

Electronic Supplementary Information (ESI)

**1,2,4-Diazaphospholide Complexes of Lanthanum(III),
Cerium(III), Neodymium(III), Praseodymium(III), and
Samarium(III): Synthesis, X-Ray Structural Characterization,
and Magnetic Susceptibility Studies**

Minggang Zhao,^a Lixia Wang,^a Pangpang Li,^a Jianping Ma,^b Wenjun Zheng^{a,c,*}

^a*Institute of Organic Chemistry & College of Chemical and Materials Science, Shanxi Normal
Univeristy, Gongyuan Street 1, Linfen, Shanxi Province, 041004, China.*

^b*College of Chemistry, Chemical Engineering and Materials Science, Shandong Normal University,
Jinan 250014, China.*

^c*Key Laboratory of Magnetic Molecules and Magnetic Information Material, Ministry of
Education, Linfen, Shanxi Province, 041004, China*

Email: wjzheng_sxnu@qq.com; wjzheng@sxnu.edu.cn

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1. ^1H , $^{31}\text{P}\{^1\text{H}\}$, $^{13}\text{C}\{^1\text{H}\}$ NMR data for **3–12**

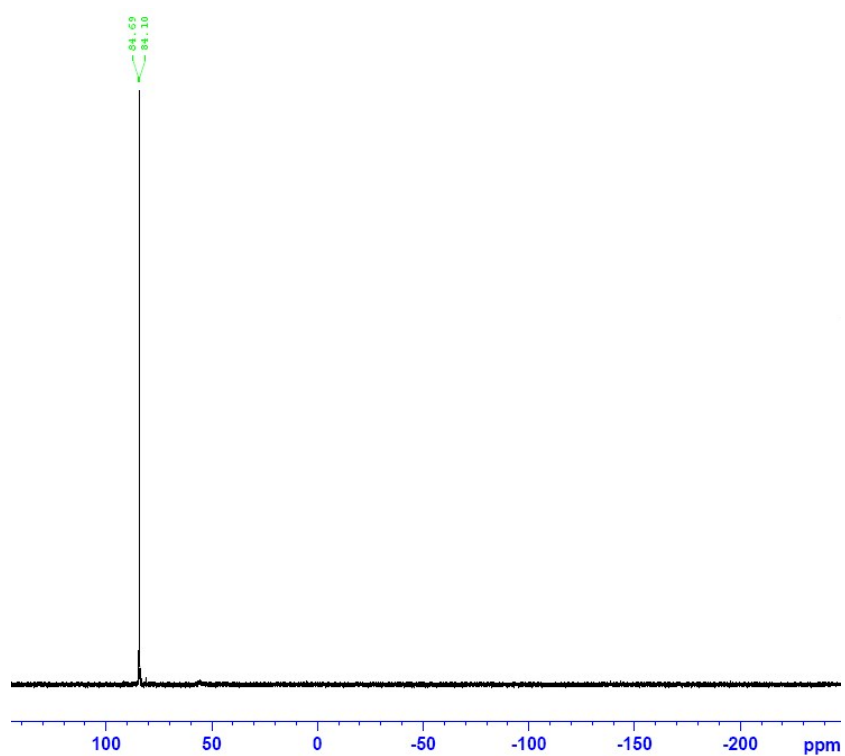


Fig. 1 The $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **3** in $\text{DMSO}-d_6$

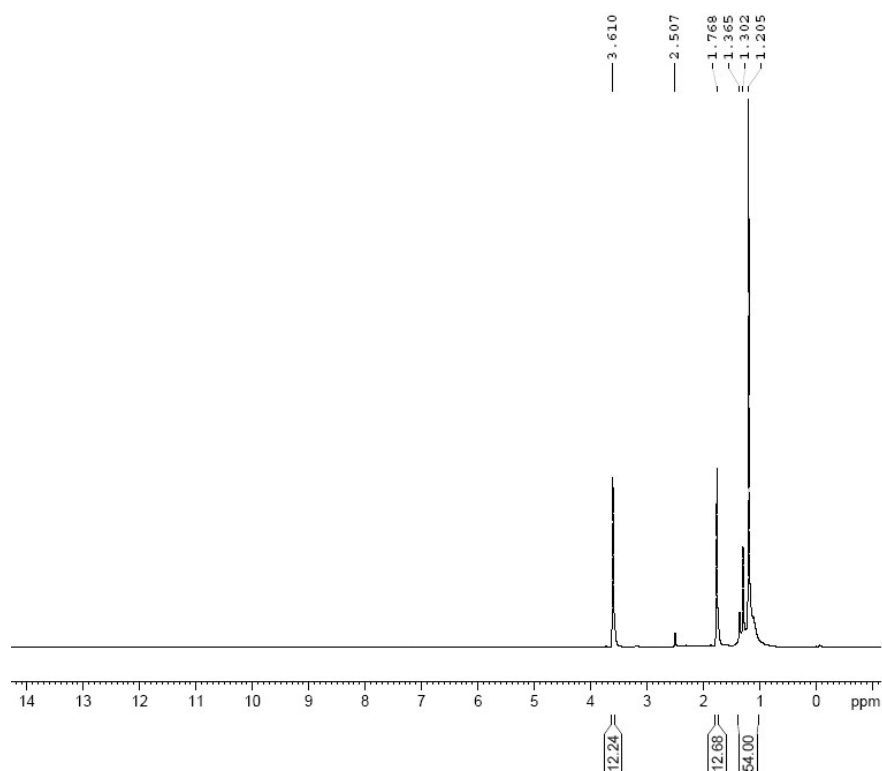


Fig. 2 The ^1H NMR spectrum of compound **3** in $\text{DMSO}-d_6$

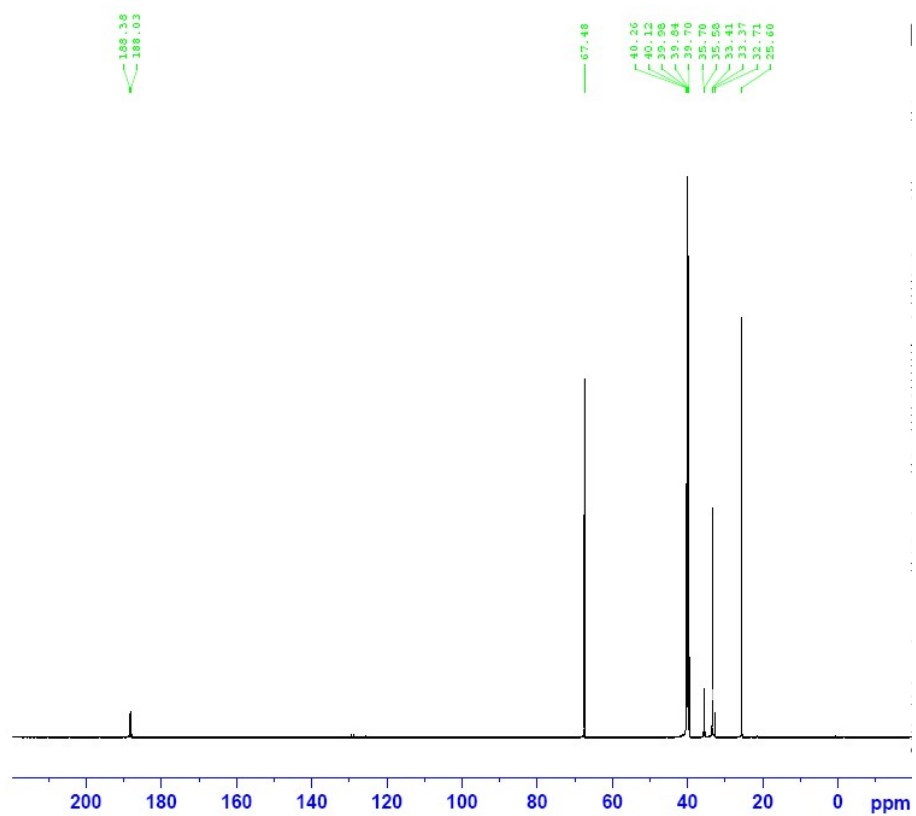


Fig. 3 The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **3** in $\text{DMSO}-d_6$

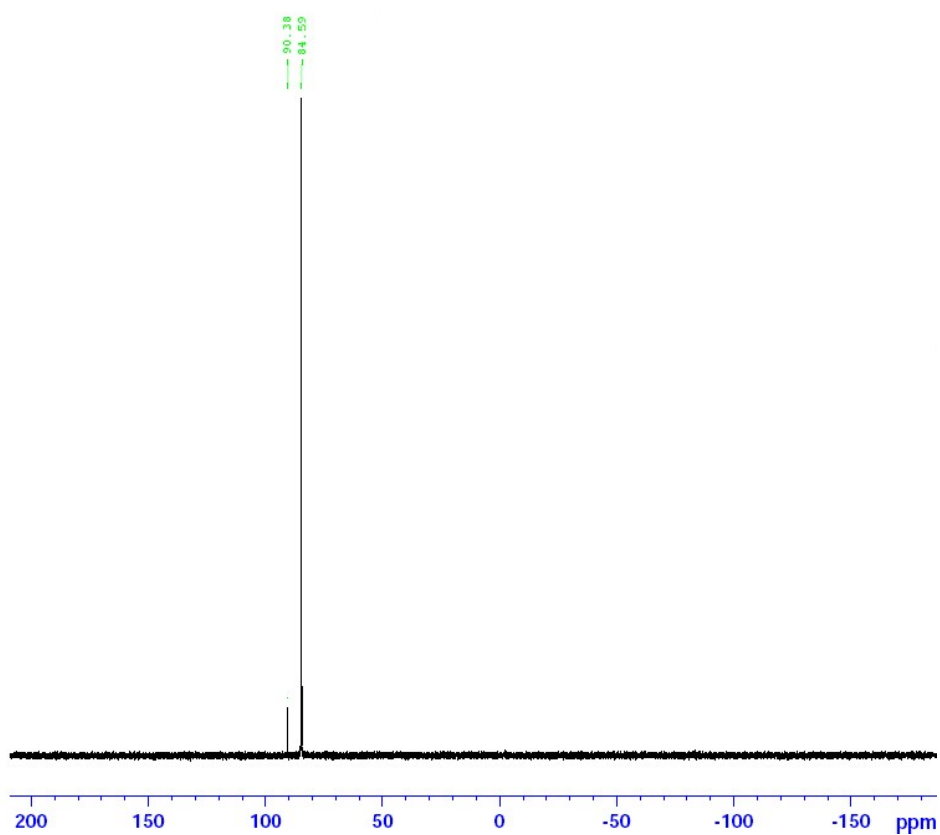


Fig. 4 The $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **4** in $\text{DMSO}-d_6$

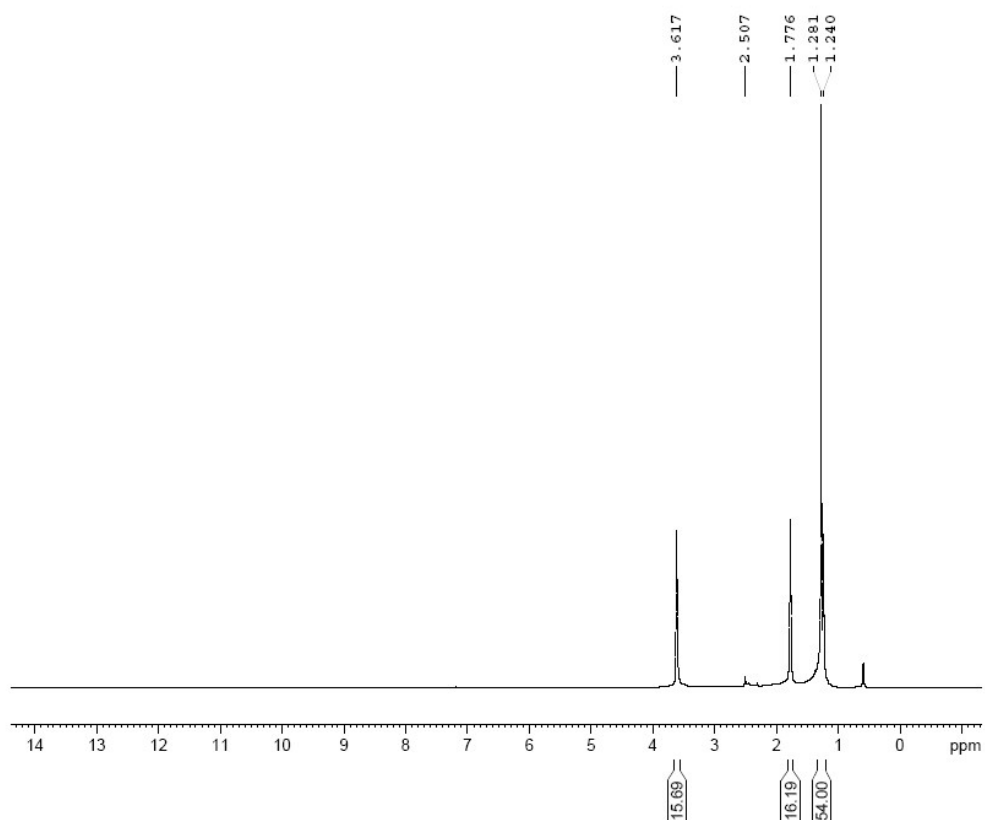


Fig. 5 The ^1H NMR spectrum of compound **4** in $\text{DMSO-}d_6$

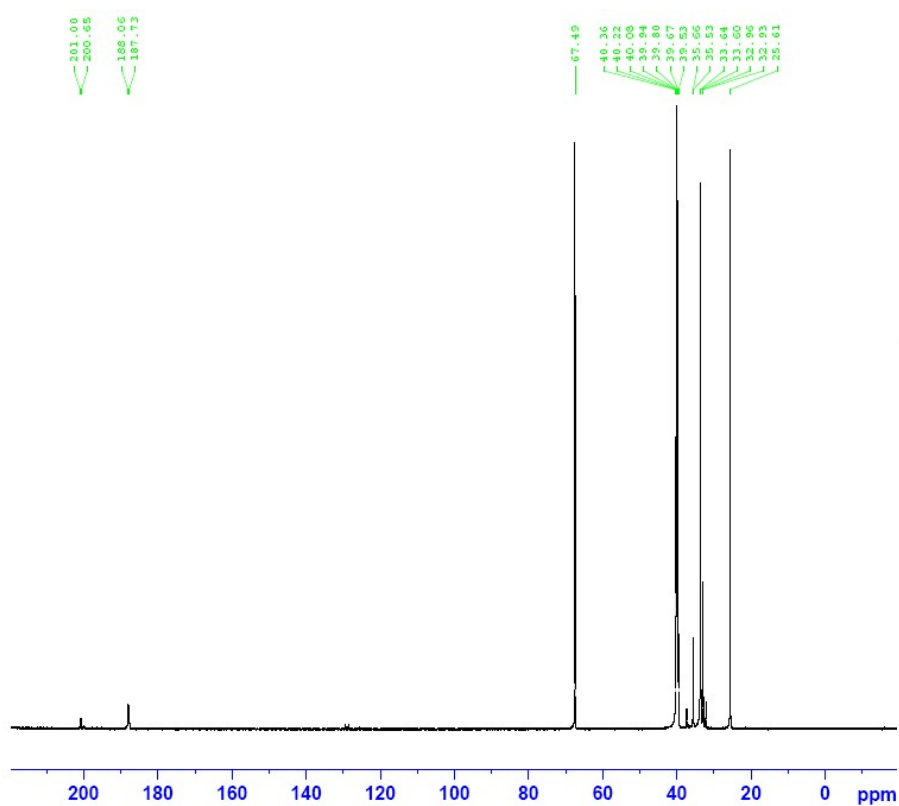


Fig. 6 The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **4** in $\text{DMSO-}d_6$

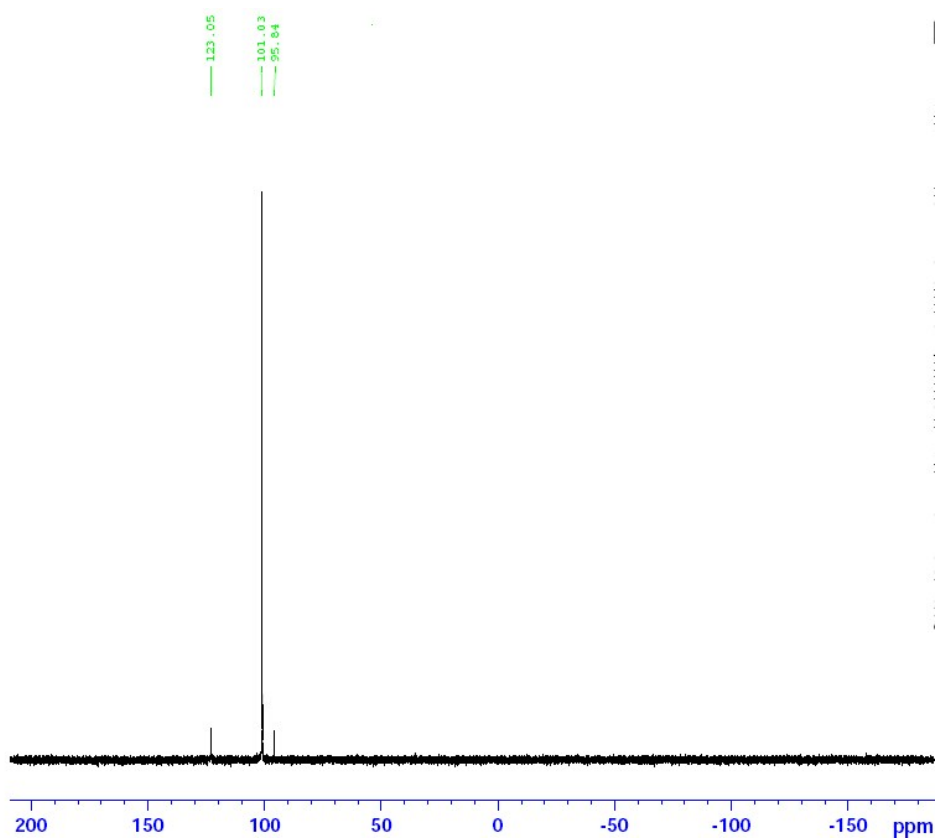


Fig. 7 The $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **5** in $\text{DMSO-}d_6$

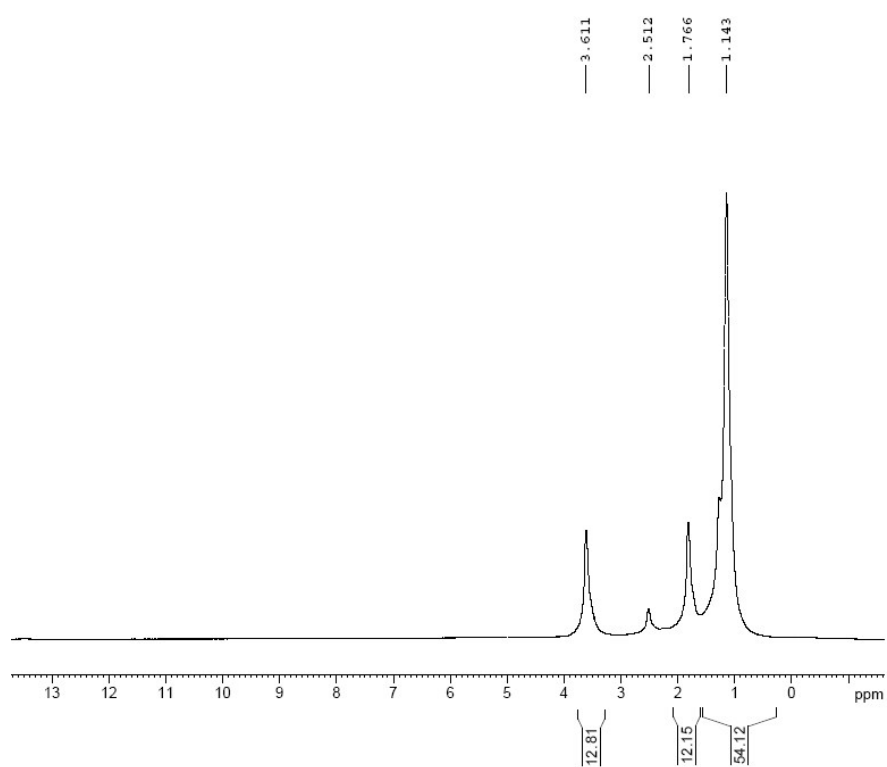


Fig. 8 The ^1H NMR spectrum of compound **5** in $\text{DMSO-}d_6$

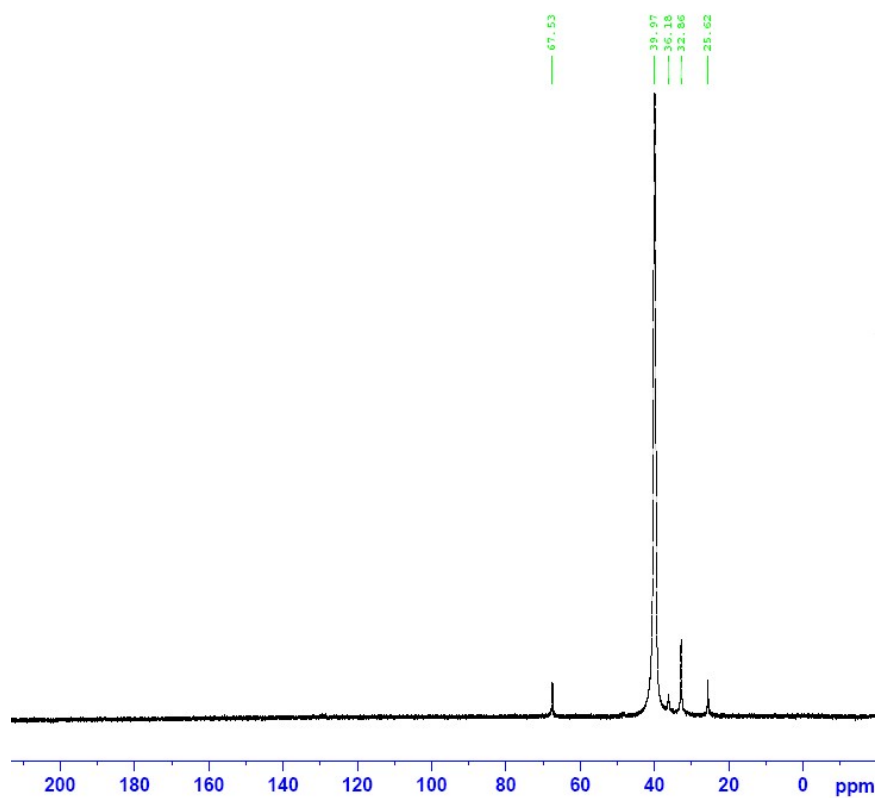


Fig. 9 The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **5** in $\text{DMSO}-d_6$

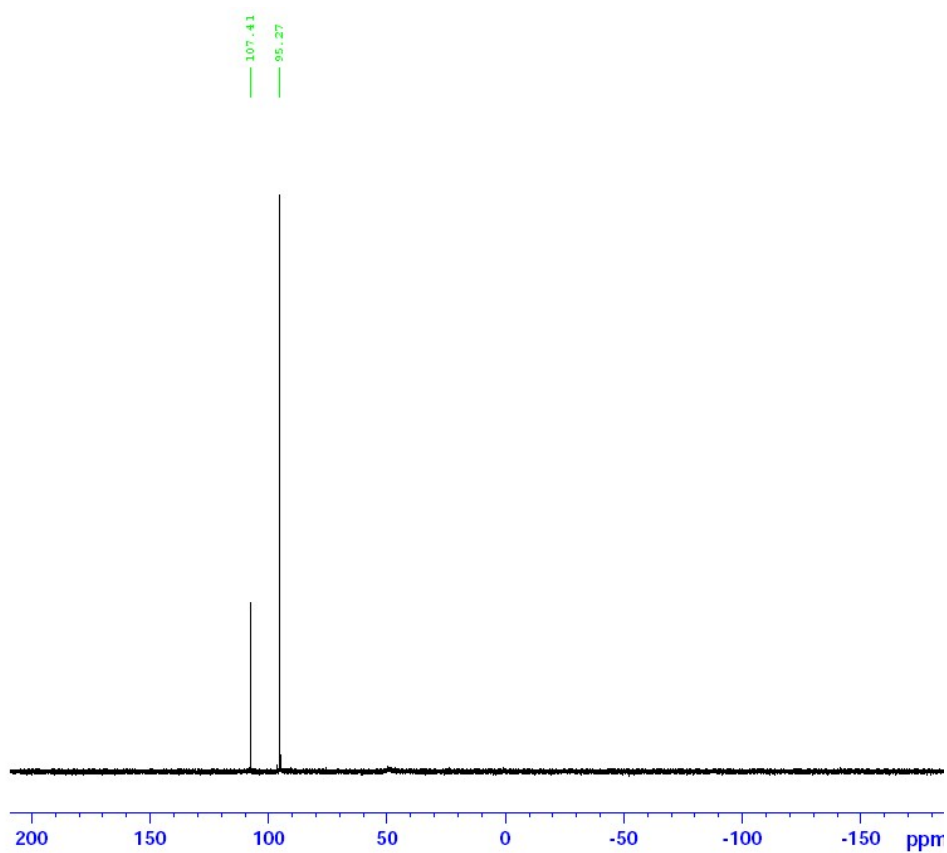


Fig. 10 The $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **6** in $\text{DMSO}-d_6$

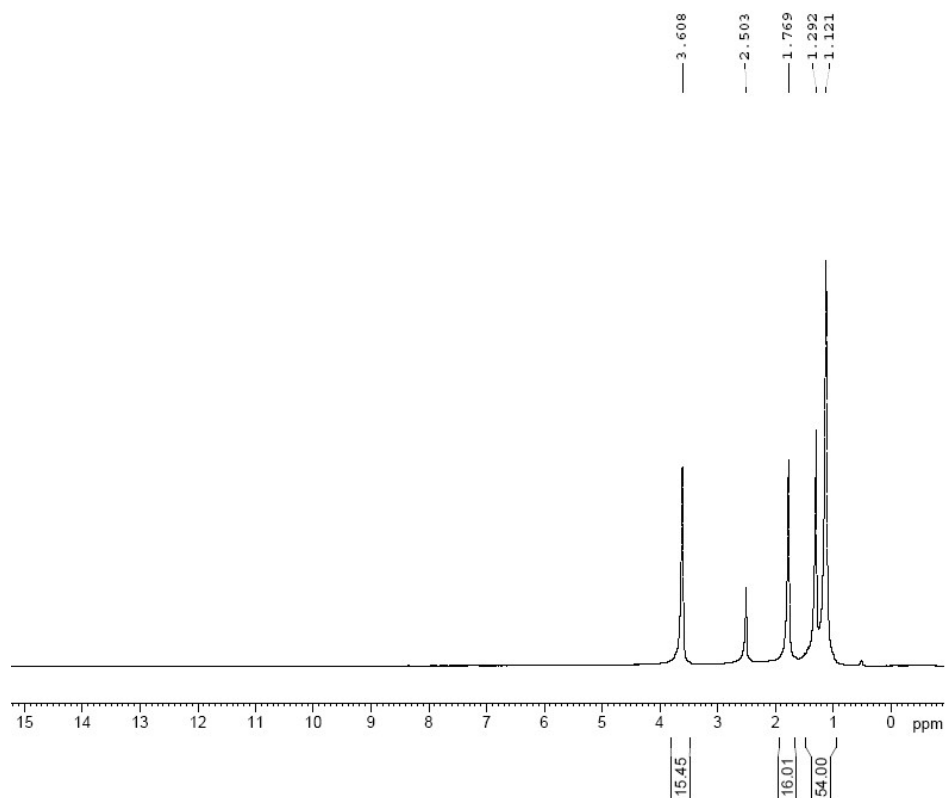


Fig. 11 The ^1H NMR spectrum of compound **6** in $\text{DMSO-}d_6$

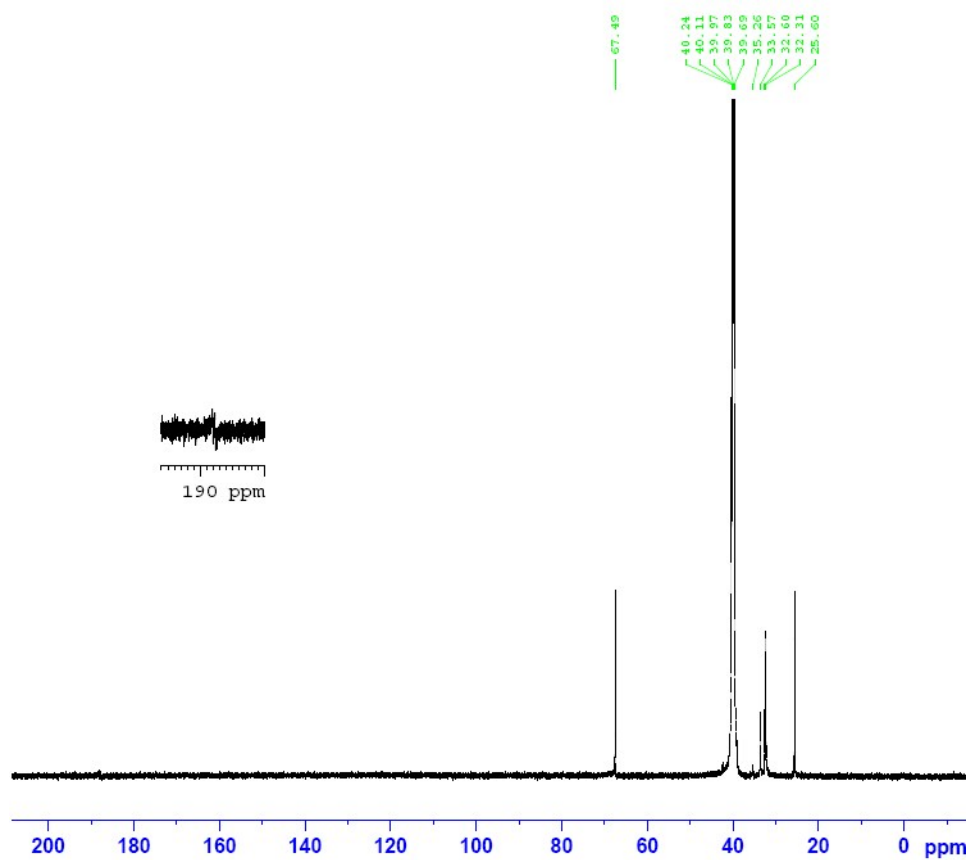


Fig. 12 The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **6** in $\text{DMSO-}d_6$

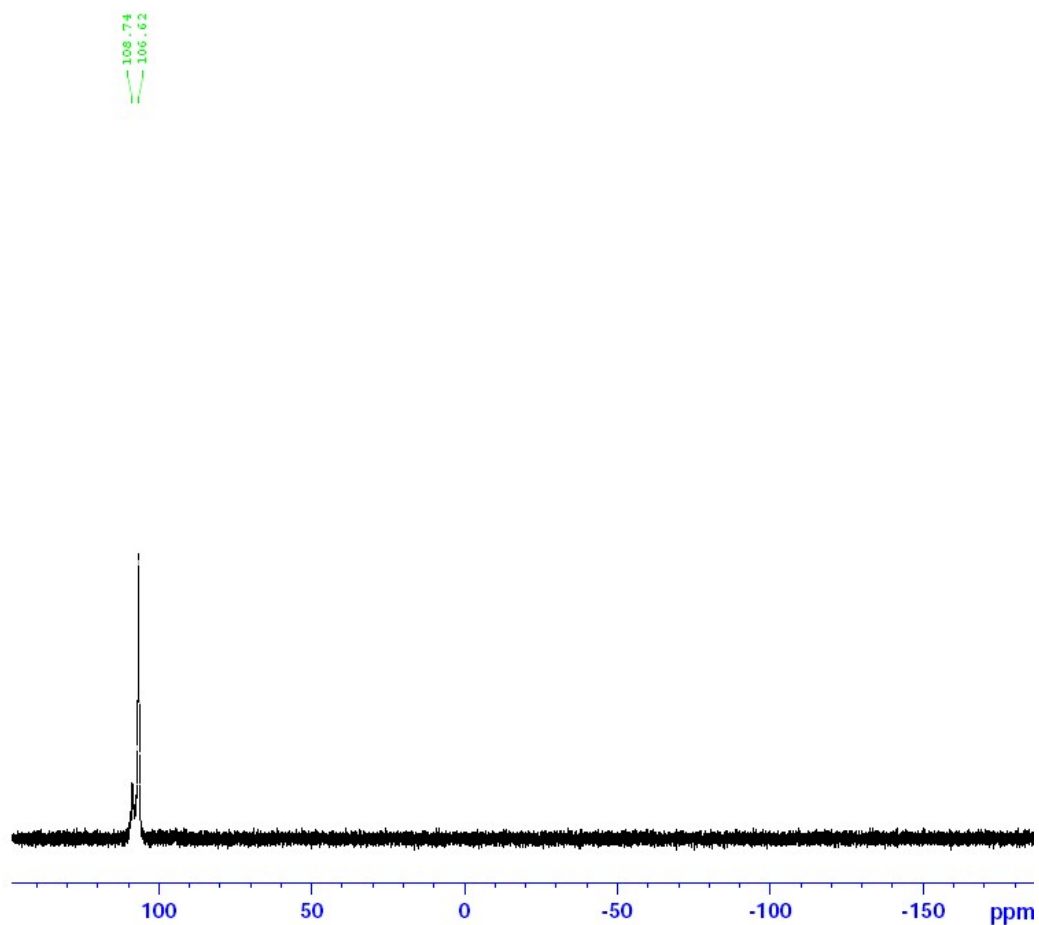


Fig. 13 The $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **7** in $\text{DMSO-}d_6$

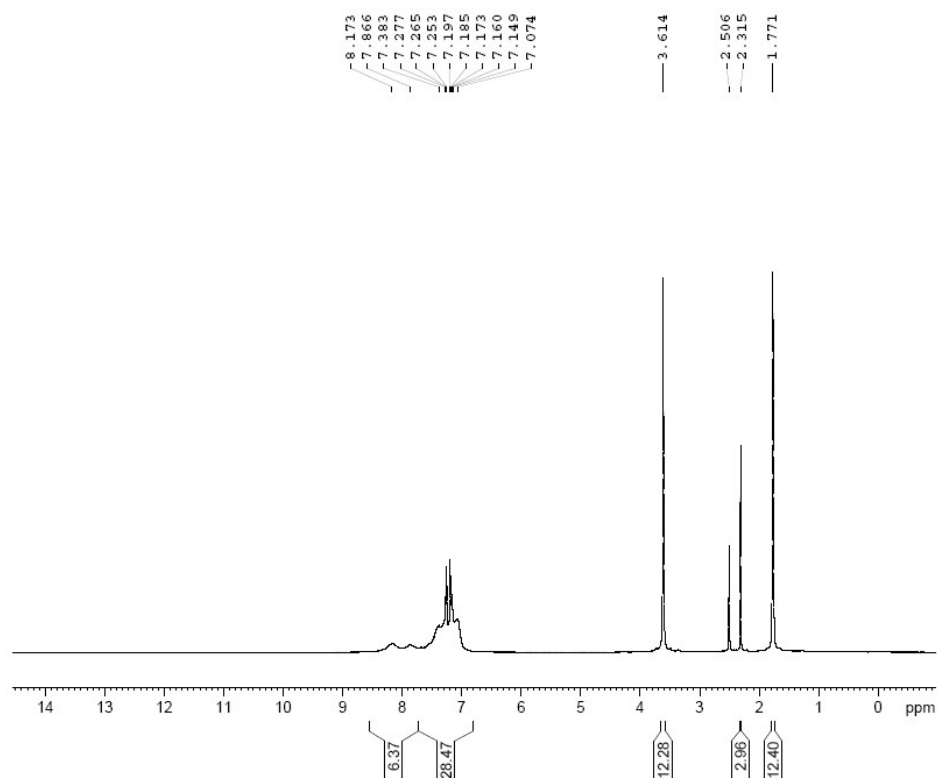


Fig. 14 The ^1H NMR spectrum of compound **7** in $\text{DMSO-}d_6$

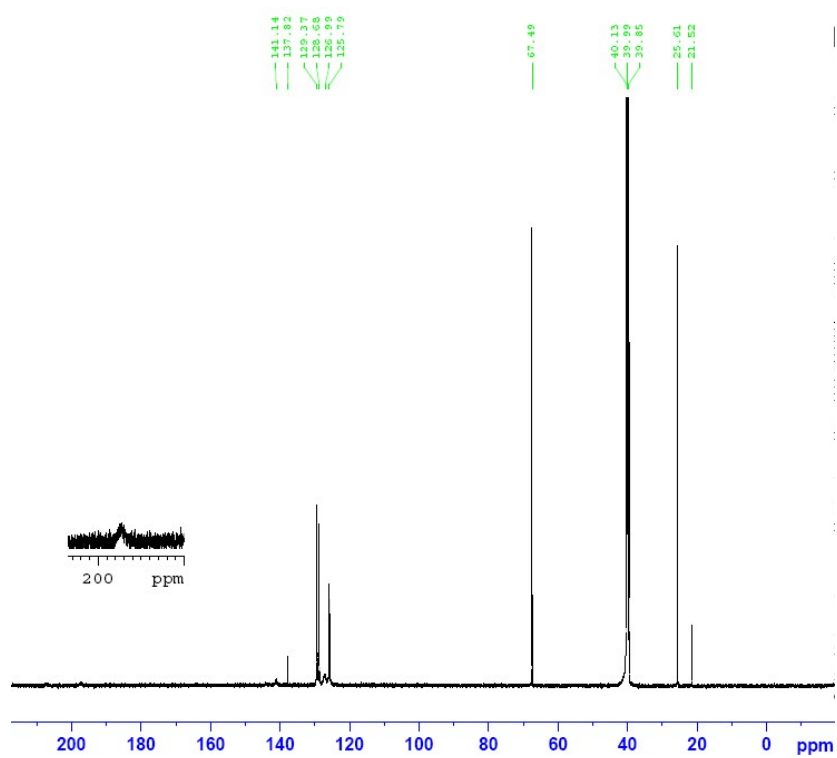


Fig. 15 The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **7** in $\text{DMSO}-d_6$

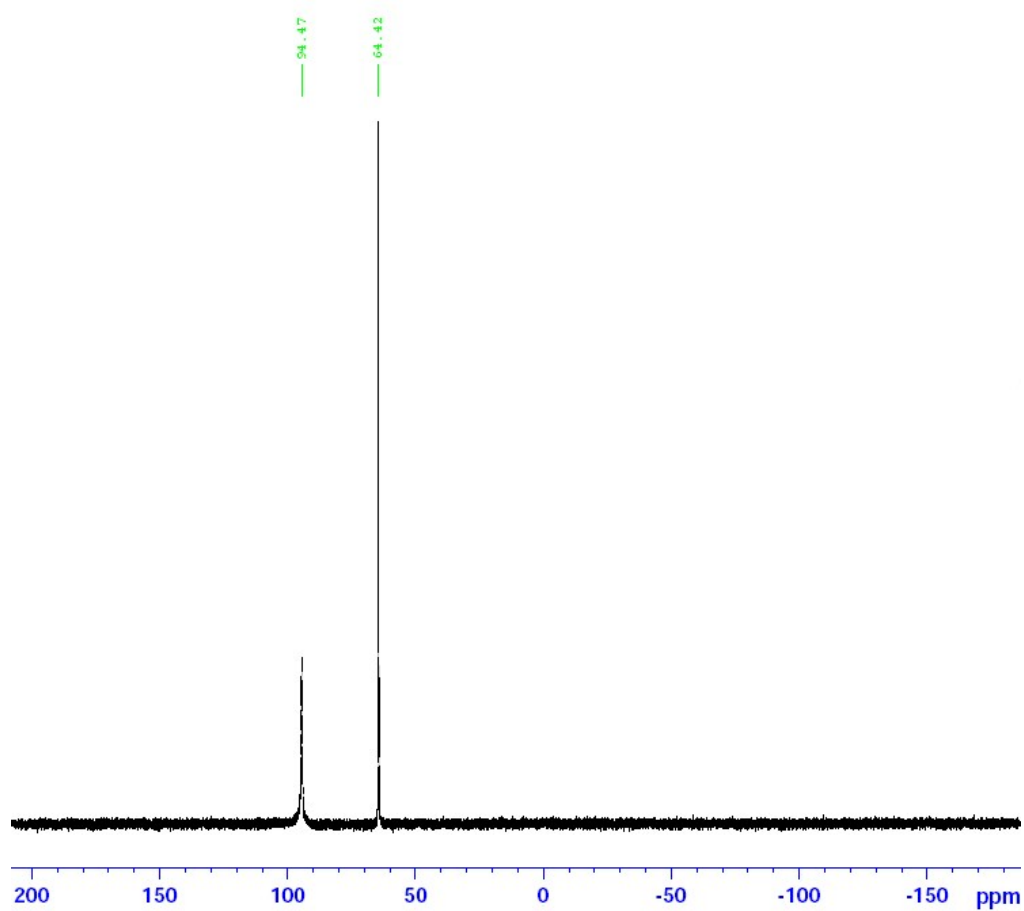


Fig. 16 The $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **8** in $\text{DMSO}-d_6$

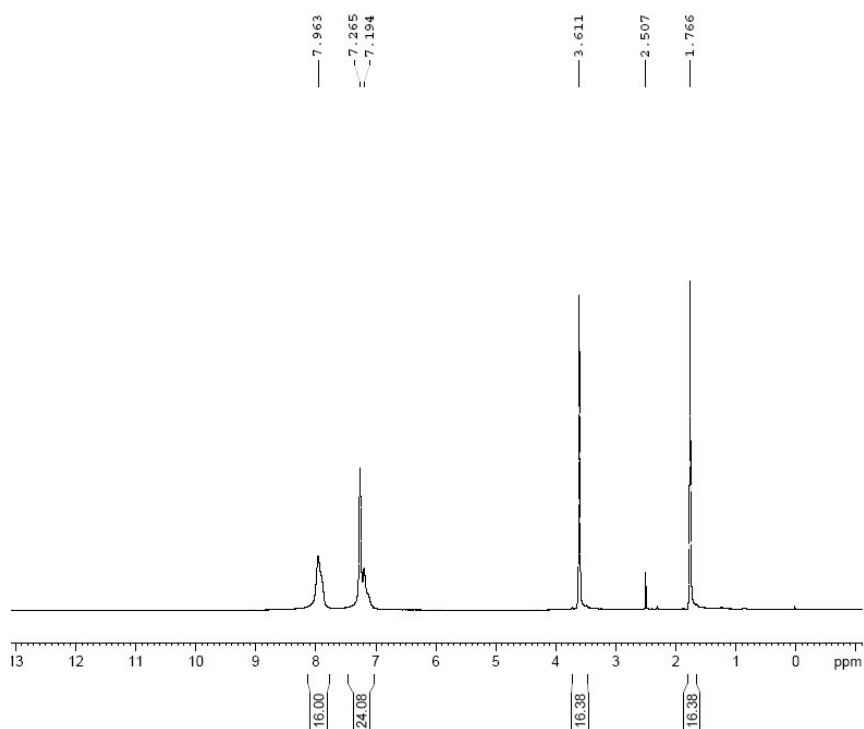


Fig. 17 The ^1H NMR spectrum of compound **8** in $\text{DMSO-}d_6$

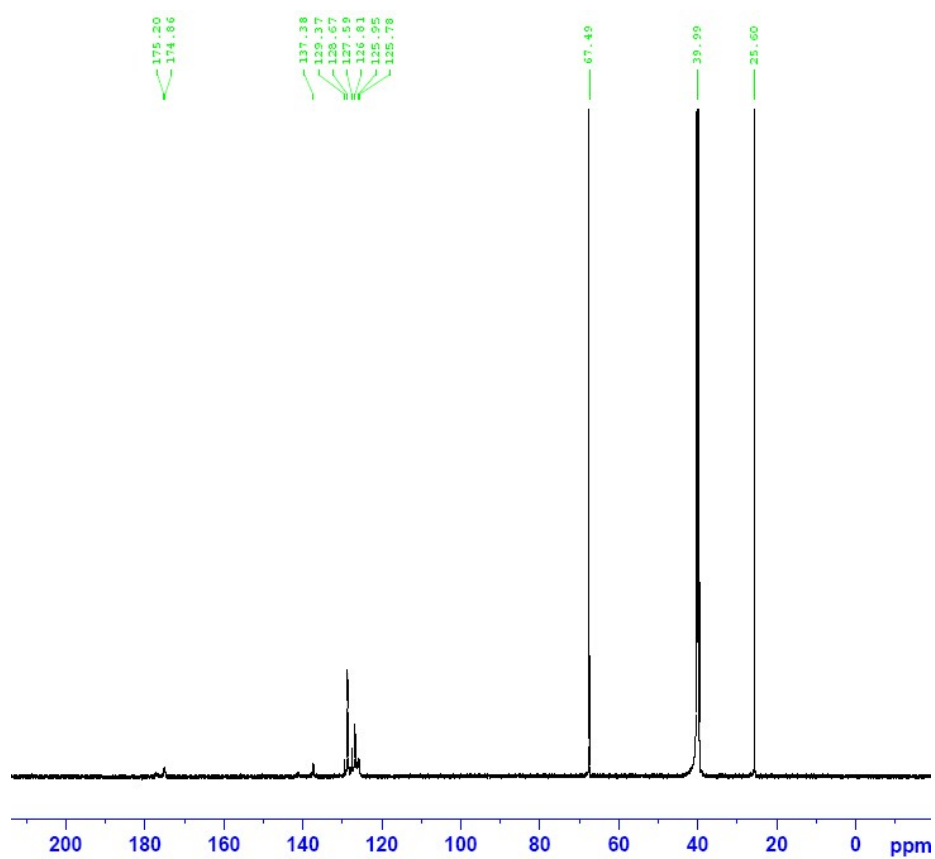


Fig. 18 The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **8** in $\text{DMSO-}d_6$

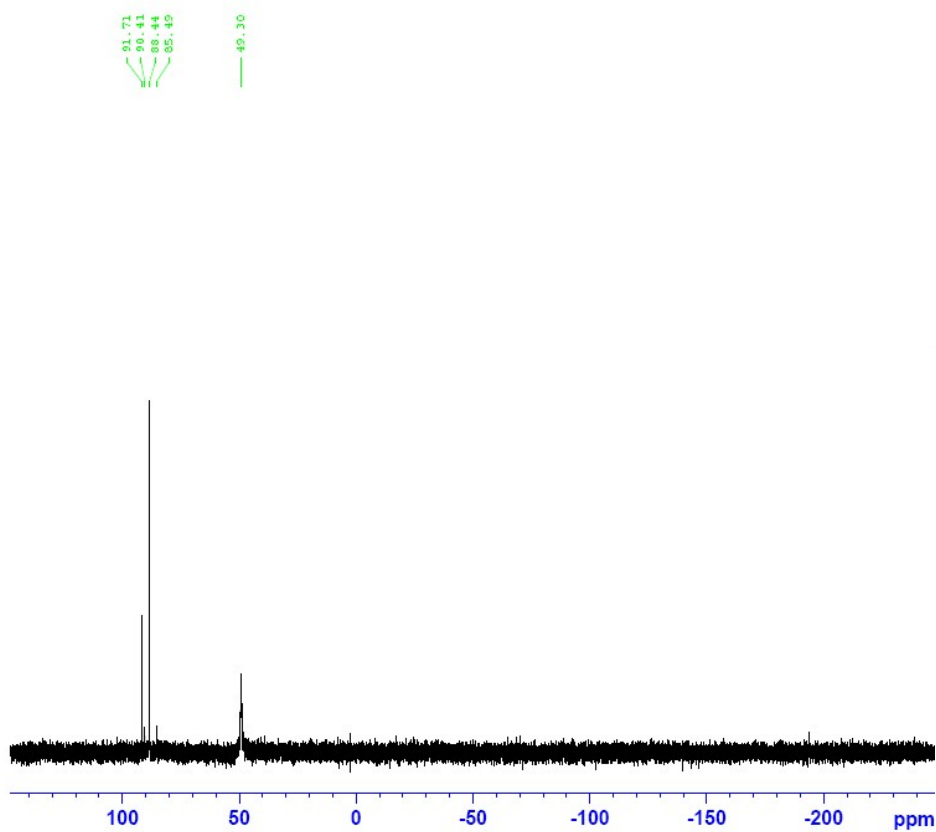


Fig. 19 The $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **9** in $\text{DMSO}-d_6$

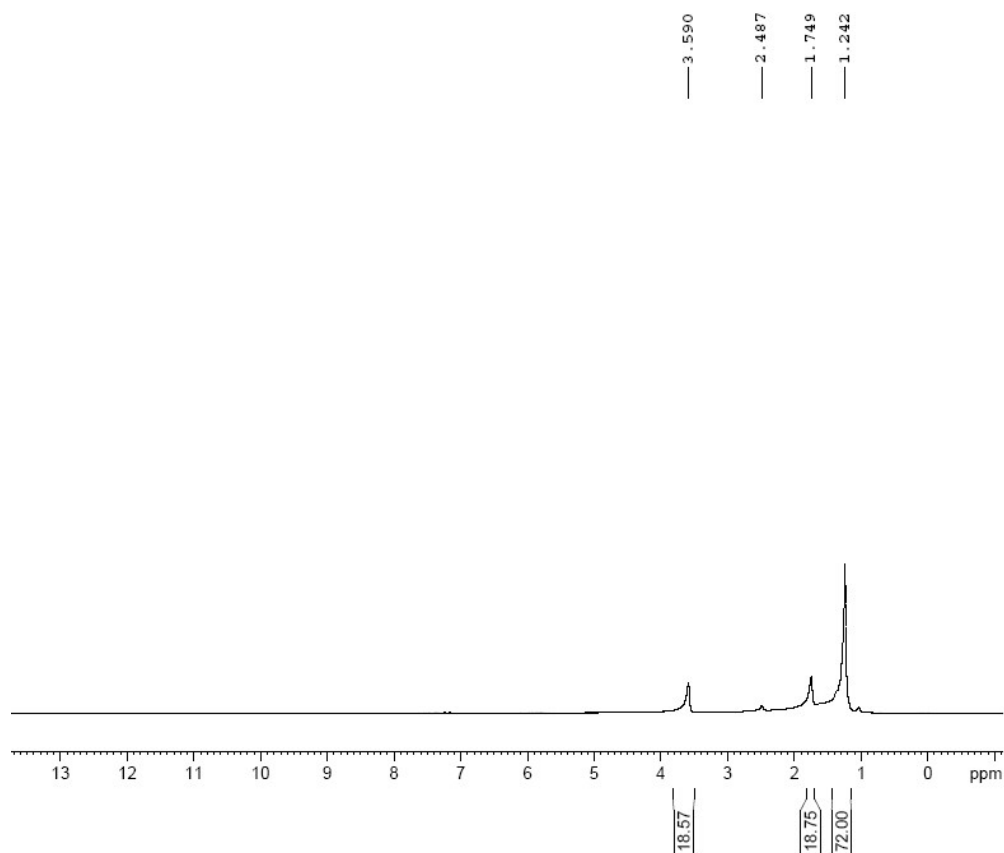


Fig. 20 The ^1H NMR spectrum of compound **9** in $\text{DMSO}-d_6$

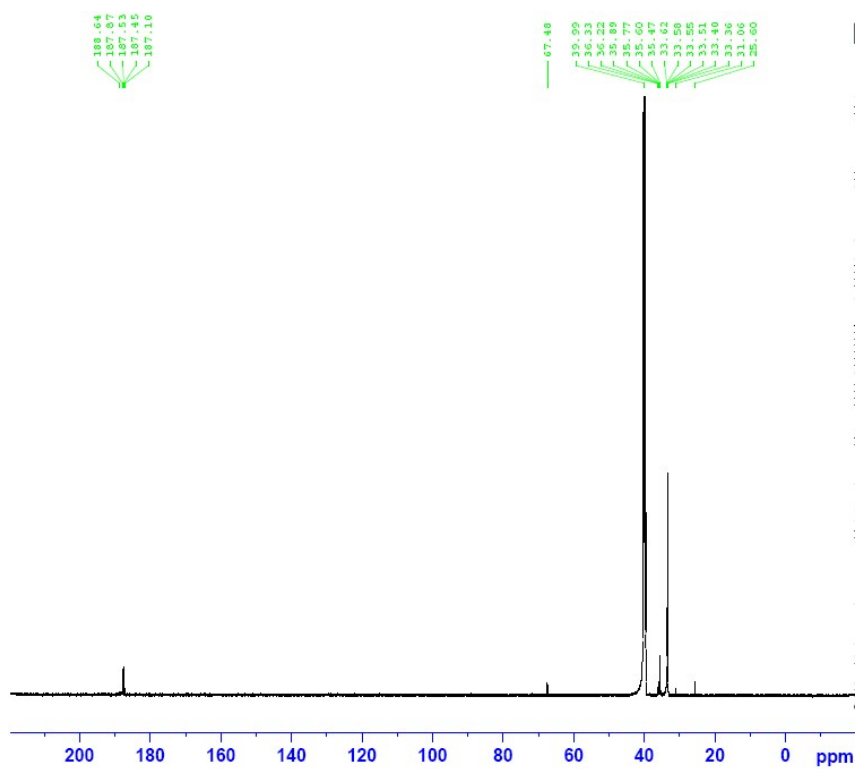


Fig. 21 The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **9** in $\text{DMSO}-d_6$

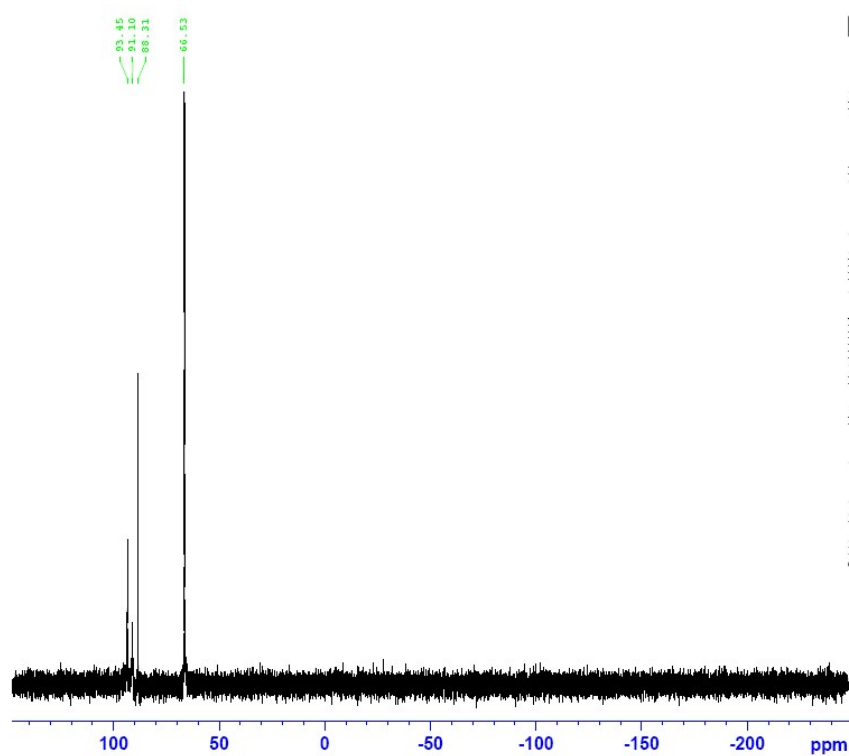


Fig. 22 The $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **10** in $\text{DMSO}-d_6$

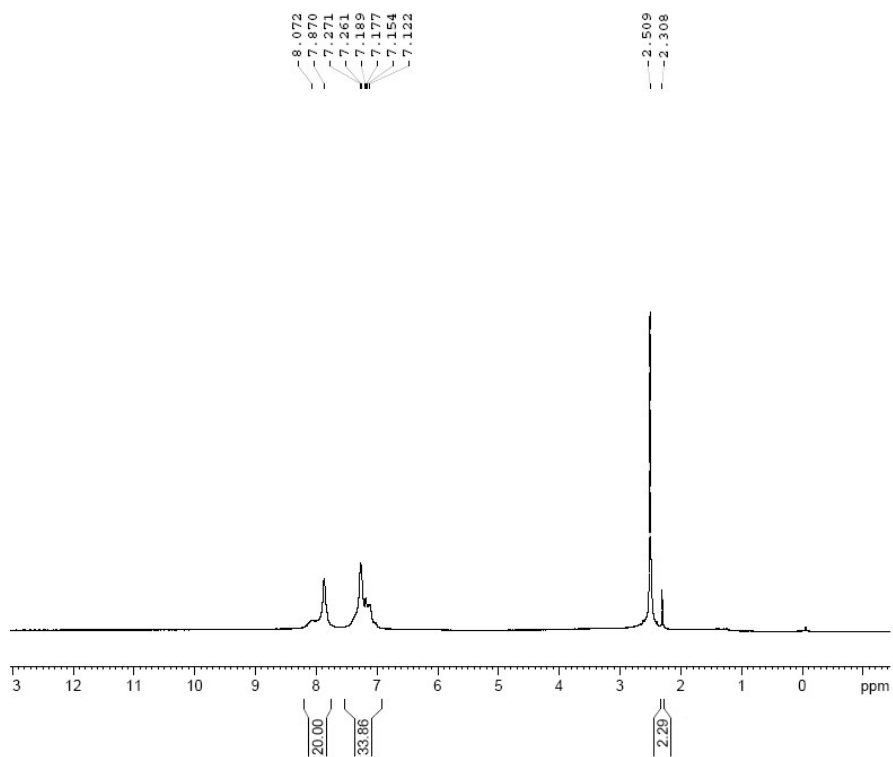


Fig. 23 The ^1H NMR spectrum of compound **10** in $\text{DMSO}-d_6$

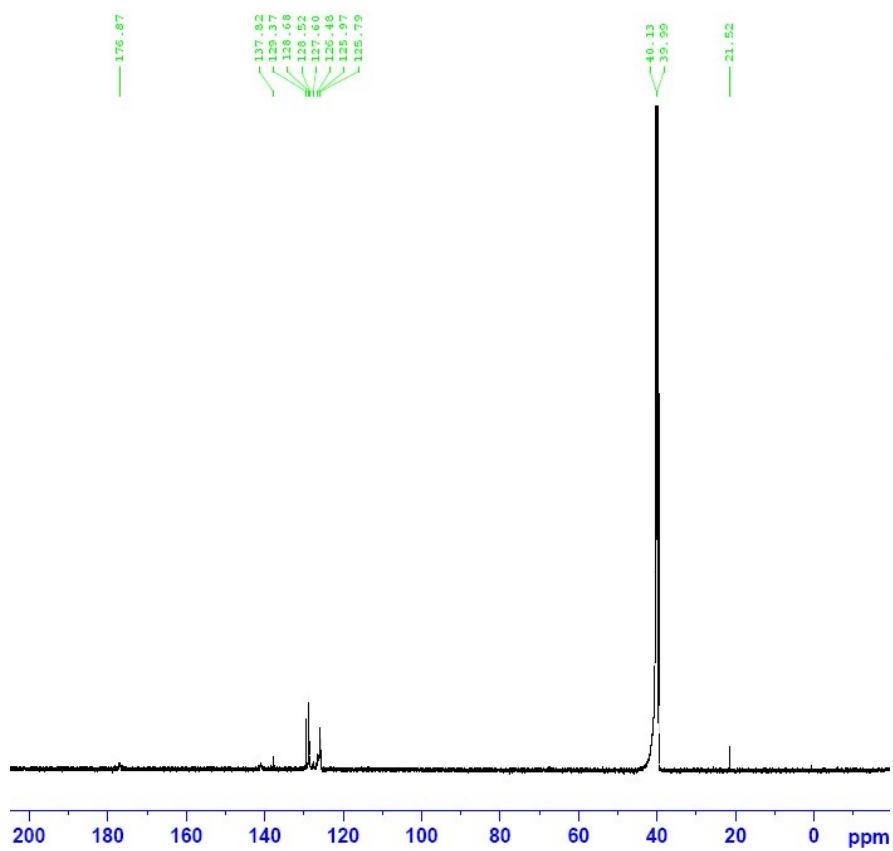


Fig. 24 The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **10** in $\text{DMSO}-d_6$

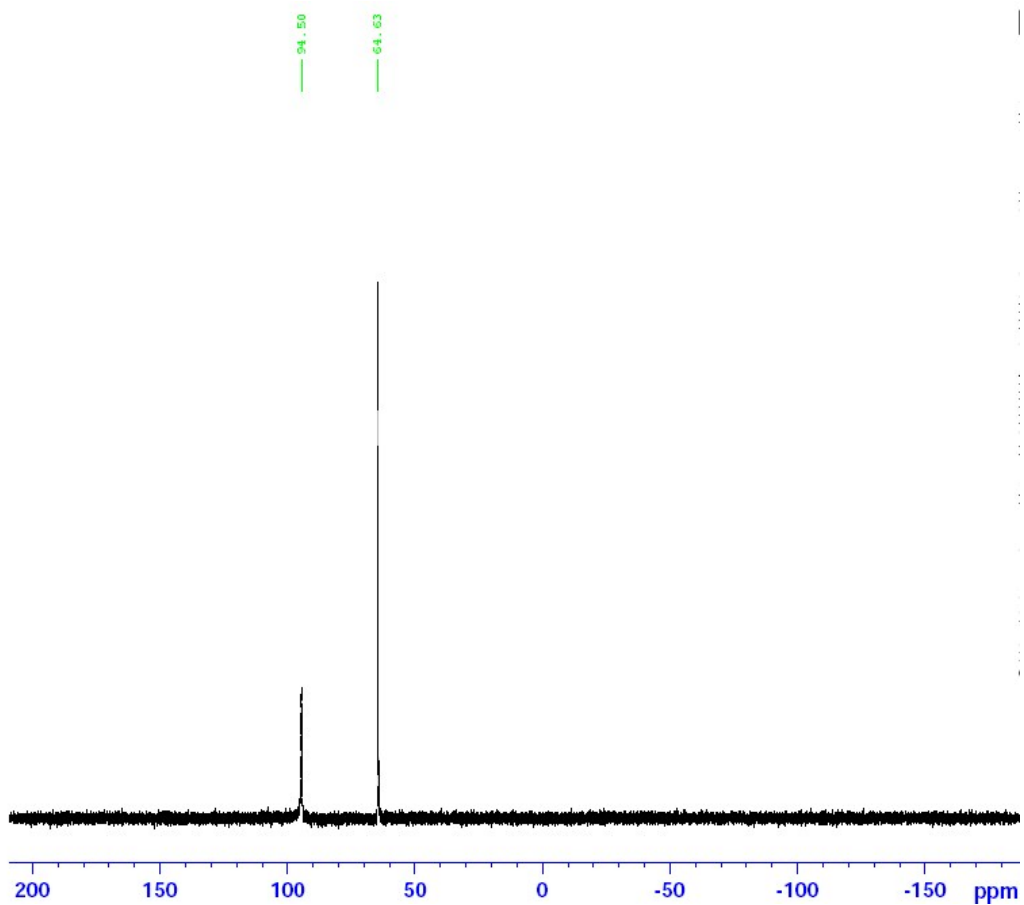


Fig. 25 The $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **11** in $\text{DMSO}-d_6$

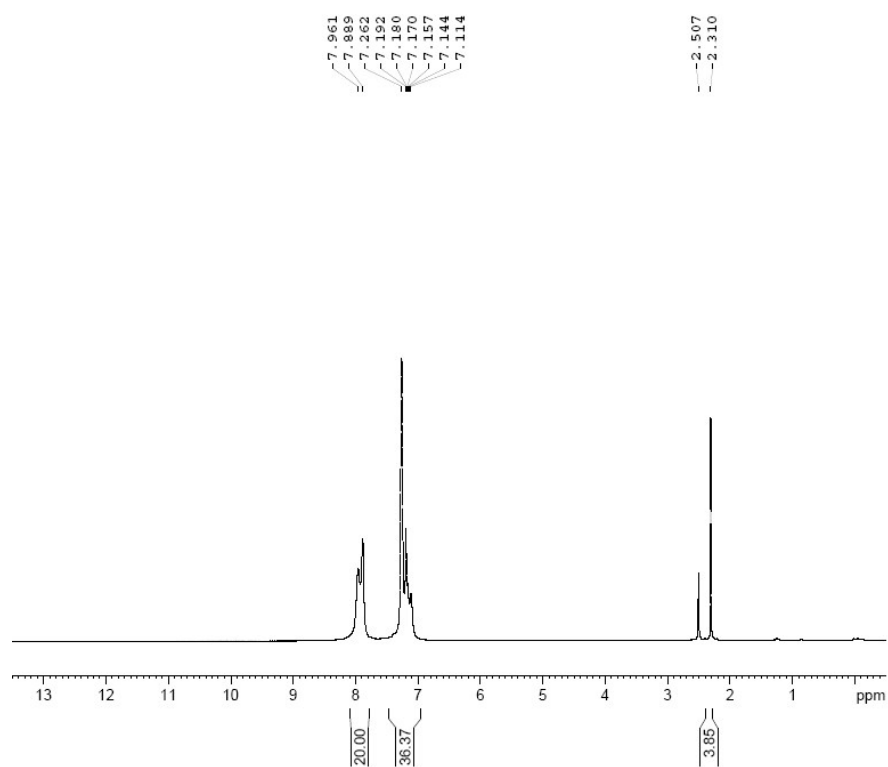


Fig. 26 The ^1H NMR spectrum of compound **11** in $\text{DMSO}-d_6$

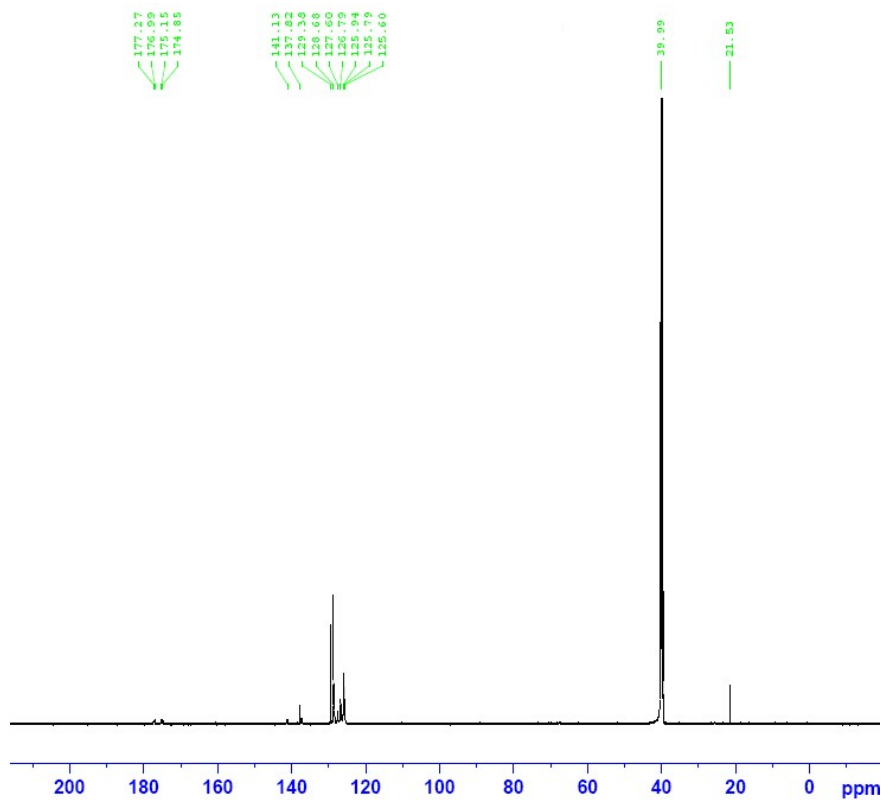


Fig. 27 The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **11** in $\text{DMSO-}d_6$

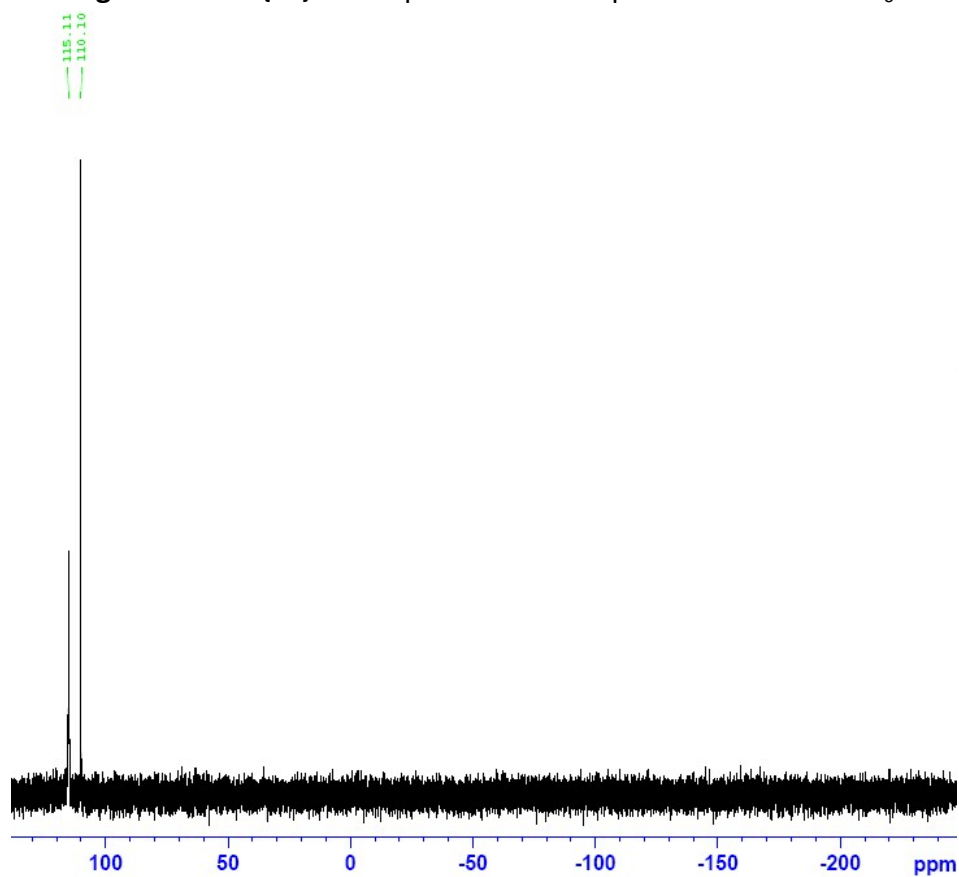


Fig. 28 The $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **12** in $\text{DMSO-}d_6$

2. The crystal structures of complexes 4–6

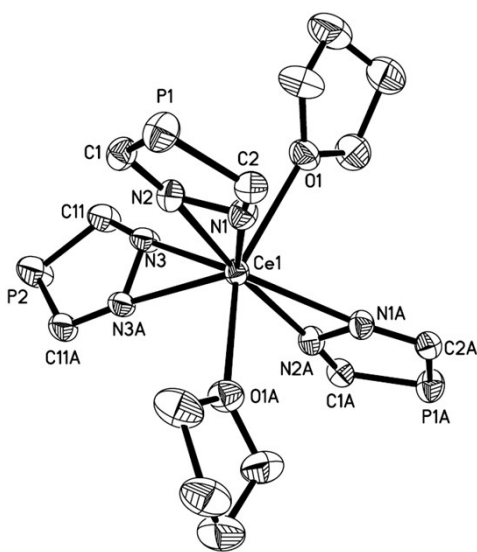


Fig. 1 The X-ray crystal structure of **4**. Drawn with ellipsoids at 30% probability, *t*Bu groups and hydrogen atoms omitted for clarity. Selected bond distances [Å] and angles (deg). Ce1–N2 2.480(3), Ce1–N3 2.504(3), Ce1–N1 2.531(3), Ce1–O1 2.532(3); N3–Ce1–N3A 32.08(14), N2–Ce1–N1 31.81(10), N2A–Ce1–N2 171.66(14), N2A–Ce1–N3 94.59(11), N2A–Ce1–N1 139.88(11), N2–Ce1–N(3) 93.42(11), N2–Ce1–O1A 91.25(10), O1A–Ce1–O1 149.88(15).

