Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information for:

Structure and Bonding of Group 4–Nickel Heterobimetallics Supported by 2-(diphenylphosphino)pyrrolide Ligands

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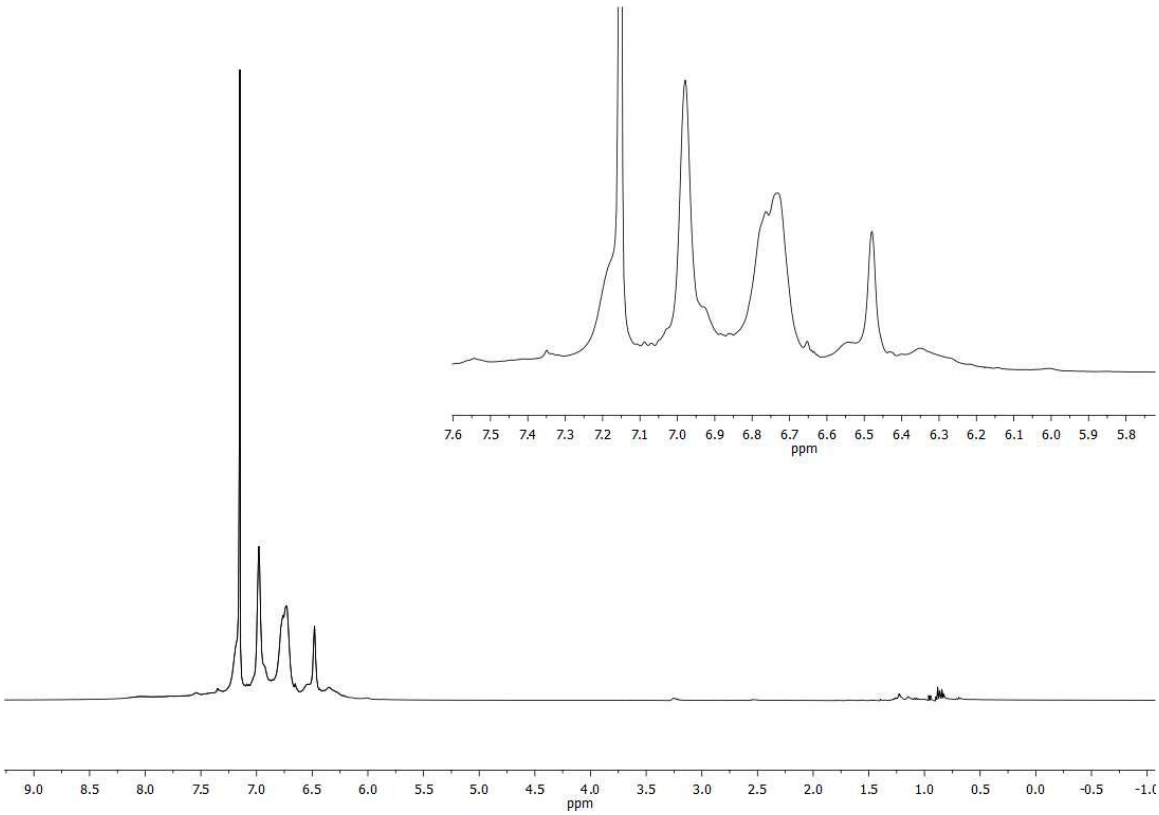

Figure 1: ^{1}H NMR of complex 3 in C_6D_6

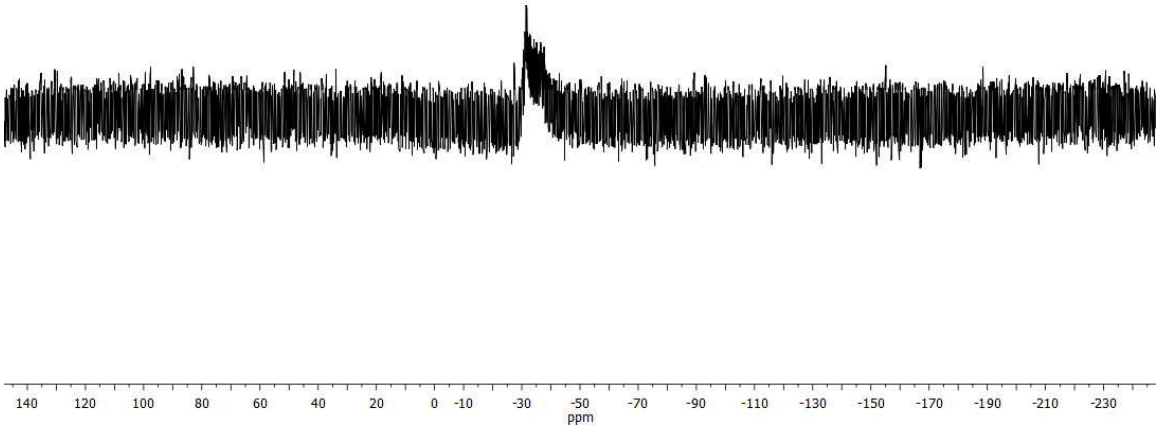

Figure 2: ^{31}P NMR of **3** in C_6D_6

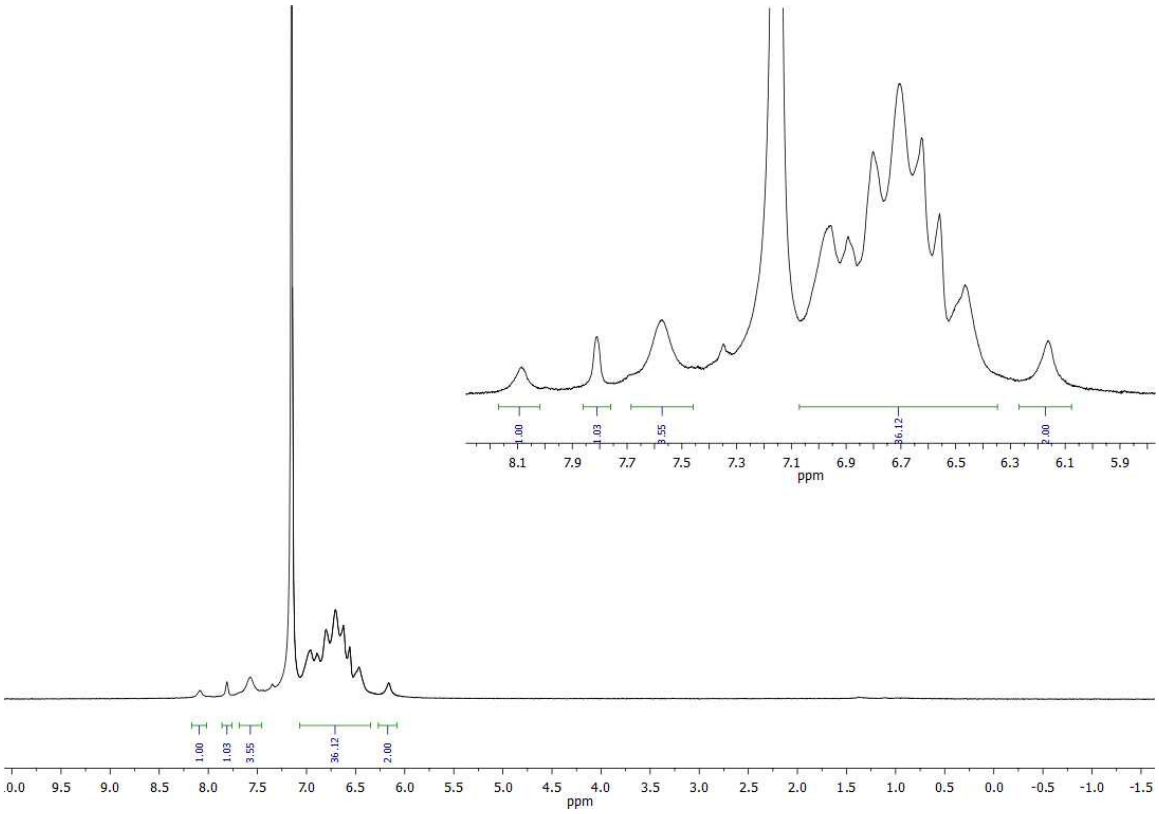

Figure 3: ^{1}H NMR of complex **4** in C_6D_6

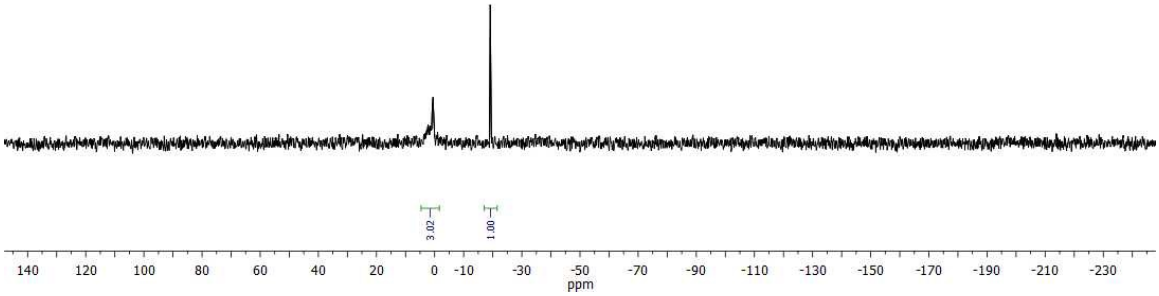

Figure 4: ^{31}P NMR of **4** in C_6D_6

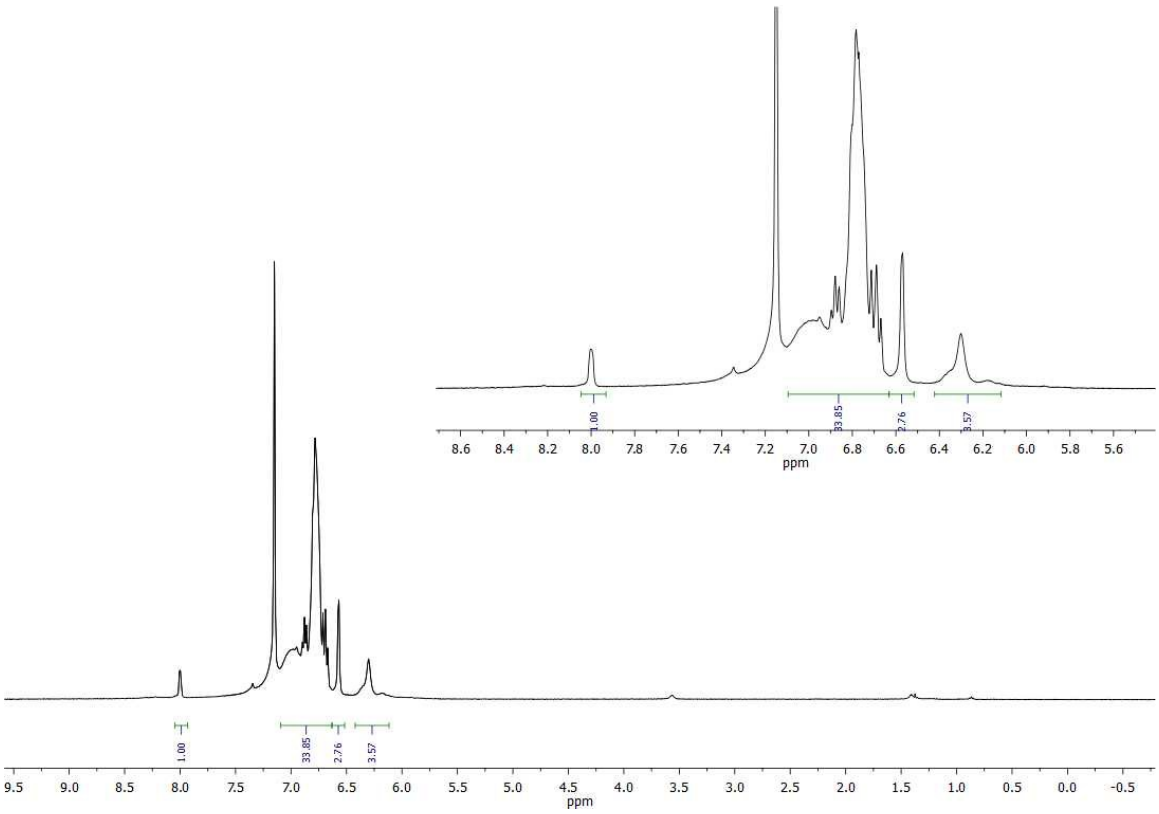

Figure 5: ^{1}H NMR of **complex** 5 in C_6D_6

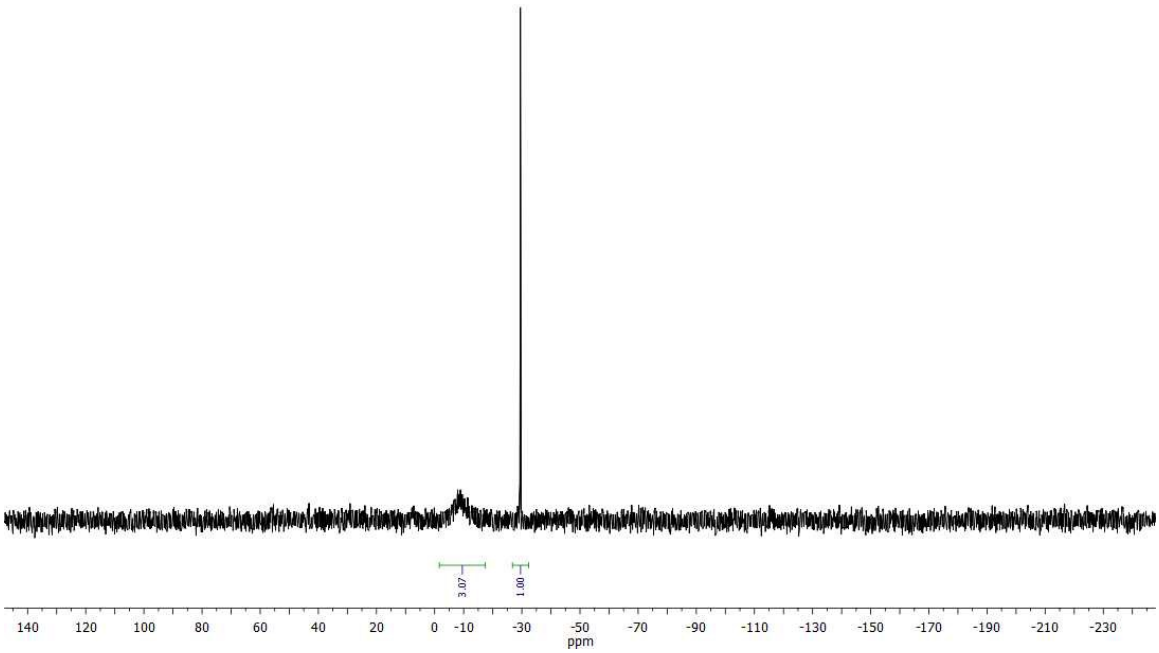

Figure 6: ^{31}P NMR of **5** in C_6D_6

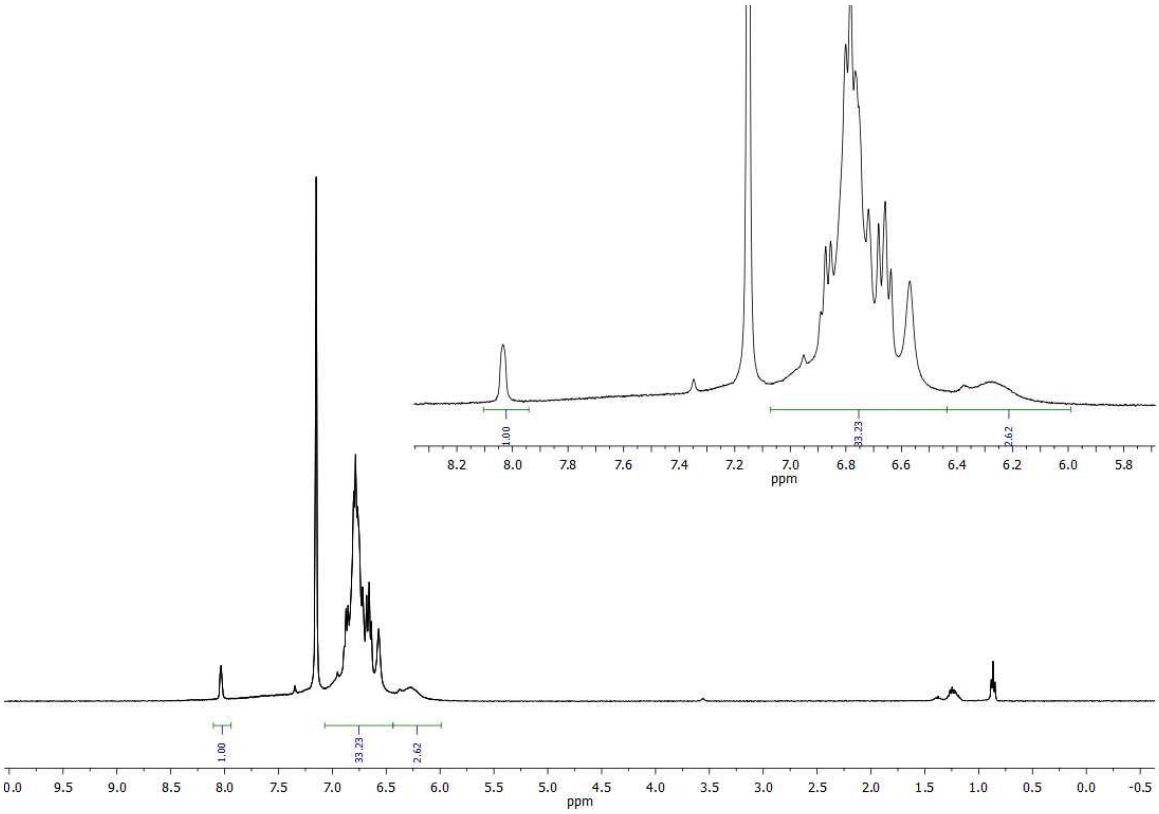

Figure 7: ^{1}H NMR of complex **6** in C_6D_6

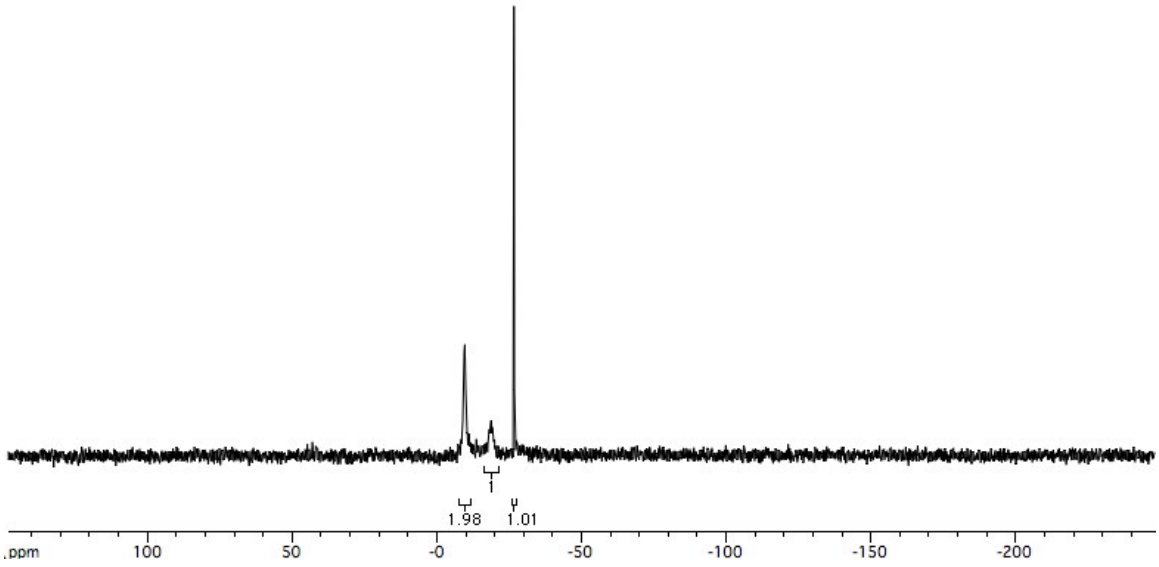

Figure 8: ^{31}P NMR of **6** in C_6D_6

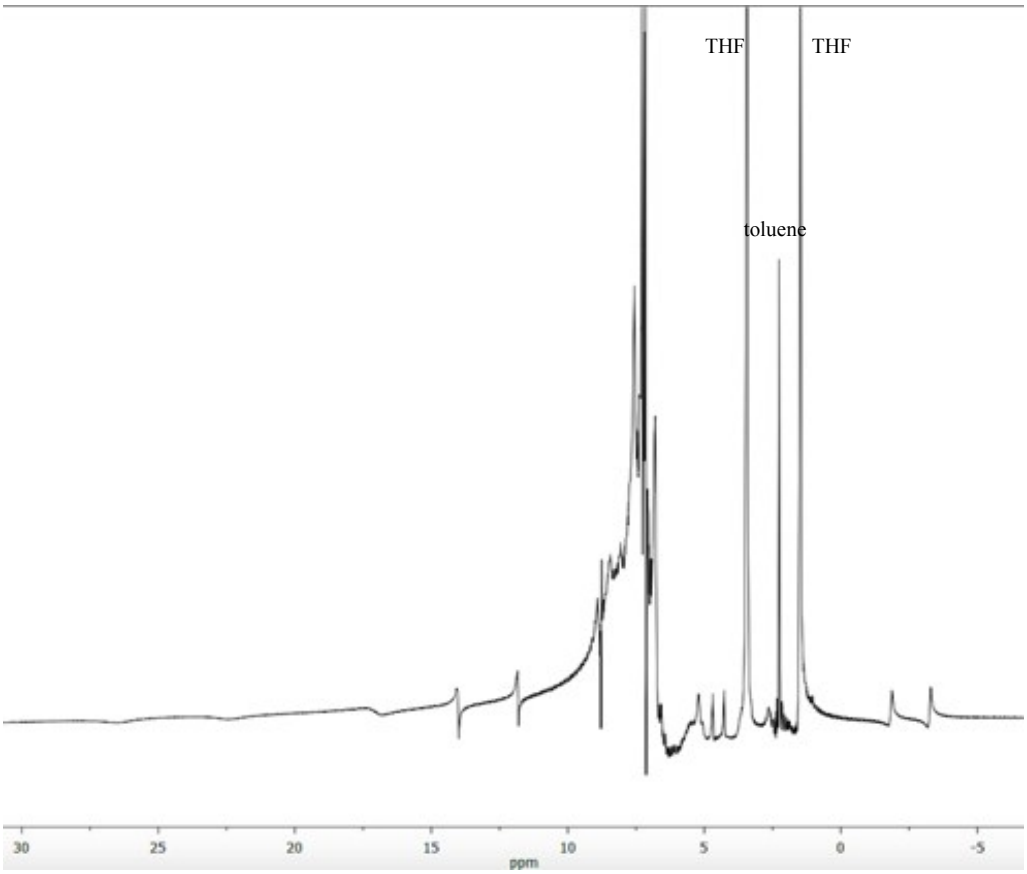

Figure 9: ^{1}H NMR of **7** in C_6D_6

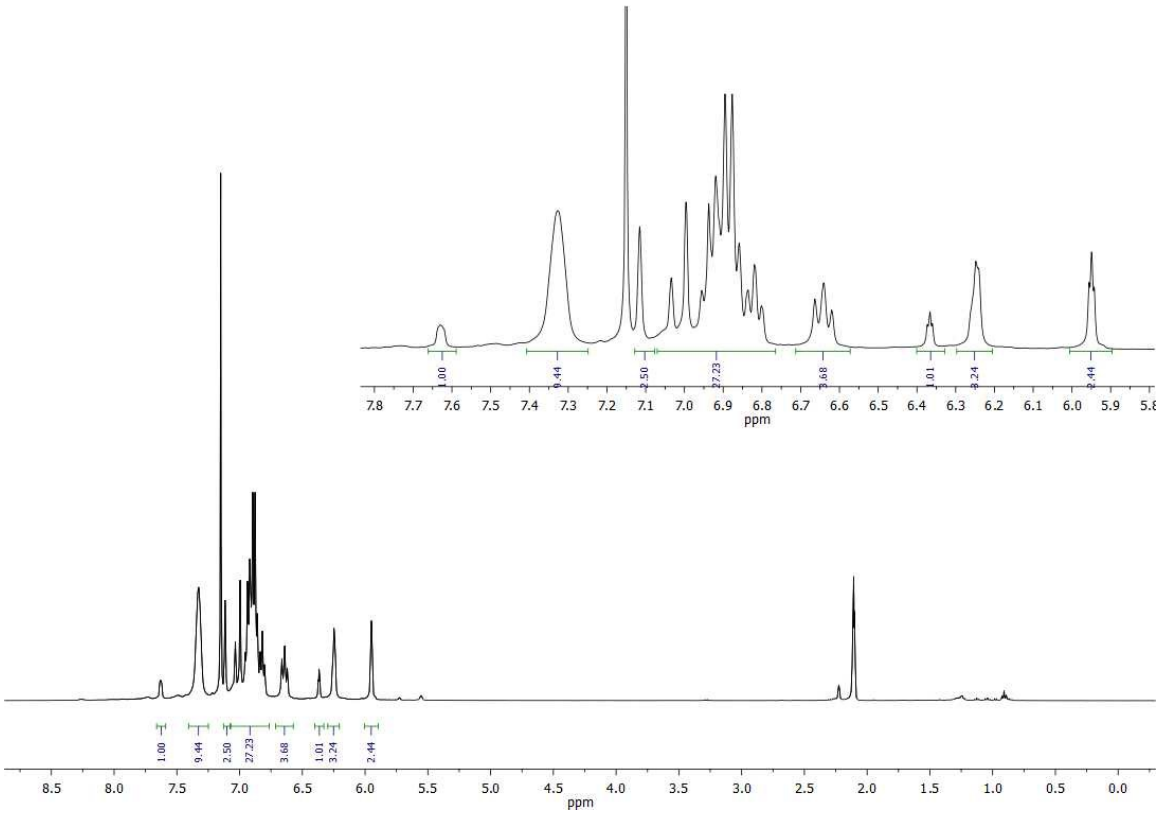

Figure 10: ^{1}H NMR of **8** in C_6D_6

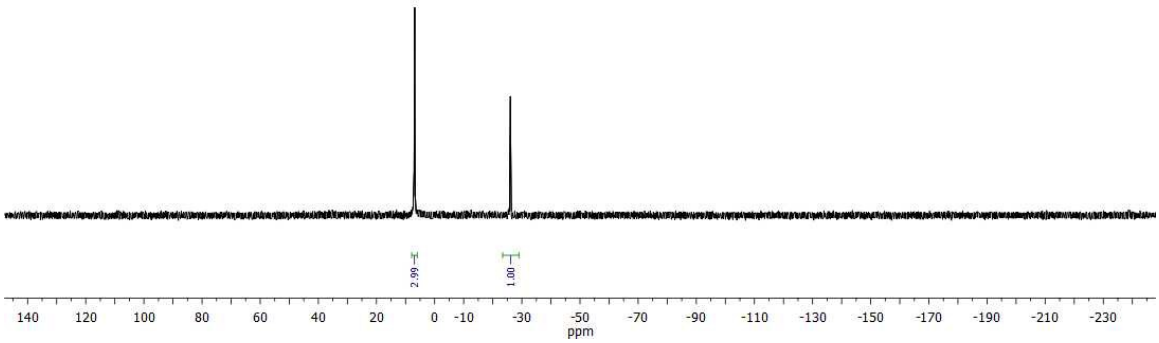

Figure 11: ^{31}P NMR of **8** in C_6D_6

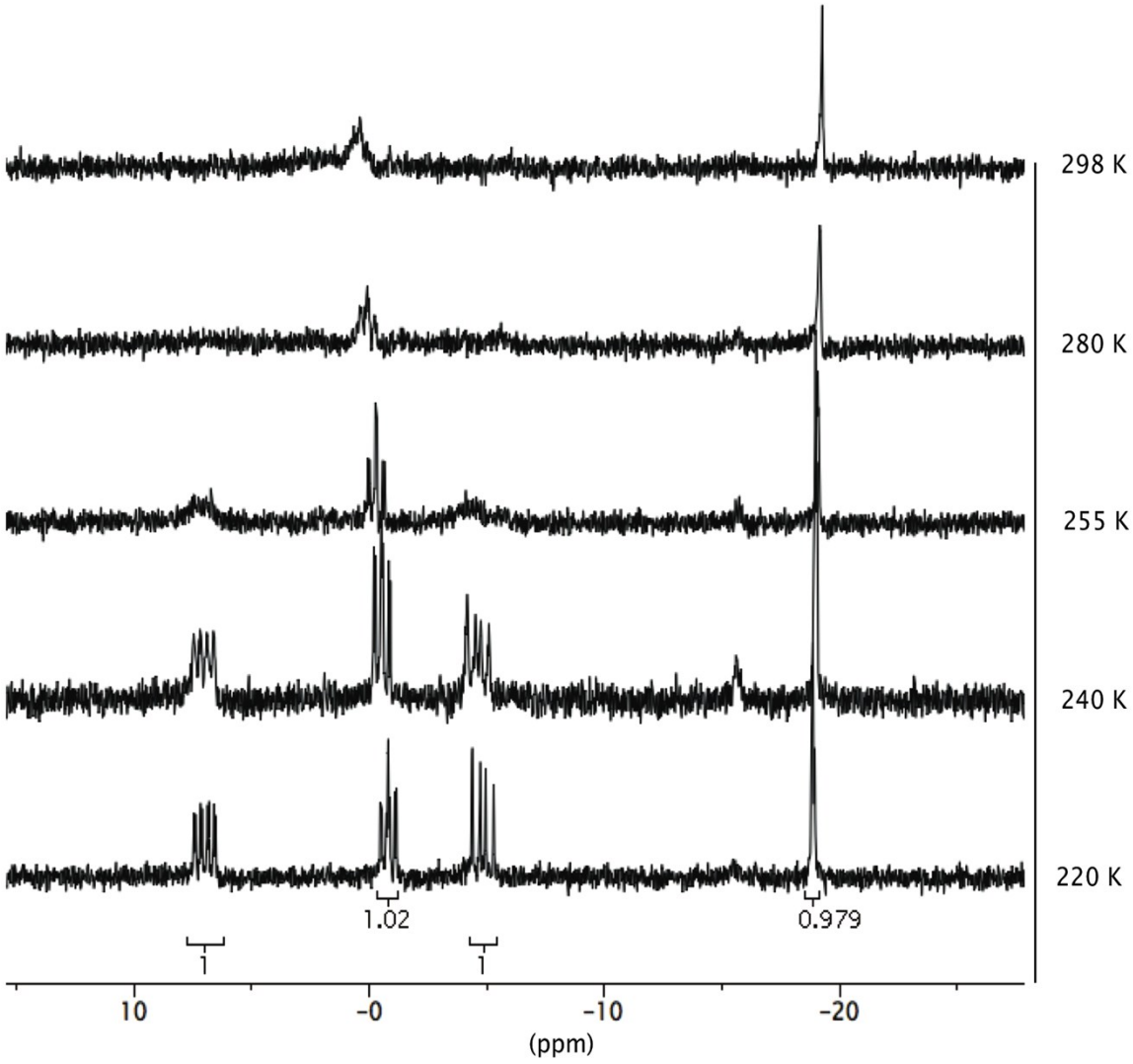

Figure 12: Variable temperature ^{31}P NMR of **4** in d_8-toluene.

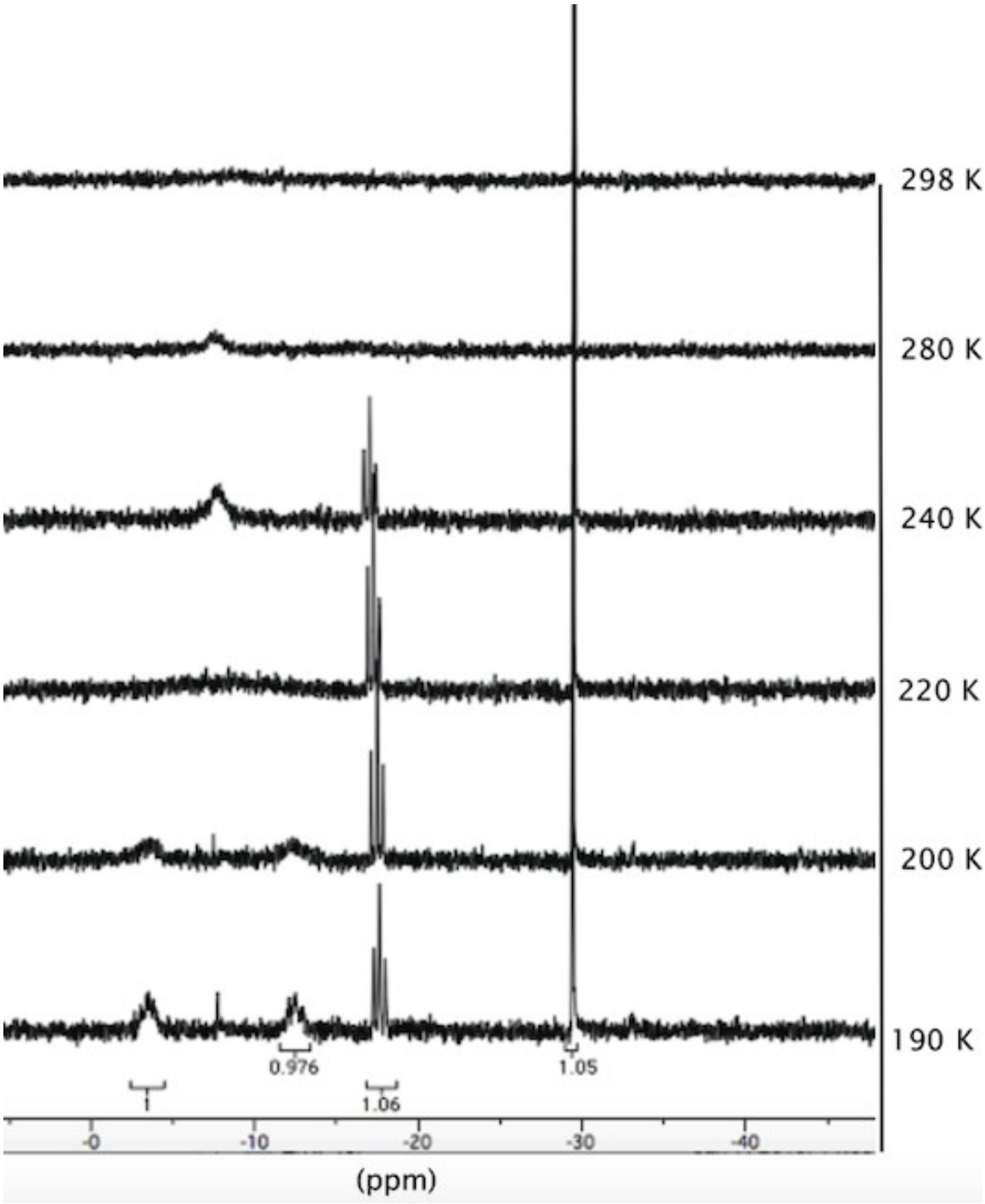

Figure 13: Variable temperature ^{31}P NMR of **5** in d_8-toluene.

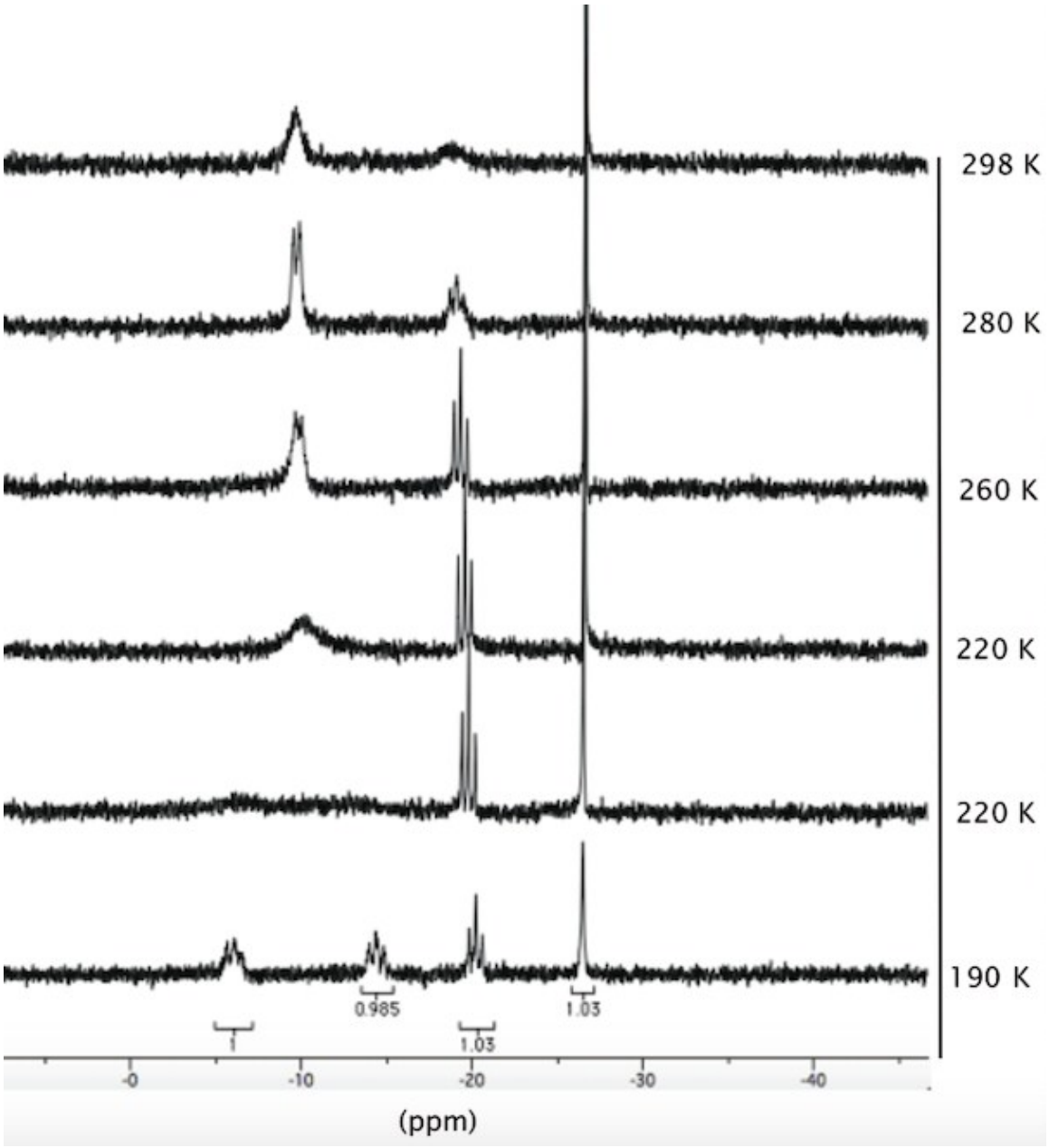

Figure 14: Variable temperature ^{31}P NMR of **6** in d_8-toluene.

