C(321)-C(326)-C(325)	-2.6(12)
P(3)-C(321)-C(326)-C(325)	177.2(7)	C(321)-P(3)-C(331)-C(336)	164.5(6)
C(311)-P(3)-C(331)-C(336)	55.5(6)	Ni(1)-P(3)-C(331)-C(336)	-78.9(6)
C(321)-P(3)-C(331)-C(332)	-17.5(7)	C(311)-P(3)-C(331)-C(332)	-126.5(7)
Ni(1)-P(3)-C(331)-C(332)	99.1(6)	C(336)-C(331)-C(332)-C(333)	-1.7(12)
P(3)-C(331)-C(332)-C(333)	-179.7(7)	C(331)-C(332)-C(333)-C(334)	1.1(14)
C(332)-C(333)-C(334)-C(335)	0.2(14)	C(333)-C(334)-C(335)-C(336)	-0.8(13)
C(332)-C(331)-C(336)-C(335)	1.0(12)	P(3)-C(331)-C(336)-C(335)	179.1(6)
C(334)-C(335)-C(336)-C(331)	0.2(13)	C(1)-Ni(2)-P(4)-C(431)	8.1(8)
P(1)-Ni(2)-P(4)-C(431)	13.4(3)	Cl(2)-Ni(2)-P(4)-C(431)	-169.7(3)
C(1)-Ni(2)-P(4)-C(411)	127.5(7)	P(1)-Ni(2)-P(4)-C(411)	132.8(3)
Cl(2)-Ni(2)-P(4)-C(411)	-50.4(3)	C(1)-Ni(2)-P(4)-C(421)	-112.8(7)
P(1)-Ni(2)-P(4)-C(421)	-107.6(3)	Cl(2)-Ni(2)-P(4)-C(421)	69.3(3)
C(431)-P(4)-C(411)-C(416)	100.9(6)	C(421)-P(4)-C(411)-C(416)	-153.3(6)
Ni(2)-P(4)-C(411)-C(416)	-26.7(7)	C(431)-P(4)-C(411)-C(412)	-76.6(7)
C(421)-P(4)-C(411)-C(412)	29.3(7)	Ni(2)-P(4)-C(411)-C(412)	155.9(6)
C(416)-C(411)-C(412)-C(413)	-1.6(12)	P(4)-C(411)-C(412)-C(413)	175.8(6)
C(411)-C(412)-C(413)-C(414)	-0.6(13)	C(412)-C(413)-C(414)-C(415)	2.3(13)
C(413)-C(414)-C(415)-C(416)	-1.7(13)	C(412)-C(411)-C(416)-C(415)	2.1(11)
P(4)-C(411)-C(416)-C(415)	-175.4(6)	C(414)-C(415)-C(416)-C(411)	-0.5(12)
C(431)-P(4)-C(421)-C(426)	9.5(7)	C(411)-P(4)-C(421)-C(426)	-96.4(6)
Ni(2)-P(4)-C(421)-C(426)	138.2(5)	C(431)-P(4)-C(421)-C(422)	-172.5(6)
C(411)-P(4)-C(421)-C(422)	81.6(6)	Ni(2)-P(4)-C(421)-C(422)	-43.8(6)
C(426)-C(421)-C(422)-C(423)	-0.4(12)	P(4)-C(421)-C(422)-C(423)	-178.5(7)
C(421)-C(422)-C(423)-C(424)	0.5(13)	C(422)-C(423)-C(424)-C(425)	-0.6(13)
C(423)-C(424)-C(425)-C(426)	0.7(12)	C(422)-C(421)-C(426)-C(425)	0.5(11)
P(4)-C(421)-C(426)-C(425)	178.5(6)	C(424)-C(425)-C(426)-C(421)	-0.7(12)
C(411)-P(4)-C(431)-C(436)	-177.9(5)	C(421)-P(4)-C(431)-C(436)	75.5(6)
Ni(2)-P(4)-C(431)-C(436)	-52.4(6)	C(411)-P(4)-C(431)-C(432)	1.8(7)
C(421)-P(4)-C(431)-C(432)	-104.8(6)	Ni(2)-P(4)-C(431)-C(432)	127.3(6)
C(436)-C(431)-C(432)-C(433)	-0.8(11)	P(4)-C(431)-C(432)-C(433)	179.4(6)
C(431)-C(432)-C(433)-C(434)	-0.1(13)	C(432)-C(433)-C(434)-C(435)	0.8(13)
C(433)-C(434)-C(435)-C(436)	-0.5(12)	C(434)-C(435)-C(436)-C(431)	-0.4(11)
C(432)-C(431)-C(436)-C(435)	1.1(10)	P(4)-C(431)-C(436)-C(435)	-179.1(5)
C(36)-C(31)-C(32)-C(33)	0.7(9)	C(37)-C(31)-C(32)-C(33)	-178.7(11)
C(31)-C(32)-C(33)-C(34)	3(2)	C(32)-C(33)-C(34)-C(35)	-4(4)
C(33)-C(34)-C(35)-C(36)	1(4)	C(32)-C(31)-C(36)-C(35)	-3(2)
C(37)-C(31)-C(36)-C(35)	176.5(13)	C(34)-C(35)-C(36)-C(31)	2(3)
C(46)-C(41)-C(42)-C(43)	-2(3)	C(47)-C(41)-C(42)-C(43)	-176(3)