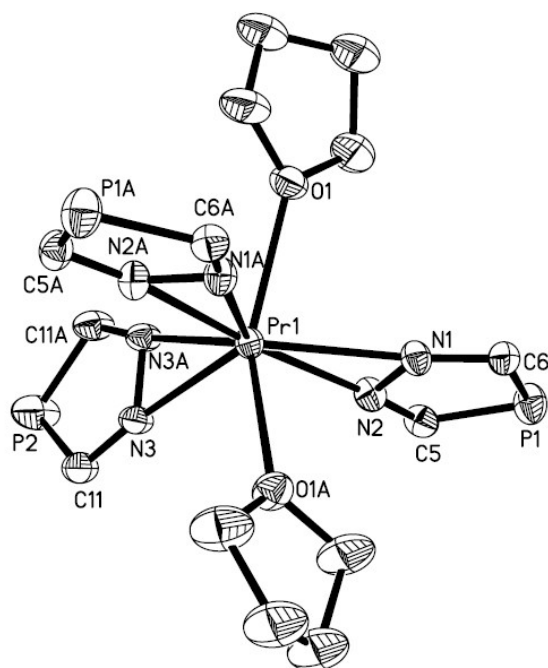


Fig. 2 The X-ray crystal structure of **5**. Drawn with ellipsoids at 30% probability, *t*Bu groups and hydrogen atoms omitted for clarity. Selected bond distances [Å] and angles (deg). Pr(1)-N(2) 2.463(3), Pr(1)-N(3) 2.479(3), Pr(1)-N(1) 2.506(3), Pr(1)-O(1) 2.508(3); N(2)-Pr(1)-N(2A) 171.87(14), N(2)-Pr(1)-N(3) 93.51(11), N(3)-Pr(1)-N(3A) 32.09(14), N(2)-Pr(1)-N(1) 32.07(9), N(2A)-Pr(1)-N(1A) 32.07(9), N(1)-Pr(1)-N(1A) 108.07(14), O(1)-Pr(1)-O(1A) 149.86(14).

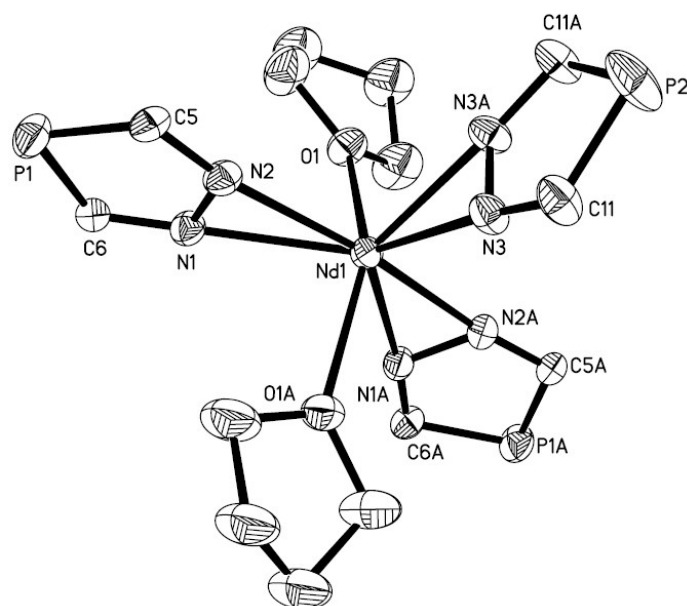


Fig. 3 The X-ray crystal structure of **6**. Drawn with ellipsoids at 30% probability, *t*Bu groups and hydrogen atoms omitted for clarity. Selected bond distances [Å] and angles (deg). Nd(1)-N(2) 2.448(4), Nd(1)-N(3) 2.469(4), Nd(1)-O(1) 2.487(3), Nd(1)-N(1) 2.491(4); N(2A)-Nd(1)-N(2) 171.84(18), N(2A)-Nd(1)-N(3) 94.22(13), N(3)-Nd(1)-N(3A) 32.43(16), O(1)-Nd(1)-O(1A) 150.06(18), N(2)-Nd(1)-N(1) 32.36(11), N(2A)-Nd(1)-N(1A) 32.36(11).

3. Crystal and Data Collection Parameters of Complexes 3-12

Table 1 Crystal and Data Collection Parameters of Complexes 3-7

Compounds	3	4	5	6	7-toluene
formula	C ₃₈ H ₇₀ LaN ₆ O ₂ P ₃	C ₃₈ H ₇₀ CeN ₆ O ₂ P ₃	C ₃₈ H ₇₀ PrN ₆ O ₂ P ₃	C ₃₈ H ₇₀ NdO ₂ P ₃	C ₆₁ H ₆₂ N ₆ O ₃ P ₃ Pr
fw	874.82	876.03	876.82	880.15	1160.99
Cryst. size (mm)	0.30×0.23×0.10	0.211×0.155×0.123	0.34×0.22×0.06	0.26×0.21×0.14	0.26×0.21×0.14
Cryst. syst.	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic
Space group	C2/c	C2/c	C2/c	C2/c	P-1
a (Å)	18.7069(5)	18.7512(14)	18.7219(9)	18.6636(8)	14.3728(3)
b (Å)	12.8790(3)	12.8964(7)	12.8523(5)	12.8610(6)	14.5000(4)
c (Å)	20.3131(5)	20.2950(11)	20.2486(8)	20.2165(8)	16.1044(4)
α (deg)	90	90	90	90	104.834(2)
β (deg)	102.571(2)	102.538(6)	102.503(5)	102.553(4)	110.391(2)
γ (deg)	90	90	90	90	93.413(2)
V (Å ³)	4776.6(2)	4790.7(5)	4756.7(3)	4736.6(4)	2999.83(13)
Z	4	4	4	4	2
D _c (g cm ⁻³)	1.216	1.215	1.224	1.234	1.285
Absor coeff (mm ⁻¹)	1.029	1.085	1.160	1.232	0.939
F (000)	1832	1836	1840	1844	1196
T (K)	298(2)	293(2)	298(2)	298(2)	298(2)
range (deg)	3.16–25.68	2.99–25.99	2.69–25.67	3.00–25.68	2.85–25.68
reflins measured	9962	10593	10431	10605	58336
unique reflins	4531	4699	4512	4499	11407
R _{int}	0.0210	0.0332	0.0331	0.0464	0.0459
min and Max	0.87734 and	0.5778 and 1.0000	0.9337 and	0.60938 and	0.67553 and
Transmn	1.0000		0.6938	1.0000	1.00000
R1, wR2 [<i>I</i> > 2σ(<i>I</i>)] ^a	0.0331, 0.0799	0.0414, 0.0982	0.0402, 0.0942	0.0466, 0.1105	0.0428, 0.1249
R1, wR2 (all data) ^b	0.0386, 0.0837	0.0533, 0.1049	0.0495, 0.0992	0.0563, 0.1202	0.0571, 0.1353
GOF	1.051	1.047	1.040	1.060	1.058
Δ(max) (eÅ ⁻³)	0.622	0.579	0.992	1.193	0.952
Δ(min) (eÅ ⁻³)	–0.521	–0.611	–0.488	–1.031	–0.790

^a R1 = $\sum |F_o| - |F_c| / \sum |F_o|$. ^b wR2 = $[\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{0.5}$.

Table 2 Crystal and Data Collection Parameters of Complexes **8–12**

Compounds	8	9	10	11-toluene	12
formula	C ₈₀ H ₈₈ KN ₈ O ₆ P ₄ Sm	C ₆₄ H ₁₂₀ KN ₈ O ₆ P ₄ Sm	C ₇₇ H ₅₈ K ₂ La N ₁₀ P ₅	C ₈₄ H ₆₆ K ₂ N ₁₀ P ₅ Sm	C ₅₆ H ₁₀₄ Cl ₂ N ₈ O ₄ P ₄ Pr ₂
fw	1570.91	1411.01	1495.29	1598.87	1430.07
Cryst. size (mm)	0.26×0.22×0.10	0.15×0.09 ×0.04	0.31 ×0.26×0.12	0.28×0.24×0.14	0.21× 0.09 ×0.06
Cryst. Syst.	Monoclinic	Monoclinic	Orthorhombic	Orthorhombic	Triclinic
Space group	<i>P</i> 121/ <i>n</i> 1	<i>C</i> 1 <i>c</i> 1	<i>P</i> 21 21 21	<i>P</i> 21 21 21	<i>P</i> -1
<i>a</i> (Å)	22.6746(10)	26.1247(9)	17.4889(6)	17.4551(2)	10.8923(10)
<i>b</i> (Å)	15.0764(5)	14.7156(4)	21.7538(6)	21.7027(3)	12.7350(12)
<i>c</i> (Å)	24.6405(11)	21.3571(7)	22.1728(8)	22.1513(3)	14.5804(9)
α (deg)	90	90	90	90	105.787(7)
β (deg)	106.253(5)	109.538(4)	90	90	104.523(7)
γ (deg)	90	90	90	90	108.687(8)
<i>V</i> (Å ³)	8086.7(6)	7737.8(4)	8435.6(5)	8391.42(19)	1712.2(3)
<i>Z</i>	4	4	4	4	1
<i>D</i> _c (g cm ⁻³)	1.290	1.211	1.177	1.266	1.387
Absor coeff (mm ⁻¹)	0.911	7.339	0.743	0.942	1.623
<i>F</i> (000)	3252	2996	3040	3260	740
<i>T</i> (K)	298(2)	100.00(10)	293(2)	298(2)	110(14)
range (deg)	2.92–25.68	3.50–67.08	2.87–26.37	2.88 –25.68	2.95–25.12
reflins measured	46231	13791	45855	162085	12116
unique reflns	15329	8714	17166	15909	6107
<i>R</i> _{int}	0.0896	0.0510	0.0689	0.0542	0.0599
min and Max	0.20144 and	0.22779 and	0.45087 and	0.42094 and	0.87808 and
Transmn	1.0000	1.0000	1.0000	1.0000	1.00000
<i>R</i> 1, <i>wR</i> 2 [<i>I</i> > 2σ(<i>I</i>)] ^a	0.0778, 0.1627	0.0603, 0.1433	0.0865, 0.2091	0.044, 0.1253	0.0782, 0.1906
<i>R</i> 1, <i>wR</i> 2 (all data) ^b	0.1398, 0.1963	0.0738, 0.1548	0.1348, 0.2453	0.0601, 0.1372	0.1029, 0.2146
GOF	1.027	1.072	1.002	1.098	1.072
Δ(max) (eÅ ⁻³)	1.423	2.599	2.627	0.692	3.180
Δ(min) (eÅ ⁻³)	−0.799	−1.223	−1.285	−0.471	−1.477

^a *R*1 = $\sum |F_o| - |F_c| / \sum |F_o|$. ^b *wR*2 = $[\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{0.5}$.

4. Crystal structural analysis data for **3-12**

4.1 Crystal structural analysis data for **3**

Table 1. Crystal data and structure refinement for 140712-2.

Identification code	140712-2
Empirical formula	C ₃₈ H ₇₀ La N ₆ O ₂ P ₃
Formula weight	874.82
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 18.7069(5) Å alpha = 90 deg. b = 12.8790(3) Å beta = 102.571(2) deg. c = 20.3131(5) Å gamma = 90 deg.
Volume	4776.6(2) Å ³
Z, Calculated density	4, 1.216 Mg/m ³
Absorption coefficient	1.029 mm ⁻¹
F(000)	1832
Crystal size	0.30 x 0.23 x 0.10 mm
Theta range for data collection	3.16 to 25.68 deg.
Limiting indices	-22 ≤ h ≤ 22, -9 ≤ k ≤ 15, -24 ≤ l ≤ 24
Reflections collected / unique	9962 / 4531 [R(int) = 0.0210]
Completeness to theta = 25.68	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.87734
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4531 / 193 / 330
Goodness-of-fit on F ²	1.051
Final R indices [I > 2σ(I)]	R1 = 0.0331, wR2 = 0.0799
R indices (all data)	R1 = 0.0386, wR2 = 0.0837
Largest diff. peak and hole	0.622 and -0.521 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 140712-2.

$U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
C(4)	8656(2)	2262(3)	9055(2)	61(1)
C(5)	8927(2)	3330(3)	8900(2)	46(1)
C(6)	9255(2)	5099(3)	8709(2)	43(1)
C(7)	9385(2)	6254(3)	8631(2)	55(1)
C(8)	8869(3)	6649(3)	7993(3)	84(1)
C(9)	9230(3)	6849(3)	9241(3)	93(2)
C(10)	10177(3)	6445(3)	8596(3)	85(1)
C(11)	9430(2)	439(3)	7096(2)	57(1)
C(12)	8739(7)	303(7)	6536(6)	87(2)
C(13)	8490(5)	-824(7)	6490(6)	96(2)
C(14)	8131(5)	1023(8)	6645(6)	91(2)
C(15)	8884(5)	573(8)	5833(4)	103(2)
C(16)	11293(7)	3952(19)	9048(5)	93(4)
C(17)	12057(5)	4373(14)	9245(6)	101(3)
C(18)	12405(7)	3916(13)	8697(7)	98(3)
C(19)	11819(6)	4017(16)	8072(7)	92(4)
C(12')	8686(9)	244(9)	6660(7)	87(2)
C(13')	8323(6)	1249(9)	6369(7)	92(2)
C(14')	8775(6)	-485(10)	6097(6)	98(2)

C(15')	8166(5)	-250(9)	7075(5)	96(2)
C(16')	11188(6)	3810(20)	9043(4)	71(3)
C(17')	11985(5)	3741(14)	9401(5)	77(3)
C(18')	12438(7)	4037(15)	8908(6)	77(3)
C(19')	11889(5)	4113(17)	8248(6)	67(3)
La(1)	10000	3280(1)	7500	35(1)
N(1)	9470(1)	4429(2)	8293(1)	41(1)
N(2)	9287(2)	3419(2)	8406(1)	43(1)
N(3)	9672(1)	1394(2)	7269(1)	46(1)
O(1)	11173(1)	3791(2)	8326(1)	59(1)
P(1)	8802(1)	4510(1)	9280(1)	57(1)
P(2)	10000	-540(1)	7500	83(1)
C(1)	8213(6)	2340(7)	9598(5)	70(3)
C(2)	9185(6)	1399(7)	9016(7)	95(3)
C(3)	7961(5)	2054(8)	8498(4)	76(3)
C(1')	8544(10)	2222(10)	9777(5)	77(4)
C(3')	8251(10)	1749(11)	8402(5)	91(4)
C(2')	9345(5)	1593(9)	9309(8)	75(4)

Table 3. Bond lengths [Å] and angles [deg] for 140712-2.

C(4)-C(2)	1.502(7)
C(4)-C(1)	1.522(6)
C(4)-C(5)	1.522(5)
C(4)-C(1')	1.527(7)
C(4)-C(3')	1.527(7)
C(4)-C(2')	1.542(7)
C(4)-C(3)	1.551(6)
C(5)-N(2)	1.329(4)
C(5)-P(1)	1.743(3)
C(6)-N(1)	1.331(4)
C(6)-C(7)	1.520(5)
C(6)-P(1)	1.751(3)
C(7)-C(10)	1.519(6)
C(7)-C(8)	1.525(6)
C(7)-C(9)	1.537(5)
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-N(3)	1.331(4)
C(11)-C(12')	1.500(17)

C(11)-C(12)	1.536(15)
C(11)-P(2)	1.737(3)
C(12)-C(14)	1.520(9)
C(12)-C(13)	1.521(9)
C(12)-C(15)	1.549(9)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-O(1)	1.448(8)
C(16)-C(17)	1.500(9)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-C(18)	1.525(9)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(18)-C(19)	1.491(8)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(19)-O(1)	1.443(8)
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(12')-C(14')	1.516(9)
C(12')-C(13')	1.521(9)
C(12')-C(15')	1.554(9)

C(13')-H(13D)	0.9600
C(13')-H(13E)	0.9600
C(13')-H(13F)	0.9600
C(14')-H(14D)	0.9600
C(14')-H(14E)	0.9600
C(14')-H(14F)	0.9600
C(15')-H(15D)	0.9600
C(15')-H(15E)	0.9600
C(15')-H(15F)	0.9600
C(16')-O(1)	1.450(8)
C(16')-C(17')	1.511(9)
C(16')-H(16C)	0.9700
C(16')-H(16D)	0.9700
C(17')-C(18')	1.494(9)
C(17')-H(17C)	0.9700
C(17')-H(17D)	0.9700
C(18')-C(19')	1.503(8)
C(18')-H(18C)	0.9700
C(18')-H(18D)	0.9700
C(19')-O(1)	1.443(8)
C(19')-H(19C)	0.9700
C(19')-H(19D)	0.9700
La(1)-N(2)	2.503(3)
La(1)-N(2)#1	2.503(3)
La(1)-N(3)	2.524(3)
La(1)-N(3)#1	2.524(3)
La(1)-N(1)	2.541(2)
La(1)-N(1)#1	2.541(2)
La(1)-O(1)	2.543(2)
La(1)-O(1)#1	2.543(2)

N(1)-N(2)	1.377(3)
N(3)-N(3)#1	1.373(5)
P(2)-C(11)#1	1.737(3)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(2)-H(2A)	0.9600
C(2)-H(2B)	0.9600
C(2)-H(2C)	0.9600
C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600
C(3)-H(3C)	0.9600
C(1')-H(1'1)	0.9600
C(1')-H(1'2)	0.9600
C(1')-H(1'3)	0.9600
C(3')-H(3'1)	0.9600
C(3')-H(3'2)	0.9600
C(3')-H(3'3)	0.9600
C(2')-H(2'1)	0.9600
C(2')-H(2'2)	0.9600
C(2')-H(2'3)	0.9600
C(2)-C(4)-C(1)	123.8(7)
C(2)-C(4)-C(5)	113.9(5)
C(1)-C(4)-C(5)	110.5(4)
C(2)-C(4)-C(1')	104.8(10)
C(1)-C(4)-C(1')	25.2(5)
C(5)-C(4)-C(1')	110.5(6)
C(2)-C(4)-C(3')	80.9(7)
C(1)-C(4)-C(3')	114.3(10)

C(5)-C(4)-C(3')	109.6(6)
C(1')-C(4)-C(3')	132.3(9)
C(2)-C(4)-C(2')	24.8(5)
C(1)-C(4)-C(2')	109.9(8)
C(5)-C(4)-C(2')	106.4(5)
C(1')-C(4)-C(2')	86.4(10)
C(3')-C(4)-C(2')	105.6(8)
C(2)-C(4)-C(3)	106.9(6)
C(1)-C(4)-C(3)	92.1(8)
C(5)-C(4)-C(3)	105.7(4)
C(1')-C(4)-C(3)	115.2(9)
C(3')-C(4)-C(3)	27.4(6)
C(2')-C(4)-C(3)	130.9(7)
N(2)-C(5)-C(4)	118.7(3)
N(2)-C(5)-P(1)	113.4(2)
C(4)-C(5)-P(1)	127.8(2)
N(1)-C(6)-C(7)	119.4(3)
N(1)-C(6)-P(1)	113.3(2)
C(7)-C(6)-P(1)	127.2(2)
C(10)-C(7)-C(6)	110.1(3)
C(10)-C(7)-C(8)	110.5(4)
C(6)-C(7)-C(8)	109.2(3)
C(10)-C(7)-C(9)	108.2(4)
C(6)-C(7)-C(9)	110.0(3)
C(8)-C(7)-C(9)	108.9(4)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5

H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(3)-C(11)-C(12')	122.0(5)
N(3)-C(11)-C(12)	119.0(4)
C(12')-C(11)-C(12)	11.3(7)
N(3)-C(11)-P(2)	114.0(2)
C(12')-C(11)-P(2)	123.5(5)
C(12)-C(11)-P(2)	126.8(4)
C(14)-C(12)-C(13)	111.3(10)
C(14)-C(12)-C(11)	110.9(8)
C(13)-C(12)-C(11)	110.5(8)
C(14)-C(12)-C(15)	106.6(10)
C(13)-C(12)-C(15)	105.7(10)
C(11)-C(12)-C(15)	111.7(8)
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5

H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(12)-C(15)-H(15A)	109.5
C(12)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(12)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
O(1)-C(16)-C(17)	104.5(8)
O(1)-C(16)-H(16A)	110.9
C(17)-C(16)-H(16A)	110.9
O(1)-C(16)-H(16B)	110.9
C(17)-C(16)-H(16B)	110.9
H(16A)-C(16)-H(16B)	108.9
C(16)-C(17)-C(18)	101.5(10)
C(16)-C(17)-H(17A)	111.5
C(18)-C(17)-H(17A)	111.5
C(16)-C(17)-H(17B)	111.5
C(18)-C(17)-H(17B)	111.5
H(17A)-C(17)-H(17B)	109.3
C(19)-C(18)-C(17)	103.7(9)
C(19)-C(18)-H(18A)	111.0
C(17)-C(18)-H(18A)	111.0
C(19)-C(18)-H(18B)	111.0
C(17)-C(18)-H(18B)	111.0

H(18A)-C(18)-H(18B)	109.0
O(1)-C(19)-C(18)	101.2(9)
O(1)-C(19)-H(19A)	111.5
C(18)-C(19)-H(19A)	111.5
O(1)-C(19)-H(19B)	111.5
C(18)-C(19)-H(19B)	111.5
H(19A)-C(19)-H(19B)	109.3
C(11)-C(12')-C(14')	108.0(9)
C(11)-C(12')-C(13')	111.4(10)
C(14')-C(12')-C(13')	110.3(11)
C(11)-C(12')-C(15')	111.0(9)
C(14')-C(12')-C(15')	109.9(11)
C(13')-C(12')-C(15')	106.3(11)
C(12')-C(13')-H(13D)	109.5
C(12')-C(13')-H(13E)	109.5
H(13D)-C(13')-H(13E)	109.5
C(12')-C(13')-H(13F)	109.5
H(13D)-C(13')-H(13F)	109.5
H(13E)-C(13')-H(13F)	109.5
C(12')-C(14')-H(14D)	109.5
C(12')-C(14')-H(14E)	109.5
H(14D)-C(14')-H(14E)	109.5
C(12')-C(14')-H(14F)	109.5
H(14D)-C(14')-H(14F)	109.5
H(14E)-C(14')-H(14F)	109.5
C(12')-C(15')-H(15D)	109.5
C(12')-C(15')-H(15E)	109.5
H(15D)-C(15')-H(15E)	109.5
C(12')-C(15')-H(15F)	109.5
H(15D)-C(15')-H(15F)	109.5

H(15E)-C(15')-H(15F)	109.5
O(1)-C(16')-C(17')	106.4(8)
O(1)-C(16')-H(16C)	110.4
C(17')-C(16')-H(16C)	110.4
O(1)-C(16')-H(16D)	110.4
C(17')-C(16')-H(16D)	110.4
H(16C)-C(16')-H(16D)	108.6
C(18')-C(17')-C(16')	107.9(9)
C(18')-C(17')-H(17C)	110.1
C(16')-C(17')-H(17C)	110.1
C(18')-C(17')-H(17D)	110.1
C(16')-C(17')-H(17D)	110.1
H(17C)-C(17')-H(17D)	108.4
C(17')-C(18')-C(19')	103.7(9)
C(17')-C(18')-H(18C)	111.0
C(19')-C(18')-H(18C)	111.0
C(17')-C(18')-H(18D)	111.0
C(19')-C(18')-H(18D)	111.0
H(18C)-C(18')-H(18D)	109.0
O(1)-C(19')-C(18')	110.7(8)
O(1)-C(19')-H(19C)	109.5
C(18')-C(19')-H(19C)	109.5
O(1)-C(19')-H(19D)	109.5
C(18')-C(19')-H(19D)	109.5
H(19C)-C(19')-H(19D)	108.1
N(2)-La(1)-N(2)#1	171.77(11)
N(2)-La(1)-N(3)	93.35(9)
N(2)#1-La(1)-N(3)	94.57(9)
N(2)-La(1)-N(3)#1	94.57(9)
N(2)#1-La(1)-N(3)#1	93.35(9)

N(3)-La(1)-N(3)#1	31.57(11)
N(2)-La(1)-N(1)	31.66(8)
N(2)#1-La(1)-N(1)	140.14(8)
N(3)-La(1)-N(1)	124.42(9)
N(3)#1-La(1)-N(1)	123.73(9)
N(2)-La(1)-N(1)#1	140.14(8)
N(2)#1-La(1)-N(1)#1	31.66(8)
N(3)-La(1)-N(1)#1	123.73(9)
N(3)#1-La(1)-N(1)#1	124.42(9)
N(1)-La(1)-N(1)#1	108.78(11)
N(2)-La(1)-O(1)	91.02(8)
N(2)#1-La(1)-O(1)	86.85(8)
N(3)-La(1)-O(1)	120.79(8)
N(3)#1-La(1)-O(1)	89.23(8)
N(1)-La(1)-O(1)	80.24(8)
N(1)#1-La(1)-O(1)	82.41(8)
N(2)-La(1)-O(1)#1	86.85(8)
N(2)#1-La(1)-O(1)#1	91.02(8)
N(3)-La(1)-O(1)#1	89.23(8)
N(3)#1-La(1)-O(1)#1	120.79(8)
N(1)-La(1)-O(1)#1	82.41(8)
N(1)#1-La(1)-O(1)#1	80.24(8)
O(1)-La(1)-O(1)#1	149.98(12)
C(6)-N(1)-N(2)	112.7(2)
C(6)-N(1)-La(1)	173.7(2)
N(2)-N(1)-La(1)	72.63(15)
C(5)-N(2)-N(1)	113.1(3)
C(5)-N(2)-La(1)	170.8(2)
N(1)-N(2)-La(1)	75.71(15)
C(11)-N(3)-N(3)#1	112.48(18)

C(11)-N(3)-La(1)	173.3(2)
N(3)#1-N(3)-La(1)	74.22(6)
C(19)-O(1)-C(19')	15.0(9)
C(19)-O(1)-C(16)	112.2(7)
C(19')-O(1)-C(16)	97.3(7)
C(19)-O(1)-C(16')	121.5(8)
C(19')-O(1)-C(16')	106.9(7)
C(16)-O(1)-C(16')	10.6(13)
C(19)-O(1)-La(1)	119.0(6)
C(19')-O(1)-La(1)	133.7(5)
C(16)-O(1)-La(1)	128.7(5)
C(16')-O(1)-La(1)	119.4(5)
C(5)-P(1)-C(6)	87.35(15)
C(11)#1-P(2)-C(11)	86.9(2)
C(4)-C(1)-H(1A)	109.5
C(4)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(4)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(4)-C(2)-H(2A)	109.5
C(4)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(4)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(4)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(4)-C(3)-H(3C)	109.5

H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(4)-C(1')-H(1'1)	109.5
C(4)-C(1')-H(1'2)	109.5
H(1'1)-C(1')-H(1'2)	109.5
C(4)-C(1')-H(1'3)	109.5
H(1'1)-C(1')-H(1'3)	109.5
H(1'2)-C(1')-H(1'3)	109.5
C(4)-C(3')-H(3'1)	109.5
C(4)-C(3')-H(3'2)	109.5
H(3'1)-C(3')-H(3'2)	109.5
C(4)-C(3')-H(3'3)	109.5
H(3'1)-C(3')-H(3'3)	109.5
H(3'2)-C(3')-H(3'3)	109.5
C(4)-C(2')-H(2'1)	109.5
C(4)-C(2')-H(2'2)	109.5
H(2'1)-C(2')-H(2'2)	109.5
C(4)-C(2')-H(2'3)	109.5
H(2'1)-C(2')-H(2'3)	109.5
H(2'2)-C(2')-H(2'3)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y,-z+3/2

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 140712-2.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
C(4)	78(2)	51(2)	61(2)	1(2)	32(2)	-15(2)
C(5)	52(2)	49(2)	39(2)	2(1)	13(1)	-6(2)
C(6)	45(2)	41(2)	43(2)	-2(1)	9(1)	0(1)
C(7)	67(2)	41(2)	60(2)	-9(2)	21(2)	-1(2)
C(8)	102(4)	54(3)	92(3)	20(2)	11(3)	5(2)
C(9)	146(5)	49(3)	94(3)	-20(2)	50(3)	-1(3)
C(10)	83(3)	53(2)	124(4)	-8(3)	33(3)	-18(2)
C(11)	47(2)	35(2)	82(2)	-11(2)	0(2)	0(1)
C(12)	64(3)	71(3)	110(4)	-25(3)	-16(3)	-5(2)
C(13)	74(3)	76(3)	120(4)	-20(3)	-20(3)	-15(3)
C(14)	63(3)	79(3)	116(4)	-21(3)	-14(3)	1(3)
C(15)	82(4)	98(4)	111(4)	-21(4)	-20(3)	-8(3)
C(16)	78(6)	119(7)	74(6)	-37(5)	-2(5)	2(5)
C(17)	80(5)	121(6)	89(5)	-32(5)	-10(4)	-14(4)
C(18)	71(5)	116(6)	93(6)	-29(5)	-12(4)	-17(4)
C(19)	64(5)	113(7)	89(7)	-25(6)	-5(5)	-18(5)
C(12')	64(3)	69(3)	111(4)	-22(3)	-17(3)	-7(2)
C(13')	68(3)	75(4)	114(4)	-16(3)	-22(3)	-4(3)
C(14')	79(3)	84(3)	114(4)	-28(3)	-16(3)	-6(3)
C(15')	68(4)	85(4)	117(5)	-12(4)	-15(4)	-16(3)

C(16')	63(6)	98(7)	42(5)	-9(5)	-11(4)	6(5)
C(17')	65(5)	99(6)	55(4)	-6(4)	-14(3)	-7(4)
C(18')	57(4)	100(6)	61(5)	-6(5)	-17(4)	-19(4)
C(19')	41(5)	99(7)	52(5)	6(5)	-11(4)	-32(4)
La(1)	39(1)	29(1)	37(1)	0	9(1)	0
N(1)	50(1)	33(1)	44(1)	0(1)	17(1)	-5(1)
N(2)	54(2)	35(1)	42(1)	2(1)	18(1)	-6(1)
N(3)	39(1)	34(1)	59(2)	-4(1)	-3(1)	1(1)
O(1)	53(1)	66(2)	54(1)	-11(1)	6(1)	-9(1)
P(1)	70(1)	57(1)	50(1)	-5(1)	29(1)	-2(1)
P(2)	66(1)	31(1)	137(2)	0	-12(1)	0
C(1)	71(3)	73(3)	70(3)	6(2)	21(2)	-4(2)
C(2)	97(4)	92(4)	97(4)	4(2)	23(2)	-2(2)
C(3)	75(3)	71(3)	80(3)	1(2)	12(2)	-7(2)
C(1')	78(4)	78(4)	76(4)	3(2)	20(2)	-2(2)
C(3')	92(5)	90(5)	91(5)	-1(2)	21(2)	-6(2)
C(2')	78(4)	71(4)	76(4)	3(2)	19(2)	-3(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 140712-2.

	x	y	z	U(eq)
H(8A)	8971	7366	7926	126
H(8B)	8371	6578	8039	126
H(8C)	8939	6250	7613	126
H(9A)	9533	6579	9648	139
H(9B)	8724	6769	9257	139
H(9C)	9337	7572	9199	139
H(10A)	10300	6018	8250	127
H(10B)	10491	6275	9023	127
H(10C)	10240	7162	8495	127
H(13A)	8347	-1017	6899	144
H(13B)	8885	-1261	6426	144
H(13C)	8081	-905	6115	144
H(14A)	7736	1009	6255	136
H(14B)	8318	1718	6719	136
H(14C)	7957	796	7032	136
H(15A)	8457	410	5491	155
H(15B)	9293	176	5757	155
H(15C)	8991	1300	5815	155
H(16A)	11250	3303	9279	112
H(16B)	10942	4444	9154	112
H(17A)	12303	4135	9690	121

H(17B)	12060	5126	9236	121
H(18A)	12838	4303	8658	118
H(18B)	12537	3195	8790	118
H(19A)	11802	4712	7886	110
H(19B)	11884	3519	7731	110
H(13D)	8598	1548	6069	138
H(13E)	8309	1727	6729	138
H(13F)	7833	1107	6126	138
H(14D)	9120	-195	5861	147
H(14E)	8311	-575	5790	147
H(14F)	8951	-1145	6285	147
H(15D)	7692	-356	6787	144
H(15E)	8123	205	7438	144
H(15F)	8362	-906	7254	144
H(16C)	10917	3222	9165	85
H(16D)	10971	4443	9165	85
H(17C)	12082	4208	9784	92
H(17D)	12104	3040	9563	92
H(18C)	12804	3512	8888	93
H(18D)	12681	4698	9028	93
H(19C)	11866	4824	8087	81
H(19D)	12044	3677	7916	81
H(1A)	8064	1658	9705	106
H(1B)	7786	2760	9437	106
H(1C)	8507	2651	9995	106
H(2A)	9665	1590	9264	143
H(2B)	9200	1276	8553	143
H(2C)	9029	778	9206	143
H(3A)	8086	2064	8064	114
H(3B)	7603	2582	8514	114

H(3C)	7762	1387	8571	114
H(1'1)	8328	1569	9852	115
H(1'2)	8226	2778	9846	115
H(1'3)	9009	2294	10087	115
H(3'1)	8564	1733	8085	136
H(3'2)	7817	2140	8216	136
H(3'3)	8118	1053	8495	136
H(2'1)	9655	1927	9689	112
H(2'2)	9606	1513	8955	112
H(2'3)	9202	923	9443	112

Table 6. Torsion angles [deg] for 140712-2.

C(2)-C(4)-C(5)-N(2)	39.6(7)
C(1)-C(4)-C(5)-N(2)	-175.8(6)
C(1')-C(4)-C(5)-N(2)	157.2(8)
C(3')-C(4)-C(5)-N(2)	-48.9(9)
C(2')-C(4)-C(5)-N(2)	64.9(7)
C(3)-C(4)-C(5)-N(2)	-77.5(6)
C(2)-C(4)-C(5)-P(1)	-142.6(7)
C(1)-C(4)-C(5)-P(1)	2.0(6)
C(1')-C(4)-C(5)-P(1)	-25.0(8)
C(3')-C(4)-C(5)-P(1)	128.9(9)
C(2')-C(4)-C(5)-P(1)	-117.3(7)
C(3)-C(4)-C(5)-P(1)	100.3(6)
N(1)-C(6)-C(7)-C(10)	-50.0(4)
P(1)-C(6)-C(7)-C(10)	133.1(3)
N(1)-C(6)-C(7)-C(8)	71.5(4)
P(1)-C(6)-C(7)-C(8)	-105.5(4)
N(1)-C(6)-C(7)-C(9)	-169.1(3)
P(1)-C(6)-C(7)-C(9)	13.9(5)
N(3)-C(11)-C(12)-C(14)	-47.4(10)
C(12')-C(11)-C(12)-C(14)	61(3)
P(2)-C(11)-C(12)-C(14)	138.6(7)
N(3)-C(11)-C(12)-C(13)	-171.3(7)
C(12')-C(11)-C(12)-C(13)	-63(3)
P(2)-C(11)-C(12)-C(13)	14.7(11)
N(3)-C(11)-C(12)-C(15)	71.3(8)
C(12')-C(11)-C(12)-C(15)	-180(4)

P(2)-C(11)-C(12)-C(15)	-102.7(7)
O(1)-C(16)-C(17)-C(18)	-26.7(18)
C(16)-C(17)-C(18)-C(19)	40.5(16)
C(17)-C(18)-C(19)-O(1)	-37.8(14)
N(3)-C(11)-C(12')-C(14')	130.1(8)
C(12)-C(11)-C(12')-C(14')	52(3)
P(2)-C(11)-C(12')-C(14')	-58.0(10)
N(3)-C(11)-C(12')-C(13')	8.9(12)
C(12)-C(11)-C(12')-C(13')	-69(3)
P(2)-C(11)-C(12')-C(13')	-179.2(8)
N(3)-C(11)-C(12')-C(15')	-109.3(8)
C(12)-C(11)-C(12')-C(15')	173(4)
P(2)-C(11)-C(12')-C(15')	62.5(9)
O(1)-C(16')-C(17')-C(18')	18(2)
C(16')-C(17')-C(18')-C(19')	-8.1(19)
C(17')-C(18')-C(19')-O(1)	-5.1(17)
C(7)-C(6)-N(1)-N(2)	-177.3(3)
P(1)-C(6)-N(1)-N(2)	0.1(3)
C(7)-C(6)-N(1)-La(1)	35(2)
P(1)-C(6)-N(1)-La(1)	-147.6(18)
N(2)-La(1)-N(1)-C(6)	149(2)
N(2)#1-La(1)-N(1)-C(6)	-32(2)
N(3)-La(1)-N(1)-C(6)	161.4(19)
N(3)#1-La(1)-N(1)-C(6)	123.1(19)
N(1)#1-La(1)-N(1)-C(6)	-37.8(19)
O(1)-La(1)-N(1)-C(6)	40.6(19)
O(1)#1-La(1)-N(1)-C(6)	-115(2)
N(2)#1-La(1)-N(1)-N(2)	178.78(4)
N(3)-La(1)-N(1)-N(2)	12.53(19)
N(3)#1-La(1)-N(1)-N(2)	-25.80(19)

N(1)#1-La(1)-N(1)-N(2)	173.29(18)
O(1)-La(1)-N(1)-N(2)	-108.25(17)
O(1)#1-La(1)-N(1)-N(2)	96.35(17)
C(4)-C(5)-N(2)-N(1)	176.9(3)
P(1)-C(5)-N(2)-N(1)	-1.2(4)
C(4)-C(5)-N(2)-La(1)	-20.1(16)
P(1)-C(5)-N(2)-La(1)	161.8(12)
C(6)-N(1)-N(2)-C(5)	0.7(4)
La(1)-N(1)-N(2)-C(5)	177.2(3)
C(6)-N(1)-N(2)-La(1)	-176.5(2)
N(2)#1-La(1)-N(2)-C(5)	-169.3(14)
N(3)-La(1)-N(2)-C(5)	26.5(14)
N(3)#1-La(1)-N(2)-C(5)	-5.1(14)
N(1)-La(1)-N(2)-C(5)	-163.9(15)
N(1)#1-La(1)-N(2)-C(5)	-173.8(13)
O(1)-La(1)-N(2)-C(5)	-94.4(14)
O(1)#1-La(1)-N(2)-C(5)	115.5(14)
N(2)#1-La(1)-N(2)-N(1)	-5.47(15)
N(3)-La(1)-N(2)-N(1)	-169.67(16)
N(3)#1-La(1)-N(2)-N(1)	158.71(16)
N(1)#1-La(1)-N(2)-N(1)	-9.9(3)
O(1)-La(1)-N(2)-N(1)	69.40(16)
O(1)#1-La(1)-N(2)-N(1)	-80.63(16)
C(12')-C(11)-N(3)-N(3)#1	173.0(6)
C(12)-C(11)-N(3)-N(3)#1	-174.3(5)
P(2)-C(11)-N(3)-N(3)#1	0.4(5)
C(12')-C(11)-N(3)-La(1)	-9(3)
C(12)-C(11)-N(3)-La(1)	4(3)
P(2)-C(11)-N(3)-La(1)	178(100)
N(2)-La(1)-N(3)-C(11)	89(2)

N(2)#1-La(1)-N(3)-C(11)	-89(2)
N(3)#1-La(1)-N(3)-C(11)	-178(100)
N(1)-La(1)-N(3)-C(11)	82(2)
N(1)#1-La(1)-N(3)-C(11)	-76(2)
O(1)-La(1)-N(3)-C(11)	-178(100)
O(1)#1-La(1)-N(3)-C(11)	2(2)
N(2)-La(1)-N(3)-N(3)#1	-93.3(2)
N(2)#1-La(1)-N(3)-N(3)#1	89.0(2)
N(1)-La(1)-N(3)-N(3)#1	-99.8(2)
N(1)#1-La(1)-N(3)-N(3)#1	102.2(2)
O(1)-La(1)-N(3)-N(3)#1	-0.1(3)
O(1)#1-La(1)-N(3)-N(3)#1	179.9(2)
C(18)-C(19)-O(1)-C(19')	29(6)
C(18)-C(19)-O(1)-C(16)	21.5(16)
C(18)-C(19)-O(1)-C(16')	15.7(19)
C(18)-C(19)-O(1)-La(1)	-161.6(7)
C(18')-C(19')-O(1)-C(19)	-151(7)
C(18')-C(19')-O(1)-C(16)	21.6(17)
C(18')-C(19')-O(1)-C(16')	16.8(17)
C(18')-C(19')-O(1)-La(1)	-164.3(8)
C(17)-C(16)-O(1)-C(19)	3.7(19)
C(17)-C(16)-O(1)-C(19')	1.7(19)
C(17)-C(16)-O(1)-C(16')	156(10)
C(17)-C(16)-O(1)-La(1)	-172.8(8)
C(17')-C(16')-O(1)-C(19)	-18(2)
C(17')-C(16')-O(1)-C(19')	-21.3(19)
C(17')-C(16')-O(1)-C(16)	-48(8)
C(17')-C(16')-O(1)-La(1)	159.6(10)
N(2)-La(1)-O(1)-C(19)	-170.3(10)
N(2)#1-La(1)-O(1)-C(19)	1.7(10)

N(3)-La(1)-O(1)-C(19)	95.2(10)
N(3)#1-La(1)-O(1)-C(19)	95.1(10)
N(1)-La(1)-O(1)-C(19)	-140.4(10)
N(1)#1-La(1)-O(1)-C(19)	-29.8(10)
O(1)#1-La(1)-O(1)-C(19)	-84.8(10)
N(2)-La(1)-O(1)-C(19')	-166.5(13)
N(2)#1-La(1)-O(1)-C(19')	5.5(12)
N(3)-La(1)-O(1)-C(19')	99.0(13)
N(3)#1-La(1)-O(1)-C(19')	98.9(13)
N(1)-La(1)-O(1)-C(19')	-136.6(13)
N(1)#1-La(1)-O(1)-C(19')	-26.0(12)
O(1)#1-La(1)-O(1)-C(19')	-81.0(12)
N(2)-La(1)-O(1)-C(16)	6.0(13)
N(2)#1-La(1)-O(1)-C(16)	178.0(13)
N(3)-La(1)-O(1)-C(16)	-88.5(13)
N(3)#1-La(1)-O(1)-C(16)	-88.6(13)
N(1)-La(1)-O(1)-C(16)	35.9(13)
N(1)#1-La(1)-O(1)-C(16)	146.5(13)
O(1)#1-La(1)-O(1)-C(16)	91.4(13)
N(2)-La(1)-O(1)-C(16')	12.3(11)
N(2)#1-La(1)-O(1)-C(16')	-175.6(11)
N(3)-La(1)-O(1)-C(16')	-82.2(11)
N(3)#1-La(1)-O(1)-C(16')	-82.2(11)
N(1)-La(1)-O(1)-C(16')	42.2(11)
N(1)#1-La(1)-O(1)-C(16')	152.9(11)
O(1)#1-La(1)-O(1)-C(16')	97.8(11)
N(2)-C(5)-P(1)-C(6)	1.0(3)
C(4)-C(5)-P(1)-C(6)	-176.9(3)
N(1)-C(6)-P(1)-C(5)	-0.6(2)
C(7)-C(6)-P(1)-C(5)	176.5(3)

N(3)-C(11)-P(2)-C(11)#1	-0.15(18)
C(12')-C(11)-P(2)-C(11)#1	-172.6(7)
C(12)-C(11)-P(2)-C(11)#1	174.1(6)

Symmetry transformations used to generate equivalent atoms:

#1 $-x+2, y, -z+3/2$

4.2 Crystal structural analysis data for **4**

Table 1. Crystal data and structure refinement for 140426-1.

Identification code	140426-1
Empirical formula	C ₃₈ H ₇₀ Ce N ₆ O ₂ P ₃
Formula weight	876.03
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, C 2/c
Unit cell dimensions	a = 18.7512(14) Å alpha = 90 deg. b = 12.8964(7) Å beta = 102.538(6) deg. c = 20.2950(11) Å gamma = 90 deg.
Volume	4790.7(5) Å ³
Z, Calculated density	4, 1.215 Mg/m ³
Absorption coefficient	1.085 mm ⁻¹
F(000)	1836
Crystal size	0.211 x 0.155 x 0.123 mm
Theta range for data collection	2.99 to 25.99 deg.
Limiting indices	-23 ≤ h ≤ 13, -14 ≤ k ≤ 15, -25 ≤ l ≤ 24
Reflections collected / unique	10593 / 4699 [R(int) = 0.0332]
Completeness to theta = 25.99	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.57788
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4699 / 83 / 275
Goodness-of-fit on F ²	1.047
Final R indices [I > 2σ(I)]	R1 = 0.0414, wR2 = 0.0982
R indices (all data)	R1 = 0.0533, wR2 = 0.1049
Largest diff. peak and hole	0.579 and -0.611 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 140426-1.

U(eq) is defined as one third of the trace of the orthogonalized

Uij tensor.

	x	y	z	U(eq)
Ce(1)	10000	3284(1)	7500	37(1)
P(1)	8804(1)	4509(1)	9274(1)	59(1)
P(2)	10000	-520(1)	7500	85(1)
N(1)	9472(2)	4432(3)	8286(2)	44(1)
N(2)	9294(2)	3423(2)	8398(2)	45(1)
N(3)	9671(2)	1417(3)	7267(2)	48(1)
O(1)	8833(2)	3794(2)	6680(1)	58(1)
C(1)	8934(2)	3336(3)	8893(2)	47(1)
C(2)	9261(2)	5095(3)	8705(2)	45(1)
C(3)	8658(3)	2257(4)	9049(2)	62(1)
C(4)	8071(5)	1939(6)	8439(4)	159(4)
C(5)	9264(5)	1492(5)	9148(5)	146(4)
C(6)	8341(4)	2309(6)	9667(3)	124(3)
C(7)	9389(3)	6255(3)	8631(2)	55(1)
C(8)	9242(4)	6850(4)	9240(3)	94(2)
C(9)	8867(4)	6649(4)	7990(3)	84(2)
C(10)	10181(3)	6448(4)	8587(3)	87(2)
C(11)	9429(2)	463(3)	7095(2)	61(1)
C(12)	8711(3)	294(4)	6588(3)	79(2)
C(13)	8199(5)	1140(7)	6529(5)	95(3)

C(14)	8944(9)	183(15)	5870(7)	151(5)
C(15)	8410(9)	-786(11)	6628(9)	129(5)
C(13')	8154(7)	-122(14)	7058(7)	109(4)
C(14')	8752(9)	909(14)	5931(8)	156(5)
C(15')	8684(10)	-695(13)	6211(9)	127(5)
C(16)	8145(3)	4058(6)	6833(3)	91(2)
C(17)	7584(3)	3985(6)	6203(3)	101(2)
C(18)	7995(6)	4385(11)	5744(6)	96(2)
C(18')	7982(6)	3756(12)	5624(6)	93(2)
C(19)	8767(3)	3878(5)	5959(2)	87(2)

Table 3. Bond lengths [Å] and angles [deg] for 140426-1.

Ce(1)-N(2)#1	2.480(3)
Ce(1)-N(2)	2.480(3)
Ce(1)-N(3)	2.504(3)
Ce(1)-N(3)#1	2.504(3)
Ce(1)-N(1)#1	2.531(3)
Ce(1)-N(1)	2.531(3)
Ce(1)-O(1)#1	2.532(3)
Ce(1)-O(1)	2.532(3)
P(1)-C(1)	1.740(4)
P(1)-C(2)	1.752(4)
P(2)-C(11)#1	1.745(5)
P(2)-C(11)	1.745(5)
N(1)-C(2)	1.324(5)
N(1)-N(2)	1.374(4)
N(2)-C(1)	1.332(5)
N(3)-C(11)	1.332(5)
N(3)-N(3)#1	1.384(6)
O(1)-C(16)	1.431(6)
O(1)-C(19)	1.447(5)
C(1)-C(3)	1.541(6)
C(2)-C(7)	1.528(6)
C(3)-C(5)	1.487(9)
C(3)-C(6)	1.501(7)
C(3)-C(4)	1.524(8)
C(4)-H(4A)	0.9600
C(4)-H(4B)	0.9600

C(4)-H(4C)	0.9600
C(5)-H(5A)	0.9600
C(5)-H(5B)	0.9600
C(5)-H(5C)	0.9600
C(6)-H(6A)	0.9600
C(6)-H(6B)	0.9600
C(6)-H(6C)	0.9600
C(7)-C(10)	1.528(7)
C(7)-C(8)	1.530(7)
C(7)-C(9)	1.534(7)
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-C(12)	1.523(6)
C(12)-C(13)	1.441(9)
C(12)-C(15')	1.483(12)
C(12)-C(15)	1.511(13)
C(12)-C(14')	1.568(15)
C(12)-C(14)	1.617(14)
C(12)-C(13')	1.650(14)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-H(14A)	0.9600

C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(13')-H(13D)	0.9600
C(13')-H(13E)	0.9600
C(13')-H(13F)	0.9600
C(14')-H(14D)	0.9600
C(14')-H(14E)	0.9600
C(14')-H(14F)	0.9600
C(15')-H(15D)	0.9600
C(15')-H(15E)	0.9600
C(15')-H(15F)	0.9600
C(16)-C(17)	1.472(7)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-C(18)	1.430(12)
C(17)-C(18')	1.552(12)
C(17)-H(17A)	0.9623
C(17)-H(17B)	0.9707
C(17)-H(17C)	0.9681
C(17)-H(17D)	0.9750
C(18)-C(19)	1.561(12)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(18')-C(19)	1.491(11)
C(18')-H(18C)	0.9700
C(18')-H(18D)	0.9700
C(19)-H(19A)	0.9776

C(19)-H(19B)	1.0096
C(19)-H(19C)	0.9626
C(19)-H(19D)	0.9490
N(2)#1-Ce(1)-N(2)	171.66(14)
N(2)#1-Ce(1)-N(3)	94.59(11)
N(2)-Ce(1)-N(3)	93.42(11)
N(2)#1-Ce(1)-N(3)#1	93.42(11)
N(2)-Ce(1)-N(3)#1	94.59(11)
N(3)-Ce(1)-N(3)#1	32.08(14)
N(2)#1-Ce(1)-N(1)#1	31.81(10)
N(2)-Ce(1)-N(1)#1	139.89(11)
N(3)-Ce(1)-N(1)#1	123.87(11)
N(3)#1-Ce(1)-N(1)#1	124.58(11)
N(2)#1-Ce(1)-N(1)	139.89(11)
N(2)-Ce(1)-N(1)	31.81(10)
N(3)-Ce(1)-N(1)	124.58(11)
N(3)#1-Ce(1)-N(1)	123.87(11)
N(1)#1-Ce(1)-N(1)	108.36(15)
N(2)#1-Ce(1)-O(1)#1	86.59(10)
N(2)-Ce(1)-O(1)#1	91.25(10)
N(3)-Ce(1)-O(1)#1	121.10(10)
N(3)#1-Ce(1)-O(1)#1	89.02(10)
N(1)#1-Ce(1)-O(1)#1	82.04(10)
N(1)-Ce(1)-O(1)#1	80.46(10)
N(2)#1-Ce(1)-O(1)	91.25(10)
N(2)-Ce(1)-O(1)	86.59(10)
N(3)-Ce(1)-O(1)	89.02(10)
N(3)#1-Ce(1)-O(1)	121.10(11)
N(1)#1-Ce(1)-O(1)	80.46(10)

N(1)-Ce(1)-O(1)	82.04(10)
O(1)#1-Ce(1)-O(1)	149.88(15)
C(1)-P(1)-C(2)	86.91(19)
C(11)#1-P(2)-C(11)	86.9(3)
C(2)-N(1)-N(2)	112.9(3)
C(2)-N(1)-Ce(1)	173.8(3)
N(2)-N(1)-Ce(1)	72.05(19)
C(1)-N(2)-N(1)	112.6(3)
C(1)-N(2)-Ce(1)	170.8(3)
N(1)-N(2)-Ce(1)	76.14(19)
C(11)-N(3)-N(3)#1	112.4(2)
C(11)-N(3)-Ce(1)	173.6(3)
N(3)#1-N(3)-Ce(1)	73.96(7)
C(16)-O(1)-C(19)	108.5(4)
C(16)-O(1)-Ce(1)	127.7(3)
C(19)-O(1)-Ce(1)	123.8(3)
N(2)-C(1)-C(3)	118.6(4)
N(2)-C(1)-P(1)	113.9(3)
C(3)-C(1)-P(1)	127.5(3)
N(1)-C(2)-C(7)	119.6(3)
N(1)-C(2)-P(1)	113.7(3)
C(7)-C(2)-P(1)	126.6(3)
C(5)-C(3)-C(6)	110.3(5)
C(5)-C(3)-C(4)	109.1(7)
C(6)-C(3)-C(4)	110.1(6)
C(5)-C(3)-C(1)	110.3(5)
C(6)-C(3)-C(1)	110.1(4)
C(4)-C(3)-C(1)	106.9(4)
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5

H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(3)-C(5)-H(5A)	109.5
C(3)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(3)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(3)-C(6)-H(6A)	109.5
C(3)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(3)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(2)-C(7)-C(10)	109.9(4)
C(2)-C(7)-C(8)	110.6(4)
C(10)-C(7)-C(8)	108.2(5)
C(2)-C(7)-C(9)	108.8(4)
C(10)-C(7)-C(9)	110.3(4)
C(8)-C(7)-C(9)	109.0(5)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5

H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(3)-C(11)-C(12)	120.6(4)
N(3)-C(11)-P(2)	114.1(3)
C(12)-C(11)-P(2)	125.2(3)
C(13)-C(12)-C(15')	131.4(8)
C(13)-C(12)-C(15)	117.0(9)
C(15')-C(12)-C(15)	42.5(8)
C(13)-C(12)-C(11)	115.1(5)
C(15')-C(12)-C(11)	113.4(7)
C(15)-C(12)-C(11)	112.4(7)
C(13)-C(12)-C(14')	72.7(9)
C(15')-C(12)-C(14')	89.9(11)
C(15)-C(12)-C(14')	126.8(9)
C(11)-C(12)-C(14')	107.6(7)
C(13)-C(12)-C(14)	107.4(9)
C(15')-C(12)-C(14)	56.2(9)
C(15)-C(12)-C(14)	98.2(8)
C(11)-C(12)-C(14)	104.4(7)
C(14')-C(12)-C(14)	37.3(8)
C(13)-C(12)-C(13')	78.5(8)
C(15')-C(12)-C(13')	93.7(10)

C(15)-C(12)-C(13')	51.6(8)
C(11)-C(12)-C(13')	103.5(6)
C(14')-C(12)-C(13')	144.2(9)
C(14)-C(12)-C(13')	145.3(8)
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
C(12)-C(15)-H(15A)	109.5
C(12)-C(15)-H(15B)	109.5
C(12)-C(15)-H(15C)	109.5
C(12)-C(13')-H(13D)	109.5
C(12)-C(13')-H(13E)	109.5
H(13D)-C(13')-H(13E)	109.5
C(12)-C(13')-H(13F)	109.5
H(13D)-C(13')-H(13F)	109.5
H(13E)-C(13')-H(13F)	109.5
C(12)-C(14')-H(14D)	109.5
C(12)-C(14')-H(14E)	109.5
H(14D)-C(14')-H(14E)	109.5
C(12)-C(14')-H(14F)	109.5
H(14D)-C(14')-H(14F)	109.5
H(14E)-C(14')-H(14F)	109.5
C(12)-C(15')-H(15D)	109.5
C(12)-C(15')-H(15E)	109.5
H(15D)-C(15')-H(15E)	109.5
C(12)-C(15')-H(15F)	109.5
H(15D)-C(15')-H(15F)	109.5

H(15E)-C(15')-H(15F)	109.5
O(1)-C(16)-C(17)	107.8(5)
O(1)-C(16)-H(16A)	110.1
C(17)-C(16)-H(16A)	110.1
O(1)-C(16)-H(16B)	110.1
C(17)-C(16)-H(16B)	110.1
H(16A)-C(16)-H(16B)	108.5
C(18)-C(17)-C(16)	99.0(7)
C(18)-C(17)-C(18')	32.6(7)
C(16)-C(17)-C(18')	107.4(6)
C(18)-C(17)-H(17A)	111.9
C(16)-C(17)-H(17A)	111.1
C(18')-C(17)-H(17A)	131.7
C(18)-C(17)-H(17B)	111.4
C(16)-C(17)-H(17B)	112.5
C(18')-C(17)-H(17B)	79.2
H(17A)-C(17)-H(17B)	110.6
C(18)-C(17)-H(17C)	85.6
C(16)-C(17)-H(17C)	110.3
C(18')-C(17)-H(17C)	111.0
H(17A)-C(17)-H(17C)	27.2
H(17B)-C(17)-H(17C)	130.2
C(18)-C(17)-H(17D)	139.1
C(16)-C(17)-H(17D)	110.1
C(18')-C(17)-H(17D)	108.9
H(17A)-C(17)-H(17D)	84.1
H(17B)-C(17)-H(17D)	30.9
H(17C)-C(17)-H(17D)	109.2
C(17)-C(18)-C(19)	105.4(8)
C(17)-C(18)-H(18A)	110.7

C(19)-C(18)-H(18A)	110.7
C(17)-C(18)-H(18B)	110.7
C(19)-C(18)-H(18B)	110.7
H(18A)-C(18)-H(18B)	108.8
C(19)-C(18')-C(17)	102.9(7)
C(19)-C(18')-H(18C)	111.2
C(17)-C(18')-H(18C)	111.2
C(19)-C(18')-H(18D)	111.2
C(17)-C(18')-H(18D)	111.2
H(18C)-C(18')-H(18D)	109.1
O(1)-C(19)-C(18')	108.2(6)
O(1)-C(19)-C(18)	100.7(6)
C(18')-C(19)-C(18)	32.1(7)
O(1)-C(19)-H(19A)	111.6
C(18')-C(19)-H(19A)	78.8
C(18)-C(19)-H(19A)	110.4
O(1)-C(19)-H(19B)	117.2
C(18')-C(19)-H(19B)	126.8
C(18)-C(19)-H(19B)	110.0
H(19A)-C(19)-H(19B)	106.9
O(1)-C(19)-H(19C)	110.6
C(18')-C(19)-H(19C)	107.3
C(18)-C(19)-H(19C)	136.7
H(19A)-C(19)-H(19C)	30.1
H(19B)-C(19)-H(19C)	81.9
O(1)-C(19)-H(19D)	109.2
C(18')-C(19)-H(19D)	110.4
C(18)-C(19)-H(19D)	84.6
H(19A)-C(19)-H(19D)	132.4
H(19B)-C(19)-H(19D)	29.7

H(19C)-C(19)-H(19D) 111.2

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y,-z+3/2

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 140426-1.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Ce(1)	40(1)	31(1)	38(1)	0	8(1)	0
P(1)	71(1)	60(1)	52(1)	-6(1)	28(1)	-3(1)
P(2)	66(1)	33(1)	141(2)	0	-14(1)	0
N(1)	49(2)	38(2)	48(2)	-3(1)	15(2)	-3(2)
N(2)	52(2)	39(2)	45(2)	1(1)	12(2)	-2(2)
N(3)	37(2)	37(2)	65(2)	-6(1)	-2(2)	2(2)
O(1)	54(2)	65(2)	50(2)	8(1)	3(1)	7(2)
C(1)	52(2)	51(2)	39(2)	1(2)	11(2)	-7(2)
C(2)	46(2)	47(2)	42(2)	-4(2)	8(2)	-2(2)
C(3)	75(3)	52(3)	64(3)	2(2)	27(2)	-14(3)
C(4)	212(10)	127(7)	114(5)	16(4)	-17(6)	-124(7)
C(5)	158(8)	70(5)	242(10)	68(5)	114(8)	22(5)
C(6)	188(8)	92(5)	123(5)	11(4)	99(5)	-38(5)
C(7)	63(3)	38(2)	66(3)	-7(2)	21(2)	-4(2)
C(8)	142(6)	54(3)	98(4)	-24(3)	49(4)	-5(4)
C(9)	100(5)	57(3)	91(4)	20(3)	9(3)	6(3)
C(10)	88(4)	57(3)	118(5)	-7(3)	28(4)	-21(3)
C(11)	49(3)	36(2)	89(3)	-10(2)	-2(2)	0(2)
C(12)	61(3)	54(3)	106(4)	-23(3)	-16(3)	-11(3)
C(13)	56(5)	68(5)	128(6)	-46(5)	-52(5)	21(4)

C(14)	120(8)	134(9)	163(9)	-61(8)	-47(7)	1(8)
C(15)	88(8)	99(7)	170(10)	-36(8)	-40(7)	-17(7)
C(13')	61(7)	105(8)	138(8)	-36(7)	-30(7)	-13(7)
C(14')	117(8)	127(8)	178(8)	-23(8)	-72(7)	0(8)
C(15')	108(9)	104(8)	143(9)	-65(8)	-27(7)	-7(7)
C(16)	59(3)	107(4)	99(3)	-5(3)	2(3)	20(3)
C(17)	72(3)	114(4)	104(3)	3(3)	-12(2)	14(3)
C(18)	78(4)	113(4)	81(3)	17(4)	-16(3)	1(4)
C(18')	76(4)	112(4)	77(3)	15(4)	-17(3)	0(4)
C(19)	78(3)	113(4)	59(2)	21(3)	-7(2)	-11(3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 140426-1.

	x	y	z	U(eq)
H(4A)	8118	2350	8056	238
H(4B)	7597	2047	8534	238
H(4C)	8129	1219	8342	238
H(5A)	9631	1680	9538	219
H(5B)	9475	1486	8757	219
H(5C)	9079	814	9213	219
H(6A)	8110	1660	9724	187
H(6B)	7985	2855	9615	187
H(6C)	8723	2443	10056	187
H(8A)	8744	6748	9272	142
H(8B)	9330	7576	9187	142
H(8C)	9562	6600	9644	142
H(9A)	8936	6251	7609	126
H(9B)	8966	7366	7921	126
H(9C)	8371	6575	8039	126
H(10A)	10499	6276	9011	130
H(10B)	10243	7165	8486	130
H(10C)	10299	6024	8237	130
H(13A)	7796	1015	6156	143
H(13B)	8437	1775	6455	143
H(13C)	8022	1195	6938	143

H(14A)	8519	40	5523	227
H(14B)	9288	-375	5892	227
H(14C)	9165	817	5767	227
H(15A)	8181	-830	7006	194
H(15B)	8802	-1280	6682	194
H(15C)	8058	-935	6220	194
H(13D)	7746	-471	6778	163
H(13E)	7981	457	7277	163
H(13F)	8410	-594	7393	163
H(14D)	9253	971	5897	235
H(14E)	8548	1588	5949	235
H(14F)	8482	545	5544	235
H(15D)	9107	-748	6018	190
H(15E)	8251	-712	5857	190
H(15F)	8677	-1266	6513	190
H(16A)	8162	4756	7012	109
H(16B)	8033	3584	7167	109
H(17A)	7170	4416	6223	121
H(17B)	7430	3276	6093	121
H(17C)	7310	4626	6123	121
H(17D)	7250	3416	6233	121
H(18A)	8030	5134	5776	115
H(18B)	7768	4198	5283	115
H(18C)	7879	3058	5451	112
H(18D)	7839	4247	5256	112
H(19A)	8771	3197	5748	104
H(19B)	9141	4317	5798	104
H(19C)	9031	3327	5798	104
H(19D)	8941	4537	5858	104

Table 6. Torsion angles [deg] for 140426-1.

N(2)#1-Ce(1)-N(1)-C(2)	-38(3)
N(2)-Ce(1)-N(1)-C(2)	143(3)
N(3)-Ce(1)-N(1)-C(2)	156(2)
N(3)#1-Ce(1)-N(1)-C(2)	117(3)
N(1)#1-Ce(1)-N(1)-C(2)	-44(2)
O(1)#1-Ce(1)-N(1)-C(2)	35(3)
O(1)-Ce(1)-N(1)-C(2)	-121(3)
N(2)#1-Ce(1)-N(1)-N(2)	178.82(5)
N(3)-Ce(1)-N(1)-N(2)	13.1(3)
N(3)#1-Ce(1)-N(1)-N(2)	-25.9(2)
N(1)#1-Ce(1)-N(1)-N(2)	173.5(2)
O(1)#1-Ce(1)-N(1)-N(2)	-108.2(2)
O(1)-Ce(1)-N(1)-N(2)	96.4(2)
C(2)-N(1)-N(2)-C(1)	1.4(5)
Ce(1)-N(1)-N(2)-C(1)	177.3(3)
C(2)-N(1)-N(2)-Ce(1)	-175.9(3)
N(2)#1-Ce(1)-N(2)-C(1)	-169.2(18)
N(3)-Ce(1)-N(2)-C(1)	26.8(18)
N(3)#1-Ce(1)-N(2)-C(1)	-5.3(18)
N(1)#1-Ce(1)-N(2)-C(1)	-173.6(17)
N(1)-Ce(1)-N(2)-C(1)	-164.0(19)
O(1)#1-Ce(1)-N(2)-C(1)	-94.4(18)
O(1)-Ce(1)-N(2)-C(1)	115.6(18)
N(2)#1-Ce(1)-N(2)-N(1)	-5.3(2)
N(3)-Ce(1)-N(2)-N(1)	-169.2(2)
N(3)#1-Ce(1)-N(2)-N(1)	158.7(2)
N(1)#1-Ce(1)-N(2)-N(1)	-9.6(4)

O(1)#1-Ce(1)-N(2)-N(1)	69.5(2)
O(1)-Ce(1)-N(2)-N(1)	-80.4(2)
N(2)#1-Ce(1)-N(3)-C(11)	-91(3)
N(2)-Ce(1)-N(3)-C(11)	87(3)
N(3)#1-Ce(1)-N(3)-C(11)	-180(100)
N(1)#1-Ce(1)-N(3)-C(11)	-77(3)
N(1)-Ce(1)-N(3)-C(11)	80(3)
O(1)#1-Ce(1)-N(3)-C(11)	-179(100)
O(1)-Ce(1)-N(3)-C(11)	0(3)
N(2)#1-Ce(1)-N(3)-N(3)#1	89.1(3)
N(2)-Ce(1)-N(3)-N(3)#1	-93.2(3)
N(1)#1-Ce(1)-N(3)-N(3)#1	102.5(3)
N(1)-Ce(1)-N(3)-N(3)#1	-100.1(3)
O(1)#1-Ce(1)-N(3)-N(3)#1	0.4(3)
O(1)-Ce(1)-N(3)-N(3)#1	-179.7(3)
N(2)#1-Ce(1)-O(1)-C(16)	-169.4(4)
N(2)-Ce(1)-O(1)-C(16)	2.5(4)
N(3)-Ce(1)-O(1)-C(16)	96.0(4)
N(3)#1-Ce(1)-O(1)-C(16)	95.8(4)
N(1)#1-Ce(1)-O(1)-C(16)	-139.4(4)
N(1)-Ce(1)-O(1)-C(16)	-29.1(4)
O(1)#1-Ce(1)-O(1)-C(16)	-84.1(4)
N(2)#1-Ce(1)-O(1)-C(19)	9.6(4)
N(2)-Ce(1)-O(1)-C(19)	-178.5(4)
N(3)-Ce(1)-O(1)-C(19)	-85.0(4)
N(3)#1-Ce(1)-O(1)-C(19)	-85.2(4)
N(1)#1-Ce(1)-O(1)-C(19)	39.6(4)
N(1)-Ce(1)-O(1)-C(19)	149.9(4)
O(1)#1-Ce(1)-O(1)-C(19)	94.9(4)
N(1)-N(2)-C(1)-C(3)	176.6(4)

Ce(1)-N(2)-C(1)-C(3)	-20(2)
N(1)-N(2)-C(1)-P(1)	-1.3(5)
Ce(1)-N(2)-C(1)-P(1)	161.8(16)
C(2)-P(1)-C(1)-N(2)	0.7(3)
C(2)-P(1)-C(1)-C(3)	-176.9(4)
N(2)-N(1)-C(2)-C(7)	-177.5(4)
Ce(1)-N(1)-C(2)-C(7)	41(3)
N(2)-N(1)-C(2)-P(1)	-0.8(4)
Ce(1)-N(1)-C(2)-P(1)	-142(2)
C(1)-P(1)-C(2)-N(1)	0.1(3)
C(1)-P(1)-C(2)-C(7)	176.4(4)
N(2)-C(1)-C(3)-C(5)	52.0(7)
P(1)-C(1)-C(3)-C(5)	-130.4(5)
N(2)-C(1)-C(3)-C(6)	173.9(5)
P(1)-C(1)-C(3)-C(6)	-8.5(7)
N(2)-C(1)-C(3)-C(4)	-66.4(7)
P(1)-C(1)-C(3)-C(4)	111.1(6)
N(1)-C(2)-C(7)-C(10)	-49.6(6)
P(1)-C(2)-C(7)-C(10)	134.2(4)
N(1)-C(2)-C(7)-C(8)	-169.0(4)
P(1)-C(2)-C(7)-C(8)	14.8(6)
N(1)-C(2)-C(7)-C(9)	71.2(5)
P(1)-C(2)-C(7)-C(9)	-104.9(4)
N(3)#1-N(3)-C(11)-C(12)	179.8(5)
Ce(1)-N(3)-C(11)-C(12)	0(3)
N(3)#1-N(3)-C(11)-P(2)	0.0(6)
Ce(1)-N(3)-C(11)-P(2)	180(100)
C(11)#1-P(2)-C(11)-N(3)	0.0(2)
C(11)#1-P(2)-C(11)-C(12)	-179.8(6)
N(3)-C(11)-C(12)-C(13)	-24.2(9)

P(2)-C(11)-C(12)-C(13)	155.6(7)
N(3)-C(11)-C(12)-C(15')	152.3(11)
P(2)-C(11)-C(12)-C(15')	-27.9(12)
N(3)-C(11)-C(12)-C(15)	-161.3(9)
P(2)-C(11)-C(12)-C(15)	18.5(11)
N(3)-C(11)-C(12)-C(14')	54.5(10)
P(2)-C(11)-C(12)-C(14')	-125.7(9)
N(3)-C(11)-C(12)-C(14)	93.3(9)
P(2)-C(11)-C(12)-C(14)	-86.9(9)
N(3)-C(11)-C(12)-C(13')	-107.6(8)
P(2)-C(11)-C(12)-C(13')	72.2(8)
C(19)-O(1)-C(16)-C(17)	17.9(7)
Ce(1)-O(1)-C(16)-C(17)	-162.9(4)
O(1)-C(16)-C(17)-C(18)	-37.8(9)
O(1)-C(16)-C(17)-C(18')	-5.4(10)
C(16)-C(17)-C(18)-C(19)	42.4(10)
C(18')-C(17)-C(18)-C(19)	-65.8(12)
C(18)-C(17)-C(18')-C(19)	70.9(12)
C(16)-C(17)-C(18')-C(19)	-8.5(11)
C(16)-O(1)-C(19)-C(18')	-23.9(9)
Ce(1)-O(1)-C(19)-C(18')	156.9(7)
C(16)-O(1)-C(19)-C(18)	8.3(8)
Ce(1)-O(1)-C(19)-C(18)	-170.9(6)
C(17)-C(18')-C(19)-O(1)	19.3(11)
C(17)-C(18')-C(19)-C(18)	-61.5(11)
C(17)-C(18)-C(19)-O(1)	-32.7(10)
C(17)-C(18)-C(19)-C(18')	74.7(13)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y,-z+3/2

4.3 Crystal structural analysis data for 5

Table 1. Crystal data and structure refinement for 130519-2.

Identification code	130519-2
Empirical formula	C ₃₈ H ₇₀ N ₆ O ₂ P ₃ Pr
Formula weight	876.82
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 18.7219(9) Å alpha = 90 deg. b = 12.8523(5) Å beta = 102.503(5) deg. c = 20.2486(8) Å gamma = 90 deg.
Volume	4756.7(3) Å ³
Z, Calculated density	4, 1.224 Mg/m ³
Absorption coefficient	1.160 mm ⁻¹
F(000)	1840
Crystal size	0.34 x 0.22 x 0.06 mm
Theta range for data collection	2.69 to 25.67 deg.
Limiting indices	-22 ≤ h ≤ 22, -15 ≤ k ≤ 14, -24 ≤ l ≤ 24
Reflections collected / unique	10431 / 4512 [R(int) = 0.0331]
Completeness to theta = 25.67	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9337 and 0.6938
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4512 / 193 / 330
Goodness-of-fit on F ²	1.040
Final R indices [I > 2σ(I)]	R1 = 0.0402, wR2 = 0.0942
R indices (all data)	R1 = 0.0495, wR2 = 0.0992
Largest diff. peak and hole	0.992 and -0.488 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 130519-2.