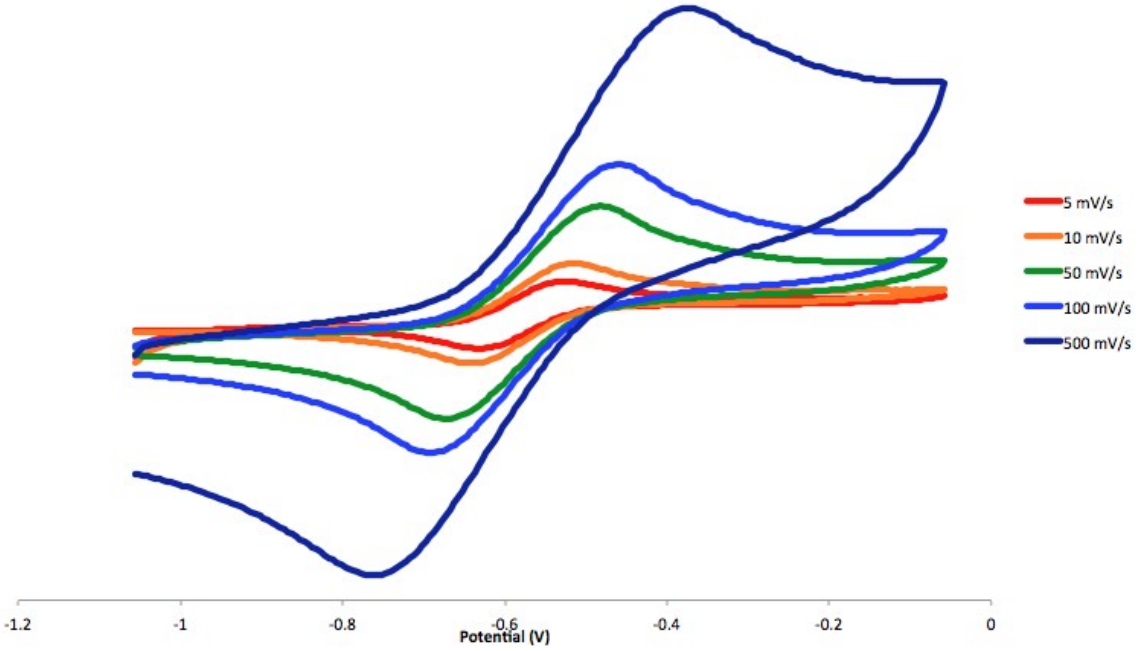

Figure 15: Cyclic voltammogram of complex **1** showing the reversible reduction. Scan rates indicated to the right.

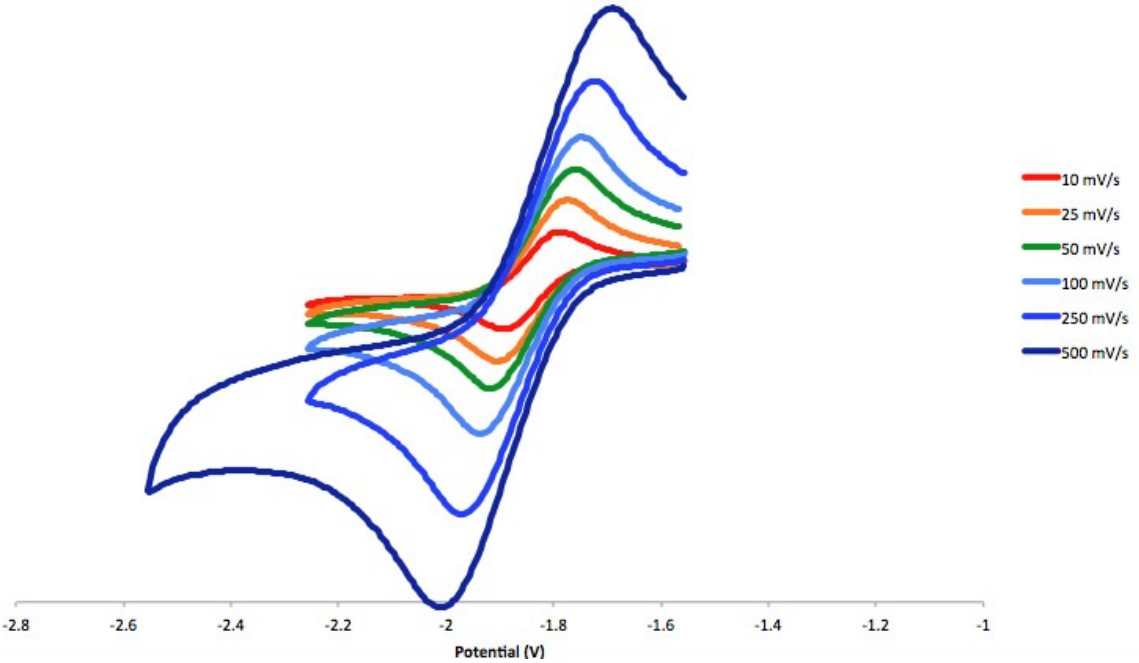

Figure 16: Cyclic voltammogram of complex **2** showing the reversible reduction. Scan rates indicated to the right.

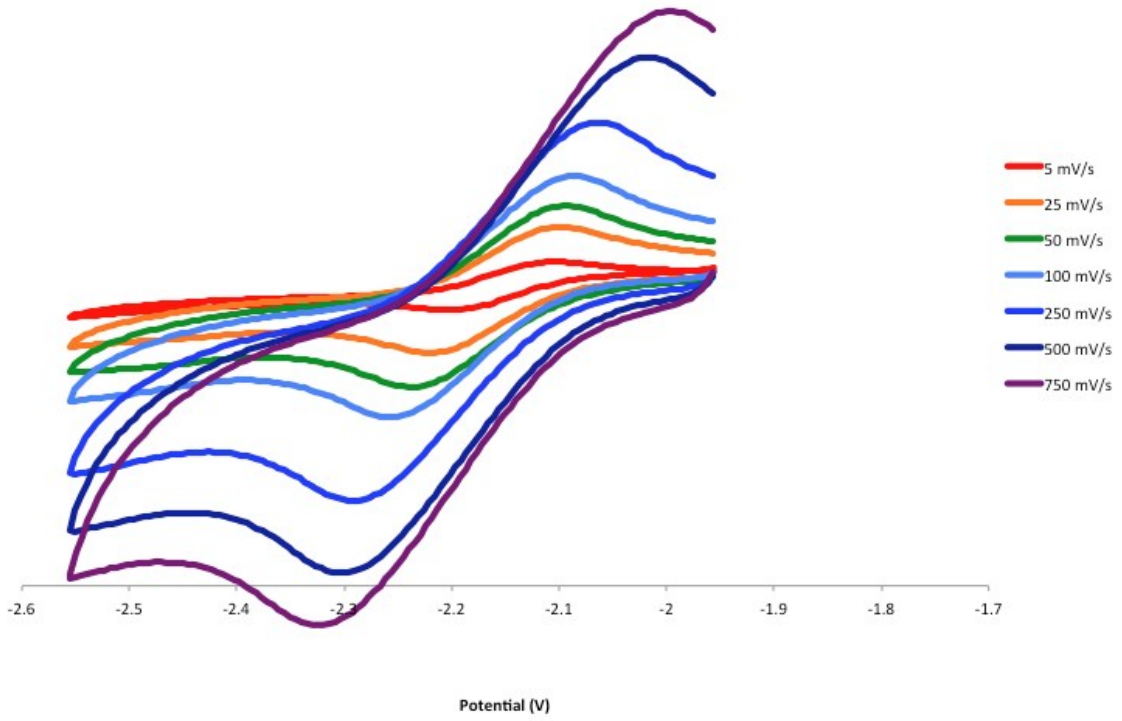

Figure 17: Cyclic voltammogram of complex **3** showing the reversible reduction. Scan rates indicated to the right.

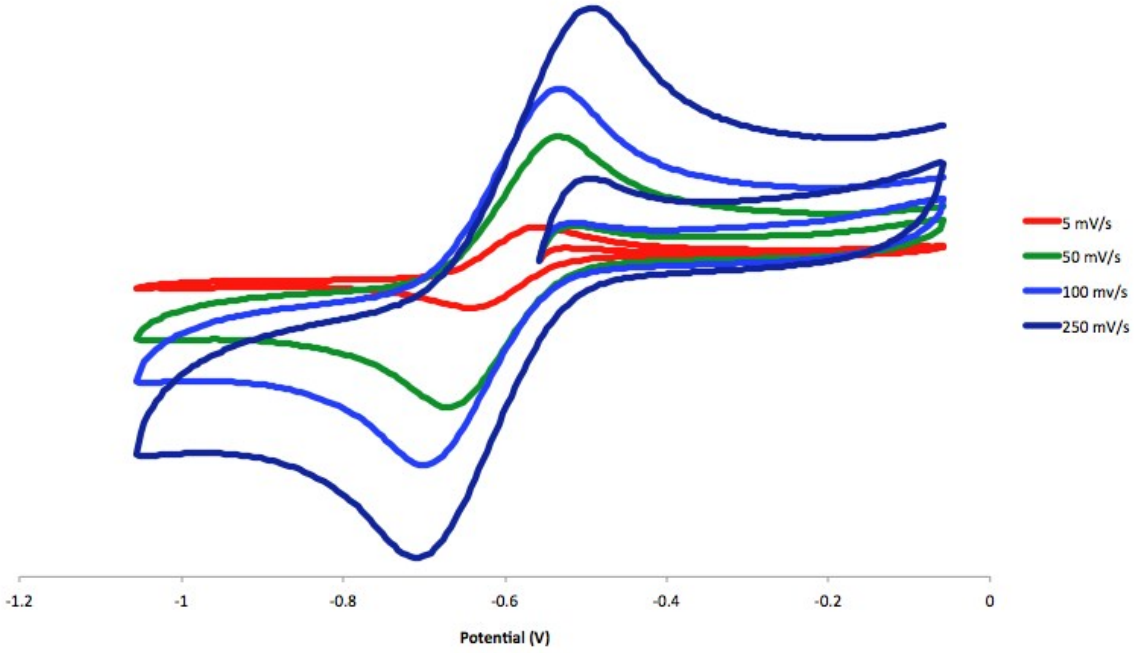

Figure 18: Cyclic voltammogram of complex **4** showing the reversible reduction. Scan rates indicated to the right.

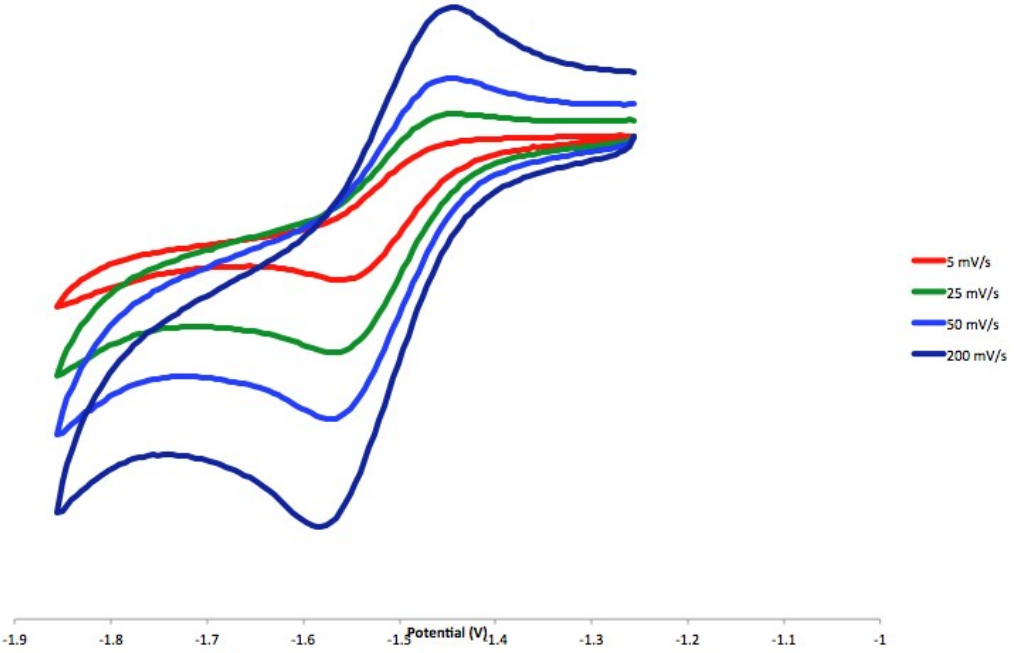

Figure 19: Cyclic voltammogram of complex **5** showing the reversible reduction. Scan rates indicated to the right.

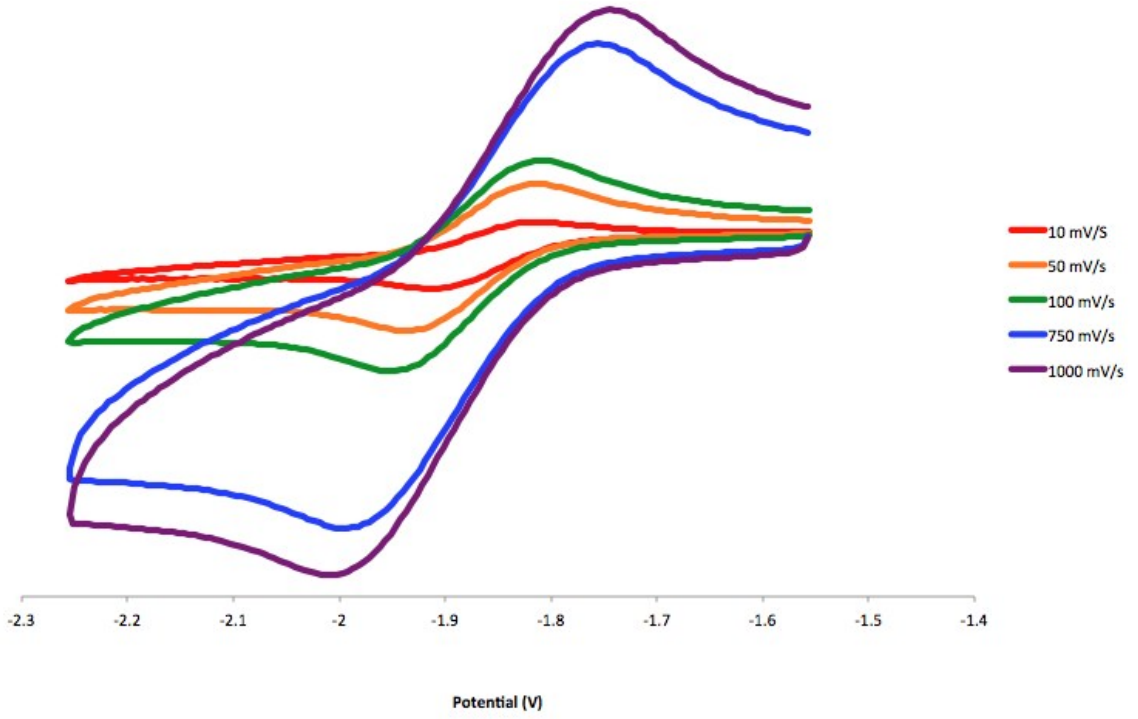

Figure 20: Cyclic voltammogram of complex **6** showing the reversible reduction. Scan rates indicated to the right.

Synthesis of $Hf(2\text{-}PPh_2)C_4H_3N)_4$, $Hf(NP)_4$ (3). Solid Li(NP) (325 mg, 1.26 mmol, 4.5 equiv) was dissolved in 5 mL Et_2O and cooled in a glovebox cold well to approximately -100 °C. Solid $HfCl_4(THF)_2$ (130.4 mg, 0.28 mmol, 1 equiv) was added to the solution and warmed to room temperature while stirring, resulting in a colorless solution with significant white precipitate. Solvent was removed *in vacuo* and the remaining solid redissolved in benzene. Following filtration over celite and removal of solvent, 245 mg of **3** was obtained as a white powder in 74 % yield. X-ray quality crystals were obtained by slow diffusion of pentane into a concentrated benzene solution of **3**. Complexes **1** and **2** were prepared in similar fashion and NMR spectra matched reported values [45]. ^{1}H NMR (400MHz, C_6D_6) δ, ppm: 6.2-6.6 (*br*, 10H). 6.7-6.82 (*br*, 17H), 6.96-7.03 (*br*, 14H), 7.15-7.25 (*br*, 5H), 7.35 (*br*, 1H), 7.55 (br 1H). ^{13}C NMR (125 MHz, C_6D_6) δ, ppm: 114.0-114.4 (*br*), 117.4-117.6 (*s*), 126.6 (*d*, *br*), 129.1 (*d*), 129.1-129.3 (*br*), 133.2-134.2 (*br*), 135.1 (*d*, *br*), 135.65 (*d*, *br*). ^{31}P NMR (121 MHz, C_6D_6) δ, ppm: -30 to -40 (*br*).

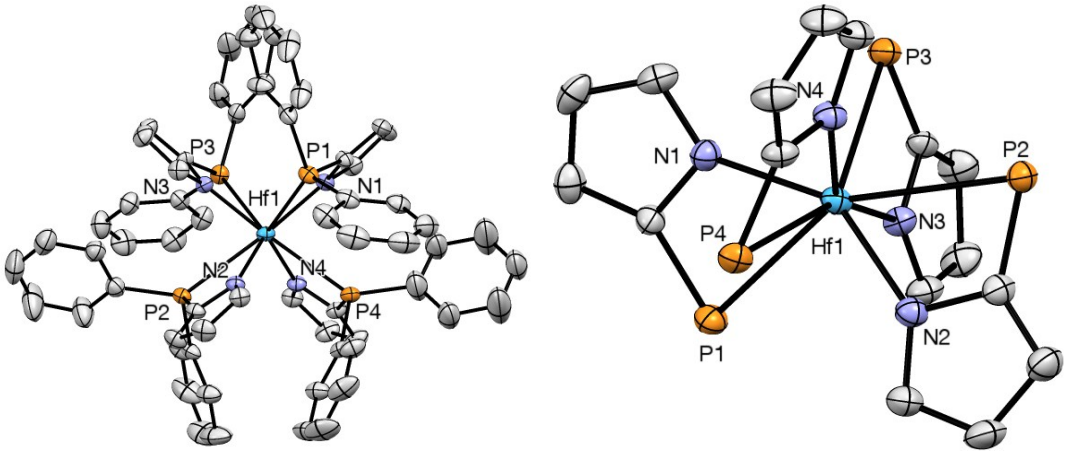

Figure 21: Thermal ellipsoid drawings of **3**. Hydrogens and phenyl rings(right) have been removed for clarity.

TABLE 1: Bond XRD and DFT bond metrics

	4	**4** DFT	**5**	**5** DFT	**6**	**6** DFT
M-M	2.267	2.266	2.373	2.396	2.413	2.437
P-Ni	2.218, 2.191, 2.235	2.193, 2.239, 2.212	2.216, 2.225, 2.198	2.235, 2.198, 2.213	2.207, 2.217, 2.195	2.192, 2.206, 2.230
<P-Ni-P	112.47, 135.91, 110.19	111.27, 112.13, 135.81	118.74, 131.62, 110.12	112.42, 134.34, 113.84	110.61, 131.52, 117.71	134.18, 112.44, 113.38
M-N	2.08, 2.043, 2.109, 2.105	2.134, 2.094, 2.063, 2.083	2.222, 2.191, 2.174, 2.228	2.195, 2.257, 2.215, 2.217	2.151, 2.176, 2.205, 2.202	2.247, 2.206, 2.205, 2.183
M-P	2.2722	2.740	2.88	2.870	2.854	2.856
<N-Ti-N	94.10, 104.42	106.95, 93.63	96.99, 103.49	95.94, 108.45	96.34, 103.02	95.72, 107.59
<N-Ti-P	83.71, 76.23	76.93, 81.05	79.32, 79.75	75.71, 79.37	80.14, 80.21	76.30, 80.00
Torsion Angles (P-	5.83, 20.71, 26.53	9.05, 27.44,	3.46, 30.80, 24.16	7.86, 22.99,	2.45, 28.68, 21.4	8.23, 25.59,

Ni-M-N)		32.05		29.75,		30.47

Table 2. **7** CASSCF spin density

	Ti	Ni
spin density	1.0061	-0.0144

Table 3. CASSCF Mulliken charges

Complex #	M	Ni
4	1.4948	0.05390
7	1.5537	-0.0992
5	2.5469	-0.2921
6	2.2678	-0.1891

Table 4. CASSCF electron count and effective oxidation state for **7**

#	type	%Ti	%Ni	total elec	Ti elec	Ni elec
	d	0	100	1.96	0	1.96
	d	0	100	1.96	0	1.96
	d’	0	100	0.03	0	0.03
	d’	0	100	0.03	0	0.03
	sigma	9.4	90.6	1.90	0.18	1.72
	d’	0	86.8	0.04	0	0.03
	sigma*	38.0	40.7	0.10	0.04	0.04
	d	0	100	1.97	0	1.97

	d’	0	90.8	0.04	0	0.03
	d	0	100	1.97	0	1.97
	d	100	0	1.00	1.00	0.00
	d’	0	100	0.01	0	0
Total elec					1.22	9.75
ox state					+2.78	+0.25

Table 5. CASSCF electron count and effective oxidation state for **4**

#	type	%Ti	%Ni	total elec	Ti elec	Ni elec
	d	0	100	1.98	0	1.98
	d	0	100	1.98	0	1.98
	sigma	5.7	94.2	1.87	0.11	1.76
	pi	28.8	71.2	1.63	0.47	1.16
	sigma *	76.5	13.8	0.12	0.09	0.02
	pi*	66.3	30.3	0.36	0.24	0.11
	d’	2.6	97.4	0.03	0.00	0.02
	d’	5.8	93.0	0.01	0.00	0.01
	d	0	100	1.97	0.00	1.97
	d’	0	100	0.02	0.0	0.02
	d’	0	100	0.02	0.0	0.02
	d’	29.0	70.9	0.01	0.0	0.01
Total elec					0.91	9.06
ox state					+3.09	+0.94

Table 6. CASSCF electron count and effective oxidation state for **5**

#	type	%Zr	%Ni	total elec	Zr elec	Ni elec
	d	0	100	1.96	0	1.96
	d	0	100	1.97	0	1.97
	d	0	100	1.97	0	1.97
	d	0	100	1.93	0	1.93
	d’	0	100	0.03	0	0.03
	sigma	5.8	94.2	1.92	0.11	1.81
	sigma*	48.1	40.4	0.07	0.03	0.03
	d’	12.5	84.4	0.04	0.01	0.04
	d’	39.2	48.0	0.06	0.03	0.03
	d’	0	100	0.03	0	0.03
	d’			0.004		
	d’			0.004		
Total elec					0.18	9.80
ox state					+3.82	+0.20

Table 7. CASSCF electron count and effective oxidation state for **6**

#	type	%Hf	%Ni	total elec	Hf elec	Ni elec
	d	0	100	1.97	0	1.97
	d	0	100	1.97	0	1.97
	d	2.2	97.7	1.94	0.04	1.89
	d	0	100	1.96	0	1.96
	sigma	6.6	93.3	1.92	0.13	1.80
	d’	29.9	57.5	0.06	0.02	0.03

	d’	0	100	0.03	0	0.03
	d’	7.2	89.6	0.04	0.00	0.04
	sigma*	40.6	43.5	0.07	0.03	0.03
	d’	0	100	0.03	0	0.03
	d’			0.003		
	d’			0.004		
Total elec					0.36	9.72
ox state					+3.64	+0.28

Table 8. **4** neutral relative spin state energies (kcal/mol)

	CASSCF	CASPT2
singlet	0.0	0.0
triplet	7.0	26.1

Table 9. **7** relative spin state energies (kcal/mol)

	CASSCF	CASPT2
doublet	0.0	0.0
quartet	31.6	42.2

Table 10. **5** relative spin state energies (kcal/mol)

	CASSCF
singlet	0.0
triplet	56.1

Table 11. **6** relative spin state energies (kcal/mol)

	CASSCF
singlet	0.0
triplet	141.7

*CASPT2 calculations were not performed since the spins states were well separated at the CASSCF level.

Table 12. DFT orbital relative energies on M06L optimized structures (eV) of **7**

	M06L	M06 (single point on M06L geom)
Ni xz	0.00	0.00
Ni yz	0.09	0.04
sigma/dz^2	0.12	0.18
Ni xy	0.50	0.93
Ni X^2-y^2	0.76	1.26
Ti xz SOMO	2.24	3.26
Ti yz LUMO	2.65	4.70

Table 13. DFT orbital relative energies on M06L optimized geometries (eV) of **4**

	M06L	M06 (Single point on M06L geom)
Ni yz	0.11	0.00
pi/xz	0.13	0.07
sigma/dz^2	0.00	0.24
Ni xy	1.19	1.84
Ni X^2-y^2 (HOMO)	1.46	1.94

Ti xz (LUMO)	3.07	5.15
Ti yz	3.17	5.28

Table 14. DFT orbital relative energies on M06L optimized structure (eV) of **5**

	M06L	M06 (single point on M06L geom)
Ni xz	0.00	0.00
Ni yz	0.08	0.04
sigma/dz^2	0.13	0.29
Ni xy	1.11	1.60
Ni X^2-y^2 (HOMO)	1.35	1.73
Zr xz (LUMO)	3.68	5.66
Zr yz	3.89	5.84

Table 15. DFT orbital relative energies on M06L optimized strucutre (eV) of **6**

	M06L	M06 (single point on M06L geom)
Ni yz	0.00	0.00
Ni xz	0.06	0.10
sigma/dz^2	0.11	0.12
Ni xy	0.98	0.80
Ni X^2-y^2 (HOMO)	1.24	1.15
Hf dz (LUMO)	3.62	3.18

Cartesian coordinates

4

Ti	-0.49036300	-0.14553300	-1.58953600
Ni	0.86626300	-0.00228600	0.22042800
P	0.88176000	-2.19799600	0.49162300
P	-0.25195800	1.67942300	1.07435000
P	2.61642700	0.71173600	-0.97929400
P	-3.10682400	-0.11830700	-0.77550300
N	-0.96224300	-2.18067800	-1.44441400
N	-0.78652700	1.96989000	-1.49253100
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C	-1.63807800	-4.30941400	-1.78189700
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C	0.98876500	2.51973300	2.11893000
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C	2.29022000	2.48399700	4.16750600
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C	-3.50846500	2.47702500	3.46076100
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C	-3.75758100	1.23498900	4.04609000
H	-4.57504600	1.12488400	4.75749300
C	-2.97496100	0.13480000	3.70682700
H	-3.17219500	-0.84246500	4.14735900
C	-1.93580400	0.28073800	2.78917600
H	-1.31135200	-0.57441800	2.51999700
C	-0.66237000	2.70230100	-0.31926800
C	-1.14694300	2.85616500	-2.46469000
H	-1.33384500	2.50740800	-3.47658700
C	-1.22278900	4.14223500	-1.94290600
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H	0.24011200	-1.51081100	-4.49298600

C	2.41777700	-0.99525700	-4.61438800
H	2.73482100	-1.38851700	-5.57461500
C	3.22379700	-0.32809500	-3.66483200
H	4.27885400	-0.08723900	-3.75259200
C	4.03293800	0.00313800	-0.08093700
C	5.00733600	-0.81842500	-0.65197200
H	4.94364600	-1.07847200	-1.70796500
C	6.03953000	-1.32553600	0.13492900
H	6.78886300	-1.97417000	-0.31658900
C	6.10950200	-1.01920500	1.49225600
H	6.91762100	-1.42227500	2.10064900
C	5.13697600	-0.20501500	2.07156400
H	5.17999300	0.03830600	3.13302500
C	4.10161000	0.29866600	1.29051600
H	3.34248700	0.94527000	1.74199000
C	3.12281300	2.44642400	-1.26694500
C	2.26930500	3.25266000	-2.03337400
H	1.37373400	2.82277900	-2.48199500
C	2.54512900	4.60377100	-2.21023700
H	1.85964700	5.21535700	-2.79507500
C	3.68238800	5.16906200	-1.63370200
H	3.89722400	6.22780900	-1.77014800
C	4.54489500	4.37080500	-0.88640500
H	5.44181400	4.80130800	-0.44219600
C	4.26692600	3.01813400	-0.69749700

H	4.94226900	2.41075100	-0.09619100
C	-3.15816500	0.04246900	-2.55799400
C	-4.23819400	1.16056400	-0.13436200
C	-4.09418100	2.47835500	-0.59181100
H	-3.34874700	2.70898900	-1.35239600
C	-4.91008100	3.48809300	-0.09366400
H	-4.78324400	4.50629100	-0.46079000
C	-5.88498500	3.19816200	0.86054500
H	-6.52993900	3.98815500	1.24322800
C	-6.02987700	1.89262900	1.32181700
H	-6.78517200	1.65764100	2.07136000
C	-5.20582700	0.87867300	0.83733100
H	-5.32083000	-0.13755400	1.21414600
C	-3.91779200	-1.68463900	-0.30809400
C	-5.02208900	-2.18030700	-1.01079400
H	-5.39877600	-1.63139900	-1.87478800
C	-5.61842500	-3.37701900	-0.62676500
H	-6.47406400	-3.75891800	-1.18186500
C	-5.11795600	-4.09047700	0.46225400
H	-5.58236500	-5.03004000	0.75777200
C	-4.01765000	-3.60493400	1.16412400
H	-3.61550400	-4.16605300	2.00810200
C	-3.41911200	-2.40729300	0.77990000
H	-2.53939700	-2.03711400	1.30910400
C	-4.08994900	0.32949900	-3.54752100

H	-5.15382700	0.49085000	-3.40058300
C	-3.37191300	0.39217100	-4.76278700
H	-3.77891900	0.59116800	-5.74889500
C	-2.03753800	0.15120800	-4.46273500
H	-1.17435600	0.13932900	-5.12147000

7

Ni	0.99366400	0.15452100	0.39459200
Ti	-0.45418200	-0.24701300	-1.74766000
P	0.49728200	2.28442200	0.51721300
P	-3.22424300	-0.20830200	-0.83787800
P	2.69206900	-0.41457300	-0.88890900
P	0.19820900	-1.64961900	1.36917200
N	-0.99893100	1.79741000	-1.72579500
C	-2.12506600	-0.99974500	-4.44723600
H	-1.25871500	-1.10934500	-5.09476300
C	-5.22593100	3.88951900	-0.06369300
H	-5.68467400	4.85825500	0.13412700
N	-0.58471100	-2.29646900	-1.13404200
C	-0.58892800	2.76039700	-0.82393700
C	-3.23782200	-0.59152400	-2.59002400
N	-1.97258700	-0.61542100	-3.15190400
C	-3.46749400	-1.22897400	-4.72881500
H	-3.87923900	-1.54723700	-5.68241500

C	-4.18294500	-0.97251900	-3.53867500
H	-5.25277300	-1.07259500	-3.37500800
C	-4.47314000	-1.37269400	-0.16745300
C	-4.31271300	-2.73908000	-0.44843300
H	-3.50631900	-3.05860800	-1.11104100
C	-5.15250400	-3.68485100	0.12749800
H	-4.99872500	-4.74125100	-0.09322300
C	-6.17816200	-3.28730500	0.98639900
H	-6.83757100	-4.02899300	1.43631600
C	-6.34901300	-1.93427200	1.26734800
H	-7.14776300	-1.61142800	1.93583600
C	-5.49798500	-0.98322700	0.70401200
H	-5.63195400	0.07163800	0.94499500
C	-4.03818200	1.41081200	-0.59059300
C	-5.02813500	1.91517900	-1.44178400
H	-5.31296300	1.34177400	-2.32558200
C	-5.61959900	3.14643100	-1.17774700
H	-6.38559000	3.53511300	-1.84903800
C	-4.23724200	3.39909300	0.78461800
H	-3.90768800	3.97896600	1.64680600
C	-3.64661400	2.16467800	0.52002200
H	-2.85894500	1.78511800	1.17361100
N	1.13606400	0.00777500	-3.04224700
C	1.13068800	0.47653600	-4.32600800
H	0.19532500	0.54664600	-4.87408600

C	2.40702300	0.85513400	-4.70613400
H	2.69568000	1.27674300	-5.66435100
C	3.25484900	0.60122100	-3.60285900
H	4.32075800	0.79637100	-3.54079000
C	2.44719800	0.08616600	-2.59628300
C	4.28340200	0.35661800	-0.38942400
C	4.33679200	1.13416800	0.77043900
H	3.42138200	1.28903200	1.34479800
C	5.52973300	1.72547200	1.18103900
H	5.54523500	2.34161600	2.07945400
C	6.68756200	1.54769300	0.42969700
H	7.62056000	2.01615500	0.74230600
C	6.65153900	0.76385200	-0.72365000
H	7.55809400	0.61305100	-1.30959500
C	5.46174500	0.16344100	-1.12389100
H	5.44359400	-0.47457400	-2.00767100
C	3.20463700	-2.18262400	-1.01032300
C	2.49930500	-3.03548500	-1.87007800
H	1.71332300	-2.62857300	-2.50602400
C	2.78366600	-4.39676800	-1.90971700
H	2.20762000	-5.04351600	-2.57088700
C	3.79085100	-4.92840100	-1.10513100
H	4.01454800	-5.99458500	-1.13790100
C	4.50443000	-4.08763300	-0.25486500
H	5.28746300	-4.49182100	0.38770600

C	4.20766500	-2.72780100	-0.19920500
H	4.75730900	-2.08695300	0.49076500
C	-1.04673600	-3.32881200	-1.89552000
H	-1.26590800	-3.16896400	-2.94853900
C	-1.21289000	-4.47355600	-1.12511600
H	-1.57252400	-5.43813400	-1.47239400
C	-0.84897000	-4.12553100	0.19083600
H	-0.88674700	-4.75768100	1.07417700
C	-0.45360100	-2.78828200	0.15471000
C	-0.98412000	-1.69787400	2.77965600
C	-2.34921000	-1.91388100	2.55161600
H	-2.68284900	-2.20551700	1.55738100
C	-3.27715500	-1.77033100	3.58097200
H	-4.33279500	-1.94187300	3.37077600
C	-2.85758700	-1.41674000	4.86176200
H	-3.58271900	-1.30527600	5.66748500
C	-1.49934400	-1.21107600	5.10525800
H	-1.15700300	-0.94162800	6.10487900
C	-0.57355000	-1.34493300	4.07505700
H	0.48356100	-1.16607700	4.27789300
C	1.67991300	-2.41052800	2.15592200
C	1.93441800	-3.78376200	2.20171100
H	1.23943800	-4.47335900	1.72358200
C	3.08872200	-4.26806900	2.81330800
H	3.27959100	-5.34128300	2.82763500

C	4.00933800	-3.38985900	3.38140900
H	4.91567900	-3.77352500	3.84938600
C	3.77583700	-2.01648800	3.32905200
H	4.49981000	-1.31730600	3.74771000
C	2.62101700	-1.53486800	2.71815200
H	2.43975700	-0.45658600	2.65995500
C	-1.76610200	2.44256300	-2.65288700
H	-2.22232700	1.88401800	-3.46519100
C	-1.85300500	3.79688900	-2.36033000
H	-2.41053100	4.54082000	-2.92177600
C	-1.09896100	4.00416000	-1.19086100
H	-0.93716200	4.94263200	-0.66756500
C	1.93750000	3.40514100	0.28766800
C	2.50090500	3.45510500	-0.99771200
H	2.00748300	2.93160400	-1.82028500
C	3.68719700	4.14243000	-1.22591000
H	4.11420300	4.15352800	-2.22867100
C	4.33055500	4.80326400	-0.17806800
H	5.26292200	5.33813300	-0.35683200
C	3.77995600	4.76219000	1.09990500
H	4.27703300	5.27199100	1.92609700
C	2.59684000	4.06061800	1.33424800
H	2.18423100	4.01948600	2.34347200
C	-0.32762200	2.97114300	2.01896300
C	-0.50915700	4.34397300	2.23882200

H	-0.08148800	5.06291400	1.53908800
C	-1.23118900	4.79684300	3.33921400
H	-1.36589800	5.86742300	3.49493600
C	-1.79049900	3.88495000	4.23567300
H	-2.36218200	4.24256200	5.09187300
C	-1.61581600	2.51872000	4.03031300
H	-2.05061700	1.79383500	4.71831600
C	-0.88250100	2.06885100	2.93325000
H	-0.75285300	0.99842400	2.75903500

ZrNi

Zr	-0.70552151	0.90490796	0.00000000
Ni	0.74201249	0.86304796	-1.90892100
P	-3.43694851	0.94376196	-0.87962400
P	2.41111449	0.12376796	-0.61881100
P	0.68385649	3.06885396	-2.07935300
P	-0.42493251	-0.77709804	-2.79158300
N	-2.29779551	0.76940796	1.53606500
N	0.96237249	1.15275096	1.40458700
N	-1.20135451	3.05827996	-0.14919200
N	-1.08587551	-1.30316104	-0.27478400
C	-4.21559551	2.54150896	-1.28936200
C	-3.68925151	3.29137796	-2.34644000
H	-2.81445751	2.91893196	-2.88316900
C	-4.25352051	4.51721596	-2.68958400