C(41)-C(42)-C(43)-C(44)	-3(3)	C(42)-C(43)-C(44)-C(45)	5(5)
C(43)-C(44)-C(45)-C(46)	-3(5)	C(42)-C(41)-C(46)-C(45)	4(5)
C(47)-C(41)-C(46)-C(45)	178(4)	C(44)-C(45)-C(46)-C(41)	-2(6)
C(46')-C(41')-C(42')-C(43')	3(3)	C(47')-C(41')-C(42')-C(43')	176(4)
C(41')-C(42')-C(43')-C(44')	-1(4)	C(42')-C(43')-C(44')-C(45')	1(7)
C(43')-C(44')-C(45')-C(46')	-4(7)	C(42')-C(41')-C(46')-C(45')	-6(5)
C(47')-C(41')-C(46')-C(45')	-179(5)	C(44')-C(45')-C(46')-C(41')	6(6)

Symmetry transformations used to generate equivalent atoms:

Table 10. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **IIIa**.

	x	y	z	U(eq)
H(11A)	1699 (45)	5140 (8)	661 (7)	59
H(11B)	1870 (39)	6042 (23)	557 (5)	59
H(11C)	521 (9)	5837 (30)	727 (5)	59
H(12A)	1182 (39)	4404 (7)	2109 (20)	68
H(12B)	-38 (10)	5056 (19)	2239 (24)	68
H(12C)	1033 (44)	4917 (23)	2787 (7)	68
H(13A)	3646 (11)	4907 (16)	1686 (24)	57
H(13B)	3472 (8)	5343 (30)	2409 (4)	57
H(13C)	3749 (9)	5820 (15)	1691 (24)	57
H(21A)	-2321 (7)	6693 (28)	1549 (18)	65
H(21B)	-1179 (41)	5970 (6)	1502 (19)	65
H(21C)	-1162 (40)	6759 (26)	1018 (5)	65
H(22A)	-2111 (9)	6762 (26)	3119 (11)	55
H(22B)	-816 (36)	6817 (24)	3432 (4)	55
H(22C)	-999 (41)	6019 (5)	3102 (11)	55
H(23A)	-781 (41)	8311 (5)	2464 (17)	63
H(23B)	-2039 (7)	8211 (5)	2132 (29)	63
H(23C)	-834 (43)	8264 (6)	1634 (12)	63
H(212)	4946 (8)	8327 (5)	-228 (5)	72
H(213)	6622 (9)	9010 (7)	-364 (7)	110
H(214)	7251 (9)	9559 (7)	606 (8)	117
H(215)	6113 (9)	9575 (5)	1662 (7)	88
H(216)	4323 (7)	8991 (5)	1783 (5)	63
H(222)	2775 (8)	9215 (5)	-193 (5)	58
H(223)	1070 (9)	9705 (5)	-879 (5)	74
H(224)	-698 (8)	9141 (5)	-742 (5)	65
H(225)	-815 (7)	8121 (5)	123 (5)	62
H(226)	880 (7)	7649 (5)	821 (4)	47
H(232)	5515 (7)	6862 (5)	1159 (4)	48
H(233)	6677 (7)	5788 (5)	571 (5)	59
H(234)	5997 (8)	5371 (5)	-437 (5)	65
H(235)	4084 (8)	6002 (5)	-870 (5)	64
H(236)	2909 (7)	7074 (5)	-298 (4)	46
H(312)	-1025 (7)	9822 (5)	4400 (4)	47
H(313)	-2944 (7)	10690 (5)	4332 (5)	61
H(314)	-3680 (8)	11143 (5)	3217 (5)	68
H(315)	-2542 (8)	10740 (6)	2212 (4)	67
H(316)	-601 (7)	9888 (5)	2267 (4)	46
H(322)	3500 (7)	8846 (5)	3257 (4)	51
H(323)	5052 (7)	9418 (5)	3690 (5)	55
H(324)	4512 (7)	10554 (5)	4345 (5)	58
H(325)	2431 (8)	11085 (5)	4577 (5)	59
H(326)	872 (7)	10512 (5)	4160 (4)	49
H(332)	2071 (7)	8491 (5)	4697 (4)	53
H(333)	1627 (8)	7685 (6)	5669 (5)	66
H(334)	-137 (9)	7101 (5)	5714 (4)	69
H(335)	-1450 (8)	7336 (5)	4766 (4)	56
H(336)	-1019 (7)	8164 (5)	3803 (4)	48