$U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
C(4)	8658(2)	2260(4)	9042(2)	60(1)
C(5)	8932(2)	3333(3)	8887(2)	45(1)
C(6)	9262(2)	5098(3)	8699(2)	42(1)
C(7)	9395(3)	6259(3)	8628(2)	55(1)
C(8)	8870(4)	6659(4)	7990(3)	82(2)
C(9)	9239(4)	6849(4)	9244(3)	92(2)
C(10)	10181(3)	6459(4)	8587(3)	84(2)
C(11)	9429(2)	472(3)	7091(2)	56(1)
C(12)	8744(8)	337(8)	6523(7)	88(2)
C(13)	8499(6)	-792(7)	6467(6)	96(2)
C(14)	8125(6)	1057(9)	6628(6)	91(2)
C(15)	8891(6)	593(9)	5814(5)	103(2)
C(16)	11274(8)	3960(20)	9040(5)	89(4)
C(17)	12045(6)	4371(16)	9247(7)	96(3)
C(18)	12400(8)	3929(15)	8696(7)	95(3)
C(19)	11810(6)	4016(19)	8068(8)	89(4)
C(12')	8693(11)	258(10)	6650(8)	89(2)
C(13')	8331(9)	1268(11)	6351(9)	92(2)
C(14')	8809(8)	-451(12)	6079(7)	97(2)

C(15')	8177(7)	-263(11)	7056(7)	97(2)
C(16')	11170(7)	3800(20)	9035(4)	63(4)
C(17')	11971(6)	3749(16)	9394(6)	70(3)
C(18')	12426(8)	4054(16)	8897(7)	72(3)
C(19')	11872(6)	4119(18)	8234(7)	62(4)
Pr(1)	10000	3290(1)	7500	34(1)
N(1)	9479(2)	4435(2)	8280(2)	41(1)
N(2)	9296(2)	3426(2)	8392(2)	43(1)
N(3)	9676(2)	1436(2)	7265(2)	44(1)
O(1)	11156(2)	3798(2)	8316(1)	54(1)
P(1)	8805(1)	4508(1)	9269(1)	56(1)
P(2)	10000	-503(1)	7500	83(1)
C(1)	8214(8)	2347(8)	9589(6)	71(3)
C(2)	9191(7)	1389(8)	9005(9)	92(4)
C(3)	7970(6)	2047(9)	8476(5)	73(3)
C(1')	8546(12)	2219(12)	9770(5)	76(4)
C(3')	8281(13)	1727(14)	8380(6)	101(6)
C(2')	9342(6)	1584(11)	9304(9)	72(4)

Table 3. Bond lengths [Å] and angles [deg] for 130519-2.

C(4)-C(2)	1.512(7)
C(4)-C(5)	1.526(6)
C(4)-C(1)	1.526(7)
C(4)-C(3')	1.535(8)
C(4)-C(1')	1.535(7)
C(4)-C(2')	1.543(7)
C(4)-C(3)	1.552(7)
C(5)-N(2)	1.333(5)
C(5)-P(1)	1.737(4)
C(6)-N(1)	1.325(5)
C(6)-C(7)	1.525(6)
C(6)-P(1)	1.751(4)
C(7)-C(10)	1.514(7)
C(7)-C(8)	1.533(7)
C(7)-C(9)	1.540(7)
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-N(3)	1.342(5)
C(11)-C(12')	1.50(2)

C(11)-C(12)	1.537(16)
C(11)-P(2)	1.736(4)
C(12)-C(13)	1.519(9)
C(12)-C(14)	1.532(9)
C(12)-C(15)	1.554(9)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-O(1)	1.449(8)
C(16)-C(17)	1.508(9)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-C(18)	1.527(9)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(18)-C(19)	1.498(9)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(19)-O(1)	1.446(9)
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(12')-C(14')	1.523(10)
C(12')-C(13')	1.527(10)
C(12')-C(15')	1.549(10)

C(13')-H(13D)	0.9600
C(13')-H(13E)	0.9600
C(13')-H(13F)	0.9600
C(14')-H(14D)	0.9600
C(14')-H(14E)	0.9600
C(14')-H(14F)	0.9600
C(15')-H(15D)	0.9600
C(15')-H(15E)	0.9600
C(15')-H(15F)	0.9600
C(16')-O(1)	1.452(9)
C(16')-C(17')	1.519(9)
C(16')-H(16C)	0.9700
C(16')-H(16D)	0.9700
C(17')-C(18')	1.505(9)
C(17')-H(17C)	0.9700
C(17')-H(17D)	0.9700
C(18')-C(19')	1.510(8)
C(18')-H(18C)	0.9700
C(18')-H(18D)	0.9700
C(19')-O(1)	1.445(8)
C(19')-H(19C)	0.9700
C(19')-H(19D)	0.9700
Pr(1)-N(2)	2.463(3)
Pr(1)-N(2)#1	2.463(3)
Pr(1)-N(3)	2.479(3)
Pr(1)-N(3)#1	2.479(3)
Pr(1)-N(1)	2.506(3)
Pr(1)-N(1)#1	2.506(3)
Pr(1)-O(1)	2.508(3)
Pr(1)-O(1)#1	2.508(3)

N(1)-N(2)	1.373(4)
N(3)-N(3)#1	1.370(6)
P(2)-C(11)#1	1.736(4)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(2)-H(2A)	0.9600
C(2)-H(2B)	0.9600
C(2)-H(2C)	0.9600
C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600
C(3)-H(3C)	0.9600
C(1')-H(1'1)	0.9600
C(1')-H(1'2)	0.9600
C(1')-H(1'3)	0.9600
C(3')-H(3'1)	0.9600
C(3')-H(3'2)	0.9600
C(3')-H(3'3)	0.9600
C(2')-H(2'1)	0.9600
C(2')-H(2'2)	0.9600
C(2')-H(2'3)	0.9600
C(2)-C(4)-C(5)	113.9(6)
C(2)-C(4)-C(1)	124.0(9)
C(5)-C(4)-C(1)	110.0(5)
C(2)-C(4)-C(3')	79.0(9)
C(5)-C(4)-C(3')	109.6(7)
C(1)-C(4)-C(3')	116.5(12)
C(2)-C(4)-C(1')	104.5(12)
C(5)-C(4)-C(1')	110.5(6)

C(1)-C(4)-C(1')	25.3(6)
C(3')-C(4)-C(1')	133.7(12)
C(2)-C(4)-C(2')	25.0(6)
C(5)-C(4)-C(2')	106.8(6)
C(1)-C(4)-C(2')	109.4(10)
C(3')-C(4)-C(2')	103.9(10)
C(1')-C(4)-C(2')	85.7(12)
C(2)-C(4)-C(3)	106.5(7)
C(5)-C(4)-C(3)	105.6(5)
C(1)-C(4)-C(3)	93.0(9)
C(3')-C(4)-C(3)	28.9(8)
C(1')-C(4)-C(3)	116.0(11)
C(2')-C(4)-C(3)	130.5(8)
N(2)-C(5)-C(4)	119.0(3)
N(2)-C(5)-P(1)	113.4(3)
C(4)-C(5)-P(1)	127.6(3)
N(1)-C(6)-C(7)	119.3(3)
N(1)-C(6)-P(1)	113.9(3)
C(7)-C(6)-P(1)	126.7(3)
C(10)-C(7)-C(6)	110.6(4)
C(10)-C(7)-C(8)	110.5(4)
C(6)-C(7)-C(8)	108.6(4)
C(10)-C(7)-C(9)	108.5(5)
C(6)-C(7)-C(9)	110.1(4)
C(8)-C(7)-C(9)	108.6(5)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5

H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(3)-C(11)-C(12')	123.1(6)
N(3)-C(11)-C(12)	119.0(5)
C(12')-C(11)-C(12)	11.6(8)
N(3)-C(11)-P(2)	113.6(3)
C(12')-C(11)-P(2)	122.9(6)
C(12)-C(11)-P(2)	127.1(5)
C(13)-C(12)-C(14)	111.3(10)
C(13)-C(12)-C(11)	110.7(9)
C(14)-C(12)-C(11)	111.2(9)
C(13)-C(12)-C(15)	104.1(10)
C(14)-C(12)-C(15)	106.9(11)
C(11)-C(12)-C(15)	112.4(9)
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5

H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(12)-C(15)-H(15A)	109.5
C(12)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(12)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
O(1)-C(16)-C(17)	105.0(8)
O(1)-C(16)-H(16A)	110.7
C(17)-C(16)-H(16A)	110.7
O(1)-C(16)-H(16B)	110.7
C(17)-C(16)-H(16B)	110.7
H(16A)-C(16)-H(16B)	108.8
C(16)-C(17)-C(18)	102.0(11)
C(16)-C(17)-H(17A)	111.4
C(18)-C(17)-H(17A)	111.4
C(16)-C(17)-H(17B)	111.4
C(18)-C(17)-H(17B)	111.4
H(17A)-C(17)-H(17B)	109.2
C(19)-C(18)-C(17)	103.5(11)
C(19)-C(18)-H(18A)	111.1
C(17)-C(18)-H(18A)	111.1
C(19)-C(18)-H(18B)	111.1
C(17)-C(18)-H(18B)	111.1

H(18A)-C(18)-H(18B)	109.0
O(1)-C(19)-C(18)	102.5(10)
O(1)-C(19)-H(19A)	111.3
C(18)-C(19)-H(19A)	111.3
O(1)-C(19)-H(19B)	111.3
C(18)-C(19)-H(19B)	111.3
H(19A)-C(19)-H(19B)	109.2
C(11)-C(12')-C(14')	107.4(12)
C(11)-C(12')-C(13')	110.6(12)
C(14')-C(12')-C(13')	109.4(14)
C(11)-C(12')-C(15')	111.3(11)
C(14')-C(12')-C(15')	110.6(14)
C(13')-C(12')-C(15')	107.6(14)
C(12')-C(13')-H(13D)	109.5
C(12')-C(13')-H(13E)	109.5
H(13D)-C(13')-H(13E)	109.5
C(12')-C(13')-H(13F)	109.5
H(13D)-C(13')-H(13F)	109.5
H(13E)-C(13')-H(13F)	109.5
C(12')-C(14')-H(14D)	109.5
C(12')-C(14')-H(14E)	109.5
H(14D)-C(14')-H(14E)	109.5
C(12')-C(14')-H(14F)	109.5
H(14D)-C(14')-H(14F)	109.5
H(14E)-C(14')-H(14F)	109.5
C(12')-C(15')-H(15D)	109.5
C(12')-C(15')-H(15E)	109.5
H(15D)-C(15')-H(15E)	109.5
C(12')-C(15')-H(15F)	109.5
H(15D)-C(15')-H(15F)	109.5

H(15E)-C(15')-H(15F)	109.5
O(1)-C(16')-C(17')	106.3(9)
O(1)-C(16')-H(16C)	110.5
C(17')-C(16')-H(16C)	110.5
O(1)-C(16')-H(16D)	110.5
C(17')-C(16')-H(16D)	110.5
H(16C)-C(16')-H(16D)	108.7
C(18')-C(17')-C(16')	108.2(10)
C(18')-C(17')-H(17C)	110.1
C(16')-C(17')-H(17C)	110.1
C(18')-C(17')-H(17D)	110.1
C(16')-C(17')-H(17D)	110.1
H(17C)-C(17')-H(17D)	108.4
C(17')-C(18')-C(19')	103.3(10)
C(17')-C(18')-H(18C)	111.1
C(19')-C(18')-H(18C)	111.1
C(17')-C(18')-H(18D)	111.1
C(19')-C(18')-H(18D)	111.1
H(18C)-C(18')-H(18D)	109.1
O(1)-C(19')-C(18')	111.0(9)
O(1)-C(19')-H(19C)	109.4
C(18')-C(19')-H(19C)	109.4
O(1)-C(19')-H(19D)	109.4
C(18')-C(19')-H(19D)	109.4
H(19C)-C(19')-H(19D)	108.0
N(2)-Pr(1)-N(2)#1	171.87(14)
N(2)-Pr(1)-N(3)	93.51(11)
N(2)#1-Pr(1)-N(3)	94.30(11)
N(2)-Pr(1)-N(3)#1	94.30(11)
N(2)#1-Pr(1)-N(3)#1	93.51(11)

N(3)-Pr(1)-N(3)#1	32.09(14)
N(2)-Pr(1)-N(1)	32.07(9)
N(2)#1-Pr(1)-N(1)	139.83(10)
N(3)-Pr(1)-N(1)	124.96(11)
N(3)#1-Pr(1)-N(1)	123.77(11)
N(2)-Pr(1)-N(1)#1	139.83(10)
N(2)#1-Pr(1)-N(1)#1	32.07(9)
N(3)-Pr(1)-N(1)#1	123.77(11)
N(3)#1-Pr(1)-N(1)#1	124.96(11)
N(1)-Pr(1)-N(1)#1	108.07(14)
N(2)-Pr(1)-O(1)	91.22(10)
N(2)#1-Pr(1)-O(1)	86.66(10)
N(3)-Pr(1)-O(1)	121.11(10)
N(3)#1-Pr(1)-O(1)	89.03(10)
N(1)-Pr(1)-O(1)	80.22(10)
N(1)#1-Pr(1)-O(1)	82.22(10)
N(2)-Pr(1)-O(1)#1	86.66(10)
N(2)#1-Pr(1)-O(1)#1	91.22(10)
N(3)-Pr(1)-O(1)#1	89.03(10)
N(3)#1-Pr(1)-O(1)#1	121.11(10)
N(1)-Pr(1)-O(1)#1	82.22(10)
N(1)#1-Pr(1)-O(1)#1	80.22(10)
O(1)-Pr(1)-O(1)#1	149.86(14)
C(6)-N(1)-N(2)	112.3(3)
C(6)-N(1)-Pr(1)	174.4(3)
N(2)-N(1)-Pr(1)	72.22(19)
C(5)-N(2)-N(1)	113.3(3)
C(5)-N(2)-Pr(1)	170.6(3)
N(1)-N(2)-Pr(1)	75.70(19)
C(11)-N(3)-N(3)#1	112.6(2)

C(11)-N(3)-Pr(1)	173.4(3)
N(3)#1-N(3)-Pr(1)	73.96(7)
C(19')-O(1)-C(19)	14.2(10)
C(19')-O(1)-C(16)	97.6(8)
C(19)-O(1)-C(16)	111.6(7)
C(19')-O(1)-C(16')	107.4(8)
C(19)-O(1)-C(16')	121.0(9)
C(16)-O(1)-C(16')	11.1(14)
C(19')-O(1)-Pr(1)	133.5(6)
C(19)-O(1)-Pr(1)	119.8(6)
C(16)-O(1)-Pr(1)	128.6(6)
C(16')-O(1)-Pr(1)	119.1(6)
C(5)-P(1)-C(6)	87.10(18)
C(11)#1-P(2)-C(11)	87.6(3)
C(4)-C(1)-H(1A)	109.5
C(4)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(4)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(4)-C(2)-H(2A)	109.5
C(4)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(4)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(4)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(4)-C(3)-H(3C)	109.5

H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(4)-C(1')-H(1'1)	109.5
C(4)-C(1')-H(1'2)	109.5
H(1'1)-C(1')-H(1'2)	109.5
C(4)-C(1')-H(1'3)	109.5
H(1'1)-C(1')-H(1'3)	109.5
H(1'2)-C(1')-H(1'3)	109.5
C(4)-C(3')-H(3'1)	109.5
C(4)-C(3')-H(3'2)	109.5
H(3'1)-C(3')-H(3'2)	109.5
C(4)-C(3')-H(3'3)	109.5
H(3'1)-C(3')-H(3'3)	109.5
H(3'2)-C(3')-H(3'3)	109.5
C(4)-C(2')-H(2'1)	109.5
C(4)-C(2')-H(2'2)	109.5
H(2'1)-C(2')-H(2'2)	109.5
C(4)-C(2')-H(2'3)	109.5
H(2'1)-C(2')-H(2'3)	109.5
H(2'2)-C(2')-H(2'3)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y,-z+3/2

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 130519-2.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
C(4)	77(3)	54(3)	56(2)	0(2)	28(2)	-18(3)
C(5)	49(2)	52(2)	36(2)	1(2)	11(2)	-9(2)
C(6)	43(2)	43(2)	41(2)	-3(2)	11(2)	1(2)
C(7)	67(3)	39(2)	60(2)	-5(2)	20(2)	-2(2)
C(8)	99(5)	52(3)	93(4)	18(3)	14(3)	5(3)
C(9)	147(6)	49(3)	92(4)	-21(3)	50(4)	-5(3)
C(10)	82(4)	49(3)	123(5)	-9(3)	29(4)	-21(3)
C(11)	42(2)	37(2)	83(3)	-9(2)	0(2)	3(2)
C(12)	67(3)	67(3)	114(4)	-27(3)	-18(3)	-7(3)
C(13)	73(4)	72(3)	124(5)	-22(3)	-20(3)	-12(3)
C(14)	65(4)	73(4)	118(5)	-23(4)	-18(3)	-1(3)
C(15)	80(4)	92(4)	117(5)	-22(4)	-20(4)	-9(4)
C(16)	71(6)	120(8)	69(6)	-32(5)	-5(5)	-3(6)
C(17)	73(5)	122(7)	81(5)	-27(5)	-11(4)	-15(5)
C(18)	67(6)	118(7)	85(6)	-27(5)	-13(5)	-20(5)
C(19)	58(6)	116(7)	82(7)	-25(6)	-8(5)	-19(6)
C(12')	67(3)	67(3)	116(4)	-24(3)	-18(3)	-7(3)
C(13')	68(4)	70(4)	118(5)	-19(4)	-23(4)	-5(3)
C(14')	76(4)	78(3)	118(5)	-27(3)	-19(3)	-6(3)
C(15')	71(4)	80(4)	122(5)	-16(4)	-17(4)	-14(4)

C(16')	61(7)	81(7)	40(5)	-8(5)	-7(5)	4(5)
C(17')	61(6)	85(7)	53(5)	-6(4)	-13(4)	-7(5)
C(18')	56(6)	90(7)	58(5)	-4(5)	-14(4)	-17(5)
C(19')	42(6)	88(7)	47(6)	8(6)	-8(5)	-27(5)
Pr(1)	39(1)	28(1)	36(1)	0	8(1)	0
N(1)	49(2)	34(2)	42(2)	-2(1)	14(1)	-3(2)
N(2)	51(2)	38(2)	41(2)	2(1)	13(1)	-5(2)
N(3)	35(2)	34(2)	59(2)	-3(2)	-2(1)	0(1)
O(1)	50(2)	59(2)	50(2)	-8(1)	5(1)	-10(2)
P(1)	70(1)	57(1)	49(1)	-5(1)	28(1)	-2(1)
P(2)	62(1)	29(1)	143(2)	0	-13(1)	0
C(1)	71(4)	72(4)	72(4)	6(2)	19(2)	-3(2)
C(2)	93(4)	90(4)	94(4)	3(2)	22(2)	-1(2)
C(3)	72(4)	69(4)	75(4)	1(2)	13(2)	-5(2)
C(1')	76(5)	76(5)	76(5)	3(2)	19(2)	-2(2)
C(3')	102(6)	100(6)	101(6)	0(2)	23(2)	-3(2)
C(2')	74(5)	69(5)	72(5)	2(2)	17(2)	-3(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 130519-2.

	x	y	z	U(eq)
H(8A)	8964	7382	7927	123
H(8B)	8374	6574	8039	123
H(8C)	8942	6270	7605	123
H(9A)	9543	6576	9651	139
H(9B)	8734	6764	9261	139
H(9C)	9343	7575	9204	139
H(10A)	10304	6030	8240	125
H(10B)	10498	6295	9014	125
H(10C)	10238	7178	8482	125
H(13A)	8354	-996	6874	144
H(13B)	8896	-1224	6401	144
H(13C)	8092	-870	6089	144
H(14A)	7733	1037	6234	137
H(14B)	8306	1756	6700	137
H(14C)	7948	829	7015	137
H(15A)	8464	429	5472	154
H(15B)	9297	187	5741	154
H(15C)	9002	1319	5792	154
H(16A)	11224	3310	9270	107
H(16B)	10926	4457	9145	107
H(17A)	12285	4118	9691	115

H(17B)	12052	5125	9247	115
H(18A)	12827	4332	8656	113
H(18B)	12544	3209	8789	113
H(19A)	11794	4709	7876	107
H(19B)	11877	3511	7731	107
H(13D)	8608	1564	6051	138
H(13E)	8315	1750	6709	138
H(13F)	7842	1124	6105	138
H(14D)	9156	-138	5854	145
H(14E)	8352	-548	5762	145
H(14F)	8991	-1112	6262	145
H(15D)	7704	-366	6765	145
H(15E)	8130	177	7427	145
H(15F)	8376	-923	7226	145
H(16C)	10906	3205	9155	76
H(16D)	10946	4430	9160	76
H(17C)	12064	4220	9777	84
H(17D)	12095	3049	9559	84
H(18C)	12795	3532	8876	86
H(18D)	12663	4719	9015	86
H(19C)	11847	4829	8068	74
H(19D)	12026	3677	7902	74
H(1A)	8064	1666	9698	107
H(1B)	7790	2770	9426	107
H(1C)	8509	2661	9986	107
H(2A)	9669	1581	9253	138
H(2B)	9206	1263	8541	138
H(2C)	9035	768	9197	138
H(3A)	8102	2059	8044	109
H(3B)	7609	2574	8488	109

H(3C)	7773	1377	8547	109
H(1'1)	8329	1565	9845	114
H(1'2)	8229	2776	9840	114
H(1'3)	9010	2290	10081	114
H(3'1)	8606	1721	8072	151
H(3'2)	7844	2102	8180	151
H(3'3)	8157	1025	8473	151
H(2'1)	9651	1921	9684	108
H(2'2)	9605	1494	8951	108
H(2'3)	9194	917	9441	108

Table 6. Torsion angles [deg] for 130519-2.

C(2)-C(4)-C(5)-N(2)	39.6(9)
C(1)-C(4)-C(5)-N(2)	-176.1(7)
C(3')-C(4)-C(5)-N(2)	-46.8(12)
C(1')-C(4)-C(5)-N(2)	156.9(10)
C(2')-C(4)-C(5)-N(2)	65.2(8)
C(3)-C(4)-C(5)-N(2)	-76.9(7)
C(2)-C(4)-C(5)-P(1)	-142.5(8)
C(1)-C(4)-C(5)-P(1)	1.8(8)
C(3')-C(4)-C(5)-P(1)	131.1(11)
C(1')-C(4)-C(5)-P(1)	-25.2(10)
C(2')-C(4)-C(5)-P(1)	-116.9(8)
C(3)-C(4)-C(5)-P(1)	101.0(7)
N(1)-C(6)-C(7)-C(10)	-49.0(6)
P(1)-C(6)-C(7)-C(10)	133.8(4)
N(1)-C(6)-C(7)-C(8)	72.4(5)
P(1)-C(6)-C(7)-C(8)	-104.9(4)
N(1)-C(6)-C(7)-C(9)	-168.9(4)
P(1)-C(6)-C(7)-C(9)	13.9(6)
N(3)-C(11)-C(12)-C(13)	-172.6(8)
C(12')-C(11)-C(12)-C(13)	-59(4)
P(2)-C(11)-C(12)-C(13)	14.3(12)
N(3)-C(11)-C(12)-C(14)	-48.4(10)
C(12')-C(11)-C(12)-C(14)	66(4)
P(2)-C(11)-C(12)-C(14)	138.5(7)
N(3)-C(11)-C(12)-C(15)	71.5(9)
C(12')-C(11)-C(12)-C(15)	-175(4)

P(2)-C(11)-C(12)-C(15)	-101.7(8)
O(1)-C(16)-C(17)-C(18)	-26(2)
C(16)-C(17)-C(18)-C(19)	38.5(19)
C(17)-C(18)-C(19)-O(1)	-36.2(17)
N(3)-C(11)-C(12')-C(14')	127.8(10)
C(12)-C(11)-C(12')-C(14')	55(3)
P(2)-C(11)-C(12')-C(14')	-59.5(12)
N(3)-C(11)-C(12')-C(13')	8.6(15)
C(12)-C(11)-C(12')-C(13')	-64(4)
P(2)-C(11)-C(12')-C(13')	-178.8(9)
N(3)-C(11)-C(12')-C(15')	-111.0(10)
C(12)-C(11)-C(12')-C(15')	176(4)
P(2)-C(11)-C(12')-C(15')	61.6(11)
O(1)-C(16')-C(17')-C(18')	18(2)
C(16')-C(17')-C(18')-C(19')	-8(2)
C(17')-C(18')-C(19')-O(1)	-4.4(19)
C(7)-C(6)-N(1)-N(2)	-177.7(4)
P(1)-C(6)-N(1)-N(2)	-0.1(4)
C(7)-C(6)-N(1)-Pr(1)	39(3)
P(1)-C(6)-N(1)-Pr(1)	-143(3)
N(2)-Pr(1)-N(1)-C(6)	144(3)
N(2)#1-Pr(1)-N(1)-C(6)	-37(3)
N(3)-Pr(1)-N(1)-C(6)	157(3)
N(3)#1-Pr(1)-N(1)-C(6)	118(3)
N(1)#1-Pr(1)-N(1)-C(6)	-43(3)
O(1)-Pr(1)-N(1)-C(6)	36(3)
O(1)#1-Pr(1)-N(1)-C(6)	-120(3)
N(2)#1-Pr(1)-N(1)-N(2)	178.79(5)
N(3)-Pr(1)-N(1)-N(2)	12.9(2)
N(3)#1-Pr(1)-N(1)-N(2)	-26.2(2)

N(1)#1-Pr(1)-N(1)-N(2)	173.2(2)
O(1)-Pr(1)-N(1)-N(2)	-108.4(2)
O(1)#1-Pr(1)-N(1)-N(2)	96.2(2)
C(4)-C(5)-N(2)-N(1)	176.9(3)
P(1)-C(5)-N(2)-N(1)	-1.3(4)
C(4)-C(5)-N(2)-Pr(1)	-19(2)
P(1)-C(5)-N(2)-Pr(1)	162.8(15)
C(6)-N(1)-N(2)-C(5)	0.9(5)
Pr(1)-N(1)-N(2)-C(5)	177.4(3)
C(6)-N(1)-N(2)-Pr(1)	-176.5(3)
N(2)#1-Pr(1)-N(2)-C(5)	-170.5(17)
N(3)-Pr(1)-N(2)-C(5)	25.6(17)
N(3)#1-Pr(1)-N(2)-C(5)	-6.6(17)
N(1)-Pr(1)-N(2)-C(5)	-165.0(18)
N(1)#1-Pr(1)-N(2)-C(5)	-175.1(17)
O(1)-Pr(1)-N(2)-C(5)	-95.7(17)
O(1)#1-Pr(1)-N(2)-C(5)	114.4(17)
N(2)#1-Pr(1)-N(2)-N(1)	-5.53(19)
N(3)-Pr(1)-N(2)-N(1)	-169.5(2)
N(3)#1-Pr(1)-N(2)-N(1)	158.4(2)
N(1)#1-Pr(1)-N(2)-N(1)	-10.1(3)
O(1)-Pr(1)-N(2)-N(1)	69.3(2)
O(1)#1-Pr(1)-N(2)-N(1)	-80.6(2)
C(12')-C(11)-N(3)-N(3)#1	172.6(7)
C(12)-C(11)-N(3)-N(3)#1	-174.7(6)
P(2)-C(11)-N(3)-N(3)#1	-0.6(6)
C(12')-C(11)-N(3)-Pr(1)	-4(3)
C(12)-C(11)-N(3)-Pr(1)	9(3)
P(2)-C(11)-N(3)-Pr(1)	-177(3)
N(2)-Pr(1)-N(3)-C(11)	84(3)

N(2)#1-Pr(1)-N(3)-C(11)	-93(3)
N(3)#1-Pr(1)-N(3)-C(11)	177(3)
N(1)-Pr(1)-N(3)-C(11)	78(3)
N(1)#1-Pr(1)-N(3)-C(11)	-80(3)
O(1)-Pr(1)-N(3)-C(11)	178(100)
O(1)#1-Pr(1)-N(3)-C(11)	-2(3)
N(2)-Pr(1)-N(3)-N(3)#1	-92.5(3)
N(2)#1-Pr(1)-N(3)-N(3)#1	89.8(3)
N(1)-Pr(1)-N(3)-N(3)#1	-99.3(3)
N(1)#1-Pr(1)-N(3)-N(3)#1	103.4(3)
O(1)-Pr(1)-N(3)-N(3)#1	1.1(3)
O(1)#1-Pr(1)-N(3)-N(3)#1	-179.1(3)
C(18')-C(19')-O(1)-C(19)	-149(8)
C(18')-C(19')-O(1)-C(16)	21.2(18)
C(18')-C(19')-O(1)-C(16')	15.7(18)
C(18')-C(19')-O(1)-Pr(1)	-164.6(9)
C(18)-C(19)-O(1)-C(19')	31(6)
C(18)-C(19)-O(1)-C(16)	20.6(18)
C(18)-C(19)-O(1)-C(16')	14(2)
C(18)-C(19)-O(1)-Pr(1)	-161.9(8)
C(17)-C(16)-O(1)-C(19')	1(2)
C(17)-C(16)-O(1)-C(19)	4(2)
C(17)-C(16)-O(1)-C(16')	153(10)
C(17)-C(16)-O(1)-Pr(1)	-173.6(9)
C(17')-C(16')-O(1)-C(19')	-20(2)
C(17')-C(16')-O(1)-C(19)	-16(2)
C(17')-C(16')-O(1)-C(16)	-49(8)
C(17')-C(16')-O(1)-Pr(1)	160.1(11)
N(2)-Pr(1)-O(1)-C(19')	-166.6(14)
N(2)#1-Pr(1)-O(1)-C(19')	5.5(14)

N(3)-Pr(1)-O(1)-C(19')	98.5(14)
N(3)#1-Pr(1)-O(1)-C(19')	99.1(14)
N(1)-Pr(1)-O(1)-C(19')	-136.4(14)
N(1)#1-Pr(1)-O(1)-C(19')	-26.4(14)
O(1)#1-Pr(1)-O(1)-C(19')	-81.2(14)
N(2)-Pr(1)-O(1)-C(19)	-171.0(11)
N(2)#1-Pr(1)-O(1)-C(19)	1.2(11)
N(3)-Pr(1)-O(1)-C(19)	94.2(12)
N(3)#1-Pr(1)-O(1)-C(19)	94.7(11)
N(1)-Pr(1)-O(1)-C(19)	-140.7(11)
N(1)#1-Pr(1)-O(1)-C(19)	-30.8(11)
O(1)#1-Pr(1)-O(1)-C(19)	-85.5(11)
N(2)-Pr(1)-O(1)-C(16)	6.0(14)
N(2)#1-Pr(1)-O(1)-C(16)	178.2(14)
N(3)-Pr(1)-O(1)-C(16)	-88.8(14)
N(3)#1-Pr(1)-O(1)-C(16)	-88.3(14)
N(1)-Pr(1)-O(1)-C(16)	36.3(14)
N(1)#1-Pr(1)-O(1)-C(16)	146.2(14)
O(1)#1-Pr(1)-O(1)-C(16)	91.5(14)
N(2)-Pr(1)-O(1)-C(16')	13.0(11)
N(2)#1-Pr(1)-O(1)-C(16')	-174.9(11)
N(3)-Pr(1)-O(1)-C(16')	-81.9(11)
N(3)#1-Pr(1)-O(1)-C(16')	-81.3(11)
N(1)-Pr(1)-O(1)-C(16')	43.2(11)
N(1)#1-Pr(1)-O(1)-C(16')	153.2(11)
O(1)#1-Pr(1)-O(1)-C(16')	98.4(11)
N(2)-C(5)-P(1)-C(6)	1.0(3)
C(4)-C(5)-P(1)-C(6)	-177.0(4)
N(1)-C(6)-P(1)-C(5)	-0.5(3)
C(7)-C(6)-P(1)-C(5)	176.9(4)

N(3)-C(11)-P(2)-C(11)#1	0.2(2)
C(12')-C(11)-P(2)-C(11)#1	-173.0(8)
C(12)-C(11)-P(2)-C(11)#1	173.7(7)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y,-z+3/2

4.4 Crystal structural analysis data for 6

Table 1. Crystal data and structure refinement for 130309-2c.

Identification code	130309-2c
Empirical formula	C ₃₈ H ₇₀ N ₆ Nd O ₂ P ₃
Formula weight	880.15
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 18.6636(8) Å alpha = 90 deg. b = 12.8610(6) Å beta = 102.553(4) deg. c = 20.2165(8) Å gamma = 90 deg.
Volume	4736.6(4) Å ³
Z, Calculated density	4, 1.234 Mg/m ³
Absorption coefficient	1.232 mm ⁻¹
F(000)	1844
Crystal size	0.26 x 0.21 x 0.14 mm
Theta range for data collection	3.00 to 25.68 deg.
Limiting indices	-22 ≤ h ≤ 22, -15 ≤ k ≤ 14, -24 ≤ l ≤ 24
Reflections collected / unique	10605 / 4499 [R(int) = 0.0464]
Completeness to theta = 25.68	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.60938
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4499 / 193 / 330
Goodness-of-fit on F ²	1.060
Final R indices [I > 2σ(I)]	R1 = 0.0466, wR2 = 0.1105
R indices (all data)	R1 = 0.0563, wR2 = 0.1202
Largest diff. peak and hole	1.193 and -1.031 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 130309-2c.

$U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
C(4)	8657(3)	2257(4)	9038(2)	59(1)
C(5)	8935(3)	3332(4)	8883(2)	44(1)
C(6)	9265(2)	5107(4)	8696(2)	43(1)
C(7)	9395(3)	6259(4)	8624(2)	56(1)
C(8)	8866(4)	6668(4)	7990(3)	80(2)
C(9)	9252(5)	6855(5)	9243(4)	89(2)
C(10)	10189(4)	6458(5)	8588(4)	85(2)
C(11)	9432(2)	484(4)	7087(3)	56(1)
C(12)	8738(8)	356(9)	6508(7)	89(2)
C(13)	8499(7)	-780(9)	6467(7)	95(2)
C(14)	8118(6)	1065(11)	6621(7)	91(2)
C(15)	8902(6)	608(11)	5805(6)	98(3)
C(16)	11278(10)	3940(20)	9040(5)	86(4)
C(17)	12038(7)	4402(19)	9242(8)	92(4)
C(18)	12386(9)	3944(17)	8690(8)	92(4)
C(19)	11796(7)	4020(20)	8056(8)	89(4)
C(12')	8696(11)	262(12)	6652(8)	90(2)
C(13')	8311(9)	1262(13)	6364(10)	91(2)
C(14')	8813(9)	-447(14)	6081(8)	96(2)

C(15')	8173(7)	-248(13)	7051(8)	95(3)
C(16')	11167(7)	3820(20)	9031(4)	65(4)
C(17')	11966(6)	3767(18)	9398(6)	70(4)
C(18')	12422(8)	4038(18)	8893(7)	70(4)
C(19')	11869(6)	4100(20)	8228(7)	61(4)
Nd(1)	10000	3289(1)	7500	36(1)
N(1)	9484(2)	4434(3)	8275(2)	42(1)
N(2)	9295(2)	3424(3)	8386(2)	43(1)
N(3)	9674(2)	1446(3)	7261(2)	47(1)
O(1)	11150(2)	3789(3)	8313(1)	55(1)
P(1)	8807(1)	4510(1)	9266(1)	56(1)
P(2)	10000	-496(2)	7500	83(1)
C(1)	8205(9)	2342(10)	9580(7)	70(4)
C(2)	9188(9)	1381(11)	9004(11)	98(5)
C(3)	7967(7)	2057(13)	8475(6)	74(4)
C(1')	8522(14)	2247(15)	9757(6)	78(5)
C(3')	8248(15)	1739(17)	8383(7)	96(7)
C(2')	9341(8)	1586(14)	9288(12)	84(6)

Table 3. Bond lengths [Å] and angles [deg] for 130309-2c.

C(4)-C(2)	1.513(8)
C(4)-C(1)	1.524(7)
C(4)-C(1')	1.527(8)
C(4)-C(3')	1.530(8)
C(4)-C(5)	1.533(7)
C(4)-C(2')	1.533(8)
C(4)-C(3)	1.545(7)
C(5)-N(2)	1.331(6)
C(5)-P(1)	1.740(5)
C(6)-N(1)	1.339(6)
C(6)-C(7)	1.514(7)
C(6)-P(1)	1.754(4)
C(7)-C(10)	1.522(8)
C(7)-C(8)	1.529(8)
C(7)-C(9)	1.540(8)
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-N(3)	1.338(6)
C(11)-C(12')	1.49(2)

C(11)-C(12)	1.554(17)
C(11)-P(2)	1.739(5)
C(12)-C(13)	1.524(9)
C(12)-C(14)	1.530(9)
C(12)-C(15)	1.550(9)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-O(1)	1.451(9)
C(16)-C(17)	1.509(9)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-C(18)	1.525(9)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(18)-C(19)	1.501(9)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(19)-O(1)	1.445(9)
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(12')-C(14')	1.523(10)
C(12')-C(13')	1.526(10)
C(12')-C(15')	1.540(10)

C(13')-H(13D)	0.9600
C(13')-H(13E)	0.9600
C(13')-H(13F)	0.9600
C(14')-H(14D)	0.9600
C(14')-H(14E)	0.9600
C(14')-H(14F)	0.9600
C(15')-H(15D)	0.9600
C(15')-H(15E)	0.9600
C(15')-H(15F)	0.9600
C(16')-O(1)	1.445(9)
C(16')-C(17')	1.517(9)
C(16')-H(16C)	0.9700
C(16')-H(16D)	0.9700
C(17')-C(18')	1.505(9)
C(17')-H(17C)	0.9700
C(17')-H(17D)	0.9700
C(18')-C(19')	1.509(8)
C(18')-H(18C)	0.9700
C(18')-H(18D)	0.9700
C(19')-O(1)	1.447(8)
C(19')-H(19C)	0.9700
C(19')-H(19D)	0.9700
Nd(1)-N(2)#1	2.448(4)
Nd(1)-N(2)	2.448(4)
Nd(1)-N(3)	2.469(4)
Nd(1)-N(3)#1	2.469(4)
Nd(1)-O(1)	2.487(3)
Nd(1)-O(1)#1	2.487(3)
Nd(1)-N(1)	2.491(4)
Nd(1)-N(1)#1	2.491(4)

N(1)-N(2)	1.377(5)
N(3)-N(3)#1	1.379(7)
P(2)-C(11)#1	1.739(5)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(2)-H(2A)	0.9600
C(2)-H(2B)	0.9600
C(2)-H(2C)	0.9600
C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600
C(3)-H(3C)	0.9600
C(1')-H(1'1)	0.9600
C(1')-H(1'2)	0.9600
C(1')-H(1'3)	0.9600
C(3')-H(3'1)	0.9600
C(3')-H(3'2)	0.9600
C(3')-H(3'3)	0.9600
C(2')-H(2'1)	0.9600
C(2')-H(2'2)	0.9600
C(2')-H(2'3)	0.9600
C(2)-C(4)-C(1)	123.8(11)
C(2)-C(4)-C(1')	106.4(14)
C(1)-C(4)-C(1')	23.9(7)
C(2)-C(4)-C(3')	81.1(10)
C(1)-C(4)-C(3')	113.8(14)
C(1')-C(4)-C(3')	131.7(14)
C(2)-C(4)-C(5)	114.0(8)
C(1)-C(4)-C(5)	110.3(6)

C(1')-C(4)-C(5)	109.6(8)
C(3')-C(4)-C(5)	110.1(8)
C(2)-C(4)-C(2')	24.2(8)
C(1)-C(4)-C(2')	110.7(12)
C(1')-C(4)-C(2')	88.8(15)
C(3')-C(4)-C(2')	105.2(11)
C(5)-C(4)-C(2')	106.2(8)
C(2)-C(4)-C(3)	107.0(9)
C(1)-C(4)-C(3)	92.3(11)
C(1')-C(4)-C(3)	114.6(13)
C(3')-C(4)-C(3)	27.1(8)
C(5)-C(4)-C(3)	105.4(6)
C(2')-C(4)-C(3)	130.6(10)
N(2)-C(5)-C(4)	119.0(4)
N(2)-C(5)-P(1)	113.5(3)
C(4)-C(5)-P(1)	127.5(3)
N(1)-C(6)-C(7)	119.6(4)
N(1)-C(6)-P(1)	113.2(4)
C(7)-C(6)-P(1)	127.1(3)
C(6)-C(7)-C(10)	110.3(5)
C(6)-C(7)-C(8)	109.3(4)
C(10)-C(7)-C(8)	111.1(5)
C(6)-C(7)-C(9)	110.4(4)
C(10)-C(7)-C(9)	107.3(5)
C(8)-C(7)-C(9)	108.4(5)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5

H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(3)-C(11)-C(12')	123.3(7)
N(3)-C(11)-C(12)	118.4(6)
C(12')-C(11)-C(12)	12.6(8)
N(3)-C(11)-P(2)	114.1(3)
C(12')-C(11)-P(2)	122.2(6)
C(12)-C(11)-P(2)	127.3(5)
C(13)-C(12)-C(14)	110.9(12)
C(13)-C(12)-C(15)	105.4(12)
C(14)-C(12)-C(15)	108.6(12)
C(13)-C(12)-C(11)	109.2(9)
C(14)-C(12)-C(11)	110.9(10)
C(15)-C(12)-C(11)	111.8(10)
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5

H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(12)-C(15)-H(15A)	109.5
C(12)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(12)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
O(1)-C(16)-C(17)	105.4(9)
O(1)-C(16)-H(16A)	110.7
C(17)-C(16)-H(16A)	110.7
O(1)-C(16)-H(16B)	110.7
C(17)-C(16)-H(16B)	110.7
H(16A)-C(16)-H(16B)	108.8
C(16)-C(17)-C(18)	100.1(13)
C(16)-C(17)-H(17A)	111.8
C(18)-C(17)-H(17A)	111.8
C(16)-C(17)-H(17B)	111.8
C(18)-C(17)-H(17B)	111.8
H(17A)-C(17)-H(17B)	109.5
C(19)-C(18)-C(17)	104.4(12)
C(19)-C(18)-H(18A)	110.9
C(17)-C(18)-H(18A)	110.9
C(19)-C(18)-H(18B)	110.9
C(17)-C(18)-H(18B)	110.9

H(18A)-C(18)-H(18B)	108.9
O(1)-C(19)-C(18)	101.1(11)
O(1)-C(19)-H(19A)	111.6
C(18)-C(19)-H(19A)	111.6
O(1)-C(19)-H(19B)	111.6
C(18)-C(19)-H(19B)	111.6
H(19A)-C(19)-H(19B)	109.4
C(11)-C(12')-C(14')	107.3(12)
C(11)-C(12')-C(13')	111.1(13)
C(14')-C(12')-C(13')	110.3(15)
C(11)-C(12')-C(15')	112.4(12)
C(14')-C(12')-C(15')	110.7(15)
C(13')-C(12')-C(15')	105.1(15)
C(12')-C(13')-H(13D)	109.5
C(12')-C(13')-H(13E)	109.5
H(13D)-C(13')-H(13E)	109.5
C(12')-C(13')-H(13F)	109.5
H(13D)-C(13')-H(13F)	109.5
H(13E)-C(13')-H(13F)	109.5
C(12')-C(14')-H(14D)	109.5
C(12')-C(14')-H(14E)	109.5
H(14D)-C(14')-H(14E)	109.5
C(12')-C(14')-H(14F)	109.5
H(14D)-C(14')-H(14F)	109.5
H(14E)-C(14')-H(14F)	109.5
C(12')-C(15')-H(15D)	109.5
C(12')-C(15')-H(15E)	109.5
H(15D)-C(15')-H(15E)	109.5
C(12')-C(15')-H(15F)	109.5
H(15D)-C(15')-H(15F)	109.5

H(15E)-C(15')-H(15F)	109.5
O(1)-C(16')-C(17')	107.2(9)
O(1)-C(16')-H(16C)	110.3
C(17')-C(16')-H(16C)	110.3
O(1)-C(16')-H(16D)	110.3
C(17')-C(16')-H(16D)	110.3
H(16C)-C(16')-H(16D)	108.5
C(18')-C(17')-C(16')	107.4(11)
C(18')-C(17')-H(17C)	110.2
C(16')-C(17')-H(17C)	110.2
C(18')-C(17')-H(17D)	110.2
C(16')-C(17')-H(17D)	110.2
H(17C)-C(17')-H(17D)	108.5
C(17')-C(18')-C(19')	103.9(10)
C(17')-C(18')-H(18C)	111.0
C(19')-C(18')-H(18C)	111.0
C(17')-C(18')-H(18D)	111.0
C(19')-C(18')-H(18D)	111.0
H(18C)-C(18')-H(18D)	109.0
O(1)-C(19')-C(18')	110.6(9)
O(1)-C(19')-H(19C)	109.5
C(18')-C(19')-H(19C)	109.5
O(1)-C(19')-H(19D)	109.5
C(18')-C(19')-H(19D)	109.5
H(19C)-C(19')-H(19D)	108.1
N(2)#1-Nd(1)-N(2)	171.84(18)
N(2)#1-Nd(1)-N(3)	94.22(13)
N(2)-Nd(1)-N(3)	93.61(13)
N(2)#1-Nd(1)-N(3)#1	93.61(13)
N(2)-Nd(1)-N(3)#1	94.22(13)

N(3)-Nd(1)-N(3)#1	32.43(16)
N(2)#1-Nd(1)-O(1)	86.63(11)
N(2)-Nd(1)-O(1)	91.27(11)
N(3)-Nd(1)-O(1)	121.18(12)
N(3)#1-Nd(1)-O(1)	88.76(12)
N(2)#1-Nd(1)-O(1)#1	91.27(11)
N(2)-Nd(1)-O(1)#1	86.63(11)
N(3)-Nd(1)-O(1)#1	88.76(12)
N(3)#1-Nd(1)-O(1)#1	121.18(12)
O(1)-Nd(1)-O(1)#1	150.06(18)
N(2)#1-Nd(1)-N(1)	139.52(13)
N(2)-Nd(1)-N(1)	32.36(11)
N(3)-Nd(1)-N(1)	125.35(13)
N(3)#1-Nd(1)-N(1)	123.84(13)
O(1)-Nd(1)-N(1)	80.08(11)
O(1)#1-Nd(1)-N(1)	82.35(11)
N(2)#1-Nd(1)-N(1)#1	32.36(11)
N(2)-Nd(1)-N(1)#1	139.52(13)
N(3)-Nd(1)-N(1)#1	123.84(13)
N(3)#1-Nd(1)-N(1)#1	125.34(13)
O(1)-Nd(1)-N(1)#1	82.35(11)
O(1)#1-Nd(1)-N(1)#1	80.08(11)
N(1)-Nd(1)-N(1)#1	107.51(17)
C(6)-N(1)-N(2)	112.5(4)
C(6)-N(1)-Nd(1)	174.4(3)
N(2)-N(1)-Nd(1)	72.1(2)
C(5)-N(2)-N(1)	113.3(4)
C(5)-N(2)-Nd(1)	170.6(3)
N(1)-N(2)-Nd(1)	75.6(2)
C(11)-N(3)-N(3)#1	112.4(3)

C(11)-N(3)-Nd(1)	173.8(3)
N(3)#1-N(3)-Nd(1)	73.79(8)
C(19)-O(1)-C(16')	121.2(9)
C(19)-O(1)-C(19')	14.3(10)
C(16')-O(1)-C(19')	107.1(8)
C(19)-O(1)-C(16)	111.7(8)
C(16')-O(1)-C(16)	10.3(15)
C(19')-O(1)-C(16)	97.5(8)
C(19)-O(1)-Nd(1)	118.9(7)
C(16')-O(1)-Nd(1)	119.8(6)
C(19')-O(1)-Nd(1)	133.1(6)
C(16)-O(1)-Nd(1)	129.3(7)
C(5)-P(1)-C(6)	87.5(2)
C(11)#1-P(2)-C(11)	87.1(3)
C(4)-C(1)-H(1A)	109.5
C(4)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(4)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(4)-C(2)-H(2A)	109.5
C(4)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(4)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(4)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(4)-C(3)-H(3C)	109.5

H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(4)-C(1')-H(1'1)	109.5
C(4)-C(1')-H(1'2)	109.5
H(1'1)-C(1')-H(1'2)	109.5
C(4)-C(1')-H(1'3)	109.5
H(1'1)-C(1')-H(1'3)	109.5
H(1'2)-C(1')-H(1'3)	109.5
C(4)-C(3')-H(3'1)	109.5
C(4)-C(3')-H(3'2)	109.5
H(3'1)-C(3')-H(3'2)	109.5
C(4)-C(3')-H(3'3)	109.5
H(3'1)-C(3')-H(3'3)	109.5
H(3'2)-C(3')-H(3'3)	109.5
C(4)-C(2')-H(2'1)	109.5
C(4)-C(2')-H(2'2)	109.5
H(2'1)-C(2')-H(2'2)	109.5
C(4)-C(2')-H(2'3)	109.5
H(2'1)-C(2')-H(2'3)	109.5
H(2'2)-C(2')-H(2'3)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y,-z+3/2

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 130309-2c.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
C(4)	75(3)	52(3)	56(3)	-1(2)	30(2)	-13(3)
C(5)	52(3)	47(3)	33(2)	4(2)	11(2)	-6(2)
C(6)	47(2)	45(3)	38(2)	3(2)	10(2)	7(2)
C(7)	69(3)	44(3)	58(3)	-8(2)	21(2)	-2(3)
C(8)	97(5)	51(4)	86(4)	19(3)	11(4)	8(3)
C(9)	136(6)	54(4)	88(5)	-21(3)	48(4)	-5(4)
C(10)	84(4)	55(4)	119(5)	-12(4)	30(4)	-19(3)
C(11)	44(3)	38(3)	81(3)	-7(2)	0(2)	-3(2)
C(12)	65(3)	73(4)	113(5)	-27(3)	-18(3)	-6(3)
C(13)	71(4)	76(4)	119(5)	-23(4)	-20(3)	-11(3)
C(14)	64(4)	76(4)	116(5)	-25(4)	-18(4)	-1(3)
C(15)	76(4)	86(5)	114(5)	-25(4)	-18(4)	-8(4)
C(16)	74(7)	113(9)	63(6)	-28(6)	-1(5)	-3(7)
C(17)	75(6)	115(8)	76(6)	-25(6)	-8(5)	-14(5)
C(18)	70(6)	113(8)	80(6)	-22(6)	-11(5)	-18(5)
C(19)	66(7)	112(9)	78(7)	-18(7)	-9(6)	-17(6)
C(12')	65(3)	73(4)	114(5)	-24(3)	-18(3)	-6(3)
C(13')	66(4)	74(4)	114(5)	-21(4)	-21(4)	-4(4)
C(14')	74(4)	80(4)	116(5)	-28(4)	-19(3)	-7(3)
C(15')	68(4)	81(5)	118(5)	-18(4)	-17(4)	-13(4)

C(16')	50(6)	93(9)	42(5)	-4(5)	-10(4)	3(6)
C(17')	54(5)	94(8)	51(5)	-4(5)	-15(4)	-8(5)
C(18')	50(5)	94(8)	53(5)	-5(5)	-14(4)	-20(5)
C(19')	40(5)	90(8)	46(6)	4(6)	-8(5)	-31(5)
Nd(1)	41(1)	32(1)	35(1)	0	8(1)	0
N(1)	48(2)	40(2)	39(2)	3(2)	14(2)	-1(2)
N(2)	49(2)	43(2)	39(2)	5(2)	12(2)	-3(2)
N(3)	37(2)	40(2)	57(2)	-5(2)	-2(2)	2(2)
O(1)	51(2)	64(2)	47(2)	-7(2)	4(1)	-8(2)
P(1)	71(1)	57(1)	48(1)	-3(1)	29(1)	-2(1)
P(2)	64(1)	31(1)	140(2)	0	-11(1)	0
C(1)	70(4)	71(4)	70(4)	4(2)	18(2)	-2(2)
C(2)	99(5)	97(6)	99(6)	2(2)	22(2)	-1(2)
C(3)	74(4)	71(4)	76(4)	1(2)	14(2)	-3(2)
C(1')	79(5)	79(5)	78(5)	2(2)	19(2)	-1(2)
C(3')	97(7)	96(7)	96(7)	-1(2)	22(2)	-2(2)
C(2')	86(6)	83(6)	84(6)	1(2)	20(2)	-2(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 130309-2c.

	x	y	z	U(eq)
H(8A)	8958	7394	7934	119
H(8B)	8370	6576	8039	119
H(8C)	8939	6291	7600	119
H(9A)	9558	6578	9648	134
H(9B)	8745	6781	9265	134
H(9C)	9362	7578	9202	134
H(10A)	10314	6031	8240	127
H(10B)	10505	6293	9016	127
H(10C)	10249	7177	8484	127
H(13A)	8356	-972	6879	143
H(13B)	8900	-1211	6406	143
H(13C)	8091	-872	6090	143
H(14A)	7723	1048	6228	137
H(14B)	8297	1763	6698	137
H(14C)	7944	827	7008	137
H(15A)	8478	448	5457	147
H(15B)	9311	199	5739	147
H(15C)	9017	1333	5785	147
H(16A)	11254	3282	9269	103
H(16B)	10916	4408	9154	103
H(17A)	12290	4177	9690	111

H(17B)	12025	5156	9225	111
H(18A)	12817	4337	8647	110
H(18B)	12526	3225	8789	110
H(19A)	11772	4717	7863	107
H(19B)	11868	3521	7718	107
H(13D)	8578	1576	6060	136
H(13E)	8293	1734	6727	136
H(13F)	7821	1104	6122	136
H(14D)	9161	-134	5855	144
H(14E)	8354	-545	5763	144
H(14F)	8996	-1107	6265	144
H(15D)	7701	-348	6756	142
H(15E)	8124	196	7421	142
H(15F)	8369	-908	7225	142
H(16C)	10899	3229	9158	78
H(16D)	10943	4452	9147	78
H(17C)	12060	4256	9772	84
H(17D)	12087	3074	9577	84
H(18C)	12785	3504	8878	84
H(18D)	12670	4698	9004	84
H(19C)	11847	4810	8059	74
H(19D)	12021	3655	7898	74
H(1A)	8056	1660	9689	105
H(1B)	7779	2761	9414	105
H(1C)	8497	2657	9980	105
H(2A)	9669	1572	9253	147
H(2B)	9203	1251	8540	147
H(2C)	9030	765	9199	147
H(3A)	8098	2068	8041	110
H(3B)	7609	2588	8489	110

H(3C)	7764	1389	8544	110
H(1'1)	8305	1596	9838	117
H(1'2)	8196	2805	9807	117
H(1'3)	8980	2334	10077	117
H(3'1)	8560	1721	8063	145
H(3'2)	7813	2129	8196	145
H(3'3)	8116	1043	8479	145
H(2'1)	9654	1918	9669	126
H(2'2)	9600	1505	8930	126
H(2'3)	9196	916	9422	126

Table 6. Torsion angles [deg] for 130309-2c.

C(2)-C(4)-C(5)-N(2)	40.4(11)
C(1)-C(4)-C(5)-N(2)	-175.0(8)
C(1')-C(4)-C(5)-N(2)	159.5(11)
C(3')-C(4)-C(5)-N(2)	-48.6(13)
C(2')-C(4)-C(5)-N(2)	64.9(11)
C(3)-C(4)-C(5)-N(2)	-76.6(9)
C(2)-C(4)-C(5)-P(1)	-142.6(10)
C(1)-C(4)-C(5)-P(1)	2.0(9)
C(1')-C(4)-C(5)-P(1)	-23.4(11)
C(3')-C(4)-C(5)-P(1)	128.5(13)
C(2')-C(4)-C(5)-P(1)	-118.1(10)
C(3)-C(4)-C(5)-P(1)	100.4(8)
N(1)-C(6)-C(7)-C(10)	-49.7(6)
P(1)-C(6)-C(7)-C(10)	133.5(4)
N(1)-C(6)-C(7)-C(8)	72.8(6)
P(1)-C(6)-C(7)-C(8)	-104.1(5)
N(1)-C(6)-C(7)-C(9)	-168.1(5)
P(1)-C(6)-C(7)-C(9)	15.1(7)
N(3)-C(11)-C(12)-C(13)	-171.8(9)
C(12')-C(11)-C(12)-C(13)	-55(4)
P(2)-C(11)-C(12)-C(13)	14.8(13)
N(3)-C(11)-C(12)-C(14)	-49.3(12)
C(12')-C(11)-C(12)-C(14)	67(4)
P(2)-C(11)-C(12)-C(14)	137.3(8)
N(3)-C(11)-C(12)-C(15)	72.0(10)
C(12')-C(11)-C(12)-C(15)	-172(4)

P(2)-C(11)-C(12)-C(15)	-101.4(9)
O(1)-C(16)-C(17)-C(18)	-28(2)
C(16)-C(17)-C(18)-C(19)	41(2)
C(17)-C(18)-C(19)-O(1)	-37.8(19)
N(3)-C(11)-C(12')-C(14')	128.1(11)
C(12)-C(11)-C(12')-C(14')	57(4)
P(2)-C(11)-C(12')-C(14')	-60.3(14)
N(3)-C(11)-C(12')-C(13')	7.5(16)
C(12)-C(11)-C(12')-C(13')	-63(4)
P(2)-C(11)-C(12')-C(13')	179.0(10)
N(3)-C(11)-C(12')-C(15')	-109.9(12)
C(12)-C(11)-C(12')-C(15')	179(5)
P(2)-C(11)-C(12')-C(15')	61.6(13)
O(1)-C(16')-C(17')-C(18')	17(3)
C(16')-C(17')-C(18')-C(19')	-7(2)
C(17')-C(18')-C(19')-O(1)	-6(2)
C(7)-C(6)-N(1)-N(2)	-177.0(4)
P(1)-C(6)-N(1)-N(2)	0.2(5)
C(7)-C(6)-N(1)-Nd(1)	39(3)
P(1)-C(6)-N(1)-Nd(1)	-143(3)
N(2)#1-Nd(1)-N(1)-C(6)	-37(3)
N(2)-Nd(1)-N(1)-C(6)	145(3)
N(3)-Nd(1)-N(1)-C(6)	158(3)
N(3)#1-Nd(1)-N(1)-C(6)	118(3)
O(1)-Nd(1)-N(1)-C(6)	36(3)
O(1)#1-Nd(1)-N(1)-C(6)	-119(3)
N(1)#1-Nd(1)-N(1)-C(6)	-42(3)
N(2)#1-Nd(1)-N(1)-N(2)	178.73(5)
N(3)-Nd(1)-N(1)-N(2)	12.8(3)
N(3)#1-Nd(1)-N(1)-N(2)	-26.8(3)

O(1)-Nd(1)-N(1)-N(2)	-108.5(2)
O(1)#1-Nd(1)-N(1)-N(2)	95.8(2)
N(1)#1-Nd(1)-N(1)-N(2)	172.8(3)
C(4)-C(5)-N(2)-N(1)	177.0(4)
P(1)-C(5)-N(2)-N(1)	-0.5(5)
C(4)-C(5)-N(2)-Nd(1)	-23(2)
P(1)-C(5)-N(2)-Nd(1)	159.7(17)
C(6)-N(1)-N(2)-C(5)	0.2(5)
Nd(1)-N(1)-N(2)-C(5)	176.7(4)
C(6)-N(1)-N(2)-Nd(1)	-176.5(3)
N(2)#1-Nd(1)-N(2)-C(5)	-167.1(19)
N(3)-Nd(1)-N(2)-C(5)	29.2(19)
N(3)#1-Nd(1)-N(2)-C(5)	-3.3(19)
O(1)-Nd(1)-N(2)-C(5)	-92.2(19)
O(1)#1-Nd(1)-N(2)-C(5)	117.7(19)
N(1)-Nd(1)-N(2)-C(5)	-161(2)
N(1)#1-Nd(1)-N(2)-C(5)	-171.8(18)
N(2)#1-Nd(1)-N(2)-N(1)	-5.8(2)
N(3)-Nd(1)-N(2)-N(1)	-169.6(2)
N(3)#1-Nd(1)-N(2)-N(1)	157.9(2)
O(1)-Nd(1)-N(2)-N(1)	69.1(2)
O(1)#1-Nd(1)-N(2)-N(1)	-81.0(2)
N(1)#1-Nd(1)-N(2)-N(1)	-10.6(4)
C(12')-C(11)-N(3)-N(3)#1	171.6(8)
C(12)-C(11)-N(3)-N(3)#1	-174.8(7)
P(2)-C(11)-N(3)-N(3)#1	-0.6(7)
C(12')-C(11)-N(3)-Nd(1)	-5(4)
C(12)-C(11)-N(3)-Nd(1)	8(4)
P(2)-C(11)-N(3)-Nd(1)	-177(3)
N(2)#1-Nd(1)-N(3)-C(11)	-93(3)

N(2)-Nd(1)-N(3)-C(11)	85(3)
N(3)#1-Nd(1)-N(3)-C(11)	177(4)
O(1)-Nd(1)-N(3)-C(11)	178(100)
O(1)#1-Nd(1)-N(3)-C(11)	-2(3)
N(1)-Nd(1)-N(3)-C(11)	78(3)
N(1)#1-Nd(1)-N(3)-C(11)	-79(3)
N(2)#1-Nd(1)-N(3)-N(3)#1	90.1(3)
N(2)-Nd(1)-N(3)-N(3)#1	-92.2(3)
O(1)-Nd(1)-N(3)-N(3)#1	1.5(4)
O(1)#1-Nd(1)-N(3)-N(3)#1	-178.7(3)
N(1)-Nd(1)-N(3)-N(3)#1	-99.0(3)
N(1)#1-Nd(1)-N(3)-N(3)#1	104.1(3)
C(18)-C(19)-O(1)-C(16')	16(2)
C(18)-C(19)-O(1)-C(19')	25(7)
C(18)-C(19)-O(1)-C(16)	20(2)
C(18)-C(19)-O(1)-Nd(1)	-162.9(9)
C(17')-C(16')-O(1)-C(19)	-18(3)
C(17')-C(16')-O(1)-C(19')	-20(2)
C(17')-C(16')-O(1)-C(16)	-41(11)
C(17')-C(16')-O(1)-Nd(1)	160.6(13)
C(18')-C(19')-O(1)-C(19)	-155(9)
C(18')-C(19')-O(1)-C(16')	16(2)
C(18')-C(19')-O(1)-C(16)	20(2)
C(18')-C(19')-O(1)-Nd(1)	-164.7(9)
C(17)-C(16)-O(1)-C(19)	6(2)
C(17)-C(16)-O(1)-C(16')	165(14)
C(17)-C(16)-O(1)-C(19')	4(2)
C(17)-C(16)-O(1)-Nd(1)	-171.0(11)
N(2)#1-Nd(1)-O(1)-C(19)	2.4(13)
N(2)-Nd(1)-O(1)-C(19)	-169.7(13)

N(3)-Nd(1)-O(1)-C(19)	95.3(13)
N(3)#1-Nd(1)-O(1)-C(19)	96.1(13)
O(1)#1-Nd(1)-O(1)-C(19)	-84.3(13)
N(1)-Nd(1)-O(1)-C(19)	-139.2(13)
N(1)#1-Nd(1)-O(1)-C(19)	-29.8(13)
N(2)#1-Nd(1)-O(1)-C(16')	-176.2(14)
N(2)-Nd(1)-O(1)-C(16')	11.7(14)
N(3)-Nd(1)-O(1)-C(16')	-83.3(14)
N(3)#1-Nd(1)-O(1)-C(16')	-82.5(14)
O(1)#1-Nd(1)-O(1)-C(16')	97.1(14)
N(1)-Nd(1)-O(1)-C(16')	42.2(14)
N(1)#1-Nd(1)-O(1)-C(16')	151.6(14)
N(2)#1-Nd(1)-O(1)-C(19')	5.0(15)
N(2)-Nd(1)-O(1)-C(19')	-167.1(15)
N(3)-Nd(1)-O(1)-C(19')	97.9(15)
N(3)#1-Nd(1)-O(1)-C(19')	98.7(15)
O(1)#1-Nd(1)-O(1)-C(19')	-81.6(15)
N(1)-Nd(1)-O(1)-C(19')	-136.6(15)
N(1)#1-Nd(1)-O(1)-C(19')	-27.2(15)
N(2)#1-Nd(1)-O(1)-C(16)	179.0(17)
N(2)-Nd(1)-O(1)-C(16)	6.9(17)
N(3)-Nd(1)-O(1)-C(16)	-88.1(17)
N(3)#1-Nd(1)-O(1)-C(16)	-87.3(17)
O(1)#1-Nd(1)-O(1)-C(16)	92.3(17)
N(1)-Nd(1)-O(1)-C(16)	37.4(17)
N(1)#1-Nd(1)-O(1)-C(16)	146.7(17)
N(2)-C(5)-P(1)-C(6)	0.5(4)
C(4)-C(5)-P(1)-C(6)	-176.7(4)
N(1)-C(6)-P(1)-C(5)	-0.4(3)
C(7)-C(6)-P(1)-C(5)	176.6(4)

N(3)-C(11)-P(2)-C(11)#1	0.2(2)
C(12')-C(11)-P(2)-C(11)#1	-172.0(9)
C(12)-C(11)-P(2)-C(11)#1	173.9(8)

Symmetry transformations used to generate equivalent atoms:

#1 $-x+2, y, -z+3/2$

4.5 Crystal structural analysis data for **7**

Table 1. Crystal data and structure refinement for 141204-1a.

Identification code	141204-1a
Empirical formula	C ₆₁ H ₆₂ N ₆ O ₃ P ₃ Pr
Formula weight	1160.99
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 14.3728(3) Å alpha = 104.834(2) deg. b = 14.5000(4) Å beta = 110.391(2) deg. c = 16.1044(4) Å gamma = 93.413(2) deg.
Volume	2999.83(13) Å ³
Z, Calculated density	2, 1.285 Mg/m ³
Absorption coefficient	0.939 mm ⁻¹
F(000)	1196
Crystal size	0.26 x 0.21 x 0.14 mm
Theta range for data collection	2.85 to 25.68 deg.
Limiting indices	-17 ≤ h ≤ 17, -17 ≤ k ≤ 17, -19 ≤ l ≤ 19
Reflections collected / unique	58336 / 11407 [R(int) = 0.0459]
Completeness to theta = 25.68	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.67553
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	11407 / 138 / 743
Goodness-of-fit on F ²	1.058
Final R indices [I > 2σ(I)]	R1 = 0.0428, wR2 = 0.1249
R indices (all data)	R1 = 0.0571, wR2 = 0.1353
Largest diff. peak and hole	0.952 and -0.790 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 141204-1a.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	10594(4)	7324(4)	8646(4)	65(1)
C(2)	11604(5)	7248(5)	8964(4)	83(2)
C(3)	11973(5)	6736(6)	9579(5)	97(2)
C(4)	11332(6)	6301(6)	9880(5)	104(3)
C(5)	10312(5)	6378(5)	9577(4)	88(2)
C(6)	9934(4)	6898(3)	8944(3)	56(1)
C(7)	8871(4)	7018(3)	8640(3)	51(1)
C(8)	7111(3)	7139(3)	8284(3)	50(1)
C(9)	6031(4)	7133(3)	8127(3)	52(1)
C(10)	5675(5)	7016(5)	8804(4)	78(2)
C(11)	4681(6)	7000(6)	8666(6)	101(2)
C(12)	4020(5)	7103(5)	7879(6)	88(2)
C(13)	4336(4)	7211(4)	7190(4)	68(1)
C(14)	5337(4)	7220(4)	7318(3)	57(1)
C(15)	6034(4)	9793(4)	8006(4)	69(1)
C(16)	6074(5)	10533(5)	8773(4)	80(2)
C(17)	5737(5)	11360(5)	8669(5)	85(2)
C(18)	5380(6)	11488(5)	7805(5)	94(2)
C(19)	5335(5)	10762(4)	7043(4)	73(2)
C(20)	5661(3)	9908(3)	7128(3)	50(1)

C(21)	5572(3)	9121(3)	6306(3)	46(1)
C(22)	5184(3)	7820(3)	4906(3)	48(1)
C(23)	4810(3)	7058(3)	4000(3)	52(1)
C(24)	3833(5)	6961(5)	3378(4)	87(2)
C(25)	3455(6)	6192(6)	2553(5)	103(2)
C(26)	4038(6)	5553(5)	2332(4)	87(2)
C(27)	4986(5)	5646(5)	2923(4)	84(2)
C(28)	5387(4)	6401(4)	3749(4)	68(1)
C(29)	8189(4)	6323(5)	3967(4)	80(2)
C(30)	7686(5)	5619(6)	3119(5)	101(2)
C(31)	8178(6)	4917(6)	2795(5)	100(2)
C(32)	9154(6)	4915(5)	3296(5)	97(2)
C(33)	9656(5)	5600(4)	4139(4)	79(2)
C(34)	9179(4)	6320(4)	4487(3)	56(1)
C(35)	9721(3)	7065(3)	5388(3)	48(1)
C(36)	10735(3)	8322(3)	6774(3)	49(1)
C(37)	11466(3)	9077(4)	7576(4)	58(1)
C(38)	12471(4)	9190(5)	7713(5)	88(2)
C(39)	13165(5)	9902(7)	8466(7)	118(3)
C(40)	12860(6)	10521(7)	9092(6)	114(3)
C(41)	11885(6)	10415(6)	8960(5)	114(3)
C(42)	11173(5)	9696(5)	8210(5)	89(2)
C(43)	6446(4)	5641(4)	5750(4)	61(1)
C(44)	6376(4)	4658(4)	5116(5)	74(2)
C(45)	7457(5)	4548(4)	5269(5)	88(2)
C(46)	8071(4)	5479(4)	5939(4)	66(1)
C(51)	8457(6)	10512(4)	7598(5)	95(2)
C(52)	8633(10)	11241(6)	8498(8)	155(4)
C(53)	9045(8)	10797(6)	9214(6)	136(4)
C(54)	8788(6)	9750(5)	8764(4)	94(2)

C(55)	4040(50)	4940(30)	9910(30)	163(5)
C(56')	4640(50)	5780(30)	10560(30)	163(5)
C(57')	5670(50)	5930(30)	10760(30)	162(5)
C(55')	6090(50)	5230(30)	10300(30)	159(5)
C(56)	5490(60)	4380(30)	9650(30)	162(5)
C(57)	4460(60)	4240(30)	9460(30)	169(5)
C(58)	3840(20)	3316(17)	8692(15)	177(6)
C(59)	9432(8)	6527(7)	1726(6)	124(3)
C(60)	10321(9)	6152(7)	1989(8)	124(3)
C(61)	11094(8)	6611(8)	2837(8)	125(3)
C(62)	10977(8)	7446(8)	3423(6)	121(3)
C(63)	10088(9)	7821(7)	3160(6)	121(3)
C(64)	9316(7)	7362(7)	2312(7)	129(3)
C(65)	8370(10)	7761(11)	2031(11)	153(4)
N(1)	8478(3)	7383(3)	7934(3)	49(1)
N(2)	7481(3)	7451(3)	7726(2)	48(1)
N(3)	6336(2)	8642(2)	6307(2)	42(1)
N(4)	6118(2)	7900(2)	5513(2)	42(1)
N(5)	9770(2)	8173(3)	6671(2)	45(1)
N(6)	9195(2)	7459(3)	5884(3)	45(1)
O(1)	7392(2)	6173(2)	5883(2)	49(1)
O(2)	7989(2)	9055(3)	5449(3)	62(1)
O(3)	8541(3)	9601(2)	7792(2)	64(1)
P(1)	7998(1)	6734(1)	9117(1)	66(1)
P(2)	4497(1)	8673(1)	5290(1)	60(1)
P(3)	11001(1)	7555(1)	5875(1)	63(1)
Pr(1)	7939(1)	8001(1)	6553(1)	38(1)
C(47)	7206(11)	9518(16)	4969(14)	95(4)
C(48)	7482(11)	9962(17)	4322(15)	102(4)
C(49)	8473(13)	9606(19)	4367(17)	104(4)

C(50)	8866(10)	9397(19)	5300(16)	97(5)
C(47')	7071(10)	9110(20)	4722(15)	95(5)
C(49')	8558(12)	10060(20)	4720(18)	101(5)
C(50')	8844(13)	9300(20)	5230(20)	99(6)
C(48')	7478(14)	9549(18)	4138(15)	98(5)

Table 3. Bond lengths [Å] and angles [deg] for 141204-1a.