H	-3.83070451	5.09866296	-3.50936000
C	-5.34519551	5.00593596	-1.97574100
H	-5.78186251	5.96841396	-2.23794100
C	-5.87076351	4.26699396	-0.91624200
H	-6.71874751	4.65167496	-0.35136000
C	-5.31014851	3.04017496	-0.57429800
H	-5.70636351	2.46993096	0.26687200
C	-4.55435251	-0.29536204	-1.61730800
C	-4.38291451	-1.64391304	-1.27225500
H	-3.62491851	-1.92470704	-0.54168700
C	-5.18585751	-2.62360304	-1.84514400
H	-5.03696451	-3.66607004	-1.56458500
C	-6.17296251	-2.27411604	-2.76636800
H	-6.80622251	-3.04169204	-3.20947800
C	-6.34376451	-0.93810904	-3.11799200
H	-7.10911451	-0.65579104	-3.84045200
C	-5.53555351	0.04784096	-2.55450000
H	-5.67267151	1.08939396	-2.84454600
C	-3.53577051	0.69268096	0.89408300
C	-2.51900351	0.48881996	2.85039700
H	-1.69416451	0.47532996	3.55735900
C	-3.86527151	0.23014796	3.06632600
H	-4.32397851	-0.02121204	4.01703600
C	-4.51526051	0.35398296	1.81968100
H	-5.56908451	0.19942396	1.60707700

C	2.89718949	-1.63476004	-0.43860500
C	4.06241549	-2.17126504	-0.99840300
H	4.76166149	-1.52744504	-1.53033800
C	4.33142349	-3.53492704	-0.89118900
H	5.24449749	-3.93731804	-1.32884800
C	3.43992149	-4.37889304	-0.23418400
H	3.64779849	-5.44530004	-0.16190900
C	2.28191849	-3.84952004	0.33548500
H	1.57338249	-4.49619604	0.85084400
C	2.01452549	-2.48865504	0.23831200
H	1.10088349	-2.09036804	0.68063700
C	3.82943649	0.86104896	-1.49262500
C	4.80313849	1.66646596	-0.89832300
H	4.74393349	1.89003896	0.16628600
C	5.82932449	2.20434996	-1.67318100
H	6.57836249	2.84022896	-1.20336000
C	5.89412049	1.94478596	-3.04037100
H	6.69783249	2.37171596	-3.63824300
C	4.92198949	1.14638096	-3.64245500
H	4.95999449	0.93789896	-4.71158700
C	3.89291449	0.61238196	-2.87400400
H	3.13484949	-0.02264804	-3.34359400
C	2.25241949	0.75613196	1.04491800
C	1.03597049	1.59044696	2.69626300
H	0.14873749	1.97474196	3.19214800

C	2.33205849	1.47448796	3.17168900
H	2.68057949	1.75486296	4.16003000
C	3.10695649	0.92891696	2.12505400
H	4.16435249	0.68381896	2.15066800
C	2.21146849	3.97542696	-1.62371700
C	2.48731949	4.08088096	-0.25158000
H	1.79706449	3.64765696	0.47572800
C	3.62414349	4.74935996	0.18694600
H	3.82175749	4.82460996	1.25577000
C	4.50213249	5.31788796	-0.73640100
H	5.39008649	5.84683396	-0.39278300
C	4.24062049	5.20443396	-2.09871800
H	4.92425649	5.64224096	-2.82533800
C	3.10188949	4.53320296	-2.54396800
H	2.90286049	4.45715096	-3.61318400
C	-0.56398251	3.86235396	-1.08396700
C	-1.99298551	3.87998196	0.59689100
H	-2.61487851	3.46411196	1.38528900
C	-1.86412851	5.19362596	0.16904900
H	-2.38338951	6.05429896	0.57745600
C	-0.94235451	5.18900396	-0.89642100
H	-0.57202551	6.04491596	-1.45376300
C	0.38360449	3.47253096	-3.83585700
C	-0.66371451	4.30416996	-4.24681000
H	-1.26534151	4.81459696	-3.49416700

C	-0.95508951	4.44956096	-5.60277900
H	-1.77990351	5.09174096	-5.91062700
C	-0.20047451	3.77689196	-6.56087300
H	-0.43569051	3.88634896	-7.61809800
C	0.85258149	2.95364596	-6.16034300
H	1.44236049	2.41752696	-6.90350900
C	1.13731649	2.79652796	-4.80801800
H	1.93913849	2.12080796	-4.49403500
C	-1.83808651	-0.55053804	-3.92816500
C	-2.08290651	0.72032696	-4.45598900
H	-1.44599051	1.55459396	-4.15286800
C	-3.12870851	0.92158596	-5.35567100
H	-3.31586751	1.91984896	-5.75128500
C	-3.93397251	-0.14979204	-5.73218400
H	-4.75838251	0.00455096	-6.42720400
C	-3.69919151	-1.41941804	-5.20334000
H	-4.34313851	-2.25285004	-5.47991300
C	-2.65911251	-1.62081904	-4.30240800
H	-2.49233051	-2.60822404	-3.86998800
C	0.83598549	-1.55363504	-3.86353800
C	1.65577849	-2.59613004	-3.41486600
H	1.46582849	-3.05565304	-2.44433800
C	2.72276349	-3.03274004	-4.19895200
H	3.35207849	-3.84443204	-3.83669400
C	2.99057049	-2.43112504	-5.42649100

H	3.82984049	-2.77166904	-6.03068800
C	2.17587049	-1.39329604	-5.88100700
H	2.37324849	-0.92294104	-6.84388700
C	1.10450049	-0.95844604	-5.10763600
H	0.46785149	-0.14621904	-5.46451300
C	-0.89224551	-1.91946204	-1.50403600
C	-1.48377751	-2.27844904	0.59180700
H	-1.72737451	-2.02477004	1.62069500
C	-1.52484351	-3.50909904	-0.05252900
H	-1.78917951	-4.46110604	0.39682600
C	-1.15684451	-3.28128704	-1.39559600
H	-1.07737751	-4.01749804	-2.19063200

HfNi

Hf	0.47646000	-0.01912300	-1.51358400
Ni	-1.02819900	-0.00569100	0.40372500
P	3.18701300	-0.07976100	-0.61683600
P	-2.65320900	0.75979000	-0.91751800
P	-0.96402700	-2.20721900	0.52659200
P	0.15798700	1.60948300	1.29294600
N	2.06279100	0.13653500	-3.03687300
N	-1.16685500	-0.22887100	-2.93578100
N	0.93843500	-2.17249600	-1.39217100
N	0.83698300	2.17782000	-1.21211600
C	2.29624600	0.43137900	-4.34607700

H	1.47562600	0.46732900	-5.05701200
C	3.64644100	0.67552000	-4.55107000
H	4.11328700	0.93466400	-5.49560700
C	4.28738300	0.52735500	-3.30295800
H	5.34160500	0.66651100	-3.08201800
C	3.29908900	0.18972500	-2.38677800
C	4.29553900	1.14901400	0.14897600
C	4.12732100	2.50198800	-0.17963800
H	3.37838400	2.79385300	-0.91529800
C	4.92258900	3.47362100	0.41719400
H	4.77594900	4.52001800	0.15045600
C	5.89862000	3.11136400	1.34516100
H	6.52558500	3.87294700	1.80711700
C	6.06626100	1.77061500	1.67976900
H	6.82274200	1.47853300	2.40760700
C	5.26554300	0.79237300	1.09272500
H	5.39892000	-0.25298200	1.37050100
C	3.95123000	-1.68584100	-0.21498100
C	3.40486000	-2.44646300	0.82412400
H	2.52422200	-2.07658500	1.35278700
C	3.95839300	-3.67913300	1.15999400
H	3.52053300	-4.26868200	1.96589700
C	5.05833300	-4.16403700	0.45646200
H	5.48639000	-5.13194000	0.71285700
C	5.60341000	-3.41446400	-0.58552800

H	6.45798800	-3.79609300	-1.14244200
C	5.05418100	-2.18044000	-0.91975900
H	5.46599600	-1.60156800	-1.74733200
C	-1.21798900	-0.63932100	-4.23844200
H	-0.32276400	-1.01548100	-4.72593700
C	-2.50471300	-0.51234200	-4.73381200
H	-2.83527300	-0.77077800	-5.73416600
C	-3.29752900	0.01140500	-3.68958300
H	-4.35407700	0.25822400	-3.72833100
C	-2.46342600	0.16151300	-2.59089900
C	0.29252800	-2.98701600	-0.47144000
C	1.73424800	-2.98835900	-2.14236400
H	2.36239400	-2.56507500	-2.92183500
C	1.60068100	-4.30574300	-1.73051700
H	2.12102300	-5.16252000	-2.14563800
C	0.67128500	-4.31114700	-0.67165600
H	0.29395200	-5.17289400	-0.12823900
C	-0.67956100	-2.64979400	2.27718200
C	0.36450600	-3.48794800	2.68325200
H	0.97408800	-3.98386300	1.92741600
C	0.64221100	-3.65929700	4.03909900
H	1.46473000	-4.30640400	4.34293100
C	-0.12330700	-3.00674300	5.00237200
H	0.10087800	-3.13688300	6.05966200
C	-1.17346400	-2.17729500	4.60691600

H	-1.77186500	-1.65669400	5.35421200
C	-1.44394000	-1.99385300	3.25500600
H	-2.24330300	-1.31287200	2.94611300
C	-2.48436300	-3.11192500	0.03896100
C	-3.38766300	-3.67992900	0.94014100
H	-3.20315600	-3.61722800	2.01283500
C	-4.52132700	-4.34423100	0.47190700
H	-5.21512700	-4.78956600	1.18420500
C	-4.76508100	-4.44109900	-0.89489700
H	-5.64910900	-4.96457200	-1.25658900
C	-3.87432200	-3.86241400	-1.79947300
H	-4.05797300	-3.92453300	-2.87165100
C	-2.74282100	-3.20053200	-1.33772200
H	-2.04294200	-2.75888200	-2.05064200
C	0.64055900	2.77263300	0.02849000
C	1.24131100	3.16883100	-2.05887900
H	1.48618500	2.93411000	-3.09190600
C	1.28530100	4.38622300	-1.39151200
H	1.55620000	5.34519500	-1.82164000
C	0.91126100	4.13445500	-0.05432400
H	0.83235400	4.85574200	0.75428600
C	1.56032200	1.36655400	2.44074100
C	2.38041200	2.42844100	2.83985500
H	2.22084000	3.42268800	2.42078700
C	3.40941200	2.21098600	3.74976800

H	4.05245200	3.03843200	4.04585700
C	3.63412500	0.93329800	4.26341200
H	4.44957900	0.76646200	4.96609400
C	2.82960400	-0.12981900	3.86274300
H	3.00828700	-1.13402000	4.24715700
C	1.79491300	0.08781200	2.95405800
H	1.15742900	-0.73931500	2.63297300
C	-1.11129700	2.37384300	2.36507600
C	-1.92541300	3.42435000	1.92454700
H	-1.72559800	3.89873400	0.96311200
C	-2.99971500	3.85015600	2.70439600
H	-3.62412700	4.66841700	2.34843200
C	-3.28136700	3.22937200	3.91930100
H	-4.12638500	3.56162000	4.52011400
C	-2.47327600	2.18274300	4.36533400
H	-2.68158900	1.69695900	5.31823300
C	-1.39437100	1.75871000	3.59638000
H	-0.76299800	0.93950200	3.94649600
C	-3.13899800	2.52086300	-1.08054600
C	-2.25376200	3.38095000	-1.74614600
H	-1.34314500	2.98438400	-2.19603500
C	-2.51486200	4.74428900	-1.82315200
H	-1.80398100	5.39528200	-2.32987500
C	-3.67032000	5.27047000	-1.24531500
H	-3.87368500	6.33867800	-1.30210500

C	-4.56503300	4.42070700	-0.60037100
H	-5.47635300	4.82053000	-0.15661800
C	-4.30146900	3.05454800	-0.51251100
H	-5.00271100	2.40616800	0.01130500
C	-4.08951100	0.00801200	-0.08535800
C	-4.17028900	0.22435700	1.30075600
H	-3.41560500	0.84528400	1.79438600
C	-5.21103500	-0.32334500	2.04330900
H	-5.26210000	-0.13974900	3.11649500
C	-6.17763100	-1.10436800	1.41026200
H	-6.99035500	-1.54236700	1.98762600
C	-6.09497700	-1.33353700	0.03860900
H	-6.83929800	-1.95680000	-0.45508800
C	-5.05717500	-0.78131200	-0.71033100
H	-4.98429700	-0.98137600	-1.77881100

X-Ray Crystallography and Structure Refinement details

Crystalline samples of 3, 4, 5, 6, 7, 8, and 9 were placed on the tip of a 0.1 mm diameter glass capillary and mounted on a Bruker APEX II CCD diffractometer or a Bruker Photon 100 CMOS diffractometer for data collection at 173(2) K or 123(2) K. The data collection was carried out using Mo Kα radiation (graphite monochromator) or Cu Kα radiation (normal parabolic mirrors). The data intensity was corrected for absorption and decay (SADABS). Final cell constants were obtained from least-squares fits of all measured reflections and the structure was solved using SHELXS-08 and refined using SHELXL-08. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E- map. Full-matrix least-squares/difference Fourier cycles were performed to locate the remaining non-hydrogen atoms and all non-hydrogen atoms were refined with anisotropic displacement parameters Hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. A disordered phenyl group in 3 was modeled using SHELXTL EADP and SIMU constraints and a disordered benzene molecule was removed from the unit cell using Platon SQUEEZE12. A disordered benzene molecule was removed from the unit cell of 7 using Platon SQUEEZE12, and a phosphine oxide impurity modeled at 27% occupation for the titanium bound phosphine. A phenyl group in 9 was modeled over two positions and geometrical restraints SADI and DFIX were used to model a disordered benzene molecule.

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 3. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Hf1	4183(1)	11874(1)	3028(1)	21(1)
P1	6562(1)	13185(1)	3678(1)	27(1)
P2	3399(1)	10079(1)	2412(1)	23(1)
P3	2757(1)	11465(1)	3996(1)	25(1)
P4	4024(1)	12694(1)	1967(1)	24(1)
C1	7516(4)	13699(2)	3223(2)	33(1)
C2	7077(4)	14383(2)	3030(2)	38(1)
C3	7786(5)	14712(3)	2637(2)	48(1)
C4	8928(5)	14367(3)	2444(2)	54(1)
C5	9388(4)	13689(3)	2641(2)	53(1)
C6	8683(4)	13354(3)	3019(2)	42(1)
C7	7734(4)	13426(2)	4541(2)	35(1)
C8	9055(4)	13902(3)	4754(2)	53(1)
C9	9791(5)	14137(3)	5434(3)	70(2)
C10	9243(5)	13902(3)	5902(3)	64(2)
C11	7950(5)	13408(3)	5701(2)	50(1)
C12	7208(4)	13166(2)	5020(2)	39(1)
C13	5061(3)	13692(2)	3827(2)	23(1)
C14	4723(4)	14450(2)	4173(2)	31(1)
C15	3268(4)	14344(2)	4123(2)	34(1)
C16	2761(4)	13526(2)	3759(2)	30(1)

N2	3860(3)	13113(2)	3585(1)	24(1)
N1	5438(3)	11174(2)	2390(1)	24(1)
C19	4926(3)	10331(2)	2141(2)	25(1)
C20	5820(4)	9911(2)	1788(2)	35(1)
C21	6910(4)	10506(2)	1809(2)	36(1)
C22	6645(3)	11266(2)	2176(2)	28(1)
C23	1923(3)	9668(2)	1662(2)	28(1)
C24	2052(4)	9644(2)	1019(2)	39(1)
C25	896(5)	9336(3)	453(2)	60(1)
C26	-381(5)	9055(3)	541(3)	70(2)
C27	-534(4)	9091(3)	1175(3)	57(1)
C28	601(4)	9400(2)	1740(2)	38(1)
C29	3790(4)	9174(2)	2707(2)	32(1)
C30	2936(5)	8418(3)	2462(3)	61(1)
C31	4490(6)	7871(3)	3239(3)	73(2)
C32	5334(5)	8599(3)	3482(2)	51(1)
C33	4993(4)	9251(2)	3229(2)	36(1)
N3	5322(3)	11416(2)	3845(1)	22(1)
C35	4501(3)	11214(2)	4249(2)	23(1)
C36	2475(4)	12134(2)	4796(2)	29(1)
C37	1491(4)	11908(2)	5119(2)	42(1)
C38	1446(5)	12403(3)	5755(2)	56(1)
C39	2375(6)	13116(3)	6077(2)	54(1)
C40	3332(5)	13353(2)	5758(2)	42(1)
C41	3376(4)	12871(2)	5115(2)	34(1)
C42	1460(3)	10550(2)	3776(2)	27(1)
C43	36(4)	10612(2)	3498(2)	35(1)

C44	-992(4)	9930(3)	3299(2)	40(1)
C45	-611(4)	9186(3)	3385(2)	48(1)
C46	800(4)	9115(3)	3661(2)	46(1)
C47	1832(4)	9798(2)	3855(2)	35(1)
C48	5365(4)	10965(2)	4761(2)	34(1)
C49	6728(4)	10985(2)	4648(2)	35(1)
C50	6668(3)	11266(2)	4087(2)	29(1)
N4	2160(3)	11781(2)	2300(1)	24(1)
C52	750(3)	11473(2)	2148(2)	28(1)
C53	-7(4)	11684(2)	1607(2)	35(1)
C54	949(4)	12152(3)	1394(2)	37(1)
C55	2271(3)	12198(2)	1828(2)	25(1)
C56	4695(3)	12219(2)	1231(2)	28(1)
C57	3968(4)	11501(2)	734(2)	37(1)
C58	4548(5)	11128(3)	192(2)	59(1)
C59	5828(5)	11476(4)	153(2)	64(2)
C60	6564(5)	12167(3)	647(2)	54(1)
C61	6004(4)	12540(3)	1189(2)	40(1)
C62	3774(6)	13742(3)	1921(3)	66(1)
C63	3291(6)	14276(3)	2428(2)	60(1)
C64	3095(9)	15078(4)	2427(3)	101(2)
C73	3287(7)	7773(3)	2727(3)	86(2)
C70	4106(6)	14043(3)	1421(2)	60(1)
C71	3455(6)	15369(3)	1950(3)	66(1)
C72	3938(9)	14858(4)	1428(3)	101(2)

Bond lengths [Å] and angles [°] for 3.

Hf(1)-N(1)	2.175(3)	C(3)-H(3A)	0.9300
Hf(1)-N(4)	2.178(3)	C(4)-C(5)	1.391(7)
Hf(1)-N(2)	2.180(3)	C(4)-H(4A)	0.9300
Hf(1)-N(3)	2.189(3)	C(5)-C(6)	1.374(6)
Hf(1)-P(1)	2.9147(9)	C(5)-H(5A)	0.9300
Hf(1)-P(3)	2.9259(9)	C(6)-H(6A)	0.9300
Hf(1)-P(4)	2.9282(9)	C(7)-C(8)	1.391(5)
Hf(1)-P(2)	2.9333(9)	C(7)-C(12)	1.392(6)
P(1)-C(13)	1.783(3)	C(8)-C(9)	1.385(6)
P(1)-C(1)	1.825(4)	C(8)-H(8A)	0.9300
P(1)-C(7)	1.841(4)	C(9)-C(10)	1.361(8)
P(2)-C(19)	1.783(3)	C(9)-H(9A)	0.9300
P(2)-C(23)	1.821(3)	C(10)-C(11)	1.383(7)
P(2)-C(29)	1.837(4)	C(10)-H(10A)	0.9300
P(3)-C(35)	1.776(3)	C(11)-C(12)	1.389(5)
P(3)-C(42)	1.826(3)	C(11)-H(11A)	0.9300
P(3)-C(36)	1.843(3)	C(12)-H(12A)	0.9300
P(4)-C(55)	1.787(3)	C(13)-N(2)	1.386(4)
P(4)-C(56)	1.822(3)	C(13)-C(14)	1.386(4)
P(4)-C(62)	1.832(5)	C(14)-C(15)	1.397(5)
C(1)-C(2)	1.388(5)	C(14)-H(14A)	0.9300
C(1)-C(6)	1.407(5)	C(15)-C(16)	1.384(5)
C(2)-C(3)	1.396(5)	C(15)-H(15A)	0.9300
C(2)-H(2A)	0.9300	C(16)-N(2)	1.376(4)
C(3)-C(4)	1.377(7)	C(16)-H(16A)	0.9300

N(1)-C(22)	1.369(4)	C(32)-H(32A)	0.9300
N(1)-C(19)	1.397(4)	C(33)-H(33A)	0.9300
C(19)-C(20)	1.374(5)	N(3)-C(50)	1.362(4)
C(20)-C(21)	1.408(5)	N(3)-C(35)	1.388(4)
C(20)-H(20A)	0.9300	C(35)-C(48)	1.392(5)
C(21)-C(22)	1.376(5)	C(36)-C(41)	1.388(5)
C(21)-H(21A)	0.9300	C(36)-C(37)	1.392(5)
C(22)-H(22A)	0.9300	C(37)-C(38)	1.383(6)
C(23)-C(24)	1.382(5)	C(37)-H(37A)	0.9300
C(23)-C(28)	1.402(5)	C(38)-C(39)	1.372(7)
C(24)-C(25)	1.396(5)	C(38)-H(38A)	0.9300
C(24)-H(24A)	0.9300	C(39)-C(40)	1.372(6)
C(25)-C(26)	1.379(7)	C(39)-H(39A)	0.9300
C(25)-H(25A)	0.9300	C(40)-C(41)	1.387(5)
C(26)-C(27)	1.366(7)	C(40)-H(40A)	0.9300
C(26)-H(26A)	0.9300	C(41)-H(41A)	0.9300
C(27)-C(28)	1.383(5)	C(42)-C(47)	1.387(5)
C(27)-H(27A)	0.9300	C(42)-C(43)	1.403(5)
C(28)-H(28A)	0.9300	C(43)-C(44)	1.389(5)
C(29)-C(30)	1.385(5)	C(43)-H(43A)	0.9300
C(29)-C(33)	1.389(5)	C(44)-C(45)	1.381(6)
C(30)-C(73)	1.385(7)	C(44)-H(44A)	0.9300
C(30)-H(30A)	0.9300	C(45)-C(46)	1.395(6)
C(31)-C(32)	1.344(7)	C(45)-H(45A)	0.9300
C(31)-C(73)	1.370(8)	C(46)-C(47)	1.392(5)
C(31)-H(31A)	0.9300	C(46)-H(46A)	0.9300
C(32)-C(33)	1.380(6)	C(47)-H(47A)	0.9300

C(48)-C(49)	1.403(5)	C(63)-H(63A)	0.9300
C(48)-H(48A)	0.9300	C(64)-C(71)	1.339(7)
C(49)-C(50)	1.386(5)	C(64)-H(64A)	0.9300
C(49)-H(49A)	0.9300	C(73)-H(73A)	0.9300
C(50)-H(50A)	0.9300	C(70)-C(72)	1.396(7)
N(4)-C(52)	1.376(4)	C(70)-H(70A)	0.9300
N(4)-C(55)	1.391(4)	C(71)-C(72)	1.392(7)
C(52)-C(53)	1.362(5)	C(71)-H(71A)	0.9300
C(52)-H(52A)	0.9300	C(72)-H(72A)	0.9300
C(53)-C(54)	1.415(5)		
C(53)-H(53A)	0.9300		
C(54)-C(55)	1.387(5)		
C(54)-H(54A)	0.9300		
C(56)-C(61)	1.391(5)		
C(56)-C(57)	1.393(5)		
C(57)-C(58)	1.398(5)		
C(57)-H(57A)	0.9300		
C(58)-C(59)	1.381(7)		
C(58)-H(58A)	0.9300		
C(59)-C(60)	1.365(7)		
C(59)-H(59A)	0.9300		
C(60)-C(61)	1.388(5)		
C(60)-H(60A)	0.9300		
C(61)-H(61A)	0.9300		
C(62)-C(70)	1.384(6)		
C(62)-C(63)	1.385(6)		
C(63)-C(64)	1.384(7)		

N(1)-Hf(1)-N(4)	102.44(10)	P(4)-Hf(1)-P(2)	110.35(2)
N(1)-Hf(1)-N(2)	144.57(10)	C(13)-P(1)-C(1)	110.17(16)
N(4)-Hf(1)-N(2)	89.06(10)	C(13)-P(1)-C(7)	102.69(16)
N(1)-Hf(1)-N(3)	87.34(10)	C(1)-P(1)-C(7)	105.16(17)
N(4)-Hf(1)-N(3)	144.95(10)	C(13)-P(1)-Hf(1)	76.41(10)
N(2)-Hf(1)-N(3)	102.34(10)	C(1)-P(1)-Hf(1)	124.66(11)
N(1)-Hf(1)-P(1)	90.22(7)	C(7)-P(1)-Hf(1)	127.59(13)
N(4)-Hf(1)-P(1)	133.19(7)	C(19)-P(2)-C(23)	108.25(15)
N(2)-Hf(1)-P(1)	59.08(7)	C(19)-P(2)-C(29)	104.18(16)
N(3)-Hf(1)-P(1)	79.46(7)	C(23)-P(2)-C(29)	103.70(16)
N(1)-Hf(1)-P(3)	131.93(7)	C(19)-P(2)-Hf(1)	74.36(10)
N(4)-Hf(1)-P(3)	91.43(7)	C(23)-P(2)-Hf(1)	120.55(11)
N(2)-Hf(1)-P(3)	80.20(7)	C(29)-P(2)-Hf(1)	134.15(12)
N(3)-Hf(1)-P(3)	58.91(7)	C(35)-P(3)-C(42)	110.20(15)
P(1)-Hf(1)-P(3)	113.06(3)	C(35)-P(3)-C(36)	103.18(15)
N(1)-Hf(1)-P(4)	77.03(7)	C(42)-P(3)-C(36)	103.89(15)
N(4)-Hf(1)-P(4)	60.62(7)	C(35)-P(3)-Hf(1)	76.44(10)
N(2)-Hf(1)-P(4)	79.98(7)	C(42)-P(3)-Hf(1)	123.49(11)
N(3)-Hf(1)-P(4)	153.55(7)	C(36)-P(3)-Hf(1)	130.01(11)
P(1)-Hf(1)-P(4)	79.40(2)	C(55)-P(4)-C(56)	108.26(15)
P(3)-Hf(1)-P(4)	145.74(2)	C(55)-P(4)-C(62)	104.5(2)
N(1)-Hf(1)-P(2)	60.63(7)	C(56)-P(4)-C(62)	104.5(2)
N(4)-Hf(1)-P(2)	76.98(7)	C(55)-P(4)-Hf(1)	74.42(11)
N(2)-Hf(1)-P(2)	154.35(7)	C(56)-P(4)-Hf(1)	118.98(12)
N(3)-Hf(1)-P(2)	79.01(7)	C(62)-P(4)-Hf(1)	134.77(16)
P(1)-Hf(1)-P(2)	144.26(2)	C(2)-C(1)-C(6)	118.8(4)
P(3)-Hf(1)-P(2)	78.77(2)	C(2)-C(1)-P(1)	122.6(3)

C(6)-C(1)-P(1)	118.5(3)	C(11)-C(10)-H(10A)	119.9
C(1)-C(2)-C(3)	120.0(4)	C(10)-C(11)-C(12)	119.3(5)
C(1)-C(2)-H(2A)	120.0	C(10)-C(11)-H(11A)	120.4
C(3)-C(2)-H(2A)	120.0	C(12)-C(11)-H(11A)	120.4
C(4)-C(3)-C(2)	120.4(4)	C(11)-C(12)-C(7)	121.0(4)
C(4)-C(3)-H(3A)	119.8	C(11)-C(12)-H(12A)	119.5
C(2)-C(3)-H(3A)	119.8	C(7)-C(12)-H(12A)	119.5
C(3)-C(4)-C(5)	120.0(4)	N(2)-C(13)-C(14)	109.6(3)
C(3)-C(4)-H(4A)	120.0	N(2)-C(13)-P(1)	109.1(2)
C(5)-C(4)-H(4A)	120.0	C(14)-C(13)-P(1)	140.7(3)
C(6)-C(5)-C(4)	119.9(4)	C(13)-C(14)-C(15)	106.7(3)
C(6)-C(5)-H(5A)	120.1	C(13)-C(14)-H(14A)	126.6
C(4)-C(5)-H(5A)	120.1	C(15)-C(14)-H(14A)	126.6
C(5)-C(6)-C(1)	120.8(4)	C(16)-C(15)-C(14)	107.5(3)
C(5)-C(6)-H(6A)	119.6	C(16)-C(15)-H(15A)	126.2
C(1)-C(6)-H(6A)	119.6	C(14)-C(15)-H(15A)	126.2
C(8)-C(7)-C(12)	118.4(4)	N(2)-C(16)-C(15)	109.6(3)
C(8)-C(7)-P(1)	124.1(3)	N(2)-C(16)-H(16A)	125.2
C(12)-C(7)-P(1)	117.3(3)	C(15)-C(16)-H(16A)	125.2
C(9)-C(8)-C(7)	120.1(5)	C(16)-N(2)-C(13)	106.5(3)
C(9)-C(8)-H(8A)	119.9	C(16)-N(2)-Hf(1)	138.4(2)
C(7)-C(8)-H(8A)	119.9	C(13)-N(2)-Hf(1)	115.04(19)
C(10)-C(9)-C(8)	120.8(4)	C(22)-N(1)-C(19)	106.4(3)
C(10)-C(9)-H(9A)	119.6	C(22)-N(1)-Hf(1)	141.4(2)
C(8)-C(9)-H(9A)	119.6	C(19)-N(1)-Hf(1)	112.0(2)
C(9)-C(10)-C(11)	120.3(4)	C(20)-C(19)-N(1)	109.5(3)
C(9)-C(10)-H(10A)	119.9	C(20)-C(19)-P(2)	137.3(3)

N(1)-C(19)-P(2)	113.0(2)	C(23)-C(28)-H(28A)	120.0
C(19)-C(20)-C(21)	106.8(3)	C(30)-C(29)-C(33)	116.8(4)
C(19)-C(20)-H(20A)	126.6	C(30)-C(29)-P(2)	124.6(3)
C(21)-C(20)-H(20A)	126.6	C(33)-C(29)-P(2)	118.5(3)
C(22)-C(21)-C(20)	107.3(3)	C(29)-C(30)-C(73)	120.9(5)
C(22)-C(21)-H(21A)	126.3	C(29)-C(30)-H(30A)	119.5
C(20)-C(21)-H(21A)	126.3	C(73)-C(30)-H(30A)	119.5
N(1)-C(22)-C(21)	110.0(3)	C(32)-C(31)-C(73)	119.5(5)
N(1)-C(22)-H(22A)	125.0	C(32)-C(31)-H(31A)	120.3
C(21)-C(22)-H(22A)	125.0	C(73)-C(31)-H(31A)	120.3
C(24)-C(23)-C(28)	119.0(3)	C(31)-C(32)-C(33)	120.8(5)
C(24)-C(23)-P(2)	121.7(3)	C(31)-C(32)-H(32A)	119.6
C(28)-C(23)-P(2)	119.3(3)	C(33)-C(32)-H(32A)	119.6
C(23)-C(24)-C(25)	120.5(4)	C(32)-C(33)-C(29)	121.4(4)
C(23)-C(24)-H(24A)	119.8	C(32)-C(33)-H(33A)	119.3
C(25)-C(24)-H(24A)	119.8	C(29)-C(33)-H(33A)	119.3
C(26)-C(25)-C(24)	119.4(5)	C(50)-N(3)-C(35)	107.5(3)
C(26)-C(25)-H(25A)	120.3	C(50)-N(3)-Hf(1)	137.6(2)
C(24)-C(25)-H(25A)	120.3	C(35)-N(3)-Hf(1)	114.91(19)
C(27)-C(26)-C(25)	120.8(4)	N(3)-C(35)-C(48)	108.9(3)
C(27)-C(26)-H(26A)	119.6	N(3)-C(35)-P(3)	109.6(2)
C(25)-C(26)-H(26A)	119.6	C(48)-C(35)-P(3)	141.1(3)
C(26)-C(27)-C(28)	120.3(4)	C(41)-C(36)-C(37)	118.8(3)
C(26)-C(27)-H(27A)	119.8	C(41)-C(36)-P(3)	117.5(3)
C(28)-C(27)-H(27A)	119.8	C(37)-C(36)-P(3)	123.4(3)
C(27)-C(28)-C(23)	120.0(4)	C(38)-C(37)-C(36)	120.0(4)
C(27)-C(28)-H(28A)	120.0	C(38)-C(37)-H(37A)	120.0

C(36)-C(37)-H(37A)	120.0	C(45)-C(46)-H(46A)	120.0
C(39)-C(38)-C(37)	120.7(4)	C(42)-C(47)-C(46)	120.2(3)
C(39)-C(38)-H(38A)	119.7	C(42)-C(47)-H(47A)	119.9
C(37)-C(38)-H(38A)	119.7	C(46)-C(47)-H(47A)	119.9
C(40)-C(39)-C(38)	119.8(4)	C(35)-C(48)-C(49)	106.7(3)
C(40)-C(39)-H(39A)	120.1	C(35)-C(48)-H(48A)	126.7
C(38)-C(39)-H(39A)	120.1	C(49)-C(48)-H(48A)	126.7
C(39)-C(40)-C(41)	120.3(4)	C(50)-C(49)-C(48)	107.4(3)
C(39)-C(40)-H(40A)	119.9	C(50)-C(49)-H(49A)	126.3
C(41)-C(40)-H(40A)	119.9	C(48)-C(49)-H(49A)	126.3
C(40)-C(41)-C(36)	120.3(3)	N(3)-C(50)-C(49)	109.5(3)
C(40)-C(41)-H(41A)	119.8	N(3)-C(50)-H(50A)	125.2
C(36)-C(41)-H(41A)	119.8	C(49)-C(50)-H(50A)	125.2
C(47)-C(42)-C(43)	119.3(3)	C(52)-N(4)-C(55)	105.9(3)
C(47)-C(42)-P(3)	122.8(3)	C(52)-N(4)-Hf(1)	142.0(2)
C(43)-C(42)-P(3)	117.9(3)	C(55)-N(4)-Hf(1)	112.09(19)
C(44)-C(43)-C(42)	120.6(4)	C(53)-C(52)-N(4)	110.5(3)
C(44)-C(43)-H(43A)	119.7	C(53)-C(52)-H(52A)	124.7
C(42)-C(43)-H(43A)	119.7	N(4)-C(52)-H(52A)	124.7
C(45)-C(44)-C(43)	119.6(4)	C(52)-C(53)-C(54)	107.7(3)
C(45)-C(44)-H(44A)	120.2	C(52)-C(53)-H(53A)	126.2
C(43)-C(44)-H(44A)	120.2	C(54)-C(53)-H(53A)	126.2
C(44)-C(45)-C(46)	120.3(4)	C(55)-C(54)-C(53)	105.9(3)
C(44)-C(45)-H(45A)	119.9	C(55)-C(54)-H(54A)	127.1
C(46)-C(45)-H(45A)	119.9	C(53)-C(54)-H(54A)	127.1
C(47)-C(46)-C(45)	120.0(4)	C(54)-C(55)-N(4)	110.0(3)
C(47)-C(46)-H(46A)	120.0	C(54)-C(55)-P(4)	137.0(3)

N(4)-C(55)-P(4)	112.9(2)	C(70)-C(62)-P(4)	123.2(4)
C(61)-C(56)-C(57)	119.3(3)	C(63)-C(62)-P(4)	118.7(4)
C(61)-C(56)-P(4)	119.6(3)	C(64)-C(63)-C(62)	121.6(5)
C(57)-C(56)-P(4)	120.9(3)	C(64)-C(63)-H(63A)	119.2
C(56)-C(57)-C(58)	119.5(4)	C(62)-C(63)-H(63A)	119.2
C(56)-C(57)-H(57A)	120.3	C(71)-C(64)-C(63)	119.7(5)
C(58)-C(57)-H(57A)	120.3	C(71)-C(64)-H(64A)	120.1
C(59)-C(58)-C(57)	119.9(4)	C(63)-C(64)-H(64A)	120.1
C(59)-C(58)-H(58A)	120.0	C(31)-C(73)-C(30)	120.5(5)
C(57)-C(58)-H(58A)	120.0	C(31)-C(73)-H(73A)	119.7
C(60)-C(59)-C(58)	120.9(4)	C(30)-C(73)-H(73A)	119.7
C(60)-C(59)-H(59A)	119.5	C(62)-C(70)-C(72)	120.4(5)
C(58)-C(59)-H(59A)	119.5	C(62)-C(70)-H(70A)	119.8
C(59)-C(60)-C(61)	119.7(4)	C(72)-C(70)-H(70A)	119.8
C(59)-C(60)-H(60A)	120.2	C(64)-C(71)-C(72)	120.9(5)
C(61)-C(60)-H(60A)	120.2	C(64)-C(71)-H(71A)	119.6
C(60)-C(61)-C(56)	120.6(4)	C(72)-C(71)-H(71A)	119.6
C(60)-C(61)-H(61A)	119.7	C(71)-C(72)-C(70)	119.2(5)
C(56)-C(61)-H(61A)	119.7	C(71)-C(72)-H(72A)	120.4
C(70)-C(62)-C(63)	118.0(4)	C(70)-C(72)-H(72A)	120.4

Symmetry transformations used to generate equivalent atoms:

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	$U_{11}U_{22}$	U_{33}	U_{23}	U_{13}	U_{12}	
Hf1	19(1)	24(1)	18(1)	3(1)	4(1)	-1(1)
P1	19(1)	27(1)	30(1)	4(1)	3(1)	-1(1)
P2	22(1)	23(1)	21(1)	2(1)	5(1)	1(1)
P3	21(1)	27(1)	28(1)	10(1)	9(1)	3(1)
P4	24(1)	28(1)	18(1)	5(1)	6(1)	1(1)
C1	23(2)	33(2)	35(2)	2(2)	6(1)	-6(1)
C2	36(2)	34(2)	35(2)	1(2)	7(2)	-5(2)
C3	60(3)	40(2)	40(2)	11(2)	13(2)	-12(2)
C4	53(3)	61(3)	39(2)	3(2)	18(2)	-23(2)
C5	32(2)	64(3)	53(3)	0(2)	18(2)	-12(2)
C6	28(2)	42(2)	51(2)	7(2)	12(2)	-3(2)
C7	28(2)	26(2)	41(2)	3(2)	-3(2)	6(1)
C8	37(2)	45(2)	67(3)	29(2)	-17(2)	-9(2)
C9	52(3)	51(3)	85(4)	34(3)	-40(3)	-18(2)
C10	66(3)	43(3)	53(3)	6(2)	-35(2)	5(2)
C11	50(2)	52(3)	34(2)	1(2)	-2(2)	17(2)
C12	29(2)	48(2)	30(2)	0(2)	1(2)	5(2)
C13	20(1)	22(2)	24(2)	4(1)	3(1)	2(1)
C14	41(2)	24(2)	24(2)	1(1)	6(2)	2(1)
C15	45(2)	34(2)	26(2)	4(2)	15(2)	17(2)
C16	24(2)	41(2)	29(2)	11(2)	10(1)	10(1)
N2	23(1)	23(1)	23(1)	3(1)	6(1)	2(1)