H(412)	6231 (6)	5475 (5)	4439 (4)	46
H(413)	8017 (7)	4507 (5)	4242 (4)	52
H(414)	8605 (7)	4080 (5)	3134 (4)	51
H(415)	7500 (7)	4671 (5)	2162 (4)	51
H(416)	5716 (6)	5662 (4)	2340 (4)	36
H(422)	5538 (8)	7639 (5)	3825 (4)	51
H(423)	5893 (9)	8260 (5)	4824 (4)	64
H(424)	5161 (8)	7863 (5)	5935 (4)	56
H(425)	4011 (8)	6841 (5)	6037 (4)	52
H(426)	3653 (7)	6210 (5)	5037 (4)	45
H(432)	4391 (6)	4647 (4)	3869 (4)	40
H(433)	2958 (7)	3878 (4)	4279 (5)	49
H(434)	889 (7)	4461 (5)	4517 (4)	51
H(435)	271 (7)	5840 (4)	4309 (4)	44
H(436)	1707 (5)	6610 (3)	3889 (3)	39
H(32)	3846 (5)	3447 (3)	2810 (3)	146
H(33)	5591 (13)	3163 (11)	2050 (8)	242
H(34)	6042 (16)	1976 (12)	1487 (10)	285
H(35)	4845 (18)	975 (10)	1774 (9)	254
H(36)	3164 (11)	1242 (7)	2595 (6)	149
H(37A)	1615 (13)	2233 (7)	3121 (7)	187
H(37B)	1864 (13)	3110 (7)	3185 (7)	187
H(37C)	2453 (13)	2414 (7)	3724 (7)	187
H(42)	1734 (21)	2094 (15)	1632 (16)	134
H(43)	2323 (25)	3038 (19)	806 (20)	143
H(44)	787 (30)	4025 (15)	325 (14)	151
H(45)	-1245 (27)	4167 (15)	798 (16)	133
H(46)	-1792 (24)	3277 (19)	1680 (20)	115
H(47A)	30 (36)	1482 (21)	2197 (23)	351
H(47B)	-1310 (36)	2023 (21)	2297 (23)	351
H(47C)	-192 (36)	2174 (21)	2735 (23)	351
H(42')	-397 (24)	3897 (19)	852 (22)	157
H(43')	-2160 (23)	3588 (28)	1467 (29)	257
H(44')	-2070 (27)	2436 (26)	2167 (24)	244
H(45')	-147 (32)	1582 (24)	2312 (21)	177
H(46')	1586 (22)	1841 (15)	1622 (19)	91
H(47D)	1705 (32)	3169 (28)	296 (30)	218
H(47E)	2582 (32)	2629 (28)	843 (30)	218
H(47F)	2125 (32)	3549 (28)	964 (30)	218

Figure 3. Fully labeled thermal ellipsoid drawing of IIIa.