C(1)-C(6)	1.382(8)
C(1)-C(2)	1.382(8)
C(1)-H(1)	0.9300
C(2)-C(3)	1.369(10)
C(2)-H(2)	0.9300
C(3)-C(4)	1.371(11)
C(3)-H(3)	0.9300
C(4)-C(5)	1.395(10)
C(4)-H(4)	0.9300
C(5)-C(6)	1.400(8)
C(5)-H(5)	0.9300
C(6)-C(7)	1.470(7)
C(7)-N(1)	1.337(6)
C(7)-P(1)	1.762(5)
C(8)-N(2)	1.344(6)
C(8)-C(9)	1.482(6)
C(8)-P(1)	1.753(5)
C(9)-C(14)	1.379(7)
C(9)-C(10)	1.397(7)
C(10)-C(11)	1.365(9)
C(10)-H(10)	0.9300
C(11)-C(12)	1.344(10)
C(11)-H(11)	0.9300
C(12)-C(13)	1.377(9)
C(12)-H(12)	0.9300
C(13)-C(14)	1.379(7)

C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(15)-C(20)	1.385(7)
C(15)-C(16)	1.394(8)
C(15)-H(15)	0.9300
C(16)-C(17)	1.348(9)
C(16)-H(16)	0.9300
C(17)-C(18)	1.371(9)
C(17)-H(17)	0.9300
C(18)-C(19)	1.375(8)
C(18)-H(18)	0.9300
C(19)-C(20)	1.373(7)
C(19)-H(19)	0.9300
C(20)-C(21)	1.470(6)
C(21)-N(3)	1.334(5)
C(21)-P(2)	1.750(4)
C(22)-N(4)	1.334(5)
C(22)-C(23)	1.481(6)
C(22)-P(2)	1.751(5)
C(23)-C(28)	1.375(7)
C(23)-C(24)	1.385(7)
C(24)-C(25)	1.403(9)
C(24)-H(24)	0.9300
C(25)-C(26)	1.348(10)
C(25)-H(25)	0.9300
C(26)-C(27)	1.337(9)
C(26)-H(26)	0.9300
C(27)-C(28)	1.394(7)
C(27)-H(27)	0.9300
C(28)-H(28)	0.9300

C(29)-C(34)	1.378(7)
C(29)-C(30)	1.393(9)
C(29)-H(29)	0.9300
C(30)-C(31)	1.371(10)
C(30)-H(30)	0.9300
C(31)-C(32)	1.354(10)
C(31)-H(31)	0.9300
C(32)-C(33)	1.376(9)
C(32)-H(32)	0.9300
C(33)-C(34)	1.387(7)
C(33)-H(33)	0.9300
C(34)-C(35)	1.479(7)
C(35)-N(6)	1.332(5)
C(35)-P(3)	1.748(4)
C(36)-N(5)	1.335(5)
C(36)-C(37)	1.472(7)
C(36)-P(3)	1.757(5)
C(37)-C(38)	1.377(7)
C(37)-C(42)	1.377(8)
C(38)-C(39)	1.387(10)
C(38)-H(38)	0.9300
C(39)-C(40)	1.381(12)
C(39)-H(39)	0.9300
C(40)-C(41)	1.334(11)
C(40)-H(40)	0.9300
C(41)-C(42)	1.400(9)
C(41)-H(41)	0.9300
C(42)-H(42)	0.9300
C(43)-O(1)	1.441(5)
C(43)-C(44)	1.500(7)

C(43)-H(43A)	0.9700
C(43)-H(43B)	0.9700
C(44)-C(45)	1.511(8)
C(44)-H(44A)	0.9700
C(44)-H(44B)	0.9700
C(45)-C(46)	1.489(8)
C(45)-H(45A)	0.9700
C(45)-H(45B)	0.9700
C(46)-O(1)	1.441(5)
C(46)-H(46A)	0.9700
C(46)-H(46B)	0.9700
C(51)-O(3)	1.435(8)
C(51)-C(52)	1.487(10)
C(51)-H(51A)	0.9700
C(51)-H(51B)	0.9700
C(52)-C(53)	1.430(13)
C(52)-H(52A)	0.9700
C(52)-H(52B)	0.9700
C(53)-C(54)	1.465(10)
C(53)-H(53A)	0.9700
C(53)-H(53B)	0.9700
C(54)-O(3)	1.433(7)
C(54)-H(54A)	0.9700
C(54)-H(54B)	0.9700
C(55)-C(55')#1	0.35(6)
C(55)-C(56)#1	1.08(6)
C(55)-C(56')	1.3900
C(55)-C(57)	1.3900
C(55)-C(57')#1	1.61(13)
C(55)-H(55A)	0.9599

C(56')-C(56)#1	0.35(6)
C(56')-C(57)#1	1.30(15)
C(56')-C(57')	1.3900
C(56')-C(55')#1	1.72(6)
C(56')-H(56A)	0.9600
C(57')-C(57)#1	0.35(5)
C(57')-C(58)#1	1.21(5)
C(57')-C(55')	1.3900
C(57')-C(56)#1	1.55(13)
C(57')-C(55)#1	1.61(12)
C(57')-H(57A)	0.9600
C(55')-C(55)#1	0.35(5)
C(55')-C(57)#1	1.23(14)
C(55')-C(56)	1.3900
C(55')-C(56')#1	1.72(6)
C(55')-H(55B)	0.9601
C(56)-C(56')#1	0.35(6)
C(56)-C(55)#1	1.08(6)
C(56)-C(57)	1.3900
C(56)-C(57')#1	1.55(14)
C(56)-H(56B)	0.9600
C(57)-C(57')#1	0.35(6)
C(57)-C(55')#1	1.23(16)
C(57)-C(56')#1	1.30(17)
C(57)-C(58)	1.534(10)
C(58)-C(57')#1	1.21(5)
C(58)-H(58A)	0.9600
C(58)-H(58B)	0.9600
C(58)-H(58C)	0.9600
C(59)-C(60)	1.3900

C(59)-C(64)	1.3900
C(59)-H(59)	0.9300
C(60)-C(61)	1.3900
C(60)-H(60)	0.9300
C(61)-C(62)	1.3900
C(61)-H(61)	0.9300
C(62)-C(63)	1.3900
C(62)-H(62)	0.9300
C(63)-C(64)	1.3900
C(63)-H(63)	0.9300
C(64)-C(65)	1.479(9)
C(65)-H(65A)	0.9600
C(65)-H(65B)	0.9600
C(65)-H(65C)	0.9600
N(1)-N(2)	1.369(5)
N(1)-Pr(1)	2.500(4)
N(2)-Pr(1)	2.494(4)
N(3)-N(4)	1.367(5)
N(3)-Pr(1)	2.477(3)
N(4)-Pr(1)	2.540(3)
N(5)-N(6)	1.363(5)
N(5)-Pr(1)	2.564(3)
N(6)-Pr(1)	2.476(3)
O(1)-Pr(1)	2.550(3)
O(2)-C(47)	1.436(8)
O(2)-C(50')	1.444(9)
O(2)-C(50)	1.446(8)
O(2)-C(47')	1.451(9)
O(2)-Pr(1)	2.639(3)
O(3)-Pr(1)	2.510(3)

C(47)-C(48)	1.503(9)
C(47)-H(47A)	0.9700
C(47)-H(47B)	0.9700
C(48)-C(49)	1.528(9)
C(48)-H(48A)	0.9700
C(48)-H(48B)	0.9700
C(49)-C(50)	1.527(10)
C(49)-H(49A)	0.9700
C(49)-H(49B)	0.9700
C(50)-H(50A)	0.9700
C(50)-H(50B)	0.9700
C(47')-C(48')	1.506(9)
C(47')-H(47C)	0.9700
C(47')-H(47D)	0.9700
C(49')-C(48')	1.528(10)
C(49')-C(50')	1.529(10)
C(49')-H(49C)	0.9700
C(49')-H(49D)	0.9700
C(50')-H(50C)	0.9700
C(50')-H(50D)	0.9700
C(48')-H(48C)	0.9700
C(48')-H(48D)	0.9700
C(6)-C(1)-C(2)	121.4(6)
C(6)-C(1)-H(1)	119.3
C(2)-C(1)-H(1)	119.3
C(3)-C(2)-C(1)	120.4(7)
C(3)-C(2)-H(2)	119.8
C(1)-C(2)-H(2)	119.8
C(2)-C(3)-C(4)	119.3(6)

C(2)-C(3)-H(3)	120.3
C(4)-C(3)-H(3)	120.3
C(3)-C(4)-C(5)	121.2(7)
C(3)-C(4)-H(4)	119.4
C(5)-C(4)-H(4)	119.4
C(4)-C(5)-C(6)	119.4(7)
C(4)-C(5)-H(5)	120.3
C(6)-C(5)-H(5)	120.3
C(1)-C(6)-C(5)	118.3(5)
C(1)-C(6)-C(7)	121.4(5)
C(5)-C(6)-C(7)	120.3(5)
N(1)-C(7)-C(6)	119.9(4)
N(1)-C(7)-P(1)	113.2(3)
C(6)-C(7)-P(1)	126.9(4)
N(2)-C(8)-C(9)	119.3(4)
N(2)-C(8)-P(1)	113.7(3)
C(9)-C(8)-P(1)	127.0(4)
C(14)-C(9)-C(10)	117.3(5)
C(14)-C(9)-C(8)	122.6(4)
C(10)-C(9)-C(8)	120.2(5)
C(11)-C(10)-C(9)	120.9(6)
C(11)-C(10)-H(10)	119.6
C(9)-C(10)-H(10)	119.6
C(12)-C(11)-C(10)	120.9(6)
C(12)-C(11)-H(11)	119.5
C(10)-C(11)-H(11)	119.5
C(11)-C(12)-C(13)	120.2(6)
C(11)-C(12)-H(12)	119.9
C(13)-C(12)-H(12)	119.9
C(12)-C(13)-C(14)	119.3(6)

C(12)-C(13)-H(13)	120.3
C(14)-C(13)-H(13)	120.3
C(9)-C(14)-C(13)	121.4(5)
C(9)-C(14)-H(14)	119.3
C(13)-C(14)-H(14)	119.3
C(20)-C(15)-C(16)	120.1(5)
C(20)-C(15)-H(15)	120.0
C(16)-C(15)-H(15)	120.0
C(17)-C(16)-C(15)	120.7(6)
C(17)-C(16)-H(16)	119.7
C(15)-C(16)-H(16)	119.7
C(16)-C(17)-C(18)	119.7(6)
C(16)-C(17)-H(17)	120.1
C(18)-C(17)-H(17)	120.1
C(17)-C(18)-C(19)	120.1(6)
C(17)-C(18)-H(18)	119.9
C(19)-C(18)-H(18)	119.9
C(20)-C(19)-C(18)	121.3(6)
C(20)-C(19)-H(19)	119.3
C(18)-C(19)-H(19)	119.3
C(19)-C(20)-C(15)	118.1(5)
C(19)-C(20)-C(21)	120.9(4)
C(15)-C(20)-C(21)	121.0(4)
N(3)-C(21)-C(20)	120.4(4)
N(3)-C(21)-P(2)	113.5(3)
C(20)-C(21)-P(2)	126.0(3)
N(4)-C(22)-C(23)	120.4(4)
N(4)-C(22)-P(2)	114.0(3)
C(23)-C(22)-P(2)	125.6(3)
C(28)-C(23)-C(24)	117.0(5)

C(28)-C(23)-C(22)	122.6(4)
C(24)-C(23)-C(22)	120.4(5)
C(23)-C(24)-C(25)	120.3(6)
C(23)-C(24)-H(24)	119.9
C(25)-C(24)-H(24)	119.9
C(26)-C(25)-C(24)	121.2(6)
C(26)-C(25)-H(25)	119.4
C(24)-C(25)-H(25)	119.4
C(27)-C(26)-C(25)	119.0(6)
C(27)-C(26)-H(26)	120.5
C(25)-C(26)-H(26)	120.5
C(26)-C(27)-C(28)	121.3(6)
C(26)-C(27)-H(27)	119.3
C(28)-C(27)-H(27)	119.3
C(23)-C(28)-C(27)	121.1(5)
C(23)-C(28)-H(28)	119.4
C(27)-C(28)-H(28)	119.4
C(34)-C(29)-C(30)	120.6(6)
C(34)-C(29)-H(29)	119.7
C(30)-C(29)-H(29)	119.7
C(31)-C(30)-C(29)	119.9(7)
C(31)-C(30)-H(30)	120.1
C(29)-C(30)-H(30)	120.1
C(32)-C(31)-C(30)	119.9(6)
C(32)-C(31)-H(31)	120.0
C(30)-C(31)-H(31)	120.0
C(31)-C(32)-C(33)	120.7(6)
C(31)-C(32)-H(32)	119.7
C(33)-C(32)-H(32)	119.7
C(32)-C(33)-C(34)	120.8(6)

C(32)-C(33)-H(33)	119.6
C(34)-C(33)-H(33)	119.6
C(29)-C(34)-C(33)	118.1(5)
C(29)-C(34)-C(35)	121.0(4)
C(33)-C(34)-C(35)	120.9(5)
N(6)-C(35)-C(34)	118.6(4)
N(6)-C(35)-P(3)	114.2(3)
C(34)-C(35)-P(3)	127.2(3)
N(5)-C(36)-C(37)	120.6(4)
N(5)-C(36)-P(3)	113.7(3)
C(37)-C(36)-P(3)	125.8(3)
C(38)-C(37)-C(42)	117.8(5)
C(38)-C(37)-C(36)	120.5(5)
C(42)-C(37)-C(36)	121.7(5)
C(37)-C(38)-C(39)	121.0(7)
C(37)-C(38)-H(38)	119.5
C(39)-C(38)-H(38)	119.5
C(40)-C(39)-C(38)	120.6(7)
C(40)-C(39)-H(39)	119.7
C(38)-C(39)-H(39)	119.7
C(41)-C(40)-C(39)	118.6(7)
C(41)-C(40)-H(40)	120.7
C(39)-C(40)-H(40)	120.7
C(40)-C(41)-C(42)	121.8(8)
C(40)-C(41)-H(41)	119.1
C(42)-C(41)-H(41)	119.1
C(37)-C(42)-C(41)	120.3(6)
C(37)-C(42)-H(42)	119.9
C(41)-C(42)-H(42)	119.9
O(1)-C(43)-C(44)	105.1(4)

O(1)-C(43)-H(43A)	110.7
C(44)-C(43)-H(43A)	110.7
O(1)-C(43)-H(43B)	110.7
C(44)-C(43)-H(43B)	110.7
H(43A)-C(43)-H(43B)	108.8
C(43)-C(44)-C(45)	104.3(4)
C(43)-C(44)-H(44A)	110.9
C(45)-C(44)-H(44A)	110.9
C(43)-C(44)-H(44B)	110.9
C(45)-C(44)-H(44B)	110.9
H(44A)-C(44)-H(44B)	108.9
C(46)-C(45)-C(44)	105.6(4)
C(46)-C(45)-H(45A)	110.6
C(44)-C(45)-H(45A)	110.6
C(46)-C(45)-H(45B)	110.6
C(44)-C(45)-H(45B)	110.6
H(45A)-C(45)-H(45B)	108.8
O(1)-C(46)-C(45)	105.5(4)
O(1)-C(46)-H(46A)	110.6
C(45)-C(46)-H(46A)	110.6
O(1)-C(46)-H(46B)	110.6
C(45)-C(46)-H(46B)	110.6
H(46A)-C(46)-H(46B)	108.8
O(3)-C(51)-C(52)	105.9(7)
O(3)-C(51)-H(51A)	110.6
C(52)-C(51)-H(51A)	110.6
O(3)-C(51)-H(51B)	110.6
C(52)-C(51)-H(51B)	110.6
H(51A)-C(51)-H(51B)	108.7
C(53)-C(52)-C(51)	107.5(8)

C(53)-C(52)-H(52A)	110.2
C(51)-C(52)-H(52A)	110.2
C(53)-C(52)-H(52B)	110.2
C(51)-C(52)-H(52B)	110.2
H(52A)-C(52)-H(52B)	108.5
C(52)-C(53)-C(54)	106.4(7)
C(52)-C(53)-H(53A)	110.5
C(54)-C(53)-H(53A)	110.5
C(52)-C(53)-H(53B)	110.5
C(54)-C(53)-H(53B)	110.5
H(53A)-C(53)-H(53B)	108.6
O(3)-C(54)-C(53)	107.1(7)
O(3)-C(54)-H(54A)	110.3
C(53)-C(54)-H(54A)	110.3
O(3)-C(54)-H(54B)	110.3
C(53)-C(54)-H(54B)	110.3
H(54A)-C(54)-H(54B)	108.6
C(55')#1-C(55)-C(56)#1	151(10)
C(55')#1-C(55)-C(56')	158(10)
C(56)#1-C(55)-C(56')	7(7)
C(55')#1-C(55)-C(57)	56(10)
C(56)#1-C(55)-C(57)	118(8)
C(56')-C(55)-C(57)	120.0
C(55')#1-C(55)-C(57')#1	46(10)
C(56)#1-C(55)-C(57')#1	126(10)
C(56')-C(55)-C(57')#1	129(5)
C(57)-C(55)-C(57')#1	10(5)
C(55')#1-C(55)-H(55A)	68.1
C(56)#1-C(55)-H(55A)	122.1
C(56')-C(55)-H(55A)	120.3

C(57)-C(55)-H(55A)	119.7
C(57')#1-C(55)-H(55A)	110.3
C(56)#1-C(56')-C(57)#1	97(10)
C(56)#1-C(56')-C(57')	111(10)
C(57)#1-C(56')-C(57')	14(3)
C(56)#1-C(56')-C(55)	22(10)
C(57)#1-C(56')-C(55)	107(2)
C(57')-C(56')-C(55)	120.0
C(56)#1-C(56')-C(55')#1	18(10)
C(57)#1-C(56')-C(55')#1	105(7)
C(57')-C(56')-C(55')#1	119(6)
C(55)-C(56')-C(55')#1	4(5)
C(56)#1-C(56')-H(56A)	124.1
C(57)#1-C(56')-H(56A)	133.1
C(57')-C(56')-H(56A)	120.0
C(55)-C(56')-H(56A)	120.0
C(55')#1-C(56')-H(56A)	121.2
C(57)#1-C(57')-C(58)#1	157(10)
C(57)#1-C(57')-C(55')	56(10)
C(58)#1-C(57')-C(55')	123(4)
C(57)#1-C(57')-C(56')	69(10)
C(58)#1-C(57')-C(56')	117(4)
C(55')-C(57')-C(56')	120.00(6)
C(57)#1-C(57')-C(56)#1	56(10)
C(58)#1-C(57')-C(56)#1	128(8)
C(55')-C(57')-C(56)#1	109(4)
C(56')-C(57')-C(56)#1	12(4)
C(57)#1-C(57')-C(55)#1	46(10)
C(58)#1-C(57')-C(55)#1	132(8)
C(55')-C(57')-C(55)#1	10(4)

C(56')-C(57')-C(55)#1	111(4)
C(56)#1-C(57')-C(55)#1	99(3)
C(57)#1-C(57')-H(57A)	158.0
C(58)#1-C(57')-H(57A)	3.4
C(55')-C(57')-H(57A)	120.0
C(56')-C(57')-H(57A)	120.0
C(56)#1-C(57')-H(57A)	131.0
C(55)#1-C(57')-H(57A)	129.2
C(55)#1-C(55')-C(57)#1	111(10)
C(55)#1-C(55')-C(57')	124(10)
C(57)#1-C(55')-C(57')	14(4)
C(55)#1-C(55')-C(56)	22(10)
C(57)#1-C(55')-C(56)	108(4)
C(57')-C(55')-C(56)	120.00(8)
C(55)#1-C(55')-C(56')#1	18(10)
C(57)#1-C(55')-C(56')#1	108(9)
C(57')-C(55')-C(56')#1	121(6)
C(56)-C(55')-C(56')#1	4(5)
C(55)#1-C(55')-H(55B)	111.5
C(57)#1-C(55')-H(55B)	132.0
C(57')-C(55')-H(55B)	120.0
C(56)-C(55')-H(55B)	120.0
C(56')#1-C(55')-H(55B)	118.6
C(56')#1-C(56)-C(55)#1	151(10)
C(56')#1-C(56)-C(57)	69(10)
C(55)#1-C(56)-C(57)	122(8)
C(56')#1-C(56)-C(55')	158(10)
C(55)#1-C(56)-C(55')	7(7)
C(57)-C(56)-C(55')	120.0
C(56')#1-C(56)-C(57')#1	56(10)

C(55)#1-C(56)-C(57')#1	132(10)
C(57)-C(56)-C(57')#1	12(4)
C(55')-C(56)-C(57')#1	131(4)
C(56')#1-C(56)-H(56B)	55.9
C(55)#1-C(56)-H(56B)	117.7
C(57)-C(56)-H(56B)	120.0
C(55')-C(56)-H(56B)	120.0
C(57')#1-C(56)-H(56B)	108.8
C(57')#1-C(57)-C(55')#1	111(10)
C(57')#1-C(57)-C(56')#1	97(10)
C(55')#1-C(57)-C(56')#1	144(7)
C(57')#1-C(57)-C(56)	111(10)
C(55')#1-C(57)-C(56)	132(4)
C(56')#1-C(57)-C(56)	14(3)
C(57')#1-C(57)-C(55)	124(10)
C(55')#1-C(57)-C(55)	14(4)
C(56')#1-C(57)-C(55)	133(3)
C(56)-C(57)-C(55)	120.0
C(57')#1-C(57)-C(58)	18(10)
C(55')#1-C(57)-C(58)	111(6)
C(56')#1-C(57)-C(58)	103(5)
C(56)-C(57)-C(58)	116(3)
C(55)-C(57)-C(58)	124(3)
C(57')#1-C(58)-C(57)	5(6)
C(57')#1-C(58)-H(58A)	109.5
C(57)-C(58)-H(58A)	110.6
C(57')#1-C(58)-H(58B)	109.5
C(57)-C(58)-H(58B)	113.1
H(58A)-C(58)-H(58B)	109.5
C(57')#1-C(58)-H(58C)	109.5

C(57)-C(58)-H(58C)	104.6
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5
C(60)-C(59)-C(64)	120.0
C(60)-C(59)-H(59)	120.0
C(64)-C(59)-H(59)	120.0
C(61)-C(60)-C(59)	120.0
C(61)-C(60)-H(60)	120.0
C(59)-C(60)-H(60)	120.0
C(60)-C(61)-C(62)	120.0
C(60)-C(61)-H(61)	120.0
C(62)-C(61)-H(61)	120.0
C(63)-C(62)-C(61)	120.0
C(63)-C(62)-H(62)	120.0
C(61)-C(62)-H(62)	120.0
C(62)-C(63)-C(64)	120.0
C(62)-C(63)-H(63)	120.0
C(64)-C(63)-H(63)	120.0
C(63)-C(64)-C(59)	120.0
C(63)-C(64)-C(65)	120.1(4)
C(59)-C(64)-C(65)	119.9(4)
C(64)-C(65)-H(65A)	109.5
C(64)-C(65)-H(65B)	109.5
H(65A)-C(65)-H(65B)	109.5
C(64)-C(65)-H(65C)	109.5
H(65A)-C(65)-H(65C)	109.5
H(65B)-C(65)-H(65C)	109.5
C(7)-N(1)-N(2)	113.5(4)
C(7)-N(1)-Pr(1)	172.2(3)
N(2)-N(1)-Pr(1)	73.8(2)

C(8)-N(2)-N(1)	112.6(4)
C(8)-N(2)-Pr(1)	172.6(3)
N(1)-N(2)-Pr(1)	74.4(2)
C(21)-N(3)-N(4)	113.3(3)
C(21)-N(3)-Pr(1)	169.7(3)
N(4)-N(3)-Pr(1)	76.7(2)
C(22)-N(4)-N(3)	112.5(3)
C(22)-N(4)-Pr(1)	175.2(3)
N(3)-N(4)-Pr(1)	71.7(2)
C(36)-N(5)-N(6)	112.9(4)
C(36)-N(5)-Pr(1)	176.1(3)
N(6)-N(5)-Pr(1)	70.8(2)
C(35)-N(6)-N(5)	112.9(3)
C(35)-N(6)-Pr(1)	169.2(3)
N(5)-N(6)-Pr(1)	77.9(2)
C(46)-O(1)-C(43)	104.7(4)
C(46)-O(1)-Pr(1)	124.5(3)
C(43)-O(1)-Pr(1)	126.1(3)
C(47)-O(2)-C(50')	105.9(9)
C(47)-O(2)-C(50)	104.8(11)
C(50')-O(2)-C(50)	6(2)
C(47)-O(2)-C(47')	23.7(12)
C(50')-O(2)-C(47')	109.4(13)
C(50)-O(2)-C(47')	110.9(11)
C(47)-O(2)-Pr(1)	128.3(6)
C(50')-O(2)-Pr(1)	125.8(8)
C(50)-O(2)-Pr(1)	126.4(7)
C(47')-O(2)-Pr(1)	120.6(7)
C(54)-O(3)-C(51)	109.3(5)
C(54)-O(3)-Pr(1)	126.0(4)

C(51)-O(3)-Pr(1)	123.2(3)
C(8)-P(1)-C(7)	87.0(2)
C(21)-P(2)-C(22)	86.7(2)
C(35)-P(3)-C(36)	86.4(2)
N(6)-Pr(1)-N(3)	146.43(12)
N(6)-Pr(1)-N(2)	128.22(12)
N(3)-Pr(1)-N(2)	82.10(12)
N(6)-Pr(1)-N(1)	99.95(12)
N(3)-Pr(1)-N(1)	112.72(12)
N(2)-Pr(1)-N(1)	31.82(12)
N(6)-Pr(1)-O(3)	113.80(12)
N(3)-Pr(1)-O(3)	79.56(11)
N(2)-Pr(1)-O(3)	83.98(12)
N(1)-Pr(1)-O(3)	81.79(12)
N(6)-Pr(1)-N(4)	120.79(11)
N(3)-Pr(1)-N(4)	31.59(11)
N(2)-Pr(1)-N(4)	93.52(11)
N(1)-Pr(1)-N(4)	124.27(12)
O(3)-Pr(1)-N(4)	110.01(11)
N(6)-Pr(1)-O(1)	76.19(11)
N(3)-Pr(1)-O(1)	104.04(10)
N(2)-Pr(1)-O(1)	73.70(11)
N(1)-Pr(1)-O(1)	75.38(11)
O(3)-Pr(1)-O(1)	156.50(12)
N(4)-Pr(1)-O(1)	79.21(10)
N(6)-Pr(1)-N(5)	31.32(11)
N(3)-Pr(1)-N(5)	150.40(12)
N(2)-Pr(1)-N(5)	120.10(12)
N(1)-Pr(1)-N(5)	88.39(12)
O(3)-Pr(1)-N(5)	83.47(11)

N(4)-Pr(1)-N(5)	145.38(11)
O(1)-Pr(1)-N(5)	101.20(10)
N(6)-Pr(1)-O(2)	73.17(11)
N(3)-Pr(1)-O(2)	78.28(10)
N(2)-Pr(1)-O(2)	158.40(11)
N(1)-Pr(1)-O(2)	159.64(12)
O(3)-Pr(1)-O(2)	83.64(12)
N(4)-Pr(1)-O(2)	74.28(10)
O(1)-Pr(1)-O(2)	119.86(11)
N(5)-Pr(1)-O(2)	75.86(10)
O(2)-C(47)-C(48)	112.5(10)
O(2)-C(47)-H(47A)	109.1
C(48)-C(47)-H(47A)	109.1
O(2)-C(47)-H(47B)	109.1
C(48)-C(47)-H(47B)	109.1
H(47A)-C(47)-H(47B)	107.8
C(47)-C(48)-C(49)	101.8(11)
C(47)-C(48)-H(48A)	111.4
C(49)-C(48)-H(48A)	111.4
C(47)-C(48)-H(48B)	111.4
C(49)-C(48)-H(48B)	111.4
H(48A)-C(48)-H(48B)	109.3
C(50)-C(49)-C(48)	103.9(13)
C(50)-C(49)-H(49A)	111.0
C(48)-C(49)-H(49A)	111.0
C(50)-C(49)-H(49B)	111.0
C(48)-C(49)-H(49B)	111.0
H(49A)-C(49)-H(49B)	109.0
O(2)-C(50)-C(49)	106.1(11)
O(2)-C(50)-H(50A)	110.5

C(49)-C(50)-H(50A)	110.5
O(2)-C(50)-H(50B)	110.5
C(49)-C(50)-H(50B)	110.5
H(50A)-C(50)-H(50B)	108.7
O(2)-C(47')-C(48')	101.8(12)
O(2)-C(47')-H(47C)	111.4
C(48')-C(47')-H(47C)	111.4
O(2)-C(47')-H(47D)	111.4
C(48')-C(47')-H(47D)	111.4
H(47C)-C(47')-H(47D)	109.3
C(48')-C(49')-C(50')	94.8(18)
C(48')-C(49')-H(49C)	112.8
C(50')-C(49')-H(49C)	112.8
C(48')-C(49')-H(49D)	112.8
C(50')-C(49')-H(49D)	112.8
H(49C)-C(49')-H(49D)	110.2
O(2)-C(50')-C(49')	105.4(12)
O(2)-C(50')-H(50C)	110.7
C(49')-C(50')-H(50C)	110.7
O(2)-C(50')-H(50D)	110.7
C(49')-C(50')-H(50D)	110.7
H(50C)-C(50')-H(50D)	108.8
C(47')-C(48')-C(49')	109.2(14)
C(47')-C(48')-H(48C)	109.8
C(49')-C(48')-H(48C)	109.8
C(47')-C(48')-H(48D)	109.8
C(49')-C(48')-H(48D)	109.8
H(48C)-C(48')-H(48D)	108.3

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 141204-1a.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
C(1)	59(3)	65(3)	61(3)	13(3)	12(2)	18(3)
C(2)	65(4)	89(5)	80(4)	11(3)	19(3)	19(3)
C(3)	65(4)	96(5)	89(5)	-1(4)	-3(4)	34(4)
C(4)	94(5)	107(6)	87(5)	38(4)	-4(4)	42(5)
C(5)	81(4)	95(5)	77(4)	38(4)	7(3)	21(4)
C(6)	59(3)	44(3)	44(2)	1(2)	4(2)	9(2)
C(7)	58(3)	42(2)	40(2)	6(2)	8(2)	5(2)
C(8)	58(3)	44(3)	44(2)	5(2)	20(2)	3(2)
C(9)	60(3)	41(2)	58(3)	10(2)	32(2)	5(2)
C(10)	85(4)	96(5)	72(4)	34(3)	44(3)	21(4)
C(11)	101(5)	137(7)	112(6)	59(5)	78(5)	33(5)
C(12)	76(4)	95(5)	127(6)	44(4)	68(4)	25(4)
C(13)	59(3)	64(3)	85(4)	20(3)	33(3)	11(3)
C(14)	56(3)	56(3)	61(3)	13(2)	30(2)	7(2)
C(15)	81(4)	59(3)	58(3)	13(3)	19(3)	16(3)
C(16)	96(4)	82(4)	54(3)	6(3)	28(3)	5(4)
C(17)	93(4)	65(4)	87(5)	-9(3)	43(4)	15(3)
C(18)	116(6)	65(4)	91(5)	8(3)	34(4)	40(4)
C(19)	82(4)	63(4)	69(3)	14(3)	24(3)	30(3)
C(20)	40(2)	53(3)	54(3)	12(2)	18(2)	13(2)

C(21)	42(2)	45(2)	49(2)	13(2)	15(2)	13(2)
C(22)	43(2)	46(3)	50(2)	13(2)	13(2)	7(2)
C(23)	52(3)	49(3)	47(2)	12(2)	12(2)	2(2)
C(24)	72(4)	78(4)	74(4)	1(3)	0(3)	19(3)
C(25)	82(5)	104(6)	70(4)	-4(4)	-8(3)	-7(4)
C(26)	100(5)	74(4)	61(4)	-10(3)	25(4)	-14(4)
C(27)	89(4)	71(4)	77(4)	-12(3)	38(4)	3(3)
C(28)	64(3)	68(4)	64(3)	3(3)	27(3)	6(3)
C(29)	62(3)	100(5)	67(4)	3(3)	27(3)	20(3)
C(30)	68(4)	147(7)	69(4)	6(4)	24(3)	2(4)
C(31)	103(5)	100(5)	80(4)	-18(4)	50(4)	-12(4)
C(32)	100(5)	78(5)	104(5)	-11(4)	55(4)	11(4)
C(33)	74(4)	70(4)	88(4)	2(3)	41(3)	18(3)
C(34)	52(3)	57(3)	64(3)	11(2)	32(2)	8(2)
C(35)	43(2)	47(3)	62(3)	16(2)	28(2)	13(2)
C(36)	40(2)	49(3)	63(3)	22(2)	21(2)	10(2)
C(37)	43(2)	55(3)	73(3)	25(3)	14(2)	5(2)
C(38)	50(3)	93(5)	105(5)	21(4)	17(3)	-3(3)
C(39)	56(4)	128(7)	134(7)	36(6)	0(4)	-27(4)
C(40)	88(6)	105(6)	103(6)	20(5)	-1(5)	-35(5)
C(41)	101(6)	99(6)	93(5)	-15(4)	16(4)	-19(5)
C(42)	65(4)	81(4)	94(5)	-2(4)	21(3)	-5(3)
C(43)	55(3)	51(3)	86(4)	17(3)	40(3)	5(2)
C(44)	66(3)	48(3)	100(4)	11(3)	31(3)	-3(3)
C(45)	78(4)	46(3)	125(6)	2(3)	39(4)	13(3)
C(46)	56(3)	51(3)	92(4)	24(3)	27(3)	19(2)
C(51)	117(6)	52(4)	99(5)	2(3)	38(4)	0(4)
C(52)	227(12)	61(5)	162(10)	-23(6)	99(9)	-2(6)
C(53)	161(9)	91(6)	91(6)	-32(5)	13(6)	14(6)
C(54)	112(5)	82(4)	55(3)	-13(3)	19(3)	9(4)

C(55)	213(15)	181(14)	133(17)	82(10)	77(14)	89(11)
C(56')	213(15)	183(14)	133(17)	83(10)	78(14)	88(11)
C(57')	214(15)	182(14)	131(17)	84(10)	77(14)	88(11)
C(55')	210(15)	183(14)	129(17)	83(10)	82(14)	90(11)
C(56)	213(15)	184(14)	131(17)	80(10)	81(14)	90(11)
C(57)	218(15)	184(14)	135(17)	79(10)	73(14)	89(11)
C(58)	224(16)	187(15)	142(16)	73(10)	67(14)	88(11)
C(59)	146(7)	128(7)	127(7)	58(6)	74(6)	-9(6)
C(60)	147(7)	126(7)	126(7)	54(6)	76(6)	-10(6)
C(61)	148(7)	127(7)	127(7)	55(6)	75(6)	-8(6)
C(62)	147(7)	120(7)	124(7)	52(5)	76(6)	-8(6)
C(63)	147(7)	122(7)	122(7)	56(6)	76(6)	-7(6)
C(64)	149(7)	132(7)	135(7)	64(5)	74(6)	-7(6)
C(65)	166(8)	148(8)	155(8)	60(7)	65(7)	-5(7)
N(1)	46(2)	50(2)	46(2)	11(2)	15(2)	9(2)
N(2)	47(2)	53(2)	44(2)	14(2)	18(2)	11(2)
N(3)	39(2)	39(2)	44(2)	11(2)	14(2)	7(2)
N(4)	39(2)	41(2)	43(2)	11(2)	14(2)	8(2)
N(5)	37(2)	44(2)	53(2)	12(2)	17(2)	6(2)
N(6)	38(2)	43(2)	55(2)	14(2)	20(2)	9(2)
O(1)	43(2)	38(2)	64(2)	10(1)	22(1)	7(1)
O(2)	51(2)	73(2)	87(2)	48(2)	36(2)	25(2)
O(3)	64(2)	52(2)	61(2)	-3(2)	21(2)	4(2)
P(1)	71(1)	76(1)	50(1)	29(1)	17(1)	6(1)
P(2)	42(1)	63(1)	61(1)	8(1)	7(1)	21(1)
P(3)	42(1)	69(1)	82(1)	17(1)	33(1)	12(1)
Pr(1)	34(1)	39(1)	41(1)	9(1)	14(1)	8(1)
C(47)	67(6)	115(8)	173(10)	112(7)	72(6)	52(5)
C(48)	76(6)	118(8)	174(9)	104(7)	71(6)	52(5)
C(49)	77(6)	120(8)	174(9)	99(7)	73(6)	46(5)

C(50)	66(7)	120(8)	172(10)	101(7)	78(7)	40(5)
C(47')	82(8)	108(10)	127(10)	93(8)	35(7)	33(6)
C(49')	92(8)	113(9)	128(9)	89(8)	38(6)	22(6)
C(50')	87(9)	115(10)	127(10)	91(8)	38(7)	22(7)
C(48')	91(8)	110(9)	126(9)	93(8)	34(6)	28(6)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 141204-1a.

	x	y	z	U(eq)
H(1)	10354	7670	8224	78
H(2)	12034	7546	8758	100
H(3)	12652	6683	9792	116
H(4)	11581	5948	10295	125
H(5)	9888	6087	9793	106
H(10)	6122	6949	9356	94
H(11)	4459	6917	9124	121
H(12)	3347	7101	7800	106
H(13)	3879	7278	6643	82
H(14)	5549	7286	6850	68
H(15)	6258	9221	8085	82
H(16)	6335	10455	9362	96
H(17)	5748	11843	9181	102
H(18)	5167	12066	7733	112
H(19)	5078	10852	6459	88
H(24)	3426	7407	3507	104
H(25)	2791	6123	2151	124
H(26)	3784	5054	1778	105
H(27)	5386	5199	2779	101
H(28)	6055	6461	4136	82
H(29)	7853	6799	4184	96

H(30)	7017	5625	2772	121
H(31)	7841	4443	2232	120
H(32)	9490	4446	3067	116
H(33)	10322	5581	4480	94
H(38)	12688	8782	7295	106
H(39)	13842	9963	8550	142
H(40)	13323	11001	9595	137
H(41)	11674	10830	9378	137
H(42)	10500	9636	8139	107
H(43A)	5891	5953	5470	74
H(43B)	6435	5594	6337	74
H(44A)	5999	4621	4475	89
H(44B)	6054	4160	5276	89
H(45A)	7634	4015	5521	105
H(45B)	7563	4429	4690	105
H(46A)	8344	5422	6562	79
H(46B)	8624	5672	5772	79
H(51A)	7792	10493	7149	114
H(51B)	8954	10665	7352	114
H(52A)	9098	11804	8589	186
H(52B)	8005	11445	8507	186
H(53A)	8758	10982	9683	163
H(53B)	9769	10993	9506	163
H(54A)	9355	9436	9013	112
H(54B)	8219	9483	8870	112
H(55A)	3327	4836	9775	195
H(56A)	4353	6263	10879	195
H(57A)	6091	6508	11206	195
H(55B)	6804	5328	10436	190
H(56B)	5778	3902	9338	195

H(58A)	4268	2952	8438	266
H(58B)	3303	3441	8201	266
H(58C)	3568	2952	8999	266
H(59)	8915	6220	1158	149
H(60)	10399	5594	1597	149
H(61)	11689	6360	3013	150
H(62)	11494	7753	3990	146
H(63)	10010	8380	3552	145
H(65A)	8396	8313	2524	230
H(65B)	7812	7277	1903	230
H(65C)	8286	7952	1484	230
H(47A)	7066	10017	5419	114
H(47B)	6597	9045	4617	114
H(48A)	7574	10663	4537	122
H(48B)	6976	9733	3698	122
H(49A)	8361	9025	3861	125
H(49B)	8941	10098	4342	125
H(50A)	9298	8908	5287	117
H(50B)	9249	9979	5792	117
H(47C)	6667	9526	4972	114
H(47D)	6673	8478	4370	114
H(49C)	8591	10694	5134	121
H(49D)	8949	10119	4347	121
H(50C)	8974	8738	4835	119
H(50D)	9441	9564	5789	119
H(48C)	7063	10006	3918	118
H(48D)	7465	9045	3603	118

Table 6. Torsion angles [deg] for 141204-1a.

C(6)-C(1)-C(2)-C(3)	0.6(9)
C(1)-C(2)-C(3)-C(4)	-0.2(10)
C(2)-C(3)-C(4)-C(5)	-0.6(12)
C(3)-C(4)-C(5)-C(6)	0.9(11)
C(2)-C(1)-C(6)-C(5)	-0.3(8)
C(2)-C(1)-C(6)-C(7)	177.1(5)
C(4)-C(5)-C(6)-C(1)	-0.4(9)
C(4)-C(5)-C(6)-C(7)	-177.9(6)
C(1)-C(6)-C(7)-N(1)	12.9(7)
C(5)-C(6)-C(7)-N(1)	-169.7(5)
C(1)-C(6)-C(7)-P(1)	-166.5(4)
C(5)-C(6)-C(7)-P(1)	10.8(7)
N(2)-C(8)-C(9)-C(14)	15.2(7)
P(1)-C(8)-C(9)-C(14)	-162.3(4)
N(2)-C(8)-C(9)-C(10)	-166.2(5)
P(1)-C(8)-C(9)-C(10)	16.4(7)
C(14)-C(9)-C(10)-C(11)	-0.7(9)
C(8)-C(9)-C(10)-C(11)	-179.4(6)
C(9)-C(10)-C(11)-C(12)	-0.5(12)
C(10)-C(11)-C(12)-C(13)	1.1(12)
C(11)-C(12)-C(13)-C(14)	-0.5(10)
C(10)-C(9)-C(14)-C(13)	1.3(8)
C(8)-C(9)-C(14)-C(13)	179.9(5)
C(12)-C(13)-C(14)-C(9)	-0.7(8)
C(20)-C(15)-C(16)-C(17)	1.0(10)
C(15)-C(16)-C(17)-C(18)	-1.9(11)

C(16)-C(17)-C(18)-C(19)	2.1(11)
C(17)-C(18)-C(19)-C(20)	-1.3(11)
C(18)-C(19)-C(20)-C(15)	0.3(9)
C(18)-C(19)-C(20)-C(21)	177.5(6)
C(16)-C(15)-C(20)-C(19)	-0.2(8)
C(16)-C(15)-C(20)-C(21)	-177.4(5)
C(19)-C(20)-C(21)-N(3)	135.8(5)
C(15)-C(20)-C(21)-N(3)	-47.1(7)
C(19)-C(20)-C(21)-P(2)	-47.8(7)
C(15)-C(20)-C(21)-P(2)	129.3(5)
N(4)-C(22)-C(23)-C(28)	1.0(7)
P(2)-C(22)-C(23)-C(28)	-179.0(4)
N(4)-C(22)-C(23)-C(24)	178.6(5)
P(2)-C(22)-C(23)-C(24)	-1.4(7)
C(28)-C(23)-C(24)-C(25)	2.9(10)
C(22)-C(23)-C(24)-C(25)	-174.9(6)
C(23)-C(24)-C(25)-C(26)	-2.2(12)
C(24)-C(25)-C(26)-C(27)	1.4(12)
C(25)-C(26)-C(27)-C(28)	-1.3(11)
C(24)-C(23)-C(28)-C(27)	-2.9(9)
C(22)-C(23)-C(28)-C(27)	174.8(5)
C(26)-C(27)-C(28)-C(23)	2.2(10)
C(34)-C(29)-C(30)-C(31)	-0.1(11)
C(29)-C(30)-C(31)-C(32)	-0.6(12)
C(30)-C(31)-C(32)-C(33)	1.4(12)
C(31)-C(32)-C(33)-C(34)	-1.3(11)
C(30)-C(29)-C(34)-C(33)	0.2(10)
C(30)-C(29)-C(34)-C(35)	179.9(6)
C(32)-C(33)-C(34)-C(29)	0.5(10)
C(32)-C(33)-C(34)-C(35)	-179.2(6)

C(29)-C(34)-C(35)-N(6)	29.1(7)
C(33)-C(34)-C(35)-N(6)	-151.3(5)
C(29)-C(34)-C(35)-P(3)	-147.3(5)
C(33)-C(34)-C(35)-P(3)	32.4(7)
N(5)-C(36)-C(37)-C(38)	175.8(5)
P(3)-C(36)-C(37)-C(38)	-4.9(7)
N(5)-C(36)-C(37)-C(42)	-4.5(8)
P(3)-C(36)-C(37)-C(42)	174.7(5)
C(42)-C(37)-C(38)-C(39)	0.1(10)
C(36)-C(37)-C(38)-C(39)	179.8(6)
C(37)-C(38)-C(39)-C(40)	-0.5(13)
C(38)-C(39)-C(40)-C(41)	0.4(14)
C(39)-C(40)-C(41)-C(42)	0.2(14)
C(38)-C(37)-C(42)-C(41)	0.4(10)
C(36)-C(37)-C(42)-C(41)	-179.2(6)
C(40)-C(41)-C(42)-C(37)	-0.6(13)
O(1)-C(43)-C(44)-C(45)	24.7(6)
C(43)-C(44)-C(45)-C(46)	-2.5(7)
C(44)-C(45)-C(46)-O(1)	-20.5(7)
O(3)-C(51)-C(52)-C(53)	13.5(12)
C(51)-C(52)-C(53)-C(54)	-19.8(13)
C(52)-C(53)-C(54)-O(3)	18.7(11)
C(55')#1-C(55)-C(56')-C(56)#1	0(11)
C(57)-C(55)-C(56')-C(56)#1	73(68)
C(57')#1-C(55)-C(56')-C(56)#1	67(66)
C(55')#1-C(55)-C(56')-C(57)#1	-67(71)
C(56)#1-C(55)-C(56')-C(57)#1	-67(67)
C(57)-C(55)-C(56')-C(57)#1	6(6)
C(57')#1-C(55)-C(56')-C(57)#1	0.0(17)
C(55')#1-C(55)-C(56')-C(57')	-73(73)

C(56)#1-C(55)-C(56')-C(57')	-73(69)
C(57)-C(55)-C(56')-C(57')	0.0
C(57')#1-C(55)-C(56')-C(57')	-6(6)
C(56)#1-C(55)-C(56')-C(55')#1	0(11)
C(57)-C(55)-C(56')-C(55')#1	73(72)
C(57')#1-C(55)-C(56')-C(55')#1	67(70)
C(56)#1-C(56')-C(57')-C(57)#1	0(3)
C(55)-C(56')-C(57')-C(57)#1	23(21)
C(55')#1-C(56')-C(57')-C(57)#1	18(17)
C(56)#1-C(56')-C(57')-C(58)#1	155(25)
C(57)#1-C(56')-C(57')-C(58)#1	155(25)
C(55)-C(56')-C(57')-C(58)#1	178(4)
C(55')#1-C(56')-C(57')-C(58)#1	173(8)
C(56)#1-C(56')-C(57')-C(55')	-23(22)
C(57)#1-C(56')-C(57')-C(55')	-23(21)
C(55)-C(56')-C(57')-C(55')	0.0
C(55')#1-C(56')-C(57')-C(55')	-5(5)
C(57)#1-C(56')-C(57')-C(56)#1	0(3)
C(55)-C(56')-C(57')-C(56)#1	23(22)
C(55')#1-C(56')-C(57')-C(56)#1	18(17)
C(56)#1-C(56')-C(57')-C(55)#1	-18(17)
C(57)#1-C(56')-C(57')-C(55)#1	-18(17)
C(55)-C(56')-C(57')-C(55)#1	5(5)
C(55')#1-C(56')-C(57')-C(55)#1	0.0(7)
C(57)#1-C(57')-C(55')-C(55)#1	0(3)
C(58)#1-C(57')-C(55')-C(55)#1	-152(28)
C(56')-C(57')-C(55')-C(55)#1	26(25)
C(56)#1-C(57')-C(55')-C(55)#1	21(21)
C(58)#1-C(57')-C(55')-C(57)#1	-152(28)
C(56')-C(57')-C(55')-C(57)#1	26(24)

C(56)#1-C(57')-C(55')-C(57)#1	21(20)
C(55)#1-C(57')-C(55')-C(57)#1	0(3)
C(57)#1-C(57')-C(55')-C(56)	-26(24)
C(58)#1-C(57')-C(55')-C(56)	-178(4)
C(56')-C(57')-C(55')-C(56)	0.0
C(56)#1-C(57')-C(55')-C(56)	-5(5)
C(55)#1-C(57')-C(55')-C(56)	-26(25)
C(57)#1-C(57')-C(55')-C(56')#1	-21(20)
C(58)#1-C(57')-C(55')-C(56')#1	-173(9)
C(56')-C(57')-C(55')-C(56')#1	5(5)
C(56)#1-C(57')-C(55')-C(56')#1	0.0(13)
C(55)#1-C(57')-C(55')-C(56')#1	-21(21)
C(55)#1-C(55')-C(56)-C(56')#1	0(7)
C(57)#1-C(55')-C(56)-C(56')#1	101(74)
C(57')-C(55')-C(56)-C(56')#1	107(73)
C(57)#1-C(55')-C(56)-C(55)#1	101(71)
C(57')-C(55')-C(56)-C(55)#1	107(70)
C(56')#1-C(55')-C(56)-C(55)#1	0(7)
C(55)#1-C(55')-C(56)-C(57)	-107(70)
C(57)#1-C(55')-C(56)-C(57)	-6(6)
C(57')-C(55')-C(56)-C(57)	0.0
C(56')#1-C(55')-C(56)-C(57)	-107(73)
C(55)#1-C(55')-C(56)-C(57')#1	-101(71)
C(57)#1-C(55')-C(56)-C(57')#1	0.0(18)
C(57')-C(55')-C(56)-C(57')#1	6(7)
C(56')#1-C(55')-C(56)-C(57')#1	-101(74)
C(56')#1-C(56)-C(57)-C(57')#1	0(3)
C(55)#1-C(56)-C(57)-C(57')#1	150(31)
C(55')-C(56)-C(57)-C(57')#1	157(24)
C(56')#1-C(56)-C(57)-C(55')#1	-150(31)

C(55)#1-C(56)-C(57)-C(55')#1	0.0(11)
C(55')-C(56)-C(57)-C(55')#1	8(8)
C(57')#1-C(56)-C(57)-C(55')#1	-150(31)
C(55)#1-C(56)-C(57)-C(56')#1	150(30)
C(55')-C(56)-C(57)-C(56')#1	157(23)
C(57')#1-C(56)-C(57)-C(56')#1	0(3)
C(56')#1-C(56)-C(57)-C(55)	-157(23)
C(55)#1-C(56)-C(57)-C(55)	-8(8)
C(55')-C(56)-C(57)-C(55)	0.0
C(57')#1-C(56)-C(57)-C(55)	-157(24)
C(56')#1-C(56)-C(57)-C(58)	19(20)
C(55)#1-C(56)-C(57)-C(58)	169(10)
C(55')-C(56)-C(57)-C(58)	176(3)
C(57')#1-C(56)-C(57)-C(58)	19(21)
C(55')#1-C(55)-C(57)-C(57')#1	0(4)
C(56)#1-C(55)-C(57)-C(57')#1	-147(34)
C(56')-C(55)-C(57)-C(57')#1	-154(27)
C(56)#1-C(55)-C(57)-C(55')#1	-147(33)
C(56')-C(55)-C(57)-C(55')#1	-154(26)
C(57')#1-C(55)-C(57)-C(55')#1	0(4)
C(55')#1-C(55)-C(57)-C(56')#1	147(33)
C(56)#1-C(55)-C(57)-C(56')#1	0.0(19)
C(56')-C(55)-C(57)-C(56')#1	-8(8)
C(57')#1-C(55)-C(57)-C(56')#1	147(34)
C(55')#1-C(55)-C(57)-C(56)	154(26)
C(56)#1-C(55)-C(57)-C(56)	8(7)
C(56')-C(55)-C(57)-C(56)	0.0
C(57')#1-C(55)-C(57)-C(56)	154(27)
C(55')#1-C(55)-C(57)-C(58)	-22(24)
C(56)#1-C(55)-C(57)-C(58)	-169(10)

C(56')-C(55)-C(57)-C(58)	-176(3)
C(57')#1-C(55)-C(57)-C(58)	-22(24)
C(55')#1-C(57)-C(58)-C(57')#1	92(82)
C(56')#1-C(57)-C(58)-C(57')#1	-74(80)
C(56)-C(57)-C(58)-C(57')#1	-79(82)
C(55)-C(57)-C(58)-C(57')#1	98(82)
C(64)-C(59)-C(60)-C(61)	0.0
C(59)-C(60)-C(61)-C(62)	0.0
C(60)-C(61)-C(62)-C(63)	0.0
C(61)-C(62)-C(63)-C(64)	0.0
C(62)-C(63)-C(64)-C(59)	0.0
C(62)-C(63)-C(64)-C(65)	-179.98(9)
C(60)-C(59)-C(64)-C(63)	0.0
C(60)-C(59)-C(64)-C(65)	179.98(9)
C(6)-C(7)-N(1)-N(2)	179.9(4)
P(1)-C(7)-N(1)-N(2)	-0.6(5)
C(6)-C(7)-N(1)-Pr(1)	20(3)
P(1)-C(7)-N(1)-Pr(1)	-160(2)
C(9)-C(8)-N(2)-N(1)	-177.8(4)
P(1)-C(8)-N(2)-N(1)	0.0(5)
C(9)-C(8)-N(2)-Pr(1)	-16(3)
P(1)-C(8)-N(2)-Pr(1)	161(2)
C(7)-N(1)-N(2)-C(8)	0.4(5)
Pr(1)-N(1)-N(2)-C(8)	177.6(4)
C(7)-N(1)-N(2)-Pr(1)	-177.2(4)
C(20)-C(21)-N(3)-N(4)	176.7(4)
P(2)-C(21)-N(3)-N(4)	-0.1(5)
C(20)-C(21)-N(3)-Pr(1)	-16(2)
P(2)-C(21)-N(3)-Pr(1)	166.7(15)
C(23)-C(22)-N(4)-N(3)	179.7(4)

P(2)-C(22)-N(4)-N(3)	-0.2(5)
C(23)-C(22)-N(4)-Pr(1)	31(4)
P(2)-C(22)-N(4)-Pr(1)	-149(3)
C(21)-N(3)-N(4)-C(22)	0.2(5)
Pr(1)-N(3)-N(4)-C(22)	-177.4(3)
C(21)-N(3)-N(4)-Pr(1)	177.6(3)
C(37)-C(36)-N(5)-N(6)	178.9(4)
P(3)-C(36)-N(5)-N(6)	-0.5(5)
C(37)-C(36)-N(5)-Pr(1)	18(5)
P(3)-C(36)-N(5)-Pr(1)	-161(4)
C(34)-C(35)-N(6)-N(5)	-176.5(4)
P(3)-C(35)-N(6)-N(5)	0.4(5)
C(34)-C(35)-N(6)-Pr(1)	-3.1(19)
P(3)-C(35)-N(6)-Pr(1)	173.7(14)
C(36)-N(5)-N(6)-C(35)	0.1(5)
Pr(1)-N(5)-N(6)-C(35)	178.7(4)
C(36)-N(5)-N(6)-Pr(1)	-178.6(3)
C(45)-C(46)-O(1)-C(43)	36.6(6)
C(45)-C(46)-O(1)-Pr(1)	-166.3(4)
C(44)-C(43)-O(1)-C(46)	-38.3(5)
C(44)-C(43)-O(1)-Pr(1)	165.1(3)
C(53)-C(54)-O(3)-C(51)	-10.4(8)
C(53)-C(54)-O(3)-Pr(1)	-176.7(5)
C(52)-C(51)-O(3)-C(54)	-1.7(9)
C(52)-C(51)-O(3)-Pr(1)	165.1(6)
N(2)-C(8)-P(1)-C(7)	-0.2(4)
C(9)-C(8)-P(1)-C(7)	177.4(4)
N(1)-C(7)-P(1)-C(8)	0.4(4)
C(6)-C(7)-P(1)-C(8)	179.9(4)
N(3)-C(21)-P(2)-C(22)	0.0(4)

C(20)-C(21)-P(2)-C(22)	-176.6(4)
N(4)-C(22)-P(2)-C(21)	0.2(4)
C(23)-C(22)-P(2)-C(21)	-179.8(4)
N(6)-C(35)-P(3)-C(36)	-0.5(4)
C(34)-C(35)-P(3)-C(36)	176.0(5)
N(5)-C(36)-P(3)-C(35)	0.5(4)
C(37)-C(36)-P(3)-C(35)	-178.8(4)
C(35)-N(6)-Pr(1)-N(3)	-50.5(17)
N(5)-N(6)-Pr(1)-N(3)	123.3(3)
C(35)-N(6)-Pr(1)-N(2)	100.1(17)
N(5)-N(6)-Pr(1)-N(2)	-86.2(2)
C(35)-N(6)-Pr(1)-N(1)	116.3(17)
N(5)-N(6)-Pr(1)-N(1)	-69.9(2)
C(35)-N(6)-Pr(1)-O(3)	-158.3(16)
N(5)-N(6)-Pr(1)-O(3)	15.4(3)
C(35)-N(6)-Pr(1)-N(4)	-24.0(17)
N(5)-N(6)-Pr(1)-N(4)	149.7(2)
C(35)-N(6)-Pr(1)-O(1)	44.2(17)
N(5)-N(6)-Pr(1)-O(1)	-142.1(2)
C(35)-N(6)-Pr(1)-N(5)	-173.7(18)
C(35)-N(6)-Pr(1)-O(2)	-83.4(17)
N(5)-N(6)-Pr(1)-O(2)	90.4(2)
C(21)-N(3)-Pr(1)-N(6)	-120.7(17)
N(4)-N(3)-Pr(1)-N(6)	46.9(3)
C(21)-N(3)-Pr(1)-N(2)	82.3(17)
N(4)-N(3)-Pr(1)-N(2)	-110.1(2)
C(21)-N(3)-Pr(1)-N(1)	73.4(17)
N(4)-N(3)-Pr(1)-N(1)	-119.0(2)
C(21)-N(3)-Pr(1)-O(3)	-3.0(17)
N(4)-N(3)-Pr(1)-O(3)	164.6(2)

C(21)-N(3)-Pr(1)-N(4)	-167.6(18)
C(21)-N(3)-Pr(1)-O(1)	153.2(17)
N(4)-N(3)-Pr(1)-O(1)	-39.2(2)
C(21)-N(3)-Pr(1)-N(5)	-59.0(18)
N(4)-N(3)-Pr(1)-N(5)	108.5(3)
C(21)-N(3)-Pr(1)-O(2)	-88.6(17)
N(4)-N(3)-Pr(1)-O(2)	79.0(2)
C(8)-N(2)-Pr(1)-N(6)	-131(2)
N(1)-N(2)-Pr(1)-N(6)	31.6(3)
C(8)-N(2)-Pr(1)-N(3)	33(2)
N(1)-N(2)-Pr(1)-N(3)	-164.4(2)
C(8)-N(2)-Pr(1)-N(1)	-162(3)
C(8)-N(2)-Pr(1)-O(3)	114(2)
N(1)-N(2)-Pr(1)-O(3)	-84.1(2)
C(8)-N(2)-Pr(1)-N(4)	4(2)
N(1)-N(2)-Pr(1)-N(4)	166.1(2)
C(8)-N(2)-Pr(1)-O(1)	-74(2)
N(1)-N(2)-Pr(1)-O(1)	88.4(2)
C(8)-N(2)-Pr(1)-N(5)	-167(2)
N(1)-N(2)-Pr(1)-N(5)	-5.3(3)
C(8)-N(2)-Pr(1)-O(2)	58(3)
N(1)-N(2)-Pr(1)-O(2)	-139.5(3)
C(7)-N(1)-Pr(1)-N(6)	5(2)
N(2)-N(1)-Pr(1)-N(6)	-155.3(2)
C(7)-N(1)-Pr(1)-N(3)	177(2)
N(2)-N(1)-Pr(1)-N(3)	16.8(3)
C(7)-N(1)-Pr(1)-N(2)	161(2)
C(7)-N(1)-Pr(1)-O(3)	-108(2)
N(2)-N(1)-Pr(1)-O(3)	91.8(2)
C(7)-N(1)-Pr(1)-N(4)	144(2)

N(2)-N(1)-Pr(1)-N(4)	-16.9(3)
C(7)-N(1)-Pr(1)-O(1)	78(2)
N(2)-N(1)-Pr(1)-O(1)	-82.5(2)
C(7)-N(1)-Pr(1)-N(5)	-24(2)
N(2)-N(1)-Pr(1)-N(5)	175.4(2)
C(7)-N(1)-Pr(1)-O(2)	-63(2)
N(2)-N(1)-Pr(1)-O(2)	136.5(3)
C(54)-O(3)-Pr(1)-N(6)	-109.1(5)
C(51)-O(3)-Pr(1)-N(6)	86.4(5)
C(54)-O(3)-Pr(1)-N(3)	103.3(5)
C(51)-O(3)-Pr(1)-N(3)	-61.2(5)
C(54)-O(3)-Pr(1)-N(2)	20.2(5)
C(51)-O(3)-Pr(1)-N(2)	-144.3(5)
C(54)-O(3)-Pr(1)-N(1)	-11.8(5)
C(51)-O(3)-Pr(1)-N(1)	-176.3(5)
C(54)-O(3)-Pr(1)-N(4)	111.8(5)
C(51)-O(3)-Pr(1)-N(4)	-52.7(5)
C(54)-O(3)-Pr(1)-O(1)	2.1(6)
C(51)-O(3)-Pr(1)-O(1)	-162.5(4)
C(54)-O(3)-Pr(1)-N(5)	-101.1(5)
C(51)-O(3)-Pr(1)-N(5)	94.4(5)
C(54)-O(3)-Pr(1)-O(2)	-177.5(5)
C(51)-O(3)-Pr(1)-O(2)	18.0(4)
C(22)-N(4)-Pr(1)-N(6)	-2(4)
N(3)-N(4)-Pr(1)-N(6)	-152.0(2)
C(22)-N(4)-Pr(1)-N(3)	150(4)
C(22)-N(4)-Pr(1)-N(2)	-141(4)
N(3)-N(4)-Pr(1)-N(2)	68.7(2)
C(22)-N(4)-Pr(1)-N(1)	-133(4)
N(3)-N(4)-Pr(1)-N(1)	77.5(2)

C(22)-N(4)-Pr(1)-O(3)	134(4)
N(3)-N(4)-Pr(1)-O(3)	-16.2(2)
C(22)-N(4)-Pr(1)-O(1)	-69(4)
N(3)-N(4)-Pr(1)-O(1)	141.4(2)
C(22)-N(4)-Pr(1)-N(5)	25(4)
N(3)-N(4)-Pr(1)-N(5)	-124.5(2)
C(22)-N(4)-Pr(1)-O(2)	57(4)
N(3)-N(4)-Pr(1)-O(2)	-93.2(2)
C(46)-O(1)-Pr(1)-N(6)	40.3(4)
C(43)-O(1)-Pr(1)-N(6)	-167.5(4)
C(46)-O(1)-Pr(1)-N(3)	-174.4(4)
C(43)-O(1)-Pr(1)-N(3)	-22.1(4)
C(46)-O(1)-Pr(1)-N(2)	-97.1(4)
C(43)-O(1)-Pr(1)-N(2)	55.1(4)
C(46)-O(1)-Pr(1)-N(1)	-64.1(4)
C(43)-O(1)-Pr(1)-N(1)	88.1(4)
C(46)-O(1)-Pr(1)-O(3)	-78.2(5)
C(43)-O(1)-Pr(1)-O(3)	74.0(5)
C(46)-O(1)-Pr(1)-N(4)	165.9(4)
C(43)-O(1)-Pr(1)-N(4)	-41.8(4)
C(46)-O(1)-Pr(1)-N(5)	21.2(4)
C(43)-O(1)-Pr(1)-N(5)	173.5(4)
C(46)-O(1)-Pr(1)-O(2)	101.3(4)
C(43)-O(1)-Pr(1)-O(2)	-106.5(4)
C(36)-N(5)-Pr(1)-N(6)	161(5)
C(36)-N(5)-Pr(1)-N(3)	51(5)
N(6)-N(5)-Pr(1)-N(3)	-110.6(3)
C(36)-N(5)-Pr(1)-N(2)	-84(5)
N(6)-N(5)-Pr(1)-N(2)	115.0(2)
C(36)-N(5)-Pr(1)-N(1)	-86(5)

N(6)-N(5)-Pr(1)-N(1)	112.3(2)
C(36)-N(5)-Pr(1)-O(3)	-5(5)
N(6)-N(5)-Pr(1)-O(3)	-165.8(2)
C(36)-N(5)-Pr(1)-N(4)	112(5)
N(6)-N(5)-Pr(1)-N(4)	-49.7(3)
C(36)-N(5)-Pr(1)-O(1)	-161(5)
N(6)-N(5)-Pr(1)-O(1)	37.5(2)
C(36)-N(5)-Pr(1)-O(2)	81(5)
N(6)-N(5)-Pr(1)-O(2)	-80.8(2)
C(47)-O(2)-Pr(1)-N(6)	153.6(13)
C(50')-O(2)-Pr(1)-N(6)	-28.1(19)
C(50)-O(2)-Pr(1)-N(6)	-35.3(14)
C(47')-O(2)-Pr(1)-N(6)	126.3(15)
C(47)-O(2)-Pr(1)-N(3)	-8.5(13)
C(50')-O(2)-Pr(1)-N(3)	169.7(19)
C(50)-O(2)-Pr(1)-N(3)	162.5(14)
C(47')-O(2)-Pr(1)-N(3)	-35.8(15)
C(47)-O(2)-Pr(1)-N(2)	-33.7(13)
C(50')-O(2)-Pr(1)-N(2)	144.5(18)
C(50)-O(2)-Pr(1)-N(2)	137.3(14)
C(47')-O(2)-Pr(1)-N(2)	-61.0(15)
C(47)-O(2)-Pr(1)-N(1)	-133.6(13)
C(50')-O(2)-Pr(1)-N(1)	44.6(19)
C(50)-O(2)-Pr(1)-N(1)	37.4(15)
C(47')-O(2)-Pr(1)-N(1)	-160.9(15)
C(47)-O(2)-Pr(1)-O(3)	-89.1(13)
C(50')-O(2)-Pr(1)-O(3)	89.1(19)
C(50)-O(2)-Pr(1)-O(3)	81.9(14)
C(47')-O(2)-Pr(1)-O(3)	-116.4(15)
C(47)-O(2)-Pr(1)-N(4)	23.8(13)

C(50')-O(2)-Pr(1)-N(4)	-158.0(19)
C(50)-O(2)-Pr(1)-N(4)	-165.2(14)
C(47')-O(2)-Pr(1)-N(4)	-3.5(15)
C(47)-O(2)-Pr(1)-O(1)	91.1(13)
C(50')-O(2)-Pr(1)-O(1)	-90.7(19)
C(50)-O(2)-Pr(1)-O(1)	-97.9(14)
C(47')-O(2)-Pr(1)-O(1)	63.8(15)
C(47)-O(2)-Pr(1)-N(5)	-174.0(13)
C(50')-O(2)-Pr(1)-N(5)	4.3(19)
C(50)-O(2)-Pr(1)-N(5)	-2.9(14)
C(47')-O(2)-Pr(1)-N(5)	158.7(15)
C(50')-O(2)-C(47)-C(48)	8(2)
C(50)-O(2)-C(47)-C(48)	13.8(19)
C(47')-O(2)-C(47)-C(48)	-94(3)
Pr(1)-O(2)-C(47)-C(48)	-173.6(9)
O(2)-C(47)-C(48)-C(49)	7(2)
C(47)-C(48)-C(49)-C(50)	-24(3)
C(47)-O(2)-C(50)-C(49)	-29(3)
C(50')-O(2)-C(50)-C(49)	72(13)
C(47')-O(2)-C(50)-C(49)	-5(3)
Pr(1)-O(2)-C(50)-C(49)	158.1(13)
C(48)-C(49)-C(50)-O(2)	34(3)
C(47)-O(2)-C(47')-C(48')	78(3)
C(50')-O(2)-C(47')-C(48')	-8(2)
C(50)-O(2)-C(47')-C(48')	-2(2)
Pr(1)-O(2)-C(47')-C(48')	-165.9(10)
C(47)-O(2)-C(50')-C(49')	9(3)
C(50)-O(2)-C(50')-C(49')	-72(13)
C(47')-O(2)-C(50')-C(49')	33(3)
Pr(1)-O(2)-C(50')-C(49')	-169.8(16)

C(48')-C(49')-C(50')-O(2)	-42(4)
O(2)-C(47')-C(48')-C(49')	-21(2)
C(50')-C(49')-C(48')-C(47')	38(3)

Symmetry transformations used to generate equivalent atoms:

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

4.6 Crystal structural analysis data for **8**

Table 1. Crystal data and structure refinement for **8**.

Identification code	150104-1b
Empirical formula	C ₈₀ H ₈₈ K N ₈ O ₆ P ₄ Sm
Formula weight	1570.91
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 1 2 ₁ /n 1
Unit cell dimensions	a = 22.6746(10) Å alpha = 90 deg. b = 15.0764(5) Å beta = 106.253(5) deg. c = 24.6405(11) Å gamma = 90 deg.
Volume	8086.7(6) Å ³
Z, Calculated density	4, 1.290 Mg/m ³
Absorption coefficient	0.911 mm ⁻¹
F(000)	3252
Crystal size	0.26 x 0.22 x 0.10 mm
Theta range for data collection	2.92 to 25.68 deg.
Limiting indices	-27 ≤ h ≤ 25, -16 ≤ k ≤ 18, -29 ≤ l ≤ 30
Reflections collected / unique	46231 / 15329 [R(int) = 0.0896]
Completeness to theta = 25.68	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.20144
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	15329 / 76 / 901
Goodness-of-fit on F ²	1.027
Final R indices [I > 2σ(I)]	R ₁ = 0.0778, wR ₂ = 0.1627
R indices (all data)	R ₁ = 0.1398, wR ₂ = 0.1963
Largest diff. peak and hole	1.423 and -0.799 e.Å ⁻³

Table 3. Bond lengths [Å] and angles [deg] for **8**.