N1	22(1)	26(1)	23(1)	5(1)	5(1)	1(1)
C19	22(2)	27(2)	22(2)	2(1)	3(1)	2(1)
C20	31(2)	33(2)	37(2)	2(2)	12(2)	7(2)
C21	25(2)	45(2)	40(2)	8(2)	16(2)	10(2)
C22	23(2)	33(2)	30(2)	9(1)	9(1)	2(1)
C23	23(2)	25(2)	26(2)	-3(1)	2(1)	3(1)
C24	33(2)	47(2)	30(2)	2(2)	3(2)	8(2)
C25	55(3)	78(3)	29(2)	-2(2)	-5(2)	16(2)
C26	37(2)	77(4)	60(3)	-10(3)	-19(2)	10(2)
C27	26(2)	55(3)	68(3)	-8(2)	2(2)	2(2)
C28	29(2)	34(2)	44(2)	1(2)	10(2)	-1(2)
C29	35(2)	29(2)	33(2)	8(2)	11(2)	6(2)
C30	57(3)	35(2)	81(4)	19(2)	-6(2)	-2(2)
C31	91(4)	54(3)	93(4)	48(3)	25(3)	26(3)
C32	56(3)	57(3)	52(3)	30(2)	19(2)	22(2)
C33	39(2)	38(2)	34(2)	13(2)	10(2)	10(2)
N3	21(1)	26(1)	21(1)	7(1)	6(1)	5(1)
C35	24(2)	25(2)	23(2)	9(1)	12(1)	4(1)
C36	30(2)	32(2)	32(2)	15(2)	15(1)	12(1)
C37	51(2)	33(2)	54(2)	16(2)	32(2)	13(2)
C38	83(3)	44(3)	65(3)	24(2)	56(3)	22(2)
C39	95(4)	38(2)	44(2)	13(2)	42(3)	25(2)
C40	55(2)	35(2)	38(2)	10(2)	13(2)	12(2)
C41	33(2)	35(2)	35(2)	11(2)	12(2)	8(2)
C42	25(2)	28(2)	31(2)	9(1)	13(1)	1(1)
C43	26(2)	43(2)	42(2)	19(2)	12(2)	6(2)
C44	26(2)	49(2)	46(2)	17(2)	11(2)	-3(2)

C45	40(2)	46(2)	56(3)	15(2)	12(2)	-14(2)
C46	46(2)	36(2)	61(3)	22(2)	15(2)	2(2)
C47	31(2)	38(2)	39(2)	17(2)	10(2)	2(2)
C48	35(2)	42(2)	30(2)	16(2)	11(2)	8(2)
C49	29(2)	43(2)	35(2)	16(2)	4(2)	12(2)
C50	20(2)	36(2)	32(2)	9(2)	8(1)	6(1)
N4	19(1)	27(1)	21(1)	4(1)	3(1)	0(1)
C52	21(2)	32(2)	30(2)	6(1)	8(1)	1(1)
C53	19(2)	52(2)	35(2)	15(2)	3(1)	5(2)
C54	27(2)	56(2)	31(2)	19(2)	7(2)	9(2)
C55	20(2)	33(2)	21(2)	8(1)	5(1)	4(1)
C56	26(2)	40(2)	19(2)	10(1)	5(1)	7(1)
C57	33(2)	46(2)	27(2)	3(2)	6(2)	9(2)
C58	64(3)	69(3)	32(2)	-6(2)	9(2)	20(2)
C59	56(3)	105(4)	38(2)	13(3)	28(2)	35(3)
C60	38(2)	97(4)	43(2)	33(3)	22(2)	22(2)
C61	34(2)	57(3)	32(2)	16(2)	11(2)	2(2)
C62	102(3)	38(2)	71(2)	24(2)	41(2)	20(2)
C63	96(3)	45(2)	57(2)	22(2)	40(2)	27(2)
C64	182(5)	64(3)	101(4)	46(3)	90(4)	57(3)
C73	82(4)	41(3)	122(5)	36(3)	-9(4)	-5(3)
C70	96(3)	45(2)	57(2)	22(2)	40(2)	27(2)
C71	102(3)	38(2)	71(2)	24(2)	41(2)	20(2)
C72	182(5)	64(3)	101(4)	46(3)	90(4)	57(3)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 4. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	zU_{eq}	
Ti1	3590(1)	3048(1)	3375(1)	10(1)
Ni1	2602(1)	2919(1)	2037(1)	10(1)
P4	1506(1)	3966(1)	2535(1)	11(1)
P3	2612(1)	1407(1)	1934(1)	11(1)
P2	3838(1)	3518(1)	1169(1)	12(1)
P1	2744(1)	1963(1)	4652(1)	13(1)
N4	2651(1)	3933(1)	4117(1)	11(1)
N3	4340(1)	1834(1)	2959(1)	12(1)
N2	4506(1)	4094(1)	2903(1)	14(1)
N1	4490(1)	2978(1)	4616(1)	14(1)
C1	1743(2)	4270(1)	3732(1)	13(1)
C2	2766(2)	4330(1)	4994(1)	15(1)
C3	1961(2)	4910(2)	5168(2)	18(1)
C4	1305(2)	4879(1)	4361(2)	18(1)
C5	1493(2)	5098(1)	2028(1)	14(1)
C6	754(2)	5318(2)	1355(2)	20(1)
C7	770(2)	6202(2)	1023(2)	24(1)
C8	1517(2)	6861(2)	1357(2)	24(1)
C9	2261(2)	6641(2)	2023(2)	22(1)
C10	2257(2)	5764(2)	2353(2)	18(1)
C11	162(2)	3484(1)	2348(2)	15(1)
C12	-111(2)	2981(2)	1516(2)	20(1)

C13	-1086(2)	2522(2)	1390(2)	27(1)
C14	-1791(2)	2551(2)	2093(2)	31(1)
C15	-1532(2)	3058(2)	2912(2)	28(1)
C16	-561(2)	3526(2)	3039(2)	21(1)
C17	2449(2)	1032(1)	703(2)	16(1)
C18	3288(2)	854(2)	153(2)	18(1)
C19	3122(2)	625(2)	-789(2)	26(1)
C20	2120(2)	579(2)	-1184(2)	36(1)
C21	1272(2)	753(2)	-639(2)	41(1)
C22	1431(2)	978(2)	300(2)	28(1)
C23	1639(2)	645(1)	2432(1)	14(1)
C24	1800(2)	-296(2)	2493(2)	21(1)
C25	1012(2)	-873(2)	2791(2)	25(1)
C26	57(2)	-526(2)	3027(2)	25(1)
C27	-104(2)	404(2)	2971(2)	22(1)
C28	688(2)	991(2)	2681(2)	17(1)
C29	3891(2)	1146(1)	2353(1)	13(1)
C30	5298(2)	1532(2)	3236(2)	16(1)
C31	5465(2)	683(2)	2807(2)	20(1)
C32	4563(2)	428(2)	2247(2)	18(1)
C33	4646(2)	4226(1)	1968(1)	13(1)
C34	5155(2)	4739(2)	3386(2)	20(1)
C35	5709(2)	5254(2)	2790(2)	22(1)
C36	5393(2)	4932(2)	1886(2)	17(1)
C37	3192(2)	4230(2)	344(1)	15(1)
C38	3356(2)	5182(2)	348(2)	17(1)
C39	2824(2)	5687(2)	-297(2)	21(1)

C40	2136(2)	5246(2)	-949(2)	27(1)
C41	1958(2)	4301(2)	-953(2)	30(1)
C42	2471(2)	3790(2)	-305(2)	23(1)
C43	4737(2)	2851(1)	464(2)	14(1)
C44	5439(2)	2310(1)	932(2)	16(1)
C45	6110(2)	1756(2)	439(2)	20(1)
C46	6096(2)	1744(2)	-519(2)	24(1)
C47	5409(2)	2283(2)	-984(2)	24(1)
C48	4728(2)	2833(2)	-500(2)	18(1)
C49	3965(2)	2396(1)	5190(2)	16(1)
C50	2680(2)	719(1)	4774(1)	16(1)
C51	3560(2)	222(2)	4583(2)	22(1)
C52	3527(2)	-728(2)	4630(2)	27(1)
C53	2609(2)	-1190(2)	4861(2)	27(1)
C54	1729(2)	-704(2)	5041(2)	26(1)
C55	1759(2)	251(2)	4998(2)	21(1)
C56	1690(2)	2368(1)	5368(2)	18(1)
C57	1821(2)	2506(2)	6326(2)	28(1)
C58	997(3)	2824(2)	6836(2)	37(1)
C59	57(2)	3014(2)	6410(2)	35(1)
C60	-81(2)	2866(2)	5463(2)	29(1)
C61	732(2)	2543(2)	4944(2)	22(1)
C62	4546(2)	2324(2)	6004(2)	24(1)
C63	5465(2)	2880(2)	5930(2)	26(1)
C64	5408(2)	3264(2)	5080(2)	19(1)

Bond lengths [Å] and angles [°] for 4.

Ti(1)-N(2)	2.0433(17)	N(2)-C(34)	1.368(3)
Ti(1)-N(4)	2.0800(17)	N(2)-C(33)	1.397(3)
Ti(1)-N(1)	2.1053(17)	N(1)-C(64)	1.366(3)
Ti(1)-N(3)	2.1089(17)	N(1)-C(49)	1.390(3)
Ti(1)-Ni(1)	2.2665(5)	C(1)-C(4)	1.385(3)
Ti(1)-P(1)	2.7224(7)	C(2)-C(3)	1.377(3)
Ni(1)-P(3)	2.1906(6)	C(2)-H(3)	0.9500
Ni(1)-P(4)	2.2181(6)	C(3)-C(4)	1.409(3)
Ni(1)-P(2)	2.2354(6)	C(3)-H(1)	0.9500
P(4)-C(1)	1.779(2)	C(4)-H(2)	0.9500
P(4)-C(11)	1.832(2)	C(5)-C(6)	1.389(3)
P(4)-C(5)	1.835(2)	C(5)-C(10)	1.395(3)
P(3)-C(29)	1.782(2)	C(6)-C(7)	1.392(3)
P(3)-C(23)	1.826(2)	C(6)-H(8)	0.9500
P(3)-C(17)	1.839(2)	C(7)-C(8)	1.377(4)
P(2)-C(33)	1.776(2)	C(7)-H(4)	0.9500
P(2)-C(37)	1.818(2)	C(8)-C(9)	1.386(3)
P(2)-C(43)	1.839(2)	C(8)-H(5)	0.9500
P(1)-C(49)	1.791(2)	C(9)-C(10)	1.383(3)
P(1)-C(50)	1.821(2)	C(9)-H(6)	0.9500
P(1)-C(56)	1.830(2)	C(10)-H(7)	0.9500
N(4)-C(2)	1.368(3)	C(11)-C(16)	1.391(3)
N(4)-C(1)	1.385(3)	C(11)-C(12)	1.400(3)
N(3)-C(30)	1.369(3)	C(12)-C(13)	1.389(3)
N(3)-C(29)	1.385(3)	C(12)-H(13)	0.9500

C(13)-C(14)	1.387(4)	C(27)-H(20)	0.9500
C(13)-H(9)	0.9500	C(28)-H(19)	0.9500
C(14)-C(15)	1.385(4)	C(29)-C(32)	1.382(3)
C(14)-H(10)	0.9500	C(30)-C(31)	1.378(3)
C(15)-C(16)	1.390(3)	C(30)-H(24)	0.9500
C(15)-H(11)	0.9500	C(31)-C(32)	1.407(3)
C(16)-H(12)	0.9500	C(31)-H(26)	0.9500
C(17)-C(18)	1.387(3)	C(32)-H(25)	0.9500
C(17)-C(22)	1.401(3)	C(33)-C(36)	1.384(3)
C(18)-C(19)	1.394(3)	C(34)-C(35)	1.373(3)
C(18)-H(18)	0.9500	C(34)-H(27)	0.9500
C(19)-C(20)	1.379(4)	C(35)-C(36)	1.406(3)
C(19)-H(14)	0.9500	C(35)-H(28)	0.9500
C(20)-C(21)	1.390(4)	C(36)-H(29)	0.9500
C(20)-H(15)	0.9500	C(37)-C(38)	1.388(3)
C(21)-C(22)	1.388(4)	C(37)-C(42)	1.399(3)
C(21)-H(16)	0.9500	C(38)-C(39)	1.391(3)
C(22)-H(17)	0.9500	C(38)-H(34)	0.9500
C(23)-C(28)	1.387(3)	C(39)-C(40)	1.378(3)
C(23)-C(24)	1.395(3)	C(39)-H(33)	0.9500
C(24)-C(25)	1.381(3)	C(40)-C(41)	1.380(4)
C(24)-H(23)	0.9500	C(40)-H(32)	0.9500
C(25)-C(26)	1.386(4)	C(41)-C(42)	1.389(3)
C(25)-H(22)	0.9500	C(41)-H(31)	0.9500
C(26)-C(27)	1.380(3)	C(42)-H(30)	0.9500
C(26)-H(21)	0.9500	C(43)-C(44)	1.395(3)
C(27)-C(28)	1.388(3)	C(43)-C(48)	1.396(3)

C(44)-C(45)	1.390(3)	C(59)-C(60)	1.381(4)
C(44)-H(39)	0.9500	C(59)-H(46)	0.9500
C(45)-C(46)	1.388(3)	C(60)-C(61)	1.389(3)
C(45)-H(38)	0.9500	C(60)-H(47)	0.9500
C(46)-C(47)	1.379(4)	C(61)-H(48)	0.9500
C(46)-H(37)	0.9500	C(62)-C(63)	1.408(4)
C(47)-C(48)	1.389(3)	C(62)-H(52)	0.9500
C(47)-H(36)	0.9500	C(63)-C(64)	1.382(3)
C(48)-H(35)	0.9500	C(63)-H(51)	0.9500
C(49)-C(62)	1.380(3)	C(64)-H(50)	0.9500
C(50)-C(51)	1.389(3)		
C(50)-C(55)	1.393(3)	N(2)-Ti(1)-N(4)	94.10(7)
C(51)-C(52)	1.381(3)	N(2)-Ti(1)-N(1)	94.14(7)
C(51)-H(44)	0.9500	N(4)-Ti(1)-N(1)	86.31(7)
C(52)-C(53)	1.390(4)	N(2)-Ti(1)-N(3)	104.42(7)
C(52)-H(43)	0.9500	N(4)-Ti(1)-N(3)	159.94(7)
C(53)-C(54)	1.377(4)	N(1)-Ti(1)-N(3)	84.76(7)
C(53)-H(42)	0.9500	N(2)-Ti(1)-Ni(1)	91.67(5)
C(54)-C(55)	1.388(3)	N(4)-Ti(1)-Ni(1)	97.93(5)
C(54)-H(41)	0.9500	N(1)-Ti(1)-Ni(1)	172.55(5)
C(55)-H(40)	0.9500	N(3)-Ti(1)-Ni(1)	89.28(5)
C(56)-C(61)	1.386(3)	N(2)-Ti(1)-P(1)	156.67(5)
C(56)-C(57)	1.395(3)	N(4)-Ti(1)-P(1)	76.23(5)
C(57)-C(58)	1.391(4)	N(1)-Ti(1)-P(1)	64.45(5)
C(57)-H(49)	0.9500	N(3)-Ti(1)-P(1)	83.72(5)
C(58)-C(59)	1.372(4)	Ni(1)-Ti(1)-P(1)	110.50(2)
C(58)-H(45)	0.9500	P(3)-Ni(1)-P(4)	135.91(2)

P(3)-Ni(1)-P(2)	110.19(2)	C(50)-P(1)-Ti(1)	133.00(7)
P(4)-Ni(1)-P(2)	112.47(2)	C(56)-P(1)-Ti(1)	121.06(7)
P(3)-Ni(1)-Ti(1)	93.82(2)	C(2)-N(4)-C(1)	106.19(16)
P(4)-Ni(1)-Ti(1)	92.78(2)	C(2)-N(4)-Ti(1)	131.55(14)
P(2)-Ni(1)-Ti(1)	95.47(2)	C(1)-N(4)-Ti(1)	122.21(13)
C(1)-P(4)-C(11)	109.02(10)	C(30)-N(3)-C(29)	106.12(16)
C(1)-P(4)-C(5)	102.48(9)	C(30)-N(3)-Ti(1)	129.65(14)
C(11)-P(4)-C(5)	104.80(9)	C(29)-N(3)-Ti(1)	124.17(13)
C(1)-P(4)-Ni(1)	111.32(7)	C(34)-N(2)-C(33)	106.23(17)
C(11)-P(4)-Ni(1)	108.64(7)	C(34)-N(2)-Ti(1)	129.56(15)
C(5)-P(4)-Ni(1)	119.99(7)	C(33)-N(2)-Ti(1)	124.01(13)
C(29)-P(3)-C(23)	109.49(9)	C(64)-N(1)-C(49)	106.35(18)
C(29)-P(3)-C(17)	109.25(10)	C(64)-N(1)-Ti(1)	144.75(16)
C(23)-P(3)-C(17)	100.87(9)	C(49)-N(1)-Ti(1)	108.87(13)
C(29)-P(3)-Ni(1)	104.63(7)	N(4)-C(1)-C(4)	110.03(18)
C(23)-P(3)-Ni(1)	124.39(7)	N(4)-C(1)-P(4)	114.84(14)
C(17)-P(3)-Ni(1)	107.66(7)	C(4)-C(1)-P(4)	134.42(16)
C(33)-P(2)-C(37)	109.87(10)	N(4)-C(2)-C(3)	110.45(18)
C(33)-P(2)-C(43)	105.89(9)	N(4)-C(2)-H(3)	124.8
C(37)-P(2)-C(43)	103.60(10)	C(3)-C(2)-H(3)	124.8
C(33)-P(2)-Ni(1)	103.95(7)	C(2)-C(3)-C(4)	107.08(18)
C(37)-P(2)-Ni(1)	107.56(7)	C(2)-C(3)-H(1)	126.5
C(43)-P(2)-Ni(1)	125.51(7)	C(4)-C(3)-H(1)	126.5
C(49)-P(1)-C(50)	106.80(10)	C(1)-C(4)-C(3)	106.24(18)
C(49)-P(1)-C(56)	107.88(10)	C(1)-C(4)-H(2)	126.9
C(50)-P(1)-C(56)	103.07(10)	C(3)-C(4)-H(2)	126.9
C(49)-P(1)-Ti(1)	76.00(7)	C(6)-C(5)-C(10)	119.3(2)

C(6)-C(5)-P(4)	123.13(17)	C(15)-C(14)-H(10)	120.1
C(10)-C(5)-P(4)	117.54(16)	C(13)-C(14)-H(10)	120.1
C(5)-C(6)-C(7)	120.0(2)	C(14)-C(15)-C(16)	120.2(2)
C(5)-C(6)-H(8)	120.0	C(14)-C(15)-H(11)	119.9
C(7)-C(6)-H(8)	120.0	C(16)-C(15)-H(11)	119.9
C(8)-C(7)-C(6)	120.4(2)	C(15)-C(16)-C(11)	120.4(2)
C(8)-C(7)-H(4)	119.8	C(15)-C(16)-H(12)	119.8
C(6)-C(7)-H(4)	119.8	C(11)-C(16)-H(12)	119.8
C(7)-C(8)-C(9)	119.7(2)	C(18)-C(17)-C(22)	119.1(2)
C(7)-C(8)-H(5)	120.1	C(18)-C(17)-P(3)	122.90(16)
C(9)-C(8)-H(5)	120.1	C(22)-C(17)-P(3)	117.88(17)
C(10)-C(9)-C(8)	120.3(2)	C(17)-C(18)-C(19)	120.5(2)
C(10)-C(9)-H(6)	119.8	C(17)-C(18)-H(18)	119.8
C(8)-C(9)-H(6)	119.8	C(19)-C(18)-H(18)	119.8
C(9)-C(10)-C(5)	120.1(2)	C(20)-C(19)-C(18)	120.2(2)
C(9)-C(10)-H(7)	119.9	C(20)-C(19)-H(14)	119.9
C(5)-C(10)-H(7)	119.9	C(18)-C(19)-H(14)	119.9
C(16)-C(11)-C(12)	119.1(2)	C(19)-C(20)-C(21)	119.8(2)
C(16)-C(11)-P(4)	121.97(16)	C(19)-C(20)-H(15)	120.1
C(12)-C(11)-P(4)	118.66(17)	C(21)-C(20)-H(15)	120.1
C(13)-C(12)-C(11)	120.2(2)	C(22)-C(21)-C(20)	120.2(2)
C(13)-C(12)-H(13)	119.9	C(22)-C(21)-H(16)	119.9
C(11)-C(12)-H(13)	119.9	C(20)-C(21)-H(16)	119.9
C(14)-C(13)-C(12)	120.2(2)	C(21)-C(22)-C(17)	120.1(2)
C(14)-C(13)-H(9)	119.9	C(21)-C(22)-H(17)	119.9
C(12)-C(13)-H(9)	119.9	C(17)-C(22)-H(17)	119.9
C(15)-C(14)-C(13)	119.9(2)	C(28)-C(23)-C(24)	119.3(2)

C(28)-C(23)-P(3)	119.40(16)	C(29)-C(32)-H(25)	126.9
C(24)-C(23)-P(3)	121.03(17)	C(31)-C(32)-H(25)	126.9
C(25)-C(24)-C(23)	119.9(2)	C(36)-C(33)-N(2)	109.46(18)
C(25)-C(24)-H(23)	120.1	C(36)-C(33)-P(2)	134.38(17)
C(23)-C(24)-H(23)	120.1	N(2)-C(33)-P(2)	116.13(14)
C(24)-C(25)-C(26)	120.6(2)	N(2)-C(34)-C(35)	110.30(19)
C(24)-C(25)-H(22)	119.7	N(2)-C(34)-H(27)	124.9
C(26)-C(25)-H(22)	119.7	C(35)-C(34)-H(27)	124.9
C(27)-C(26)-C(25)	119.7(2)	C(34)-C(35)-C(36)	107.48(19)
C(27)-C(26)-H(21)	120.2	C(34)-C(35)-H(28)	126.3
C(25)-C(26)-H(21)	120.2	C(36)-C(35)-H(28)	126.3
C(26)-C(27)-C(28)	120.1(2)	C(33)-C(36)-C(35)	106.51(19)
C(26)-C(27)-H(20)	119.9	C(33)-C(36)-H(29)	126.7
C(28)-C(27)-H(20)	119.9	C(35)-C(36)-H(29)	126.7
C(23)-C(28)-C(27)	120.3(2)	C(38)-C(37)-C(42)	119.2(2)
C(23)-C(28)-H(19)	119.8	C(38)-C(37)-P(2)	123.22(16)
C(27)-C(28)-H(19)	119.8	C(42)-C(37)-P(2)	117.60(17)
C(32)-C(29)-N(3)	110.19(18)	C(37)-C(38)-C(39)	120.2(2)
C(32)-C(29)-P(3)	137.21(16)	C(37)-C(38)-H(34)	119.9
N(3)-C(29)-P(3)	112.59(14)	C(39)-C(38)-H(34)	119.9
N(3)-C(30)-C(31)	110.24(19)	C(40)-C(39)-C(38)	120.3(2)
N(3)-C(30)-H(24)	124.9	C(40)-C(39)-H(33)	119.8
C(31)-C(30)-H(24)	124.9	C(38)-C(39)-H(33)	119.8
C(30)-C(31)-C(32)	107.20(19)	C(39)-C(40)-C(41)	119.9(2)
C(30)-C(31)-H(26)	126.4	C(39)-C(40)-H(32)	120.0
C(32)-C(31)-H(26)	126.4	C(41)-C(40)-H(32)	120.0
C(29)-C(32)-C(31)	106.23(19)	C(40)-C(41)-C(42)	120.4(2)

C(40)-C(41)-H(31)	119.8	C(51)-C(50)-P(1)	118.57(17)
C(42)-C(41)-H(31)	119.8	C(55)-C(50)-P(1)	121.81(17)
C(41)-C(42)-C(37)	119.9(2)	C(52)-C(51)-C(50)	120.2(2)
C(41)-C(42)-H(30)	120.0	C(52)-C(51)-H(44)	119.9
C(37)-C(42)-H(30)	120.0	C(50)-C(51)-H(44)	119.9
C(44)-C(43)-C(48)	119.07(19)	C(51)-C(52)-C(53)	120.1(2)
C(44)-C(43)-P(2)	116.97(16)	C(51)-C(52)-H(43)	120.0
C(48)-C(43)-P(2)	123.92(16)	C(53)-C(52)-H(43)	120.0
C(45)-C(44)-C(43)	120.0(2)	C(54)-C(53)-C(52)	120.1(2)
C(45)-C(44)-H(39)	120.0	C(54)-C(53)-H(42)	120.0
C(43)-C(44)-H(39)	120.0	C(52)-C(53)-H(42)	120.0
C(46)-C(45)-C(44)	120.5(2)	C(53)-C(54)-C(55)	120.1(2)
C(46)-C(45)-H(38)	119.8	C(53)-C(54)-H(41)	120.0
C(44)-C(45)-H(38)	119.8	C(55)-C(54)-H(41)	120.0
C(47)-C(46)-C(45)	119.6(2)	C(54)-C(55)-C(50)	120.1(2)
C(47)-C(46)-H(37)	120.2	C(54)-C(55)-H(40)	120.0
C(45)-C(46)-H(37)	120.2	C(50)-C(55)-H(40)	120.0
C(46)-C(47)-C(48)	120.5(2)	C(61)-C(56)-C(57)	119.1(2)
C(46)-C(47)-H(36)	119.8	C(61)-C(56)-P(1)	118.88(17)
C(48)-C(47)-H(36)	119.8	C(57)-C(56)-P(1)	122.06(19)
C(47)-C(48)-C(43)	120.3(2)	C(58)-C(57)-C(56)	119.7(3)
C(47)-C(48)-H(35)	119.8	C(58)-C(57)-H(49)	120.2
C(43)-C(48)-H(35)	119.8	C(56)-C(57)-H(49)	120.2
C(62)-C(49)-N(1)	110.17(19)	C(59)-C(58)-C(57)	120.9(3)
C(62)-C(49)-P(1)	139.15(19)	C(59)-C(58)-H(45)	119.6
N(1)-C(49)-P(1)	110.68(15)	C(57)-C(58)-H(45)	119.6
C(51)-C(50)-C(55)	119.5(2)	C(58)-C(59)-C(60)	119.6(2)

C(58)-C(59)-H(46)	120.2	C(49)-C(62)-H(52)	127.0
C(60)-C(59)-H(46)	120.2	C(63)-C(62)-H(52)	127.0
C(59)-C(60)-C(61)	120.2(3)	C(64)-C(63)-C(62)	107.6(2)
C(59)-C(60)-H(47)	119.9	C(64)-C(63)-H(51)	126.2
C(61)-C(60)-H(47)	119.9	C(62)-C(63)-H(51)	126.2
C(56)-C(61)-C(60)	120.5(2)	N(1)-C(64)-C(63)	109.8(2)
C(56)-C(61)-H(48)	119.7	N(1)-C(64)-H(50)	125.1
C(60)-C(61)-H(48)	119.7	C(63)-C(64)-H(50)	125.1
C(49)-C(62)-C(63)	106.0(2)		

Symmetry transformations used to generate equivalent atoms:

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 4. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	$U_{11}U_{22}$	U_{33}	U_{23}	U_{13}	U_{12}	
Ti1	9(1) 10(1)	9(1)	0(1)	0(1)	0(1)	
Ni1	9(1) 10(1)	11(1)	0(1)	1(1)	1(1)	
P4	10(1)	11(1)	12(1)	1(1)	2(1)	3(1)
P3	11(1)	9(1)	13(1)	-1(1)	1(1)	0(1)
P2	12(1)	10(1)	12(1)	0(1)	3(1)	0(1)
P1	15(1)	13(1)	11(1)	0(1)	1(1)	0(1)
N4	11(1)	11(1)	12(1)	-2(1)	2(1)	0(1)
N3	13(1)	11(1)	13(1)	0(1)	1(1)	1(1)
N2	15(1)	12(1)	14(1)	-1(1)	2(1)	-2(1)
N1	14(1)	14(1)	13(1)	-2(1)	-2(1)	1(1)
C1	14(1)	12(1)	13(1)	3(1)	2(1)	1(1)
C2	16(1)	16(1)	13(1)	-2(1)	0(1)	-2(1)
C3	23(1)	15(1)	16(1)	-5(1)	6(1)	-1(1)
C4	18(1)	15(1)	20(1)	1(1)	4(1)	4(1)
C5	14(1)	15(1)	15(1)	2(1)	5(1)	5(1)
C6	21(1)	20(1)	20(1)	5(1)	1(1)	3(1)
C7	28(1)	25(1)	21(1)	9(1)	0(1)	7(1)
C8	34(1)	17(1)	23(1)	7(1)	10(1)	6(1)
C9	27(1)	18(1)	21(1)	2(1)	7(1)	-4(1)
C10	18(1)	20(1)	18(1)	2(1)	2(1)	2(1)
C11	14(1)	13(1)	19(1)	3(1)	-2(1)	3(1)
C12	21(1)	21(1)	18(1)	1(1)	-3(1)	4(1)

C13	25(1)	26(1)	28(1)	-1(1)	-12(1)	-2(1)
C14	18(1)	34(1)	38(2)	4(1)	-7(1)	-7(1)
C15	16(1)	39(1)	30(1)	3(1)	4(1)	-3(1)
C16	16(1)	25(1)	22(1)	0(1)	1(1)	2(1)
C17	18(1)	14(1)	15(1)	0(1)	0(1)	-1(1)
C18	17(1)	18(1)	19(1)	-4(1)	1(1)	-3(1)
C19	27(1)	29(1)	20(1)	-6(1)	7(1)	-3(1)
C20	35(2)	54(2)	16(1)	-11(1)	-3(1)	-2(1)
C21	25(1)	73(2)	22(1)	-8(1)	-8(1)	1(1)
C22	18(1)	46(2)	21(1)	-4(1)	-1(1)	3(1)
C23	16(1)	14(1)	12(1)	-2(1)	-1(1)	-2(1)
C24	24(1)	15(1)	24(1)	-1(1)	6(1)	1(1)
C25	36(1)	14(1)	25(1)	0(1)	7(1)	-4(1)
C26	27(1)	26(1)	22(1)	2(1)	5(1)	-12(1)
C27	16(1)	29(1)	22(1)	2(1)	4(1)	-3(1)
C28	17(1)	19(1)	15(1)	2(1)	1(1)	-1(1)
C29	14(1)	12(1)	13(1)	0(1)	1(1)	0(1)
C30	13(1)	18(1)	17(1)	1(1)	-2(1)	1(1)
C31	17(1)	21(1)	22(1)	1(1)	0(1)	7(1)
C32	18(1)	14(1)	22(1)	-3(1)	2(1)	4(1)
C33	14(1)	12(1)	12(1)	0(1)	4(1)	0(1)
C34	26(1)	17(1)	15(1)	-3(1)	-1(1)	-7(1)
C35	25(1)	20(1)	21(1)	-1(1)	1(1)	-11(1)
C36	18(1)	17(1)	17(1)	2(1)	4(1)	-4(1)
C37	14(1)	18(1)	12(1)	0(1)	4(1)	2(1)
C38	16(1)	18(1)	16(1)	1(1)	6(1)	1(1)
C39	21(1)	21(1)	23(1)	7(1)	7(1)	4(1)

C40	25(1)	34(1)	22(1)	6(1)	0(1)	12(1)
C41	25(1)	35(1)	28(1)	-6(1)	-10(1)	6(1)
C42	21(1)	20(1)	28(1)	-5(1)	-3(1)	1(1)
C43	12(1)	12(1)	18(1)	-2(1)	5(1)	-3(1)
C44	14(1)	15(1)	20(1)	-2(1)	3(1)	-3(1)
C45	13(1)	16(1)	32(1)	-4(1)	3(1)	-1(1)
C46	17(1)	23(1)	31(1)	-12(1)	10(1)	-2(1)
C47	26(1)	27(1)	18(1)	-8(1)	7(1)	-5(1)
C48	19(1)	18(1)	17(1)	-2(1)	4(1)	-2(1)
C49	20(1)	13(1)	16(1)	-1(1)	-2(1)	0(1)
C50	20(1)	15(1)	12(1)	1(1)	-1(1)	-1(1)
C51	21(1)	19(1)	26(1)	2(1)	-2(1)	-1(1)
C52	25(1)	21(1)	35(1)	3(1)	-3(1)	4(1)
C53	35(1)	15(1)	31(1)	5(1)	-3(1)	-1(1)
C54	30(1)	20(1)	28(1)	1(1)	6(1)	-8(1)
C55	23(1)	19(1)	22(1)	-1(1)	4(1)	-1(1)
C56	23(1)	11(1)	20(1)	-1(1)	9(1)	-2(1)
C57	39(2)	27(1)	19(1)	-3(1)	7(1)	-6(1)
C58	60(2)	29(1)	23(1)	-7(1)	22(1)	-6(1)
C59	45(2)	18(1)	44(2)	1(1)	33(1)	3(1)
C60	27(1)	17(1)	45(2)	5(1)	19(1)	3(1)
C61	24(1)	14(1)	26(1)	0(1)	8(1)	0(1)
C62	32(1)	21(1)	20(1)	3(1)	-8(1)	2(1)
C63	26(1)	23(1)	27(1)	-2(1)	-16(1)	2(1)
C64	14(1)	15(1)	27(1)	-4(1)	-5(1)	0(1)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 5. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Zr1	2573(1)	3529(1)	2931(1)	12(1)
Ni1	1790(1)	4389(1)	2467(1)	12(1)
P1	1350(1)	3202(1)	3867(1)	15(1)
P2	2466(1)	4180(1)	1642(1)	15(1)
P4	2956(1)	4926(1)	3162(1)	13(1)
P3	-85(1)	4082(1)	2372(1)	13(1)
N1	3038(1)	2704(1)	3397(1)	16(1)
N2	3934(1)	3449(1)	2389(1)	18(1)
N4	3749(1)	3936(1)	3715(1)	14(1)
N3	970(1)	3073(1)	2390(1)	16(1)
C1	1851(2)	3471(1)	4634(1)	18(1)
C2	2026(2)	4049(1)	4714(1)	24(1)
C3	2443(2)	4273(1)	5289(1)	31(1)
C4	2684(2)	3925(1)	5787(1)	36(1)
C5	2500(2)	3348(1)	5714(1)	36(1)
C6	2085(2)	3121(1)	5140(1)	26(1)
C7	-181(2)	2932(1)	3848(1)	20(1)
C8	-701(2)	2541(1)	3410(1)	30(1)
C9	-1886(2)	2357(1)	3373(1)	39(1)
C10	-2559(2)	2556(1)	3768(1)	40(1)
C11	-2056(2)	2948(1)	4198(1)	36(1)
C12	-869(2)	3139(1)	4241(1)	26(1)

C13	2269(2)	2600(1)	3789(1)	17(1)
C14	3653(2)	2211(1)	3366(1)	21(1)
C15	3292(2)	1805(1)	3724(1)	26(1)
C16	2404(2)	2050(1)	3994(1)	24(1)
C17	1483(2)	3897(1)	949(1)	20(1)
C18	1040(2)	4228(1)	443(1)	27(1)
C19	280(2)	3995(1)	-69(1)	35(1)
C20	-47(2)	3433(1)	-76(1)	33(1)
C21	387(2)	3101(1)	428(1)	29(1)
C22	1148(2)	3328(1)	939(1)	24(1)
C23	3009(2)	4839(1)	1378(1)	22(1)
C24	4035(2)	4886(1)	1136(1)	36(1)
C25	4376(2)	5414(1)	955(1)	50(1)
C26	3709(2)	5886(1)	1011(1)	48(1)
C27	2681(2)	5844(1)	1242(1)	42(1)
C28	2335(2)	5321(1)	1428(1)	30(1)
C29	3686(2)	3680(1)	1811(1)	20(1)
C30	4888(2)	3080(1)	2410(1)	23(1)
C31	5223(2)	3069(1)	1863(1)	31(1)
C32	4451(2)	3447(1)	1480(1)	33(1)
C33	4058(2)	5402(1)	2934(1)	17(1)
C34	4971(2)	5154(1)	2699(1)	24(1)
C35	5867(2)	5482(1)	2533(1)	32(1)
C36	5839(2)	6063(1)	2594(1)	34(1)
C37	4935(2)	6315(1)	2821(1)	34(1)
C38	4038(2)	5986(1)	2994(1)	26(1)
C39	3878(1)	4519(1)	3754(1)	14(1)

C40	4547(2)	3719(1)	4209(1)	17(1)
C41	5171(2)	4149(1)	4554(1)	19(1)
C42	4753(2)	4661(1)	4264(1)	18(1)
C43	2028(2)	5401(1)	3514(1)	18(1)
C44	2165(2)	5443(1)	4137(1)	22(1)
C45	1358(2)	5767(1)	4381(1)	33(1)
C46	412(2)	6047(1)	4004(1)	39(1)
C47	271(2)	6013(1)	3385(1)	37(1)
C48	1078(2)	5694(1)	3138(1)	28(1)
C49	-1009(2)	4185(1)	2930(1)	16(1)
C50	-544(2)	4502(1)	3444(1)	20(1)
C51	-1255(2)	4615(1)	3859(1)	27(1)
C52	-2429(2)	4404(1)	3763(1)	27(1)
C53	-2891(2)	4076(1)	3257(1)	25(1)
C54	-2196(2)	3971(1)	2838(1)	21(1)
C55	-975(2)	4472(1)	1728(1)	19(1)
C56	-1359(2)	4244(1)	1151(1)	29(1)
C57	-1995(2)	4579(1)	681(1)	41(1)
C58	-2224(2)	5138(1)	779(1)	45(1)
C59	-1836(2)	5370(1)	1347(1)	45(1)
C60	-1221(2)	5037(1)	1823(1)	30(1)
C61	-129(2)	3349(1)	2185(1)	16(1)
C62	768(2)	2518(1)	2223(1)	21(1)
C63	-429(2)	2447(1)	1913(1)	25(1)
C64	-1005(2)	2975(1)	1896(1)	22(1)
C65	2564(2)	7466(1)	4426(1)	42(1)
C66	3107(2)	7940(1)	4719(1)	40(1)

C67	4361(2)	7978(1)	4871(1)	41(1)
C68	5059(2)	7544(1)	4731(1)	43(1)
C69	3263(2)	7034(1)	4277(1)	37(1)
C70	4518(2)	7074(1)	4432(1)	38(1)

Bond lengths [Å] and angles [°] for 5.