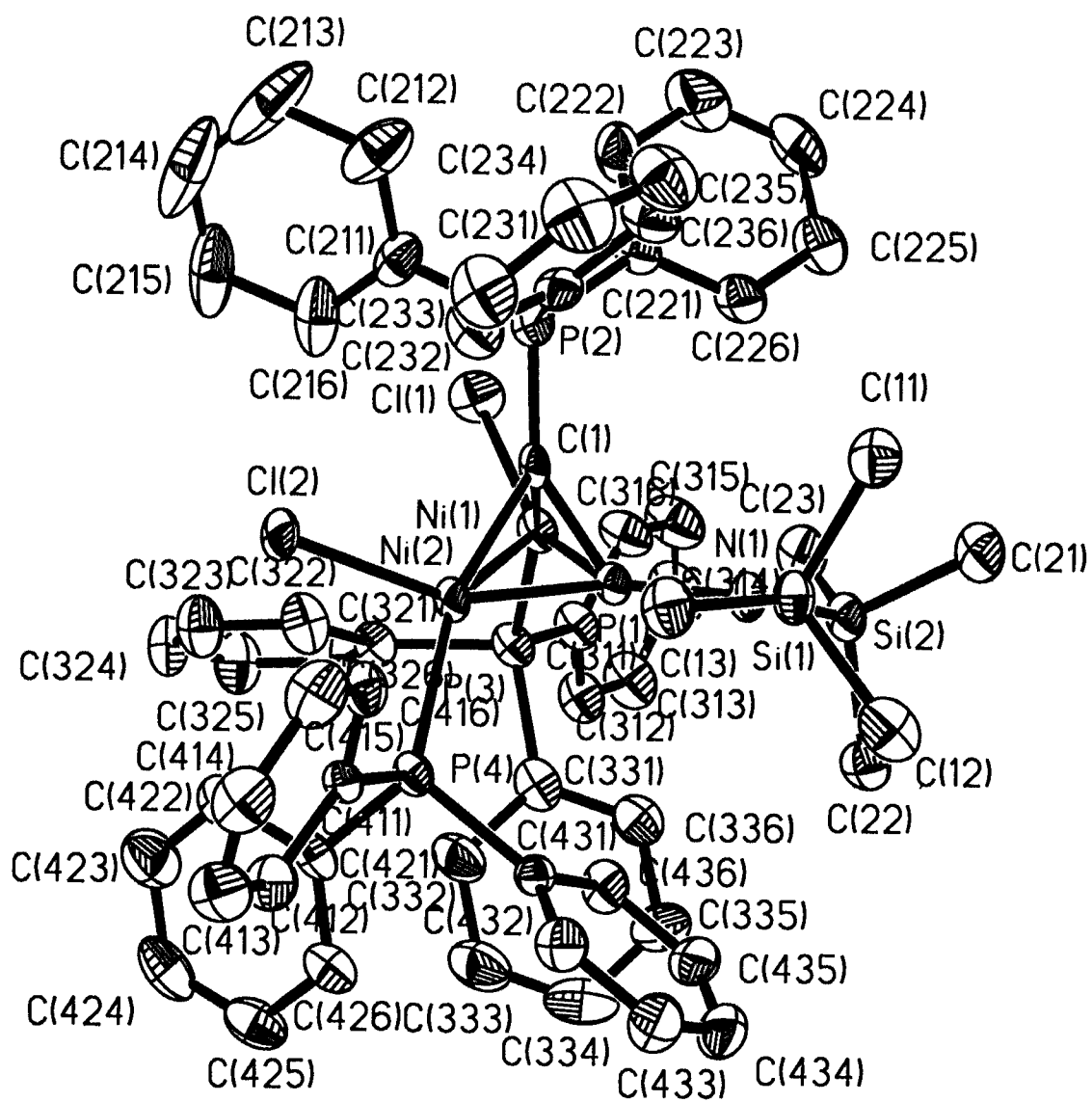


Figure 4. Unit cell and packing diagram for **IIIa**.