C(1)-C(6)	1.364(13)
C(1)-C(2)	1.372(14)
C(1)-H(1)	0.9300
C(2)-C(3)	1.374(15)
C(2)-H(2)	0.9300
C(3)-C(4)	1.341(15)
C(3)-H(3)	0.9300
C(4)-C(5)	1.372(14)
C(4)-H(4)	0.9300
C(5)-C(6)	1.387(11)
C(5)-H(5)	0.9300
C(6)-C(7)	1.474(12)
C(7)-N(3)	1.320(9)
C(7)-P(1)	1.754(8)
C(8)-N(4)	1.336(9)
C(8)-C(9)	1.444(13)
C(8)-P(1)	1.756(10)
C(9)-C(14)	1.357(13)
C(9)-C(10)	1.360(16)
C(10)-C(11)	1.416(16)
C(10)-H(10)	0.9300
C(11)-C(12)	1.383(18)
C(11)-H(11)	0.9300
C(12)-C(13)	1.349(19)
C(12)-H(12)	0.9300
C(13)-C(14)	1.360(17)
C(13)-H(13)	0.9300

C(14)-H(14)	0.9300
C(15)-C(20)	1.378(12)
C(15)-C(16)	1.392(13)
C(15)-H(15)	0.9300
C(16)-C(17)	1.390(13)
C(16)-H(16)	0.9300
C(17)-C(18)	1.346(14)
C(17)-H(17)	0.9300
C(18)-C(19)	1.359(14)
C(18)-H(18)	0.9300
C(19)-C(20)	1.376(11)
C(19)-H(19)	0.9300
C(20)-C(21)	1.462(11)
C(21)-N(7)	1.332(9)
C(21)-P(3)	1.757(8)
C(22)-N(8)	1.345(9)
C(22)-C(23)	1.480(11)
C(22)-P(3)	1.729(9)
C(23)-C(28)	1.385(12)
C(23)-C(24)	1.392(11)
C(24)-C(25)	1.366(14)
C(24)-H(24)	0.9300
C(25)-C(26)	1.354(16)
C(25)-H(25)	0.9300
C(26)-C(27)	1.371(15)
C(26)-H(26)	0.9300
C(27)-C(28)	1.405(14)
C(27)-H(27)	0.9300
C(28)-H(28)	0.9300
C(29)-C(34)	1.377(11)

C(29)-C(30)	1.397(11)
C(29)-H(29)	0.9300
C(30)-C(31)	1.384(14)
C(30)-H(30)	0.9300
C(31)-C(32)	1.364(14)
C(31)-H(31)	0.9300
C(32)-C(33)	1.376(12)
C(32)-H(32)	0.9300
C(33)-C(34)	1.378(11)
C(33)-H(33)	0.9300
C(34)-C(35)	1.483(9)
C(35)-N(2)	1.319(8)
C(35)-P(2)	1.755(7)
C(36)-N(1)	1.341(9)
C(36)-C(37)	1.478(10)
C(36)-P(2)	1.744(7)
C(37)-C(42)	1.371(11)
C(37)-C(38)	1.377(11)
C(38)-C(39)	1.410(12)
C(38)-H(38)	0.9300
C(39)-C(40)	1.355(14)
C(39)-H(39)	0.9300
C(40)-C(41)	1.331(14)
C(40)-H(40)	0.9300
C(41)-C(42)	1.386(12)
C(41)-H(41)	0.9300
C(42)-H(42)	0.9300
C(43)-C(48)	1.365(12)
C(43)-C(44)	1.393(13)
C(43)-H(43)	0.9300

C(44)-C(45)	1.361(14)
C(44)-H(44)	0.9300
C(45)-C(46)	1.345(15)
C(45)-H(45)	0.9300
C(46)-C(47)	1.383(14)
C(46)-H(46)	0.9300
C(47)-C(48)	1.383(11)
C(47)-H(47)	0.9300
C(48)-C(49)	1.482(11)
C(49)-N(5)	1.327(8)
C(49)-P(4)	1.729(8)
C(50)-N(6)	1.350(9)
C(50)-C(51)	1.492(11)
C(50)-P(4)	1.744(8)
C(51)-C(52)	1.367(12)
C(51)-C(56)	1.371(12)
C(52)-C(53)	1.411(13)
C(52)-H(52)	0.9300
C(53)-C(54)	1.372(16)
C(53)-H(53)	0.9300
C(54)-C(55)	1.347(17)
C(54)-H(54)	0.9300
C(55)-C(56)	1.367(15)
C(55)-H(55)	0.9300
C(56)-H(56)	0.9300
C(57)-O(1)	1.389(11)
C(57)-C(58)	1.527(16)
C(57)-H(57A)	0.9700
C(57)-H(57B)	0.9700
C(58)-C(59)	1.476(9)

C(58)-H(58A)	0.9700
C(58)-H(58B)	0.9700
C(59)-C(60)	1.475(12)
C(59)-H(59A)	0.9700
C(59)-H(59B)	0.9700
C(60)-O(1)	1.428(10)
C(60)-H(60A)	0.9700
C(60)-H(60B)	0.9700
C(61)-O(5)	1.337(19)
C(61)-C(62)	1.37(2)
C(61)-H(61A)	0.9700
C(61)-H(61B)	0.9700
C(62)-C(63)	1.508(9)
C(62)-H(62A)	0.9700
C(62)-H(62B)	0.9700
C(63)-C(64)	1.40(2)
C(63)-H(63A)	0.9700
C(63)-H(63B)	0.9700
C(64)-O(5)	1.365(19)
C(64)-H(64A)	0.9700
C(64)-H(64B)	0.9700
C(70)-C(69)	1.42(2)
C(70)-C(71)	1.43(3)
C(70)-H(70A)	0.9700
C(70)-H(70B)	0.9700
C(71)-C(72)	1.511(10)
C(71)-H(71A)	0.9700
C(71)-H(71B)	0.9700
C(72)-O(3)	1.380(19)
C(72)-H(72A)	0.9700

C(72)-H(72B)	0.9700
C(73)-O(4)	1.354(19)
C(73)-C(74)	1.498(10)
C(73)-H(73A)	0.9700
C(73)-H(73B)	0.9700
C(74)-C(75)	1.520(10)
C(74)-H(74A)	0.9700
C(74)-H(74B)	0.9700
C(75)-C(76)	1.517(10)
C(75)-H(75A)	0.9700
C(75)-H(75B)	0.9700
C(76)-O(4)	1.33(2)
C(76)-H(76A)	0.9700
C(76)-H(76B)	0.9700
C(77)-C(78)	1.37(2)
C(77)-O(2)	1.39(2)
C(77)-H(77A)	0.9700
C(77)-H(77B)	0.9700
C(78)-C(79)	1.49(3)
C(78)-H(78A)	0.9700
C(78)-H(78B)	0.9700
C(79)-C(80)	1.43(2)
C(79)-H(79A)	0.9700
C(79)-H(79B)	0.9700
C(80)-O(2)	1.40(2)
C(80)-H(80A)	0.9700
C(80)-H(80B)	0.9700
K(1)-O(4)	2.593(12)
K(1)-O(2)	2.619(11)
K(1)-O(6)	2.636(10)

K(1)-O(5)	2.747(11)
K(1)-O(3)	2.763(11)
N(1)-N(2)	1.322(7)
N(1)-Sm(1)	2.483(6)
N(2)-Sm(1)	2.506(6)
N(3)-N(4)	1.341(8)
N(3)-Sm(1)	2.458(6)
N(4)-Sm(1)	2.452(6)
N(5)-N(6)	1.352(8)
N(5)-Sm(1)	2.457(6)
N(6)-Sm(1)	2.470(6)
N(7)-N(8)	1.366(8)
N(7)-Sm(1)	2.461(6)
N(8)-Sm(1)	2.468(5)
O(1)-Sm(1)	2.581(5)
O(3)-C(69)	1.361(18)
O(6)-C(68)	1.23(2)
O(6)-C(65)	1.314(19)
C(65)-C(66)	1.477(9)
C(65)-H(65A)	0.9700
C(65)-H(65B)	0.9700
C(66)-C(67)	1.507(9)
C(66)-H(66A)	0.9700
C(66)-H(66B)	0.9700
C(67)-C(68)	1.47(3)
C(67)-H(67A)	0.9700
C(67)-H(67B)	0.9700
C(68)-H(68A)	0.9700
C(68)-H(68B)	0.9700
C(69)-H(69A)	0.9700

C(69)-H(69B)	0.9700
C(6)-C(1)-C(2)	121.9(10)
C(6)-C(1)-H(1)	119.0
C(2)-C(1)-H(1)	119.0
C(1)-C(2)-C(3)	119.5(12)
C(1)-C(2)-H(2)	120.2
C(3)-C(2)-H(2)	120.2
C(4)-C(3)-C(2)	119.8(12)
C(4)-C(3)-H(3)	120.1
C(2)-C(3)-H(3)	120.1
C(3)-C(4)-C(5)	120.5(10)
C(3)-C(4)-H(4)	119.7
C(5)-C(4)-H(4)	119.7
C(4)-C(5)-C(6)	121.1(11)
C(4)-C(5)-H(5)	119.4
C(6)-C(5)-H(5)	119.4
C(1)-C(6)-C(5)	117.1(10)
C(1)-C(6)-C(7)	121.3(8)
C(5)-C(6)-C(7)	121.5(9)
N(3)-C(7)-C(6)	120.5(7)
N(3)-C(7)-P(1)	113.3(6)
C(6)-C(7)-P(1)	126.2(6)
N(4)-C(8)-C(9)	121.5(9)
N(4)-C(8)-P(1)	112.6(7)
C(9)-C(8)-P(1)	125.8(7)
C(14)-C(9)-C(10)	112.6(12)
C(14)-C(9)-C(8)	124.7(12)
C(10)-C(9)-C(8)	122.4(9)
C(9)-C(10)-C(11)	126.8(13)

C(9)-C(10)-H(10)	116.6
C(11)-C(10)-H(10)	116.6
C(12)-C(11)-C(10)	114.5(15)
C(12)-C(11)-H(11)	122.7
C(10)-C(11)-H(11)	122.7
C(13)-C(12)-C(11)	120.5(16)
C(13)-C(12)-H(12)	119.7
C(11)-C(12)-H(12)	119.7
C(12)-C(13)-C(14)	120.0(14)
C(12)-C(13)-H(13)	120.0
C(14)-C(13)-H(13)	120.0
C(9)-C(14)-C(13)	125.0(14)
C(9)-C(14)-H(14)	117.5
C(13)-C(14)-H(14)	117.5
C(20)-C(15)-C(16)	120.7(10)
C(20)-C(15)-H(15)	119.6
C(16)-C(15)-H(15)	119.6
C(17)-C(16)-C(15)	120.8(11)
C(17)-C(16)-H(16)	119.6
C(15)-C(16)-H(16)	119.6
C(18)-C(17)-C(16)	117.5(11)
C(18)-C(17)-H(17)	121.3
C(16)-C(17)-H(17)	121.3
C(17)-C(18)-C(19)	121.8(11)
C(17)-C(18)-H(18)	119.1
C(19)-C(18)-H(18)	119.1
C(18)-C(19)-C(20)	122.6(10)
C(18)-C(19)-H(19)	118.7
C(20)-C(19)-H(19)	118.7
C(19)-C(20)-C(15)	116.6(9)

C(19)-C(20)-C(21)	121.8(9)
C(15)-C(20)-C(21)	121.7(8)
N(7)-C(21)-C(20)	121.4(7)
N(7)-C(21)-P(3)	112.9(6)
C(20)-C(21)-P(3)	125.7(6)
N(8)-C(22)-C(23)	118.3(7)
N(8)-C(22)-P(3)	115.7(6)
C(23)-C(22)-P(3)	126.0(6)
C(28)-C(23)-C(24)	117.6(10)
C(28)-C(23)-C(22)	121.0(8)
C(24)-C(23)-C(22)	121.5(9)
C(25)-C(24)-C(23)	122.5(12)
C(25)-C(24)-H(24)	118.7
C(23)-C(24)-H(24)	118.7
C(26)-C(25)-C(24)	119.8(12)
C(26)-C(25)-H(25)	120.1
C(24)-C(25)-H(25)	120.1
C(25)-C(26)-C(27)	119.9(12)
C(25)-C(26)-H(26)	120.1
C(27)-C(26)-H(26)	120.1
C(26)-C(27)-C(28)	121.0(13)
C(26)-C(27)-H(27)	119.5
C(28)-C(27)-H(27)	119.5
C(23)-C(28)-C(27)	119.2(11)
C(23)-C(28)-H(28)	120.4
C(27)-C(28)-H(28)	120.4
C(34)-C(29)-C(30)	121.1(8)
C(34)-C(29)-H(29)	119.4
C(30)-C(29)-H(29)	119.4
C(31)-C(30)-C(29)	116.9(9)

C(31)-C(30)-H(30)	121.5
C(29)-C(30)-H(30)	121.5
C(32)-C(31)-C(30)	123.2(9)
C(32)-C(31)-H(31)	118.4
C(30)-C(31)-H(31)	118.4
C(31)-C(32)-C(33)	118.2(9)
C(31)-C(32)-H(32)	120.9
C(33)-C(32)-H(32)	120.9
C(32)-C(33)-C(34)	121.4(9)
C(32)-C(33)-H(33)	119.3
C(34)-C(33)-H(33)	119.3
C(29)-C(34)-C(33)	119.2(8)
C(29)-C(34)-C(35)	119.7(7)
C(33)-C(34)-C(35)	121.0(8)
N(2)-C(35)-C(34)	124.7(7)
N(2)-C(35)-P(2)	110.5(5)
C(34)-C(35)-P(2)	124.8(5)
N(1)-C(36)-C(37)	119.7(7)
N(1)-C(36)-P(2)	113.9(5)
C(37)-C(36)-P(2)	126.4(6)
C(42)-C(37)-C(38)	117.3(8)
C(42)-C(37)-C(36)	123.9(8)
C(38)-C(37)-C(36)	118.8(8)
C(37)-C(38)-C(39)	121.0(9)
C(37)-C(38)-H(38)	119.5
C(39)-C(38)-H(38)	119.5
C(40)-C(39)-C(38)	120.3(10)
C(40)-C(39)-H(39)	119.9
C(38)-C(39)-H(39)	119.9
C(41)-C(40)-C(39)	118.3(10)

C(41)-C(40)-H(40)	120.9
C(39)-C(40)-H(40)	120.9
C(40)-C(41)-C(42)	123.1(10)
C(40)-C(41)-H(41)	118.4
C(42)-C(41)-H(41)	118.4
C(37)-C(42)-C(41)	120.0(9)
C(37)-C(42)-H(42)	120.0
C(41)-C(42)-H(42)	120.0
C(48)-C(43)-C(44)	122.0(9)
C(48)-C(43)-H(43)	119.0
C(44)-C(43)-H(43)	119.0
C(45)-C(44)-C(43)	120.4(12)
C(45)-C(44)-H(44)	119.8
C(43)-C(44)-H(44)	119.8
C(46)-C(45)-C(44)	118.0(11)
C(46)-C(45)-H(45)	121.0
C(44)-C(45)-H(45)	121.0
C(45)-C(46)-C(47)	122.5(11)
C(45)-C(46)-H(46)	118.8
C(47)-C(46)-H(46)	118.8
C(48)-C(47)-C(46)	120.3(10)
C(48)-C(47)-H(47)	119.9
C(46)-C(47)-H(47)	119.9
C(43)-C(48)-C(47)	116.8(9)
C(43)-C(48)-C(49)	121.9(8)
C(47)-C(48)-C(49)	121.2(9)
N(5)-C(49)-C(48)	118.8(7)
N(5)-C(49)-P(4)	115.3(6)
C(48)-C(49)-P(4)	125.9(6)
N(6)-C(50)-C(51)	121.5(7)

N(6)-C(50)-P(4)	113.5(6)
C(51)-C(50)-P(4)	124.9(6)
C(52)-C(51)-C(56)	119.9(9)
C(52)-C(51)-C(50)	120.2(8)
C(56)-C(51)-C(50)	119.8(9)
C(51)-C(52)-C(53)	119.6(10)
C(51)-C(52)-H(52)	120.2
C(53)-C(52)-H(52)	120.2
C(54)-C(53)-C(52)	119.1(12)
C(54)-C(53)-H(53)	120.4
C(52)-C(53)-H(53)	120.4
C(55)-C(54)-C(53)	119.9(12)
C(55)-C(54)-H(54)	120.0
C(53)-C(54)-H(54)	120.0
C(54)-C(55)-C(56)	121.5(13)
C(54)-C(55)-H(55)	119.2
C(56)-C(55)-H(55)	119.2
C(55)-C(56)-C(51)	119.8(12)
C(55)-C(56)-H(56)	120.1
C(51)-C(56)-H(56)	120.1
O(1)-C(57)-C(58)	112.7(10)
O(1)-C(57)-H(57A)	109.0
C(58)-C(57)-H(57A)	109.0
O(1)-C(57)-H(57B)	109.0
C(58)-C(57)-H(57B)	109.0
H(57A)-C(57)-H(57B)	107.8
C(59)-C(58)-C(57)	101.6(11)
C(59)-C(58)-H(58A)	111.4
C(57)-C(58)-H(58A)	111.4
C(59)-C(58)-H(58B)	111.4

C(57)-C(58)-H(58B)	111.4
H(58A)-C(58)-H(58B)	109.3
C(60)-C(59)-C(58)	108.4(10)
C(60)-C(59)-H(59A)	110.0
C(58)-C(59)-H(59A)	110.0
C(60)-C(59)-H(59B)	110.0
C(58)-C(59)-H(59B)	110.0
H(59A)-C(59)-H(59B)	108.4
O(1)-C(60)-C(59)	109.3(8)
O(1)-C(60)-H(60A)	109.8
C(59)-C(60)-H(60A)	109.8
O(1)-C(60)-H(60B)	109.8
C(59)-C(60)-H(60B)	109.8
H(60A)-C(60)-H(60B)	108.3
O(5)-C(61)-C(62)	110(2)
O(5)-C(61)-H(61A)	109.7
C(62)-C(61)-H(61A)	109.7
O(5)-C(61)-H(61B)	109.7
C(62)-C(61)-H(61B)	109.7
H(61A)-C(61)-H(61B)	108.2
C(61)-C(62)-C(63)	105.7(19)
C(61)-C(62)-H(62A)	110.6
C(63)-C(62)-H(62A)	110.6
C(61)-C(62)-H(62B)	110.6
C(63)-C(62)-H(62B)	110.6
H(62A)-C(62)-H(62B)	108.7
C(64)-C(63)-C(62)	99.1(18)
C(64)-C(63)-H(63A)	111.9
C(62)-C(63)-H(63A)	111.9
C(64)-C(63)-H(63B)	111.9

C(62)-C(63)-H(63B)	111.9
H(63A)-C(63)-H(63B)	109.6
O(5)-C(64)-C(63)	113.8(18)
O(5)-C(64)-H(64A)	108.8
C(63)-C(64)-H(64A)	108.8
O(5)-C(64)-H(64B)	108.8
C(63)-C(64)-H(64B)	108.8
H(64A)-C(64)-H(64B)	107.7
C(69)-C(70)-C(71)	109(2)
C(69)-C(70)-H(70A)	109.8
C(71)-C(70)-H(70A)	109.8
C(69)-C(70)-H(70B)	109.8
C(71)-C(70)-H(70B)	109.8
H(70A)-C(70)-H(70B)	108.2
C(70)-C(71)-C(72)	101(2)
C(70)-C(71)-H(71A)	111.5
C(72)-C(71)-H(71A)	111.5
C(70)-C(71)-H(71B)	111.5
C(72)-C(71)-H(71B)	111.5
H(71A)-C(71)-H(71B)	109.3
O(3)-C(72)-C(71)	108.9(18)
O(3)-C(72)-H(72A)	109.9
C(71)-C(72)-H(72A)	109.9
O(3)-C(72)-H(72B)	109.9
C(71)-C(72)-H(72B)	109.9
H(72A)-C(72)-H(72B)	108.3
O(4)-C(73)-C(74)	112.9(13)
O(4)-C(73)-H(73A)	109.0
C(74)-C(73)-H(73A)	109.0
O(4)-C(73)-H(73B)	109.0

C(74)-C(73)-H(73B)	109.0
H(73A)-C(73)-H(73B)	107.8
C(73)-C(74)-C(75)	102.5(10)
C(73)-C(74)-H(74A)	111.3
C(75)-C(74)-H(74A)	111.3
C(73)-C(74)-H(74B)	111.3
C(75)-C(74)-H(74B)	111.3
H(74A)-C(74)-H(74B)	109.2
C(76)-C(75)-C(74)	100.0(12)
C(76)-C(75)-H(75A)	111.8
C(74)-C(75)-H(75A)	111.8
C(76)-C(75)-H(75B)	111.8
C(74)-C(75)-H(75B)	111.8
H(75A)-C(75)-H(75B)	109.5
O(4)-C(76)-C(75)	112.2(13)
O(4)-C(76)-H(76A)	109.2
C(75)-C(76)-H(76A)	109.2
O(4)-C(76)-H(76B)	109.2
C(75)-C(76)-H(76B)	109.2
H(76A)-C(76)-H(76B)	107.9
C(78)-C(77)-O(2)	118.2(19)
C(78)-C(77)-H(77A)	107.8
O(2)-C(77)-H(77A)	107.8
C(78)-C(77)-H(77B)	107.8
O(2)-C(77)-H(77B)	107.8
H(77A)-C(77)-H(77B)	107.1
C(77)-C(78)-C(79)	101.7(13)
C(77)-C(78)-H(78A)	111.4
C(79)-C(78)-H(78A)	111.4
C(77)-C(78)-H(78B)	111.4

C(79)-C(78)-H(78B)	111.4
H(78A)-C(78)-H(78B)	109.3
C(80)-C(79)-C(78)	102.8(13)
C(80)-C(79)-H(79A)	111.2
C(78)-C(79)-H(79A)	111.2
C(80)-C(79)-H(79B)	111.2
C(78)-C(79)-H(79B)	111.2
H(79A)-C(79)-H(79B)	109.1
O(2)-C(80)-C(79)	113.3(19)
O(2)-C(80)-H(80A)	108.9
C(79)-C(80)-H(80A)	108.9
O(2)-C(80)-H(80B)	108.9
C(79)-C(80)-H(80B)	108.9
H(80A)-C(80)-H(80B)	107.7
O(4)-K(1)-O(2)	85.2(5)
O(4)-K(1)-O(6)	153.0(5)
O(2)-K(1)-O(6)	119.2(5)
O(4)-K(1)-O(5)	113.2(5)
O(2)-K(1)-O(5)	85.9(4)
O(6)-K(1)-O(5)	81.9(4)
O(4)-K(1)-O(3)	86.0(4)
O(2)-K(1)-O(3)	87.7(4)
O(6)-K(1)-O(3)	83.9(4)
O(5)-K(1)-O(3)	159.1(4)
N(2)-N(1)-C(36)	110.5(6)
N(2)-N(1)-Sm(1)	75.6(4)
C(36)-N(1)-Sm(1)	172.7(5)
C(35)-N(2)-N(1)	117.8(6)
C(35)-N(2)-Sm(1)	168.5(5)
N(1)-N(2)-Sm(1)	73.7(4)

C(7)-N(3)-N(4)	113.8(6)
C(7)-N(3)-Sm(1)	172.0(6)
N(4)-N(3)-Sm(1)	73.9(4)
C(8)-N(4)-N(3)	113.6(7)
C(8)-N(4)-Sm(1)	171.6(6)
N(3)-N(4)-Sm(1)	74.4(4)
C(49)-N(5)-N(6)	112.2(6)
C(49)-N(5)-Sm(1)	172.8(5)
N(6)-N(5)-Sm(1)	74.6(3)
C(50)-N(6)-N(5)	112.6(6)
C(50)-N(6)-Sm(1)	173.8(5)
N(5)-N(6)-Sm(1)	73.5(3)
C(21)-N(7)-N(8)	114.5(6)
C(21)-N(7)-Sm(1)	171.2(5)
N(8)-N(7)-Sm(1)	74.2(3)
C(22)-N(8)-N(7)	110.4(6)
C(22)-N(8)-Sm(1)	176.0(6)
N(7)-N(8)-Sm(1)	73.6(3)
C(57)-O(1)-C(60)	106.4(8)
C(57)-O(1)-Sm(1)	128.4(6)
C(60)-O(1)-Sm(1)	124.2(5)
C(77)-O(2)-C(80)	99.6(14)
C(77)-O(2)-K(1)	123.7(13)
C(80)-O(2)-K(1)	135.8(15)
C(69)-O(3)-C(72)	109.0(14)
C(69)-O(3)-K(1)	125.8(14)
C(72)-O(3)-K(1)	124.9(13)
C(76)-O(4)-C(73)	106.0(11)
C(76)-O(4)-K(1)	124.2(12)
C(73)-O(4)-K(1)	129.2(11)

C(61)-O(5)-C(64)	105.6(16)
C(61)-O(5)-K(1)	124.9(13)
C(64)-O(5)-K(1)	129.3(13)
C(68)-O(6)-C(65)	97.9(13)
C(68)-O(6)-K(1)	126.4(14)
C(65)-O(6)-K(1)	135.6(11)
O(6)-C(65)-C(66)	117.0(14)
O(6)-C(65)-H(65A)	108.0
C(66)-C(65)-H(65A)	108.0
O(6)-C(65)-H(65B)	108.0
C(66)-C(65)-H(65B)	108.0
H(65A)-C(65)-H(65B)	107.3
C(65)-C(66)-C(67)	98.7(11)
C(65)-C(66)-H(66A)	112.0
C(67)-C(66)-H(66A)	112.0
C(65)-C(66)-H(66B)	112.0
C(67)-C(66)-H(66B)	112.0
H(66A)-C(66)-H(66B)	109.7
C(68)-C(67)-C(66)	93.2(13)
C(68)-C(67)-H(67A)	113.1
C(66)-C(67)-H(67A)	113.1
C(68)-C(67)-H(67B)	113.1
C(66)-C(67)-H(67B)	113.1
H(67A)-C(67)-H(67B)	110.5
O(6)-C(68)-C(67)	121(2)
O(6)-C(68)-H(68A)	107.0
C(67)-C(68)-H(68A)	107.0
O(6)-C(68)-H(68B)	107.0
C(67)-C(68)-H(68B)	107.0
H(68A)-C(68)-H(68B)	106.8

O(3)-C(69)-C(70)	107.9(19)
O(3)-C(69)-H(69A)	110.1
C(70)-C(69)-H(69A)	110.1
O(3)-C(69)-H(69B)	110.1
C(70)-C(69)-H(69B)	110.1
H(69A)-C(69)-H(69B)	108.4
C(7)-P(1)-C(8)	86.7(4)
C(36)-P(2)-C(35)	87.1(3)
C(22)-P(3)-C(21)	86.4(4)
C(49)-P(4)-C(50)	86.3(4)
N(4)-Sm(1)-N(5)	88.9(2)
N(4)-Sm(1)-N(3)	31.69(19)
N(5)-Sm(1)-N(3)	91.5(2)
N(4)-Sm(1)-N(7)	87.8(2)
N(5)-Sm(1)-N(7)	155.20(19)
N(3)-Sm(1)-N(7)	98.4(2)
N(4)-Sm(1)-N(8)	118.6(2)
N(5)-Sm(1)-N(8)	137.4(2)
N(3)-Sm(1)-N(8)	129.4(2)
N(7)-Sm(1)-N(8)	32.17(19)
N(4)-Sm(1)-N(6)	117.94(19)
N(5)-Sm(1)-N(6)	31.87(18)
N(3)-Sm(1)-N(6)	122.98(19)
N(7)-Sm(1)-N(6)	135.4(2)
N(8)-Sm(1)-N(6)	107.3(2)
N(4)-Sm(1)-N(1)	121.0(2)
N(5)-Sm(1)-N(1)	86.30(18)
N(3)-Sm(1)-N(1)	89.72(19)
N(7)-Sm(1)-N(1)	116.27(17)
N(8)-Sm(1)-N(1)	103.15(19)

N(6)-Sm(1)-N(1)	82.66(18)
N(4)-Sm(1)-N(2)	115.3(2)
N(5)-Sm(1)-N(2)	116.87(19)
N(3)-Sm(1)-N(2)	86.15(18)
N(7)-Sm(1)-N(2)	86.60(18)
N(8)-Sm(1)-N(2)	81.97(19)
N(6)-Sm(1)-N(2)	110.16(18)
N(1)-Sm(1)-N(2)	30.72(17)
N(4)-Sm(1)-O(1)	80.7(2)
N(5)-Sm(1)-O(1)	77.43(18)
N(3)-Sm(1)-O(1)	112.05(19)
N(7)-Sm(1)-O(1)	77.79(18)
N(8)-Sm(1)-O(1)	76.08(18)
N(6)-Sm(1)-O(1)	72.00(18)
N(1)-Sm(1)-O(1)	152.84(18)
N(2)-Sm(1)-O(1)	157.37(19)

Symmetry transformations used to generate equivalent atoms:

Table 6. Torsion angles [deg] for **8**.

C(6)-C(1)-C(2)-C(3)	-2(2)
C(1)-C(2)-C(3)-C(4)	3(2)
C(2)-C(3)-C(4)-C(5)	-2(2)
C(3)-C(4)-C(5)-C(6)	-0.2(18)
C(2)-C(1)-C(6)-C(5)	-0.1(18)
C(2)-C(1)-C(6)-C(7)	-177.5(11)
C(4)-C(5)-C(6)-C(1)	1.1(15)
C(4)-C(5)-C(6)-C(7)	178.4(9)
C(1)-C(6)-C(7)-N(3)	-7.9(13)
C(5)-C(6)-C(7)-N(3)	174.9(8)
C(1)-C(6)-C(7)-P(1)	171.8(8)
C(5)-C(6)-C(7)-P(1)	-5.4(12)
N(4)-C(8)-C(9)-C(14)	-162.9(11)
P(1)-C(8)-C(9)-C(14)	20.5(16)
N(4)-C(8)-C(9)-C(10)	22.9(16)
P(1)-C(8)-C(9)-C(10)	-153.7(10)
C(14)-C(9)-C(10)-C(11)	2(2)
C(8)-C(9)-C(10)-C(11)	177.3(13)
C(9)-C(10)-C(11)-C(12)	4(2)
C(10)-C(11)-C(12)-C(13)	-8(2)
C(11)-C(12)-C(13)-C(14)	6(3)
C(10)-C(9)-C(14)-C(13)	-5(2)
C(8)-C(9)-C(14)-C(13)	-179.5(13)
C(12)-C(13)-C(14)-C(9)	1(3)
C(20)-C(15)-C(16)-C(17)	0.1(17)
C(15)-C(16)-C(17)-C(18)	0.5(18)
C(16)-C(17)-C(18)-C(19)	-0.6(19)

C(17)-C(18)-C(19)-C(20)	0.1(19)
C(18)-C(19)-C(20)-C(15)	0.4(15)
C(18)-C(19)-C(20)-C(21)	179.9(10)
C(16)-C(15)-C(20)-C(19)	-0.6(15)
C(16)-C(15)-C(20)-C(21)	179.9(9)
C(19)-C(20)-C(21)-N(7)	-165.7(8)
C(15)-C(20)-C(21)-N(7)	13.7(12)
C(19)-C(20)-C(21)-P(3)	13.5(12)
C(15)-C(20)-C(21)-P(3)	-167.0(7)
N(8)-C(22)-C(23)-C(28)	17.0(13)
P(3)-C(22)-C(23)-C(28)	-160.9(8)
N(8)-C(22)-C(23)-C(24)	-161.8(8)
P(3)-C(22)-C(23)-C(24)	20.3(12)
C(28)-C(23)-C(24)-C(25)	1.8(15)
C(22)-C(23)-C(24)-C(25)	-179.4(9)
C(23)-C(24)-C(25)-C(26)	-2.2(18)
C(24)-C(25)-C(26)-C(27)	2(2)
C(25)-C(26)-C(27)-C(28)	-2(2)
C(24)-C(23)-C(28)-C(27)	-1.5(16)
C(22)-C(23)-C(28)-C(27)	179.6(10)
C(26)-C(27)-C(28)-C(23)	2(2)
C(34)-C(29)-C(30)-C(31)	-0.7(15)
C(29)-C(30)-C(31)-C(32)	0.2(19)
C(30)-C(31)-C(32)-C(33)	0(2)
C(31)-C(32)-C(33)-C(34)	0.9(19)
C(30)-C(29)-C(34)-C(33)	1.2(14)
C(30)-C(29)-C(34)-C(35)	176.7(8)
C(32)-C(33)-C(34)-C(29)	-1.3(16)
C(32)-C(33)-C(34)-C(35)	-176.8(10)
C(29)-C(34)-C(35)-N(2)	26.9(12)

C(33)-C(34)-C(35)-N(2)	-157.6(8)
C(29)-C(34)-C(35)-P(2)	-156.2(7)
C(33)-C(34)-C(35)-P(2)	19.3(12)
N(1)-C(36)-C(37)-C(42)	-1.8(13)
P(2)-C(36)-C(37)-C(42)	176.5(8)
N(1)-C(36)-C(37)-C(38)	178.7(8)
P(2)-C(36)-C(37)-C(38)	-3.0(12)
C(42)-C(37)-C(38)-C(39)	-1.0(16)
C(36)-C(37)-C(38)-C(39)	178.6(10)
C(37)-C(38)-C(39)-C(40)	-0.5(19)
C(38)-C(39)-C(40)-C(41)	0(2)
C(39)-C(40)-C(41)-C(42)	1(2)
C(38)-C(37)-C(42)-C(41)	2.5(16)
C(36)-C(37)-C(42)-C(41)	-177.0(10)
C(40)-C(41)-C(42)-C(37)	-3(2)
C(48)-C(43)-C(44)-C(45)	-1(2)
C(43)-C(44)-C(45)-C(46)	1(3)
C(44)-C(45)-C(46)-C(47)	-1(3)
C(45)-C(46)-C(47)-C(48)	1(2)
C(44)-C(43)-C(48)-C(47)	1.3(18)
C(44)-C(43)-C(48)-C(49)	-177.9(11)
C(46)-C(47)-C(48)-C(43)	-1.1(18)
C(46)-C(47)-C(48)-C(49)	178.0(12)
C(43)-C(48)-C(49)-N(5)	-11.1(14)
C(47)-C(48)-C(49)-N(5)	169.8(9)
C(43)-C(48)-C(49)-P(4)	167.0(9)
C(47)-C(48)-C(49)-P(4)	-12.2(13)
N(6)-C(50)-C(51)-C(52)	30.2(12)
P(4)-C(50)-C(51)-C(52)	-146.1(8)
N(6)-C(50)-C(51)-C(56)	-153.1(9)

P(4)-C(50)-C(51)-C(56)	30.6(12)
C(56)-C(51)-C(52)-C(53)	-1.2(15)
C(50)-C(51)-C(52)-C(53)	175.5(9)
C(51)-C(52)-C(53)-C(54)	2.3(17)
C(52)-C(53)-C(54)-C(55)	-3(2)
C(53)-C(54)-C(55)-C(56)	3(2)
C(54)-C(55)-C(56)-C(51)	-2(2)
C(52)-C(51)-C(56)-C(55)	1.2(16)
C(50)-C(51)-C(56)-C(55)	-175.5(10)
O(1)-C(57)-C(58)-C(59)	2.6(17)
C(57)-C(58)-C(59)-C(60)	5.2(17)
C(58)-C(59)-C(60)-O(1)	-11.4(17)
O(5)-C(61)-C(62)-C(63)	-26(3)
C(61)-C(62)-C(63)-C(64)	20(3)
C(62)-C(63)-C(64)-O(5)	-8(3)
C(69)-C(70)-C(71)-C(72)	16(3)
C(70)-C(71)-C(72)-O(3)	-8(3)
O(4)-C(73)-C(74)-C(75)	4(4)
C(73)-C(74)-C(75)-C(76)	-16(3)
C(74)-C(75)-C(76)-O(4)	26(3)
O(2)-C(77)-C(78)-C(79)	-15(4)
C(77)-C(78)-C(79)-C(80)	20(3)
C(78)-C(79)-C(80)-O(2)	-20(3)
C(37)-C(36)-N(1)-N(2)	-178.3(7)
P(2)-C(36)-N(1)-N(2)	3.2(8)
C(37)-C(36)-N(1)-Sm(1)	-33(4)
P(2)-C(36)-N(1)-Sm(1)	149(3)
C(34)-C(35)-N(2)-N(1)	-178.9(7)
P(2)-C(35)-N(2)-N(1)	3.8(8)
C(34)-C(35)-N(2)-Sm(1)	0(3)

P(2)-C(35)-N(2)-Sm(1)	-178(2)
C(36)-N(1)-N(2)-C(35)	-4.6(9)
Sm(1)-N(1)-N(2)-C(35)	179.7(6)
C(36)-N(1)-N(2)-Sm(1)	175.7(5)
C(6)-C(7)-N(3)-N(4)	179.0(6)
P(1)-C(7)-N(3)-N(4)	-0.7(8)
C(6)-C(7)-N(3)-Sm(1)	-15(4)
P(1)-C(7)-N(3)-Sm(1)	165(3)
C(9)-C(8)-N(4)-N(3)	-177.1(7)
P(1)-C(8)-N(4)-N(3)	-0.1(8)
C(9)-C(8)-N(4)-Sm(1)	20(4)
P(1)-C(8)-N(4)-Sm(1)	-163(3)
C(7)-N(3)-N(4)-C(8)	0.5(9)
Sm(1)-N(3)-N(4)-C(8)	-177.4(6)
C(7)-N(3)-N(4)-Sm(1)	177.9(6)
C(48)-C(49)-N(5)-N(6)	176.0(7)
P(4)-C(49)-N(5)-N(6)	-2.3(8)
C(48)-C(49)-N(5)-Sm(1)	16(5)
P(4)-C(49)-N(5)-Sm(1)	-162(4)
C(51)-C(50)-N(6)-N(5)	-177.9(7)
P(4)-C(50)-N(6)-N(5)	-1.2(8)
C(51)-C(50)-N(6)-Sm(1)	-1(5)
P(4)-C(50)-N(6)-Sm(1)	175(4)
C(49)-N(5)-N(6)-C(50)	2.2(9)
Sm(1)-N(5)-N(6)-C(50)	179.6(6)
C(49)-N(5)-N(6)-Sm(1)	-177.4(6)
C(20)-C(21)-N(7)-N(8)	178.3(6)
P(3)-C(21)-N(7)-N(8)	-1.0(8)
C(20)-C(21)-N(7)-Sm(1)	5(4)
P(3)-C(21)-N(7)-Sm(1)	-174(3)

C(23)-C(22)-N(8)-N(7)	-178.5(6)
P(3)-C(22)-N(8)-N(7)	-0.3(8)
C(23)-C(22)-N(8)-Sm(1)	-1(8)
P(3)-C(22)-N(8)-Sm(1)	177(100)
C(21)-N(7)-N(8)-C(22)	0.9(8)
Sm(1)-N(7)-N(8)-C(22)	179.8(6)
C(21)-N(7)-N(8)-Sm(1)	-178.9(6)
C(58)-C(57)-O(1)-C(60)	-9.6(14)
C(58)-C(57)-O(1)-Sm(1)	-178.3(8)
C(59)-C(60)-O(1)-C(57)	12.8(14)
C(59)-C(60)-O(1)-Sm(1)	-177.9(8)
C(78)-C(77)-O(2)-C(80)	4(3)
C(78)-C(77)-O(2)-K(1)	174.6(19)
C(79)-C(80)-O(2)-C(77)	11(3)
C(79)-C(80)-O(2)-K(1)	-158.2(17)
O(4)-K(1)-O(2)-C(77)	35.6(17)
O(6)-K(1)-O(2)-C(77)	-156.6(16)
O(5)-K(1)-O(2)-C(77)	-78.2(17)
O(3)-K(1)-O(2)-C(77)	121.7(17)
O(4)-K(1)-O(2)-C(80)	-157.5(18)
O(6)-K(1)-O(2)-C(80)	10.3(18)
O(5)-K(1)-O(2)-C(80)	88.7(17)
O(3)-K(1)-O(2)-C(80)	-71.4(17)
C(71)-C(72)-O(3)-C(69)	-4(3)
C(71)-C(72)-O(3)-K(1)	-178.1(14)
O(4)-K(1)-O(3)-C(69)	-89.2(15)
O(2)-K(1)-O(3)-C(69)	-174.6(15)
O(6)-K(1)-O(3)-C(69)	65.7(15)
O(5)-K(1)-O(3)-C(69)	113.2(18)
O(4)-K(1)-O(3)-C(72)	83.9(16)

O(2)-K(1)-O(3)-C(72)	-1.5(15)
O(6)-K(1)-O(3)-C(72)	-121.2(16)
O(5)-K(1)-O(3)-C(72)	-73.7(19)
C(75)-C(76)-O(4)-C(73)	-24(3)
C(75)-C(76)-O(4)-K(1)	163.5(18)
C(74)-C(73)-O(4)-C(76)	12(3)
C(74)-C(73)-O(4)-K(1)	-176.0(19)
O(2)-K(1)-O(4)-C(76)	-104.8(19)
O(6)-K(1)-O(4)-C(76)	99(2)
O(5)-K(1)-O(4)-C(76)	-21(2)
O(3)-K(1)-O(4)-C(76)	167.2(19)
O(2)-K(1)-O(4)-C(73)	85(2)
O(6)-K(1)-O(4)-C(73)	-71(3)
O(5)-K(1)-O(4)-C(73)	169(2)
O(3)-K(1)-O(4)-C(73)	-3(2)
C(62)-C(61)-O(5)-C(64)	21(3)
C(62)-C(61)-O(5)-K(1)	-153.9(16)
C(63)-C(64)-O(5)-C(61)	-7(3)
C(63)-C(64)-O(5)-K(1)	167.5(16)
O(4)-K(1)-O(5)-C(61)	-94.6(17)
O(2)-K(1)-O(5)-C(61)	-11.6(17)
O(6)-K(1)-O(5)-C(61)	108.7(17)
O(3)-K(1)-O(5)-C(61)	61(2)
O(4)-K(1)-O(5)-C(64)	92.2(18)
O(2)-K(1)-O(5)-C(64)	175.2(18)
O(6)-K(1)-O(5)-C(64)	-64.5(18)
O(3)-K(1)-O(5)-C(64)	-112(2)
O(4)-K(1)-O(6)-C(68)	100(3)
O(2)-K(1)-O(6)-C(68)	-52(3)
O(5)-K(1)-O(6)-C(68)	-133(3)

O(3)-K(1)-O(6)-C(68)	32(3)
O(4)-K(1)-O(6)-C(65)	-74(3)
O(2)-K(1)-O(6)-C(65)	134(2)
O(5)-K(1)-O(6)-C(65)	53(3)
O(3)-K(1)-O(6)-C(65)	-142(3)
C(68)-O(6)-C(65)-C(66)	-5(4)
K(1)-O(6)-C(65)-C(66)	169.6(18)
O(6)-C(65)-C(66)-C(67)	-16(4)
C(65)-C(66)-C(67)-C(68)	25(3)
C(65)-O(6)-C(68)-C(67)	29(4)
K(1)-O(6)-C(68)-C(67)	-146.5(19)
C(66)-C(67)-C(68)-O(6)	-38(4)
C(72)-O(3)-C(69)-C(70)	14(3)
K(1)-O(3)-C(69)-C(70)	-171.6(14)
C(71)-C(70)-C(69)-O(3)	-20(3)
N(3)-C(7)-P(1)-C(8)	0.6(6)
C(6)-C(7)-P(1)-C(8)	-179.2(7)
N(4)-C(8)-P(1)-C(7)	-0.3(6)
C(9)-C(8)-P(1)-C(7)	176.6(8)
N(1)-C(36)-P(2)-C(35)	-1.0(6)
C(37)-C(36)-P(2)-C(35)	-179.4(7)
N(2)-C(35)-P(2)-C(36)	-1.5(6)
C(34)-C(35)-P(2)-C(36)	-178.8(7)
N(8)-C(22)-P(3)-C(21)	-0.2(6)
C(23)-C(22)-P(3)-C(21)	177.8(7)
N(7)-C(21)-P(3)-C(22)	0.7(6)
C(20)-C(21)-P(3)-C(22)	-178.6(7)
N(5)-C(49)-P(4)-C(50)	1.3(7)
C(48)-C(49)-P(4)-C(50)	-176.8(8)
N(6)-C(50)-P(4)-C(49)	-0.1(6)

C(51)-C(50)-P(4)-C(49)	176.5(8)
C(8)-N(4)-Sm(1)-N(5)	69(4)
N(3)-N(4)-Sm(1)-N(5)	-94.6(4)
C(8)-N(4)-Sm(1)-N(3)	163(4)
C(8)-N(4)-Sm(1)-N(7)	-87(4)
N(3)-N(4)-Sm(1)-N(7)	109.9(4)
C(8)-N(4)-Sm(1)-N(8)	-77(4)
N(3)-N(4)-Sm(1)-N(8)	119.5(4)
C(8)-N(4)-Sm(1)-N(6)	55(4)
N(3)-N(4)-Sm(1)-N(6)	-108.3(4)
C(8)-N(4)-Sm(1)-N(1)	154(4)
N(3)-N(4)-Sm(1)-N(1)	-9.6(4)
C(8)-N(4)-Sm(1)-N(2)	-172(4)
N(3)-N(4)-Sm(1)-N(2)	24.8(4)
C(8)-N(4)-Sm(1)-O(1)	-9(4)
N(3)-N(4)-Sm(1)-O(1)	-172.1(4)
C(49)-N(5)-Sm(1)-N(4)	4(4)
N(6)-N(5)-Sm(1)-N(4)	-156.7(4)
C(49)-N(5)-Sm(1)-N(3)	-28(4)
N(6)-N(5)-Sm(1)-N(3)	171.7(4)
C(49)-N(5)-Sm(1)-N(7)	86(4)
N(6)-N(5)-Sm(1)-N(7)	-74.5(6)
C(49)-N(5)-Sm(1)-N(8)	137(4)
N(6)-N(5)-Sm(1)-N(8)	-23.4(5)
C(49)-N(5)-Sm(1)-N(6)	161(4)
C(49)-N(5)-Sm(1)-N(1)	-117(4)
N(6)-N(5)-Sm(1)-N(1)	82.0(4)
C(49)-N(5)-Sm(1)-N(2)	-114(4)
N(6)-N(5)-Sm(1)-N(2)	85.2(4)
C(49)-N(5)-Sm(1)-O(1)	85(4)

N(6)-N(5)-Sm(1)-O(1)	-76.1(4)
C(7)-N(3)-Sm(1)-N(4)	-166(4)
C(7)-N(3)-Sm(1)-N(5)	-81(4)
N(4)-N(3)-Sm(1)-N(5)	85.5(4)
C(7)-N(3)-Sm(1)-N(7)	122(4)
N(4)-N(3)-Sm(1)-N(7)	-71.7(4)
C(7)-N(3)-Sm(1)-N(8)	112(4)
N(4)-N(3)-Sm(1)-N(8)	-81.4(4)
C(7)-N(3)-Sm(1)-N(6)	-76(4)
N(4)-N(3)-Sm(1)-N(6)	90.7(4)
C(7)-N(3)-Sm(1)-N(1)	5(4)
N(4)-N(3)-Sm(1)-N(1)	171.8(4)
C(7)-N(3)-Sm(1)-N(2)	36(4)
N(4)-N(3)-Sm(1)-N(2)	-157.7(4)
C(7)-N(3)-Sm(1)-O(1)	-158(4)
N(4)-N(3)-Sm(1)-O(1)	8.4(4)
C(21)-N(7)-Sm(1)-N(4)	-22(3)
N(8)-N(7)-Sm(1)-N(4)	164.1(4)
C(21)-N(7)-Sm(1)-N(5)	-105(3)
N(8)-N(7)-Sm(1)-N(5)	81.7(6)
C(21)-N(7)-Sm(1)-N(3)	8(3)
N(8)-N(7)-Sm(1)-N(3)	-165.9(3)
C(21)-N(7)-Sm(1)-N(8)	174(3)
C(21)-N(7)-Sm(1)-N(6)	-151(3)
N(8)-N(7)-Sm(1)-N(6)	35.3(4)
C(21)-N(7)-Sm(1)-N(1)	101(3)
N(8)-N(7)-Sm(1)-N(1)	-72.1(4)
C(21)-N(7)-Sm(1)-N(2)	93(3)
N(8)-N(7)-Sm(1)-N(2)	-80.3(4)
C(21)-N(7)-Sm(1)-O(1)	-103(3)

N(8)-N(7)-Sm(1)-O(1)	83.2(4)
C(22)-N(8)-Sm(1)-N(4)	164(7)
N(7)-N(8)-Sm(1)-N(4)	-18.1(4)
C(22)-N(8)-Sm(1)-N(5)	40(8)
N(7)-N(8)-Sm(1)-N(5)	-142.2(3)
C(22)-N(8)-Sm(1)-N(3)	-159(7)
N(7)-N(8)-Sm(1)-N(3)	18.2(4)
C(22)-N(8)-Sm(1)-N(7)	-177(100)
C(22)-N(8)-Sm(1)-N(6)	28(8)
N(7)-N(8)-Sm(1)-N(6)	-154.9(3)
C(22)-N(8)-Sm(1)-N(1)	-59(7)
N(7)-N(8)-Sm(1)-N(1)	118.8(3)
C(22)-N(8)-Sm(1)-N(2)	-81(7)
N(7)-N(8)-Sm(1)-N(2)	96.4(4)
C(22)-N(8)-Sm(1)-O(1)	93(7)
N(7)-N(8)-Sm(1)-O(1)	-89.1(3)
C(50)-N(6)-Sm(1)-N(4)	-150(5)
N(5)-N(6)-Sm(1)-N(4)	26.5(4)
C(50)-N(6)-Sm(1)-N(5)	-177(100)
C(50)-N(6)-Sm(1)-N(3)	173(5)
N(5)-N(6)-Sm(1)-N(3)	-9.9(4)
C(50)-N(6)-Sm(1)-N(7)	-32(5)
N(5)-N(6)-Sm(1)-N(7)	144.9(3)
C(50)-N(6)-Sm(1)-N(8)	-13(5)
N(5)-N(6)-Sm(1)-N(8)	163.6(4)
C(50)-N(6)-Sm(1)-N(1)	89(5)
N(5)-N(6)-Sm(1)-N(1)	-94.8(4)
C(50)-N(6)-Sm(1)-N(2)	75(5)
N(5)-N(6)-Sm(1)-N(2)	-108.7(4)
C(50)-N(6)-Sm(1)-O(1)	-81(5)

N(5)-N(6)-Sm(1)-O(1)	95.1(4)
N(2)-N(1)-Sm(1)-N(4)	88.0(4)
C(36)-N(1)-Sm(1)-N(4)	-59(4)
N(2)-N(1)-Sm(1)-N(5)	174.4(4)
C(36)-N(1)-Sm(1)-N(5)	27(4)
N(2)-N(1)-Sm(1)-N(3)	82.9(4)
C(36)-N(1)-Sm(1)-N(3)	-64(4)
N(2)-N(1)-Sm(1)-N(7)	-16.3(4)
C(36)-N(1)-Sm(1)-N(7)	-163(4)
N(2)-N(1)-Sm(1)-N(8)	-47.6(4)
C(36)-N(1)-Sm(1)-N(8)	165(4)
N(2)-N(1)-Sm(1)-N(6)	-153.8(4)
C(36)-N(1)-Sm(1)-N(6)	59(4)
C(36)-N(1)-Sm(1)-N(2)	-147(4)
N(2)-N(1)-Sm(1)-O(1)	-132.7(4)
C(36)-N(1)-Sm(1)-O(1)	80(4)
C(35)-N(2)-Sm(1)-N(4)	73(3)
N(1)-N(2)-Sm(1)-N(4)	-108.7(4)
C(35)-N(2)-Sm(1)-N(5)	175(2)
N(1)-N(2)-Sm(1)-N(5)	-6.2(4)
C(35)-N(2)-Sm(1)-N(3)	85(2)
N(1)-N(2)-Sm(1)-N(3)	-96.0(4)
C(35)-N(2)-Sm(1)-N(7)	-13(2)
N(1)-N(2)-Sm(1)-N(7)	165.4(4)
C(35)-N(2)-Sm(1)-N(8)	-45(2)
N(1)-N(2)-Sm(1)-N(8)	133.4(4)
C(35)-N(2)-Sm(1)-N(6)	-151(2)
N(1)-N(2)-Sm(1)-N(6)	27.9(4)
C(35)-N(2)-Sm(1)-N(1)	-179(3)
C(35)-N(2)-Sm(1)-O(1)	-59(3)

N(1)-N(2)-Sm(1)-O(1)	119.3(5)
C(57)-O(1)-Sm(1)-N(4)	-117.5(8)
C(60)-O(1)-Sm(1)-N(4)	75.6(8)
C(57)-O(1)-Sm(1)-N(5)	151.5(8)
C(60)-O(1)-Sm(1)-N(5)	-15.3(8)
C(57)-O(1)-Sm(1)-N(3)	-122.0(8)
C(60)-O(1)-Sm(1)-N(3)	71.1(8)
C(57)-O(1)-Sm(1)-N(7)	-27.8(8)
C(60)-O(1)-Sm(1)-N(7)	165.3(8)
C(57)-O(1)-Sm(1)-N(8)	5.2(8)
C(60)-O(1)-Sm(1)-N(8)	-161.7(8)
C(57)-O(1)-Sm(1)-N(6)	118.9(8)
C(60)-O(1)-Sm(1)-N(6)	-47.9(8)
C(57)-O(1)-Sm(1)-N(1)	96.9(9)
C(60)-O(1)-Sm(1)-N(1)	-69.9(9)
C(57)-O(1)-Sm(1)-N(2)	19.6(10)
C(60)-O(1)-Sm(1)-N(2)	-147.3(8)

Symmetry transformations used to generate equivalent atoms:

4.7 Crystal structural analysis data for **9**

Table 1. Crystal data and structure refinement for **9**.

Identification code	exp_1064
Empirical formula	C ₆₄ H ₁₂₀ K N ₈ O ₆ P ₄ Sm
Formula weight	1411.01
Temperature	100.00(10) K
Wavelength	1.54184 Å
Crystal system, space group	Monoclinic, C 1 c 1
Unit cell dimensions	a = 26.1247(9) Å alpha = 90 deg. b = 14.7156(4) Å beta = 109.538(4) deg. c = 21.3571(7) Å gamma = 90 deg.
Volume	7737.8(4) Å ³
Z, Calculated density	4, 1.211 Mg/m ³
Absorption coefficient	7.339 mm ⁻¹
F(000)	2996
Crystal size	0.1500 x 0.0900 x 0.0400 mm
Theta range for data collection	3.50 to 67.08 deg.
Limiting indices	-30 ≤ h ≤ 31, -17 ≤ k ≤ 13, -25 ≤ l ≤ 25
Reflections collected / unique	13791 / 8714 [R(int) = 0.0510]
Completeness to theta = 67.08	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.22779
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8714 / 20 / 778
Goodness-of-fit on F ²	1.072
Final R indices [I > 2sigma(I)]	R1 = 0.0603, wR2 = 0.1433
R indices (all data)	R1 = 0.0738, wR2 = 0.1548
Absolute structure parameter	0.097(5)
Largest diff. peak and hole	2.599 and -1.223 e.Å ⁻³

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

C(1)-C(4)	1.511(18)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(2)-C(4)	1.539(17)
C(2)-H(2A)	0.9600
C(2)-H(2B)	0.9600
C(2)-H(2C)	0.9600
C(3)-C(4)	1.523(18)
C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600
C(3)-H(3C)	0.9600
C(4)-C(5)	1.506(17)
C(5)-N(5)	1.325(14)
C(5)-P(4)	1.770(12)
C(6)-N(6)	1.338(14)
C(6)-C(7)	1.530(17)
C(6)-P(4)	1.745(12)
C(7)-C(8)	1.491(18)
C(7)-C(10)	1.506(18)
C(7)-C(9)	1.561(18)
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600

C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-C(14)	1.566(19)
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(12)-C(14)	1.505(19)
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-C(14)	1.51(2)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-C(15)	1.512(17)
C(15)-N(8)	1.357(15)
C(15)-P(3)	1.745(13)
C(16)-N(7)	1.322(15)
C(16)-C(17)	1.512(18)
C(16)-P(3)	1.754(12)
C(17)-C(19)	1.526(19)
C(17)-C(18)	1.537(19)
C(17)-C(20)	1.538(19)
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600

C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(21)-C(24)	1.564(16)
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-C(24)	1.559(18)
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(23)-C(24)	1.500(17)
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(24)-C(25)	1.538(16)
C(25)-N(2)	1.317(13)
C(25)-P(1)	1.769(11)
C(26)-N(1)	1.347(14)
C(26)-C(27)	1.526(18)
C(26)-P(1)	1.742(12)
C(27)-C(30)	1.490(19)
C(27)-C(28)	1.541(17)
C(27)-C(29)	1.560(18)
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600
C(29)-H(29A)	0.9600
C(29)-H(29B)	0.9600
C(29)-H(29C)	0.9600

C(30)-H(30A)	0.9600
C(30)-H(30B)	0.9600
C(30)-H(30C)	0.9600
C(31)-C(34)	1.515(18)
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600
C(31)-H(31C)	0.9600
C(32)-C(34)	1.531(17)
C(32)-H(32A)	0.9600
C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
C(33)-C(34)	1.506(18)
C(33)-H(33A)	0.9600
C(33)-H(33B)	0.9600
C(33)-H(33C)	0.9600
C(34)-C(35)	1.510(16)
C(35)-N(4)	1.372(13)
C(35)-P(2)	1.764(12)
C(36)-N(3)	1.329(14)
C(36)-C(37)	1.543(18)
C(36)-P(2)	1.737(13)
C(37)-C(38)	1.495(19)
C(37)-C(39)	1.522(18)
C(37)-C(40)	1.534(18)
C(38)-H(38A)	0.9600
C(38)-H(38B)	0.9600
C(38)-H(38C)	0.9600
C(39)-H(39A)	0.9600
C(39)-H(39B)	0.9600
C(39)-H(39C)	0.9600

C(40)-H(40A)	0.9600
C(40)-H(40B)	0.9600
C(40)-H(40C)	0.9600
C(41)-O(3)	1.414(17)
C(41)-C(42)	1.49(2)
C(41)-H(41A)	0.9700
C(41)-H(41B)	0.9700
C(42)-C(43)	1.46(2)
C(42)-H(42A)	0.9700
C(42)-H(42B)	0.9700
C(43)-C(44)	1.50(3)
C(43)-H(43A)	0.9700
C(43)-H(43B)	0.9700
C(44)-O(3)	1.428(19)
C(44)-H(44A)	0.9700
C(44)-H(44B)	0.9700
C(45)-O(6)	1.436(16)
C(45)-C(46)	1.513(18)
C(45)-H(45A)	0.9700
C(45)-H(45B)	0.9700
C(46)-C(47)	1.484(17)
C(46)-H(46A)	0.9700
C(46)-H(46B)	0.9700
C(47)-C(48)	1.489(19)
C(47)-H(47A)	0.9700
C(47)-H(47B)	0.9700
C(48)-O(6)	1.437(15)
C(48)-H(48A)	0.9700
C(48)-H(48B)	0.9700
C(49)-O(4)	1.42(2)

C(49)-C(50)	1.48(2)
C(49)-H(49A)	0.9700
C(49)-H(49B)	0.9700
C(50)-C(51)	1.49(2)
C(50)-H(50A)	0.9700
C(50)-H(50B)	0.9700
C(51)-C(52)	1.50(2)
C(51)-H(51A)	0.9700
C(51)-H(51B)	0.9700
C(52)-O(4)	1.438(18)
C(52)-H(52A)	0.9700
C(52)-H(52B)	0.9700
C(53)-O(2)	1.417(16)
C(53)-C(54)	1.510(18)
C(53)-H(53A)	0.9700
C(53)-H(53B)	0.9700
C(54)-C(55)	1.510(17)
C(54)-H(54A)	0.9700
C(54)-H(54B)	0.9700
C(55)-C(56)	1.527(18)
C(55)-H(55A)	0.9700
C(55)-H(55B)	0.9700
C(56)-O(2)	1.454(15)
C(56)-H(56A)	0.9700
C(56)-H(56B)	0.9700
C(57)-O(5)	1.397(16)
C(57)-C(58)	1.54(2)
C(57)-H(57A)	0.9700
C(57)-H(57B)	0.9700
C(58)-C(59)	1.48(3)

C(58)-H(58A)	0.9700
C(58)-H(58B)	0.9700
C(59)-C(60)	1.47(2)
C(59)-H(59A)	0.9700
C(59)-H(59B)	0.9700
C(60)-O(5)	1.421(18)
C(60)-H(60A)	0.9700
C(60)-H(60B)	0.9700
C(61)-O(1)	1.438(17)
C(61)-C(62)	1.48(2)
C(61)-H(61A)	0.9700
C(61)-H(61B)	0.9700
C(62)-C(63)	1.49(2)
C(62)-H(62A)	0.9700
C(62)-H(62B)	0.9700
C(63)-C(64)	1.48(2)
C(63)-H(63A)	0.9700
C(63)-H(63B)	0.9700
C(64)-O(1)	1.432(17)
C(64)-H(64A)	0.9700
C(64)-H(64B)	0.9700
K(1)-O(6)	2.665(10)
K(1)-O(2)	2.676(10)
K(1)-O(4)	2.684(12)
K(1)-O(3)	2.689(11)
K(1)-O(1)	2.695(11)
K(1)-O(5)	2.699(11)
N(1)-N(2)	1.387(12)
N(1)-Sm(1)	2.445(9)
N(2)-Sm(1)	2.450(10)

N(3)-N(4)	1.360(12)
N(3)-Sm(1)	2.458(8)
N(4)-Sm(1)	2.439(8)
N(5)-N(6)	1.364(12)
N(5)-Sm(1)	2.444(9)
N(6)-Sm(1)	2.424(8)
N(7)-N(8)	1.382(11)
N(7)-Sm(1)	2.426(9)
N(8)-Sm(1)	2.444(10)

C(4)-C(1)-H(1A)	109.5
C(4)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(4)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(4)-C(2)-H(2A)	109.5
C(4)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(4)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(4)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(4)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(5)-C(4)-C(1)	111.0(11)
C(5)-C(4)-C(3)	110.2(10)

C(1)-C(4)-C(3)	108.0(12)
C(5)-C(4)-C(2)	109.4(11)
C(1)-C(4)-C(2)	108.9(11)
C(3)-C(4)-C(2)	109.2(11)
N(5)-C(5)-C(4)	122.1(11)
N(5)-C(5)-P(4)	112.4(8)
C(4)-C(5)-P(4)	125.5(9)
N(6)-C(6)-C(7)	118.1(10)
N(6)-C(6)-P(4)	113.2(8)
C(7)-C(6)-P(4)	128.4(9)
C(8)-C(7)-C(10)	112.3(12)
C(8)-C(7)-C(6)	110.2(11)
C(10)-C(7)-C(6)	109.9(11)
C(8)-C(7)-C(9)	108.7(11)
C(10)-C(7)-C(9)	109.5(12)
C(6)-C(7)-C(9)	106.0(11)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5

H(10A)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(14)-C(11)-H(11A)	109.5
C(14)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(14)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(14)-C(12)-H(12A)	109.5
C(14)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(14)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(14)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-C(15)	111.2(11)
C(12)-C(14)-C(13)	110.2(15)
C(15)-C(14)-C(13)	110.2(11)
C(12)-C(14)-C(11)	107.9(13)
C(15)-C(14)-C(11)	108.6(12)
C(13)-C(14)-C(11)	108.7(13)
N(8)-C(15)-C(14)	118.0(11)
N(8)-C(15)-P(3)	114.1(9)

C(14)-C(15)-P(3)	127.9(9)
N(7)-C(16)-C(17)	117.8(11)
N(7)-C(16)-P(3)	113.6(9)
C(17)-C(16)-P(3)	128.5(9)
C(16)-C(17)-C(19)	110.3(11)
C(16)-C(17)-C(18)	111.0(11)
C(19)-C(17)-C(18)	109.2(12)
C(16)-C(17)-C(20)	110.7(11)
C(19)-C(17)-C(20)	108.5(11)
C(18)-C(17)-C(20)	107.0(12)
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(17)-C(20)-H(20A)	109.5
C(17)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(17)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(24)-C(21)-H(21A)	109.5
C(24)-C(21)-H(21B)	109.5

H(21A)-C(21)-H(21B)	109.5
C(24)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(24)-C(22)-H(22A)	109.5
C(24)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(24)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(24)-C(23)-H(23A)	109.5
C(24)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(24)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(23)-C(24)-C(25)	111.8(10)
C(23)-C(24)-C(22)	110.7(11)
C(25)-C(24)-C(22)	108.6(10)
C(23)-C(24)-C(21)	108.7(11)
C(25)-C(24)-C(21)	108.8(10)
C(22)-C(24)-C(21)	108.0(10)
N(2)-C(25)-C(24)	119.5(10)
N(2)-C(25)-P(1)	114.2(8)
C(24)-C(25)-P(1)	126.3(8)
N(1)-C(26)-C(27)	117.5(11)
N(1)-C(26)-P(1)	113.3(8)
C(27)-C(26)-P(1)	129.1(9)
C(30)-C(27)-C(26)	112.9(11)
C(30)-C(27)-C(28)	110.3(12)

C(26)-C(27)-C(28)	108.3(11)
C(30)-C(27)-C(29)	110.1(12)
C(26)-C(27)-C(29)	106.5(11)
C(28)-C(27)-C(29)	108.6(11)
C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-H(29A)	109.5
C(27)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(27)-C(30)-H(30A)	109.5
C(27)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(27)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(34)-C(31)-H(31A)	109.5
C(34)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(34)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(34)-C(32)-H(32A)	109.5
C(34)-C(32)-H(32B)	109.5

H(32A)-C(32)-H(32B)	109.5
C(34)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(34)-C(33)-H(33A)	109.5
C(34)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(34)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(33)-C(34)-C(35)	109.8(11)
C(33)-C(34)-C(31)	109.5(12)
C(35)-C(34)-C(31)	110.3(10)
C(33)-C(34)-C(32)	108.3(12)
C(35)-C(34)-C(32)	109.2(11)
C(31)-C(34)-C(32)	109.6(13)
N(4)-C(35)-C(34)	120.0(10)
N(4)-C(35)-P(2)	111.9(8)
C(34)-C(35)-P(2)	128.2(8)
N(3)-C(36)-C(37)	119.1(11)
N(3)-C(36)-P(2)	112.9(9)
C(37)-C(36)-P(2)	128.0(9)
C(38)-C(37)-C(39)	110.7(12)
C(38)-C(37)-C(40)	109.6(12)
C(39)-C(37)-C(40)	109.1(12)
C(38)-C(37)-C(36)	108.7(11)
C(39)-C(37)-C(36)	109.3(11)
C(40)-C(37)-C(36)	109.5(10)
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5

H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(37)-C(40)-H(40A)	109.5
C(37)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(37)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
O(3)-C(41)-C(42)	106.7(12)
O(3)-C(41)-H(41A)	110.4
C(42)-C(41)-H(41A)	110.4
O(3)-C(41)-H(41B)	110.4
C(42)-C(41)-H(41B)	110.4
H(41A)-C(41)-H(41B)	108.6
C(43)-C(42)-C(41)	101.3(15)
C(43)-C(42)-H(42A)	111.5
C(41)-C(42)-H(42A)	111.5
C(43)-C(42)-H(42B)	111.5
C(41)-C(42)-H(42B)	111.5
H(42A)-C(42)-H(42B)	109.3
C(42)-C(43)-C(44)	103.7(14)
C(42)-C(43)-H(43A)	111.0

C(44)-C(43)-H(43A)	111.0
C(42)-C(43)-H(43B)	111.0
C(44)-C(43)-H(43B)	111.0
H(43A)-C(43)-H(43B)	109.0
O(3)-C(44)-C(43)	104.5(14)
O(3)-C(44)-H(44A)	110.9
C(43)-C(44)-H(44A)	110.9
O(3)-C(44)-H(44B)	110.9
C(43)-C(44)-H(44B)	110.9
H(44A)-C(44)-H(44B)	108.9
O(6)-C(45)-C(46)	106.1(10)
O(6)-C(45)-H(45A)	110.5
C(46)-C(45)-H(45A)	110.5
O(6)-C(45)-H(45B)	110.5
C(46)-C(45)-H(45B)	110.5
H(45A)-C(45)-H(45B)	108.7
C(47)-C(46)-C(45)	103.3(11)
C(47)-C(46)-H(46A)	111.1
C(45)-C(46)-H(46A)	111.1
C(47)-C(46)-H(46B)	111.1
C(45)-C(46)-H(46B)	111.1
H(46A)-C(46)-H(46B)	109.1
C(46)-C(47)-C(48)	101.6(11)
C(46)-C(47)-H(47A)	111.4
C(48)-C(47)-H(47A)	111.4
C(46)-C(47)-H(47B)	111.4
C(48)-C(47)-H(47B)	111.4
H(47A)-C(47)-H(47B)	109.3
O(6)-C(48)-C(47)	106.4(11)
O(6)-C(48)-H(48A)	110.4

C(47)-C(48)-H(48A)	110.4
O(6)-C(48)-H(48B)	110.4
C(47)-C(48)-H(48B)	110.4
H(48A)-C(48)-H(48B)	108.6
O(4)-C(49)-C(50)	107.4(13)
O(4)-C(49)-H(49A)	110.2
C(50)-C(49)-H(49A)	110.2
O(4)-C(49)-H(49B)	110.2
C(50)-C(49)-H(49B)	110.2
H(49A)-C(49)-H(49B)	108.5
C(49)-C(50)-C(51)	104.0(14)
C(49)-C(50)-H(50A)	111.0
C(51)-C(50)-H(50A)	111.0
C(49)-C(50)-H(50B)	111.0
C(51)-C(50)-H(50B)	111.0
H(50A)-C(50)-H(50B)	109.0
C(50)-C(51)-C(52)	104.5(13)
C(50)-C(51)-H(51A)	110.8
C(52)-C(51)-H(51A)	110.8
C(50)-C(51)-H(51B)	110.8
C(52)-C(51)-H(51B)	110.8
H(51A)-C(51)-H(51B)	108.9
O(4)-C(52)-C(51)	102.7(12)
O(4)-C(52)-H(52A)	111.2
C(51)-C(52)-H(52A)	111.2
O(4)-C(52)-H(52B)	111.2
C(51)-C(52)-H(52B)	111.2
H(52A)-C(52)-H(52B)	109.1
O(2)-C(53)-C(54)	107.4(10)
O(2)-C(53)-H(53A)	110.2

C(54)-C(53)-H(53A)	110.2
O(2)-C(53)-H(53B)	110.2
C(54)-C(53)-H(53B)	110.2
H(53A)-C(53)-H(53B)	108.5
C(53)-C(54)-C(55)	102.4(10)
C(53)-C(54)-H(54A)	111.3
C(55)-C(54)-H(54A)	111.3
C(53)-C(54)-H(54B)	111.3
C(55)-C(54)-H(54B)	111.3
H(54A)-C(54)-H(54B)	109.2
C(54)-C(55)-C(56)	101.6(10)
C(54)-C(55)-H(55A)	111.4
C(56)-C(55)-H(55A)	111.4
C(54)-C(55)-H(55B)	111.4
C(56)-C(55)-H(55B)	111.4
H(55A)-C(55)-H(55B)	109.3
O(2)-C(56)-C(55)	104.2(10)
O(2)-C(56)-H(56A)	110.9
C(55)-C(56)-H(56A)	110.9
O(2)-C(56)-H(56B)	110.9
C(55)-C(56)-H(56B)	110.9
H(56A)-C(56)-H(56B)	108.9
O(5)-C(57)-C(58)	104.8(12)
O(5)-C(57)-H(57A)	110.8
C(58)-C(57)-H(57A)	110.8
O(5)-C(57)-H(57B)	110.8
C(58)-C(57)-H(57B)	110.8
H(57A)-C(57)-H(57B)	108.9
C(59)-C(58)-C(57)	100.9(14)
C(59)-C(58)-H(58A)	111.6

C(57)-C(58)-H(58A)	111.6
C(59)-C(58)-H(58B)	111.6
C(57)-C(58)-H(58B)	111.6
H(58A)-C(58)-H(58B)	109.4
C(60)-C(59)-C(58)	105.8(14)
C(60)-C(59)-H(59A)	110.6
C(58)-C(59)-H(59A)	110.6
C(60)-C(59)-H(59B)	110.6
C(58)-C(59)-H(59B)	110.6
H(59A)-C(59)-H(59B)	108.7
O(5)-C(60)-C(59)	107.8(14)
O(5)-C(60)-H(60A)	110.1
C(59)-C(60)-H(60A)	110.1
O(5)-C(60)-H(60B)	110.1
C(59)-C(60)-H(60B)	110.1
H(60A)-C(60)-H(60B)	108.5
O(1)-C(61)-C(62)	104.7(13)
O(1)-C(61)-H(61A)	110.8
C(62)-C(61)-H(61A)	110.8
O(1)-C(61)-H(61B)	110.8
C(62)-C(61)-H(61B)	110.8
H(61A)-C(61)-H(61B)	108.9
C(61)-C(62)-C(63)	103.9(14)
C(61)-C(62)-H(62A)	111.0
C(63)-C(62)-H(62A)	111.0
C(61)-C(62)-H(62B)	111.0
C(63)-C(62)-H(62B)	111.0
H(62A)-C(62)-H(62B)	109.0
C(64)-C(63)-C(62)	102.3(13)
C(64)-C(63)-H(63A)	111.3

C(62)-C(63)-H(63A)	111.3
C(64)-C(63)-H(63B)	111.3
C(62)-C(63)-H(63B)	111.3
H(63A)-C(63)-H(63B)	109.2
O(1)-C(64)-C(63)	107.5(13)
O(1)-C(64)-H(64A)	110.2
C(63)-C(64)-H(64A)	110.2
O(1)-C(64)-H(64B)	110.2
C(63)-C(64)-H(64B)	110.2
H(64A)-C(64)-H(64B)	108.5
O(6)-K(1)-O(2)	167.5(3)
O(6)-K(1)-O(4)	91.1(4)
O(2)-K(1)-O(4)	101.0(4)
O(6)-K(1)-O(3)	85.5(3)
O(2)-K(1)-O(3)	97.3(3)
O(4)-K(1)-O(3)	91.8(4)
O(6)-K(1)-O(1)	85.5(3)
O(2)-K(1)-O(1)	82.3(3)
O(4)-K(1)-O(1)	175.9(4)
O(3)-K(1)-O(1)	90.2(3)
O(6)-K(1)-O(5)	92.4(3)
O(2)-K(1)-O(5)	84.9(3)
O(4)-K(1)-O(5)	87.3(4)
O(3)-K(1)-O(5)	177.8(4)
O(1)-K(1)-O(5)	90.6(3)
C(26)-N(1)-N(2)	113.2(9)
C(26)-N(1)-Sm(1)	168.3(7)
N(2)-N(1)-Sm(1)	73.7(5)
C(25)-N(2)-N(1)	112.3(9)
C(25)-N(2)-Sm(1)	169.8(7)

N(1)-N(2)-Sm(1)	73.3(5)
C(36)-N(3)-N(4)	115.1(9)
C(36)-N(3)-Sm(1)	167.0(8)
N(4)-N(3)-Sm(1)	73.1(5)
N(3)-N(4)-C(35)	112.0(8)
N(3)-N(4)-Sm(1)	74.6(5)
C(35)-N(4)-Sm(1)	168.5(7)
C(5)-N(5)-N(6)	114.0(9)
C(5)-N(5)-Sm(1)	171.0(8)
N(6)-N(5)-Sm(1)	72.9(5)
C(6)-N(6)-N(5)	113.0(9)
C(6)-N(6)-Sm(1)	170.2(8)
N(5)-N(6)-Sm(1)	74.6(5)
C(16)-N(7)-N(8)	114.1(10)
C(16)-N(7)-Sm(1)	171.6(8)
N(8)-N(7)-Sm(1)	74.2(6)
C(15)-N(8)-N(7)	111.1(10)
C(15)-N(8)-Sm(1)	176.0(8)
N(7)-N(8)-Sm(1)	72.8(6)
C(64)-O(1)-C(61)	108.6(11)
C(64)-O(1)-K(1)	121.9(9)
C(61)-O(1)-K(1)	125.5(8)
C(53)-O(2)-C(56)	109.4(10)
C(53)-O(2)-K(1)	113.3(7)
C(56)-O(2)-K(1)	115.8(8)
C(41)-O(3)-C(44)	108.9(12)
C(41)-O(3)-K(1)	115.3(9)
C(44)-O(3)-K(1)	128.5(9)
C(49)-O(4)-C(52)	109.9(12)
C(49)-O(4)-K(1)	121.6(10)

C(52)-O(4)-K(1)	128.1(9)
C(57)-O(5)-C(60)	108.5(12)
C(57)-O(5)-K(1)	138.7(9)
C(60)-O(5)-K(1)	111.0(9)
C(45)-O(6)-C(48)	108.0(10)
C(45)-O(6)-K(1)	136.6(8)
C(48)-O(6)-K(1)	113.5(8)
C(26)-P(1)-C(25)	87.0(5)
C(36)-P(2)-C(35)	88.2(5)
C(15)-P(3)-C(16)	87.2(5)
C(6)-P(4)-C(5)	87.3(5)
N(6)-Sm(1)-N(7)	80.4(3)
N(6)-Sm(1)-N(4)	117.9(3)
N(7)-Sm(1)-N(4)	134.1(3)
N(6)-Sm(1)-N(8)	89.0(3)
N(7)-Sm(1)-N(8)	33.0(3)
N(4)-Sm(1)-N(8)	102.1(3)
N(6)-Sm(1)-N(5)	32.5(3)
N(7)-Sm(1)-N(5)	88.3(3)
N(4)-Sm(1)-N(5)	130.6(3)
N(8)-Sm(1)-N(5)	111.1(3)
N(6)-Sm(1)-N(1)	134.0(3)
N(7)-Sm(1)-N(1)	114.6(3)
N(4)-Sm(1)-N(1)	83.8(3)
N(8)-Sm(1)-N(1)	128.0(3)
N(5)-Sm(1)-N(1)	102.0(3)
N(6)-Sm(1)-N(2)	149.5(3)
N(7)-Sm(1)-N(2)	86.8(3)
N(4)-Sm(1)-N(2)	90.9(3)
N(8)-Sm(1)-N(2)	95.1(3)

N(5)-Sm(1)-N(2)	120.3(3)
N(1)-Sm(1)-N(2)	32.9(3)
N(6)-Sm(1)-N(3)	89.9(3)
N(7)-Sm(1)-N(3)	150.3(3)
N(4)-Sm(1)-N(3)	32.2(3)
N(8)-Sm(1)-N(3)	119.8(3)
N(5)-Sm(1)-N(3)	98.4(3)
N(1)-Sm(1)-N(3)	92.3(3)
N(2)-Sm(1)-N(3)	113.6(3)

Symmetry transformations used to generate equivalent atoms:

Table 6. Torsion angles [deg] for **9**.