Zr(1)-N(2)	2.1747(14)	N(4)-C(40)	1.371(2)
Zr(1)-N(4)	2.1926(13)	N(4)-C(39)	1.390(2)
Zr(1)-N(3)	2.2234(13)	N(3)-C(62)	1.374(2)
Zr(1)-N(1)	2.2283(13)	N(3)-C(61)	1.385(2)
Zr(1)-Ni(1)	2.3724(3)	C(1)-C(2)	1.391(3)
Zr(1)-P(1)	2.8799(4)	C(1)-C(6)	1.394(3)
Ni(1)-P(3)	2.1979(5)	C(2)-C(3)	1.388(3)
Ni(1)-P(4)	2.2160(5)	C(2)-H(1)	0.9500
Ni(1)-P(2)	2.2257(5)	C(3)-C(4)	1.377(3)
P(1)-C(13)	1.7926(17)	C(3)-H(5)	0.9500
P(1)-C(1)	1.8221(17)	C(4)-C(5)	1.387(3)
P(1)-C(7)	1.8308(18)	C(4)-H(4)	0.9500
P(2)-C(29)	1.7897(18)	C(5)-C(6)	1.391(3)
P(2)-C(23)	1.8250(18)	C(5)-H(2)	0.9500
P(2)-C(17)	1.8384(18)	C(6)-H(3)	0.9500
P(4)-C(39)	1.7864(17)	C(7)-C(8)	1.390(3)
P(4)-C(43)	1.8347(17)	C(7)-C(12)	1.392(3)
P(4)-C(33)	1.8349(17)	C(8)-C(9)	1.388(3)
P(3)-C(61)	1.7867(17)	C(8)-H(10)	0.9500
P(3)-C(49)	1.8247(17)	C(9)-C(10)	1.378(4)
P(3)-C(55)	1.8274(17)	C(9)-H(9)	0.9500
N(1)-C(14)	1.366(2)	C(10)-C(11)	1.376(4)
N(1)-C(13)	1.393(2)	C(10)-H(8)	0.9500
N(2)-C(30)	1.377(2)	C(11)-C(12)	1.393(3)
N(2)-C(29)	1.391(2)	C(11)-H(7)	0.9500

C(12)-H(6)	0.9500	C(27)-H(21)	0.9500
C(13)-C(16)	1.380(2)	C(28)-H(22)	0.9500
C(14)-C(15)	1.378(3)	C(29)-C(32)	1.378(3)
C(14)-H(11)	0.9500	C(30)-C(31)	1.373(3)
C(15)-C(16)	1.409(3)	C(30)-H(24)	0.9500
C(15)-H(12)	0.9500	C(31)-C(32)	1.407(3)
C(16)-H(13)	0.9500	C(31)-H(25)	0.9500
C(17)-C(18)	1.388(3)	C(32)-H(26)	0.9500
C(17)-C(22)	1.397(3)	C(33)-C(34)	1.389(3)
C(18)-C(19)	1.395(3)	C(33)-C(38)	1.391(2)
C(18)-H(18)	0.9500	C(34)-C(35)	1.391(3)
C(19)-C(20)	1.382(3)	C(34)-H(31)	0.9500
C(19)-H(14)	0.9500	C(35)-C(36)	1.384(3)
C(20)-C(21)	1.383(3)	C(35)-H(30)	0.9500
C(20)-H(15)	0.9500	C(36)-C(37)	1.372(3)
C(21)-C(22)	1.389(3)	C(36)-H(29)	0.9500
C(21)-H(16)	0.9500	C(37)-C(38)	1.398(3)
C(22)-H(17)	0.9500	C(37)-H(27)	0.9500
C(23)-C(24)	1.388(3)	C(38)-H(28)	0.9500
C(23)-C(28)	1.391(3)	C(39)-C(42)	1.385(2)
C(24)-C(25)	1.396(3)	C(40)-C(41)	1.378(2)
C(24)-H(23)	0.9500	C(40)-H(32)	0.9500
C(25)-C(26)	1.367(4)	C(41)-C(42)	1.410(2)
C(25)-H(19)	0.9500	C(41)-H(34)	0.9500
C(26)-C(27)	1.375(4)	C(42)-H(33)	0.9500
C(26)-H(20)	0.9500	C(43)-C(44)	1.391(3)
C(27)-C(28)	1.390(3)	C(43)-C(48)	1.397(3)

C(44)-C(45)	1.394(3)	C(58)-H(46)	0.9500
C(44)-H(39)	0.9500	C(59)-C(60)	1.391(3)
C(45)-C(46)	1.380(3)	C(59)-H(47)	0.9500
C(45)-H(38)	0.9500	C(60)-H(48)	0.9500
C(46)-C(47)	1.379(4)	C(61)-C(64)	1.379(2)
C(46)-H(37)	0.9500	C(62)-C(63)	1.384(3)
C(47)-C(48)	1.392(3)	C(62)-H(52)	0.9500
C(47)-H(36)	0.9500	C(63)-C(64)	1.405(3)
C(48)-H(35)	0.9500	C(63)-H(51)	0.9500
C(49)-C(50)	1.388(2)	C(64)-H(50)	0.9500
C(49)-C(54)	1.401(2)	C(65)-C(66)	1.377(4)
C(50)-C(51)	1.390(2)	C(65)-C(69)	1.377(3)
C(50)-H(44)	0.9500	C(65)-H(53)	0.9500
C(51)-C(52)	1.383(3)	C(66)-C(67)	1.380(3)
C(51)-H(40)	0.9500	C(66)-H(58)	0.9500
C(52)-C(53)	1.389(3)	C(67)-C(68)	1.373(3)
C(52)-H(43)	0.9500	C(67)-H(55)	0.9500
C(53)-C(54)	1.381(3)	C(68)-C(70)	1.375(4)
C(53)-H(41)	0.9500	C(68)-H(54)	0.9500
C(54)-H(42)	0.9500	C(69)-C(70)	1.381(3)
C(55)-C(56)	1.393(3)	C(69)-H(57)	0.9500
C(55)-C(60)	1.394(3)	C(70)-H(56)	0.9500
C(56)-C(57)	1.394(3)		
C(56)-H(49)	0.9500	N(2)-Zr(1)-N(4)	97.00(5)
C(57)-C(58)	1.377(4)	N(2)-Zr(1)-N(3)	103.50(5)
C(57)-H(45)	0.9500	N(4)-Zr(1)-N(3)	158.72(5)
C(58)-C(59)	1.380(4)	N(2)-Zr(1)-N(1)	94.05(5)

N(4)-Zr(1)-N(1)	87.94(5)	C(23)-P(2)-Ni(1)	106.73(6)
N(3)-Zr(1)-N(1)	85.03(5)	C(17)-P(2)-Ni(1)	123.18(6)
N(2)-Zr(1)-Ni(1)	93.62(4)	C(39)-P(4)-C(43)	107.25(8)
N(4)-Zr(1)-Ni(1)	94.63(4)	C(39)-P(4)-C(33)	103.13(8)
N(3)-Zr(1)-Ni(1)	89.75(4)	C(43)-P(4)-C(33)	103.35(8)
N(1)-Zr(1)-Ni(1)	171.55(4)	C(39)-P(4)-Ni(1)	112.32(5)
N(2)-Zr(1)-P(1)	154.77(4)	C(43)-P(4)-Ni(1)	110.91(6)
N(4)-Zr(1)-P(1)	79.72(4)	C(33)-P(4)-Ni(1)	118.89(5)
N(3)-Zr(1)-P(1)	79.30(4)	C(61)-P(3)-C(49)	107.71(8)
N(1)-Zr(1)-P(1)	60.98(4)	C(61)-P(3)-C(55)	108.69(8)
Ni(1)-Zr(1)-P(1)	111.537(11)	C(49)-P(3)-C(55)	101.06(8)
P(3)-Ni(1)-P(4)	131.631(19)	C(61)-P(3)-Ni(1)	108.68(6)
P(3)-Ni(1)-P(2)	110.103(19)	C(49)-P(3)-Ni(1)	124.79(6)
P(4)-Ni(1)-P(2)	117.840(19)	C(55)-P(3)-Ni(1)	104.83(6)
P(3)-Ni(1)-Zr(1)	90.801(14)	C(14)-N(1)-C(13)	106.01(14)
P(4)-Ni(1)-Zr(1)	94.214(15)	C(14)-N(1)-Zr(1)	142.43(12)
P(2)-Ni(1)-Zr(1)	91.114(15)	C(13)-N(1)-Zr(1)	110.10(10)
C(13)-P(1)-C(1)	108.02(8)	C(30)-N(2)-C(29)	105.92(14)
C(13)-P(1)-C(7)	106.33(8)	C(30)-N(2)-Zr(1)	132.70(12)
C(1)-P(1)-C(7)	103.55(8)	C(29)-N(2)-Zr(1)	118.56(11)
C(13)-P(1)-Zr(1)	76.18(6)	C(40)-N(4)-C(39)	106.26(13)
C(1)-P(1)-Zr(1)	120.85(6)	C(40)-N(4)-Zr(1)	131.88(11)
C(7)-P(1)-Zr(1)	132.73(6)	C(39)-N(4)-Zr(1)	121.61(10)
C(29)-P(2)-C(23)	109.85(9)	C(62)-N(3)-C(61)	106.05(14)
C(29)-P(2)-C(17)	103.29(8)	C(62)-N(3)-Zr(1)	132.99(12)
C(23)-P(2)-C(17)	102.30(8)	C(61)-N(3)-Zr(1)	120.83(10)
C(29)-P(2)-Ni(1)	110.84(6)	C(2)-C(1)-C(6)	118.88(17)

C(2)-C(1)-P(1)	118.42(14)	C(11)-C(10)-H(8)	120.2
C(6)-C(1)-P(1)	122.69(14)	C(9)-C(10)-H(8)	120.2
C(3)-C(2)-C(1)	120.52(19)	C(10)-C(11)-C(12)	120.4(2)
C(3)-C(2)-H(1)	119.7	C(10)-C(11)-H(7)	119.8
C(1)-C(2)-H(1)	119.7	C(12)-C(11)-H(7)	119.8
C(4)-C(3)-C(2)	120.4(2)	C(7)-C(12)-C(11)	120.1(2)
C(4)-C(3)-H(5)	119.8	C(7)-C(12)-H(6)	119.9
C(2)-C(3)-H(5)	119.8	C(11)-C(12)-H(6)	119.9
C(3)-C(4)-C(5)	119.66(18)	C(16)-C(13)-N(1)	110.14(15)
C(3)-C(4)-H(4)	120.2	C(16)-C(13)-P(1)	137.74(14)
C(5)-C(4)-H(4)	120.2	N(1)-C(13)-P(1)	112.07(11)
C(4)-C(5)-C(6)	120.2(2)	N(1)-C(14)-C(15)	110.31(16)
C(4)-C(5)-H(2)	119.9	N(1)-C(14)-H(11)	124.8
C(6)-C(5)-H(2)	119.9	C(15)-C(14)-H(11)	124.8
C(5)-C(6)-C(1)	120.25(19)	C(14)-C(15)-C(16)	107.38(15)
C(5)-C(6)-H(3)	119.9	C(14)-C(15)-H(12)	126.3
C(1)-C(6)-H(3)	119.9	C(16)-C(15)-H(12)	126.3
C(8)-C(7)-C(12)	119.10(17)	C(13)-C(16)-C(15)	106.15(16)
C(8)-C(7)-P(1)	119.64(15)	C(13)-C(16)-H(13)	126.9
C(12)-C(7)-P(1)	121.12(14)	C(15)-C(16)-H(13)	126.9
C(9)-C(8)-C(7)	120.0(2)	C(18)-C(17)-C(22)	119.04(17)
C(9)-C(8)-H(10)	120.0	C(18)-C(17)-P(2)	122.60(14)
C(7)-C(8)-H(10)	120.0	C(22)-C(17)-P(2)	118.35(14)
C(10)-C(9)-C(8)	120.7(2)	C(17)-C(18)-C(19)	120.45(19)
C(10)-C(9)-H(9)	119.6	C(17)-C(18)-H(18)	119.8
C(8)-C(9)-H(9)	119.6	C(19)-C(18)-H(18)	119.8
C(11)-C(10)-C(9)	119.56(19)	C(20)-C(19)-C(18)	120.2(2)

C(20)-C(19)-H(14)	119.9	C(27)-C(28)-H(22)	119.6
C(18)-C(19)-H(14)	119.9	C(23)-C(28)-H(22)	119.6
C(19)-C(20)-C(21)	119.63(18)	C(32)-C(29)-N(2)	109.68(16)
C(19)-C(20)-H(15)	120.2	C(32)-C(29)-P(2)	133.69(15)
C(21)-C(20)-H(15)	120.2	N(2)-C(29)-P(2)	116.60(12)
C(20)-C(21)-C(22)	120.63(19)	C(31)-C(30)-N(2)	110.44(17)
C(20)-C(21)-H(16)	119.7	C(31)-C(30)-H(24)	124.8
C(22)-C(21)-H(16)	119.7	N(2)-C(30)-H(24)	124.8
C(21)-C(22)-C(17)	120.08(19)	C(30)-C(31)-C(32)	106.91(17)
C(21)-C(22)-H(17)	120.0	C(30)-C(31)-H(25)	126.5
C(17)-C(22)-H(17)	120.0	C(32)-C(31)-H(25)	126.5
C(24)-C(23)-C(28)	118.83(19)	C(29)-C(32)-C(31)	107.03(18)
C(24)-C(23)-P(2)	124.60(16)	C(29)-C(32)-H(26)	126.5
C(28)-C(23)-P(2)	116.56(14)	C(31)-C(32)-H(26)	126.5
C(23)-C(24)-C(25)	119.7(2)	C(34)-C(33)-C(38)	119.23(16)
C(23)-C(24)-H(23)	120.1	C(34)-C(33)-P(4)	116.83(13)
C(25)-C(24)-H(23)	120.1	C(38)-C(33)-P(4)	123.93(14)
C(26)-C(25)-C(24)	120.8(2)	C(33)-C(34)-C(35)	120.65(18)
C(26)-C(25)-H(19)	119.6	C(33)-C(34)-H(31)	119.7
C(24)-C(25)-H(19)	119.6	C(35)-C(34)-H(31)	119.7
C(25)-C(26)-C(27)	120.1(2)	C(36)-C(35)-C(34)	119.6(2)
C(25)-C(26)-H(20)	119.9	C(36)-C(35)-H(30)	120.2
C(27)-C(26)-H(20)	119.9	C(34)-C(35)-H(30)	120.2
C(26)-C(27)-C(28)	119.7(2)	C(37)-C(36)-C(35)	120.32(18)
C(26)-C(27)-H(21)	120.1	C(37)-C(36)-H(29)	119.8
C(28)-C(27)-H(21)	120.1	C(35)-C(36)-H(29)	119.8
C(27)-C(28)-C(23)	120.8(2)	C(36)-C(37)-C(38)	120.34(19)

C(36)-C(37)-H(27)	119.8	C(47)-C(46)-H(37)	119.9
C(38)-C(37)-H(27)	119.8	C(45)-C(46)-H(37)	119.9
C(33)-C(38)-C(37)	119.83(19)	C(46)-C(47)-C(48)	120.2(2)
C(33)-C(38)-H(28)	120.1	C(46)-C(47)-H(36)	119.9
C(37)-C(38)-H(28)	120.1	C(48)-C(47)-H(36)	119.9
C(42)-C(39)-N(4)	109.82(14)	C(47)-C(48)-C(43)	120.2(2)
C(42)-C(39)-P(4)	133.20(13)	C(47)-C(48)-H(35)	119.9
N(4)-C(39)-P(4)	116.97(11)	C(43)-C(48)-H(35)	119.9
N(4)-C(40)-C(41)	110.33(15)	C(50)-C(49)-C(54)	119.47(16)
N(4)-C(40)-H(32)	124.8	C(50)-C(49)-P(3)	119.21(13)
C(41)-C(40)-H(32)	124.8	C(54)-C(49)-P(3)	121.26(13)
C(40)-C(41)-C(42)	107.12(15)	C(49)-C(50)-C(51)	120.40(16)
C(40)-C(41)-H(34)	126.4	C(49)-C(50)-H(44)	119.8
C(42)-C(41)-H(34)	126.4	C(51)-C(50)-H(44)	119.8
C(39)-C(42)-C(41)	106.47(14)	C(52)-C(51)-C(50)	119.78(17)
C(39)-C(42)-H(33)	126.8	C(52)-C(51)-H(40)	120.1
C(41)-C(42)-H(33)	126.8	C(50)-C(51)-H(40)	120.1
C(44)-C(43)-C(48)	118.93(17)	C(51)-C(52)-C(53)	120.16(17)
C(44)-C(43)-P(4)	122.66(14)	C(51)-C(52)-H(43)	119.9
C(48)-C(43)-P(4)	118.18(14)	C(53)-C(52)-H(43)	119.9
C(43)-C(44)-C(45)	120.43(19)	C(54)-C(53)-C(52)	120.27(17)
C(43)-C(44)-H(39)	119.8	C(54)-C(53)-H(41)	119.9
C(45)-C(44)-H(39)	119.8	C(52)-C(53)-H(41)	119.9
C(46)-C(45)-C(44)	120.0(2)	C(53)-C(54)-C(49)	119.90(17)
C(46)-C(45)-H(38)	120.0	C(53)-C(54)-H(42)	120.0
C(44)-C(45)-H(38)	120.0	C(49)-C(54)-H(42)	120.0
C(47)-C(46)-C(45)	120.12(19)	C(56)-C(55)-C(60)	119.09(17)

C(56)-C(55)-P(3)	123.79(14)	C(62)-C(63)-H(51)	126.3
C(60)-C(55)-P(3)	117.04(14)	C(64)-C(63)-H(51)	126.3
C(55)-C(56)-C(57)	119.9(2)	C(61)-C(64)-C(63)	106.32(16)
C(55)-C(56)-H(49)	120.1	C(61)-C(64)-H(50)	126.8
C(57)-C(56)-H(49)	120.1	C(63)-C(64)-H(50)	126.8
C(58)-C(57)-C(56)	120.5(2)	C(66)-C(65)-C(69)	120.5(2)
C(58)-C(57)-H(45)	119.7	C(66)-C(65)-H(53)	119.8
C(56)-C(57)-H(45)	119.7	C(69)-C(65)-H(53)	119.8
C(57)-C(58)-C(59)	120.0(2)	C(65)-C(66)-C(67)	119.6(2)
C(57)-C(58)-H(46)	120.0	C(65)-C(66)-H(58)	120.2
C(59)-C(58)-H(46)	120.0	C(67)-C(66)-H(58)	120.2
C(58)-C(59)-C(60)	120.0(2)	C(68)-C(67)-C(66)	120.0(2)
C(58)-C(59)-H(47)	120.0	C(68)-C(67)-H(55)	120.0
C(60)-C(59)-H(47)	120.0	C(66)-C(67)-H(55)	120.0
C(59)-C(60)-C(55)	120.4(2)	C(67)-C(68)-C(70)	120.4(2)
C(59)-C(60)-H(48)	119.8	C(67)-C(68)-H(54)	119.8
C(55)-C(60)-H(48)	119.8	C(70)-C(68)-H(54)	119.8
C(64)-C(61)-N(3)	110.43(14)	C(65)-C(69)-C(70)	119.7(2)
C(64)-C(61)-P(3)	135.79(14)	C(65)-C(69)-H(57)	120.2
N(3)-C(61)-P(3)	113.75(11)	C(70)-C(69)-H(57)	120.2
N(3)-C(62)-C(63)	109.88(15)	C(68)-C(70)-C(69)	119.8(2)
N(3)-C(62)-H(52)	125.1	C(68)-C(70)-H(56)	120.1
C(63)-C(62)-H(52)	125.1	C(69)-C(70)-H(56)	120.1
C(62)-C(63)-C(64)	107.31(15)		

Symmetry transformations used to generate equivalent atoms:

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 5. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	$U_{11}U_{22}$	U_{33}	U_{23}	U_{13}	U_{12}	
Zr1	14(1)	9(1)	12(1)	-2(1)	2(1)	0(1)
Ni1	13(1)	10(1)	13(1)	-1(1)	3(1)	-1(1)
P1	16(1)	12(1)	16(1)	-1(1)	4(1)	-1(1)
P2	16(1)	18(1)	12(1)	-1(1)	5(1)	-2(1)
P4	15(1)	10(1)	15(1)	-2(1)	3(1)	-2(1)
P3	12(1)	12(1)	16(1)	-2(1)	3(1)	0(1)
N1	19(1)	10(1)	19(1)	0(1)	2(1)	2(1)
N2	14(1)	20(1)	18(1)	-3(1)	5(1)	1(1)
N4	15(1)	12(1)	13(1)	-3(1)	2(1)	-2(1)
N3	16(1)	13(1)	16(1)	-4(1)	1(1)	-2(1)
C1	15(1)	24(1)	18(1)	-3(1)	7(1)	0(1)
C2	23(1)	26(1)	24(1)	-5(1)	10(1)	-3(1)
C3	25(1)	38(1)	31(1)	-19(1)	11(1)	-6(1)
C4	25(1)	60(2)	22(1)	-15(1)	3(1)	6(1)
C5	31(1)	58(1)	18(1)	4(1)	5(1)	17(1)
C6	24(1)	32(1)	23(1)	2(1)	7(1)	7(1)
C7	18(1)	19(1)	22(1)	7(1)	2(1)	-2(1)
C8	31(1)	31(1)	25(1)	4(1)	3(1)	-11(1)
C9	35(1)	42(1)	34(1)	11(1)	-7(1)	-19(1)
C10	19(1)	53(1)	45(1)	28(1)	-2(1)	-9(1)
C11	21(1)	47(1)	43(1)	19(1)	10(1)	4(1)
C12	20(1)	27(1)	32(1)	7(1)	6(1)	3(1)

C13	18(1)	14(1)	17(1)	-1(1)	2(1)	-1(1)
C14	20(1)	14(1)	28(1)	-4(1)	4(1)	4(1)
C15	27(1)	11(1)	37(1)	1(1)	4(1)	3(1)
C16	29(1)	16(1)	29(1)	3(1)	6(1)	-1(1)
C17	17(1)	28(1)	16(1)	-6(1)	7(1)	-4(1)
C18	29(1)	33(1)	18(1)	0(1)	3(1)	-5(1)
C19	32(1)	51(1)	19(1)	0(1)	-1(1)	-4(1)
C20	25(1)	50(1)	24(1)	-16(1)	4(1)	-9(1)
C21	25(1)	34(1)	31(1)	-14(1)	12(1)	-9(1)
C22	26(1)	27(1)	22(1)	-5(1)	10(1)	-3(1)
C23	24(1)	27(1)	14(1)	2(1)	1(1)	-7(1)
C24	30(1)	46(1)	34(1)	8(1)	10(1)	-9(1)
C25	39(1)	66(2)	45(1)	18(1)	9(1)	-24(1)
C26	57(2)	42(1)	37(1)	17(1)	-6(1)	-27(1)
C27	60(2)	26(1)	32(1)	7(1)	-6(1)	-6(1)
C28	38(1)	26(1)	24(1)	3(1)	3(1)	-4(1)
C29	19(1)	25(1)	17(1)	-1(1)	7(1)	0(1)
C30	16(1)	22(1)	32(1)	-1(1)	4(1)	3(1)
C31	24(1)	31(1)	43(1)	-5(1)	16(1)	6(1)
C32	36(1)	40(1)	28(1)	0(1)	18(1)	10(1)
C33	20(1)	16(1)	15(1)	2(1)	1(1)	-6(1)
C34	23(1)	24(1)	25(1)	1(1)	6(1)	-5(1)
C35	26(1)	42(1)	29(1)	6(1)	12(1)	-6(1)
C36	33(1)	40(1)	29(1)	14(1)	5(1)	-16(1)
C37	44(1)	21(1)	37(1)	9(1)	5(1)	-13(1)
C38	31(1)	19(1)	29(1)	2(1)	7(1)	-6(1)
C39	15(1)	12(1)	15(1)	-3(1)	5(1)	-2(1)

C40	18(1)	16(1)	16(1)	1(1)	3(1)	1(1)
C41	16(1)	23(1)	16(1)	-2(1)	2(1)	-2(1)
C42	17(1)	17(1)	19(1)	-4(1)	4(1)	-5(1)
C43	17(1)	10(1)	30(1)	-3(1)	7(1)	-3(1)
C44	23(1)	16(1)	31(1)	-7(1)	12(1)	-4(1)
C45	36(1)	25(1)	45(1)	-12(1)	23(1)	-5(1)
C46	29(1)	21(1)	72(2)	-12(1)	26(1)	-1(1)
C47	21(1)	16(1)	73(2)	1(1)	6(1)	3(1)
C48	25(1)	16(1)	40(1)	0(1)	3(1)	-2(1)
C49	15(1)	13(1)	20(1)	1(1)	6(1)	1(1)
C50	19(1)	19(1)	24(1)	-4(1)	9(1)	-4(1)
C51	31(1)	28(1)	28(1)	-10(1)	15(1)	-7(1)
C52	26(1)	27(1)	35(1)	-4(1)	20(1)	-1(1)
C53	15(1)	26(1)	36(1)	2(1)	11(1)	-2(1)
C54	17(1)	21(1)	26(1)	-3(1)	4(1)	-4(1)
C55	13(1)	22(1)	23(1)	5(1)	6(1)	3(1)
C56	27(1)	37(1)	22(1)	3(1)	4(1)	7(1)
C57	37(1)	61(2)	23(1)	9(1)	5(1)	14(1)
C58	38(1)	59(2)	40(1)	31(1)	13(1)	21(1)
C59	45(1)	32(1)	59(2)	21(1)	17(1)	18(1)
C60	32(1)	24(1)	36(1)	5(1)	9(1)	6(1)
C61	16(1)	15(1)	16(1)	-3(1)	2(1)	-1(1)
C62	27(1)	11(1)	24(1)	-5(1)	1(1)	1(1)
C63	29(1)	16(1)	29(1)	-8(1)	0(1)	-4(1)
C64	18(1)	20(1)	26(1)	-6(1)	0(1)	-2(1)
C65	24(1)	70(2)	30(1)	4(1)	4(1)	6(1)
C66	39(1)	54(1)	30(1)	6(1)	11(1)	20(1)

C67	42(1)	46(1)	36(1)	-2(1)	10(1)	0(1)
C68	26(1)	54(2)	48(1)	3(1)	7(1)	4(1)
C69	37(1)	44(1)	32(1)	4(1)	11(1)	-2(1)
C70	36(1)	37(1)	45(1)	10(1)	13(1)	10(1)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 6. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	zU_{eq}	
Hf1	7471(1)	6488(1)	7057(1)	20(1)
Ni1	8260(1)	5611(1)	7536(1)	18(1)
P1	8658(1)	6809(1)	6132(1)	25(1)
P2	7578(1)	5834(1)	8341(1)	23(1)
P3	7069(1)	5082(1)	6838(1)	19(1)
P4	10127(1)	5926(1)	7628(1)	19(1)
N1	6990(3)	7308(1)	6608(1)	25(1)
N2	6121(3)	6570(1)	7584(2)	24(1)
N3	6266(3)	6077(1)	6285(1)	19(1)
N4	9072(3)	6938(1)	7606(1)	21(1)
C1	6391(4)	7799(2)	6640(2)	33(1)
C2	6720(4)	8206(2)	6272(2)	39(1)
C3	7592(4)	7961(2)	6001(2)	36(1)
C4	7739(3)	7411(2)	6210(2)	28(1)
C5	10194(3)	7079(2)	6154(2)	28(1)
C6	10733(4)	7470(2)	6597(2)	37(1)
C7	11927(4)	7655(2)	6633(2)	46(1)
C8	12578(4)	7462(2)	6232(2)	52(2)
C9	12060(4)	7067(2)	5803(2)	49(1)
C10	10873(4)	6877(2)	5762(2)	38(1)
C11	8133(4)	6537(2)	5363(2)	30(1)
C12	7998(4)	5954(2)	5286(2)	30(1)

C13	7558(4)	5731(2)	4714(2)	36(1)
C14	7268(5)	6076(2)	4218(2)	48(1)
C15	7447(6)	6650(2)	4290(2)	56(1)
C16	7879(5)	6878(2)	4863(2)	47(1)
C17	5155(4)	6938(2)	7546(2)	35(1)
C18	4796(4)	6945(2)	8079(2)	42(1)
C19	5572(4)	6569(2)	8472(2)	40(1)
C20	6350(4)	6339(2)	8159(2)	28(1)
C21	6136(3)	5495(1)	6244(2)	20(1)
C22	5466(3)	6294(1)	5789(2)	22(1)
C23	4823(3)	5865(2)	5441(2)	22(1)
C24	5250(3)	5352(1)	5731(2)	21(1)
C25	7992(3)	4605(1)	6486(2)	24(1)
C26	7845(4)	4569(2)	5866(2)	27(1)
C27	8658(4)	4246(2)	5630(2)	39(1)
C28	9601(4)	3962(2)	6002(3)	45(1)
C29	9752(4)	3988(2)	6618(3)	44(1)
C30	8942(4)	4305(2)	6864(2)	34(1)
C31	5954(3)	4607(1)	7056(2)	22(1)
C32	5993(4)	4021(2)	7014(2)	33(1)
C33	5102(4)	3696(2)	7185(2)	40(1)
C34	4180(4)	3950(2)	7395(2)	41(1)
C35	4140(4)	4532(2)	7442(2)	38(1)
C36	5034(4)	4858(2)	7276(2)	28(1)
C37	10186(3)	6661(1)	7816(2)	22(1)
C38	9278(4)	7490(2)	7779(2)	29(1)
C39	10478(4)	7561(2)	8100(2)	33(1)

C40	11063(4)	7032(2)	8117(2)	30(1)
C41	11044(3)	5825(1)	7074(2)	20(1)
C42	12233(3)	6048(2)	7165(2)	25(1)
C43	12912(4)	5943(2)	6749(2)	29(1)
C44	12443(4)	5613(2)	6245(2)	30(1)
C45	11272(4)	5393(2)	6151(2)	31(1)
C46	10576(3)	5501(2)	6565(2)	25(1)
C47	11019(3)	5535(2)	8275(2)	24(1)
C48	11384(4)	5758(2)	8855(2)	33(1)
C49	11998(4)	5418(2)	9328(2)	44(1)
C50	12219(4)	4860(2)	9232(2)	52(1)
C51	11847(5)	4630(2)	8658(3)	49(1)
C52	11259(4)	4966(2)	8177(2)	34(1)
C53	8558(3)	6122(2)	9041(2)	27(1)
C54	8901(4)	6686(2)	9052(2)	33(1)
C55	9662(4)	6914(2)	9574(2)	40(1)
C56	10073(4)	6586(2)	10075(2)	44(1)
C57	9741(4)	6025(2)	10072(2)	41(1)
C58	8977(4)	5789(2)	9551(2)	32(1)
C59	7004(4)	5181(2)	8602(2)	29(1)
C60	7683(4)	4693(2)	8569(2)	37(1)
C61	7322(5)	4176(2)	8749(2)	48(1)
C62	6276(5)	4142(2)	8968(2)	56(2)
C63	5608(5)	4616(3)	9008(3)	60(2)
C64	5969(4)	5139(2)	8828(2)	44(1)
C65	13128(6)	7933(3)	4717(3)	66(2)
C66	14356(5)	8000(3)	4850(3)	63(2)

C67	15062(6)	7563(3)	4703(3)	64(2)
C68	14509(6)	7070(2)	4410(3)	59(1)
C69	13312(5)	7027(3)	4275(3)	64(2)
C70	12568(6)	7442(3)	4434(3)	63(2)

Bond lengths [Å] and angles [°] for 6.

Hf(1)-N(2)	2.156(3)	N(3)-C(22)	1.365(4)
Hf(1)-N(3)	2.178(3)	N(3)-C(21)	1.387(4)
Hf(1)-N(4)	2.203(3)	N(4)-C(38)	1.369(4)
Hf(1)-N(1)	2.203(3)	N(4)-C(37)	1.391(4)
Hf(1)-Ni(1)	2.4123(6)	C(1)-C(2)	1.383(6)
Hf(1)-P(1)	2.8543(11)	C(1)-H(13)	0.9500
Ni(1)-P(4)	2.1849(10)	C(2)-C(3)	1.400(7)
Ni(1)-P(3)	2.2072(10)	C(2)-H(12)	0.9500
Ni(1)-P(2)	2.2171(11)	C(3)-C(4)	1.383(5)
P(1)-C(4)	1.792(4)	C(3)-H(11)	0.9500
P(1)-C(5)	1.827(4)	C(5)-C(10)	1.391(6)
P(1)-C(11)	1.831(4)	C(5)-C(6)	1.398(6)
P(2)-C(20)	1.796(4)	C(6)-C(7)	1.393(6)
P(2)-C(59)	1.827(4)	C(6)-H(1)	0.9500
P(2)-C(53)	1.841(4)	C(7)-C(8)	1.377(8)
P(3)-C(21)	1.791(4)	C(7)-H(2)	0.9500
P(3)-C(31)	1.837(4)	C(8)-C(9)	1.378(8)
P(3)-C(25)	1.841(4)	C(8)-H(3)	0.9500
P(4)-C(37)	1.789(3)	C(9)-C(10)	1.386(6)
P(4)-C(41)	1.825(4)	C(9)-H(4)	0.9500
P(4)-C(47)	1.827(4)	C(10)-H(5)	0.9500
N(1)-C(1)	1.353(5)	C(11)-C(16)	1.373(6)
N(1)-C(4)	1.398(5)	C(11)-C(12)	1.393(5)
N(2)-C(17)	1.376(5)	C(12)-C(13)	1.384(6)
N(2)-C(20)	1.389(5)	C(12)-H(10)	0.9500

C(13)-C(14)	1.371(7)	C(29)-C(30)	1.395(6)
C(13)-H(9)	0.9500	C(29)-H(20)	0.9500
C(14)-C(15)	1.378(8)	C(30)-H(19)	0.9500
C(14)-H(8)	0.9500	C(31)-C(36)	1.386(6)
C(15)-C(16)	1.391(7)	C(31)-C(32)	1.392(5)
C(15)-H(7)	0.9500	C(32)-C(33)	1.388(6)
C(16)-H(6)	0.9500	C(32)-H(28)	0.9500
C(17)-C(18)	1.371(7)	C(33)-C(34)	1.378(7)
C(17)-H(14)	0.9500	C(33)-H(27)	0.9500
C(18)-C(19)	1.407(7)	C(34)-C(35)	1.383(6)
C(18)-H(15)	0.9500	C(34)-H(26)	0.9500
C(19)-C(20)	1.366(6)	C(35)-C(36)	1.388(5)
C(19)-H(52)	0.9500	C(35)-H(25)	0.9500
C(21)-C(24)	1.384(5)	C(36)-H(24)	0.9500
C(22)-C(23)	1.380(5)	C(37)-C(40)	1.375(5)
C(22)-H(16)	0.9500	C(38)-C(39)	1.380(5)
C(23)-C(24)	1.412(5)	C(38)-H(29)	0.9500
C(23)-H(17)	0.9500	C(39)-C(40)	1.411(5)
C(24)-H(18)	0.9500	C(39)-H(30)	0.9500
C(25)-C(26)	1.388(6)	C(40)-H(31)	0.9500
C(25)-C(30)	1.394(5)	C(41)-C(46)	1.386(5)
C(26)-C(27)	1.393(6)	C(41)-C(42)	1.402(5)
C(26)-H(23)	0.9500	C(42)-C(43)	1.374(6)
C(27)-C(28)	1.365(7)	C(42)-H(36)	0.9500
C(27)-H(22)	0.9500	C(43)-C(44)	1.387(6)
C(28)-C(29)	1.377(8)	C(43)-H(35)	0.9500
C(28)-H(21)	0.9500	C(44)-C(45)	1.381(6)

C(44)-H(34)	0.9500	C(59)-C(60)	1.396(6)
C(45)-C(46)	1.386(5)	C(60)-C(61)	1.382(6)
C(45)-H(33)	0.9500	C(60)-H(51)	0.9500
C(46)-H(32)	0.9500	C(61)-C(62)	1.382(8)
C(47)-C(48)	1.393(6)	C(61)-H(47)	0.9500
C(47)-C(52)	1.401(5)	C(62)-C(63)	1.363(8)
C(48)-C(49)	1.390(6)	C(62)-H(48)	0.9500
C(48)-H(41)	0.9500	C(63)-C(64)	1.395(7)
C(49)-C(50)	1.373(7)	C(63)-H(49)	0.9500
C(49)-H(37)	0.9500	C(64)-H(50)	0.9500
C(50)-C(51)	1.387(8)	C(65)-C(66)	1.347(8)
C(50)-H(38)	0.9500	C(65)-C(70)	1.403(9)
C(51)-C(52)	1.389(6)	C(65)-H(53)	0.9500
C(51)-H(39)	0.9500	C(66)-C(67)	1.393(8)
C(52)-H(40)	0.9500	C(66)-H(57)	0.9500
C(53)-C(54)	1.388(6)	C(67)-C(68)	1.414(8)
C(53)-C(58)	1.392(6)	C(67)-H(58)	0.9500
C(54)-C(55)	1.397(6)	C(68)-C(69)	1.308(8)
C(54)-H(46)	0.9500	C(68)-H(54)	0.9500
C(55)-C(56)	1.367(7)	C(69)-C(70)	1.392(9)
C(55)-H(42)	0.9500	C(69)-H(55)	0.9500
C(56)-C(57)	1.380(7)	C(70)-H(56)	0.9500
C(56)-H(43)	0.9500		
C(57)-C(58)	1.404(6)		
C(57)-H(44)	0.9500		
C(58)-H(45)	0.9500		
C(59)-C(64)	1.382(6)		

N(2)-Hf(1)-N(3)	96.28(11)	C(20)-P(2)-C(59)	109.16(19)
N(2)-Hf(1)-N(4)	102.98(11)	C(20)-P(2)-C(53)	102.72(18)
N(3)-Hf(1)-N(4)	160.07(12)	C(59)-P(2)-C(53)	102.38(18)
N(2)-Hf(1)-N(1)	93.02(12)	C(20)-P(2)-Ni(1)	111.29(14)
N(3)-Hf(1)-N(1)	88.93(11)	C(59)-P(2)-Ni(1)	106.71(13)
N(4)-Hf(1)-N(1)	85.02(11)	C(53)-P(2)-Ni(1)	123.73(12)
N(2)-Hf(1)-Ni(1)	93.19(9)	C(21)-P(3)-C(31)	103.11(16)
N(3)-Hf(1)-Ni(1)	94.12(7)	C(21)-P(3)-C(25)	106.99(17)
N(4)-Hf(1)-Ni(1)	89.92(8)	C(31)-P(3)-C(25)	103.39(16)
N(1)-Hf(1)-Ni(1)	172.74(9)	C(21)-P(3)-Ni(1)	112.38(11)
N(2)-Hf(1)-P(1)	154.41(9)	C(31)-P(3)-Ni(1)	119.01(12)
N(3)-Hf(1)-P(1)	80.14(8)	C(25)-P(3)-Ni(1)	110.91(12)
N(4)-Hf(1)-P(1)	80.27(9)	C(37)-P(4)-C(41)	107.36(17)
N(1)-Hf(1)-P(1)	61.73(9)	C(37)-P(4)-C(47)	108.44(17)
Ni(1)-Hf(1)-P(1)	112.29(2)	C(41)-P(4)-C(47)	101.77(16)
P(4)-Ni(1)-P(3)	131.53(4)	C(37)-P(4)-Ni(1)	109.51(12)
P(4)-Ni(1)-P(2)	110.61(4)	C(41)-P(4)-Ni(1)	125.08(12)
P(3)-Ni(1)-P(2)	117.68(4)	C(47)-P(4)-Ni(1)	103.42(12)
P(4)-Ni(1)-Hf(1)	89.38(3)	C(1)-N(1)-C(4)	105.6(3)
P(3)-Ni(1)-Hf(1)	93.89(3)	C(1)-N(1)-Hf(1)	143.3(3)
P(2)-Ni(1)-Hf(1)	90.57(3)	C(4)-N(1)-Hf(1)	109.7(2)
C(4)-P(1)-C(5)	106.27(18)	C(17)-N(2)-C(20)	105.9(3)
C(4)-P(1)-C(11)	108.34(18)	C(17)-N(2)-Hf(1)	132.0(3)
C(5)-P(1)-C(11)	103.55(19)	C(20)-N(2)-Hf(1)	119.7(2)
C(4)-P(1)-Hf(1)	75.99(14)	C(22)-N(3)-C(21)	106.3(3)
C(5)-P(1)-Hf(1)	132.52(13)	C(22)-N(3)-Hf(1)	131.4(2)
C(11)-P(1)-Hf(1)	121.06(14)	C(21)-N(3)-Hf(1)	122.2(2)

C(38)-N(4)-C(37)	106.0(3)	C(8)-C(9)-C(10)	120.2(5)
C(38)-N(4)-Hf(1)	133.3(2)	C(8)-C(9)-H(4)	119.9
C(37)-N(4)-Hf(1)	120.6(2)	C(10)-C(9)-H(4)	119.9
N(1)-C(1)-C(2)	110.9(4)	C(9)-C(10)-C(5)	120.6(5)
N(1)-C(1)-H(13)	124.6	C(9)-C(10)-H(5)	119.7
C(2)-C(1)-H(13)	124.6	C(5)-C(10)-H(5)	119.7
C(1)-C(2)-C(3)	107.2(3)	C(16)-C(11)-C(12)	118.9(4)
C(1)-C(2)-H(12)	126.4	C(16)-C(11)-P(1)	123.1(3)
C(3)-C(2)-H(12)	126.4	C(12)-C(11)-P(1)	118.1(3)
C(4)-C(3)-C(2)	106.0(4)	C(13)-C(12)-C(11)	120.0(4)
C(4)-C(3)-H(11)	127.0	C(13)-C(12)-H(10)	120.0
C(2)-C(3)-H(11)	127.0	C(11)-C(12)-H(10)	120.0
C(3)-C(4)-N(1)	110.3(4)	C(14)-C(13)-C(12)	120.8(4)
C(3)-C(4)-P(1)	137.6(4)	C(14)-C(13)-H(9)	119.6
N(1)-C(4)-P(1)	112.1(3)	C(12)-C(13)-H(9)	119.6
C(10)-C(5)-C(6)	119.0(4)	C(13)-C(14)-C(15)	119.4(4)
C(10)-C(5)-P(1)	121.3(3)	C(13)-C(14)-H(8)	120.3
C(6)-C(5)-P(1)	119.5(3)	C(15)-C(14)-H(8)	120.3
C(7)-C(6)-C(5)	119.5(5)	C(14)-C(15)-C(16)	120.2(5)
C(7)-C(6)-H(1)	120.2	C(14)-C(15)-H(7)	119.9
C(5)-C(6)-H(1)	120.2	C(16)-C(15)-H(7)	119.9
C(8)-C(7)-C(6)	120.8(5)	C(11)-C(16)-C(15)	120.7(5)
C(8)-C(7)-H(2)	119.6	C(11)-C(16)-H(6)	119.7
C(6)-C(7)-H(2)	119.6	C(15)-C(16)-H(6)	119.7
C(7)-C(8)-C(9)	119.8(4)	C(18)-C(17)-N(2)	110.2(4)
C(7)-C(8)-H(3)	120.1	C(18)-C(17)-H(14)	124.9
C(9)-C(8)-H(3)	120.1	N(2)-C(17)-H(14)	124.9

C(17)-C(18)-C(19)	106.9(4)	C(28)-C(27)-C(26)	120.7(5)
C(17)-C(18)-H(15)	126.6	C(28)-C(27)-H(22)	119.7
C(19)-C(18)-H(15)	126.6	C(26)-C(27)-H(22)	119.7
C(20)-C(19)-C(18)	107.2(4)	C(27)-C(28)-C(29)	120.1(4)
C(20)-C(19)-H(52)	126.4	C(27)-C(28)-H(21)	119.9
C(18)-C(19)-H(52)	126.4	C(29)-C(28)-H(21)	119.9
C(19)-C(20)-N(2)	109.8(4)	C(28)-C(29)-C(30)	120.1(4)
C(19)-C(20)-P(2)	134.0(4)	C(28)-C(29)-H(20)	119.9
N(2)-C(20)-P(2)	116.1(3)	C(30)-C(29)-H(20)	119.9
C(24)-C(21)-N(3)	110.0(3)	C(25)-C(30)-C(29)	120.0(4)
C(24)-C(21)-P(3)	132.7(3)	C(25)-C(30)-H(19)	120.0
N(3)-C(21)-P(3)	117.2(2)	C(29)-C(30)-H(19)	120.0
N(3)-C(22)-C(23)	110.5(3)	C(36)-C(31)-C(32)	119.4(4)
N(3)-C(22)-H(16)	124.8	C(36)-C(31)-P(3)	116.7(3)
C(23)-C(22)-H(16)	124.8	C(32)-C(31)-P(3)	123.9(3)
C(22)-C(23)-C(24)	106.9(3)	C(33)-C(32)-C(31)	119.8(4)
C(22)-C(23)-H(17)	126.5	C(33)-C(32)-H(28)	120.1
C(24)-C(23)-H(17)	126.5	C(31)-C(32)-H(28)	120.1
C(21)-C(24)-C(23)	106.3(3)	C(34)-C(33)-C(32)	120.4(4)
C(21)-C(24)-H(18)	126.8	C(34)-C(33)-H(27)	119.8
C(23)-C(24)-H(18)	126.8	C(32)-C(33)-H(27)	119.8
C(26)-C(25)-C(30)	119.1(4)	C(33)-C(34)-C(35)	120.1(4)
C(26)-C(25)-P(3)	122.7(3)	C(33)-C(34)-H(26)	119.9
C(30)-C(25)-P(3)	118.0(3)	C(35)-C(34)-H(26)	119.9
C(25)-C(26)-C(27)	119.9(4)	C(34)-C(35)-C(36)	119.7(4)
C(25)-C(26)-H(23)	120.0	C(34)-C(35)-H(25)	120.2
C(27)-C(26)-H(23)	120.0	C(36)-C(35)-H(25)	120.2

C(31)-C(36)-C(35)	120.6(4)	C(44)-C(45)-C(46)	119.6(4)
C(31)-C(36)-H(24)	119.7	C(44)-C(45)-H(33)	120.2
C(35)-C(36)-H(24)	119.7	C(46)-C(45)-H(33)	120.2
C(40)-C(37)-N(4)	110.3(3)	C(45)-C(46)-C(41)	120.8(3)
C(40)-C(37)-P(4)	136.3(3)	C(45)-C(46)-H(32)	119.6
N(4)-C(37)-P(4)	113.5(2)	C(41)-C(46)-H(32)	119.6
N(4)-C(38)-C(39)	110.2(3)	C(48)-C(47)-C(52)	119.5(4)
N(4)-C(38)-H(29)	124.9	C(48)-C(47)-P(4)	123.9(3)
C(39)-C(38)-H(29)	124.9	C(52)-C(47)-P(4)	116.5(3)
C(38)-C(39)-C(40)	107.1(3)	C(49)-C(48)-C(47)	119.9(4)
C(38)-C(39)-H(30)	126.4	C(49)-C(48)-H(41)	120.1
C(40)-C(39)-H(30)	126.4	C(47)-C(48)-H(41)	120.1
C(37)-C(40)-C(39)	106.4(3)	C(50)-C(49)-C(48)	120.5(5)
C(37)-C(40)-H(31)	126.8	C(50)-C(49)-H(37)	119.8
C(39)-C(40)-H(31)	126.8	C(48)-C(49)-H(37)	119.8
C(46)-C(41)-C(42)	119.2(3)	C(49)-C(50)-C(51)	120.2(4)
C(46)-C(41)-P(4)	119.3(3)	C(49)-C(50)-H(38)	119.9
C(42)-C(41)-P(4)	121.5(3)	C(51)-C(50)-H(38)	119.9
C(43)-C(42)-C(41)	119.6(3)	C(50)-C(51)-C(52)	120.1(5)
C(43)-C(42)-H(36)	120.2	C(50)-C(51)-H(39)	119.9
C(41)-C(42)-H(36)	120.2	C(52)-C(51)-H(39)	119.9
C(42)-C(43)-C(44)	120.8(4)	C(51)-C(52)-C(47)	119.8(4)
C(42)-C(43)-H(35)	119.6	C(51)-C(52)-H(40)	120.1
C(44)-C(43)-H(35)	119.6	C(47)-C(52)-H(40)	120.1
C(45)-C(44)-C(43)	119.9(4)	C(54)-C(53)-C(58)	119.6(4)
C(45)-C(44)-H(34)	120.0	C(54)-C(53)-P(2)	118.5(3)
C(43)-C(44)-H(34)	120.0	C(58)-C(53)-P(2)	121.9(3)

C(53)-C(54)-C(55)	119.8(4)	C(61)-C(62)-H(48)	119.9
C(53)-C(54)-H(46)	120.1	C(62)-C(63)-C(64)	120.5(5)
C(55)-C(54)-H(46)	120.1	C(62)-C(63)-H(49)	119.7
C(56)-C(55)-C(54)	120.6(4)	C(64)-C(63)-H(49)	119.7
C(56)-C(55)-H(42)	119.7	C(59)-C(64)-C(63)	120.2(5)
C(54)-C(55)-H(42)	119.7	C(59)-C(64)-H(50)	119.9
C(55)-C(56)-C(57)	120.4(4)	C(63)-C(64)-H(50)	119.9
C(55)-C(56)-H(43)	119.8	C(66)-C(65)-C(70)	121.5(6)
C(57)-C(56)-H(43)	119.8	C(66)-C(65)-H(53)	119.2
C(56)-C(57)-C(58)	119.8(4)	C(70)-C(65)-H(53)	119.2
C(56)-C(57)-H(44)	120.1	C(65)-C(66)-C(67)	117.9(6)
C(58)-C(57)-H(44)	120.1	C(65)-C(66)-H(57)	121.1
C(53)-C(58)-C(57)	119.9(4)	C(67)-C(66)-H(57)	121.1
C(53)-C(58)-H(45)	120.1	C(66)-C(67)-C(68)	121.2(6)
C(57)-C(58)-H(45)	120.1	C(66)-C(67)-H(58)	119.4
C(64)-C(59)-C(60)	118.5(4)	C(68)-C(67)-H(58)	119.4
C(64)-C(59)-P(2)	125.1(3)	C(69)-C(68)-C(67)	119.0(6)
C(60)-C(59)-P(2)	116.3(3)	C(69)-C(68)-H(54)	120.5
C(61)-C(60)-C(59)	121.0(5)	C(67)-C(68)-H(54)	120.5
C(61)-C(60)-H(51)	119.5	C(68)-C(69)-C(70)	122.0(7)
C(59)-C(60)-H(51)	119.5	C(68)-C(69)-H(55)	119.0
C(62)-C(61)-C(60)	119.5(5)	C(70)-C(69)-H(55)	119.0
C(62)-C(61)-H(47)	120.2	C(69)-C(70)-C(65)	118.3(6)
C(60)-C(61)-H(47)	120.2	C(69)-C(70)-H(56)	120.8
C(63)-C(62)-C(61)	120.3(5)	C(65)-C(70)-H(56)	120.
C(63)-C(62)-H(48)	119.9		

Symmetry transformations used to generate equivalent atoms:

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 7. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	zU_{eq}	
Ni1	2039(1)	1770(1)	2318(1)	13(1)
Ti1	2535(1)	3292(1)	3576(1)	16(1)
P2	2617(1)	2483(1)	1463(1)	14(1)
P3	2919(1)	1035(1)	3293(1)	16(1)
P4	566(1)	1637(1)	2410(1)	16(1)
Na1	5154(1)	3099(1)	3527(1)	28(1)
N1	7144(2)	5511(1)	5430(1)	20(1)
O1	6182(1)	2179(1)	3062(1)	32(1)
C78	7666(2)	4804(2)	5698(2)	20(1)
C77	6711(2)	5258(2)	4541(2)	21(1)
C76	-88(2)	2092(2)	3952(2)	24(1)
C75	6940(2)	4407(2)	4244(2)	21(1)
N4	1392(1)	2759(1)	3995(1)	18(1)
C73	569(2)	2146(2)	3486(2)	19(1)
C72	1232(2)	3062(2)	4781(2)	23(1)
C1	1803(2)	3068(2)	651(1)	16(1)
C2	2149(2)	3561(2)	107(2)	21(1)
C3	1540(2)	4057(2)	-441(2)	24(1)
C4	578(2)	4063(2)	-459(2)	26(1)
C5	226(2)	3560(2)	63(2)	28(1)
C6	840(2)	3070(2)	617(2)	21(1)
C7	3172(2)	1820(2)	720(2)	17(1)

C8	4170(2)	1789(2)	915(2)	24(1)
C9	4521(2)	1260(2)	322(2)	29(1)
C10	3896(2)	732(2)	-444(2)	28(1)
C11	2897(2)	732(2)	-629(2)	28(1)
C12	2538(2)	1283(2)	-52(2)	22(1)
C13	3543(2)	3415(2)	2098(2)	18(1)
C14	6311(3)	1303(2)	3346(3)	50(1)
C15	7008(2)	862(2)	2934(2)	39(1)
C16	7106(2)	1448(2)	2270(2)	32(1)
C17	6902(2)	2375(2)	2646(2)	34(1)
C18	3882(2)	1810(2)	4140(2)	19(1)
C19	3602(2)	175(2)	2889(2)	21(1)
C20	4177(2)	-350(2)	3442(2)	24(1)
C21	4763(2)	-920(2)	3135(2)	31(1)
C22	4763(2)	-988(2)	2268(2)	36(1)
C23	4164(2)	-503(2)	1701(2)	32(1)
C24	3585(2)	79(2)	2013(2)	25(1)
C25	2327(2)	382(2)	3931(2)	22(1)
C26	1986(2)	-553(2)	3634(2)	28(1)
C27	1463(2)	-1024(2)	4074(2)	40(1)
C28	1258(2)	-564(2)	4788(2)	46(1)
C29	1588(3)	361(3)	5081(2)	46(1)
C30	2125(2)	835(2)	4654(2)	34(1)
C31	4796(2)	1694(2)	4668(2)	26(1)
C32	5236(2)	2569(2)	5173(2)	26(1)
C33	4570(2)	3171(2)	4937(2)	24(1)
N3	3735(1)	2723(1)	4301(1)	20(1)

C35	7554(2)	4114(2)	4984(2)	25(1)
C36	4147(2)	4589(2)	3204(2)	25(1)
N2	3450(1)	3831(1)	2891(1)	18(1)
C38	4300(2)	3910(2)	1926(2)	25(1)
C39	4683(2)	4651(2)	2635(2)	28(1)
C40	-553(2)	1978(2)	1687(2)	19(1)
C41	-1124(2)	1417(2)	899(2)	26(1)
C42	-1944(2)	1717(2)	360(2)	33(1)
C43	-2199(2)	2574(2)	596(2)	36(1)
C44	-1620(2)	3147(2)	1370(2)	33(1)
C45	-801(2)	2851(2)	1908(2)	26(1)
C46	219(2)	385(2)	2206(2)	21(1)
C47	538(2)	-131(2)	1574(2)	27(1)
C48	299(2)	-1085(2)	1352(2)	36(1)
C49	-257(2)	-1531(2)	1771(2)	37(1)
C50	-560(2)	-1030(2)	2408(2)	36(1)
C51	-332(2)	-77(2)	2624(2)	27(1)
C52	340(2)	2669(2)	4780(2)	26(1)
C54	7959(2)	4249(2)	7409(2)	22(1)
C55	7634(2)	3330(2)	7011(2)	34(1)
C56	7290(2)	2724(2)	7456(2)	37(1)
C57	7277(2)	3019(2)	8306(2)	30(1)
C58	7596(2)	3927(2)	8703(2)	34(1)
C59	7929(2)	4542(2)	8251(2)	26(1)
C60	9580(2)	4743(2)	6817(2)	24(1)
C61	10028(2)	4084(2)	7265(2)	30(1)
C62	10952(2)	3907(2)	7255(2)	34(1)

C63	11433(2)	4392(2)	6798(2)	32(1)
C64	10979(2)	5032(2)	6337(2)	32(1)
C65	10058(2)	5212(2)	6339(2)	28(1)
P1	8393(4)	5124(4)	6851(4)	17(1)
O2	8463(4)	5895(4)	7174(4)	16(2)
P1A	8417(13)	4908(9)	6782(12)	19(2)

Bond lengths [Å] and angles [°] for 7.

Ni(1)-P(2)	2.1651(6)	Na(1)-C(13)	2.869(3)
Ni(1)-P(4)	2.1810(7)	Na(1)-C(39)	2.901(3)
Ni(1)-P(3)	2.1898(7)	Na(1)-C(38)	2.974(3)
Ni(1)-Ti(1)	2.6892(5)	Na(1)-C(18)	3.016(2)
Ti(1)-N(3)	2.098(2)	Na(1)-C(31)	3.080(3)
Ti(1)-N(4)	2.1068(19)	N(1)-C(77)	1.361(3)
Ti(1)-N(1)#1	2.1263(19)	N(1)-C(78)	1.384(3)
Ti(1)-N(2)	2.1390(19)	N(1)-Ti(1)#1	2.1264(19)
Ti(1)-O(2)#1	2.158(6)	O(1)-C(17)	1.433(3)
Ti(1)-P(1)#1	2.863(5)	O(1)-C(14)	1.443(4)
P(2)-C(13)	1.794(2)	C(78)-C(35)	1.383(3)
P(2)-C(7)	1.845(2)	C(78)-P(1A)	1.735(18)
P(2)-C(1)	1.850(2)	C(78)-P(1)	1.809(7)
P(3)-C(18)	1.808(2)	C(77)-C(75)	1.384(3)
P(3)-C(19)	1.837(2)	C(77)-H(77A)	0.9500
P(3)-C(25)	1.846(2)	C(76)-C(73)	1.383(3)
P(4)-C(73)	1.786(2)	C(76)-C(52)	1.408(3)
P(4)-C(46)	1.835(2)	C(76)-H(76A)	0.9500
P(4)-C(40)	1.847(2)	C(75)-C(35)	1.406(4)
Na(1)-O(1)	2.311(2)	C(75)-H(75A)	0.9500
Na(1)-C(33)	2.644(3)	N(4)-C(72)	1.374(3)
Na(1)-N(2)	2.749(2)	N(4)-C(73)	1.394(3)
Na(1)-C(36)	2.766(3)	C(72)-C(52)	1.375(4)
Na(1)-N(3)	2.767(2)	C(72)-H(72A)	0.9500
Na(1)-C(32)	2.846(3)	C(1)-C(6)	1.381(3)

C(1)-C(2)	1.395(3)	C(15)-H(15A)	0.9900
C(2)-C(3)	1.386(3)	C(15)-H(15B)	0.9900
C(2)-H(2A)	0.9500	C(16)-C(17)	1.505(4)
C(3)-C(4)	1.386(4)	C(16)-H(16A)	0.9900
C(3)-H(3A)	0.9500	C(16)-H(16B)	0.9900
C(4)-C(5)	1.379(4)	C(17)-H(17A)	0.9900
C(4)-H(4A)	0.9500	C(17)-H(17B)	0.9900
C(5)-C(6)	1.389(3)	C(18)-C(31)	1.383(3)
C(5)-H(5A)	0.9500	C(18)-N(3)	1.384(3)
C(6)-H(6A)	0.9500	C(19)-C(24)	1.390(4)
C(7)-C(12)	1.391(3)	C(19)-C(20)	1.397(3)
C(7)-C(8)	1.393(3)	C(20)-C(21)	1.387(4)
C(8)-C(9)	1.387(3)	C(20)-H(20A)	0.9500
C(8)-H(8A)	0.9500	C(21)-C(22)	1.386(4)
C(9)-C(10)	1.375(4)	C(21)-H(21A)	0.9500
C(9)-H(9A)	0.9500	C(22)-C(23)	1.385(4)
C(10)-C(11)	1.388(4)	C(22)-H(22A)	0.9500
C(10)-H(10A)	0.9500	C(23)-C(24)	1.393(4)
C(11)-C(12)	1.392(3)	C(23)-H(23A)	0.9500
C(11)-H(11A)	0.9500	C(24)-H(24A)	0.9500
C(12)-H(12A)	0.9500	C(25)-C(30)	1.380(4)
C(13)-N(2)	1.386(3)	C(25)-C(26)	1.394(4)
C(13)-C(38)	1.390(3)	C(26)-C(27)	1.394(4)
C(14)-C(15)	1.508(4)	C(26)-H(26A)	0.9500
C(14)-H(14A)	0.9900	C(27)-C(28)	1.373(5)
C(14)-H(14B)	0.9900	C(27)-H(27A)	0.9500
C(15)-C(16)	1.502(4)	C(28)-C(29)	1.378(5)

C(28)-H(28A)	0.9500	C(45)-H(45A)	0.9500
C(29)-C(30)	1.394(4)	C(46)-C(51)	1.389(4)
C(29)-H(29A)	0.9500	C(46)-C(47)	1.396(4)
C(30)-H(30A)	0.9500	C(47)-C(48)	1.393(4)
C(31)-C(32)	1.412(4)	C(47)-H(47A)	0.9500
C(31)-H(31A)	1.0000	C(48)-C(49)	1.383(4)
C(32)-C(33)	1.373(4)	C(48)-H(48A)	0.9500
C(32)-H(32A)	1.0000	C(49)-C(50)	1.378(5)
C(33)-N(3)	1.373(3)	C(49)-H(49A)	0.9500
C(33)-H(33A)	1.0000	C(50)-C(51)	1.389(4)
C(35)-H(35A)	0.9500	C(50)-H(50A)	0.9500
C(36)-N(2)	1.371(3)	C(51)-H(51A)	0.9500
C(36)-C(39)	1.376(4)	C(52)-H(52A)	0.9500
C(36)-H(36A)	1.0000	C(54)-C(59)	1.378(3)
C(38)-C(39)	1.404(4)	C(54)-C(55)	1.394(4)
C(38)-H(38A)	1.0000	C(54)-P(1A)	1.731(18)
C(39)-H(39A)	1.0000	C(54)-P(1)	1.851(6)
C(40)-C(41)	1.393(3)	C(55)-C(56)	1.376(4)
C(40)-C(45)	1.394(4)	C(55)-H(55A)	0.9500
C(41)-C(42)	1.394(4)	C(56)-C(57)	1.383(4)
C(41)-H(41A)	0.9500	C(56)-H(56A)	0.9500
C(42)-C(43)	1.382(4)	C(57)-C(58)	1.379(4)
C(42)-H(42A)	0.9500	C(57)-H(57A)	0.9500
C(43)-C(44)	1.389(4)	C(58)-C(59)	1.387(4)
C(43)-H(43A)	0.9500	C(58)-H(58A)	0.9500
C(44)-C(45)	1.389(4)	C(59)-H(59A)	0.9500
C(44)-H(44A)	0.9500	C(60)-C(61)	1.386(4)

C(60)-C(65)	1.397(4)	N(1)#1-Ti(1)-N(2)	94.32(7)
C(60)-P(1A)	1.707(17)	N(3)-Ti(1)-O(2)#1	167.68(17)
C(60)-P(1)	1.867(6)	N(4)-Ti(1)-O(2)#1	88.24(17)
C(61)-C(62)	1.390(4)	N(1)#1-Ti(1)-O(2)#1	82.73(17)
C(61)-H(61A)	0.9500	N(2)-Ti(1)-O(2)#1	81.60(17)
C(62)-C(63)	1.388(4)	N(3)-Ti(1)-Ni(1)	90.16(6)
C(62)-H(62A)	0.9500	N(4)-Ti(1)-Ni(1)	86.17(5)
C(63)-C(64)	1.376(4)	N(1)#1-Ti(1)-Ni(1)	177.18(6)
C(63)-H(63A)	0.9500	N(2)-Ti(1)-Ni(1)	87.89(5)
C(64)-C(65)	1.384(4)	O(2)#1-Ti(1)-Ni(1)	95.87(16)
C(64)-H(64A)	0.9500	N(3)-Ti(1)-P(1)#1	149.71(14)
C(65)-H(65A)	0.9500	N(4)-Ti(1)-P(1)#1	92.18(13)
P(1)-Ti(1)#1	2.863(5)	N(1)#1-Ti(1)-P(1)#1	61.49(14)
O(2)-P(1A)	1.493(12)	N(2)-Ti(1)-P(1)#1	80.93(13)
O(2)-Ti(1)#1	2.158(6)	O(2)#1-Ti(1)-P(1)#1	21.5(2)
		Ni(1)-Ti(1)-P(1)#1	117.25(13)
P(2)-Ni(1)-P(4)	129.33(3)	C(13)-P(2)-C(7)	105.08(11)
P(2)-Ni(1)-P(3)	123.31(3)	C(13)-P(2)-C(1)	101.66(10)
P(4)-Ni(1)-P(3)	107.36(3)	C(7)-P(2)-C(1)	98.82(10)
P(2)-Ni(1)-Ti(1)	91.00(2)	C(13)-P(2)-Ni(1)	110.79(8)
P(4)-Ni(1)-Ti(1)	90.05(2)	C(7)-P(2)-Ni(1)	118.56(7)
P(3)-Ni(1)-Ti(1)	88.27(2)	C(1)-P(2)-Ni(1)	119.66(8)
N(3)-Ti(1)-N(4)	102.91(8)	C(18)-P(3)-C(19)	101.94(11)
N(3)-Ti(1)-N(1)#1	91.67(8)	C(18)-P(3)-C(25)	103.41(11)
N(4)-Ti(1)-N(1)#1	91.33(8)	C(19)-P(3)-C(25)	101.49(11)
N(3)-Ti(1)-N(2)	87.92(8)	C(18)-P(3)-Ni(1)	111.58(8)
N(4)-Ti(1)-N(2)	167.64(8)	C(19)-P(3)-Ni(1)	116.71(8)

C(25)-P(3)-Ni(1)	119.48(8)	C(32)-Na(1)-C(13)	131.46(8)
C(73)-P(4)-C(46)	110.95(11)	O(1)-Na(1)-C(39)	116.20(8)
C(73)-P(4)-C(40)	102.35(11)	C(33)-Na(1)-C(39)	112.38(9)
C(46)-P(4)-C(40)	99.86(11)	N(2)-Na(1)-C(39)	46.92(7)
C(73)-P(4)-Ni(1)	110.66(8)	C(36)-Na(1)-C(39)	27.97(8)
C(46)-P(4)-Ni(1)	103.10(8)	N(3)-Na(1)-C(39)	108.03(7)
C(40)-P(4)-Ni(1)	129.00(7)	C(32)-Na(1)-C(39)	138.82(9)
O(1)-Na(1)-C(33)	130.39(9)	C(13)-Na(1)-C(39)	45.69(7)
O(1)-Na(1)-N(2)	141.54(8)	O(1)-Na(1)-C(38)	101.15(8)
C(33)-Na(1)-N(2)	81.65(7)	C(33)-Na(1)-C(38)	127.30(8)
O(1)-Na(1)-C(36)	143.98(8)	N(2)-Na(1)-C(38)	46.45(6)
C(33)-Na(1)-C(36)	85.37(8)	C(36)-Na(1)-C(38)	45.72(7)
N(2)-Na(1)-C(36)	28.80(6)	N(3)-Na(1)-C(38)	109.56(7)
O(1)-Na(1)-N(3)	131.49(8)	C(32)-Na(1)-C(38)	155.50(8)
C(33)-Na(1)-N(3)	29.28(6)	C(13)-Na(1)-C(38)	27.44(7)
N(2)-Na(1)-N(3)	64.44(6)	C(39)-Na(1)-C(38)	27.61(7)
C(36)-Na(1)-N(3)	80.94(7)	O(1)-Na(1)-C(18)	104.42(8)
O(1)-Na(1)-C(32)	101.88(8)	C(33)-Na(1)-C(18)	45.24(7)
C(33)-Na(1)-C(32)	28.67(8)	N(2)-Na(1)-C(18)	83.16(7)
N(2)-Na(1)-C(32)	109.08(7)	C(36)-Na(1)-C(18)	105.58(8)
C(36)-Na(1)-C(32)	113.40(8)	N(3)-Na(1)-C(18)	27.25(6)
N(3)-Na(1)-C(32)	47.42(7)	C(32)-Na(1)-C(18)	44.87(7)
O(1)-Na(1)-C(13)	113.13(8)	C(13)-Na(1)-C(18)	92.88(7)
C(33)-Na(1)-C(13)	107.39(8)	C(39)-Na(1)-C(18)	130.01(8)
N(2)-Na(1)-C(13)	28.47(6)	C(38)-Na(1)-C(18)	120.23(7)
C(36)-Na(1)-C(13)	46.12(7)	O(1)-Na(1)-C(31)	89.43(8)
N(3)-Na(1)-C(13)	84.04(7)	C(33)-Na(1)-C(31)	45.17(8)

N(2)-Na(1)-C(31)	107.99(7)	C(77)-C(75)-H(75A)	126.5
C(36)-Na(1)-C(31)	125.58(8)	C(35)-C(75)-H(75A)	126.5
N(3)-Na(1)-C(31)	45.16(7)	C(72)-N(4)-C(73)	105.86(19)
C(32)-Na(1)-C(31)	27.21(7)	C(72)-N(4)-Ti(1)	126.23(16)
C(13)-Na(1)-C(31)	118.78(7)	C(73)-N(4)-Ti(1)	127.15(15)
C(39)-Na(1)-C(31)	153.17(8)	C(76)-C(73)-N(4)	109.5(2)
C(38)-Na(1)-C(31)	145.75(8)	C(76)-C(73)-P(4)	134.40(18)
C(18)-Na(1)-C(31)	26.20(6)	N(4)-C(73)-P(4)	116.12(16)
C(77)-N(1)-C(78)	106.11(19)	N(4)-C(72)-C(52)	110.9(2)
C(77)-N(1)-Ti(1)#1	139.16(17)	N(4)-C(72)-H(72A)	124.6
C(78)-N(1)-Ti(1)#1	113.37(15)	C(52)-C(72)-H(72A)	124.6
C(17)-O(1)-C(14)	107.9(2)	C(6)-C(1)-C(2)	118.6(2)
C(17)-O(1)-Na(1)	131.11(16)	C(6)-C(1)-P(2)	119.60(17)
C(14)-O(1)-Na(1)	119.89(17)	C(2)-C(1)-P(2)	121.71(18)
C(35)-C(78)-N(1)	110.3(2)	C(3)-C(2)-C(1)	120.3(2)
C(35)-C(78)-P(1A)	128.9(4)	C(3)-C(2)-H(2A)	119.9
N(1)-C(78)-P(1A)	120.5(4)	C(1)-C(2)-H(2A)	119.9
C(35)-C(78)-P(1)	139.1(3)	C(2)-C(3)-C(4)	120.5(2)
N(1)-C(78)-P(1)	110.1(2)	C(2)-C(3)-H(3A)	119.7
P(1A)-C(78)-P(1)	10.5(5)	C(4)-C(3)-H(3A)	119.7
N(1)-C(77)-C(75)	110.5(2)	C(5)-C(4)-C(3)	119.5(2)
N(1)-C(77)-H(77A)	124.8	C(5)-C(4)-H(4A)	120.3
C(75)-C(77)-H(77A)	124.8	C(3)-C(4)-H(4A)	120.3
C(73)-C(76)-C(52)	107.2(2)	C(4)-C(5)-C(6)	119.9(2)
C(73)-C(76)-H(76A)	126.4	C(4)-C(5)-H(5A)	120.0
C(52)-C(76)-H(76A)	126.4	C(6)-C(5)-H(5A)	120.0
C(77)-C(75)-C(35)	107.0(2)	C(1)-C(6)-C(5)	121.2(2)

C(1)-C(6)-H(6A)	119.4	O(1)-C(14)-H(14A)	110.2
C(5)-C(6)-H(6A)	119.4	C(15)-C(14)-H(14A)	110.2
C(12)-C(7)-C(8)	119.0(2)	O(1)-C(14)-H(14B)	110.2
C(12)-C(7)-P(2)	117.04(18)	C(15)-C(14)-H(14B)	110.2
C(8)-C(7)-P(2)	123.85(18)	H(14A)-C(14)-H(14B)	108.5
C(9)-C(8)-C(7)	119.9(2)	C(16)-C(15)-C(14)	104.3(2)
C(9)-C(8)-H(8A)	120.0	C(16)-C(15)-H(15A)	110.9
C(7)-C(8)-H(8A)	120.0	C(14)-C(15)-H(15A)	110.9
C(10)-C(9)-C(8)	121.1(2)	C(16)-C(15)-H(15B)	110.9
C(10)-C(9)-H(9A)	119.5	C(14)-C(15)-H(15B)	110.9
C(8)-C(9)-H(9A)	119.5	H(15A)-C(15)-H(15B)	108.9
C(9)-C(10)-C(11)	119.4(2)	C(15)-C(16)-C(17)	103.3(2)
C(9)-C(10)-H(10A)	120.3	C(15)-C(16)-H(16A)	111.1
C(11)-C(10)-H(10A)	120.3	C(17)-C(16)-H(16A)	111.1
C(10)-C(11)-C(12)	120.0(2)	C(15)-C(16)-H(16B)	111.1
C(10)-C(11)-H(11A)	120.0	C(17)-C(16)-H(16B)	111.1
C(12)-C(11)-H(11A)	120.0	H(16A)-C(16)-H(16B)	109.1
C(7)-C(12)-C(11)	120.5(2)	O(1)-C(17)-C(16)	105.2(2)
C(7)-C(12)-H(12A)	119.7	O(1)-C(17)-H(17A)	110.7
C(11)-C(12)-H(12A)	119.7	C(16)-C(17)-H(17A)	110.7
N(2)-C(13)-C(38)	109.5(2)	O(1)-C(17)-H(17B)	110.7
N(2)-C(13)-P(2)	116.36(17)	C(16)-C(17)-H(17B)	110.7
C(38)-C(13)-P(2)	133.63(18)	H(17A)-C(17)-H(17B)	108.8
N(2)-C(13)-Na(1)	70.97(12)	C(31)-C(18)-N(3)	109.8(2)
C(38)-C(13)-Na(1)	80.50(14)	C(31)-C(18)-P(3)	133.0(2)
P(2)-C(13)-Na(1)	120.38(11)	N(3)-C(18)-P(3)	117.14(17)
O(1)-C(14)-C(15)	107.7(2)	C(31)-C(18)-Na(1)	79.45(14)