C(1)-C(4)-C(5)-N(5)	153.3(11)
C(3)-C(4)-C(5)-N(5)	33.7(16)
C(2)-C(4)-C(5)-N(5)	-86.5(14)
C(1)-C(4)-C(5)-P(4)	-26.0(16)
C(3)-C(4)-C(5)-P(4)	-145.7(10)
C(2)-C(4)-C(5)-P(4)	94.2(13)
N(6)-C(6)-C(7)-C(8)	49.2(16)
P(4)-C(6)-C(7)-C(8)	-136.3(11)
N(6)-C(6)-C(7)-C(10)	173.5(11)
P(4)-C(6)-C(7)-C(10)	-12.0(17)
N(6)-C(6)-C(7)-C(9)	-68.3(13)
P(4)-C(6)-C(7)-C(9)	106.3(12)
C(12)-C(14)-C(15)-N(8)	170.4(13)
C(13)-C(14)-C(15)-N(8)	47.9(17)
C(11)-C(14)-C(15)-N(8)	-71.0(15)
C(12)-C(14)-C(15)-P(3)	-9.1(18)
C(13)-C(14)-C(15)-P(3)	-131.5(13)
C(11)-C(14)-C(15)-P(3)	109.5(13)
N(7)-C(16)-C(17)-C(19)	-65.7(15)
P(3)-C(16)-C(17)-C(19)	110.1(13)
N(7)-C(16)-C(17)-C(18)	55.5(16)
P(3)-C(16)-C(17)-C(18)	-128.7(12)
N(7)-C(16)-C(17)-C(20)	174.1(11)
P(3)-C(16)-C(17)-C(20)	-10.1(18)
C(23)-C(24)-C(25)-N(2)	-16.4(16)
C(22)-C(24)-C(25)-N(2)	106.1(11)
C(21)-C(24)-C(25)-N(2)	-136.4(10)
C(23)-C(24)-C(25)-P(1)	163.8(9)

C(22)-C(24)-C(25)-P(1)	-73.7(12)
C(21)-C(24)-C(25)-P(1)	43.7(14)
N(1)-C(26)-C(27)-C(30)	-45.4(15)
P(1)-C(26)-C(27)-C(30)	138.7(11)
N(1)-C(26)-C(27)-C(28)	-167.9(10)
P(1)-C(26)-C(27)-C(28)	16.2(16)
N(1)-C(26)-C(27)-C(29)	75.5(14)
P(1)-C(26)-C(27)-C(29)	-100.4(12)
C(33)-C(34)-C(35)-N(4)	-86.4(14)
C(31)-C(34)-C(35)-N(4)	34.4(15)
C(32)-C(34)-C(35)-N(4)	154.9(12)
C(33)-C(34)-C(35)-P(2)	93.4(13)
C(31)-C(34)-C(35)-P(2)	-145.8(10)
C(32)-C(34)-C(35)-P(2)	-25.2(16)
N(3)-C(36)-C(37)-C(38)	-68.5(15)
P(2)-C(36)-C(37)-C(38)	109.4(12)
N(3)-C(36)-C(37)-C(39)	170.7(11)
P(2)-C(36)-C(37)-C(39)	-11.5(16)
N(3)-C(36)-C(37)-C(40)	51.2(15)
P(2)-C(36)-C(37)-C(40)	-130.9(11)
O(3)-C(41)-C(42)-C(43)	32.6(18)
C(41)-C(42)-C(43)-C(44)	-38(2)
C(42)-C(43)-C(44)-O(3)	31(2)
O(6)-C(45)-C(46)-C(47)	26.5(14)
C(45)-C(46)-C(47)-C(48)	-36.9(13)
C(46)-C(47)-C(48)-O(6)	35.2(14)
O(4)-C(49)-C(50)-C(51)	-14.0(18)
C(49)-C(50)-C(51)-C(52)	29.6(17)
C(50)-C(51)-C(52)-O(4)	-34.0(16)
O(2)-C(53)-C(54)-C(55)	26.7(14)

C(53)-C(54)-C(55)-C(56)	-37.4(13)
C(54)-C(55)-C(56)-O(2)	35.6(14)
O(5)-C(57)-C(58)-C(59)	-34.9(17)
C(57)-C(58)-C(59)-C(60)	28.5(18)
C(58)-C(59)-C(60)-O(5)	-13.2(19)
O(1)-C(61)-C(62)-C(63)	33.4(18)
C(61)-C(62)-C(63)-C(64)	-35.2(19)
C(62)-C(63)-C(64)-O(1)	24.5(19)
C(27)-C(26)-N(1)-N(2)	-175.6(9)
P(1)-C(26)-N(1)-N(2)	0.9(11)
C(27)-C(26)-N(1)-Sm(1)	-51(4)
P(1)-C(26)-N(1)-Sm(1)	126(3)
C(24)-C(25)-N(2)-N(1)	-179.3(9)
P(1)-C(25)-N(2)-N(1)	0.5(11)
C(24)-C(25)-N(2)-Sm(1)	59(5)
P(1)-C(25)-N(2)-Sm(1)	-121(4)
C(26)-N(1)-N(2)-C(25)	-0.9(12)
Sm(1)-N(1)-N(2)-C(25)	-170.9(8)
C(26)-N(1)-N(2)-Sm(1)	170.0(8)
C(37)-C(36)-N(3)-N(4)	177.3(10)
P(2)-C(36)-N(3)-N(4)	-0.9(12)
C(37)-C(36)-N(3)-Sm(1)	51(4)
P(2)-C(36)-N(3)-Sm(1)	-128(3)
C(36)-N(3)-N(4)-C(35)	0.9(13)
Sm(1)-N(3)-N(4)-C(35)	170.0(8)
C(36)-N(3)-N(4)-Sm(1)	-169.1(9)
C(34)-C(35)-N(4)-N(3)	179.3(10)
P(2)-C(35)-N(4)-N(3)	-0.6(11)
C(34)-C(35)-N(4)-Sm(1)	-57(4)
P(2)-C(35)-N(4)-Sm(1)	123(3)

C(4)-C(5)-N(5)-N(6)	-179.4(10)
P(4)-C(5)-N(5)-N(6)	0.0(12)
C(4)-C(5)-N(5)-Sm(1)	-40(5)
P(4)-C(5)-N(5)-Sm(1)	139(4)
C(7)-C(6)-N(6)-N(5)	174.7(10)
P(4)-C(6)-N(6)-N(5)	-0.7(12)
C(7)-C(6)-N(6)-Sm(1)	35(5)
P(4)-C(6)-N(6)-Sm(1)	-140(4)
C(5)-N(5)-N(6)-C(6)	0.4(13)
Sm(1)-N(5)-N(6)-C(6)	-173.4(9)
C(5)-N(5)-N(6)-Sm(1)	173.8(9)
C(17)-C(16)-N(7)-N(8)	178.2(10)
P(3)-C(16)-N(7)-N(8)	1.8(12)
C(17)-C(16)-N(7)-Sm(1)	-7(7)
P(3)-C(16)-N(7)-Sm(1)	176(5)
C(14)-C(15)-N(8)-N(7)	-178.2(10)
P(3)-C(15)-N(8)-N(7)	1.4(11)
C(14)-C(15)-N(8)-Sm(1)	-14(13)
P(3)-C(15)-N(8)-Sm(1)	165(11)
C(16)-N(7)-N(8)-C(15)	-2.0(11)
Sm(1)-N(7)-N(8)-C(15)	178.8(9)
C(16)-N(7)-N(8)-Sm(1)	179.2(9)
C(63)-C(64)-O(1)-C(61)	-4.2(18)
C(63)-C(64)-O(1)-K(1)	-162.7(10)
C(62)-C(61)-O(1)-C(64)	-18.2(17)
C(62)-C(61)-O(1)-K(1)	139.3(11)
O(6)-K(1)-O(1)-C(64)	155.1(11)
O(2)-K(1)-O(1)-C(64)	-27.7(11)
O(4)-K(1)-O(1)-C(64)	-172(6)
O(3)-K(1)-O(1)-C(64)	69.6(11)

O(5)-K(1)-O(1)-C(64)	-112.5(11)
O(6)-K(1)-O(1)-C(61)	0.4(11)
O(2)-K(1)-O(1)-C(61)	177.5(11)
O(4)-K(1)-O(1)-C(61)	33(7)
O(3)-K(1)-O(1)-C(61)	-85.2(11)
O(5)-K(1)-O(1)-C(61)	92.8(11)
C(54)-C(53)-O(2)-C(56)	-4.2(14)
C(54)-C(53)-O(2)-K(1)	-135.1(8)
C(55)-C(56)-O(2)-C(53)	-19.8(14)
C(55)-C(56)-O(2)-K(1)	109.7(10)
O(6)-K(1)-O(2)-C(53)	-123.0(15)
O(4)-K(1)-O(2)-C(53)	41.4(9)
O(3)-K(1)-O(2)-C(53)	134.6(8)
O(1)-K(1)-O(2)-C(53)	-136.2(9)
O(5)-K(1)-O(2)-C(53)	-44.9(8)
O(6)-K(1)-O(2)-C(56)	109.4(16)
O(4)-K(1)-O(2)-C(56)	-86.2(9)
O(3)-K(1)-O(2)-C(56)	7.0(9)
O(1)-K(1)-O(2)-C(56)	96.2(8)
O(5)-K(1)-O(2)-C(56)	-172.5(8)
C(42)-C(41)-O(3)-C(44)	-13.6(17)
C(42)-C(41)-O(3)-K(1)	139.1(10)
C(43)-C(44)-O(3)-C(41)	-10.7(19)
C(43)-C(44)-O(3)-K(1)	-158.8(13)
O(6)-K(1)-O(3)-C(41)	-60.5(10)
O(2)-K(1)-O(3)-C(41)	107.2(10)
O(4)-K(1)-O(3)-C(41)	-151.5(10)
O(1)-K(1)-O(3)-C(41)	25.0(10)
O(5)-K(1)-O(3)-C(41)	-85(8)
O(6)-K(1)-O(3)-C(44)	85.8(13)

O(2)-K(1)-O(3)-C(44)	-106.4(12)
O(4)-K(1)-O(3)-C(44)	-5.1(13)
O(1)-K(1)-O(3)-C(44)	171.4(12)
O(5)-K(1)-O(3)-C(44)	61(9)
C(50)-C(49)-O(4)-C(52)	-7.8(19)
C(50)-C(49)-O(4)-K(1)	165.0(10)
C(51)-C(52)-O(4)-C(49)	26.0(17)
C(51)-C(52)-O(4)-K(1)	-146.2(10)
O(6)-K(1)-O(4)-C(49)	15.6(13)
O(2)-K(1)-O(4)-C(49)	-161.1(12)
O(3)-K(1)-O(4)-C(49)	101.1(13)
O(1)-K(1)-O(4)-C(49)	-17(7)
O(5)-K(1)-O(4)-C(49)	-76.8(13)
O(6)-K(1)-O(4)-C(52)	-173.1(12)
O(2)-K(1)-O(4)-C(52)	10.2(13)
O(3)-K(1)-O(4)-C(52)	-87.5(13)
O(1)-K(1)-O(4)-C(52)	154(5)
O(5)-K(1)-O(4)-C(52)	94.5(13)
C(58)-C(57)-O(5)-C(60)	28.2(17)
C(58)-C(57)-O(5)-K(1)	-134.2(13)
C(59)-C(60)-O(5)-C(57)	-10.0(18)
C(59)-C(60)-O(5)-K(1)	157.7(11)
O(6)-K(1)-O(5)-C(57)	-100.9(14)
O(2)-K(1)-O(5)-C(57)	91.4(14)
O(4)-K(1)-O(5)-C(57)	-9.9(14)
O(3)-K(1)-O(5)-C(57)	-76(9)
O(1)-K(1)-O(5)-C(57)	173.6(14)
O(6)-K(1)-O(5)-C(60)	97.0(10)
O(2)-K(1)-O(5)-C(60)	-70.7(10)
O(4)-K(1)-O(5)-C(60)	-172.0(10)

O(3)-K(1)-O(5)-C(60)	122(8)
O(1)-K(1)-O(5)-C(60)	11.5(10)
C(46)-C(45)-O(6)-C(48)	-4.6(15)
C(46)-C(45)-O(6)-K(1)	-167.4(9)
C(47)-C(48)-O(6)-C(45)	-19.2(16)
C(47)-C(48)-O(6)-K(1)	148.0(9)
O(2)-K(1)-O(6)-C(45)	-117.9(16)
O(4)-K(1)-O(6)-C(45)	77.4(13)
O(3)-K(1)-O(6)-C(45)	-14.3(13)
O(1)-K(1)-O(6)-C(45)	-104.8(13)
O(5)-K(1)-O(6)-C(45)	164.7(13)
O(2)-K(1)-O(6)-C(48)	80.0(19)
O(4)-K(1)-O(6)-C(48)	-84.7(10)
O(3)-K(1)-O(6)-C(48)	-176.4(10)
O(1)-K(1)-O(6)-C(48)	93.1(10)
O(5)-K(1)-O(6)-C(48)	2.7(10)
N(1)-C(26)-P(1)-C(25)	-0.5(8)
C(27)-C(26)-P(1)-C(25)	175.5(11)
N(2)-C(25)-P(1)-C(26)	0.0(8)
C(24)-C(25)-P(1)-C(26)	179.8(10)
N(3)-C(36)-P(2)-C(35)	0.4(9)
C(37)-C(36)-P(2)-C(35)	-177.5(11)
N(4)-C(35)-P(2)-C(36)	0.1(9)
C(34)-C(35)-P(2)-C(36)	-179.8(11)
N(8)-C(15)-P(3)-C(16)	-0.4(10)
C(14)-C(15)-P(3)-C(16)	179.1(11)
N(7)-C(16)-P(3)-C(15)	-0.8(11)
C(17)-C(16)-P(3)-C(15)	-176.7(11)
N(6)-C(6)-P(4)-C(5)	0.5(9)
C(7)-C(6)-P(4)-C(5)	-174.2(11)

N(5)-C(5)-P(4)-C(6)	-0.3(9)
C(4)-C(5)-P(4)-C(6)	179.1(11)
C(6)-N(6)-Sm(1)-N(7)	39(5)
N(5)-N(6)-Sm(1)-N(7)	-102.2(6)
C(6)-N(6)-Sm(1)-N(4)	-96(5)
N(5)-N(6)-Sm(1)-N(4)	122.7(5)
C(6)-N(6)-Sm(1)-N(8)	7(5)
N(5)-N(6)-Sm(1)-N(8)	-134.2(6)
C(6)-N(6)-Sm(1)-N(5)	142(5)
C(6)-N(6)-Sm(1)-N(1)	154(4)
N(5)-N(6)-Sm(1)-N(1)	12.8(7)
C(6)-N(6)-Sm(1)-N(2)	106(5)
N(5)-N(6)-Sm(1)-N(2)	-35.8(9)
C(6)-N(6)-Sm(1)-N(3)	-112(5)
N(5)-N(6)-Sm(1)-N(3)	106.0(6)
C(16)-N(7)-Sm(1)-N(6)	82(6)
N(8)-N(7)-Sm(1)-N(6)	-103.3(5)
C(16)-N(7)-Sm(1)-N(4)	-158(6)
N(8)-N(7)-Sm(1)-N(4)	16.5(6)
C(16)-N(7)-Sm(1)-N(8)	-175(6)
C(16)-N(7)-Sm(1)-N(5)	50(6)
N(8)-N(7)-Sm(1)-N(5)	-135.0(5)
C(16)-N(7)-Sm(1)-N(1)	-52(6)
N(8)-N(7)-Sm(1)-N(1)	122.6(5)
C(16)-N(7)-Sm(1)-N(2)	-70(6)
N(8)-N(7)-Sm(1)-N(2)	104.5(5)
C(16)-N(7)-Sm(1)-N(3)	154(6)
N(8)-N(7)-Sm(1)-N(3)	-30.8(8)
N(3)-N(4)-Sm(1)-N(6)	-32.6(6)
C(35)-N(4)-Sm(1)-N(6)	-159(4)

N(3)-N(4)-Sm(1)-N(7)	-137.0(6)
C(35)-N(4)-Sm(1)-N(7)	96(4)
N(3)-N(4)-Sm(1)-N(8)	-127.9(6)
C(35)-N(4)-Sm(1)-N(8)	106(4)
N(3)-N(4)-Sm(1)-N(5)	4.0(7)
C(35)-N(4)-Sm(1)-N(5)	-123(4)
N(3)-N(4)-Sm(1)-N(1)	104.5(6)
C(35)-N(4)-Sm(1)-N(1)	-22(4)
N(3)-N(4)-Sm(1)-N(2)	136.7(6)
C(35)-N(4)-Sm(1)-N(2)	10(4)
C(35)-N(4)-Sm(1)-N(3)	-127(4)
C(15)-N(8)-Sm(1)-N(6)	-91(12)
N(7)-N(8)-Sm(1)-N(6)	73.7(5)
C(15)-N(8)-Sm(1)-N(7)	-164(12)
C(15)-N(8)-Sm(1)-N(4)	28(12)
N(7)-N(8)-Sm(1)-N(4)	-168.0(5)
C(15)-N(8)-Sm(1)-N(5)	-115(12)
N(7)-N(8)-Sm(1)-N(5)	49.3(5)
C(15)-N(8)-Sm(1)-N(1)	119(12)
N(7)-N(8)-Sm(1)-N(1)	-76.5(5)
C(15)-N(8)-Sm(1)-N(2)	120(12)
N(7)-N(8)-Sm(1)-N(2)	-76.0(5)
C(15)-N(8)-Sm(1)-N(3)	-1(12)
N(7)-N(8)-Sm(1)-N(3)	163.0(5)
C(5)-N(5)-Sm(1)-N(6)	-141(5)
C(5)-N(5)-Sm(1)-N(7)	-67(5)
N(6)-N(5)-Sm(1)-N(7)	74.6(6)
C(5)-N(5)-Sm(1)-N(4)	140(5)
N(6)-N(5)-Sm(1)-N(4)	-78.5(6)
C(5)-N(5)-Sm(1)-N(8)	-91(5)

N(6)-N(5)-Sm(1)-N(8)	50.2(6)
C(5)-N(5)-Sm(1)-N(1)	48(5)
N(6)-N(5)-Sm(1)-N(1)	-170.6(5)
C(5)-N(5)-Sm(1)-N(2)	19(5)
N(6)-N(5)-Sm(1)-N(2)	159.9(5)
C(5)-N(5)-Sm(1)-N(3)	142(5)
N(6)-N(5)-Sm(1)-N(3)	-76.4(6)
C(26)-N(1)-Sm(1)-N(6)	96(4)
N(2)-N(1)-Sm(1)-N(6)	-135.4(5)
C(26)-N(1)-Sm(1)-N(7)	-163(4)
N(2)-N(1)-Sm(1)-N(7)	-34.7(6)
C(26)-N(1)-Sm(1)-N(4)	-27(4)
N(2)-N(1)-Sm(1)-N(4)	101.4(5)
C(26)-N(1)-Sm(1)-N(8)	-127(4)
N(2)-N(1)-Sm(1)-N(8)	0.9(6)
C(26)-N(1)-Sm(1)-N(5)	103(4)
N(2)-N(1)-Sm(1)-N(5)	-128.4(5)
C(26)-N(1)-Sm(1)-N(2)	-128(4)
C(26)-N(1)-Sm(1)-N(3)	4(4)
N(2)-N(1)-Sm(1)-N(3)	132.5(5)
C(25)-N(2)-Sm(1)-N(6)	-151(4)
N(1)-N(2)-Sm(1)-N(6)	84.0(7)
C(25)-N(2)-Sm(1)-N(7)	-86(4)
N(1)-N(2)-Sm(1)-N(7)	148.8(5)
C(25)-N(2)-Sm(1)-N(4)	48(4)
N(1)-N(2)-Sm(1)-N(4)	-77.1(5)
C(25)-N(2)-Sm(1)-N(8)	-55(4)
N(1)-N(2)-Sm(1)-N(8)	-179.3(5)
C(25)-N(2)-Sm(1)-N(5)	-173(4)
N(1)-N(2)-Sm(1)-N(5)	62.6(5)

C(25)-N(2)-Sm(1)-N(1)	125(5)
C(25)-N(2)-Sm(1)-N(3)	71(5)
N(1)-N(2)-Sm(1)-N(3)	-53.5(5)
C(36)-N(3)-Sm(1)-N(6)	-78(4)
N(4)-N(3)-Sm(1)-N(6)	151.6(6)
C(36)-N(3)-Sm(1)-N(7)	-148(3)
N(4)-N(3)-Sm(1)-N(7)	81.6(8)
C(36)-N(3)-Sm(1)-N(4)	131(4)
C(36)-N(3)-Sm(1)-N(8)	-167(4)
N(4)-N(3)-Sm(1)-N(8)	62.8(6)
C(36)-N(3)-Sm(1)-N(5)	-46(4)
N(4)-N(3)-Sm(1)-N(5)	-176.9(5)
C(36)-N(3)-Sm(1)-N(1)	56(4)
N(4)-N(3)-Sm(1)-N(1)	-74.4(6)
C(36)-N(3)-Sm(1)-N(2)	82(4)
N(4)-N(3)-Sm(1)-N(2)	-48.5(6)

Symmetry transformations used to generate equivalent atoms:

4.8 Crystal structural analysis data for **10**

Table 1. Crystal data and structure refinement for 140905-1.

Identification code	140905-1
Empirical formula	C ₇₇ H ₅₈ K ₂ La N ₁₀ P ₅
Formula weight	1495.29
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P 21 21 21
Unit cell dimensions	a = 17.4889(6) Å alpha = 90 deg. b = 21.7538(6) Å beta = 90 deg. c = 22.1728(8) Å gamma = 90 deg.
Volume	8435.6(5) Å ³
Z, Calculated density	4, 1.177 Mg/m ³
Absorption coefficient	0.743 mm ⁻¹
F(000)	3040
Crystal size	0.31 x 0.26 x 0.12 mm
Theta range for data collection	2.87 to 26.37 deg.
Limiting indices	-21 ≤ h ≤ 20, -27 ≤ k ≤ 27, -27 ≤ l ≤ 26
Reflections collected / unique	45855 / 17166 [R(int) = 0.0689]
Completeness to theta = 26.37	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.45087
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	17166 / 209 / 762
Goodness-of-fit on F ²	1.002
Final R indices [I > 2σ(I)]	R1 = 0.0865, wR2 = 0.2091
R indices (all data)	R1 = 0.1348, wR2 = 0.2453
Absolute structure parameter	-0.03(2)
Largest diff. peak and hole	2.627 and -1.285 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 140905-1.

$U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
C(1)	-694(6)	4781(6)	4563(5)	87(3)
C(2)	-1149(7)	5027(7)	4120(5)	101(4)
C(3)	-1360(8)	5644(8)	4206(6)	106(4)
C(4)	-1162(8)	5937(7)	4709(6)	109(4)
C(5)	-714(7)	5665(5)	5134(5)	83(3)
C(6)	-462(5)	5065(5)	5069(4)	64(2)
C(7)	-12(5)	4749(4)	5531(4)	55(2)
C(8)	685(5)	4118(4)	6240(4)	54(2)
C(9)	1052(6)	3686(4)	6661(4)	70(2)
C(10)	1578(6)	3876(5)	7092(5)	74(2)
C(11)	1903(7)	3466(5)	7470(5)	84(2)
C(12)	1750(7)	2845(6)	7405(5)	90(2)
C(13)	1233(7)	2652(5)	6958(5)	93(2)
C(14)	908(7)	3065(5)	6607(5)	83(2)
C(15)	-615(7)	4366(5)	7511(6)	81(3)
C(16)	-1313(8)	4093(6)	7509(6)	96(4)
C(17)	-1719(8)	3897(6)	8049(8)	113(5)
C(18)	-1328(9)	3969(7)	8571(7)	107(4)
C(19)	-636(9)	4246(5)	8603(6)	100(4)
C(20)	-250(7)	4435(5)	8073(5)	75(3)

C(21)	493(6)	4738(5)	8108(4)	69(3)
C(22)	1770(6)	5127(4)	8256(5)	70(2)
C(23)	2535(6)	5340(5)	8402(4)	72(3)
C(24)	2980(7)	5016(6)	8841(5)	87(3)
C(25)	3709(8)	5256(7)	8975(6)	107(4)
C(26)	3980(8)	5796(6)	8679(7)	113(4)
C(27)	3526(7)	6089(6)	8263(7)	109(4)
C(28)	2829(6)	5852(5)	8132(5)	80(3)
C(29)	43(4)	6306(3)	8522(3)	105(3)
C(30)	-500(4)	6170(4)	8960(3)	111(3)
C(31)	-552(4)	6529(4)	9477(3)	111(3)
C(32)	-60(5)	7024(4)	9556(3)	115(3)
C(33)	483(5)	7161(3)	9118(3)	108(3)
C(34)	535(3)	6801(3)	8601(2)	103(3)
C(35)	1100(4)	6975(4)	8133(3)	80(3)
C(36)	2133(6)	7234(4)	7462(5)	76(3)
C(37)	2812(4)	7456(4)	7130(4)	109(3)
C(38)	3312(5)	7870(4)	7399(4)	122(3)
C(39)	3972(5)	8051(4)	7098(5)	129(3)
C(40)	4132(4)	7818(5)	6529(5)	129(3)
C(41)	3632(6)	7403(4)	6260(4)	126(3)
C(42)	2972(5)	7222(4)	6561(4)	116(3)
C(43)	-2349(5)	6200(5)	6553(3)	120(3)
C(44)	-2942(4)	5860(5)	6805(4)	123(3)
C(45)	-2818(4)	5522(5)	7328(4)	127(3)
C(46)	-2102(5)	5525(4)	7600(3)	122(3)
C(47)	-1509(4)	5864(5)	7348(4)	115(3)
C(48)	-1633(4)	6202(5)	6825(4)	108(3)
C(49)	-994(7)	6539(5)	6528(4)	76(3)
C(50)	-96(6)	7144(4)	5947(4)	65(2)

C(51)	367(5)	7556(3)	5586(3)	92(4)
C(52)	26(5)	7993(4)	5217(4)	117(5)
C(53)	475(7)	8369(4)	4855(4)	148(7)
C(54)	1267(7)	8308(4)	4862(4)	132(7)
C(55)	1608(5)	7871(4)	5232(5)	121(5)
C(56)	1158(5)	7495(3)	5594(3)	90(4)
C(57)	2423(7)	6598(5)	4443(5)	78(3)
C(58)	2058(7)	6838(6)	3946(5)	86(3)
C(59)	1299(8)	6721(7)	3859(6)	104(4)
C(60)	883(7)	6431(6)	4271(5)	87(3)
C(61)	1254(6)	6191(5)	4787(5)	75(3)
C(62)	2020(6)	6281(5)	4872(4)	64(2)
C(63)	2415(6)	6016(5)	5406(4)	73(3)
C(64)	3154(6)	5576(5)	6225(5)	72(3)
C(65)	3682(4)	5334(5)	6680(4)	110(3)
C(66)	4410(5)	5585(4)	6727(4)	122(3)
C(67)	4929(4)	5345(5)	7139(4)	131(3)
C(68)	4719(5)	4855(5)	7506(4)	128(3)
C(69)	3990(5)	4604(4)	7459(4)	123(3)
C(70)	3472(4)	4844(5)	7047(4)	114(3)
C(77)	4035(15)	4304(13)	4619(11)	143(7)
C(71)	2369(15)	3242(14)	4961(10)	126(6)
C(72)	2408(13)	3201(11)	5586(10)	132(6)
C(73)	2973(15)	3517(13)	5899(7)	132(6)
C(74)	3499(13)	3875(12)	5587(7)	133(6)
C(75)	3461(11)	3916(9)	4962(8)	129(6)
C(76)	2896(15)	3599(13)	4649(7)	124(6)
C(77')	1826(11)	2843(11)	4800(10)	93(4)
C(71')	2475(11)	3234(10)	5084(8)	92(4)
C(72')	2723(10)	3266(8)	5679(6)	74(6)

C(73')	3307(11)	3668(9)	5837(6)	93(4)
C(74')	3643(9)	4039(8)	5401(8)	94(4)
C(75')	3395(10)	4008(9)	4807(7)	91(4)
C(76')	2811(13)	3606(11)	4648(6)	92(4)
K(1)	306(2)	7840(1)	7128(1)	98(1)
K(2)	1966(2)	4641(1)	5359(1)	94(1)
La(1)	1026(1)	5832(1)	6768(1)	51(1)
N(1)	1999(4)	5887(4)	5906(3)	60(2)
N(2)	421(4)	5084(4)	5924(4)	62(2)
N(3)	809(4)	4743(3)	6325(3)	59(2)
N(4)	724(4)	5124(3)	7666(3)	53(2)
N(5)	-272(5)	6366(4)	6590(3)	70(2)
N(6)	224(5)	6695(4)	6280(3)	66(2)
N(7)	1068(4)	6679(3)	7583(3)	55(2)
N(8)	1647(5)	6834(3)	7210(3)	67(2)
N(9)	1430(4)	5340(3)	7745(3)	59(2)
N(10)	2415(4)	5645(4)	6363(3)	63(2)
P(1)	63(2)	3965(1)	5648(1)	72(1)
P(2)	1182(2)	4626(1)	8669(1)	83(1)
P(3)	1865(2)	7473(1)	8197(2)	90(1)
P(4)	-1090(2)	7179(2)	6022(1)	95(1)
P(5)	3384(2)	5843(2)	5496(1)	80(1)

Table 3. Bond lengths [Å] and angles [deg] for 140905-1.

C(1)-C(6)	1.343(14)
C(1)-C(2)	1.372(15)
C(1)-H(1A)	0.9300
C(2)-C(3)	1.405(18)
C(2)-H(2A)	0.9300
C(3)-C(4)	1.330(18)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.362(16)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.385(14)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.463(13)
C(7)-N(2)	1.366(11)
C(7)-P(1)	1.731(10)
C(7)-K(2)	3.489(9)
C(8)-N(3)	1.390(10)
C(8)-C(9)	1.471(12)
C(8)-P(1)	1.736(9)
C(8)-K(2)	3.182(9)
C(9)-C(14)	1.379(14)
C(9)-C(10)	1.391(13)
C(10)-C(11)	1.349(13)
C(10)-H(10A)	0.9300
C(11)-C(12)	1.384(15)
C(11)-H(11A)	0.9300
C(12)-C(13)	1.406(16)

C(12)-H(12A)	0.9300
C(13)-C(14)	1.317(14)
C(13)-K(1)#1	3.393(13)
C(13)-H(13A)	0.9300
C(14)-H(14A)	0.9300
C(15)-C(16)	1.357(16)
C(15)-C(20)	1.408(15)
C(15)-K(1)#1	3.458(11)
C(15)-H(15)	0.9300
C(16)-C(17)	1.457(18)
C(16)-K(1)#1	3.344(12)
C(16)-H(16A)	0.9300
C(17)-C(18)	1.353(19)
C(17)-K(1)#1	3.398(15)
C(17)-H(17)	0.9300
C(18)-C(19)	1.354(19)
C(18)-K(1)#1	3.411(15)
C(18)-H(18A)	0.9300
C(19)-C(20)	1.416(14)
C(19)-K(1)#1	3.510(13)
C(19)-H(19A)	0.9300
C(20)-C(21)	1.460(15)
C(20)-K(1)#1	3.500(11)
C(21)-N(4)	1.353(12)
C(21)-P(2)	1.750(10)
C(22)-N(9)	1.361(12)
C(22)-C(23)	1.452(14)
C(22)-P(2)	1.756(11)
C(23)-C(28)	1.363(14)
C(23)-C(24)	1.432(14)

C(24)-C(25)	1.409(17)
C(24)-K(2)#2	3.449(11)
C(24)-H(24A)	0.9300
C(25)-C(26)	1.426(17)
C(25)-K(2)#2	3.295(15)
C(25)-H(25A)	0.9300
C(26)-C(27)	1.375(17)
C(26)-H(26A)	0.9300
C(27)-C(28)	1.356(15)
C(27)-H(27A)	0.9300
C(28)-H(28A)	0.9300
C(29)-C(30)	1.3900
C(29)-C(34)	1.3900
C(29)-H(29)	0.9300
C(30)-C(31)	1.3900
C(30)-H(30)	0.9300
C(31)-C(32)	1.3900
C(31)-H(31)	0.9300
C(32)-C(33)	1.3900
C(32)-H(32)	0.9300
C(33)-C(34)	1.3900
C(33)-H(33)	0.9300
C(34)-C(35)	1.4827
C(35)-N(7)	1.381(10)
C(35)-P(3)	1.727(8)
C(35)-K(1)	3.229(8)
C(36)-N(8)	1.338(12)
C(36)-C(37)	1.477(13)
C(36)-P(3)	1.774(12)
C(36)-K(1)	3.534(11)

C(37)-C(38)	1.3900
C(37)-C(42)	1.3900
C(38)-C(39)	1.3900
C(38)-H(38)	0.9300
C(39)-C(40)	1.3900
C(39)-H(39)	0.9300
C(40)-C(41)	1.3900
C(40)-H(40)	0.9300
C(41)-C(42)	1.3900
C(41)-H(41)	0.9300
C(42)-H(42)	0.9300
C(43)-C(44)	1.3900
C(43)-C(48)	1.3900
C(43)-H(43)	0.9300
C(44)-C(45)	1.3900
C(44)-H(44)	0.9300
C(45)-C(46)	1.3900
C(45)-H(45)	0.9300
C(46)-C(47)	1.3900
C(46)-H(46)	0.9300
C(47)-C(48)	1.3900
C(47)-H(47)	0.9300
C(48)-C(49)	1.491(13)
C(49)-N(5)	1.324(13)
C(49)-P(4)	1.796(11)
C(50)-N(6)	1.346(11)
C(50)-C(51)	1.449(12)
C(50)-P(4)	1.748(11)
C(50)-K(1)	3.106(9)
C(51)-C(52)	1.3900

C(51)-C(56)	1.3900
C(51)-K(1)	3.477(8)
C(52)-C(53)	1.3900
C(52)-H(52)	0.9300
C(53)-C(54)	1.3900
C(53)-H(53)	0.9300
C(54)-C(55)	1.3900
C(54)-H(54)	0.9300
C(55)-C(56)	1.3900
C(55)-H(55)	0.9300
C(56)-H(56)	0.9300
C(57)-C(62)	1.371(13)
C(57)-C(58)	1.375(15)
C(57)-H(57A)	0.9300
C(58)-C(59)	1.365(17)
C(58)-H(58A)	0.9300
C(59)-C(60)	1.327(16)
C(59)-H(59A)	0.9300
C(60)-C(61)	1.417(15)
C(60)-H(60A)	0.9300
C(61)-C(62)	1.366(13)
C(61)-H(61A)	0.9300
C(62)-C(63)	1.487(14)
C(63)-N(1)	1.357(11)
C(63)-P(5)	1.747(11)
C(63)-K(2)	3.094(10)
C(64)-N(10)	1.338(12)
C(64)-C(65)	1.466(12)
C(64)-P(5)	1.764(10)
C(64)-K(2)	3.484(11)

C(65)-C(66)	1.3900
C(65)-C(70)	1.3900
C(66)-C(67)	1.3900
C(66)-H(66)	0.9300
C(67)-C(68)	1.3900
C(67)-H(67)	0.9300
C(68)-C(69)	1.3900
C(68)-H(68)	0.9300
C(69)-C(70)	1.3900
C(69)-H(69)	0.9300
C(70)-H(70)	0.9300
C(77)-C(75)	1.516(10)
C(77)-H(77A)	0.9600
C(77)-H(77B)	0.9600
C(77)-H(77C)	0.9600
C(71)-C(72)	1.3900
C(71)-C(76)	1.3900
C(71)-K(2)	3.25(3)
C(71)-H(71A)	0.9800
C(72)-C(73)	1.3900
C(72)-K(2)	3.27(2)
C(72)-H(72A)	0.9800
C(73)-C(74)	1.3900
C(73)-K(2)	3.24(3)
C(73)-H(73A)	0.9800
C(74)-C(75)	1.3900
C(74)-K(2)	3.20(3)
C(74)-H(74A)	0.9800
C(75)-C(76)	1.3900
C(75)-K(2)	3.18(2)

C(76)-K(2)	3.20(3)
C(76)-H(76A)	0.9800
C(77')-C(71')	1.554(10)
C(77')-H(77D)	0.9600
C(77')-H(77E)	0.9600
C(77')-H(77F)	0.9600
C(71')-C(72')	1.3900
C(71')-C(76')	1.3900
C(71')-K(2)	3.24(3)
C(72')-C(73')	1.3900
C(72')-K(2)	3.347(19)
C(72')-H(72B)	0.9800
C(73')-C(74')	1.3900
C(73')-K(2)	3.33(2)
C(73')-H(73B)	0.9800
C(74')-C(75')	1.3900
C(74')-K(2)	3.21(2)
C(74')-H(74B)	0.9800
C(75')-C(76')	1.3900
C(75')-K(2)	3.10(2)
C(75')-H(75A)	0.9800
C(76')-K(2)	3.12(3)
C(76')-H(76B)	0.9800
K(1)-N(7)	3.028(7)
K(1)-N(6)	3.124(9)
K(1)-N(8)	3.212(9)
K(1)-C(16)#3	3.344(13)
K(1)-C(13)#3	3.393(13)
K(1)-C(17)#3	3.398(15)
K(1)-C(18)#3	3.411(15)

K(1)-C(15)#3	3.458(11)
K(1)-C(20)#3	3.500(11)
K(2)-N(3)	2.954(8)
K(2)-N(1)	2.970(8)
K(2)-N(2)	3.131(7)
K(2)-N(10)	3.216(8)
La(1)-N(9)	2.519(7)
La(1)-N(1)	2.560(6)
La(1)-N(4)	2.573(7)
La(1)-N(6)	2.580(7)
La(1)-N(5)	2.581(8)
La(1)-N(7)	2.582(7)
La(1)-N(3)	2.592(7)
La(1)-N(10)	2.620(7)
La(1)-N(8)	2.626(8)
La(1)-N(2)	2.696(8)
N(1)-N(10)	1.354(10)
N(2)-N(3)	1.342(9)
N(4)-N(9)	1.333(10)
N(5)-N(6)	1.317(11)
N(7)-N(8)	1.350(10)

C(6)-C(1)-C(2)	126.4(13)
C(6)-C(1)-H(1A)	116.8
C(2)-C(1)-H(1A)	116.8
C(1)-C(2)-C(3)	115.4(12)
C(1)-C(2)-H(2A)	122.3
C(3)-C(2)-H(2A)	122.3
C(4)-C(3)-C(2)	120.1(13)
C(4)-C(3)-H(3A)	120.0

C(2)-C(3)-H(3A)	120.0
C(3)-C(4)-C(5)	121.6(14)
C(3)-C(4)-H(4A)	119.2
C(5)-C(4)-H(4A)	119.2
C(4)-C(5)-C(6)	121.3(12)
C(4)-C(5)-H(5A)	119.3
C(6)-C(5)-H(5A)	119.3
C(1)-C(6)-C(5)	115.1(10)
C(1)-C(6)-C(7)	122.1(10)
C(5)-C(6)-C(7)	122.7(9)
N(2)-C(7)-C(6)	119.6(8)
N(2)-C(7)-P(1)	112.9(7)
C(6)-C(7)-P(1)	127.6(7)
N(2)-C(7)-K(2)	63.6(4)
C(6)-C(7)-K(2)	119.2(6)
P(1)-C(7)-K(2)	82.8(3)
N(3)-C(8)-C(9)	118.1(7)
N(3)-C(8)-P(1)	112.8(6)
C(9)-C(8)-P(1)	129.0(6)
N(3)-C(8)-K(2)	67.9(5)
C(9)-C(8)-K(2)	108.1(6)
P(1)-C(8)-K(2)	92.6(3)
C(14)-C(9)-C(10)	118.1(10)
C(14)-C(9)-C(8)	119.4(9)
C(10)-C(9)-C(8)	122.4(9)
C(11)-C(10)-C(9)	120.7(10)
C(11)-C(10)-H(10A)	119.6
C(9)-C(10)-H(10A)	119.6
C(10)-C(11)-C(12)	119.9(11)
C(10)-C(11)-H(11A)	120.1

C(12)-C(11)-H(11A)	120.1
C(11)-C(12)-C(13)	119.3(11)
C(11)-C(12)-H(12A)	120.3
C(13)-C(12)-H(12A)	120.3
C(14)-C(13)-C(12)	119.4(12)
C(14)-C(13)-K(1)#1	86.0(8)
C(12)-C(13)-K(1)#1	93.1(8)
C(14)-C(13)-H(13A)	120.3
C(12)-C(13)-H(13A)	120.3
K(1)#1-C(13)-H(13A)	90.9
C(13)-C(14)-C(9)	122.6(12)
C(13)-C(14)-H(14A)	118.7
C(9)-C(14)-H(14A)	118.7
C(16)-C(15)-C(20)	117.2(12)
C(16)-C(15)-K(1)#1	73.8(7)
C(20)-C(15)-K(1)#1	80.0(6)
C(16)-C(15)-H(15)	121.4
C(20)-C(15)-H(15)	121.4
K(1)#1-C(15)-H(15)	115.7
C(15)-C(16)-C(17)	124.3(12)
C(15)-C(16)-K(1)#1	83.2(7)
C(17)-C(16)-K(1)#1	79.6(8)
C(15)-C(16)-H(16A)	117.9
C(17)-C(16)-H(16A)	117.9
K(1)#1-C(16)-H(16A)	108.6
C(18)-C(17)-C(16)	115.1(13)
C(18)-C(17)-K(1)#1	79.1(10)
C(16)-C(17)-K(1)#1	75.5(7)
C(18)-C(17)-H(17)	122.5
C(16)-C(17)-H(17)	122.5

K(1)#1-C(17)-H(17)	114.2
C(17)-C(18)-C(19)	123.2(13)
C(17)-C(18)-K(1)#1	78.0(9)
C(19)-C(18)-K(1)#1	82.8(9)
C(17)-C(18)-H(18A)	118.4
C(19)-C(18)-H(18A)	118.4
K(1)#1-C(18)-H(18A)	110.5
C(18)-C(19)-C(20)	120.9(13)
C(18)-C(19)-K(1)#1	74.7(8)
C(20)-C(19)-K(1)#1	78.0(7)
C(18)-C(19)-H(19A)	119.6
C(20)-C(19)-H(19A)	119.6
K(1)#1-C(19)-H(19A)	118.6
C(15)-C(20)-C(19)	119.1(12)
C(15)-C(20)-C(21)	120.0(9)
C(19)-C(20)-C(21)	120.8(11)
C(15)-C(20)-K(1)#1	76.6(6)
C(19)-C(20)-K(1)#1	78.7(7)
C(21)-C(20)-K(1)#1	118.7(7)
N(4)-C(21)-C(20)	120.5(9)
N(4)-C(21)-P(2)	113.4(7)
C(20)-C(21)-P(2)	126.1(8)
N(9)-C(22)-C(23)	118.6(9)
N(9)-C(22)-P(2)	112.9(7)
C(23)-C(22)-P(2)	128.4(8)
C(28)-C(23)-C(24)	119.7(11)
C(28)-C(23)-C(22)	120.6(9)
C(24)-C(23)-C(22)	119.6(11)
C(25)-C(24)-C(23)	116.9(12)
C(25)-C(24)-K(2)#2	71.9(7)

C(23)-C(24)-K(2)#2	125.0(7)
C(25)-C(24)-H(24A)	121.5
C(23)-C(24)-H(24A)	121.5
K(2)#2-C(24)-H(24A)	75.5
C(24)-C(25)-C(26)	120.6(12)
C(24)-C(25)-K(2)#2	84.1(8)
C(26)-C(25)-K(2)#2	119.5(10)
C(24)-C(25)-H(25A)	119.7
C(26)-C(25)-H(25A)	119.7
K(2)#2-C(25)-H(25A)	66.9
C(27)-C(26)-C(25)	119.9(13)
C(27)-C(26)-H(26A)	120.0
C(25)-C(26)-H(26A)	120.0
C(28)-C(27)-C(26)	119.1(12)
C(28)-C(27)-H(27A)	120.4
C(26)-C(27)-H(27A)	120.4
C(27)-C(28)-C(23)	123.8(11)
C(27)-C(28)-H(28A)	118.1
C(23)-C(28)-H(28A)	118.1
C(30)-C(29)-C(34)	120.0
C(30)-C(29)-H(29)	120.0
C(34)-C(29)-H(29)	120.0
C(31)-C(30)-C(29)	120.0
C(31)-C(30)-H(30)	120.0
C(29)-C(30)-H(30)	120.0
C(30)-C(31)-C(32)	120.0
C(30)-C(31)-H(31)	120.0
C(32)-C(31)-H(31)	120.0
C(31)-C(32)-C(33)	120.0
C(31)-C(32)-H(32)	120.0

C(33)-C(32)-H(32)	120.0
C(34)-C(33)-C(32)	120.0
C(34)-C(33)-H(33)	120.0
C(32)-C(33)-H(33)	120.0
C(33)-C(34)-C(29)	120.0
C(33)-C(34)-C(35)	118.4
C(29)-C(34)-C(35)	121.5
N(7)-C(35)-C(34)	118.1(5)
N(7)-C(35)-P(3)	113.4(5)
C(34)-C(35)-P(3)	128.3(4)
N(7)-C(35)-K(1)	69.2(4)
C(34)-C(35)-K(1)	110.2(3)
P(3)-C(35)-K(1)	91.4(3)
N(8)-C(36)-C(37)	121.0(10)
N(8)-C(36)-P(3)	113.9(9)
C(37)-C(36)-P(3)	125.0(7)
N(8)-C(36)-K(1)	65.2(5)
C(37)-C(36)-K(1)	120.1(6)
P(3)-C(36)-K(1)	81.0(4)
C(38)-C(37)-C(42)	120.0
C(38)-C(37)-C(36)	120.2(7)
C(42)-C(37)-C(36)	119.7(7)
C(37)-C(38)-C(39)	120.0
C(37)-C(38)-H(38)	120.0
C(39)-C(38)-H(38)	120.0
C(38)-C(39)-C(40)	120.0
C(38)-C(39)-H(39)	120.0
C(40)-C(39)-H(39)	120.0
C(41)-C(40)-C(39)	120.0
C(41)-C(40)-H(40)	120.0

C(39)-C(40)-H(40)	120.0
C(42)-C(41)-C(40)	120.0
C(42)-C(41)-H(41)	120.0
C(40)-C(41)-H(41)	120.0
C(41)-C(42)-C(37)	120.0
C(41)-C(42)-H(42)	120.0
C(37)-C(42)-H(42)	120.0
C(44)-C(43)-C(48)	120.0
C(44)-C(43)-H(43)	120.0
C(48)-C(43)-H(43)	120.0
C(45)-C(44)-C(43)	120.0
C(45)-C(44)-H(44)	120.0
C(43)-C(44)-H(44)	120.0
C(44)-C(45)-C(46)	120.0
C(44)-C(45)-H(45)	120.0
C(46)-C(45)-H(45)	120.0
C(45)-C(46)-C(47)	120.0
C(45)-C(46)-H(46)	120.0
C(47)-C(46)-H(46)	120.0
C(48)-C(47)-C(46)	120.0
C(48)-C(47)-H(47)	120.0
C(46)-C(47)-H(47)	120.0
C(47)-C(48)-C(43)	120.0
C(47)-C(48)-C(49)	120.8(7)
C(43)-C(48)-C(49)	119.1(7)
N(5)-C(49)-C(48)	122.0(10)
N(5)-C(49)-P(4)	112.0(8)
C(48)-C(49)-P(4)	126.0(8)
N(6)-C(50)-C(51)	121.3(9)
N(6)-C(50)-P(4)	113.2(8)

C(51)-C(50)-P(4)	125.5(7)
N(6)-C(50)-K(1)	78.3(5)
C(51)-C(50)-K(1)	92.2(5)
P(4)-C(50)-K(1)	97.1(4)
C(52)-C(51)-C(56)	120.0
C(52)-C(51)-C(50)	120.6(7)
C(56)-C(51)-C(50)	119.4(7)
C(52)-C(51)-K(1)	116.5(4)
C(56)-C(51)-K(1)	92.0(4)
C(50)-C(51)-K(1)	63.2(5)
C(53)-C(52)-C(51)	120.0
C(53)-C(52)-H(52)	120.0
C(51)-C(52)-H(52)	120.0
C(52)-C(53)-C(54)	120.0
C(52)-C(53)-H(53)	120.0
C(54)-C(53)-H(53)	120.0
C(53)-C(54)-C(55)	120.0
C(53)-C(54)-H(54)	120.0
C(55)-C(54)-H(54)	120.0
C(56)-C(55)-C(54)	120.0
C(56)-C(55)-H(55)	120.0
C(54)-C(55)-H(55)	120.0
C(55)-C(56)-C(51)	120.0
C(55)-C(56)-H(56)	120.0
C(51)-C(56)-H(56)	120.0
C(62)-C(57)-C(58)	120.6(11)
C(62)-C(57)-H(57A)	119.7
C(58)-C(57)-H(57A)	119.7
C(59)-C(58)-C(57)	119.5(11)
C(59)-C(58)-H(58A)	120.2

C(57)-C(58)-H(58A)	120.2
C(60)-C(59)-C(58)	121.7(12)
C(60)-C(59)-H(59A)	119.1
C(58)-C(59)-H(59A)	119.1
C(59)-C(60)-C(61)	118.6(11)
C(59)-C(60)-H(60A)	120.7
C(61)-C(60)-H(60A)	120.7
C(62)-C(61)-C(60)	120.6(10)
C(62)-C(61)-H(61A)	119.7
C(60)-C(61)-H(61A)	119.7
C(61)-C(62)-C(57)	118.7(10)
C(61)-C(62)-C(63)	120.7(9)
C(57)-C(62)-C(63)	120.6(10)
N(1)-C(63)-C(62)	118.8(9)
N(1)-C(63)-P(5)	112.5(8)
C(62)-C(63)-P(5)	128.7(7)
N(1)-C(63)-K(2)	72.0(5)
C(62)-C(63)-K(2)	103.3(6)
P(5)-C(63)-K(2)	92.4(4)
N(10)-C(64)-C(65)	119.3(9)
N(10)-C(64)-P(5)	113.2(8)
C(65)-C(64)-P(5)	127.4(7)
N(10)-C(64)-K(2)	67.4(5)
C(65)-C(64)-K(2)	123.0(7)
P(5)-C(64)-K(2)	79.9(4)
C(66)-C(65)-C(70)	120.0
C(66)-C(65)-C(64)	119.1(7)
C(70)-C(65)-C(64)	120.8(7)
C(65)-C(66)-C(67)	120.0
C(65)-C(66)-H(66)	120.0

C(67)-C(66)-H(66)	120.0
C(68)-C(67)-C(66)	120.0
C(68)-C(67)-H(67)	120.0
C(66)-C(67)-H(67)	120.0
C(67)-C(68)-C(69)	120.0
C(67)-C(68)-H(68)	120.0
C(69)-C(68)-H(68)	120.0
C(68)-C(69)-C(70)	120.0
C(68)-C(69)-H(69)	120.0
C(70)-C(69)-H(69)	120.0
C(69)-C(70)-C(65)	120.0
C(69)-C(70)-H(70)	120.0
C(65)-C(70)-H(70)	120.0
C(75)-C(77)-H(77A)	109.5
C(75)-C(77)-H(77B)	109.5
H(77A)-C(77)-H(77B)	109.5
C(75)-C(77)-H(77C)	109.5
H(77A)-C(77)-H(77C)	109.5
H(77B)-C(77)-H(77C)	109.5
C(72)-C(71)-C(76)	120.0
C(72)-C(71)-K(2)	78.4(10)
C(76)-C(71)-K(2)	75.8(6)
C(72)-C(71)-H(71A)	119.9
C(76)-C(71)-H(71A)	119.9
K(2)-C(71)-H(71A)	119.9
C(73)-C(72)-C(71)	120.0
C(73)-C(72)-K(2)	76.7(10)
C(71)-C(72)-K(2)	76.9(10)
C(73)-C(72)-H(72A)	120.0
C(71)-C(72)-H(72A)	120.0

K(2)-C(72)-H(72A)	120.0
C(72)-C(73)-C(74)	120.0
C(72)-C(73)-K(2)	78.7(10)
C(74)-C(73)-K(2)	75.8(6)
C(72)-C(73)-H(73A)	119.9
C(74)-C(73)-H(73A)	119.9
K(2)-C(73)-H(73A)	119.9
C(73)-C(74)-C(75)	120.0
C(73)-C(74)-K(2)	79.3(6)
C(75)-C(74)-K(2)	76.6(10)
C(73)-C(74)-H(74A)	119.9
C(75)-C(74)-H(74A)	119.9
K(2)-C(74)-H(74A)	119.9
C(76)-C(75)-C(74)	120.0
C(76)-C(75)-C(77)	119.8(4)
C(74)-C(75)-C(77)	120.2(4)
C(76)-C(75)-K(2)	78.4(10)
C(74)-C(75)-K(2)	78.2(10)
C(77)-C(75)-K(2)	114.1(6)
C(75)-C(76)-C(71)	120.0
C(75)-C(76)-K(2)	76.4(9)
C(71)-C(76)-K(2)	79.3(6)
C(75)-C(76)-H(76A)	119.9
C(71)-C(76)-H(76A)	119.9
K(2)-C(76)-H(76A)	119.9
C(71')-C(77')-H(77D)	109.5
C(71')-C(77')-H(77E)	109.5
H(77D)-C(77')-H(77E)	109.5
C(71')-C(77')-H(77F)	109.5
H(77D)-C(77')-H(77F)	109.5

H(77E)-C(77')-H(77F)	109.5
C(72')-C(71')-C(76')	120.0
C(72')-C(71')-C(77')	129.8(14)
C(76')-C(71')-C(77')	110.2(14)
C(72')-C(71')-K(2)	82.0(8)
C(76')-C(71')-K(2)	72.5(6)
C(77')-C(71')-K(2)	113.1(15)
C(71')-C(72')-C(73')	120.0
C(71')-C(72')-K(2)	73.7(8)
C(73')-C(72')-K(2)	77.4(7)
C(71')-C(72')-H(72B)	120.0
C(73')-C(72')-H(72B)	120.0
K(2)-C(72')-H(72B)	120.0
C(72')-C(73')-C(74')	120.0
C(72')-C(73')-K(2)	78.6(7)
C(74')-C(73')-K(2)	73.0(6)
C(72')-C(73')-H(73B)	120.0
C(74')-C(73')-H(73B)	120.0
K(2)-C(73')-H(73B)	120.0
C(75')-C(74')-C(73')	120.0
C(75')-C(74')-K(2)	73.0(8)
C(73')-C(74')-K(2)	82.6(6)
C(75')-C(74')-H(74B)	119.9
C(73')-C(74')-H(74B)	119.9
K(2)-C(74')-H(74B)	119.9
C(74')-C(75')-C(76')	120.0
C(74')-C(75')-K(2)	81.7(8)
C(76')-C(75')-K(2)	77.8(8)
C(74')-C(75')-H(75A)	119.6
C(76')-C(75')-H(75A)	119.6

K(2)-C(75')-H(75A)	119.6
C(75')-C(76')-C(71')	120.0
C(75')-C(76')-K(2)	76.4(7)
C(71')-C(76')-K(2)	82.4(6)
C(75')-C(76')-H(76B)	119.7
C(71')-C(76')-H(76B)	119.7
K(2)-C(76')-H(76B)	119.7
N(7)-K(1)-C(50)	88.5(2)
N(7)-K(1)-N(6)	63.62(19)
C(50)-K(1)-N(6)	25.0(2)
N(7)-K(1)-N(8)	24.76(18)
C(50)-K(1)-N(8)	83.2(2)
N(6)-K(1)-N(8)	61.6(2)
N(7)-K(1)-C(35)	25.24(18)
C(50)-K(1)-C(35)	113.3(2)
N(6)-K(1)-C(35)	88.3(2)
N(8)-K(1)-C(35)	41.46(19)
N(7)-K(1)-C(16)#3	111.6(3)
C(50)-K(1)-C(16)#3	136.0(3)
N(6)-K(1)-C(16)#3	145.0(3)
N(8)-K(1)-C(16)#3	99.1(3)
C(35)-K(1)-C(16)#3	94.7(3)
N(7)-K(1)-C(13)#3	92.9(3)
C(50)-K(1)-C(13)#3	105.4(3)
N(6)-K(1)-C(13)#3	103.1(3)
N(8)-K(1)-C(13)#3	117.6(3)
C(35)-K(1)-C(13)#3	81.9(3)
C(16)#3-K(1)-C(13)#3	111.8(3)
N(7)-K(1)-C(17)#3	106.4(3)
C(50)-K(1)-C(17)#3	113.4(4)

N(6)-K(1)-C(17)#3	120.2(3)
N(8)-K(1)-C(17)#3	86.4(3)
C(35)-K(1)-C(17)#3	99.3(3)
C(16)#3-K(1)-C(17)#3	24.9(3)
C(13)#3-K(1)-C(17)#3	136.7(3)
N(7)-K(1)-C(18)#3	121.4(3)
C(50)-K(1)-C(18)#3	95.0(3)
N(6)-K(1)-C(18)#3	108.9(3)
N(8)-K(1)-C(18)#3	97.7(3)
C(35)-K(1)-C(18)#3	120.5(3)
C(16)#3-K(1)-C(18)#3	41.1(3)
C(13)#3-K(1)-C(18)#3	140.7(3)
C(17)#3-K(1)-C(18)#3	22.9(3)
N(7)-K(1)-C(15)#3	130.9(3)
C(50)-K(1)-C(15)#3	134.3(3)
N(6)-K(1)-C(15)#3	155.8(3)
N(8)-K(1)-C(15)#3	121.8(3)
C(35)-K(1)-C(15)#3	109.4(3)
C(16)#3-K(1)-C(15)#3	22.9(3)
C(13)#3-K(1)-C(15)#3	95.8(3)
C(17)#3-K(1)-C(15)#3	42.5(3)
C(18)#3-K(1)-C(15)#3	48.1(3)
N(7)-K(1)-C(51)	99.54(19)
C(50)-K(1)-C(51)	24.6(2)
N(6)-K(1)-C(51)	42.91(18)
N(8)-K(1)-C(51)	85.0(2)
C(35)-K(1)-C(51)	124.2(2)
C(16)#3-K(1)-C(51)	111.4(3)
C(13)#3-K(1)-C(51)	126.2(3)
C(17)#3-K(1)-C(51)	89.1(3)

C(18)#3-K(1)-C(51)	70.4(3)
C(15)#3-K(1)-C(51)	113.2(2)
N(7)-K(1)-C(20)#3	151.8(3)
C(50)-K(1)-C(20)#3	111.7(3)
N(6)-K(1)-C(20)#3	135.4(2)
N(8)-K(1)-C(20)#3	134.7(3)
C(35)-K(1)-C(20)#3	132.6(3)
C(16)#3-K(1)-C(20)#3	40.3(3)
C(13)#3-K(1)-C(20)#3	100.0(3)
C(17)#3-K(1)-C(20)#3	48.3(3)
C(18)#3-K(1)-C(20)#3	40.8(3)
C(15)#3-K(1)-C(20)#3	23.3(3)
C(51)-K(1)-C(20)#3	93.0(2)
N(3)-K(2)-N(1)	69.4(2)
N(3)-K(2)-C(63)	94.4(2)
N(1)-K(2)-C(63)	25.8(2)
N(3)-K(2)-C(75')	150.6(3)
N(1)-K(2)-C(75')	123.4(3)
C(63)-K(2)-C(75')	103.7(3)
N(3)-K(2)-C(76')	138.2(4)
N(1)-K(2)-C(76')	148.8(4)
C(63)-K(2)-C(76')	126.4(4)
C(75')-K(2)-C(76')	25.80(19)
N(3)-K(2)-N(2)	25.26(18)
N(1)-K(2)-N(2)	64.7(2)
C(63)-K(2)-N(2)	84.7(2)
C(75')-K(2)-N(2)	171.5(3)
C(76')-K(2)-N(2)	146.4(4)
N(3)-K(2)-C(75)	143.3(3)
N(1)-K(2)-C(75)	123.4(4)

C(63)-K(2)-C(75)	106.3(4)
C(75')-K(2)-C(75)	7.5(4)
C(76')-K(2)-C(75)	27.4(5)
N(2)-K(2)-C(75)	166.9(4)
N(3)-K(2)-C(8)	25.8(2)
N(1)-K(2)-C(8)	95.1(2)
C(63)-K(2)-C(8)	120.2(2)
C(75')-K(2)-C(8)	130.6(3)
C(76')-K(2)-C(8)	112.7(4)
N(2)-K(2)-C(8)	42.0(2)
C(75)-K(2)-C(8)	124.9(4)
N(3)-K(2)-C(74)	120.0(4)
N(1)-K(2)-C(74)	113.3(4)
C(63)-K(2)-C(74)	106.6(4)
C(75')-K(2)-C(74)	32.5(4)
C(76')-K(2)-C(74)	46.1(5)
N(2)-K(2)-C(74)	145.3(4)
C(75)-K(2)-C(74)	25.19(16)
C(8)-K(2)-C(74)	107.9(4)
N(3)-K(2)-C(76)	139.2(4)
N(1)-K(2)-C(76)	146.8(4)
C(63)-K(2)-C(76)	124.9(4)
C(75')-K(2)-C(76)	23.6(5)
C(76')-K(2)-C(76)	2.3(5)
N(2)-K(2)-C(76)	148.5(4)
C(75)-K(2)-C(76)	25.16(19)
C(8)-K(2)-C(76)	114.0(4)
C(74)-K(2)-C(76)	44.2(2)
N(3)-K(2)-C(74')	129.4(4)
N(1)-K(2)-C(74')	110.0(3)

C(63)-K(2)-C(74')	99.3(3)
C(75')-K(2)-C(74')	25.35(14)
C(76')-K(2)-C(74')	44.7(2)
N(2)-K(2)-C(74')	154.4(4)
C(75)-K(2)-C(74')	19.1(5)
C(8)-K(2)-C(74')	118.7(3)
C(74)-K(2)-C(74')	10.7(4)
C(76)-K(2)-C(74')	42.5(5)
N(3)-K(2)-N(10)	67.31(19)
N(1)-K(2)-N(10)	24.88(18)
C(63)-K(2)-N(10)	42.1(2)
C(75')-K(2)-N(10)	112.2(4)
C(76')-K(2)-N(10)	136.4(3)
N(2)-K(2)-N(10)	74.0(2)
C(75)-K(2)-N(10)	109.2(4)
C(8)-K(2)-N(10)	89.4(2)
C(74)-K(2)-N(10)	92.3(4)
C(76)-K(2)-N(10)	134.2(4)
C(74')-K(2)-N(10)	92.0(3)
N(9)-La(1)-N(1)	118.4(2)
N(9)-La(1)-N(4)	30.3(2)
N(1)-La(1)-N(4)	137.9(2)
N(9)-La(1)-N(6)	145.3(3)
N(1)-La(1)-N(6)	90.9(2)
N(4)-La(1)-N(6)	130.4(2)
N(9)-La(1)-N(5)	124.7(2)
N(1)-La(1)-N(5)	116.7(2)
N(4)-La(1)-N(5)	101.9(3)
N(6)-La(1)-N(5)	29.6(2)
N(9)-La(1)-N(7)	72.1(2)

N(1)-La(1)-N(7)	118.0(2)
N(4)-La(1)-N(7)	83.7(2)
N(6)-La(1)-N(7)	77.9(2)
N(5)-La(1)-N(7)	79.1(2)
N(9)-La(1)-N(3)	88.8(2)
N(1)-La(1)-N(3)	81.8(2)
N(4)-La(1)-N(3)	73.5(2)
N(6)-La(1)-N(3)	115.2(2)
N(5)-La(1)-N(3)	103.0(2)
N(7)-La(1)-N(3)	157.1(2)
N(9)-La(1)-N(10)	88.2(2)
N(1)-La(1)-N(10)	30.3(2)
N(4)-La(1)-N(10)	111.3(2)
N(6)-La(1)-N(10)	118.3(3)
N(5)-La(1)-N(10)	146.4(2)
N(7)-La(1)-N(10)	108.9(2)
N(3)-La(1)-N(10)	82.2(2)
N(9)-La(1)-N(8)	85.1(2)
N(1)-La(1)-N(8)	88.0(3)
N(4)-La(1)-N(8)	107.0(2)
N(6)-La(1)-N(8)	77.1(3)
N(5)-La(1)-N(8)	92.7(3)
N(7)-La(1)-N(8)	30.0(2)
N(3)-La(1)-N(8)	163.9(2)
N(10)-La(1)-N(8)	82.7(3)
N(9)-La(1)-N(2)	116.8(2)
N(1)-La(1)-N(2)	76.8(2)
N(4)-La(1)-N(2)	95.5(2)
N(6)-La(1)-N(2)	86.3(2)
N(5)-La(1)-N(2)	79.6(2)

N(7)-La(1)-N(2)	158.1(2)
N(3)-La(1)-N(2)	29.3(2)
N(10)-La(1)-N(2)	91.9(2)
N(8)-La(1)-N(2)	157.3(2)
N(9)-La(1)-K(2)	104.88(18)
N(1)-La(1)-K(2)	41.06(18)
N(4)-La(1)-K(2)	105.98(16)
N(6)-La(1)-K(2)	109.64(18)
N(5)-La(1)-K(2)	119.20(17)
N(7)-La(1)-K(2)	155.63(18)
N(3)-La(1)-K(2)	40.88(17)
N(10)-La(1)-K(2)	46.84(17)
N(8)-La(1)-K(2)	127.1(2)
N(2)-La(1)-K(2)	45.21(15)
N(9)-La(1)-K(1)	109.25(18)
N(1)-La(1)-K(1)	105.46(18)
N(4)-La(1)-K(1)	112.08(16)
N(6)-La(1)-K(1)	40.18(19)
N(5)-La(1)-K(1)	50.2(2)
N(7)-La(1)-K(1)	37.94(15)
N(3)-La(1)-K(1)	152.92(15)
N(10)-La(1)-K(1)	117.34(18)
N(8)-La(1)-K(1)	42.48(19)
N(2)-La(1)-K(1)	125.74(16)
K(2)-La(1)-K(1)	141.84(6)
N(10)-N(1)-C(63)	113.9(8)
N(10)-N(1)-La(1)	77.3(4)
C(63)-N(1)-La(1)	167.5(7)
N(10)-N(1)-K(2)	87.8(5)
C(63)-N(1)-K(2)	82.3(5)