N(3)-C(18)-Na(1)	66.30(12)	C(28)-C(27)-H(27A)	119.9
P(3)-C(18)-Na(1)	116.97(10)	C(26)-C(27)-H(27A)	119.9
C(24)-C(19)-C(20)	119.0(2)	C(27)-C(28)-C(29)	119.8(3)
C(24)-C(19)-P(3)	118.71(18)	C(27)-C(28)-H(28A)	120.1
C(20)-C(19)-P(3)	122.22(19)	C(29)-C(28)-H(28A)	120.1
C(21)-C(20)-C(19)	120.4(2)	C(28)-C(29)-C(30)	120.3(3)
C(21)-C(20)-H(20A)	119.8	C(28)-C(29)-H(29A)	119.8
C(19)-C(20)-H(20A)	119.8	C(30)-C(29)-H(29A)	119.8
C(22)-C(21)-C(20)	120.0(3)	C(25)-C(30)-C(29)	120.3(3)
C(22)-C(21)-H(21A)	120.0	C(25)-C(30)-H(30A)	119.8
C(20)-C(21)-H(21A)	120.0	C(29)-C(30)-H(30A)	119.8
C(23)-C(22)-C(21)	120.1(3)	C(18)-C(31)-C(32)	106.7(2)
C(23)-C(22)-H(22A)	119.9	C(18)-C(31)-Na(1)	74.35(14)
C(21)-C(22)-H(22A)	119.9	C(32)-C(31)-Na(1)	67.12(14)
C(22)-C(23)-C(24)	119.8(3)	C(18)-C(31)-H(31A)	126.6
C(22)-C(23)-H(23A)	120.1	C(32)-C(31)-H(31A)	126.6
C(24)-C(23)-H(23A)	120.1	Na(1)-C(31)-H(31A)	126.6
C(19)-C(24)-C(23)	120.5(2)	C(33)-C(32)-C(31)	106.7(2)
C(19)-C(24)-H(24A)	119.7	C(33)-C(32)-Na(1)	67.49(14)
C(23)-C(24)-H(24A)	119.7	C(31)-C(32)-Na(1)	85.67(15)
C(30)-C(25)-C(26)	119.0(2)	C(33)-C(32)-H(32A)	125.5
C(30)-C(25)-P(3)	120.1(2)	C(31)-C(32)-H(32A)	125.5
C(26)-C(25)-P(3)	120.5(2)	Na(1)-C(32)-H(32A)	125.5
C(27)-C(26)-C(25)	120.2(3)	N(3)-C(33)-C(32)	110.6(2)
C(27)-C(26)-H(26A)	119.9	N(3)-C(33)-Na(1)	80.34(14)
C(25)-C(26)-H(26A)	119.9	C(32)-C(33)-Na(1)	83.83(15)
C(28)-C(27)-C(26)	120.3(3)	N(3)-C(33)-H(33A)	122.6

C(32)-C(33)-H(33A)	122.6	C(39)-C(38)-H(38A)	126.4
Na(1)-C(33)-H(33A)	122.6	Na(1)-C(38)-H(38A)	126.4
C(33)-N(3)-C(18)	106.2(2)	C(36)-C(39)-C(38)	107.2(2)
C(33)-N(3)-Ti(1)	128.39(17)	C(36)-C(39)-Na(1)	70.52(16)
C(18)-N(3)-Ti(1)	124.99(15)	C(38)-C(39)-Na(1)	79.07(16)
C(33)-N(3)-Na(1)	70.38(13)	C(36)-C(39)-H(39A)	125.8
C(18)-N(3)-Na(1)	86.45(13)	C(38)-C(39)-H(39A)	125.8
Ti(1)-N(3)-Na(1)	103.89(8)	Na(1)-C(39)-H(39A)	125.8
C(78)-C(35)-C(75)	106.1(2)	C(41)-C(40)-C(45)	118.7(2)
C(78)-C(35)-H(35A)	126.9	C(41)-C(40)-P(4)	122.31(19)
C(75)-C(35)-H(35A)	126.9	C(45)-C(40)-P(4)	118.87(18)
N(2)-C(36)-C(39)	110.2(2)	C(40)-C(41)-C(42)	120.2(3)
N(2)-C(36)-Na(1)	74.93(14)	C(40)-C(41)-H(41A)	119.9
C(39)-C(36)-Na(1)	81.51(17)	C(42)-C(41)-H(41A)	119.9
N(2)-C(36)-H(36A)	123.9	C(43)-C(42)-C(41)	120.6(3)
C(39)-C(36)-H(36A)	123.9	C(43)-C(42)-H(42A)	119.7
Na(1)-C(36)-H(36A)	123.9	C(41)-C(42)-H(42A)	119.7
C(36)-N(2)-C(13)	106.46(19)	C(42)-C(43)-C(44)	119.5(3)
C(36)-N(2)-Ti(1)	126.68(16)	C(42)-C(43)-H(43A)	120.2
C(13)-N(2)-Ti(1)	126.35(15)	C(44)-C(43)-H(43A)	120.2
C(36)-N(2)-Na(1)	76.27(14)	C(45)-C(44)-C(43)	120.0(3)
C(13)-N(2)-Na(1)	80.57(13)	C(45)-C(44)-H(44A)	120.0
Ti(1)-N(2)-Na(1)	103.34(8)	C(43)-C(44)-H(44A)	120.0
C(13)-C(38)-C(39)	106.6(2)	C(44)-C(45)-C(40)	120.9(2)
C(13)-C(38)-Na(1)	72.06(14)	C(44)-C(45)-H(45A)	119.6
C(39)-C(38)-Na(1)	73.31(15)	C(40)-C(45)-H(45A)	119.6
C(13)-C(38)-H(38A)	126.4	C(51)-C(46)-C(47)	118.4(2)

C(51)-C(46)-P(4)	125.3(2)	C(56)-C(55)-H(55A)	119.8
C(47)-C(46)-P(4)	116.30(19)	C(54)-C(55)-H(55A)	119.8
C(48)-C(47)-C(46)	121.2(3)	C(55)-C(56)-C(57)	120.3(2)
C(48)-C(47)-H(47A)	119.4	C(55)-C(56)-H(56A)	119.8
C(46)-C(47)-H(47A)	119.4	C(57)-C(56)-H(56A)	119.8
C(49)-C(48)-C(47)	119.5(3)	C(58)-C(57)-C(56)	119.6(2)
C(49)-C(48)-H(48A)	120.2	C(58)-C(57)-H(57A)	120.2
C(47)-C(48)-H(48A)	120.2	C(56)-C(57)-H(57A)	120.2
C(50)-C(49)-C(48)	119.7(3)	C(57)-C(58)-C(59)	120.2(3)
C(50)-C(49)-H(49A)	120.1	C(57)-C(58)-H(58A)	119.9
C(48)-C(49)-H(49A)	120.1	C(59)-C(58)-H(58A)	119.9
C(49)-C(50)-C(51)	121.0(3)	C(54)-C(59)-C(58)	120.4(2)
C(49)-C(50)-H(50A)	119.5	C(54)-C(59)-H(59A)	119.8
C(51)-C(50)-H(50A)	119.5	C(58)-C(59)-H(59A)	119.8
C(46)-C(51)-C(50)	120.2(3)	C(61)-C(60)-C(65)	119.2(2)
C(46)-C(51)-H(51A)	119.9	C(61)-C(60)-P(1A)	119.8(6)
C(50)-C(51)-H(51A)	119.9	C(65)-C(60)-P(1A)	120.8(6)
C(72)-C(52)-C(76)	106.6(2)	C(61)-C(60)-P(1)	124.9(3)
C(72)-C(52)-H(52A)	126.7	C(65)-C(60)-P(1)	115.7(3)
C(76)-C(52)-H(52A)	126.7	P(1A)-C(60)-P(1)	9.3(6)
C(59)-C(54)-C(55)	119.1(2)	C(60)-C(61)-C(62)	120.3(3)
C(59)-C(54)-P(1A)	126.2(5)	C(60)-C(61)-H(61A)	119.9
C(55)-C(54)-P(1A)	114.6(5)	C(62)-C(61)-H(61A)	119.9
C(59)-C(54)-P(1)	117.3(3)	C(63)-C(62)-C(61)	120.2(3)
C(55)-C(54)-P(1)	123.6(3)	C(63)-C(62)-H(62A)	119.9
P(1A)-C(54)-P(1)	9.9(5)	C(61)-C(62)-H(62A)	119.9
C(56)-C(55)-C(54)	120.4(3)	C(64)-C(63)-C(62)	119.6(3)

C(64)-C(63)-H(63A)	120.2	C(78)-P(1)-Ti(1)#1	74.9(2)
C(62)-C(63)-H(63A)	120.2	C(54)-P(1)-Ti(1)#1	124.8(3)
C(63)-C(64)-C(65)	120.8(3)	C(60)-P(1)-Ti(1)#1	133.6(3)
C(63)-C(64)-H(64A)	119.6	P(1A)-O(2)-Ti(1)#1	117.9(7)
C(65)-C(64)-H(64A)	119.6	O(2)-P(1A)-C(60)	106.3(11)
C(64)-C(65)-C(60)	120.0(3)	O(2)-P(1A)-C(54)	107.1(9)
C(64)-C(65)-H(65A)	120.0	C(60)-P(1A)-C(54)	113.2(9)
C(60)-C(65)-H(65A)	120.0	O(2)-P(1A)-C(78)	104.4(9)
C(78)-P(1)-C(54)	105.3(3)	C(60)-P(1A)-C(78)	110.9(9)
C(78)-P(1)-C(60)	100.9(3)	C(54)-P(1A)-C(78)	114.1(10)
C(54)-P(1)-C(60)	101.1(3)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 7. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	$U_{11}U_{22}$	U_{33}	U_{23}	U_{13}	U_{12}	
Ni1	13(1)	14(1)	12(1)	1(1)	4(1)	0(1)
Ti1	18(1)	15(1)	17(1)	-1(1)	8(1)	-2(1)
P2	14(1)	17(1)	13(1)	2(1)	5(1)	1(1)
P3	16(1)	15(1)	16(1)	5(1)	4(1)	1(1)
P4	12(1)	18(1)	15(1)	2(1)	4(1)	-2(1)
Na1	25(1)	37(1)	27(1)	6(1)	13(1)	8(1)
N1	22(1)	18(1)	15(1)	-4(1)	6(1)	-4(1)
O1	29(1)	29(1)	44(1)	3(1)	22(1)	2(1)
C78	19(1)	24(1)	19(1)	2(1)	8(1)	0(1)
C77	22(1)	23(1)	16(1)	-1(1)	6(1)	-1(1)
C76	21(1)	30(1)	21(1)	2(1)	8(1)	-4(1)
C75	20(1)	25(1)	15(1)	-6(1)	7(1)	-4(1)
N4	18(1)	20(1)	14(1)	1(1)	6(1)	-2(1)
C73	19(1)	20(1)	15(1)	2(1)	4(1)	-3(1)
C72	27(1)	26(1)	16(1)	0(1)	8(1)	-2(1)
C1	19(1)	14(1)	13(1)	-2(1)	4(1)	1(1)
C2	23(1)	23(1)	18(1)	4(1)	9(1)	2(1)
C3	36(1)	20(1)	17(1)	7(1)	8(1)	2(1)
C4	34(1)	23(1)	21(1)	6(1)	6(1)	11(1)
C5	22(1)	32(1)	29(1)	5(1)	7(1)	9(1)
C6	20(1)	22(1)	22(1)	7(1)	7(1)	3(1)
C7	19(1)	18(1)	16(1)	5(1)	7(1)	2(1)

C8	21(1)	32(1)	19(1)	2(1)	6(1)	5(1)
C9	22(1)	38(1)	31(1)	4(1)	11(1)	10(1)
C10	34(1)	28(1)	27(1)	1(1)	16(1)	13(1)
C11	30(1)	27(1)	25(1)	-4(1)	7(1)	6(1)
C12	18(1)	23(1)	24(1)	-1(1)	6(1)	3(1)
C13	18(1)	23(1)	14(1)	1(1)	6(1)	0(1)
C14	52(2)	38(2)	76(2)	18(2)	42(2)	9(2)
C15	31(2)	37(2)	56(2)	14(1)	20(1)	9(1)
C16	32(1)	32(1)	34(1)	-2(1)	15(1)	8(1)
C17	36(2)	29(1)	46(2)	2(1)	27(1)	2(1)
C18	21(1)	20(1)	16(1)	6(1)	6(1)	-2(1)
C19	18(1)	18(1)	25(1)	4(1)	6(1)	1(1)
C20	24(1)	21(1)	28(1)	8(1)	7(1)	1(1)
C21	26(1)	26(1)	45(2)	14(1)	12(1)	9(1)
C22	31(1)	30(1)	57(2)	13(1)	25(1)	12(1)
C23	35(2)	33(1)	38(2)	10(1)	21(1)	10(1)
C24	23(1)	25(1)	28(1)	5(1)	10(1)	3(1)
C25	20(1)	24(1)	23(1)	10(1)	5(1)	0(1)
C26	25(1)	26(1)	33(1)	12(1)	5(1)	-1(1)
C27	34(2)	34(2)	51(2)	24(1)	7(1)	-7(1)
C28	42(2)	56(2)	51(2)	38(2)	18(2)	0(2)
C29	57(2)	55(2)	41(2)	23(2)	31(2)	10(2)
C30	50(2)	30(1)	32(1)	13(1)	23(1)	6(1)
C31	23(1)	30(1)	23(1)	9(1)	2(1)	0(1)
C32	19(1)	39(1)	18(1)	4(1)	2(1)	-3(1)
C33	20(1)	30(1)	16(1)	-4(1)	4(1)	-6(1)
N3	18(1)	21(1)	18(1)	2(1)	3(1)	-2(1)

C35	28(1)	24(1)	25(1)	-1(1)	12(1)	7(1)
C36	24(1)	24(1)	21(1)	-3(1)	5(1)	-7(1)
N2	17(1)	19(1)	16(1)	0(1)	6(1)	-3(1)
C38	22(1)	32(1)	18(1)	5(1)	6(1)	-5(1)
C39	22(1)	34(1)	22(1)	4(1)	5(1)	-12(1)
C40	15(1)	26(1)	16(1)	5(1)	6(1)	-1(1)
C41	22(1)	32(1)	20(1)	2(1)	5(1)	0(1)
C42	24(1)	50(2)	21(1)	6(1)	0(1)	2(1)
C43	26(1)	56(2)	29(1)	20(1)	8(1)	14(1)
C44	33(1)	34(1)	37(2)	15(1)	14(1)	12(1)
C45	28(1)	26(1)	25(1)	5(1)	10(1)	2(1)
C46	14(1)	23(1)	21(1)	2(1)	1(1)	-2(1)
C47	25(1)	27(1)	26(1)	-1(1)	8(1)	-2(1)
C48	36(2)	26(1)	36(2)	-6(1)	6(1)	2(1)
C49	38(2)	19(1)	41(2)	-3(1)	-1(1)	-5(1)
C50	36(2)	26(1)	42(2)	11(1)	7(1)	-10(1)
C51	24(1)	28(1)	29(1)	4(1)	8(1)	-4(1)
C52	30(1)	31(1)	20(1)	4(1)	14(1)	-2(1)
C54	19(1)	24(1)	21(1)	1(1)	6(1)	-1(1)
C55	35(2)	32(1)	29(1)	-8(1)	13(1)	-10(1)
C56	40(2)	21(1)	44(2)	-5(1)	13(1)	-8(1)
C57	34(1)	23(1)	35(1)	10(1)	12(1)	-3(1)
C58	50(2)	28(1)	26(1)	3(1)	20(1)	-5(1)
C59	37(1)	19(1)	26(1)	1(1)	15(1)	0(1)
C60	20(1)	33(1)	16(1)	0(1)	4(1)	-2(1)
C61	25(1)	44(2)	21(1)	7(1)	8(1)	6(1)
C62	33(2)	46(2)	22(1)	5(1)	9(1)	13(1)

C63	22(1)	49(2)	22(1)	-6(1)	9(1)	5(1)
C64	26(1)	38(2)	34(1)	2(1)	17(1)	0(1)
C65	27(1)	31(1)	26(1)	4(1)	10(1)	1(1)
P1	16(1)	20(2)	15(1)	0(1)	7(1)	-2(1)
O2	17(3)	9(4)	20(3)	-2(3)	3(2)	1(2)
P1A	21(2)	22(6)	12(2)	-5(3)	7(1)	2(3)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 8. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	zU_{eq}	
Ti01	4484(1)	5897(1)	8072(1)	15(1)
Ni1	4210(1)	8161(1)	7592(1)	23(1)
P1	4421(1)	8251(1)	8578(1)	17(1)
P4	5027(1)	4550(1)	7106(1)	18(1)
P3	6029(1)	7445(1)	6976(1)	16(1)
P2	2271(1)	8371(1)	7490(1)	19(1)
N4	4910(2)	4056(2)	8377(1)	19(1)
N3	6434(2)	5488(2)	7904(1)	17(1)
N2	2756(2)	5987(2)	7952(1)	18(1)
C6	1858(2)	7041(2)	7708(1)	20(1)
C5	5992(3)	7943(2)	8752(1)	19(1)
N1	3851(2)	6193(2)	8987(1)	21(1)
C4	5300(2)	3485(2)	7848(1)	20(1)
C3	7356(3)	4505(2)	8177(1)	20(1)
C2	5198(3)	3170(3)	8910(1)	22(1)
C020	2176(3)	5135(3)	8172(2)	22(1)
C00H	6106(3)	7126(2)	6178(1)	20(1)
C00I	3811(2)	7212(2)	9182(1)	19(1)
C00J	7887(3)	6583(3)	9176(2)	29(1)
C00K	2754(3)	6247(3)	9996(2)	28(1)
C00L	8344(3)	5596(2)	7397(2)	22(1)
C00M	7262(3)	6587(3)	5813(2)	26(1)

C00N	8081(3)	9537(3)	6982(2)	33(1)
C00O	907(3)	8908(3)	8671(2)	29(1)
C00P	7626(3)	8585(3)	7117(2)	25(1)
C00Q	6268(3)	3890(3)	5893(2)	27(1)
C00R	3154(3)	7265(3)	9796(1)	24(1)
C00S	1561(3)	4353(3)	6495(2)	34(1)
C00T	7708(3)	8639(3)	8700(2)	29(1)
C00U	3708(3)	4421(3)	6834(1)	22(1)
C00V	7056(2)	6145(2)	7421(1)	19(1)
C00W	6827(3)	8561(3)	6739(2)	27(1)
C00X	2306(4)	11859(3)	9321(2)	45(1)
C00Y	7591(3)	3666(3)	6658(2)	25(1)
C00Z	5758(3)	2060(3)	8724(2)	26(1)
C010	6390(3)	3973(2)	6504(1)	21(1)
C011	3194(3)	5621(3)	9492(2)	26(1)
C012	5015(3)	7486(3)	5911(2)	28(1)
C013	6684(3)	6806(3)	9056(2)	24(1)
C014	939(3)	5639(3)	8072(2)	27(1)
C015	8650(3)	3264(3)	6207(2)	29(1)
C016	6512(3)	8858(3)	8574(2)	26(1)
C017	1893(3)	9096(3)	6667(2)	31(1)
C018	735(3)	6852(3)	7778(2)	27(1)
C019	3807(3)	9845(3)	9438(2)	28(1)
O1	4253(3)	10681(3)	7057(2)	58(1)
C01B	5825(3)	2253(3)	8044(2)	26(1)
C01C	8530(3)	4551(2)	7883(2)	22(1)
C01D	-672(3)	11189(3)	8207(2)	43(1)

C01E	3387(3)	3385(3)	7036(2)	32(1)
C01F	8523(3)	3176(3)	5598(2)	31(1)
C01G	2955(3)	5423(3)	6453(2)	27(1)
C01H	7301(3)	6430(3)	5192(2)	32(1)
C01I	8397(3)	7500(3)	8998(2)	29(1)
C01J	7333(3)	3491(3)	5444(2)	32(1)
C01K	225(3)	10497(3)	7771(2)	33(1)
C01L	1023(2)	9349(3)	8005(2)	23(1)
C01M	5066(4)	7330(4)	5290(2)	39(1)
C01N	6207(4)	6806(3)	4927(2)	37(1)
C01O	2053(4)	11718(3)	8763(2)	45(1)
C01P	3181(3)	10917(3)	9664(2)	38(1)
C01Q	2313(3)	3356(3)	6865(2)	37(1)
C01R	1364(3)	8623(4)	6334(2)	43(1)
C01S	3575(3)	9692(3)	8864(2)	23(1)
C01T	1878(3)	5383(3)	6286(2)	32(1)
C01U	22(3)	9618(4)	9098(2)	40(1)
C01V	2686(3)	10636(3)	8529(2)	34(1)
C01W	-758(3)	10758(4)	8861(2)	48(1)
C01X	6607(5)	9454(4)	6187(2)	47(1)
C01Y	7778(5)	10448(4)	6472(2)	50(1)
C01Z	2161(4)	10130(4)	6350(3)	56(1)
C1	4171(4)	9765(3)	7251(2)	40(1)
C021	1892(5)	10653(5)	5699(3)	81(2)
C022	1392(6)	10145(7)	5397(3)	82(2)
C023	1137(5)	9141(6)	5700(2)	71(2)
C024	7099(5)	10374(4)	6055(2)	54(1)

Bond lengths [Å] and angles [°] for 8.

Ti(01)-N(1)	2.014(2)	N(3)-C(00V)	1.383(4)
Ti(01)-N(2)	2.039(2)	N(2)-C(020)	1.373(4)
Ti(01)-N(4)	2.068(2)	N(2)-C(6)	1.383(4)
Ti(01)-N(3)	2.087(2)	C(6)-C(018)	1.375(4)
Ti(01)-Ni(1)	2.6136(8)	C(5)-C(013)	1.391(4)
Ti(01)-P(4)	2.7888(9)	C(5)-C(016)	1.393(4)
Ni(1)-C(1)	1.894(4)	N(1)-C(011)	1.373(4)
Ni(1)-P(3)	2.2109(8)	N(1)-C(00I)	1.392(4)
Ni(1)-P(2)	2.2217(8)	C(4)-C(01B)	1.383(4)
Ni(1)-P(1)	2.2285(9)	C(3)-C(01C)	1.379(4)
P(1)-C(00I)	1.793(3)	C(3)-H(3A)	0.9500
P(1)-C(5)	1.824(3)	C(2)-C(00Z)	1.381(4)
P(1)-C(01S)	1.844(3)	C(2)-H(2A)	0.9500
P(4)-C(4)	1.790(3)	C(020)-C(014)	1.375(4)
P(4)-C(00U)	1.831(3)	C(020)-H(1A)	0.9500
P(4)-C(010)	1.833(3)	C(00H)-C(012)	1.382(4)
P(3)-C(00V)	1.782(3)	C(00H)-C(00M)	1.400(4)
P(3)-C(00W)	1.831(3)	C(00I)-C(00R)	1.369(4)
P(3)-C(00H)	1.834(3)	C(00J)-C(01I)	1.388(5)
P(2)-C(6)	1.783(3)	C(00J)-C(013)	1.389(4)
P(2)-C(01L)	1.838(3)	C(00J)-H(00A)	0.9500
P(2)-C(017)	1.841(3)	C(00K)-C(011)	1.377(5)
N(4)-C(2)	1.367(4)	C(00K)-C(00R)	1.419(5)
N(4)-C(4)	1.385(4)	C(00K)-H(00B)	0.9500
N(3)-C(3)	1.375(4)	C(00L)-C(00V)	1.381(4)

C(00L)-C(01C)	1.409(4)	C(00X)-H(00L)	0.9500
C(00L)-H(00C)	0.9500	C(00Y)-C(015)	1.391(5)
C(00M)-C(01H)	1.387(5)	C(00Y)-C(010)	1.395(4)
C(00M)-H(00D)	0.9500	C(00Y)-H(00M)	0.9500
C(00N)-C(01Y)	1.351(6)	C(00Z)-C(01B)	1.413(5)
C(00N)-C(00P)	1.391(4)	C(00Z)-H(00N)	0.9500
C(00N)-H(00E)	0.9500	C(011)-H(01A)	0.9500
C(00O)-C(01L)	1.392(5)	C(012)-C(01M)	1.384(5)
C(00O)-C(01U)	1.397(5)	C(012)-H(01B)	0.9500
C(00O)-H(00F)	0.9500	C(013)-H(01C)	0.9500
C(00P)-C(00W)	1.379(5)	C(014)-C(018)	1.405(5)
C(00P)-H(00G)	0.9500	C(014)-H(01D)	0.9500
C(00Q)-C(010)	1.388(5)	C(015)-C(01F)	1.388(5)
C(00Q)-C(01J)	1.392(5)	C(015)-H(01E)	0.9500
C(00Q)-H(00H)	0.9500	C(016)-H(01F)	0.9500
C(00R)-H(00I)	0.9500	C(017)-C(01R)	1.381(6)
C(00S)-C(01Q)	1.378(6)	C(017)-C(01Z)	1.383(6)
C(00S)-C(01T)	1.379(6)	C(018)-H(01G)	0.9500
C(00S)-H(00J)	0.9500	C(019)-C(01P)	1.386(5)
C(00T)-C(01I)	1.387(5)	C(019)-C(01S)	1.393(5)
C(00T)-C(016)	1.387(5)	C(019)-H(01H)	0.9500
C(00T)-H(00K)	0.9500	O(1)-C(1)	1.121(5)
C(00U)-C(01E)	1.388(5)	C(01B)-H(01I)	0.9500
C(00U)-C(01G)	1.394(5)	C(01C)-H(01J)	0.9500
C(00W)-C(01X)	1.391(5)	C(01D)-C(01W)	1.368(7)
C(00X)-C(01O)	1.368(7)	C(01D)-C(01K)	1.404(5)
C(00X)-C(01P)	1.388(7)	C(01D)-H(01K)	0.9500

C(01E)-C(01Q)	1.393(5)	C(01X)-C(024)	1.383(6)
C(01E)-H(01L)	0.9500	C(01X)-H(02C)	0.9500
C(01F)-C(01J)	1.382(5)	C(01Y)-C(024)	1.363(7)
C(01F)-H(01M)	0.9500	C(01Y)-H(02D)	0.9500
C(01G)-C(01T)	1.398(5)	C(01Z)-C(021)	1.438(9)
C(01G)-H(01N)	0.9500	C(01Z)-H(02E)	0.9500
C(01H)-C(01N)	1.382(6)	C(021)-C(022)	1.339(12)
C(01H)-H(01O)	0.9500	C(021)-H(02F)	0.9500
C(01I)-H(01P)	0.9500	C(022)-C(023)	1.339(11)
C(01J)-H(01Q)	0.9500	C(022)-H(02G)	0.9500
C(01K)-C(01L)	1.396(4)	C(023)-H(02H)	0.9500
C(01K)-H(01R)	0.9500	C(024)-H(02I)	0.9500
C(01M)-C(01N)	1.382(6)		
C(01M)-H(01S)	0.9500	N(1)-Ti(01)-N(2)	91.85(10)
C(01N)-H(01T)	0.9500	N(1)-Ti(01)-N(4)	91.90(10)
C(01O)-C(01V)	1.403(5)	N(2)-Ti(01)-N(4)	87.97(9)
C(01O)-H(01U)	0.9500	N(1)-Ti(01)-N(3)	108.09(9)
C(01P)-H(01V)	0.9500	N(2)-Ti(01)-N(3)	158.87(9)
C(01Q)-H(01W)	0.9500	N(4)-Ti(01)-N(3)	84.55(9)
C(01R)-C(023)	1.391(6)	N(1)-Ti(01)-Ni(1)	93.22(7)
C(01R)-H(01X)	0.9500	N(2)-Ti(01)-Ni(1)	96.61(7)
C(01S)-C(01V)	1.389(5)	N(4)-Ti(01)-Ni(1)	173.01(7)
C(01T)-H(01Y)	0.9500	N(3)-Ti(01)-Ni(1)	89.34(6)
C(01U)-C(01W)	1.383(7)	N(1)-Ti(01)-P(4)	152.80(7)
C(01U)-H(01Z)	0.9500	N(2)-Ti(01)-P(4)	76.43(7)
C(01V)-H(02A)	0.9500	N(4)-Ti(01)-P(4)	63.63(7)
C(01W)-H(02B)	0.9500	N(3)-Ti(01)-P(4)	82.54(7)

Ni(1)-Ti(01)-P(4)	112.26(2)	C(00W)-P(3)-Ni(1)	109.43(10)
C(1)-Ni(1)-P(3)	91.26(12)	C(00H)-P(3)-Ni(1)	121.61(9)
C(1)-Ni(1)-P(2)	99.28(12)	C(6)-P(2)-C(01L)	101.30(13)
P(3)-Ni(1)-P(2)	130.50(3)	C(6)-P(2)-C(017)	107.03(15)
C(1)-Ni(1)-P(1)	92.79(13)	C(01L)-P(2)-C(017)	103.16(14)
P(3)-Ni(1)-P(1)	113.26(3)	C(6)-P(2)-Ni(1)	116.95(9)
P(2)-Ni(1)-P(1)	114.32(3)	C(01L)-P(2)-Ni(1)	114.13(10)
C(1)-Ni(1)-Ti(01)	174.63(12)	C(017)-P(2)-Ni(1)	112.79(11)
P(3)-Ni(1)-Ti(01)	84.91(3)	C(2)-N(4)-C(4)	106.5(2)
P(2)-Ni(1)-Ti(01)	86.07(3)	C(2)-N(4)-Ti(01)	141.2(2)
P(1)-Ni(1)-Ti(01)	85.29(3)	C(4)-N(4)-Ti(01)	110.32(17)
C(00I)-P(1)-C(5)	105.26(13)	C(3)-N(3)-C(00V)	106.0(2)
C(00I)-P(1)-C(01S)	102.97(13)	C(3)-N(3)-Ti(01)	129.65(18)
C(5)-P(1)-C(01S)	100.05(13)	C(00V)-N(3)-Ti(01)	124.05(18)
C(00I)-P(1)-Ni(1)	110.27(10)	C(020)-N(2)-C(6)	106.5(2)
C(5)-P(1)-Ni(1)	118.84(9)	C(020)-N(2)-Ti(01)	129.36(19)
C(01S)-P(1)-Ni(1)	117.60(10)	C(6)-N(2)-Ti(01)	123.44(18)
C(4)-P(4)-C(00U)	107.00(13)	C(018)-C(6)-N(2)	109.7(2)
C(4)-P(4)-C(010)	105.76(13)	C(018)-C(6)-P(2)	132.7(2)
C(00U)-P(4)-C(010)	104.43(13)	N(2)-C(6)-P(2)	116.8(2)
C(4)-P(4)-Ti(01)	73.74(9)	C(013)-C(5)-C(016)	119.4(3)
C(00U)-P(4)-Ti(01)	118.06(9)	C(013)-C(5)-P(1)	121.1(2)
C(010)-P(4)-Ti(01)	135.93(10)	C(016)-C(5)-P(1)	119.6(2)
C(00V)-P(3)-C(00W)	105.73(14)	C(011)-N(1)-C(00I)	106.3(2)
C(00V)-P(3)-C(00H)	107.94(13)	C(011)-N(1)-Ti(01)	129.6(2)
C(00W)-P(3)-C(00H)	99.93(13)	C(00I)-N(1)-Ti(01)	123.12(18)
C(00V)-P(3)-Ni(1)	110.72(9)	C(01B)-C(4)-N(4)	110.4(3)

C(01B)-C(4)-P(4)	138.2(2)	C(01H)-C(00M)-H(00D)	120.0
N(4)-C(4)-P(4)	111.39(19)	C(00H)-C(00M)-H(00D)	120.0
N(3)-C(3)-C(01C)	110.1(2)	C(01Y)-C(00N)-C(00P)	121.2(4)
N(3)-C(3)-H(3A)	124.9	C(01Y)-C(00N)-H(00E)	119.4
C(01C)-C(3)-H(3A)	124.9	C(00P)-C(00N)-H(00E)	119.4
N(4)-C(2)-C(00Z)	109.8(3)	C(01L)-C(00O)-C(01U)	120.3(3)
N(4)-C(2)-H(2A)	125.1	C(01L)-C(00O)-H(00F)	119.9
C(00Z)-C(2)-H(2A)	125.1	C(01U)-C(00O)-H(00F)	119.9
N(2)-C(020)-C(014)	109.8(3)	C(00W)-C(00P)-C(00N)	120.5(3)
N(2)-C(020)-H(1A)	125.1	C(00W)-C(00P)-H(00G)	119.7
C(014)-C(020)-H(1A)	125.1	C(00N)-C(00P)-H(00G)	119.7
C(012)-C(00H)-C(00M)	119.0(3)	C(010)-C(00Q)-C(01J)	120.2(3)
C(012)-C(00H)-P(3)	119.8(2)	C(010)-C(00Q)-H(00H)	119.9
C(00M)-C(00H)-P(3)	121.1(2)	C(01J)-C(00Q)-H(00H)	119.9
C(00R)-C(00I)-N(1)	110.0(2)	C(00I)-C(00R)-C(00K)	106.8(3)
C(00R)-C(00I)-P(1)	133.1(2)	C(00I)-C(00R)-H(00I)	126.6
N(1)-C(00I)-P(1)	116.4(2)	C(00K)-C(00R)-H(00I)	126.6
C(01I)-C(00J)-C(013)	120.0(3)	C(01Q)-C(00S)-C(01T)	120.0(3)
C(01I)-C(00J)-H(00A)	120.0	C(01Q)-C(00S)-H(00J)	120.0
C(013)-C(00J)-H(00A)	120.0	C(01T)-C(00S)-H(00J)	120.0
C(011)-C(00K)-C(00R)	106.8(3)	C(01I)-C(00T)-C(016)	119.9(3)
C(011)-C(00K)-H(00B)	126.6	C(01I)-C(00T)-H(00K)	120.0
C(00R)-C(00K)-H(00B)	126.6	C(016)-C(00T)-H(00K)	120.0
C(00V)-C(00L)-C(01C)	106.2(2)	C(01E)-C(00U)-C(01G)	119.4(3)
C(00V)-C(00L)-H(00C)	126.9	C(01E)-C(00U)-P(4)	121.7(2)
C(01C)-C(00L)-H(00C)	126.9	C(01G)-C(00U)-P(4)	118.8(2)
C(01H)-C(00M)-C(00H)	120.0(3)	C(00L)-C(00V)-N(3)	110.4(2)

C(00L)-C(00V)-P(3)	135.9(2)	C(020)-C(014)-H(01D)	126.5
N(3)-C(00V)-P(3)	113.65(19)	C(018)-C(014)-H(01D)	126.5
C(00P)-C(00W)-C(01X)	117.3(3)	C(01F)-C(015)-C(00Y)	120.5(3)
C(00P)-C(00W)-P(3)	121.2(2)	C(01F)-C(015)-H(01E)	119.8
C(01X)-C(00W)-P(3)	121.4(3)	C(00Y)-C(015)-H(01E)	119.8
C(01O)-C(00X)-C(01P)	119.6(3)	C(00T)-C(016)-C(5)	120.4(3)
C(01O)-C(00X)-H(00L)	120.2	C(00T)-C(016)-H(01F)	119.8
C(01P)-C(00X)-H(00L)	120.2	C(5)-C(016)-H(01F)	119.8
C(015)-C(00Y)-C(010)	120.1(3)	C(01R)-C(017)-C(01Z)	117.2(4)
C(015)-C(00Y)-H(00M)	120.0	C(01R)-C(017)-P(2)	121.9(3)
C(010)-C(00Y)-H(00M)	120.0	C(01Z)-C(017)-P(2)	120.8(4)
C(2)-C(00Z)-C(01B)	107.6(3)	C(6)-C(018)-C(014)	106.9(3)
C(2)-C(00Z)-H(00N)	126.2	C(6)-C(018)-H(01G)	126.6
C(01B)-C(00Z)-H(00N)	126.2	C(014)-C(018)-H(01G)	126.6
C(00Q)-C(010)-C(00Y)	119.3(3)	C(01P)-C(019)-C(01S)	120.9(3)
C(00Q)-C(010)-P(4)	122.4(2)	C(01P)-C(019)-H(01H)	119.6
C(00Y)-C(010)-P(4)	118.2(2)	C(01S)-C(019)-H(01H)	119.6
N(1)-C(011)-C(00K)	110.2(3)	C(4)-C(01B)-C(00Z)	105.7(3)
N(1)-C(011)-H(01A)	124.9	C(4)-C(01B)-H(01I)	127.2
C(00K)-C(011)-H(01A)	124.9	C(00Z)-C(01B)-H(01I)	127.2
C(00H)-C(012)-C(01M)	120.5(3)	C(3)-C(01C)-C(00L)	107.3(2)
C(00H)-C(012)-H(01B)	119.7	C(3)-C(01C)-H(01J)	126.4
C(01M)-C(012)-H(01B)	119.7	C(00L)-C(01C)-H(01J)	126.4
C(00J)-C(013)-C(5)	120.3(3)	C(01W)-C(01D)-C(01K)	120.6(3)
C(00J)-C(013)-H(01C)	119.9	C(01W)-C(01D)-H(01K)	119.7
C(5)-C(013)-H(01C)	119.9	C(01K)-C(01D)-H(01K)	119.7
C(020)-C(014)-C(018)	107.1(3)	C(00U)-C(01E)-C(01Q)	120.1(3)

C(00U)-C(01E)-H(01L)	119.9	C(01H)-C(01N)-H(01T)	120.4
C(01Q)-C(01E)-H(01L)	119.9	C(01M)-C(01N)-H(01T)	120.4
C(01J)-C(01F)-C(015)	119.4(3)	C(00X)-C(01O)-C(01V)	120.5(4)
C(01J)-C(01F)-H(01M)	120.3	C(00X)-C(01O)-H(01U)	119.8
C(015)-C(01F)-H(01M)	120.3	C(01V)-C(01O)-H(01U)	119.8
C(00U)-C(01G)-C(01T)	120.0(3)	C(019)-C(01P)-C(00X)	120.2(4)
C(00U)-C(01G)-H(01N)	120.0	C(019)-C(01P)-H(01V)	119.9
C(01T)-C(01G)-H(01N)	120.0	C(00X)-C(01P)-H(01V)	119.9
C(01N)-C(01H)-C(00M)	120.6(3)	C(00S)-C(01Q)-C(01E)	120.4(3)
C(01N)-C(01H)-H(01O)	119.7	C(00S)-C(01Q)-H(01W)	119.8
C(00M)-C(01H)-H(01O)	119.7	C(01E)-C(01Q)-H(01W)	119.8
C(00T)-C(01I)-C(00J)	120.0(3)	C(017)-C(01R)-C(023)	121.7(5)
C(00T)-C(01I)-H(01P)	120.0	C(017)-C(01R)-H(01X)	119.1
C(00J)-C(01I)-H(01P)	120.0	C(023)-C(01R)-H(01X)	119.2
C(01F)-C(01J)-C(00Q)	120.6(3)	C(01V)-C(01S)-C(019)	118.4(3)
C(01F)-C(01J)-H(01Q)	119.7	C(01V)-C(01S)-P(1)	121.9(2)
C(00Q)-C(01J)-H(01Q)	119.7	C(019)-C(01S)-P(1)	119.7(2)
C(01L)-C(01K)-C(01D)	119.7(4)	C(00S)-C(01T)-C(01G)	120.1(3)
C(01L)-C(01K)-H(01R)	120.1	C(00S)-C(01T)-H(01Y)	119.9
C(01D)-C(01K)-H(01R)	120.1	C(01G)-C(01T)-H(01Y)	119.9
C(00O)-C(01L)-C(01K)	119.1(3)	C(01W)-C(01U)-C(00O)	120.1(4)
C(00O)-C(01L)-P(2)	116.7(2)	C(01W)-C(01U)-H(01Z)	119.9
C(01K)-C(01L)-P(2)	124.1(3)	C(00O)-C(01U)-H(01Z)	119.9
C(01N)-C(01M)-C(012)	120.6(3)	C(01S)-C(01V)-C(01O)	120.4(4)
C(01N)-C(01M)-H(01S)	119.7	C(01S)-C(01V)-H(02A)	119.8
C(012)-C(01M)-H(01S)	119.7	C(01O)-C(01V)-H(02A)	119.8
C(01H)-C(01N)-C(01M)	119.3(3)	C(01D)-C(01W)-C(01U)	120.1(3)

C(01D)-C(01W)-H(02B)	120.0	C(022)-C(021)-C(01Z)	120.6(5)
C(01U)-C(01W)-H(02B)	120.0	C(022)-C(021)-H(02F)	119.7
C(024)-C(01X)-C(00W)	120.8(4)	C(01Z)-C(021)-H(02F)	119.7
C(024)-C(01X)-H(02C)	119.6	C(021)-C(022)-C(023)	120.1(5)
C(00W)-C(01X)-H(02C)	119.6	C(021)-C(022)-H(02G)	119.9
C(00N)-C(01Y)-C(024)	118.8(3)	C(023)-C(022)-H(02G)	119.9
C(00N)-C(01Y)-H(02D)	120.6	C(022)-C(023)-C(01R)	120.8(6)
C(024)-C(01Y)-H(02D)	120.6	C(022)-C(023)-H(02H)	119.6
C(017)-C(01Z)-C(021)	119.5(6)	C(01R)-C(023)-H(02H)	119.6
C(017)-C(01Z)-H(02E)	120.3	C(01Y)-C(024)-C(01X)	120.8(4)
C(021)-C(01Z)-H(02E)	120.3	C(01Y)-C(024)-H(02I)	119.6
O(1)-C(1)-Ni(1)	174.1(4)	C(01X)-C(024)-H(02I)	119.6

Symmetry transformations used to generate equivalent atoms:

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 8. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	$U_{11}U_{22}$	U_{33}	U_{23}	U_{13}	U_{12}	
Ti01	14(1)	13(1)	18(1)	-4(1)	-3(1)	-4(1)
Ni1	15(1)	36(1)	21(1)	-14(1)	-2(1)	-5(1)
P1	19(1)	16(1)	17(1)	-5(1)	-3(1)	-5(1)
P4	18(1)	16(1)	20(1)	-5(1)	-5(1)	-5(1)
P3	15(1)	16(1)	16(1)	-4(1)	-3(1)	-4(1)
P2	15(1)	16(1)	26(1)	-6(1)	-6(1)	-2(1)
N4	17(1)	17(1)	22(1)	-3(1)	-4(1)	-6(1)
N3	16(1)	16(1)	20(1)	-4(1)	-5(1)	-5(1)
N2	16(1)	16(1)	24(1)	-6(1)	-4(1)	-4(1)
C6	17(1)	21(1)	24(1)	-10(1)	-5(1)	-3(1)
C5	20(1)	21(1)	17(1)	-7(1)	-1(1)	-6(1)
N1	22(1)	22(1)	19(1)	-5(1)	-2(1)	-8(1)
C4	19(1)	17(1)	23(1)	-5(1)	-4(1)	-6(1)
C3	20(1)	16(1)	24(1)	-4(1)	-9(1)	-4(1)
C2	22(1)	22(1)	23(1)	-1(1)	-5(1)	-8(1)
C020	21(1)	21(1)	28(1)	-7(1)	-3(1)	-9(1)
C00H	24(1)	18(1)	17(1)	-4(1)	-2(1)	-8(1)
C00I	18(1)	18(1)	20(1)	-5(1)	-3(1)	-5(1)
C00J	24(1)	26(1)	35(2)	-6(1)	-9(1)	-4(1)
C00K	29(1)	31(2)	21(1)	-5(1)	1(1)	-11(1)
C00L	16(1)	22(1)	31(2)	-9(1)	-4(1)	-6(1)
C00M	26(1)	27(1)	25(1)	-7(1)	-1(1)	-8(1)

C00N	31(2)	31(2)	44(2)	-13(1)	-2(1)	-16(1)
C00O	19(1)	35(2)	38(2)	-17(1)	1(1)	-9(1)
C00P	20(1)	22(1)	31(2)	-7(1)	0(1)	-6(1)
C00Q	28(1)	28(1)	26(1)	-7(1)	-4(1)	-10(1)
C00R	27(1)	25(1)	21(1)	-8(1)	-2(1)	-7(1)
C00S	25(1)	52(2)	34(2)	-23(2)	-4(1)	-14(1)
C00T	30(2)	35(2)	30(2)	-9(1)	-2(1)	-18(1)
C00U	21(1)	28(1)	22(1)	-12(1)	-3(1)	-8(1)
C00V	17(1)	18(1)	22(1)	-6(1)	-2(1)	-6(1)
C00W	37(2)	23(1)	23(1)	-2(1)	-6(1)	-15(1)
C00X	36(2)	35(2)	70(3)	-33(2)	0(2)	-8(1)
C00Y	25(1)	23(1)	28(2)	-7(1)	-4(1)	-9(1)
C00Z	30(1)	17(1)	29(2)	0(1)	-7(1)	-7(1)
C010	23(1)	16(1)	24(1)	-5(1)	-2(1)	-6(1)
C011	29(1)	24(1)	25(1)	-4(1)	-1(1)	-12(1)
C012	24(1)	32(2)	27(2)	-11(1)	-5(1)	-5(1)
C013	23(1)	22(1)	28(1)	-6(1)	-4(1)	-7(1)
C014	20(1)	27(1)	38(2)	-11(1)	-1(1)	-11(1)
C015	25(1)	22(1)	39(2)	-9(1)	-1(1)	-8(1)
C016	29(1)	23(1)	27(1)	-4(1)	-6(1)	-10(1)
C017	19(1)	30(2)	31(2)	1(1)	-4(1)	2(1)
C018	16(1)	27(1)	37(2)	-10(1)	-6(1)	-4(1)
C019	28(1)	31(2)	28(2)	-14(1)	-1(1)	-9(1)
O1	67(2)	28(1)	73(2)	-5(1)	-2(2)	-19(1)
C01B	28(1)	17(1)	30(2)	-7(1)	-2(1)	-5(1)
C01C	18(1)	19(1)	32(2)	-7(1)	-10(1)	-3(1)
C01D	24(2)	28(2)	78(3)	-27(2)	-7(2)	1(1)

C01E	36(2)	29(2)	40(2)	-9(1)	-14(1)	-14(1)
C01F	31(2)	28(1)	32(2)	-9(1)	6(1)	-12(1)
C01G	25(1)	32(2)	24(1)	-5(1)	-5(1)	-9(1)
C01H	36(2)	31(2)	26(2)	-12(1)	5(1)	-10(1)
C01I	22(1)	39(2)	30(2)	-14(1)	-3(1)	-9(1)
C01J	37(2)	36(2)	25(2)	-10(1)	-1(1)	-14(1)
C01K	23(1)	22(1)	54(2)	-13(1)	-9(1)	-2(1)
C01L	14(1)	21(1)	37(2)	-13(1)	-4(1)	-4(1)
C01M	38(2)	50(2)	31(2)	-14(2)	-14(1)	-8(2)
C01N	48(2)	43(2)	21(2)	-12(1)	-5(1)	-14(2)
C01O	35(2)	25(2)	77(3)	-18(2)	-18(2)	2(1)
C01P	37(2)	44(2)	41(2)	-27(2)	3(1)	-15(2)
C01Q	36(2)	39(2)	48(2)	-17(2)	-8(2)	-19(1)
C01R	28(2)	60(2)	31(2)	-10(2)	-12(1)	0(2)
C01S	23(1)	21(1)	28(1)	-12(1)	-2(1)	-6(1)
C01T	26(1)	43(2)	28(2)	-9(1)	-10(1)	-7(1)
C01U	27(2)	55(2)	47(2)	-31(2)	6(1)	-18(2)
C01V	35(2)	21(1)	51(2)	-12(1)	-18(2)	-4(1)
C01W	25(2)	50(2)	76(3)	-46(2)	8(2)	-8(2)
C01X	68(3)	41(2)	40(2)	5(2)	-20(2)	-28(2)
C01Y	86(3)	43(2)	40(2)	1(2)	-13(2)	-46(2)
C01Z	52(2)	43(2)	57(3)	10(2)	-4(2)	-14(2)
C1	39(2)	36(2)	43(2)	-10(2)	-7(2)	-9(1)
C021	61(3)	59(3)	73(4)	37(3)	1(3)	-4(2)
C022	66(3)	102(5)	44(3)	11(3)	-21(2)	1(3)
C023	49(2)	106(5)	37(2)	-11(3)	-19(2)	2(3)
C024	77(3)	42(2)	44(2)	6(2)	-13(2)	-29(2)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 9. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
P2	567(1)	6892(1)	9084(1)	23(1)
Ti1	494(1)	5472(1)	9501(1)	19(1)
Ni1	1154(1)	6095(1)	8870(1)	22(1)
N2	-296(1)	5998(1)	9289(1)	24(1)
P3	2038(1)	5869(1)	9370(1)	25(1)
N3	1100(1)	5682(1)	10203(1)	26(1)
P1	837(1)	5549(1)	8096(1)	24(1)
C99	978(2)	5698(1)	10813(1)	31(1)
O1	0	5000	10000	24(1)
C2	-842(2)	6888(1)	9239(1)	33(1)
C3	-1292(1)	6414(1)	9333(1)	35(1)
C4	-947(1)	5884(1)	9361(1)	29(1)
C5	-238(1)	6619(1)	9205(1)	25(1)
C6	700(1)	7448(1)	9688(1)	28(1)
C7	910(2)	7263(2)	10241(2)	53(1)
C8	994(3)	7679(2)	10711(2)	61(1)
C9	860(2)	8280(2)	10622(2)	47(1)
C10	645(2)	8470(2)	10063(2)	44(1)
C11	564(2)	8057(1)	9595(2)	37(1)
C12	2702(2)	6422(1)	9407(1)	34(1)
C13	2535(2)	7034(2)	9473(2)	51(1)
C14	3019(2)	7474(2)	9528(2)	65(1)

C15	3662(2)	7305(2)	9510(2)	56(1)
C16	3823(2)	6709(2)	9459(2)	52(1)
C17	3344(2)	6267(2)	9401(2)	44(1)
C18	1749(1)	5836(1)	10131(1)	29(1)
C19	1534(2)	5867(2)	11118(1)	42(1)
C20	2025(2)	5954(2)	10683(1)	43(1)
C21	2458(1)	5150(1)	9240(1)	32(1)
C22	2664(2)	5014(2)	8658(2)	45(1)
C23	3003(2)	4486(2)	8548(2)	61(1)
C24	3115(2)	4082(2)	9009(3)	69(1)
C25	2903(2)	4202(2)	9582(3)	72(1)
C26	2574(2)	4742(2)	9701(2)	54(1)
C27	771(1)	4789(1)	8364(1)	27(1)
C28	738(2)	4216(1)	8119(1)	41(1)
C29	697(2)	3803(1)	8604(1)	39(1)
C30	683(2)	4136(1)	9120(1)	32(1)
N1	725(1)	4743(1)	8988(1)	26(1)
C32	77(1)	5703(1)	7697(1)	30(1)
C33	-488(2)	5402(2)	7858(2)	44(1)
C34	-1073(2)	5550(2)	7584(2)	58(1)
C35	-1097(2)	5996(2)	7148(2)	59(1)
C36	-541(2)	6297(2)	6987(2)	56(1)
C37	45(2)	6156(2)	7264(2)	42(1)
C43	559(1)	7348(1)	8394(1)	29(1)
C44	1146(2)	7579(2)	8188(2)	44(1)
C45	1173(2)	7906(2)	7649(2)	51(1)
C46	622(2)	8004(2)	7320(2)	50(1)

C47	42(2)	7768(2)	7516(2)	46(1)
C48	10(2)	7433(1)	8049(1)	38(1)
C49	-9859(3)	-14(2)	10833(3)	84(2)
C50	-10200(2)	233(2)	11306(2)	64(1)
C51	-10010(2)	779(2)	11545(2)	59(1)
C52	-9484(2)	1073(2)	11325(2)	62(1)
C53	-9331(3)	279(3)	10607(3)	93(2)
C54	-9132(3)	829(3)	10847(2)	77(1)
C55	2971(3)	8122(2)	7985(3)	82(2)
C56	3147(3)	7552(2)	7816(3)	85(2)
C57	3217(3)	7409(2)	7218(3)	86(2)
C58	3078(3)	7845(3)	6774(3)	107(2)
C59	2932(3)	8439(2)	6984(2)	76(1)
C60	2902(2)	8544(3)	7594(2)	73(1)
C80	1421(2)	5577(2)	7500(1)	22(1)
C81	1724(4)	6131(2)	7409(2)	52(2)
C82	2175(4)	6197(2)	6945(3)	69(2)
C83	2322(2)	5709(3)	6573(2)	59(2)
C84	2019(3)	5154(2)	6664(3)	64(3)
C85	1568(3)	5088(2)	7128(3)	47(2)
C80"	1362(4)	5222(4)	6935(4)	22(1)
C81"	1451(4)	5581(4)	7445(3)	52(2)
C82"	2000(5)	5943(5)	7496(4)	40(3)
C83"	2460(5)	5946(7)	7036(5)	70(5)
C84"	2372(5)	5587(7)	6526(5)	69(7)
C85"	1823(5)	5225(5)	6475(4)	59(5)

Table 3. Bond lengths [Å] and angles [°] for 9.

P(2)-C(5)	1.784(3)	C(2)-C(5)	1.381(4)
P(2)-C(43)	1.826(3)	C(2)-C(3)	1.411(4)
P(2)-C(6)	1.835(3)	C(2)-H(2A)	0.9500
P(2)-Ni(1)	2.1877(7)	C(3)-C(4)	1.372(4)
Ti(1)-O(1)	1.8273(4)	C(3)-H(3A)	0.9500
Ti(1)-N(1)	2.026(2)	C(4)-H(4A)	0.9500
Ti(1)-N(3)	2.043(2)	C(6)-C(7)	1.359(4)
Ti(1)-N(2)	2.053(2)	C(6)-C(11)	1.389(4)
Ti(1)-Ni(1)	2.3846(6)	C(7)-C(8)	1.400(5)
Ni(1)-P(3)	2.1889(8)	C(7)-H(7A)	0.9500
Ni(1)-P(1)	2.1925(7)	C(8)-C(9)	1.370(5)
N(2)-C(4)	1.373(4)	C(8)-H(8A)	0.9500
N(2)-C(5)	1.391(3)	C(9)-C(10)	1.377(5)
P(3)-C(18)	1.785(3)	C(9)-H(9A)	0.9500
P(3)-C(21)	1.831(3)	C(10)-C(11)	1.388(4)
P(3)-C(12)	1.835(3)	C(10)-H(10B)	0.9500
N(3)-C(99)	1.372(3)	C(11)-H(11A)	0.9500
N(3)-C(18)	1.389(4)	C(12)-C(17)	1.367(5)
P(1)-C(80)	1.783(3)	C(12)-C(13)	1.403(5)
P(1)-C(27)	1.785(3)	C(13)-C(14)	1.398(5)
P(1)-C(32)	1.829(3)	C(13)-H(13A)	0.9500
P(1)-C(81")	1.915(7)	C(14)-C(15)	1.378(7)
C(99)-C(19)	1.381(4)	C(14)-H(14A)	0.9500
C(99)-H(10A)	0.9500	C(15)-C(16)	1.364(6)
O(1)-Ti(1)#1	1.8273(4)	C(15)-H(15A)	0.9500

C(16)-C(17)	1.395(5)	C(32)-C(33)	1.387(5)
C(16)-H(16A)	0.9500	C(33)-C(34)	1.387(5)
C(17)-H(17A)	0.9500	C(33)-H(33A)	0.9500
C(18)-C(20)	1.372(4)	C(34)-C(35)	1.378(6)
C(19)-C(20)	1.407(5)	C(34)-H(34A)	0.9500
C(19)-H(19A)	0.9500	C(35)-C(36)	1.372(6)
C(20)-H(20A)	0.9500	C(35)-H(35A)	0.9500
C(21)-C(26)	1.380(5)	C(36)-C(37)	1.390(5)
C(21)-C(22)	1.386(5)	C(36)-H(36A)	0.9500
C(22)-C(23)	1.380(5)	C(37)-H(37A)	0.9500
C(22)-H(22A)	0.9500	C(43)-C(48)	1.378(4)
C(23)-C(24)	1.372(7)	C(43)-C(44)	1.389(5)
C(23)-H(23A)	0.9500	C(44)-C(45)	1.392(5)
C(24)-C(25)	1.366(8)	C(44)-H(44A)	0.9500
C(24)-H(24A)	0.9500	C(45)-C(46)	1.366(6)
C(25)-C(26)	1.397(6)	C(45)-H(45A)	0.9500
C(25)-H(25A)	0.9500	C(46)-C(47)	1.372(6)
C(26)-H(26A)	0.9500	C(46)-H(46A)	0.9500
C(27)-C(28)	1.378(4)	C(47)-C(48)	1.391(4)
C(27)-N(1)	1.386(3)	C(47)-H(47A)	0.9500
C(28)-C(29)	1.408(5)	C(48)-H(48A)	0.9500
C(28)-H(28A)	0.9500	C(49)-C(53)	1.362(8)
C(29)-C(30)	1.357(4)	C(49)-C(50)	1.371(6)
C(29)-H(29A)	0.9500	C(49)-H(49A)	0.9500
C(30)-N(1)	1.374(4)	C(50)-C(51)	1.374(7)
C(30)-H(30A)	0.9500	C(50)-H(50A)	0.9500
C(32)-C(37)	1.385(4)	C(51)-C(52)	1.354(7)

C(51)-H(51A)	0.9500	C(84)-H(84A)	0.9500
C(52)-C(54)	1.390(7)	C(85)-H(85A)	0.9500
C(52)-H(52A)	0.9500	C(80")-C(81")	1.3900
C(53)-C(54)	1.387(8)	C(80")-C(85")	1.3900
C(53)-H(53A)	0.9500	C(80")-H(80A)	0.9500
C(54)-H(54A)	0.9500	C(81")-C(82")	1.3900
C(55)-C(60)	1.278(7)	C(82")-C(83")	1.3900
C(55)-C(56)	1.363(5)	C(82")-H(82B)	0.9500
C(55)-H(55A)	0.9500	C(83")-C(84")	1.3900
C(56)-C(57)	1.365(6)	C(83")-H(83B)	0.9500
C(56)-H(56A)	0.9500	C(84")-C(85")	1.3900
C(57)-C(58)	1.405(6)	C(84")-H(84B)	0.9500
C(57)-H(57A)	0.9500	C(85")-H(85B)	0.9500
C(58)-C(59)	1.423(6)		
C(58)-H(58A)	0.9500	C(5)-P(2)-C(43)	107.68(13)
C(59)-C(60)	1.368(5)	C(5)-P(2)-C(6)	104.79(12)
C(59)-H(59A)	0.9500	C(43)-P(2)-C(6)	103.84(13)
C(60)-H(60A)	0.9500	C(5)-P(2)-Ni(1)	105.97(9)
C(80)-C(81)	1.3900	C(43)-P(2)-Ni(1)	105.51(9)
C(80)-C(85)	1.3900	C(6)-P(2)-Ni(1)	127.85(10)
C(81)-C(82)	1.3900	O(1)-Ti(1)-N(1)	90.81(7)
C(81)-H(81A)	0.9500	O(1)-Ti(1)-N(3)	90.71(7)
C(82)-C(83)	1.3900	N(1)-Ti(1)-N(3)	117.48(9)
C(82)-H(82A)	0.9500	O(1)-Ti(1)-N(2)	91.06(7)
C(83)-C(84)	1.3900	N(1)-Ti(1)-N(2)	120.49(9)
C(83)-H(83A)	0.9500	N(3)-Ti(1)-N(2)	121.97(9)
C(84)-C(85)	1.3900	O(1)-Ti(1)-Ni(1)	178.67(3)

N(1)-Ti(1)-Ni(1)	89.86(7)	C(80)-P(1)-Ni(1)	110.79(11)
N(3)-Ti(1)-Ni(1)	87.96(7)	C(27)-P(1)-Ni(1)	106.35(9)
N(2)-Ti(1)-Ni(1)	89.59(7)	C(32)-P(1)-Ni(1)	121.88(9)
P(2)-Ni(1)-P(3)	122.34(3)	C(81")-P(1)-Ni(1)	111.6(2)
P(2)-Ni(1)-P(1)	116.53(3)	N(3)-C(99)-C(19)	109.5(3)
P(3)-Ni(1)-P(1)	121.07(3)	N(3)-C(99)-H(10A)	125.3
P(2)-Ni(1)-Ti(1)	91.26(3)	C(19)-C(99)-H(10A)	125.3
P(3)-Ni(1)-Ti(1)	92.76(3)	Ti(1)-O(1)-Ti(1)#1	180.00(2)
P(1)-Ni(1)-Ti(1)	88.22(3)	C(5)-C(2)-C(3)	106.4(2)
C(4)-N(2)-C(5)	106.3(2)	C(5)-C(2)-H(2A)	126.8
C(4)-N(2)-Ti(1)	130.11(18)	C(3)-C(2)-H(2A)	126.8
C(5)-N(2)-Ti(1)	121.32(18)	C(4)-C(3)-C(2)	107.4(3)
C(18)-P(3)-C(21)	105.64(14)	C(4)-C(3)-H(3A)	126.3
C(18)-P(3)-C(12)	103.56(13)	C(2)-C(3)-H(3A)	126.3
C(21)-P(3)-C(12)	103.45(14)	C(3)-C(4)-N(2)	110.1(3)
C(18)-P(3)-Ni(1)	101.89(9)	C(3)-C(4)-H(4A)	124.9
C(21)-P(3)-Ni(1)	120.80(10)	N(2)-C(4)-H(4A)	124.9
C(12)-P(3)-Ni(1)	119.42(10)	C(2)-C(5)-N(2)	109.8(2)
C(99)-N(3)-C(18)	106.4(2)	C(2)-C(5)-P(2)	134.5(2)
C(99)-N(3)-Ti(1)	129.8(2)	N(2)-C(5)-P(2)	115.67(19)
C(18)-N(3)-Ti(1)	123.80(18)	C(7)-C(6)-C(11)	119.3(3)
C(80)-P(1)-C(27)	109.19(14)	C(7)-C(6)-P(2)	119.9(2)
C(80)-P(1)-C(32)	102.52(14)	C(11)-C(6)-P(2)	120.7(2)
C(27)-P(1)-C(32)	105.61(14)	C(6)-C(7)-C(8)	120.5(3)
C(80)-P(1)-C(81")	1.1(3)	C(6)-C(7)-H(7A)	119.7
C(27)-P(1)-C(81")	109.5(3)	C(8)-C(7)-H(7A)	119.7
C(32)-P(1)-C(81")	101.4(3)	C(9)-C(8)-C(7)	120.3(3)

C(9)-C(8)-H(8A)	119.8	C(12)-C(17)-H(17A)	119.7
C(7)-C(8)-H(8A)	119.8	C(16)-C(17)-H(17A)	119.7
C(8)-C(9)-C(10)	119.3(3)	C(20)-C(18)-N(3)	110.1(3)
C(8)-C(9)-H(9A)	120.3	C(20)-C(18)-P(3)	133.7(3)
C(10)-C(9)-H(9A)	120.3	N(3)-C(18)-P(3)	116.13(19)
C(9)-C(10)-C(11)	120.4(3)	C(99)-C(19)-C(20)	107.5(3)
C(9)-C(10)-H(10B)	119.8	C(99)-C(19)-H(19A)	126.2
C(11)-C(10)-H(10B)	119.8	C(20)-C(19)-H(19A)	126.2
C(10)-C(11)-C(6)	120.1(3)	C(18)-C(20)-C(19)	106.4(3)
C(10)-C(11)-H(11A)	119.9	C(18)-C(20)-H(20A)	126.8
C(6)-C(11)-H(11A)	119.9	C(19)-C(20)-H(20A)	126.8
C(17)-C(12)-C(13)	118.7(3)	C(26)-C(21)-C(22)	119.3(3)
C(17)-C(12)-P(3)	123.6(3)	C(26)-C(21)-P(3)	122.1(3)
C(13)-C(12)-P(3)	117.6(3)	C(22)-C(21)-P(3)	118.6(2)
C(14)-C(13)-C(12)	120.2(4)	C(23)-C(22)-C(21)	120.1(4)
C(14)-C(13)-H(13A)	119.9	C(23)-C(22)-H(22A)	120.0
C(12)-C(13)-H(13A)	119.9	C(21)-C(22)-H(22A)	120.0
C(15)-C(14)-C(13)	119.8(4)	C(24)-C(23)-C(22)	120.3(4)
C(15)-C(14)-H(14A)	120.1	C(24)-C(23)-H(23A)	119.9
C(13)-C(14)-H(14A)	120.1	C(22)-C(23)-H(23A)	119.9
C(16)-C(15)-C(14)	119.9(4)	C(25)-C(24)-C(23)	120.5(4)
C(16)-C(15)-H(15A)	120.1	C(25)-C(24)-H(24A)	119.8
C(14)-C(15)-H(15A)	120.1	C(23)-C(24)-H(24A)	119.8
C(15)-C(16)-C(17)	120.7(4)	C(24)-C(25)-C(26)	119.7(4)
C(15)-C(16)-H(16A)	119.6	C(24)-C(25)-H(25A)	120.2
C(17)-C(16)-H(16A)	119.6	C(26)-C(25)-H(25A)	120.2
C(12)-C(17)-C(16)	120.6(4)	C(21)-C(26)-C(25)	120.2(4)

C(21)-C(26)-H(26A)	119.9	C(36)-C(35)-H(35A)	120.1
C(25)-C(26)-H(26A)	119.9	C(34)-C(35)-H(35A)	120.1
C(28)-C(27)-N(1)	108.6(3)	C(35)-C(36)-C(37)	120.2(4)
C(28)-C(27)-P(1)	137.6(2)	C(35)-C(36)-H(36A)	119.9
N(1)-C(27)-P(1)	113.83(19)	C(37)-C(36)-H(36A)	119.9
C(27)-C(28)-C(29)	107.4(3)	C(32)-C(37)-C(36)	120.5(4)
C(27)-C(28)-H(28A)	126.3	C(32)-C(37)-H(37A)	119.8
C(29)-C(28)-H(28A)	126.3	C(36)-C(37)-H(37A)	119.8
C(30)-C(29)-C(28)	106.8(3)	C(48)-C(43)-C(44)	118.8(3)
C(30)-C(29)-H(29A)	126.6	C(48)-C(43)-P(2)	123.0(2)
C(28)-C(29)-H(29A)	126.6	C(44)-C(43)-P(2)	118.0(2)
C(29)-C(30)-N(1)	110.4(3)	C(43)-C(44)-C(45)	120.5(3)
C(29)-C(30)-H(30A)	124.8	C(43)-C(44)-H(44A)	119.8
N(1)-C(30)-H(30A)	124.8	C(45)-C(44)-H(44A)	119.8
C(30)-N(1)-C(27)	106.7(2)	C(46)-C(45)-C(44)	120.1(3)
C(30)-N(1)-Ti(1)	129.92(19)	C(46)-C(45)-H(45A)	119.9
C(27)-N(1)-Ti(1)	120.98(18)	C(44)-C(45)-H(45A)	119.9
C(37)-C(32)-C(33)	118.9(3)	C(45)-C(46)-C(47)	119.8(3)
C(37)-C(32)-P(1)	120.4(2)	C(45)-C(46)-H(46A)	120.1
C(33)-C(32)-P(1)	120.4(2)	C(47)-C(46)-H(46A)	120.1
C(34)-C(33)-C(32)	120.3(3)	C(46)-C(47)-C(48)	120.6(3)
C(34)-C(33)-H(33A)	119.8	C(46)-C(47)-H(47A)	119.7
C(32)-C(33)-H(33A)	119.8	C(48)-C(47)-H(47A)	119.7
C(35)-C(34)-C(33)	120.2(4)	C(43)-C(48)-C(47)	120.1(3)
C(35)-C(34)-H(34A)	119.9	C(43)-C(48)-H(48A)	119.9
C(33)-C(34)-H(34A)	119.9	C(47)-C(48)-H(48A)	119.9
C(36)-C(35)-C(34)	119.9(3)	C(53)-C(49)-C(50)	120.0(5)

C(53)-C(49)-H(49A)	120.0	C(57)-C(58)-H(58A)	121.8
C(50)-C(49)-H(49A)	120.0	C(59)-C(58)-H(58A)	121.8
C(49)-C(50)-C(51)	119.7(5)	C(60)-C(59)-C(58)	119.2(5)
C(49)-C(50)-H(50A)	120.1	C(60)-C(59)-H(59A)	120.4
C(51)-C(50)-H(50A)	120.1	C(58)-C(59)-H(59A)	120.4
C(52)-C(51)-C(50)	120.8(4)	C(55)-C(60)-C(59)	122.5(6)
C(52)-C(51)-H(51A)	119.6	C(55)-C(60)-H(60A)	118.8
C(50)-C(51)-H(51A)	119.6	C(59)-C(60)-H(60A)	118.8
C(51)-C(52)-C(54)	120.3(5)	C(81)-C(80)-C(85)	120.0
C(51)-C(52)-H(52A)	119.9	C(81)-C(80)-P(1)	116.2(2)
C(54)-C(52)-H(52A)	119.9	C(85)-C(80)-P(1)	123.8(2)
C(49)-C(53)-C(54)	120.8(5)	C(80)-C(81)-C(82)	120.0
C(49)-C(53)-H(53A)	119.6	C(80)-C(81)-H(81A)	120.0
C(54)-C(53)-H(53A)	119.6	C(82)-C(81)-H(81A)	120.0
C(53)-C(54)-C(52)	118.4(5)	C(83)-C(82)-C(81)	120.0
C(53)-C(54)-H(54A)	120.8	C(83)-C(82)-H(82A)	120.0
C(52)-C(54)-H(54A)	120.8	C(81)-C(82)-H(82A)	120.0
C(60)-C(55)-C(56)	121.2(6)	C(84)-C(83)-C(82)	120.0
C(60)-C(55)-H(55A)	119.4	C(84)-C(83)-H(83A)	120.0
C(56)-C(55)-H(55A)	119.4	C(82)-C(83)-H(83A)	120.0
C(55)-C(56)-C(57)	120.5(6)	C(83)-C(84)-C(85)	120.0
C(55)-C(56)-H(56A)	119.8	C(83)-C(84)-H(84A)	120.0
C(57)-C(56)-H(56A)	119.8	C(85)-C(84)-H(84A)	120.0
C(56)-C(57)-C(58)	119.7(5)	C(84)-C(85)-C(80)	120.0
C(56)-C(57)-H(57A)	120.1	C(84)-C(85)-H(85A)	120.0
C(58)-C(57)-H(57A)	120.1	C(80)-C(85)-H(85A)	120.0
C(57)-C(58)-C(59)	116.5(5)	C(81")-C(80")-C(85")	120.0

C(81")-C(80")-H(80A)	120.0	C(84")-C(83")-H(83B)	120.0
C(85")-C(80")-H(80A)	120.0	C(82")-C(83")-H(83B)	120.0
C(80")-C(81")-C(82")	120.0	C(83")-C(84")-C(85")	120.0
C(80")-C(81")-P(1)	120.0(5)	C(83")-C(84")-H(84B)	120.0
C(82")-C(81")-P(1)	119.9(5)	C(85")-C(84")-H(84B)	120.0
C(83")-C(82")-C(81")	120.0	C(84")-C(85")-C(80")	120.0
C(83")-C(82")-H(82B)	120.0	C(84")-C(85")-H(85B)	120.0
C(81")-C(82")-H(82B)	120.0	C(80")-C(85")-H(85B)	120.0
C(84")-C(83")-C(82")	120.0		

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 9. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	$U_{11}U_{22}$	U_{33}	U_{23}	U_{13}	U_{12}	
P2	31(1)	18(1)	21(1)	0(1)	-2(1)	4(1)
Ti1	24(1)	18(1)	15(1)	0(1)	-1(1)	2(1)
Ni1	26(1)	21(1)	19(1)	-2(1)	-4(1)	3(1)
N2	29(1)	22(1)	22(1)	1(1)	-3(1)	4(1)
P3	24(1)	27(1)	25(1)	-2(1)	-6(1)	2(1)
N3	32(1)	24(1)	21(1)	-1(1)	-4(1)	4(1)
P1	27(1)	26(1)	19(1)	-5(1)	-6(1)	5(1)
C99	42(2)	31(1)	20(1)	-1(1)	-2(1)	4(1)
O1	30(1)	22(1)	21(1)	0(1)	-1(1)	4(1)
C2	37(2)	26(1)	35(2)	0(1)	-1(1)	10(1)
C3	28(1)	39(2)	37(2)	1(1)	0(1)	7(1)
C4	28(1)	32(1)	28(1)	2(1)	-1(1)	1(1)
C5	30(1)	21(1)	23(1)	-1(1)	-3(1)	6(1)
C6	33(1)	24(1)	29(1)	-4(1)	3(1)	-1(1)
C7	100(3)	26(2)	33(2)	-7(1)	-10(2)	8(2)
C8	109(4)	47(2)	27(2)	-5(2)	-12(2)	3(2)
C9	60(2)	40(2)	41(2)	-19(2)	7(2)	-5(2)
C10	57(2)	27(1)	50(2)	-11(1)	0(2)	2(1)
C11	43(2)	26(1)	41(2)	-6(1)	-5(1)	3(1)
C12	38(2)	39(2)	25(1)	-3(1)	-6(1)	-9(1)
C13	47(2)	44(2)	64(2)	-7(2)	-11(2)	-6(2)
C14	80(3)	44(2)	71(3)	-10(2)	-14(2)	-16(2)

C15	62(2)	62(2)	45(2)	-4(2)	-9(2)	-31(2)
C16	38(2)	74(3)	46(2)	-4(2)	-4(2)	-17(2)
C17	37(2)	53(2)	42(2)	0(2)	-3(1)	-8(2)
C18	30(1)	34(1)	24(1)	-1(1)	-8(1)	3(1)
C19	49(2)	54(2)	22(1)	-3(1)	-9(1)	4(2)
C20	34(2)	65(2)	31(2)	-4(2)	-11(1)	1(2)
C21	19(1)	31(1)	47(2)	-2(1)	-5(1)	1(1)
C22	37(2)	47(2)	52(2)	-12(2)	-6(2)	11(1)
C23	48(2)	57(2)	78(3)	-24(2)	2(2)	15(2)
C24	46(2)	41(2)	120(4)	-11(2)	10(2)	14(2)
C25	51(2)	50(2)	114(4)	25(3)	8(2)	16(2)
C26	47(2)	48(2)	68(2)	14(2)	9(2)	14(2)
C27	31(1)	31(1)	20(1)	-6(1)	-6(1)	5(1)
C28	67(2)	32(2)	25(1)	-9(1)	-8(1)	7(2)
C29	56(2)	26(1)	35(2)	-8(1)	-4(1)	4(1)
C30	41(2)	23(1)	31(1)	-3(1)	-1(1)	6(1)
N1	31(1)	23(1)	22(1)	-5(1)	-1(1)	3(1)
C32	32(1)	39(2)	20(1)	-8(1)	-7(1)	10(1)
C33	36(2)	63(2)	35(2)	4(2)	-9(1)	1(2)
C34	33(2)	89(3)	51(2)	-2(2)	-12(2)	3(2)
C35	43(2)	73(3)	60(2)	-5(2)	-26(2)	19(2)
C36	63(2)	53(2)	51(2)	4(2)	-27(2)	18(2)
C37	44(2)	40(2)	40(2)	2(1)	-13(1)	7(1)
C43	42(2)	22(1)	24(1)	0(1)	2(1)	5(1)
C44	47(2)	45(2)	42(2)	8(2)	1(2)	-4(2)
C45	60(2)	50(2)	43(2)	8(2)	10(2)	-10(2)
C46	80(3)	38(2)	30(2)	10(1)	5(2)	-2(2)

C47	65(2)	41(2)	33(2)	12(1)	-10(2)	0(2)
C48	49(2)	34(2)	31(2)	6(1)	-5(1)	-2(1)
C49	101(4)	62(3)	90(4)	-24(3)	30(3)	-3(3)
C50	75(3)	57(2)	60(2)	8(2)	11(2)	13(2)
C51	71(3)	62(2)	44(2)	4(2)	2(2)	28(2)
C52	76(3)	49(2)	60(2)	4(2)	-13(2)	17(2)
C53	103(4)	106(4)	70(3)	-31(3)	32(3)	-4(4)
C54	77(3)	98(4)	55(3)	22(3)	6(2)	0(3)
C55	63(3)	89(4)	95(4)	5(3)	0(3)	-4(3)
C56	72(3)	84(4)	97(4)	8(3)	-1(3)	9(3)
C57	75(3)	67(3)	117(5)	-8(3)	-4(3)	11(3)
C58	97(4)	146(6)	79(4)	-15(4)	29(3)	22(4)
C59	73(3)	89(4)	68(3)	12(3)	-9(2)	13(3)
C60	62(3)	87(3)	70(3)	-1(3)	9(2)	-5(2)
C80	16(2)	31(2)	18(2)	-5(2)	-4(1)	2(1)
C81	65(5)	41(3)	52(3)	0(3)	15(3)	-13(3)
C82	79(6)	71(5)	59(4)	6(4)	21(4)	-35(4)
C83	36(4)	99(6)	41(5)	9(4)	13(4)	-19(4)
C84	75(5)	56(4)	62(5)	-18(4)	38(5)	-9(4)
C85	50(4)	44(3)	48(4)	-8(3)	17(3)	-7(3)
C80"	16(2)	31(2)	18(2)	-5(2)	-4(1)	2(1)
C81"	65(5)	41(3)	52(3)	0(3)	15(3)	-13(3)
C82"	31(6)	45(7)	46(6)	-3(5)	-11(5)	-5(5)
C83"	33(7)	85(12)	92(12)	33(10)	1(7)	-14(7)
C84"	48(12)	96(14)	64(14)	-6(12)	15(11)	-3(11)
C85"	62(9)	62(9)	54(8)	2(7)	34(8)	13(7)