La(1)-N(1)-K(2)	104.4(3)
N(3)-N(2)-C(7)	114.1(8)
N(3)-N(2)-La(1)	71.0(5)
C(7)-N(2)-La(1)	169.4(6)
N(3)-N(2)-K(2)	70.0(4)
C(7)-N(2)-K(2)	93.4(5)
La(1)-N(2)-K(2)	97.1(2)
N(2)-N(3)-C(8)	111.9(7)
N(2)-N(3)-La(1)	79.6(5)
C(8)-N(3)-La(1)	165.5(6)
N(2)-N(3)-K(2)	84.8(5)
C(8)-N(3)-K(2)	86.3(5)
La(1)-N(3)-K(2)	104.1(2)
N(9)-N(4)-C(21)	113.5(7)
N(9)-N(4)-La(1)	72.6(4)
C(21)-N(4)-La(1)	173.9(6)
N(6)-N(5)-C(49)	114.9(9)
N(6)-N(5)-La(1)	75.2(5)
C(49)-N(5)-La(1)	169.2(8)
N(5)-N(6)-C(50)	113.9(8)
N(5)-N(6)-La(1)	75.3(5)
C(50)-N(6)-La(1)	169.5(7)
N(5)-N(6)-K(1)	98.6(5)
C(50)-N(6)-K(1)	76.8(5)
La(1)-N(6)-K(1)	107.6(3)
N(8)-N(7)-C(35)	113.2(7)
N(8)-N(7)-La(1)	76.8(4)
C(35)-N(7)-La(1)	162.3(5)
N(8)-N(7)-K(1)	85.3(5)
C(35)-N(7)-K(1)	85.5(4)

La(1)-N(7)-K(1)	110.4(2)
C(36)-N(8)-N(7)	112.6(8)
C(36)-N(8)-La(1)	163.4(7)
N(7)-N(8)-La(1)	73.2(4)
C(36)-N(8)-K(1)	92.5(6)
N(7)-N(8)-K(1)	70.0(5)
La(1)-N(8)-K(1)	104.0(3)
N(4)-N(9)-C(22)	113.3(8)
N(4)-N(9)-La(1)	77.1(4)
C(22)-N(9)-La(1)	169.6(7)
C(64)-N(10)-N(1)	113.0(8)
C(64)-N(10)-La(1)	172.7(7)
N(1)-N(10)-La(1)	72.4(4)
C(64)-N(10)-K(2)	90.1(6)
N(1)-N(10)-K(2)	67.4(5)
La(1)-N(10)-K(2)	96.7(2)
C(7)-P(1)-C(8)	88.4(4)
C(7)-P(1)-K(2)	69.5(3)
C(8)-P(1)-K(2)	59.4(3)
C(21)-P(2)-C(22)	86.9(5)
C(35)-P(3)-C(36)	86.9(4)
C(35)-P(3)-K(1)	60.8(3)
C(36)-P(3)-K(1)	70.7(3)
C(50)-P(4)-C(49)	86.1(5)
C(50)-P(4)-K(1)	55.3(3)
C(49)-P(4)-K(1)	80.1(3)
C(63)-P(5)-C(64)	87.4(5)
C(63)-P(5)-K(2)	58.7(3)
C(64)-P(5)-K(2)	71.5(4)

Symmetry transformations used to generate equivalent atoms:

#1 $-x, y-1/2, -z+3/2$ #2 $-x+1/2, -y+1, z+1/2$

#3 $-x, y+1/2, -z+3/2$

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 140905-1.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
C(1)	81(7)	116(10)	64(6)	0(6)	-10(5)	19(7)
C(2)	92(9)	135(12)	77(7)	-12(7)	-26(6)	9(9)
C(3)	95(9)	134(13)	88(9)	5(8)	-16(7)	26(9)
C(4)	111(10)	117(11)	99(9)	2(8)	-22(8)	8(9)
C(5)	85(7)	69(7)	94(8)	14(6)	-8(6)	27(6)
C(6)	60(6)	75(7)	57(6)	-3(5)	-8(4)	1(5)
C(7)	43(4)	62(5)	59(5)	1(4)	2(4)	-15(4)
C(8)	55(4)	39(4)	68(5)	-7(4)	0(4)	-7(4)
C(9)	65(4)	55(3)	90(4)	3(3)	-9(4)	2(4)
C(10)	76(4)	56(4)	91(4)	-1(3)	-15(4)	6(4)
C(11)	86(4)	64(4)	102(5)	5(4)	-19(4)	8(4)
C(12)	90(5)	72(4)	107(5)	18(4)	-9(4)	6(4)
C(13)	97(5)	71(4)	112(5)	26(4)	-1(4)	4(4)
C(14)	82(4)	68(4)	101(4)	15(4)	-10(4)	1(4)
C(15)	71(7)	67(7)	104(9)	-4(6)	-1(6)	4(6)
C(16)	102(9)	72(8)	114(9)	-5(7)	-16(7)	-3(7)
C(17)	87(9)	87(9)	163(14)	0(9)	34(10)	-23(8)
C(18)	115(11)	96(10)	111(11)	23(8)	29(9)	-11(9)
C(19)	131(11)	73(8)	96(8)	28(7)	22(7)	-24(8)
C(20)	91(8)	51(5)	81(7)	8(5)	24(6)	-5(6)

C(21)	76(6)	55(5)	75(7)	6(5)	-1(5)	8(5)
C(22)	88(7)	57(5)	65(6)	-9(5)	-8(6)	1(5)
C(23)	78(7)	81(7)	56(6)	-11(5)	-11(5)	18(6)
C(24)	105(9)	84(8)	73(7)	-7(6)	-25(6)	0(7)
C(25)	107(10)	107(10)	108(9)	24(8)	-34(8)	8(9)
C(26)	82(8)	107(10)	150(12)	11(9)	-22(8)	-16(10)
C(27)	81(8)	88(8)	159(12)	44(9)	-18(9)	3(7)
C(28)	89(7)	74(7)	77(7)	12(6)	-19(5)	-15(7)
C(29)	118(6)	120(6)	78(4)	-2(5)	20(4)	31(5)
C(30)	122(6)	126(6)	84(5)	3(5)	19(4)	28(5)
C(31)	122(6)	130(6)	81(4)	3(5)	14(5)	32(5)
C(32)	128(6)	134(6)	83(4)	-3(5)	3(4)	35(5)
C(33)	123(6)	125(6)	75(4)	-4(4)	4(4)	38(5)
C(34)	120(6)	117(6)	70(4)	-5(4)	11(4)	34(5)
C(35)	114(9)	53(5)	73(6)	3(5)	-26(7)	14(6)
C(36)	80(7)	47(5)	100(8)	10(5)	-30(6)	-3(5)
C(37)	93(5)	95(6)	138(6)	24(5)	-36(5)	-41(5)
C(38)	107(5)	112(6)	147(6)	19(5)	-36(5)	-44(5)
C(39)	114(5)	122(6)	153(6)	21(5)	-27(5)	-46(5)
C(40)	112(5)	124(6)	153(6)	29(5)	-14(5)	-46(5)
C(41)	111(5)	118(6)	149(6)	25(5)	-11(5)	-42(5)
C(42)	99(5)	106(6)	144(6)	22(5)	-17(5)	-44(5)
C(43)	76(4)	169(7)	114(5)	19(5)	1(4)	-11(5)
C(44)	78(4)	173(7)	119(6)	18(5)	6(4)	-9(5)
C(45)	87(5)	164(7)	131(6)	17(5)	10(5)	-6(5)
C(46)	86(5)	154(7)	126(6)	14(5)	5(4)	0(5)
C(47)	78(4)	151(7)	116(5)	11(5)	2(4)	1(5)
C(48)	67(4)	152(7)	104(5)	12(5)	4(4)	-1(5)
C(49)	69(6)	73(6)	85(7)	-20(5)	-11(6)	12(6)
C(50)	90(7)	47(5)	59(5)	-2(4)	-4(5)	17(5)

C(51)	130(11)	47(6)	99(8)	9(6)	12(8)	13(7)
C(52)	150(13)	96(10)	104(10)	23(8)	-9(9)	26(10)
C(53)	210(20)	118(13)	117(13)	50(10)	-22(13)	-29(14)
C(54)	184(18)	83(10)	128(12)	16(9)	66(12)	-6(11)
C(55)	154(14)	59(7)	149(12)	-3(8)	36(11)	33(9)
C(56)	116(10)	50(6)	104(8)	26(6)	42(7)	4(7)
C(57)	78(7)	77(7)	78(7)	0(5)	21(6)	-6(6)
C(58)	90(8)	95(8)	73(7)	22(6)	15(6)	12(7)
C(59)	100(10)	126(11)	85(8)	22(8)	-4(7)	10(9)
C(60)	70(7)	104(9)	88(8)	18(7)	14(6)	1(7)
C(61)	68(7)	58(6)	97(8)	12(5)	18(5)	6(5)
C(62)	63(6)	64(6)	64(6)	-3(5)	8(5)	-4(5)
C(63)	75(6)	72(7)	72(6)	-19(5)	15(5)	-9(5)
C(64)	57(5)	77(7)	83(7)	-1(5)	11(5)	0(5)
C(65)	69(4)	148(7)	114(6)	22(5)	-6(4)	15(5)
C(66)	76(4)	162(7)	127(6)	29(5)	-11(4)	9(5)
C(67)	87(5)	173(7)	133(6)	27(5)	-13(5)	10(5)
C(68)	90(5)	167(7)	127(6)	25(5)	-15(5)	17(5)
C(69)	92(5)	156(7)	121(6)	22(5)	-8(5)	19(5)
C(70)	79(5)	148(7)	114(6)	20(5)	-9(4)	17(5)
K(1)	110(2)	81(2)	102(2)	-8(1)	-20(2)	9(2)
K(2)	89(2)	77(2)	116(2)	-18(2)	32(2)	-3(2)
La(1)	51(1)	51(1)	52(1)	2(1)	0(1)	0(1)
N(1)	50(4)	76(5)	53(4)	10(4)	6(3)	1(4)
N(2)	42(4)	64(5)	80(5)	13(4)	5(4)	2(4)
N(3)	50(4)	58(5)	70(5)	4(4)	-18(3)	3(4)
N(4)	72(5)	43(4)	45(4)	-2(3)	-2(3)	-4(4)
N(5)	65(5)	80(6)	64(5)	-3(4)	13(4)	27(5)
N(6)	61(5)	73(5)	65(5)	11(4)	1(4)	15(4)
N(7)	56(4)	57(4)	53(4)	-3(3)	5(4)	8(4)

N(8)	85(6)	53(5)	64(5)	0(4)	-8(4)	-7(4)
N(9)	66(5)	59(4)	52(4)	1(3)	-8(3)	-20(4)
N(10)	48(4)	78(6)	64(4)	1(4)	4(3)	-5(4)
P(1)	73(2)	66(2)	76(2)	-9(1)	-13(1)	-3(1)
P(2)	108(2)	77(2)	64(2)	17(1)	-11(2)	-7(2)
P(3)	114(2)	68(2)	87(2)	-9(2)	-30(2)	-7(2)
P(4)	99(2)	95(2)	92(2)	-1(2)	-16(2)	39(2)
P(5)	57(1)	92(2)	90(2)	7(2)	17(1)	2(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 140905-1.

	x	y	z	U(eq)
H(1A)	-532	4378	4508	104
H(2A)	-1306	4802	3787	122
H(3A)	-1639	5849	3910	127
H(4A)	-1334	6336	4772	131
H(5A)	-574	5886	5476	99
H(10A)	1707	4290	7121	89
H(11A)	2230	3600	7774	101
H(12A)	1988	2559	7653	108
H(13A)	1120	2237	6911	112
H(14A)	570	2933	6310	100
H(15)	-388	4502	7156	97
H(16A)	-1548	4027	7138	115
H(17)	-2210	3734	8037	135
H(18A)	-1546	3821	8925	128
H(19A)	-411	4313	8977	120
H(24A)	2796	4664	9030	105
H(25A)	4015	5061	9260	129
H(26A)	4464	5949	8768	136
H(27A)	3695	6445	8073	131
H(28A)	2534	6049	7842	96
H(29)	77	6065	8176	126

H(30)	-829	5838	8907	133
H(31)	-915	6438	9769	133
H(32)	-94	7265	9901	138
H(33)	812	7492	9171	129
H(38)	3205	8026	7780	147
H(39)	4306	8328	7278	155
H(40)	4574	7939	6327	155
H(41)	3739	7247	5879	151
H(42)	2638	6945	6381	140
H(43)	-2432	6426	6203	144
H(44)	-3421	5859	6623	148
H(45)	-3215	5295	7496	152
H(46)	-2019	5299	7950	146
H(47)	-1030	5866	7530	138
H(52)	-504	8033	5211	140
H(53)	247	8661	4607	178
H(54)	1567	8559	4620	158
H(55)	2137	7830	5237	145
H(56)	1387	7202	5841	108
H(57A)	2947	6652	4488	93
H(58A)	2327	7079	3672	103
H(59A)	1068	6848	3503	124
H(60A)	358	6387	4221	105
H(61A)	975	5970	5071	89
H(66)	4551	5913	6482	146
H(67)	5417	5513	7170	157
H(68)	5066	4694	7782	154
H(69)	3850	4276	7704	148
H(70)	2984	4676	7016	136
H(77A)	4501	4076	4568	215

H(77B)	4139	4673	4842	215
H(77C)	3830	4409	4231	215
H(71A)	1992	2997	4739	152
H(72A)	2053	2932	5804	158
H(73A)	3022	3465	6336	159
H(74A)	3927	4065	5803	159
H(76A)	2898	3597	4207	149
H(77D)	2012	2436	4718	140
H(77E)	1660	3030	4430	140
H(77F)	1403	2819	5075	140
H(72B)	2487	3004	5986	89
H(73B)	3486	3686	6256	112
H(74B)	4086	4294	5506	113
H(75A)	3686	4218	4490	109
H(76B)	2692	3539	4221	110

Table 6. Torsion angles [deg] for 140905-1.

C(6)-C(1)-C(2)-C(3)	2(2)
C(1)-C(2)-C(3)-C(4)	-4(2)
C(2)-C(3)-C(4)-C(5)	4(2)
C(3)-C(4)-C(5)-C(6)	-2(2)
C(2)-C(1)-C(6)-C(5)	-0.2(18)
C(2)-C(1)-C(6)-C(7)	176.4(11)
C(4)-C(5)-C(6)-C(1)	-0.3(17)
C(4)-C(5)-C(6)-C(7)	-176.8(11)
C(1)-C(6)-C(7)-N(2)	158.2(9)
C(5)-C(6)-C(7)-N(2)	-25.5(14)
C(1)-C(6)-C(7)-P(1)	-20.6(14)
C(5)-C(6)-C(7)-P(1)	155.7(9)
C(1)-C(6)-C(7)-K(2)	83.7(11)
C(5)-C(6)-C(7)-K(2)	-100.0(10)
N(3)-C(8)-C(9)-C(14)	176.8(9)
P(1)-C(8)-C(9)-C(14)	-0.1(15)
K(2)-C(8)-C(9)-C(14)	-109.2(10)
N(3)-C(8)-C(9)-C(10)	-7.2(14)
P(1)-C(8)-C(9)-C(10)	175.9(8)
K(2)-C(8)-C(9)-C(10)	66.8(11)
C(14)-C(9)-C(10)-C(11)	-3.9(17)
C(8)-C(9)-C(10)-C(11)	-179.9(10)
C(9)-C(10)-C(11)-C(12)	4.1(18)
C(10)-C(11)-C(12)-C(13)	-2.4(19)
C(11)-C(12)-C(13)-C(14)	0.6(19)
C(11)-C(12)-C(13)-K(1)#1	-86.5(11)

C(12)-C(13)-C(14)-C(9)	-0.5(19)
K(1)#1-C(13)-C(14)-C(9)	90.8(11)
C(10)-C(9)-C(14)-C(13)	2.0(18)
C(8)-C(9)-C(14)-C(13)	178.2(11)
C(20)-C(15)-C(16)-C(17)	3.1(19)
K(1)#1-C(15)-C(16)-C(17)	72.5(12)
C(20)-C(15)-C(16)-K(1)#1	-69.4(10)
C(15)-C(16)-C(17)-C(18)	-4(2)
K(1)#1-C(16)-C(17)-C(18)	70.3(13)
C(15)-C(16)-C(17)-K(1)#1	-74.3(12)
C(16)-C(17)-C(18)-C(19)	5(2)
K(1)#1-C(17)-C(18)-C(19)	73.1(14)
C(16)-C(17)-C(18)-K(1)#1	-68.1(11)
C(17)-C(18)-C(19)-C(20)	-5(2)
K(1)#1-C(18)-C(19)-C(20)	65.4(12)
C(17)-C(18)-C(19)-K(1)#1	-70.6(15)
C(16)-C(15)-C(20)-C(19)	-2.9(16)
K(1)#1-C(15)-C(20)-C(19)	-68.8(10)
C(16)-C(15)-C(20)-C(21)	-178.5(10)
K(1)#1-C(15)-C(20)-C(21)	115.6(9)
C(16)-C(15)-C(20)-K(1)#1	65.9(10)
C(18)-C(19)-C(20)-C(15)	3.9(18)
K(1)#1-C(19)-C(20)-C(15)	67.6(9)
C(18)-C(19)-C(20)-C(21)	179.4(12)
K(1)#1-C(19)-C(20)-C(21)	-116.8(10)
C(18)-C(19)-C(20)-K(1)#1	-63.7(12)
C(15)-C(20)-C(21)-N(4)	21.7(15)
C(19)-C(20)-C(21)-N(4)	-153.8(10)
K(1)#1-C(20)-C(21)-N(4)	112.4(8)
C(15)-C(20)-C(21)-P(2)	-154.6(9)

C(19)-C(20)-C(21)-P(2)	29.8(15)
K(1)#1-C(20)-C(21)-P(2)	-64.0(10)
N(9)-C(22)-C(23)-C(28)	17.0(14)
P(2)-C(22)-C(23)-C(28)	-161.5(8)
N(9)-C(22)-C(23)-C(24)	-164.3(9)
P(2)-C(22)-C(23)-C(24)	17.3(14)
C(28)-C(23)-C(24)-C(25)	0.6(16)
C(22)-C(23)-C(24)-C(25)	-178.2(10)
C(28)-C(23)-C(24)-K(2)#2	86.6(12)
C(22)-C(23)-C(24)-K(2)#2	-92.2(11)
C(23)-C(24)-C(25)-C(26)	-0.2(19)
K(2)#2-C(24)-C(25)-C(26)	-120.9(14)
C(23)-C(24)-C(25)-K(2)#2	120.7(9)
C(24)-C(25)-C(26)-C(27)	1(2)
K(2)#2-C(25)-C(26)-C(27)	-100.8(14)
C(25)-C(26)-C(27)-C(28)	-1(2)
C(26)-C(27)-C(28)-C(23)	2(2)
C(24)-C(23)-C(28)-C(27)	-1.3(18)
C(22)-C(23)-C(28)-C(27)	177.4(12)
C(34)-C(29)-C(30)-C(31)	0.0
C(29)-C(30)-C(31)-C(32)	0.0
C(30)-C(31)-C(32)-C(33)	0.0
C(31)-C(32)-C(33)-C(34)	0.0
C(32)-C(33)-C(34)-C(29)	0.0
C(32)-C(33)-C(34)-C(35)	177.6
C(30)-C(29)-C(34)-C(33)	0.0
C(30)-C(29)-C(34)-C(35)	-177.5
C(33)-C(34)-C(35)-N(7)	-170.0(6)
C(29)-C(34)-C(35)-N(7)	7.6(6)
C(33)-C(34)-C(35)-P(3)	15.4(6)

C(29)-C(34)-C(35)-P(3)	-167.0(6)
C(33)-C(34)-C(35)-K(1)	-93.4(4)
C(29)-C(34)-C(35)-K(1)	84.2(4)
N(8)-C(36)-C(37)-C(38)	-179.8(7)
P(3)-C(36)-C(37)-C(38)	2.0(11)
K(1)-C(36)-C(37)-C(38)	102.7(7)
N(8)-C(36)-C(37)-C(42)	-3.3(12)
P(3)-C(36)-C(37)-C(42)	178.5(6)
K(1)-C(36)-C(37)-C(42)	-80.8(8)
C(42)-C(37)-C(38)-C(39)	0.0
C(36)-C(37)-C(38)-C(39)	176.5(9)
C(37)-C(38)-C(39)-C(40)	0.0
C(38)-C(39)-C(40)-C(41)	0.0
C(39)-C(40)-C(41)-C(42)	0.0
C(40)-C(41)-C(42)-C(37)	0.0
C(38)-C(37)-C(42)-C(41)	0.0
C(36)-C(37)-C(42)-C(41)	-176.5(9)
C(48)-C(43)-C(44)-C(45)	0.0
C(43)-C(44)-C(45)-C(46)	0.0
C(44)-C(45)-C(46)-C(47)	0.0
C(45)-C(46)-C(47)-C(48)	0.0
C(46)-C(47)-C(48)-C(43)	0.0
C(46)-C(47)-C(48)-C(49)	-176.3(10)
C(44)-C(43)-C(48)-C(47)	0.0
C(44)-C(43)-C(48)-C(49)	176.4(9)
C(47)-C(48)-C(49)-N(5)	25.8(13)
C(43)-C(48)-C(49)-N(5)	-150.6(8)
C(47)-C(48)-C(49)-P(4)	-158.0(6)
C(43)-C(48)-C(49)-P(4)	25.6(11)
N(6)-C(50)-C(51)-C(52)	176.1(7)

P(4)-C(50)-C(51)-C(52)	-6.0(10)
K(1)-C(50)-C(51)-C(52)	-106.3(5)
N(6)-C(50)-C(51)-C(56)	-1.4(12)
P(4)-C(50)-C(51)-C(56)	176.5(6)
K(1)-C(50)-C(51)-C(56)	76.2(6)
N(6)-C(50)-C(51)-K(1)	-77.6(8)
P(4)-C(50)-C(51)-K(1)	100.3(7)
C(56)-C(51)-C(52)-C(53)	0.0
C(50)-C(51)-C(52)-C(53)	-177.5(8)
K(1)-C(51)-C(52)-C(53)	109.4(4)
C(51)-C(52)-C(53)-C(54)	0.0
C(52)-C(53)-C(54)-C(55)	0.0
C(53)-C(54)-C(55)-C(56)	0.0
C(54)-C(55)-C(56)-C(51)	0.0
C(52)-C(51)-C(56)-C(55)	0.0
C(50)-C(51)-C(56)-C(55)	177.5(8)
K(1)-C(51)-C(56)-C(55)	-122.3(4)
C(62)-C(57)-C(58)-C(59)	-4.7(18)
C(57)-C(58)-C(59)-C(60)	7(2)
C(58)-C(59)-C(60)-C(61)	-6(2)
C(59)-C(60)-C(61)-C(62)	2.9(18)
C(60)-C(61)-C(62)-C(57)	-1.2(16)
C(60)-C(61)-C(62)-C(63)	-178.4(9)
C(58)-C(57)-C(62)-C(61)	2.1(16)
C(58)-C(57)-C(62)-C(63)	179.4(10)
C(61)-C(62)-C(63)-N(1)	-24.1(14)
C(57)-C(62)-C(63)-N(1)	158.7(9)
C(61)-C(62)-C(63)-P(5)	156.7(9)
C(57)-C(62)-C(63)-P(5)	-20.5(15)
C(61)-C(62)-C(63)-K(2)	52.5(10)

C(57)-C(62)-C(63)-K(2)	-124.7(9)
N(10)-C(64)-C(65)-C(66)	-140.5(9)
P(5)-C(64)-C(65)-C(66)	35.5(12)
K(2)-C(64)-C(65)-C(66)	138.9(6)
N(10)-C(64)-C(65)-C(70)	42.1(13)
P(5)-C(64)-C(65)-C(70)	-141.9(7)
K(2)-C(64)-C(65)-C(70)	-38.5(9)
C(70)-C(65)-C(66)-C(67)	0.0
C(64)-C(65)-C(66)-C(67)	-177.4(9)
C(65)-C(66)-C(67)-C(68)	0.0
C(66)-C(67)-C(68)-C(69)	0.0
C(67)-C(68)-C(69)-C(70)	0.0
C(68)-C(69)-C(70)-C(65)	0.0
C(66)-C(65)-C(70)-C(69)	0.0
C(64)-C(65)-C(70)-C(69)	177.4(9)
C(76)-C(71)-C(72)-C(73)	0.0
K(2)-C(71)-C(72)-C(73)	-66.0(7)
C(76)-C(71)-C(72)-K(2)	65.9(7)
C(71)-C(72)-C(73)-C(74)	0.0
K(2)-C(72)-C(73)-C(74)	-66.1(7)
C(71)-C(72)-C(73)-K(2)	66.1(7)
C(72)-C(73)-C(74)-C(75)	0.0
K(2)-C(73)-C(74)-C(75)	-67.6(11)
C(72)-C(73)-C(74)-K(2)	67.6(11)
C(73)-C(74)-C(75)-C(76)	0.0
K(2)-C(74)-C(75)-C(76)	-69.1(8)
C(73)-C(74)-C(75)-C(77)	-179.8(3)
K(2)-C(74)-C(75)-C(77)	111.1(8)
C(73)-C(74)-C(75)-K(2)	69.1(8)
C(74)-C(75)-C(76)-C(71)	0.0

C(77)-C(75)-C(76)-C(71)	179.8(3)
K(2)-C(75)-C(76)-C(71)	-68.9(8)
C(74)-C(75)-C(76)-K(2)	68.9(8)
C(77)-C(75)-C(76)-K(2)	-111.2(8)
C(72)-C(71)-C(76)-C(75)	0.0
K(2)-C(71)-C(76)-C(75)	67.4(10)
C(72)-C(71)-C(76)-K(2)	-67.4(10)
C(76')-C(71')-C(72')-C(73')	0.0
C(77')-C(71')-C(72')-C(73')	-178(3)
K(2)-C(71')-C(72')-C(73')	-64.4(6)
C(76')-C(71')-C(72')-K(2)	64.4(6)
C(77')-C(71')-C(72')-K(2)	-114(2)
C(71')-C(72')-C(73')-C(74')	0.0
K(2)-C(72')-C(73')-C(74')	-62.5(7)
C(71')-C(72')-C(73')-K(2)	62.5(7)
C(72')-C(73')-C(74')-C(75')	0.0
K(2)-C(73')-C(74')-C(75')	-65.5(8)
C(72')-C(73')-C(74')-K(2)	65.5(8)
C(73')-C(74')-C(75')-C(76')	0.0
K(2)-C(74')-C(75')-C(76')	-70.6(6)
C(73')-C(74')-C(75')-K(2)	70.6(6)
C(74')-C(75')-C(76')-C(71')	0.0
K(2)-C(75')-C(76')-C(71')	-72.7(7)
C(74')-C(75')-C(76')-K(2)	72.7(7)
C(72')-C(71')-C(76')-C(75')	0.0
C(77')-C(71')-C(76')-C(75')	178(2)
K(2)-C(71')-C(76')-C(75')	69.5(8)
C(72')-C(71')-C(76')-K(2)	-69.5(8)
C(77')-C(71')-C(76')-K(2)	108.8(16)
N(6)-C(50)-K(1)-N(7)	4.5(6)

C(51)-C(50)-K(1)-N(7)	-117.1(5)
P(4)-C(50)-K(1)-N(7)	116.8(4)
C(51)-C(50)-K(1)-N(6)	-121.5(9)
P(4)-C(50)-K(1)-N(6)	112.3(8)
N(6)-C(50)-K(1)-N(8)	28.7(6)
C(51)-C(50)-K(1)-N(8)	-92.8(5)
P(4)-C(50)-K(1)-N(8)	141.0(4)
N(6)-C(50)-K(1)-C(35)	-0.4(7)
C(51)-C(50)-K(1)-C(35)	-122.0(5)
P(4)-C(50)-K(1)-C(35)	111.9(4)
N(6)-C(50)-K(1)-C(16)#3	124.7(6)
C(51)-C(50)-K(1)-C(16)#3	3.1(8)
P(4)-C(50)-K(1)-C(16)#3	-123.0(5)
N(6)-C(50)-K(1)-C(13)#3	-88.1(6)
C(51)-C(50)-K(1)-C(13)#3	150.3(5)
P(4)-C(50)-K(1)-C(13)#3	24.2(5)
N(6)-C(50)-K(1)-C(17)#3	111.7(6)
C(51)-C(50)-K(1)-C(17)#3	-9.8(6)
P(4)-C(50)-K(1)-C(17)#3	-136.0(4)
N(6)-C(50)-K(1)-C(18)#3	125.9(6)
C(51)-C(50)-K(1)-C(18)#3	4.3(6)
P(4)-C(50)-K(1)-C(18)#3	-121.8(4)
N(6)-C(50)-K(1)-C(15)#3	157.3(5)
C(51)-C(50)-K(1)-C(15)#3	35.8(7)
P(4)-C(50)-K(1)-C(15)#3	-90.4(5)
N(6)-C(50)-K(1)-C(51)	121.5(9)
P(4)-C(50)-K(1)-C(51)	-126.2(7)
N(6)-C(50)-K(1)-C(20)#3	164.3(6)
C(51)-C(50)-K(1)-C(20)#3	42.7(6)
P(4)-C(50)-K(1)-C(20)#3	-83.4(4)

C(34)-C(35)-K(1)-N(7)	-113.5(5)
P(3)-C(35)-K(1)-N(7)	114.5(5)
N(7)-C(35)-K(1)-C(50)	11.5(5)
C(34)-C(35)-K(1)-C(50)	-101.9(3)
P(3)-C(35)-K(1)-C(50)	126.1(3)
N(7)-C(35)-K(1)-N(6)	11.4(5)
C(34)-C(35)-K(1)-N(6)	-102.1(3)
P(3)-C(35)-K(1)-N(6)	125.9(3)
N(7)-C(35)-K(1)-N(8)	-35.4(4)
C(34)-C(35)-K(1)-N(8)	-148.8(4)
P(3)-C(35)-K(1)-N(8)	79.1(3)
N(7)-C(35)-K(1)-C(16)#3	-133.7(5)
C(34)-C(35)-K(1)-C(16)#3	112.8(3)
P(3)-C(35)-K(1)-C(16)#3	-19.2(4)
N(7)-C(35)-K(1)-C(13)#3	114.9(5)
C(34)-C(35)-K(1)-C(13)#3	1.4(3)
P(3)-C(35)-K(1)-C(13)#3	-130.6(3)
N(7)-C(35)-K(1)-C(17)#3	-109.0(5)
C(34)-C(35)-K(1)-C(17)#3	137.5(3)
P(3)-C(35)-K(1)-C(17)#3	5.5(4)
N(7)-C(35)-K(1)-C(18)#3	-99.7(5)
C(34)-C(35)-K(1)-C(18)#3	146.8(3)
P(3)-C(35)-K(1)-C(18)#3	14.8(4)
N(7)-C(35)-K(1)-C(15)#3	-151.8(5)
C(34)-C(35)-K(1)-C(15)#3	94.8(3)
P(3)-C(35)-K(1)-C(15)#3	-37.3(4)
N(7)-C(35)-K(1)-C(51)	-13.7(5)
C(34)-C(35)-K(1)-C(51)	-127.2(3)
P(3)-C(35)-K(1)-C(51)	100.8(3)
N(7)-C(35)-K(1)-C(20)#3	-149.0(5)

C(34)-C(35)-K(1)-C(20)#3	97.5(4)
P(3)-C(35)-K(1)-C(20)#3	-34.5(4)
C(52)-C(51)-K(1)-N(7)	177.2(4)
C(56)-C(51)-K(1)-N(7)	-57.6(3)
C(50)-C(51)-K(1)-N(7)	64.5(6)
C(52)-C(51)-K(1)-C(50)	112.7(7)
C(56)-C(51)-K(1)-C(50)	-122.1(7)
C(52)-C(51)-K(1)-N(6)	144.6(5)
C(56)-C(51)-K(1)-N(6)	-90.3(4)
C(50)-C(51)-K(1)-N(6)	31.9(5)
C(52)-C(51)-K(1)-N(8)	-162.7(4)
C(56)-C(51)-K(1)-N(8)	-37.6(3)
C(50)-C(51)-K(1)-N(8)	84.6(5)
C(52)-C(51)-K(1)-C(35)	-176.9(4)
C(56)-C(51)-K(1)-C(35)	-51.8(4)
C(50)-C(51)-K(1)-C(35)	70.4(6)
C(52)-C(51)-K(1)-C(16)#3	-65.0(5)
C(56)-C(51)-K(1)-C(16)#3	60.2(4)
C(50)-C(51)-K(1)-C(16)#3	-177.7(6)
C(52)-C(51)-K(1)-C(13)#3	76.4(4)
C(56)-C(51)-K(1)-C(13)#3	-158.4(4)
C(50)-C(51)-K(1)-C(13)#3	-36.2(6)
C(52)-C(51)-K(1)-C(17)#3	-76.3(4)
C(56)-C(51)-K(1)-C(17)#3	48.9(4)
C(50)-C(51)-K(1)-C(17)#3	171.0(6)
C(52)-C(51)-K(1)-C(18)#3	-62.7(4)
C(56)-C(51)-K(1)-C(18)#3	62.4(4)
C(50)-C(51)-K(1)-C(18)#3	-175.4(6)
C(52)-C(51)-K(1)-C(15)#3	-40.2(5)
C(56)-C(51)-K(1)-C(15)#3	85.0(4)

C(50)-C(51)-K(1)-C(15)#3	-152.9(6)
C(52)-C(51)-K(1)-C(20)#3	-28.2(4)
C(56)-C(51)-K(1)-C(20)#3	97.0(4)
C(50)-C(51)-K(1)-C(20)#3	-140.8(6)
N(1)-C(63)-K(2)-N(3)	13.8(6)
C(62)-C(63)-K(2)-N(3)	-102.6(6)
P(5)-C(63)-K(2)-N(3)	126.7(4)
C(62)-C(63)-K(2)-N(1)	-116.3(9)
P(5)-C(63)-K(2)-N(1)	112.9(7)
N(1)-C(63)-K(2)-C(75')	-142.9(6)
C(62)-C(63)-K(2)-C(75')	100.8(6)
P(5)-C(63)-K(2)-C(75')	-30.0(5)
N(1)-C(63)-K(2)-C(76')	-156.6(5)
C(62)-C(63)-K(2)-C(76')	87.1(7)
P(5)-C(63)-K(2)-C(76')	-43.7(6)
N(1)-C(63)-K(2)-N(2)	37.1(5)
C(62)-C(63)-K(2)-N(2)	-79.2(6)
P(5)-C(63)-K(2)-N(2)	150.0(4)
N(1)-C(63)-K(2)-C(75)	-135.6(6)
C(62)-C(63)-K(2)-C(75)	108.1(6)
P(5)-C(63)-K(2)-C(75)	-22.7(5)
N(1)-C(63)-K(2)-C(8)	13.7(7)
C(62)-C(63)-K(2)-C(8)	-102.6(6)
P(5)-C(63)-K(2)-C(8)	126.6(3)
N(1)-C(63)-K(2)-C(74)	-109.4(6)
C(62)-C(63)-K(2)-C(74)	134.3(6)
P(5)-C(63)-K(2)-C(74)	3.6(5)
N(1)-C(63)-K(2)-C(76)	-154.6(6)
C(62)-C(63)-K(2)-C(76)	89.1(7)
P(5)-C(63)-K(2)-C(76)	-41.7(6)

N(1)-C(63)-K(2)-C(74')	-117.4(6)
C(62)-C(63)-K(2)-C(74')	126.3(6)
P(5)-C(63)-K(2)-C(74')	-4.5(5)
N(1)-C(63)-K(2)-N(10)	-34.8(4)
C(62)-C(63)-K(2)-N(10)	-151.1(7)
P(5)-C(63)-K(2)-N(10)	78.1(4)
C(74')-C(75')-K(2)-N(3)	-43.8(11)
C(76')-C(75')-K(2)-N(3)	79.5(11)
C(74')-C(75')-K(2)-N(1)	64.3(5)
C(76')-C(75')-K(2)-N(1)	-172.4(5)
C(74')-C(75')-K(2)-C(63)	82.6(6)
C(76')-C(75')-K(2)-C(63)	-154.1(6)
C(74')-C(75')-K(2)-C(76')	-123.29(19)
C(74')-C(75')-K(2)-N(2)	-97(3)
C(76')-C(75')-K(2)-N(2)	26(3)
C(74')-C(75')-K(2)-C(75)	-28(4)
C(76')-C(75')-K(2)-C(75)	95(4)
C(74')-C(75')-K(2)-C(8)	-70.5(8)
C(76')-C(75')-K(2)-C(8)	52.8(8)
C(74')-C(75')-K(2)-C(74)	-16.8(9)
C(76')-C(75')-K(2)-C(74)	106.5(9)
C(74')-C(75')-K(2)-C(76)	-122.0(14)
C(76')-C(75')-K(2)-C(76)	1.3(14)
C(76')-C(75')-K(2)-C(74')	123.29(19)
C(74')-C(75')-K(2)-N(10)	39.1(6)
C(76')-C(75')-K(2)-N(10)	162.4(6)
C(75')-C(76')-K(2)-N(3)	-133.6(7)
C(71')-C(76')-K(2)-N(3)	-10.1(8)
C(75')-C(76')-K(2)-N(1)	12.4(8)
C(71')-C(76')-K(2)-N(1)	135.8(8)

C(75')-C(76')-K(2)-C(63)	31.9(7)
C(71')-C(76')-K(2)-C(63)	155.3(6)
C(71')-C(76')-K(2)-C(75')	123.4(2)
C(75')-C(76')-K(2)-N(2)	-173.3(7)
C(71')-C(76')-K(2)-N(2)	-49.9(7)
C(75')-C(76')-K(2)-C(75)	-16.3(9)
C(71')-C(76')-K(2)-C(75)	107.1(9)
C(75')-C(76')-K(2)-C(8)	-139.0(6)
C(71')-C(76')-K(2)-C(8)	-15.6(6)
C(75')-C(76')-K(2)-C(74)	-45.6(6)
C(71')-C(76')-K(2)-C(74)	77.9(6)
C(75')-C(76')-K(2)-C(76)	-14(15)
C(71')-C(76')-K(2)-C(76)	110(15)
C(75')-C(76')-K(2)-C(74')	-30.61(14)
C(71')-C(76')-K(2)-C(74')	92.8(3)
C(75')-C(76')-K(2)-N(10)	-24.0(8)
C(71')-C(76')-K(2)-N(10)	99.4(8)
C(76)-C(75)-K(2)-N(3)	97.1(10)
C(74)-C(75)-K(2)-N(3)	-27.2(9)
C(77)-C(75)-K(2)-N(3)	-145.2(8)
C(76)-C(75)-K(2)-N(1)	-162.5(7)
C(74)-C(75)-K(2)-N(1)	73.2(7)
C(77)-C(75)-K(2)-N(1)	-44.8(7)
C(76)-C(75)-K(2)-C(63)	-141.1(7)
C(74)-C(75)-K(2)-C(63)	94.5(7)
C(77)-C(75)-K(2)-C(63)	-23.4(7)
C(76)-C(75)-K(2)-C(75')	-70(4)
C(74)-C(75)-K(2)-C(75')	166(4)
C(77)-C(75)-K(2)-C(75')	48(4)
C(76)-C(75)-K(2)-C(76')	0.2(13)

C(74)-C(75)-K(2)-C(76')	-124.1(12)
C(77)-C(75)-K(2)-C(76')	117.9(12)
C(76)-C(75)-K(2)-N(2)	72.6(19)
C(74)-C(75)-K(2)-N(2)	-51.8(19)
C(77)-C(75)-K(2)-N(2)	-169.7(17)
C(76)-C(75)-K(2)-C(8)	71.4(8)
C(74)-C(75)-K(2)-C(8)	-53.0(8)
C(77)-C(75)-K(2)-C(8)	-171.0(7)
C(76)-C(75)-K(2)-C(74)	124.3(2)
C(77)-C(75)-K(2)-C(74)	-118.0(6)
C(74)-C(75)-K(2)-C(76)	-124.3(2)
C(77)-C(75)-K(2)-C(76)	117.7(6)
C(76)-C(75)-K(2)-C(74')	148.1(14)
C(74)-C(75)-K(2)-C(74')	23.8(14)
C(77)-C(75)-K(2)-C(74')	-94.2(14)
C(76)-C(75)-K(2)-N(10)	174.6(7)
C(74)-C(75)-K(2)-N(10)	50.3(7)
C(77)-C(75)-K(2)-N(10)	-67.7(7)
C(9)-C(8)-K(2)-N(3)	-113.7(8)
P(1)-C(8)-K(2)-N(3)	113.6(6)
N(3)-C(8)-K(2)-N(1)	6.0(5)
C(9)-C(8)-K(2)-N(1)	-107.7(6)
P(1)-C(8)-K(2)-N(1)	119.6(3)
N(3)-C(8)-K(2)-C(63)	0.1(6)
C(9)-C(8)-K(2)-C(63)	-113.7(6)
P(1)-C(8)-K(2)-C(63)	113.7(4)
N(3)-C(8)-K(2)-C(75')	149.6(6)
C(9)-C(8)-K(2)-C(75')	35.8(8)
P(1)-C(8)-K(2)-C(75')	-96.8(5)
N(3)-C(8)-K(2)-C(76')	171.6(5)

C(9)-C(8)-K(2)-C(76')	57.9(6)
P(1)-C(8)-K(2)-C(76')	-74.8(4)
N(3)-C(8)-K(2)-N(2)	-36.1(4)
C(9)-C(8)-K(2)-N(2)	-149.9(7)
P(1)-C(8)-K(2)-N(2)	77.5(4)
N(3)-C(8)-K(2)-C(75)	143.4(6)
C(9)-C(8)-K(2)-C(75)	29.7(7)
P(1)-C(8)-K(2)-C(75)	-102.9(5)
N(3)-C(8)-K(2)-C(74)	122.5(5)
C(9)-C(8)-K(2)-C(74)	8.8(7)
P(1)-C(8)-K(2)-C(74)	-123.9(4)
N(3)-C(8)-K(2)-C(76)	169.6(5)
C(9)-C(8)-K(2)-C(76)	55.9(7)
P(1)-C(8)-K(2)-C(76)	-76.8(5)
N(3)-C(8)-K(2)-C(74')	122.2(5)
C(9)-C(8)-K(2)-C(74')	8.4(7)
P(1)-C(8)-K(2)-C(74')	-124.2(4)
N(3)-C(8)-K(2)-N(10)	30.3(5)
C(9)-C(8)-K(2)-N(10)	-83.5(6)
P(1)-C(8)-K(2)-N(10)	143.9(3)
C(73)-C(74)-K(2)-N(3)	37.0(6)
C(75)-C(74)-K(2)-N(3)	161.6(6)
C(73)-C(74)-K(2)-N(1)	115.9(5)
C(75)-C(74)-K(2)-N(1)	-119.5(6)
C(73)-C(74)-K(2)-C(63)	142.4(6)
C(75)-C(74)-K(2)-C(63)	-93.0(6)
C(73)-C(74)-K(2)-C(75')	-128.1(10)
C(75)-C(74)-K(2)-C(75')	-3.5(10)
C(73)-C(74)-K(2)-C(76')	-92.7(8)
C(75)-C(74)-K(2)-C(76')	31.9(8)

C(73)-C(74)-K(2)-N(2)	37.2(7)
C(75)-C(74)-K(2)-N(2)	161.8(7)
C(73)-C(74)-K(2)-C(75)	-124.6(4)
C(73)-C(74)-K(2)-C(8)	11.9(6)
C(75)-C(74)-K(2)-C(8)	136.5(6)
C(73)-C(74)-K(2)-C(76)	-94.4(3)
C(75)-C(74)-K(2)-C(76)	30.24(18)
C(73)-C(74)-K(2)-C(74')	-170(3)
C(75)-C(74)-K(2)-C(74')	-45(3)
C(73)-C(74)-K(2)-N(10)	102.0(6)
C(75)-C(74)-K(2)-N(10)	-133.4(6)
C(75)-C(76)-K(2)-N(3)	-114.8(7)
C(71)-C(76)-K(2)-N(3)	9.9(7)
C(75)-C(76)-K(2)-N(1)	27.3(10)
C(71)-C(76)-K(2)-N(1)	152.0(9)
C(75)-C(76)-K(2)-C(63)	47.2(8)
C(71)-C(76)-K(2)-C(63)	171.9(7)
C(75)-C(76)-K(2)-C(75')	17.7(11)
C(71)-C(76)-K(2)-C(75')	142.4(11)
C(75)-C(76)-K(2)-C(76')	-177(15)
C(71)-C(76)-K(2)-C(76')	-53(15)
C(75)-C(76)-K(2)-N(2)	-155.5(7)
C(71)-C(76)-K(2)-N(2)	-30.9(7)
C(71)-C(76)-K(2)-C(75)	124.7(3)
C(75)-C(76)-K(2)-C(8)	-121.7(7)
C(71)-C(76)-K(2)-C(8)	2.9(6)
C(75)-C(76)-K(2)-C(74)	-30.27(18)
C(71)-C(76)-K(2)-C(74)	94.4(3)
C(75)-C(76)-K(2)-C(74')	-14.8(7)
C(71)-C(76)-K(2)-C(74')	109.9(6)

C(75)-C(76)-K(2)-N(10)	-7.1(9)
C(71)-C(76)-K(2)-N(10)	117.6(8)
C(75')-C(74')-K(2)-N(3)	153.9(6)
C(73')-C(74')-K(2)-N(3)	29.3(6)
C(75')-C(74')-K(2)-N(1)	-126.8(5)
C(73')-C(74')-K(2)-N(1)	108.7(5)
C(75')-C(74')-K(2)-C(63)	-102.5(6)
C(73')-C(74')-K(2)-C(63)	132.9(5)
C(73')-C(74')-K(2)-C(75')	-124.5(3)
C(75')-C(74')-K(2)-C(76')	31.17(19)
C(73')-C(74')-K(2)-C(76')	-93.4(3)
C(75')-C(74')-K(2)-N(2)	160.3(8)
C(73')-C(74')-K(2)-N(2)	35.7(8)
C(75')-C(74')-K(2)-C(75)	10.8(14)
C(73')-C(74')-K(2)-C(75)	-113.7(14)
C(75')-C(74')-K(2)-C(8)	125.3(6)
C(73')-C(74')-K(2)-C(8)	0.8(6)
C(75')-C(74')-K(2)-C(74)	124(3)
C(73')-C(74')-K(2)-C(74)	-1(3)
C(75')-C(74')-K(2)-C(76)	30.2(9)
C(73')-C(74')-K(2)-C(76)	-94.3(8)
C(75')-C(74')-K(2)-N(10)	-144.3(6)
C(73')-C(74')-K(2)-N(10)	91.2(5)
N(3)-K(2)-La(1)-N(9)	70.1(3)
N(1)-K(2)-La(1)-N(9)	-116.4(3)
C(63)-K(2)-La(1)-N(9)	-121.7(3)
C(75')-K(2)-La(1)-N(9)	-55.5(5)
C(76')-K(2)-La(1)-N(9)	-2.4(13)
N(2)-K(2)-La(1)-N(9)	113.2(3)
C(75)-K(2)-La(1)-N(9)	-45.2(6)

C(8)-K(2)-La(1)-N(9)	64.9(3)
C(74)-K(2)-La(1)-N(9)	-29.4(5)
C(76)-K(2)-La(1)-N(9)	-9.7(14)
C(74')-K(2)-La(1)-N(9)	-41.4(4)
N(10)-K(2)-La(1)-N(9)	-72.9(3)
N(3)-K(2)-La(1)-N(1)	-173.6(3)
C(63)-K(2)-La(1)-N(1)	-5.4(3)
C(75')-K(2)-La(1)-N(1)	60.8(6)
C(76')-K(2)-La(1)-N(1)	114.0(13)
N(2)-K(2)-La(1)-N(1)	-130.5(3)
C(75)-K(2)-La(1)-N(1)	71.2(6)
C(8)-K(2)-La(1)-N(1)	-178.7(3)
C(74)-K(2)-La(1)-N(1)	87.0(5)
C(76)-K(2)-La(1)-N(1)	106.7(14)
C(74')-K(2)-La(1)-N(1)	74.9(4)
N(10)-K(2)-La(1)-N(1)	43.4(3)
N(3)-K(2)-La(1)-N(4)	38.6(3)
N(1)-K(2)-La(1)-N(4)	-147.8(3)
C(63)-K(2)-La(1)-N(4)	-153.2(3)
C(75')-K(2)-La(1)-N(4)	-87.0(5)
C(76')-K(2)-La(1)-N(4)	-33.8(13)
N(2)-K(2)-La(1)-N(4)	81.7(3)
C(75)-K(2)-La(1)-N(4)	-76.6(6)
C(8)-K(2)-La(1)-N(4)	33.5(3)
C(74)-K(2)-La(1)-N(4)	-60.9(5)
C(76)-K(2)-La(1)-N(4)	-41.1(14)
C(74')-K(2)-La(1)-N(4)	-72.9(4)
N(10)-K(2)-La(1)-N(4)	-104.4(3)
N(3)-K(2)-La(1)-N(6)	-106.2(3)
N(1)-K(2)-La(1)-N(6)	67.3(3)

C(63)-K(2)-La(1)-N(6)	62.0(3)
C(75')-K(2)-La(1)-N(6)	128.2(6)
C(76')-K(2)-La(1)-N(6)	-178.7(13)
N(2)-K(2)-La(1)-N(6)	-63.1(3)
C(75)-K(2)-La(1)-N(6)	138.5(6)
C(8)-K(2)-La(1)-N(6)	-111.3(3)
C(74)-K(2)-La(1)-N(6)	154.3(5)
C(76)-K(2)-La(1)-N(6)	174.0(14)
C(74')-K(2)-La(1)-N(6)	142.3(4)
N(10)-K(2)-La(1)-N(6)	110.8(3)
N(3)-K(2)-La(1)-N(5)	-75.4(3)
N(1)-K(2)-La(1)-N(5)	98.2(3)
C(63)-K(2)-La(1)-N(5)	92.8(3)
C(75')-K(2)-La(1)-N(5)	159.0(6)
C(76')-K(2)-La(1)-N(5)	-147.8(13)
N(2)-K(2)-La(1)-N(5)	-32.3(3)
C(75)-K(2)-La(1)-N(5)	169.4(6)
C(8)-K(2)-La(1)-N(5)	-80.5(3)
C(74)-K(2)-La(1)-N(5)	-174.9(5)
C(76)-K(2)-La(1)-N(5)	-155.1(14)
C(74')-K(2)-La(1)-N(5)	173.1(4)
N(10)-K(2)-La(1)-N(5)	141.6(3)
N(3)-K(2)-La(1)-N(7)	149.5(4)
N(1)-K(2)-La(1)-N(7)	-37.0(4)
C(63)-K(2)-La(1)-N(7)	-42.3(5)
C(75')-K(2)-La(1)-N(7)	23.9(7)
C(76')-K(2)-La(1)-N(7)	77.0(13)
N(2)-K(2)-La(1)-N(7)	-167.4(4)
C(75)-K(2)-La(1)-N(7)	34.3(7)
C(8)-K(2)-La(1)-N(7)	144.4(4)

C(74)-K(2)-La(1)-N(7)	50.0(6)
C(76)-K(2)-La(1)-N(7)	69.7(14)
C(74')-K(2)-La(1)-N(7)	38.0(5)
N(10)-K(2)-La(1)-N(7)	6.5(4)
N(1)-K(2)-La(1)-N(3)	173.6(3)
C(63)-K(2)-La(1)-N(3)	168.2(3)
C(75')-K(2)-La(1)-N(3)	-125.6(6)
C(76')-K(2)-La(1)-N(3)	-72.5(13)
N(2)-K(2)-La(1)-N(3)	43.1(3)
C(75)-K(2)-La(1)-N(3)	-115.2(6)
C(8)-K(2)-La(1)-N(3)	-5.1(3)
C(74)-K(2)-La(1)-N(3)	-99.5(5)
C(76)-K(2)-La(1)-N(3)	-79.7(14)
C(74')-K(2)-La(1)-N(3)	-111.5(4)
N(10)-K(2)-La(1)-N(3)	-143.0(3)
N(3)-K(2)-La(1)-N(10)	143.0(3)
N(1)-K(2)-La(1)-N(10)	-43.4(3)
C(63)-K(2)-La(1)-N(10)	-48.8(3)
C(75')-K(2)-La(1)-N(10)	17.4(6)
C(76')-K(2)-La(1)-N(10)	70.5(13)
N(2)-K(2)-La(1)-N(10)	-173.9(3)
C(75)-K(2)-La(1)-N(10)	27.8(6)
C(8)-K(2)-La(1)-N(10)	137.9(3)
C(74)-K(2)-La(1)-N(10)	43.5(5)
C(76)-K(2)-La(1)-N(10)	63.3(14)
C(74')-K(2)-La(1)-N(10)	31.5(4)
N(3)-K(2)-La(1)-N(8)	165.3(3)
N(1)-K(2)-La(1)-N(8)	-21.1(3)
C(63)-K(2)-La(1)-N(8)	-26.5(3)
C(75')-K(2)-La(1)-N(8)	39.7(6)

C(76')-K(2)-La(1)-N(8)	92.8(13)
N(2)-K(2)-La(1)-N(8)	-151.6(3)
C(75)-K(2)-La(1)-N(8)	50.1(6)
C(8)-K(2)-La(1)-N(8)	160.2(3)
C(74)-K(2)-La(1)-N(8)	65.8(5)
C(76)-K(2)-La(1)-N(8)	85.5(14)
C(74')-K(2)-La(1)-N(8)	53.8(4)
N(10)-K(2)-La(1)-N(8)	22.3(3)
N(3)-K(2)-La(1)-N(2)	-43.1(3)
N(1)-K(2)-La(1)-N(2)	130.5(3)
C(63)-K(2)-La(1)-N(2)	125.1(3)
C(75')-K(2)-La(1)-N(2)	-168.7(6)
C(76')-K(2)-La(1)-N(2)	-115.5(13)
C(75)-K(2)-La(1)-N(2)	-158.3(6)
C(8)-K(2)-La(1)-N(2)	-48.2(3)
C(74)-K(2)-La(1)-N(2)	-142.6(5)
C(76)-K(2)-La(1)-N(2)	-122.8(14)
C(74')-K(2)-La(1)-N(2)	-154.6(4)
N(10)-K(2)-La(1)-N(2)	173.9(3)
N(3)-K(2)-La(1)-K(1)	-137.0(2)
N(1)-K(2)-La(1)-K(1)	36.5(3)
C(63)-K(2)-La(1)-K(1)	31.2(3)
C(75')-K(2)-La(1)-K(1)	97.4(5)
C(76')-K(2)-La(1)-K(1)	150.5(13)
N(2)-K(2)-La(1)-K(1)	-94.0(2)
C(75)-K(2)-La(1)-K(1)	107.7(5)
C(8)-K(2)-La(1)-K(1)	-142.16(19)
C(74)-K(2)-La(1)-K(1)	123.5(5)
C(76)-K(2)-La(1)-K(1)	143.2(14)
C(74')-K(2)-La(1)-K(1)	111.4(4)

N(10)-K(2)-La(1)-K(1)	80.0(2)
N(7)-K(1)-La(1)-N(9)	12.2(3)
C(50)-K(1)-La(1)-N(9)	-164.3(3)
N(6)-K(1)-La(1)-N(9)	-159.4(3)
N(8)-K(1)-La(1)-N(9)	59.1(3)
C(35)-K(1)-La(1)-N(9)	8.3(2)
C(16)#3-K(1)-La(1)-N(9)	71.0(4)
C(13)#3-K(1)-La(1)-N(9)	-63.6(3)
C(17)#3-K(1)-La(1)-N(9)	93.0(4)
C(18)#3-K(1)-La(1)-N(9)	118.4(4)
C(15)#3-K(1)-La(1)-N(9)	70.5(6)
C(51)-K(1)-La(1)-N(9)	172.0(2)
C(20)#3-K(1)-La(1)-N(9)	130.5(6)
N(7)-K(1)-La(1)-N(1)	-116.0(3)
C(50)-K(1)-La(1)-N(1)	67.4(3)
N(6)-K(1)-La(1)-N(1)	72.3(3)
N(8)-K(1)-La(1)-N(1)	-69.2(3)
C(35)-K(1)-La(1)-N(1)	-120.0(2)
C(16)#3-K(1)-La(1)-N(1)	-57.3(4)
C(13)#3-K(1)-La(1)-N(1)	168.1(3)
C(17)#3-K(1)-La(1)-N(1)	-35.3(4)
C(18)#3-K(1)-La(1)-N(1)	-9.8(4)
C(15)#3-K(1)-La(1)-N(1)	-57.7(5)
C(51)-K(1)-La(1)-N(1)	43.7(2)
C(20)#3-K(1)-La(1)-N(1)	2.2(6)
N(7)-K(1)-La(1)-N(4)	44.6(3)
C(50)-K(1)-La(1)-N(4)	-132.0(3)
N(6)-K(1)-La(1)-N(4)	-127.1(3)
N(8)-K(1)-La(1)-N(4)	91.4(3)
C(35)-K(1)-La(1)-N(4)	40.6(2)

C(16)#3-K(1)-La(1)-N(4)	103.3(4)
C(13)#3-K(1)-La(1)-N(4)	-31.3(3)
C(17)#3-K(1)-La(1)-N(4)	125.3(4)
C(18)#3-K(1)-La(1)-N(4)	150.8(4)
C(15)#3-K(1)-La(1)-N(4)	102.9(6)
C(51)-K(1)-La(1)-N(4)	-155.7(2)
C(20)#3-K(1)-La(1)-N(4)	162.8(6)
N(7)-K(1)-La(1)-N(6)	171.6(4)
C(50)-K(1)-La(1)-N(6)	-4.9(4)
N(8)-K(1)-La(1)-N(6)	-141.5(4)
C(35)-K(1)-La(1)-N(6)	167.7(3)
C(16)#3-K(1)-La(1)-N(6)	-129.6(4)
C(13)#3-K(1)-La(1)-N(6)	95.8(4)
C(17)#3-K(1)-La(1)-N(6)	-107.6(5)
C(18)#3-K(1)-La(1)-N(6)	-82.2(4)
C(15)#3-K(1)-La(1)-N(6)	-130.1(6)
C(51)-K(1)-La(1)-N(6)	-28.6(3)
C(20)#3-K(1)-La(1)-N(6)	-70.1(6)
N(7)-K(1)-La(1)-N(5)	131.9(4)
C(50)-K(1)-La(1)-N(5)	-44.7(3)
N(6)-K(1)-La(1)-N(5)	-39.8(3)
N(8)-K(1)-La(1)-N(5)	178.7(3)
C(35)-K(1)-La(1)-N(5)	127.9(3)
C(16)#3-K(1)-La(1)-N(5)	-169.4(4)
C(13)#3-K(1)-La(1)-N(5)	56.0(3)
C(17)#3-K(1)-La(1)-N(5)	-147.4(4)
C(18)#3-K(1)-La(1)-N(5)	-121.9(4)
C(15)#3-K(1)-La(1)-N(5)	-169.8(6)
C(51)-K(1)-La(1)-N(5)	-68.4(3)
C(20)#3-K(1)-La(1)-N(5)	-109.9(6)

C(50)-K(1)-La(1)-N(7)	-176.6(4)
N(6)-K(1)-La(1)-N(7)	-171.6(4)
N(8)-K(1)-La(1)-N(7)	46.8(3)
C(35)-K(1)-La(1)-N(7)	-3.9(3)
C(16)#3-K(1)-La(1)-N(7)	58.7(4)
C(13)#3-K(1)-La(1)-N(7)	-75.9(4)
C(17)#3-K(1)-La(1)-N(7)	80.8(4)
C(18)#3-K(1)-La(1)-N(7)	106.2(4)
C(15)#3-K(1)-La(1)-N(7)	58.3(6)
C(51)-K(1)-La(1)-N(7)	159.7(3)
C(20)#3-K(1)-La(1)-N(7)	118.3(6)
N(7)-K(1)-La(1)-N(3)	141.5(5)
C(50)-K(1)-La(1)-N(3)	-35.1(5)
N(6)-K(1)-La(1)-N(3)	-30.1(5)
N(8)-K(1)-La(1)-N(3)	-171.6(5)
C(35)-K(1)-La(1)-N(3)	137.6(4)
C(16)#3-K(1)-La(1)-N(3)	-159.7(5)
C(13)#3-K(1)-La(1)-N(3)	65.7(4)
C(17)#3-K(1)-La(1)-N(3)	-137.7(5)
C(18)#3-K(1)-La(1)-N(3)	-112.3(5)
C(15)#3-K(1)-La(1)-N(3)	-160.2(6)
C(51)-K(1)-La(1)-N(3)	-58.7(4)
C(20)#3-K(1)-La(1)-N(3)	-100.2(7)
N(7)-K(1)-La(1)-N(10)	-86.0(3)
C(50)-K(1)-La(1)-N(10)	97.4(3)
N(6)-K(1)-La(1)-N(10)	102.4(3)
N(8)-K(1)-La(1)-N(10)	-39.2(3)
C(35)-K(1)-La(1)-N(10)	-89.9(2)
C(16)#3-K(1)-La(1)-N(10)	-27.2(4)
C(13)#3-K(1)-La(1)-N(10)	-161.8(3)

C(17)#3-K(1)-La(1)-N(10)	-5.2(4)
C(18)#3-K(1)-La(1)-N(10)	20.2(4)
C(15)#3-K(1)-La(1)-N(10)	-27.7(6)
C(51)-K(1)-La(1)-N(10)	73.8(2)
C(20)#3-K(1)-La(1)-N(10)	32.3(6)
N(7)-K(1)-La(1)-N(8)	-46.8(3)
C(50)-K(1)-La(1)-N(8)	136.6(4)
N(6)-K(1)-La(1)-N(8)	141.5(4)
C(35)-K(1)-La(1)-N(8)	-50.8(3)
C(16)#3-K(1)-La(1)-N(8)	11.9(4)
C(13)#3-K(1)-La(1)-N(8)	-122.7(3)
C(17)#3-K(1)-La(1)-N(8)	33.9(4)
C(18)#3-K(1)-La(1)-N(8)	59.4(4)
C(15)#3-K(1)-La(1)-N(8)	11.5(6)
C(51)-K(1)-La(1)-N(8)	112.9(3)
C(20)#3-K(1)-La(1)-N(8)	71.4(6)
N(7)-K(1)-La(1)-N(2)	159.3(3)
C(50)-K(1)-La(1)-N(2)	-17.3(3)
N(6)-K(1)-La(1)-N(2)	-12.3(3)
N(8)-K(1)-La(1)-N(2)	-153.9(3)
C(35)-K(1)-La(1)-N(2)	155.4(2)
C(16)#3-K(1)-La(1)-N(2)	-141.9(4)
C(13)#3-K(1)-La(1)-N(2)	83.5(3)
C(17)#3-K(1)-La(1)-N(2)	-119.9(4)
C(18)#3-K(1)-La(1)-N(2)	-94.5(4)
C(15)#3-K(1)-La(1)-N(2)	-142.4(5)
C(51)-K(1)-La(1)-N(2)	-40.9(2)
C(20)#3-K(1)-La(1)-N(2)	-82.4(6)
N(7)-K(1)-La(1)-K(2)	-140.0(3)
C(50)-K(1)-La(1)-K(2)	43.5(3)

N(6)-K(1)-La(1)-K(2)	48.4(3)
N(8)-K(1)-La(1)-K(2)	-93.1(3)
C(35)-K(1)-La(1)-K(2)	-143.89(16)
C(16)#3-K(1)-La(1)-K(2)	-81.2(3)
C(13)#3-K(1)-La(1)-K(2)	144.2(2)
C(17)#3-K(1)-La(1)-K(2)	-59.2(4)
C(18)#3-K(1)-La(1)-K(2)	-33.8(4)
C(15)#3-K(1)-La(1)-K(2)	-81.7(5)
C(51)-K(1)-La(1)-K(2)	19.80(18)
C(20)#3-K(1)-La(1)-K(2)	-21.7(6)
C(62)-C(63)-N(1)-N(10)	179.7(8)
P(5)-C(63)-N(1)-N(10)	-0.9(10)
K(2)-C(63)-N(1)-N(10)	84.1(7)
C(62)-C(63)-N(1)-La(1)	-28(3)
P(5)-C(63)-N(1)-La(1)	152(3)
K(2)-C(63)-N(1)-La(1)	-123(3)
C(62)-C(63)-N(1)-K(2)	95.6(8)
P(5)-C(63)-N(1)-K(2)	-85.0(6)
N(9)-La(1)-N(1)-N(10)	-4.5(6)
N(4)-La(1)-N(1)-N(10)	-34.5(6)
N(6)-La(1)-N(1)-N(10)	156.1(5)
N(5)-La(1)-N(1)-N(10)	171.0(5)
N(7)-La(1)-N(1)-N(10)	79.4(5)
N(3)-La(1)-N(1)-N(10)	-88.6(5)
N(8)-La(1)-N(1)-N(10)	79.0(5)
N(2)-La(1)-N(1)-N(10)	-118.0(5)
K(2)-La(1)-N(1)-N(10)	-84.3(5)
K(1)-La(1)-N(1)-N(10)	118.1(4)
N(9)-La(1)-N(1)-C(63)	-159(3)
N(4)-La(1)-N(1)-C(63)	171(3)

N(6)-La(1)-N(1)-C(63)	2(3)
N(5)-La(1)-N(1)-C(63)	17(3)
N(7)-La(1)-N(1)-C(63)	-75(3)
N(3)-La(1)-N(1)-C(63)	117(3)
N(10)-La(1)-N(1)-C(63)	-154(3)
N(8)-La(1)-N(1)-C(63)	-75(3)
N(2)-La(1)-N(1)-C(63)	88(3)
K(2)-La(1)-N(1)-C(63)	121(3)
K(1)-La(1)-N(1)-C(63)	-36(3)
N(9)-La(1)-N(1)-K(2)	79.9(3)
N(4)-La(1)-N(1)-K(2)	49.8(4)
N(6)-La(1)-N(1)-K(2)	-119.6(3)
N(5)-La(1)-N(1)-K(2)	-104.7(3)
N(7)-La(1)-N(1)-K(2)	163.7(2)
N(3)-La(1)-N(1)-K(2)	-4.3(2)
N(10)-La(1)-N(1)-K(2)	84.3(5)
N(8)-La(1)-N(1)-K(2)	163.3(3)
N(2)-La(1)-N(1)-K(2)	-33.7(2)
K(1)-La(1)-N(1)-K(2)	-157.57(16)
N(3)-K(2)-N(1)-N(10)	80.2(4)
C(63)-K(2)-N(1)-N(10)	-114.4(7)
C(75')-K(2)-N(1)-N(10)	-69.8(6)
C(76')-K(2)-N(1)-N(10)	-76.2(7)
N(2)-K(2)-N(1)-N(10)	107.2(4)
C(75)-K(2)-N(1)-N(10)	-60.9(6)
C(8)-K(2)-N(1)-N(10)	77.4(4)
C(74)-K(2)-N(1)-N(10)	-34.6(6)
C(76)-K(2)-N(1)-N(10)	-74.4(8)
C(74')-K(2)-N(1)-N(10)	-45.6(5)
N(3)-K(2)-N(1)-C(63)	-165.3(6)

C(75')-K(2)-N(1)-C(63)	44.6(7)
C(76')-K(2)-N(1)-C(63)	38.2(9)
N(2)-K(2)-N(1)-C(63)	-138.3(6)
C(75)-K(2)-N(1)-C(63)	53.5(7)
C(8)-K(2)-N(1)-C(63)	-168.1(6)
C(74)-K(2)-N(1)-C(63)	79.9(7)
C(76)-K(2)-N(1)-C(63)	40.0(9)
C(74')-K(2)-N(1)-C(63)	68.8(7)
N(10)-K(2)-N(1)-C(63)	114.4(7)
N(3)-K(2)-N(1)-La(1)	3.9(2)
C(63)-K(2)-N(1)-La(1)	169.3(7)
C(75')-K(2)-N(1)-La(1)	-146.1(4)
C(76')-K(2)-N(1)-La(1)	-152.5(6)
N(2)-K(2)-N(1)-La(1)	30.9(2)
C(75)-K(2)-N(1)-La(1)	-137.2(4)
C(8)-K(2)-N(1)-La(1)	1.2(3)
C(74)-K(2)-N(1)-La(1)	-110.9(4)
C(76)-K(2)-N(1)-La(1)	-150.7(6)
C(74')-K(2)-N(1)-La(1)	-121.9(4)
N(10)-K(2)-N(1)-La(1)	-76.3(4)
C(6)-C(7)-N(2)-N(3)	-179.7(8)
P(1)-C(7)-N(2)-N(3)	-0.7(9)
K(2)-C(7)-N(2)-N(3)	-69.6(6)
C(6)-C(7)-N(2)-La(1)	63(4)
P(1)-C(7)-N(2)-La(1)	-118(3)
K(2)-C(7)-N(2)-La(1)	174(3)
C(6)-C(7)-N(2)-K(2)	-110.2(7)
P(1)-C(7)-N(2)-K(2)	68.8(5)
N(9)-La(1)-N(2)-N(3)	-18.6(5)
N(1)-La(1)-N(2)-N(3)	96.8(5)

N(4)-La(1)-N(2)-N(3)	-41.2(5)
N(6)-La(1)-N(2)-N(3)	-171.4(5)
N(5)-La(1)-N(2)-N(3)	-142.4(5)
N(7)-La(1)-N(2)-N(3)	-128.0(6)
N(10)-La(1)-N(2)-N(3)	70.4(5)
N(8)-La(1)-N(2)-N(3)	145.9(7)
K(2)-La(1)-N(2)-N(3)	65.9(4)
K(1)-La(1)-N(2)-N(3)	-163.5(4)
N(9)-La(1)-N(2)-C(7)	102(3)
N(1)-La(1)-N(2)-C(7)	-143(3)
N(4)-La(1)-N(2)-C(7)	79(3)
N(6)-La(1)-N(2)-C(7)	-51(3)
N(5)-La(1)-N(2)-C(7)	-22(3)
N(7)-La(1)-N(2)-C(7)	-7(4)
N(3)-La(1)-N(2)-C(7)	121(3)
N(10)-La(1)-N(2)-C(7)	-169(3)
N(8)-La(1)-N(2)-C(7)	-94(3)
K(2)-La(1)-N(2)-C(7)	-174(3)
K(1)-La(1)-N(2)-C(7)	-43(3)
N(9)-La(1)-N(2)-K(2)	-84.5(3)
N(1)-La(1)-N(2)-K(2)	30.9(2)
N(4)-La(1)-N(2)-K(2)	-107.1(2)
N(6)-La(1)-N(2)-K(2)	122.6(2)
N(5)-La(1)-N(2)-K(2)	151.7(3)
N(7)-La(1)-N(2)-K(2)	166.1(5)
N(3)-La(1)-N(2)-K(2)	-65.9(4)
N(10)-La(1)-N(2)-K(2)	4.4(2)
N(8)-La(1)-N(2)-K(2)	80.0(7)
K(1)-La(1)-N(2)-K(2)	130.58(14)
N(1)-K(2)-N(2)-N(3)	-95.3(5)

C(63)-K(2)-N(2)-N(3)	-112.1(5)
C(75')-K(2)-N(2)-N(3)	68(2)
C(76')-K(2)-N(2)-N(3)	88.0(7)
C(75)-K(2)-N(2)-N(3)	35.5(18)
C(8)-K(2)-N(2)-N(3)	37.0(4)
C(74)-K(2)-N(2)-N(3)	-0.4(9)
C(76)-K(2)-N(2)-N(3)	86.5(9)
C(74')-K(2)-N(2)-N(3)	-11.6(9)
N(10)-K(2)-N(2)-N(3)	-70.6(5)
N(3)-K(2)-N(2)-C(7)	-114.4(7)
N(1)-K(2)-N(2)-C(7)	150.3(6)
C(63)-K(2)-N(2)-C(7)	133.5(5)
C(75')-K(2)-N(2)-C(7)	-47(2)
C(76')-K(2)-N(2)-C(7)	-26.4(8)
C(75)-K(2)-N(2)-C(7)	-78.9(17)
C(8)-K(2)-N(2)-C(7)	-77.4(6)
C(74)-K(2)-N(2)-C(7)	-114.8(8)
C(76)-K(2)-N(2)-C(7)	-27.9(9)
C(74')-K(2)-N(2)-C(7)	-126.0(8)
N(10)-K(2)-N(2)-C(7)	175.1(5)
N(3)-K(2)-N(2)-La(1)	66.8(4)
N(1)-K(2)-N(2)-La(1)	-28.5(2)
C(63)-K(2)-N(2)-La(1)	-45.3(3)
C(75')-K(2)-N(2)-La(1)	135(2)
C(76')-K(2)-N(2)-La(1)	154.8(5)
C(75)-K(2)-N(2)-La(1)	102.3(16)
C(8)-K(2)-N(2)-La(1)	103.8(3)
C(74)-K(2)-N(2)-La(1)	66.4(7)
C(76)-K(2)-N(2)-La(1)	153.3(7)
C(74')-K(2)-N(2)-La(1)	55.2(7)

N(10)-K(2)-N(2)-La(1)	-3.8(2)
C(7)-N(2)-N(3)-C(8)	0.7(10)
La(1)-N(2)-N(3)-C(8)	170.8(7)
K(2)-N(2)-N(3)-C(8)	-83.9(6)
C(7)-N(2)-N(3)-La(1)	-170.0(6)
K(2)-N(2)-N(3)-La(1)	105.36(19)
C(7)-N(2)-N(3)-K(2)	84.6(6)
La(1)-N(2)-N(3)-K(2)	-105.36(19)
C(9)-C(8)-N(3)-N(2)	-177.8(8)
P(1)-C(8)-N(3)-N(2)	-0.4(9)
K(2)-C(8)-N(3)-N(2)	82.9(6)
C(9)-C(8)-N(3)-La(1)	-37(3)
P(1)-C(8)-N(3)-La(1)	140.5(19)
K(2)-C(8)-N(3)-La(1)	-136(2)
C(9)-C(8)-N(3)-K(2)	99.3(8)
P(1)-C(8)-N(3)-K(2)	-83.3(5)
N(9)-La(1)-N(3)-N(2)	163.5(5)
N(1)-La(1)-N(3)-N(2)	-77.6(4)
N(4)-La(1)-N(3)-N(2)	136.9(5)
N(6)-La(1)-N(3)-N(2)	9.5(5)
N(5)-La(1)-N(3)-N(2)	38.0(5)
N(7)-La(1)-N(3)-N(2)	130.7(6)
N(10)-La(1)-N(3)-N(2)	-108.2(5)
N(8)-La(1)-N(3)-N(2)	-128.8(8)
K(2)-La(1)-N(3)-N(2)	-81.9(5)
K(1)-La(1)-N(3)-N(2)	30.4(7)
N(9)-La(1)-N(3)-C(8)	20(2)
N(1)-La(1)-N(3)-C(8)	139(2)
N(4)-La(1)-N(3)-C(8)	-7(2)
N(6)-La(1)-N(3)-C(8)	-134(2)

N(5)-La(1)-N(3)-C(8)	-105(2)
N(7)-La(1)-N(3)-C(8)	-13(3)
N(10)-La(1)-N(3)-C(8)	108(2)
N(8)-La(1)-N(3)-C(8)	88(2)
N(2)-La(1)-N(3)-C(8)	-144(2)
K(2)-La(1)-N(3)-C(8)	135(2)
K(1)-La(1)-N(3)-C(8)	-113(2)
N(9)-La(1)-N(3)-K(2)	-114.7(3)
N(1)-La(1)-N(3)-K(2)	4.3(2)
N(4)-La(1)-N(3)-K(2)	-141.3(3)
N(6)-La(1)-N(3)-K(2)	91.3(3)
N(5)-La(1)-N(3)-K(2)	119.9(2)
N(7)-La(1)-N(3)-K(2)	-147.4(5)
N(10)-La(1)-N(3)-K(2)	-26.3(2)
N(8)-La(1)-N(3)-K(2)	-47.0(9)
N(2)-La(1)-N(3)-K(2)	81.9(5)
K(1)-La(1)-N(3)-K(2)	112.3(3)
N(1)-K(2)-N(3)-N(2)	74.0(5)
C(63)-K(2)-N(3)-N(2)	67.7(5)
C(75')-K(2)-N(3)-N(2)	-163.9(8)
C(76')-K(2)-N(3)-N(2)	-124.0(6)
C(75)-K(2)-N(3)-N(2)	-167.3(7)
C(8)-K(2)-N(3)-N(2)	-112.4(7)
C(74)-K(2)-N(3)-N(2)	179.8(6)
C(76)-K(2)-N(3)-N(2)	-127.0(7)
C(74')-K(2)-N(3)-N(2)	173.5(5)
N(10)-K(2)-N(3)-N(2)	100.7(5)
N(1)-K(2)-N(3)-C(8)	-173.6(5)
C(63)-K(2)-N(3)-C(8)	-179.9(5)
C(75')-K(2)-N(3)-C(8)	-51.5(9)

C(76')-K(2)-N(3)-C(8)	-11.6(7)
N(2)-K(2)-N(3)-C(8)	112.4(7)
C(75)-K(2)-N(3)-C(8)	-54.9(8)
C(74)-K(2)-N(3)-C(8)	-67.9(6)
C(76)-K(2)-N(3)-C(8)	-14.6(7)
C(74')-K(2)-N(3)-C(8)	-74.1(6)
N(10)-K(2)-N(3)-C(8)	-146.9(5)
N(1)-K(2)-N(3)-La(1)	-3.9(2)
C(63)-K(2)-N(3)-La(1)	-10.2(3)
C(75')-K(2)-N(3)-La(1)	118.2(7)
C(76')-K(2)-N(3)-La(1)	158.1(4)
N(2)-K(2)-N(3)-La(1)	-77.9(5)
C(75)-K(2)-N(3)-La(1)	114.8(6)
C(8)-K(2)-N(3)-La(1)	169.7(6)
C(74)-K(2)-N(3)-La(1)	101.8(5)
C(76)-K(2)-N(3)-La(1)	155.1(5)
C(74')-K(2)-N(3)-La(1)	95.6(4)
N(10)-K(2)-N(3)-La(1)	22.8(2)
C(20)-C(21)-N(4)-N(9)	-176.6(8)
P(2)-C(21)-N(4)-N(9)	0.2(10)
C(20)-C(21)-N(4)-La(1)	-1(6)
P(2)-C(21)-N(4)-La(1)	176(5)
N(1)-La(1)-N(4)-N(9)	60.8(5)
N(6)-La(1)-N(4)-N(9)	-133.1(5)
N(5)-La(1)-N(4)-N(9)	-142.3(5)
N(7)-La(1)-N(4)-N(9)	-64.9(5)
N(3)-La(1)-N(4)-N(9)	117.5(5)
N(10)-La(1)-N(4)-N(9)	43.0(5)
N(8)-La(1)-N(4)-N(9)	-45.7(5)
N(2)-La(1)-N(4)-N(9)	137.1(5)

K(2)-La(1)-N(4)-N(9)	92.3(4)
K(1)-La(1)-N(4)-N(9)	-90.6(4)
N(9)-La(1)-N(4)-C(21)	-176(6)
N(1)-La(1)-N(4)-C(21)	-115(6)
N(6)-La(1)-N(4)-C(21)	51(6)
N(5)-La(1)-N(4)-C(21)	42(6)
N(7)-La(1)-N(4)-C(21)	120(6)
N(3)-La(1)-N(4)-C(21)	-58(6)
N(10)-La(1)-N(4)-C(21)	-133(6)
N(8)-La(1)-N(4)-C(21)	139(6)
N(2)-La(1)-N(4)-C(21)	-38(6)
K(2)-La(1)-N(4)-C(21)	-83(6)
K(1)-La(1)-N(4)-C(21)	94(6)
C(48)-C(49)-N(5)-N(6)	177.4(8)
P(4)-C(49)-N(5)-N(6)	0.7(11)
C(48)-C(49)-N(5)-La(1)	20(4)
P(4)-C(49)-N(5)-La(1)	-156(3)
N(9)-La(1)-N(5)-N(6)	143.6(5)
N(1)-La(1)-N(5)-N(6)	-31.5(6)
N(4)-La(1)-N(5)-N(6)	165.7(5)
N(7)-La(1)-N(5)-N(6)	84.6(5)
N(3)-La(1)-N(5)-N(6)	-118.7(5)
N(10)-La(1)-N(5)-N(6)	-23.3(8)
N(8)-La(1)-N(5)-N(6)	57.7(5)
N(2)-La(1)-N(5)-N(6)	-100.8(5)
K(2)-La(1)-N(5)-N(6)	-78.2(5)
K(1)-La(1)-N(5)-N(6)	56.8(5)
N(9)-La(1)-N(5)-C(49)	-58(4)
N(1)-La(1)-N(5)-C(49)	127(3)
N(4)-La(1)-N(5)-C(49)	-36(4)

N(6)-La(1)-N(5)-C(49)	159(4)
N(7)-La(1)-N(5)-C(49)	-117(4)
N(3)-La(1)-N(5)-C(49)	40(4)
N(10)-La(1)-N(5)-C(49)	135(3)
N(8)-La(1)-N(5)-C(49)	-144(4)
N(2)-La(1)-N(5)-C(49)	58(4)
K(2)-La(1)-N(5)-C(49)	80(4)
K(1)-La(1)-N(5)-C(49)	-145(4)
C(49)-N(5)-N(6)-C(50)	-1.0(12)
La(1)-N(5)-N(6)-C(50)	174.7(8)
C(49)-N(5)-N(6)-La(1)	-175.7(8)
C(49)-N(5)-N(6)-K(1)	78.3(8)
La(1)-N(5)-N(6)-K(1)	-106.1(3)
C(51)-C(50)-N(6)-N(5)	179.0(8)
P(4)-C(50)-N(6)-N(5)	0.8(10)
K(1)-C(50)-N(6)-N(5)	93.6(7)
C(51)-C(50)-N(6)-La(1)	-31(4)
P(4)-C(50)-N(6)-La(1)	151(3)
K(1)-C(50)-N(6)-La(1)	-116(4)
C(51)-C(50)-N(6)-K(1)	85.4(8)
P(4)-C(50)-N(6)-K(1)	-92.8(5)
N(9)-La(1)-N(6)-N(5)	-58.8(7)
N(1)-La(1)-N(6)-N(5)	152.2(5)
N(4)-La(1)-N(6)-N(5)	-18.5(6)
N(7)-La(1)-N(6)-N(5)	-89.3(5)
N(3)-La(1)-N(6)-N(5)	70.9(5)
N(10)-La(1)-N(6)-N(5)	165.6(5)
N(8)-La(1)-N(6)-N(5)	-120.0(5)
N(2)-La(1)-N(6)-N(5)	75.5(5)
K(2)-La(1)-N(6)-N(5)	114.9(5)

K(1)-La(1)-N(6)-N(5)	-94.5(5)
N(9)-La(1)-N(6)-C(50)	149(4)
N(1)-La(1)-N(6)-C(50)	0(4)
N(4)-La(1)-N(6)-C(50)	-171(4)
N(5)-La(1)-N(6)-C(50)	-152(4)
N(7)-La(1)-N(6)-C(50)	119(4)
N(3)-La(1)-N(6)-C(50)	-81(4)
N(10)-La(1)-N(6)-C(50)	14(4)
N(8)-La(1)-N(6)-C(50)	88(4)
N(2)-La(1)-N(6)-C(50)	-77(4)
K(2)-La(1)-N(6)-C(50)	-37(4)
K(1)-La(1)-N(6)-C(50)	113(4)
N(9)-La(1)-N(6)-K(1)	35.7(6)
N(1)-La(1)-N(6)-K(1)	-113.3(3)
N(4)-La(1)-N(6)-K(1)	76.0(4)
N(5)-La(1)-N(6)-K(1)	94.5(5)
N(7)-La(1)-N(6)-K(1)	5.2(3)
N(3)-La(1)-N(6)-K(1)	165.4(2)
N(10)-La(1)-N(6)-K(1)	-99.9(3)
N(8)-La(1)-N(6)-K(1)	-25.5(3)
N(2)-La(1)-N(6)-K(1)	170.0(3)
K(2)-La(1)-N(6)-K(1)	-150.62(18)
N(7)-K(1)-N(6)-N(5)	72.3(5)
C(50)-K(1)-N(6)-N(5)	-112.7(8)
N(8)-K(1)-N(6)-N(5)	100.2(5)
C(35)-K(1)-N(6)-N(5)	66.9(5)
C(16)#3-K(1)-N(6)-N(5)	162.8(6)
C(13)#3-K(1)-N(6)-N(5)	-14.4(6)
C(17)#3-K(1)-N(6)-N(5)	166.7(6)
C(18)#3-K(1)-N(6)-N(5)	-171.3(6)

C(15)#3-K(1)-N(6)-N(5)	-154.9(6)
C(51)-K(1)-N(6)-N(5)	-144.1(6)
C(20)#3-K(1)-N(6)-N(5)	-133.7(5)
N(7)-K(1)-N(6)-C(50)	-175.0(7)
N(8)-K(1)-N(6)-C(50)	-147.2(7)
C(35)-K(1)-N(6)-C(50)	179.6(6)
C(16)#3-K(1)-N(6)-C(50)	-84.5(8)
C(13)#3-K(1)-N(6)-C(50)	98.3(6)
C(17)#3-K(1)-N(6)-C(50)	-80.6(7)
C(18)#3-K(1)-N(6)-C(50)	-58.6(7)
C(15)#3-K(1)-N(6)-C(50)	-42.2(9)
C(51)-K(1)-N(6)-C(50)	-31.4(6)
C(20)#3-K(1)-N(6)-C(50)	-21.0(7)
N(7)-K(1)-N(6)-La(1)	-4.9(2)
C(50)-K(1)-N(6)-La(1)	170.2(7)
N(8)-K(1)-N(6)-La(1)	23.0(2)
C(35)-K(1)-N(6)-La(1)	-10.3(3)
C(16)#3-K(1)-N(6)-La(1)	85.6(5)
C(13)#3-K(1)-N(6)-La(1)	-91.6(3)
C(17)#3-K(1)-N(6)-La(1)	89.5(4)
C(18)#3-K(1)-N(6)-La(1)	111.6(4)
C(15)#3-K(1)-N(6)-La(1)	128.0(6)
C(51)-K(1)-N(6)-La(1)	138.7(4)
C(20)#3-K(1)-N(6)-La(1)	149.1(3)
C(34)-C(35)-N(7)-N(8)	-174.7(5)
P(3)-C(35)-N(7)-N(8)	0.7(9)
K(1)-C(35)-N(7)-N(8)	82.9(6)
C(34)-C(35)-N(7)-La(1)	-53(2)
P(3)-C(35)-N(7)-La(1)	122.3(17)
K(1)-C(35)-N(7)-La(1)	-155(2)

C(34)-C(35)-N(7)-K(1)	102.4(4)
P(3)-C(35)-N(7)-K(1)	-82.2(5)
N(9)-La(1)-N(7)-N(8)	112.4(5)
N(1)-La(1)-N(7)-N(8)	-0.8(5)
N(4)-La(1)-N(7)-N(8)	141.1(5)
N(6)-La(1)-N(7)-N(8)	-85.3(5)
N(5)-La(1)-N(7)-N(8)	-115.4(5)
N(3)-La(1)-N(7)-N(8)	147.0(6)
N(10)-La(1)-N(7)-N(8)	30.7(5)
N(2)-La(1)-N(7)-N(8)	-129.8(6)
K(2)-La(1)-N(7)-N(8)	25.8(7)
K(1)-La(1)-N(7)-N(8)	-79.8(5)
N(9)-La(1)-N(7)-C(35)	-14.1(19)
N(1)-La(1)-N(7)-C(35)	-127.3(19)
N(4)-La(1)-N(7)-C(35)	14.6(19)
N(6)-La(1)-N(7)-C(35)	148.3(19)
N(5)-La(1)-N(7)-C(35)	118.1(19)
N(3)-La(1)-N(7)-C(35)	21(2)
N(10)-La(1)-N(7)-C(35)	-95.7(19)
N(8)-La(1)-N(7)-C(35)	-126(2)
N(2)-La(1)-N(7)-C(35)	103.7(19)
K(2)-La(1)-N(7)-C(35)	-100.7(19)
K(1)-La(1)-N(7)-C(35)	154(2)
N(9)-La(1)-N(7)-K(1)	-167.9(3)
N(1)-La(1)-N(7)-K(1)	78.9(3)
N(4)-La(1)-N(7)-K(1)	-139.1(3)
N(6)-La(1)-N(7)-K(1)	-5.5(3)
N(5)-La(1)-N(7)-K(1)	-35.7(3)
N(3)-La(1)-N(7)-K(1)	-133.2(5)
N(10)-La(1)-N(7)-K(1)	110.5(3)

N(8)-La(1)-N(7)-K(1)	79.8(5)
N(2)-La(1)-N(7)-K(1)	-50.1(7)
K(2)-La(1)-N(7)-K(1)	105.5(4)
C(50)-K(1)-N(7)-N(8)	76.8(5)
N(6)-K(1)-N(7)-N(8)	78.9(5)
C(35)-K(1)-N(7)-N(8)	-113.8(7)
C(16)#3-K(1)-N(7)-N(8)	-63.0(5)
C(13)#3-K(1)-N(7)-N(8)	-177.8(5)
C(17)#3-K(1)-N(7)-N(8)	-37.1(6)
C(18)#3-K(1)-N(7)-N(8)	-18.0(6)
C(15)#3-K(1)-N(7)-N(8)	-77.6(5)
C(51)-K(1)-N(7)-N(8)	54.8(5)
C(20)#3-K(1)-N(7)-N(8)	-60.4(7)
C(50)-K(1)-N(7)-C(35)	-169.4(5)
N(6)-K(1)-N(7)-C(35)	-167.3(5)
N(8)-K(1)-N(7)-C(35)	113.8(7)
C(16)#3-K(1)-N(7)-C(35)	50.8(5)
C(13)#3-K(1)-N(7)-C(35)	-64.1(5)
C(17)#3-K(1)-N(7)-C(35)	76.6(5)
C(18)#3-K(1)-N(7)-C(35)	95.7(5)
C(15)#3-K(1)-N(7)-C(35)	36.2(6)
C(51)-K(1)-N(7)-C(35)	168.5(4)
C(20)#3-K(1)-N(7)-C(35)	53.4(7)
C(50)-K(1)-N(7)-La(1)	2.9(3)
N(6)-K(1)-N(7)-La(1)	5.0(2)
N(8)-K(1)-N(7)-La(1)	-74.0(4)
C(35)-K(1)-N(7)-La(1)	172.3(6)
C(16)#3-K(1)-N(7)-La(1)	-136.9(3)
C(13)#3-K(1)-N(7)-La(1)	108.2(3)
C(17)#3-K(1)-N(7)-La(1)	-111.1(4)

C(18)#3-K(1)-N(7)-La(1)	-92.0(4)
C(15)#3-K(1)-N(7)-La(1)	-151.6(3)
C(51)-K(1)-N(7)-La(1)	-19.2(3)
C(20)#3-K(1)-N(7)-La(1)	-134.4(4)
C(37)-C(36)-N(8)-N(7)	179.2(8)
P(3)-C(36)-N(8)-N(7)	-2.5(10)
K(1)-C(36)-N(8)-N(7)	-69.3(6)
C(37)-C(36)-N(8)-La(1)	72(3)
P(3)-C(36)-N(8)-La(1)	-110(2)
K(1)-C(36)-N(8)-La(1)	-177(3)
C(37)-C(36)-N(8)-K(1)	-111.5(8)
P(3)-C(36)-N(8)-K(1)	66.9(6)
C(35)-N(7)-N(8)-C(36)	1.1(11)
La(1)-N(7)-N(8)-C(36)	-163.5(7)
K(1)-N(7)-N(8)-C(36)	84.2(7)
C(35)-N(7)-N(8)-La(1)	164.6(6)
K(1)-N(7)-N(8)-La(1)	-112.3(2)
C(35)-N(7)-N(8)-K(1)	-83.1(6)
La(1)-N(7)-N(8)-K(1)	112.3(2)
N(9)-La(1)-N(8)-C(36)	51(3)
N(1)-La(1)-N(8)-C(36)	-68(3)
N(4)-La(1)-N(8)-C(36)	72(3)
N(6)-La(1)-N(8)-C(36)	-159(3)
N(5)-La(1)-N(8)-C(36)	176(3)
N(7)-La(1)-N(8)-C(36)	113(3)
N(3)-La(1)-N(8)-C(36)	-17(3)
N(10)-La(1)-N(8)-C(36)	-38(3)
N(2)-La(1)-N(8)-C(36)	-115(2)
K(2)-La(1)-N(8)-C(36)	-54(3)
K(1)-La(1)-N(8)-C(36)	177(3)

N(9)-La(1)-N(8)-N(7)	-62.0(5)
N(1)-La(1)-N(8)-N(7)	179.3(5)
N(4)-La(1)-N(8)-N(7)	-40.7(5)
N(6)-La(1)-N(8)-N(7)	87.9(5)
N(5)-La(1)-N(8)-N(7)	62.6(5)
N(3)-La(1)-N(8)-N(7)	-130.2(8)
N(10)-La(1)-N(8)-N(7)	-150.8(5)
N(2)-La(1)-N(8)-N(7)	131.8(6)
K(2)-La(1)-N(8)-N(7)	-167.0(4)
K(1)-La(1)-N(8)-N(7)	63.6(4)
N(9)-La(1)-N(8)-K(1)	-125.6(3)
N(1)-La(1)-N(8)-K(1)	115.6(3)
N(4)-La(1)-N(8)-K(1)	-104.4(3)
N(6)-La(1)-N(8)-K(1)	24.3(2)
N(5)-La(1)-N(8)-K(1)	-1.0(3)
N(7)-La(1)-N(8)-K(1)	-63.6(4)
N(3)-La(1)-N(8)-K(1)	166.2(7)
N(10)-La(1)-N(8)-K(1)	145.6(3)
N(2)-La(1)-N(8)-K(1)	68.2(7)
K(2)-La(1)-N(8)-K(1)	129.36(19)
N(7)-K(1)-N(8)-C(36)	-113.1(8)
C(50)-K(1)-N(8)-C(36)	145.5(6)
N(6)-K(1)-N(8)-C(36)	158.8(7)
C(35)-K(1)-N(8)-C(36)	-77.0(6)
C(16)#3-K(1)-N(8)-C(36)	9.9(7)
C(13)#3-K(1)-N(8)-C(36)	-110.7(6)
C(17)#3-K(1)-N(8)-C(36)	31.4(7)
C(18)#3-K(1)-N(8)-C(36)	51.4(7)
C(15)#3-K(1)-N(8)-C(36)	6.6(7)
C(51)-K(1)-N(8)-C(36)	120.8(6)

C(20)#3-K(1)-N(8)-C(36)	31.6(7)
C(50)-K(1)-N(8)-N(7)	-101.4(5)
N(6)-K(1)-N(8)-N(7)	-88.0(5)
C(35)-K(1)-N(8)-N(7)	36.1(4)
C(16)#3-K(1)-N(8)-N(7)	123.0(5)
C(13)#3-K(1)-N(8)-N(7)	2.4(5)
C(17)#3-K(1)-N(8)-N(7)	144.6(5)
C(18)#3-K(1)-N(8)-N(7)	164.5(5)
C(15)#3-K(1)-N(8)-N(7)	119.8(5)
C(51)-K(1)-N(8)-N(7)	-126.0(5)
C(20)#3-K(1)-N(8)-N(7)	144.8(5)
N(7)-K(1)-N(8)-La(1)	65.9(4)
C(50)-K(1)-N(8)-La(1)	-35.4(3)
N(6)-K(1)-N(8)-La(1)	-22.1(2)
C(35)-K(1)-N(8)-La(1)	102.0(4)
C(16)#3-K(1)-N(8)-La(1)	-171.1(3)
C(13)#3-K(1)-N(8)-La(1)	68.4(3)
C(17)#3-K(1)-N(8)-La(1)	-149.5(4)
C(18)#3-K(1)-N(8)-La(1)	-129.6(3)
C(15)#3-K(1)-N(8)-La(1)	-174.3(3)
C(51)-K(1)-N(8)-La(1)	-60.1(2)
C(20)#3-K(1)-N(8)-La(1)	-149.3(3)
C(21)-N(4)-N(9)-C(22)	-0.2(10)
La(1)-N(4)-N(9)-C(22)	-179.7(8)
C(21)-N(4)-N(9)-La(1)	179.5(7)
C(23)-C(22)-N(9)-N(4)	-178.5(8)
P(2)-C(22)-N(9)-N(4)	0.1(10)
C(23)-C(22)-N(9)-La(1)	3(4)
P(2)-C(22)-N(9)-La(1)	-178(3)
N(1)-La(1)-N(9)-N(4)	-138.3(4)

N(6)-La(1)-N(9)-N(4)	77.6(6)
N(5)-La(1)-N(9)-N(4)	46.7(5)
N(7)-La(1)-N(9)-N(4)	108.9(5)
N(3)-La(1)-N(9)-N(4)	-58.3(4)
N(10)-La(1)-N(9)-N(4)	-140.5(5)
N(8)-La(1)-N(9)-N(4)	136.6(5)
N(2)-La(1)-N(9)-N(4)	-49.3(5)
K(2)-La(1)-N(9)-N(4)	-96.3(4)
K(1)-La(1)-N(9)-N(4)	101.0(4)
N(1)-La(1)-N(9)-C(22)	40(4)
N(4)-La(1)-N(9)-C(22)	178(100)
N(6)-La(1)-N(9)-C(22)	-104(4)
N(5)-La(1)-N(9)-C(22)	-135(4)
N(7)-La(1)-N(9)-C(22)	-73(4)
N(3)-La(1)-N(9)-C(22)	120(4)
N(10)-La(1)-N(9)-C(22)	38(4)
N(8)-La(1)-N(9)-C(22)	-45(4)
N(2)-La(1)-N(9)-C(22)	129(4)
K(2)-La(1)-N(9)-C(22)	82(4)
K(1)-La(1)-N(9)-C(22)	-80(4)
C(65)-C(64)-N(10)-N(1)	178.5(9)
P(5)-C(64)-N(10)-N(1)	2.0(11)
K(2)-C(64)-N(10)-N(1)	-65.3(6)
C(65)-C(64)-N(10)-La(1)	42(6)
P(5)-C(64)-N(10)-La(1)	-135(5)
K(2)-C(64)-N(10)-La(1)	158(6)
C(65)-C(64)-N(10)-K(2)	-116.2(9)
P(5)-C(64)-N(10)-K(2)	67.2(7)
C(63)-N(1)-N(10)-C(64)	-0.7(12)
La(1)-N(1)-N(10)-C(64)	-174.8(8)

K(2)-N(1)-N(10)-C(64)	79.9(8)
C(63)-N(1)-N(10)-La(1)	174.1(8)
K(2)-N(1)-N(10)-La(1)	-105.3(2)
C(63)-N(1)-N(10)-K(2)	-80.5(7)
La(1)-N(1)-N(10)-K(2)	105.3(2)
N(9)-La(1)-N(10)-C(64)	-45(6)
N(1)-La(1)-N(10)-C(64)	139(6)
N(4)-La(1)-N(10)-C(64)	-65(6)
N(6)-La(1)-N(10)-C(64)	111(6)
N(5)-La(1)-N(10)-C(64)	124(6)
N(7)-La(1)-N(10)-C(64)	25(6)
N(3)-La(1)-N(10)-C(64)	-134(6)
N(8)-La(1)-N(10)-C(64)	40(6)
N(2)-La(1)-N(10)-C(64)	-162(6)
K(2)-La(1)-N(10)-C(64)	-158(6)
K(1)-La(1)-N(10)-C(64)	66(6)
N(9)-La(1)-N(10)-N(1)	176.1(5)
N(4)-La(1)-N(10)-N(1)	155.9(5)
N(6)-La(1)-N(10)-N(1)	-27.4(6)
N(5)-La(1)-N(10)-N(1)	-14.6(7)
N(7)-La(1)-N(10)-N(1)	-113.5(5)
N(3)-La(1)-N(10)-N(1)	87.1(5)
N(8)-La(1)-N(10)-N(1)	-98.6(5)
N(2)-La(1)-N(10)-N(1)	59.3(5)
K(2)-La(1)-N(10)-N(1)	63.6(4)
K(1)-La(1)-N(10)-N(1)	-73.1(5)
N(9)-La(1)-N(10)-K(2)	112.4(2)
N(1)-La(1)-N(10)-K(2)	-63.6(4)
N(4)-La(1)-N(10)-K(2)	92.3(2)
N(6)-La(1)-N(10)-K(2)	-91.1(3)

N(5)-La(1)-N(10)-K(2)	-78.3(5)
N(7)-La(1)-N(10)-K(2)	-177.18(19)
N(3)-La(1)-N(10)-K(2)	23.4(2)
N(8)-La(1)-N(10)-K(2)	-162.2(2)
N(2)-La(1)-N(10)-K(2)	-4.3(2)
K(1)-La(1)-N(10)-K(2)	-136.77(13)
N(3)-K(2)-N(10)-C(64)	155.2(6)
N(1)-K(2)-N(10)-C(64)	-115.0(8)
C(63)-K(2)-N(10)-C(64)	-78.9(7)
C(75')-K(2)-N(10)-C(64)	7.1(7)
C(76')-K(2)-N(10)-C(64)	18.2(8)
N(2)-K(2)-N(10)-C(64)	-178.9(6)
C(75)-K(2)-N(10)-C(64)	14.4(7)
C(8)-K(2)-N(10)-C(64)	141.5(6)
C(74)-K(2)-N(10)-C(64)	33.5(7)
C(76)-K(2)-N(10)-C(64)	17.6(9)
C(74'')-K(2)-N(10)-C(64)	22.8(7)
N(3)-K(2)-N(10)-N(1)	-89.8(4)
C(63)-K(2)-N(10)-N(1)	36.1(5)
C(75')-K(2)-N(10)-N(1)	122.1(5)
C(76')-K(2)-N(10)-N(1)	133.2(6)
N(2)-K(2)-N(10)-N(1)	-63.9(4)
C(75)-K(2)-N(10)-N(1)	129.4(5)
C(8)-K(2)-N(10)-N(1)	-103.5(4)
C(74)-K(2)-N(10)-N(1)	148.5(6)
C(76)-K(2)-N(10)-N(1)	132.6(6)
C(74'')-K(2)-N(10)-N(1)	137.8(5)
N(3)-K(2)-N(10)-La(1)	-22.0(2)
N(1)-K(2)-N(10)-La(1)	67.8(4)
C(63)-K(2)-N(10)-La(1)	103.9(4)

C(75')-K(2)-N(10)-La(1)	-170.1(3)
C(76')-K(2)-N(10)-La(1)	-159.1(5)
N(2)-K(2)-N(10)-La(1)	3.9(2)
C(75)-K(2)-N(10)-La(1)	-162.8(4)
C(8)-K(2)-N(10)-La(1)	-35.8(2)
C(74)-K(2)-N(10)-La(1)	-143.7(4)
C(76)-K(2)-N(10)-La(1)	-159.6(5)
C(74')-K(2)-N(10)-La(1)	-154.4(4)
N(2)-C(7)-P(1)-C(8)	0.4(7)
C(6)-C(7)-P(1)-C(8)	179.3(8)
K(2)-C(7)-P(1)-C(8)	57.7(3)
N(2)-C(7)-P(1)-K(2)	-57.3(6)
C(6)-C(7)-P(1)-K(2)	121.5(8)
N(3)-C(8)-P(1)-C(7)	0.0(7)
C(9)-C(8)-P(1)-C(7)	177.1(9)
K(2)-C(8)-P(1)-C(7)	-67.1(3)
N(3)-C(8)-P(1)-K(2)	67.1(6)
C(9)-C(8)-P(1)-K(2)	-115.9(9)
N(3)-K(2)-P(1)-C(7)	66.0(4)
N(1)-K(2)-P(1)-C(7)	35.1(4)
C(63)-K(2)-P(1)-C(7)	15.8(4)
C(75')-K(2)-P(1)-C(7)	-152.6(5)
C(76')-K(2)-P(1)-C(7)	-145.3(4)
N(2)-K(2)-P(1)-C(7)	29.4(4)
C(75)-K(2)-P(1)-C(7)	-161.7(5)
C(8)-K(2)-P(1)-C(7)	100.7(5)
C(74)-K(2)-P(1)-C(7)	168.4(5)
C(76)-K(2)-P(1)-C(7)	-146.4(5)
C(74')-K(2)-P(1)-C(7)	174.5(5)
N(10)-K(2)-P(1)-C(7)	61.3(4)

N(3)-K(2)-P(1)-C(8)	-34.7(4)
N(1)-K(2)-P(1)-C(8)	-65.6(4)
C(63)-K(2)-P(1)-C(8)	-84.9(4)
C(75')-K(2)-P(1)-C(8)	106.7(5)
C(76')-K(2)-P(1)-C(8)	113.9(4)
N(2)-K(2)-P(1)-C(8)	-71.3(4)
C(75)-K(2)-P(1)-C(8)	97.6(5)
C(74)-K(2)-P(1)-C(8)	67.7(5)
C(76)-K(2)-P(1)-C(8)	112.9(5)
C(74')-K(2)-P(1)-C(8)	73.8(5)
N(10)-K(2)-P(1)-C(8)	-39.4(4)
N(4)-C(21)-P(2)-C(22)	-0.1(7)
C(20)-C(21)-P(2)-C(22)	176.5(9)
N(9)-C(22)-P(2)-C(21)	0.0(8)
C(23)-C(22)-P(2)-C(21)	178.5(9)
N(7)-C(35)-P(3)-C(36)	-1.7(6)
C(34)-C(35)-P(3)-C(36)	173.1(5)
K(1)-C(35)-P(3)-C(36)	-69.6(3)
N(7)-C(35)-P(3)-K(1)	67.9(5)
C(34)-C(35)-P(3)-K(1)	-117.3(5)
N(8)-C(36)-P(3)-C(35)	2.4(7)
C(37)-C(36)-P(3)-C(35)	-179.3(9)
K(1)-C(36)-P(3)-C(35)	60.1(3)
N(8)-C(36)-P(3)-K(1)	-57.7(7)
C(37)-C(36)-P(3)-K(1)	120.6(9)
N(7)-K(1)-P(3)-C(35)	-33.8(3)
C(50)-K(1)-P(3)-C(35)	-68.4(4)
N(6)-K(1)-P(3)-C(35)	-56.7(3)
N(8)-K(1)-P(3)-C(35)	-69.8(4)
C(16)#3-K(1)-P(3)-C(35)	159.4(4)

C(13)#3-K(1)-P(3)-C(35)	49.8(3)
C(17)#3-K(1)-P(3)-C(35)	-174.2(4)
C(18)#3-K(1)-P(3)-C(35)	-167.3(4)
C(15)#3-K(1)-P(3)-C(35)	145.1(4)
C(51)-K(1)-P(3)-C(35)	-98.8(3)
C(20)#3-K(1)-P(3)-C(35)	154.0(3)
N(7)-K(1)-P(3)-C(36)	63.6(4)
C(50)-K(1)-P(3)-C(36)	29.1(4)
N(6)-K(1)-P(3)-C(36)	40.8(4)
N(8)-K(1)-P(3)-C(36)	27.7(4)
C(35)-K(1)-P(3)-C(36)	97.5(5)
C(16)#3-K(1)-P(3)-C(36)	-103.1(4)
C(13)#3-K(1)-P(3)-C(36)	147.3(4)
C(17)#3-K(1)-P(3)-C(36)	-76.8(4)
C(18)#3-K(1)-P(3)-C(36)	-69.8(4)
C(15)#3-K(1)-P(3)-C(36)	-117.4(4)
C(51)-K(1)-P(3)-C(36)	-1.3(4)
C(20)#3-K(1)-P(3)-C(36)	-108.6(4)
N(6)-C(50)-P(4)-C(49)	-0.4(7)
C(51)-C(50)-P(4)-C(49)	-178.5(8)
K(1)-C(50)-P(4)-C(49)	-80.6(4)
N(6)-C(50)-P(4)-K(1)	80.3(7)
C(51)-C(50)-P(4)-K(1)	-97.8(8)
N(5)-C(49)-P(4)-C(50)	-0.2(7)
C(48)-C(49)-P(4)-C(50)	-176.7(9)
N(5)-C(49)-P(4)-K(1)	-55.6(7)
C(48)-C(49)-P(4)-K(1)	127.8(9)
N(7)-K(1)-P(4)-C(50)	-65.3(4)
N(6)-K(1)-P(4)-C(50)	-34.8(4)
N(8)-K(1)-P(4)-C(50)	-40.2(4)

C(35)-K(1)-P(4)-C(50)	-82.0(4)
C(16)#3-K(1)-P(4)-C(50)	89.8(6)
C(13)#3-K(1)-P(4)-C(50)	-156.4(5)
C(17)#3-K(1)-P(4)-C(50)	57.8(5)
C(18)#3-K(1)-P(4)-C(50)	63.3(5)
C(15)#3-K(1)-P(4)-C(50)	114.0(5)
C(51)-K(1)-P(4)-C(50)	27.8(4)
C(20)#3-K(1)-P(4)-C(50)	106.0(4)
N(7)-K(1)-P(4)-C(49)	26.8(4)
C(50)-K(1)-P(4)-C(49)	92.1(5)
N(6)-K(1)-P(4)-C(49)	57.3(4)
N(8)-K(1)-P(4)-C(49)	51.9(4)
C(35)-K(1)-P(4)-C(49)	10.1(4)
C(16)#3-K(1)-P(4)-C(49)	-178.2(6)
C(13)#3-K(1)-P(4)-C(49)	-64.3(4)
C(17)#3-K(1)-P(4)-C(49)	149.9(5)
C(18)#3-K(1)-P(4)-C(49)	155.4(4)
C(15)#3-K(1)-P(4)-C(49)	-153.9(4)
C(51)-K(1)-P(4)-C(49)	119.9(4)
C(20)#3-K(1)-P(4)-C(49)	-161.9(4)
N(1)-C(63)-P(5)-C(64)	1.6(8)
C(62)-C(63)-P(5)-C(64)	-179.1(10)
K(2)-C(63)-P(5)-C(64)	-69.8(4)
N(1)-C(63)-P(5)-K(2)	71.5(7)
C(62)-C(63)-P(5)-K(2)	-109.2(9)
N(10)-C(64)-P(5)-C(63)	-2.0(8)
C(65)-C(64)-P(5)-C(63)	-178.2(10)
K(2)-C(64)-P(5)-C(63)	57.8(4)
N(10)-C(64)-P(5)-K(2)	-59.8(7)
C(65)-C(64)-P(5)-K(2)	124.0(10)

N(3)-K(2)-P(5)-C(63)	-58.8(4)
N(1)-K(2)-P(5)-C(63)	-34.5(4)
C(75')-K(2)-P(5)-C(63)	150.3(5)
C(76')-K(2)-P(5)-C(63)	145.1(5)
N(2)-K(2)-P(5)-C(63)	-31.9(4)
C(75)-K(2)-P(5)-C(63)	157.9(5)
C(8)-K(2)-P(5)-C(63)	-73.3(5)
C(74)-K(2)-P(5)-C(63)	-176.5(5)
C(76)-K(2)-P(5)-C(63)	146.1(5)
C(74')-K(2)-P(5)-C(63)	175.3(5)
N(10)-K(2)-P(5)-C(63)	-70.2(4)
N(3)-K(2)-P(5)-C(64)	39.7(4)
N(1)-K(2)-P(5)-C(64)	64.0(4)
C(63)-K(2)-P(5)-C(64)	98.5(5)
C(75')-K(2)-P(5)-C(64)	-111.2(5)
C(76')-K(2)-P(5)-C(64)	-116.4(5)
N(2)-K(2)-P(5)-C(64)	66.6(4)
C(75)-K(2)-P(5)-C(64)	-103.7(5)
C(8)-K(2)-P(5)-C(64)	25.2(5)
C(74)-K(2)-P(5)-C(64)	-78.0(5)
C(76)-K(2)-P(5)-C(64)	-115.4(5)
C(74')-K(2)-P(5)-C(64)	-86.2(5)
N(10)-K(2)-P(5)-C(64)	28.3(4)

Symmetry transformations used to generate equivalent atoms:

#1 $-x, y-1/2, -z+3/2$ #2 $-x+1/2, -y+1, z+1/2$

#3 $-x, y+1/2, -z+3/2$

4.9 Crystal structural analysis data for **11**

Table 1. Crystal data and structure refinement for 150429-1c.

Identification code	150429-1c
Empirical formula	C ₈₄ H ₆₆ K ₂ N ₁₀ P ₅ Sm
Formula weight	1598.87
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P 21 21 21
Unit cell dimensions	a = 17.4551(2) Å alpha = 90 deg. b = 21.7027(3) Å beta = 90 deg. c = 22.1513(3) Å gamma = 90 deg.
Volume	8391.42(19) Å ³
Z, Calculated density	4, 1.266 Mg/m ³
Absorption coefficient	0.942 mm ⁻¹
F(000)	3260
Crystal size	0.28 x 0.24 x 0.14 mm
Theta range for data collection	2.88 to 25.68 deg.
Limiting indices	-21 ≤ h ≤ 21, -26 ≤ k ≤ 26, -27 ≤ l ≤ 26
Reflections collected / unique	162085 / 15909 [R(int) = 0.0542]
Completeness to theta = 25.68	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.42094
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	15909 / 236 / 893
Goodness-of-fit on F ²	1.098
Final R indices [I > 2sigma(I)]	R1 = 0.0440, wR2 = 0.1253
R indices (all data)	R1 = 0.0601, wR2 = 0.1372
Absolute structure parameter	-0.025(11)
Largest diff. peak and hole	0.692 and -0.471 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 150429-1c.

$U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
C(1)	7524(5)	3393(3)	5533(3)	65(2)
C(2)	7865(6)	3158(4)	6038(4)	82(3)
C(3)	8643(6)	3240(5)	6121(4)	89(3)
C(4)	9073(5)	3549(4)	5707(4)	81(2)
C(5)	8715(4)	3787(3)	5186(3)	63(2)
C(6)	7938(4)	3718(3)	5096(3)	52(2)
C(7)	7567(4)	3977(3)	4561(3)	52(2)
C(8)	6835(4)	4432(4)	3755(3)	60(2)
C(9)	6291(3)	4696(4)	3314(3)	100(2)
C(10)	5555(3)	4454(3)	3277(3)	119(2)
C(11)	5035(3)	4695(4)	2865(4)	131(2)
C(12)	5251(4)	5178(4)	2489(3)	127(2)
C(13)	5987(4)	5419(3)	2526(3)	117(2)
C(14)	6507(3)	5178(3)	2938(3)	104(2)
C(15)	7009(5)	4968(4)	1189(4)	78(2)
C(16)	6298(5)	4761(4)	1031(4)	84(3)
C(17)	5999(6)	4238(5)	1304(5)	103(3)
C(18)	6418(5)	3938(4)	1740(5)	94(3)
C(19)	7127(4)	4141(4)	1888(3)	70(2)

C(20)	7439(4)	4669(3)	1624(3)	60(2)
C(21)	8221(4)	4863(3)	1782(3)	53(1)
C(22)	9501(4)	5239(3)	1931(3)	53(2)
C(23)	10259(2)	5531(2)	1967(2)	60(2)
C(24)	10616(3)	5725(3)	1439(2)	85(3)
C(25)	11330(3)	6008(3)	1465(3)	104(3)
C(26)	11687(3)	6097(3)	2020(3)	103(4)
C(27)	11330(3)	5902(3)	2547(2)	90(3)
C(28)	10616(3)	5620(3)	2521(2)	70(2)
C(29)	9971(6)	3691(4)	1518(4)	86(2)
C(30)	10520(7)	3831(5)	1080(4)	100(2)
C(31)	10546(7)	3481(5)	565(5)	102(2)
C(32)	10062(6)	2998(5)	482(4)	98(2)
C(33)	9526(6)	2846(5)	914(4)	86(2)
C(34)	9474(5)	3199(4)	1444(3)	74(2)
C(35)	8896(5)	3047(3)	1900(3)	59(2)
C(36)	7858(4)	2767(3)	2541(3)	59(2)
C(37)	7140(3)	2568(3)	2885(3)	93(2)
C(38)	6955(4)	2814(3)	3445(3)	106(2)
C(39)	6290(4)	2627(3)	3739(3)	118(2)
C(40)	5811(3)	2194(4)	3471(4)	122(2)
C(41)	5997(4)	1948(3)	2911(4)	123(2)
C(42)	6661(4)	2135(3)	2617(3)	111(2)
C(43)	8722(3)	2496(2)	4349(3)	84(3)
C(44)	8264(4)	2118(3)	4706(4)	106(3)
C(45)	8600(6)	1699(3)	5100(3)	138(6)
C(46)	9393(6)	1657(3)	5137(3)	144(6)
C(47)	9851(4)	2034(3)	4780(3)	115(4)
C(48)	9515(3)	2454(2)	4386(2)	75(2)
C(49)	10008(5)	2855(3)	4024(3)	62(2)

C(50)	10935(4)	3471(4)	3468(3)	63(2)
C(51)	11571(5)	3797(5)	3189(5)	95(2)
C(52)	11469(5)	4131(6)	2663(5)	102(2)
C(53)	12080(6)	4453(6)	2401(6)	116(2)
C(54)	12760(7)	4460(7)	2667(6)	129(2)
C(55)	12901(7)	4088(7)	3148(6)	134(2)
C(56)	12289(6)	3719(7)	3424(5)	120(2)
C(57)	10674(4)	4284(4)	4858(3)	66(2)
C(58)	11140(5)	3998(4)	5294(4)	89(3)
C(59)	11353(5)	4316(5)	5797(4)	93(3)
C(60)	11139(6)	4914(5)	5858(4)	93(3)
C(61)	10691(5)	5204(4)	5430(3)	73(2)
C(62)	10450(4)	4891(3)	4919(3)	54(2)
C(63)	9968(3)	5206(3)	4459(3)	47(1)
C(64)	9282(3)	5831(3)	3751(3)	46(1)
C(65)	8916(4)	6280(3)	3342(3)	50(1)
C(66)	8375(5)	6099(3)	2922(3)	64(2)
C(67)	8031(6)	6527(4)	2536(4)	85(3)
C(68)	8202(6)	7150(4)	2591(4)	85(3)
C(69)	8743(6)	7334(4)	3008(5)	94(3)
C(70)	9088(5)	6910(3)	3385(3)	74(2)
C(71)	7117(5)	6387(4)	5359(3)	108(4)
C(72)	6537(5)	6019(3)	5125(6)	131(5)
C(73)	6384(5)	6026(5)	4509(6)	174(8)
C(74)	6810(8)	6401(6)	4128(3)	205(12)
C(75)	7390(7)	6770(4)	4362(4)	148(7)
C(76)	7543(5)	6763(3)	4978(5)	127(5)
C(77)	8189(10)	7142(7)	5231(12)	233(11)
C(78)	1819(12)	4084(7)	8973(7)	175(7)
C(79)	2386(11)	4382(9)	9303(9)	175(7)

C(80)	2190(14)	4841(8)	9712(7)	175(7)
C(81)	1426(15)	5002(7)	9792(7)	176(7)
C(82)	858(12)	4704(8)	9462(8)	177(6)
C(83)	1055(11)	4245(7)	9053(6)	175(6)
C(84)	445(14)	3927(11)	8702(9)	177(6)
C(85)	3360(11)	3178(7)	1775(9)	178(7)
C(86)	3994(13)	2947(8)	2080(9)	182(7)
C(87)	4640(11)	2766(7)	1759(12)	181(7)
C(88)	4653(10)	2815(7)	1134(12)	178(7)
C(89)	4019(12)	3046(7)	829(9)	175(7)
C(90)	3373(10)	3227(7)	1149(9)	177(7)
C(91)	2711(13)	3505(10)	828(13)	182(7)
K(1)	8018(1)	5349(1)	4652(1)	82(1)
K(2)	9686(1)	2149(1)	2853(1)	90(1)
N(1)	7576(3)	4365(2)	3617(2)	51(1)
N(2)	7978(2)	4110(2)	4071(2)	45(1)
N(3)	9542(3)	4876(2)	4077(2)	46(1)
N(4)	9146(3)	5225(2)	3678(2)	44(1)
N(5)	9695(3)	3327(2)	3712(2)	49(1)
N(6)	10213(3)	3659(3)	3392(2)	56(1)
N(7)	8308(3)	3191(2)	2796(2)	53(1)
N(8)	8914(3)	3341(2)	2439(2)	49(1)
N(9)	9276(3)	4860(2)	2369(2)	45(1)
N(10)	8547(3)	4660(2)	2284(2)	48(1)
P(1)	6594(1)	4172(1)	4483(1)	69(1)
P(2)	8819(1)	5366(1)	1364(1)	68(1)
P(3)	8130(1)	2534(1)	1825(1)	76(1)
P(4)	11010(2)	2816(1)	3944(1)	83(1)
P(5)	9913(1)	6004(1)	4341(1)	59(1)
Sm(1)	8930(1)	4168(1)	3239(1)	37(1)

Table 3. Bond lengths [Å] and angles [deg] for 150429-1c.

C(1)-C(2)	1.367(12)
C(1)-C(6)	1.398(9)
C(1)-H(1)	0.9300
C(2)-C(3)	1.381(13)
C(2)-H(2)	0.9300
C(3)-C(4)	1.363(12)
C(3)-H(3)	0.9300
C(4)-C(5)	1.412(11)
C(4)-H(4)	0.9300
C(5)-C(6)	1.378(10)
C(5)-H(5)	0.9300
C(6)-C(7)	1.464(9)
C(7)-N(2)	1.333(7)
C(7)-P(1)	1.758(7)
C(7)-K(1)	3.086(7)
C(8)-N(1)	1.337(8)
C(8)-C(9)	1.476(8)
C(8)-P(1)	1.759(7)
C(8)-K(1)	3.489(8)
C(9)-C(10)	1.3900
C(9)-C(14)	1.3900
C(10)-C(11)	1.3900
C(10)-H(10)	0.9300
C(11)-C(12)	1.3900
C(11)-H(11)	0.9300
C(12)-C(13)	1.3900

C(12)-H(12)	0.9300
C(13)-C(14)	1.3900
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(15)-C(16)	1.365(12)
C(15)-C(20)	1.383(10)
C(15)-K(1)#1	3.473(9)
C(15)-H(15)	0.9800
C(16)-C(17)	1.387(13)
C(16)-K(1)#1	3.288(10)
C(16)-H(16)	0.9800
C(17)-C(18)	1.374(13)
C(17)-H(17)	0.9300
C(18)-C(19)	1.355(11)
C(18)-H(18)	0.9300
C(19)-C(20)	1.395(11)
C(19)-H(19)	0.9300
C(20)-C(21)	1.471(10)
C(21)-N(10)	1.323(8)
C(21)-P(2)	1.772(7)
C(22)-N(9)	1.330(8)
C(22)-C(23)	1.470(8)
C(22)-P(2)	1.751(7)
C(23)-C(24)	1.3900
C(23)-C(28)	1.3900
C(23)-K(2)#2	3.534(5)
C(24)-C(25)	1.3900
C(24)-K(2)#2	3.503(6)
C(24)-H(24)	0.9300
C(25)-C(26)	1.3900

C(25)-K(2)#2	3.398(7)
C(25)-H(25)	0.9300
C(26)-C(27)	1.3900
C(26)-K(2)#2	3.322(7)
C(26)-H(26)	0.9300
C(27)-C(28)	1.3900
C(27)-K(2)#2	3.354(7)
C(27)-H(27)	0.9300
C(28)-K(2)#2	3.461(6)
C(28)-H(28)	0.9300
C(29)-C(34)	1.385(13)
C(29)-C(30)	1.397(13)
C(29)-H(29)	0.9300
C(30)-C(31)	1.370(14)
C(30)-H(30)	0.9300
C(31)-C(32)	1.359(15)
C(31)-H(31)	0.9300
C(32)-C(33)	1.378(13)
C(32)-H(32)	0.9300
C(33)-C(34)	1.405(11)
C(33)-H(33)	0.9300
C(34)-C(35)	1.464(11)
C(35)-N(8)	1.355(7)
C(35)-P(3)	1.748(8)
C(35)-K(2)	3.189(6)
C(36)-N(7)	1.335(8)
C(36)-C(37)	1.529(9)
C(36)-P(3)	1.730(8)
C(36)-K(2)	3.531(8)
C(37)-C(38)	1.3900

C(37)-C(42)	1.3900
C(38)-C(39)	1.3900
C(38)-H(38)	0.9300
C(39)-C(40)	1.3900
C(39)-H(39)	0.9300
C(40)-C(41)	1.3900
C(40)-H(40)	0.9300
C(41)-C(42)	1.3900
C(41)-H(41)	0.9300
C(42)-H(42)	0.9300
C(43)-C(44)	1.3900
C(43)-C(48)	1.3900
C(43)-H(43)	0.9300
C(44)-C(45)	1.3900
C(44)-H(44)	0.9300
C(45)-C(46)	1.3900
C(45)-H(45)	0.9300
C(46)-C(47)	1.3900
C(46)-H(46)	0.9300
C(47)-C(48)	1.3900
C(47)-H(47)	0.9300
C(48)-C(49)	1.463(9)
C(48)-K(2)	3.473(6)
C(49)-N(5)	1.353(8)
C(49)-P(4)	1.760(8)
C(49)-K(2)	3.065(7)
C(50)-N(6)	1.335(8)
C(50)-C(51)	1.454(12)
C(50)-P(4)	1.776(8)
C(51)-C(56)	1.368(14)

C(51)-C(52)	1.384(15)
C(52)-C(53)	1.401(15)
C(52)-H(52)	0.9300
C(53)-C(54)	1.325(16)
C(53)-H(53)	0.9300
C(54)-C(55)	1.360(17)
C(54)-H(54)	0.9300
C(55)-C(56)	1.469(16)
C(55)-H(55)	0.9300
C(56)-H(56)	0.9300
C(57)-C(62)	1.379(10)
C(57)-C(58)	1.408(11)
C(57)-H(57)	0.9300
C(58)-C(59)	1.363(13)
C(58)-H(58)	0.9300
C(59)-C(60)	1.358(14)
C(59)-H(59)	0.9300
C(60)-C(61)	1.379(12)
C(60)-H(60)	0.9300
C(61)-C(62)	1.386(10)
C(61)-H(61)	0.9300
C(62)-C(63)	1.489(9)
C(63)-N(3)	1.335(8)
C(63)-P(5)	1.754(7)
C(63)-K(1)	3.446(6)
C(64)-N(4)	1.345(8)
C(64)-C(65)	1.476(9)
C(64)-P(5)	1.750(6)
C(64)-K(1)	3.155(6)
C(65)-C(66)	1.382(9)

C(65)-C(70)	1.404(9)
C(66)-C(67)	1.398(11)
C(66)-H(66)	0.9300
C(67)-C(68)	1.392(12)
C(67)-H(67)	0.9300
C(68)-C(69)	1.379(13)
C(68)-H(68)	0.9300
C(69)-C(70)	1.381(11)
C(69)-K(2)#2	3.364(10)
C(69)-H(69)	0.9800
C(70)-K(2)#2	3.517(9)
C(70)-H(70)	0.9800
C(71)-C(72)	1.3900
C(71)-C(76)	1.3900
C(71)-K(1)	3.163(7)
C(71)-H(71)	0.9800
C(72)-C(73)	1.3900
C(72)-K(1)	3.144(7)
C(72)-H(72)	0.9800
C(73)-C(74)	1.3900
C(73)-K(1)	3.223(8)
C(73)-H(73)	0.9800
C(74)-C(75)	1.3900
C(74)-K(1)	3.318(8)
C(74)-H(74)	0.9800
C(75)-C(76)	1.3900
C(75)-K(1)	3.336(8)
C(75)-H(75)	0.9800
C(76)-C(77)	1.504(17)
C(76)-K(1)	3.260(7)

C(77)-H(77A)	0.9600
C(77)-H(77B)	0.9600
C(77)-H(77C)	0.9600
C(78)-C(79)	1.3900
C(78)-C(83)	1.3900
C(78)-H(78)	0.9300
C(79)-C(80)	1.3900
C(79)-H(79)	0.9300
C(80)-C(81)	1.3900
C(80)-H(80)	0.9300
C(81)-C(82)	1.3900
C(81)-H(81)	0.9300
C(82)-C(83)	1.3900
C(82)-H(82)	0.9300
C(83)-C(84)	1.489(10)
C(84)-H(84A)	0.9600
C(84)-H(84B)	0.9600
C(84)-H(84C)	0.9600
C(85)-C(86)	1.3900
C(85)-C(90)	1.3900
C(85)-H(85)	0.9300
C(86)-C(87)	1.3900
C(86)-H(86)	0.9300
C(87)-C(88)	1.3900
C(87)-H(87)	0.9300
C(88)-C(89)	1.3900
C(88)-H(88)	0.9300
C(89)-C(90)	1.3900
C(89)-H(89)	0.9300
C(90)-C(91)	1.484(10)

C(91)-H(91A)	0.9600
C(91)-H(91B)	0.9600
C(91)-H(91C)	0.9600
K(1)-N(4)	2.935(5)
K(1)-N(2)	2.982(5)
K(1)-N(3)	3.123(5)
K(1)-N(1)	3.227(5)
K(1)-C(16)#3	3.288(10)
K(2)-N(8)	3.058(5)
K(2)-N(5)	3.187(6)
K(2)-N(7)	3.304(6)
K(2)-C(26)#4	3.32(4)
K(2)-C(27)#4	3.35(3)
K(2)-C(69)#4	3.364(10)
K(2)-C(25)#4	3.40(4)
K(2)-C(28)#4	3.461(17)
K(2)-C(24)#4	3.50(3)
N(1)-N(2)	1.347(7)
N(1)-Sm(1)	2.544(5)
N(2)-Sm(1)	2.484(4)
N(3)-N(4)	1.354(7)
N(3)-Sm(1)	2.636(5)
N(4)-Sm(1)	2.521(5)
N(5)-N(6)	1.356(8)
N(5)-Sm(1)	2.493(5)
N(6)-Sm(1)	2.522(5)
N(7)-N(8)	1.359(8)
N(7)-Sm(1)	2.576(5)
N(8)-Sm(1)	2.522(5)
N(9)-N(10)	1.359(7)

N(9)-Sm(1)	2.517(5)
N(10)-Sm(1)	2.462(5)
C(2)-C(1)-C(6)	122.0(8)
C(2)-C(1)-H(1)	119.0
C(6)-C(1)-H(1)	119.0
C(1)-C(2)-C(3)	119.3(8)
C(1)-C(2)-H(2)	120.3
C(3)-C(2)-H(2)	120.3
C(4)-C(3)-C(2)	121.0(8)
C(4)-C(3)-H(3)	119.5
C(2)-C(3)-H(3)	119.5
C(3)-C(4)-C(5)	119.1(8)
C(3)-C(4)-H(4)	120.5
C(5)-C(4)-H(4)	120.5
C(6)-C(5)-C(4)	121.0(7)
C(6)-C(5)-H(5)	119.5
C(4)-C(5)-H(5)	119.5
C(5)-C(6)-C(1)	117.6(7)
C(5)-C(6)-C(7)	120.7(6)
C(1)-C(6)-C(7)	121.7(6)
N(2)-C(7)-C(6)	120.3(5)
N(2)-C(7)-P(1)	112.8(5)
C(6)-C(7)-P(1)	126.9(4)
N(2)-C(7)-K(1)	73.0(3)
C(6)-C(7)-K(1)	101.8(4)
P(1)-C(7)-K(1)	91.1(3)
N(1)-C(8)-C(9)	120.9(6)
N(1)-C(8)-P(1)	113.9(5)
C(9)-C(8)-P(1)	125.2(5)

N(1)-C(8)-K(1)	67.7(4)
C(9)-C(8)-K(1)	122.4(5)
P(1)-C(8)-K(1)	78.5(2)
C(10)-C(9)-C(14)	120.0
C(10)-C(9)-C(8)	119.1(5)
C(14)-C(9)-C(8)	120.9(5)
C(11)-C(10)-C(9)	120.0
C(11)-C(10)-H(10)	120.0
C(9)-C(10)-H(10)	120.0
C(10)-C(11)-C(12)	120.0
C(10)-C(11)-H(11)	120.0
C(12)-C(11)-H(11)	120.0
C(13)-C(12)-C(11)	120.0
C(13)-C(12)-H(12)	120.0
C(11)-C(12)-H(12)	120.0
C(14)-C(13)-C(12)	120.0
C(14)-C(13)-H(13)	120.0
C(12)-C(13)-H(13)	120.0
C(13)-C(14)-C(9)	120.0
C(13)-C(14)-H(14)	120.0
C(9)-C(14)-H(14)	120.0
C(16)-C(15)-C(20)	121.2(8)
C(16)-C(15)-K(1)#1	70.8(5)
C(20)-C(15)-K(1)#1	126.7(6)
C(16)-C(15)-H(15)	110.8
C(20)-C(15)-H(15)	110.8
K(1)#1-C(15)-H(15)	110.8
C(15)-C(16)-C(17)	119.9(8)
C(15)-C(16)-K(1)#1	86.1(6)
C(17)-C(16)-K(1)#1	118.9(7)

C(15)-C(16)-H(16)	110.0
C(17)-C(16)-H(16)	110.0
K(1)#1-C(16)-H(16)	110.0
C(18)-C(17)-C(16)	119.6(9)
C(18)-C(17)-H(17)	120.2
C(16)-C(17)-H(17)	120.2
C(19)-C(18)-C(17)	120.1(9)
C(19)-C(18)-H(18)	120.0
C(17)-C(18)-H(18)	120.0
C(18)-C(19)-C(20)	121.5(7)
C(18)-C(19)-H(19)	119.3
C(20)-C(19)-H(19)	119.3
C(15)-C(20)-C(19)	117.7(7)
C(15)-C(20)-C(21)	122.3(7)
C(19)-C(20)-C(21)	119.8(6)
N(10)-C(21)-C(20)	120.2(6)
N(10)-C(21)-P(2)	113.0(5)
C(20)-C(21)-P(2)	126.8(5)
N(9)-C(22)-C(23)	119.5(6)
N(9)-C(22)-P(2)	114.8(5)
C(23)-C(22)-P(2)	125.6(4)
C(24)-C(23)-C(28)	120.0
C(24)-C(23)-C(22)	119.3(4)
C(28)-C(23)-C(22)	120.7(4)
C(24)-C(23)-K(2)#2	77.4(2)
C(28)-C(23)-K(2)#2	75.6(2)
C(22)-C(23)-K(2)#2	117.3(4)
C(23)-C(24)-C(25)	120.0
C(23)-C(24)-K(2)#2	79.8(2)
C(25)-C(24)-K(2)#2	74.2(2)

C(23)-C(24)-H(24)	120.0
C(25)-C(24)-H(24)	120.0
K(2)#2-C(24)-H(24)	116.7
C(24)-C(25)-C(26)	120.0
C(24)-C(25)-K(2)#2	82.7(2)
C(26)-C(25)-K(2)#2	75.0(2)
C(24)-C(25)-H(25)	120.0
C(26)-C(25)-H(25)	120.0
K(2)#2-C(25)-H(25)	112.7
C(27)-C(26)-C(25)	120.0
C(27)-C(26)-K(2)#2	79.3(2)
C(25)-C(26)-K(2)#2	81.2(2)
C(27)-C(26)-H(26)	120.0
C(25)-C(26)-H(26)	120.0
K(2)#2-C(26)-H(26)	109.9
C(26)-C(27)-C(28)	120.0
C(26)-C(27)-K(2)#2	76.7(2)
C(28)-C(27)-K(2)#2	82.6(2)
C(26)-C(27)-H(27)	120.0
C(28)-C(27)-H(27)	120.0
K(2)#2-C(27)-H(27)	111.1
C(27)-C(28)-C(23)	120.0
C(27)-C(28)-K(2)#2	74.0(2)
C(23)-C(28)-K(2)#2	81.5(2)
C(27)-C(28)-H(28)	120.0
C(23)-C(28)-H(28)	120.0
K(2)#2-C(28)-H(28)	115.1
C(34)-C(29)-C(30)	121.0(9)
C(34)-C(29)-H(29)	119.5
C(30)-C(29)-H(29)	119.5

C(31)-C(30)-C(29)	118.8(11)
C(31)-C(30)-H(30)	120.6
C(29)-C(30)-H(30)	120.6
C(32)-C(31)-C(30)	121.2(10)
C(32)-C(31)-H(31)	119.4
C(30)-C(31)-H(31)	119.4
C(31)-C(32)-C(33)	120.9(10)
C(31)-C(32)-H(32)	119.6
C(33)-C(32)-H(32)	119.6
C(32)-C(33)-C(34)	119.6(11)
C(32)-C(33)-H(33)	120.2
C(34)-C(33)-H(33)	120.2
C(29)-C(34)-C(33)	118.5(9)
C(29)-C(34)-C(35)	121.6(7)
C(33)-C(34)-C(35)	119.9(9)
N(8)-C(35)-C(34)	119.1(7)
N(8)-C(35)-P(3)	113.6(6)
C(34)-C(35)-P(3)	127.2(5)
N(8)-C(35)-K(2)	72.1(3)
C(34)-C(35)-K(2)	107.3(5)
P(3)-C(35)-K(2)	90.2(2)
N(7)-C(36)-C(37)	117.8(6)
N(7)-C(36)-P(3)	115.3(6)
C(37)-C(36)-P(3)	126.8(5)
N(7)-C(36)-K(2)	69.3(4)
C(37)-C(36)-K(2)	122.4(4)
P(3)-C(36)-K(2)	79.6(3)
C(38)-C(37)-C(42)	120.0
C(38)-C(37)-C(36)	121.8(5)
C(42)-C(37)-C(36)	118.2(5)

C(37)-C(38)-C(39)	120.0
C(37)-C(38)-H(38)	120.0
C(39)-C(38)-H(38)	120.0
C(40)-C(39)-C(38)	120.0
C(40)-C(39)-H(39)	120.0
C(38)-C(39)-H(39)	120.0
C(39)-C(40)-C(41)	120.0
C(39)-C(40)-H(40)	120.0
C(41)-C(40)-H(40)	120.0
C(42)-C(41)-C(40)	120.0
C(42)-C(41)-H(41)	120.0
C(40)-C(41)-H(41)	120.0
C(41)-C(42)-C(37)	120.0
C(41)-C(42)-H(42)	120.0
C(37)-C(42)-H(42)	120.0
C(44)-C(43)-C(48)	120.0
C(44)-C(43)-H(43)	120.0
C(48)-C(43)-H(43)	120.0
C(45)-C(44)-C(43)	120.0
C(45)-C(44)-H(44)	120.0
C(43)-C(44)-H(44)	120.0
C(46)-C(45)-C(44)	120.0
C(46)-C(45)-H(45)	120.0
C(44)-C(45)-H(45)	120.0
C(47)-C(46)-C(45)	120.0
C(47)-C(46)-H(46)	120.0
C(45)-C(46)-H(46)	120.0
C(46)-C(47)-C(48)	120.0
C(46)-C(47)-H(47)	120.0
C(48)-C(47)-H(47)	120.0

C(47)-C(48)-C(43)	120.0
C(47)-C(48)-C(49)	119.0(5)
C(43)-C(48)-C(49)	121.0(5)
C(47)-C(48)-K(2)	116.9(3)
C(43)-C(48)-K(2)	92.3(3)
C(49)-C(48)-K(2)	61.8(3)
N(5)-C(49)-C(48)	119.6(6)
N(5)-C(49)-P(4)	112.7(6)
C(48)-C(49)-P(4)	127.7(5)
N(5)-C(49)-K(2)	82.6(4)
C(48)-C(49)-K(2)	93.4(4)
P(4)-C(49)-K(2)	94.2(3)
N(6)-C(50)-C(51)	121.2(7)
N(6)-C(50)-P(4)	112.9(6)
C(51)-C(50)-P(4)	125.9(6)
C(56)-C(51)-C(52)	120.2(10)
C(56)-C(51)-C(50)	118.5(10)
C(52)-C(51)-C(50)	120.9(8)
C(51)-C(52)-C(53)	120.8(10)
C(51)-C(52)-H(52)	119.6
C(53)-C(52)-H(52)	119.6
C(54)-C(53)-C(52)	120.2(12)
C(54)-C(53)-H(53)	119.9
C(52)-C(53)-H(53)	119.9
C(53)-C(54)-C(55)	120.2(13)
C(53)-C(54)-H(54)	119.9
C(55)-C(54)-H(54)	119.9
C(54)-C(55)-C(56)	121.3(12)
C(54)-C(55)-H(55)	119.4
C(56)-C(55)-H(55)	119.4

C(51)-C(56)-C(55)	116.1(12)
C(51)-C(56)-H(56)	122.0
C(55)-C(56)-H(56)	122.0
C(62)-C(57)-C(58)	121.2(8)
C(62)-C(57)-H(57)	119.4
C(58)-C(57)-H(57)	119.4
C(59)-C(58)-C(57)	119.7(9)
C(59)-C(58)-H(58)	120.2
C(57)-C(58)-H(58)	120.2
C(60)-C(59)-C(58)	119.3(8)
C(60)-C(59)-H(59)	120.3
C(58)-C(59)-H(59)	120.3
C(59)-C(60)-C(61)	121.6(9)
C(59)-C(60)-H(60)	119.2
C(61)-C(60)-H(60)	119.2
C(60)-C(61)-C(62)	120.6(9)
C(60)-C(61)-H(61)	119.7
C(62)-C(61)-H(61)	119.7
C(57)-C(62)-C(61)	117.6(7)
C(57)-C(62)-C(63)	122.1(6)
C(61)-C(62)-C(63)	120.4(7)
N(3)-C(63)-C(62)	120.2(6)
N(3)-C(63)-P(5)	113.9(5)
C(62)-C(63)-P(5)	125.9(5)
N(3)-C(63)-K(1)	64.9(3)
C(62)-C(63)-K(1)	121.0(4)
P(5)-C(63)-K(1)	82.8(2)
N(4)-C(64)-C(65)	119.7(5)
N(4)-C(64)-P(5)	114.2(5)
C(65)-C(64)-P(5)	126.1(5)

N(4)-C(64)-K(1)	68.2(3)
C(65)-C(64)-K(1)	107.7(4)
P(5)-C(64)-K(1)	92.2(2)
C(66)-C(65)-C(70)	117.9(6)
C(66)-C(65)-C(64)	121.4(6)
C(70)-C(65)-C(64)	120.6(6)
C(65)-C(66)-C(67)	121.1(7)
C(65)-C(66)-H(66)	119.5
C(67)-C(66)-H(66)	119.5
C(68)-C(67)-C(66)	120.0(8)
C(68)-C(67)-H(67)	120.0
C(66)-C(67)-H(67)	120.0
C(69)-C(68)-C(67)	119.2(8)
C(69)-C(68)-H(68)	120.4
C(67)-C(68)-H(68)	120.4
C(68)-C(69)-C(70)	120.7(8)
C(68)-C(69)-K(2)#2	98.3(7)
C(70)-C(69)-K(2)#2	84.7(6)
C(68)-C(69)-H(69)	115.7
C(70)-C(69)-H(69)	115.7
K(2)#2-C(69)-H(69)	115.7
C(69)-C(70)-C(65)	121.0(8)
C(69)-C(70)-K(2)#2	72.3(5)
C(65)-C(70)-K(2)#2	102.7(5)
C(69)-C(70)-H(70)	116.9
C(65)-C(70)-H(70)	116.9
K(2)#2-C(70)-H(70)	116.9
C(72)-C(71)-C(76)	120.0
C(72)-C(71)-K(1)	76.5(3)
C(76)-C(71)-K(1)	81.4(3)

C(72)-C(71)-H(71)	119.7
C(76)-C(71)-H(71)	119.7
K(1)-C(71)-H(71)	119.7
C(71)-C(72)-C(73)	120.0
C(71)-C(72)-K(1)	78.0(3)
C(73)-C(72)-K(1)	80.6(3)
C(71)-C(72)-H(72)	119.7
C(73)-C(72)-H(72)	119.7
K(1)-C(72)-H(72)	119.7
C(74)-C(73)-C(72)	120.0
C(74)-C(73)-K(1)	81.6(3)
C(72)-C(73)-K(1)	74.3(3)
C(74)-C(73)-H(73)	119.9
C(72)-C(73)-H(73)	119.9
K(1)-C(73)-H(73)	119.9
C(73)-C(74)-C(75)	120.0
C(73)-C(74)-K(1)	73.9(2)
C(75)-C(74)-K(1)	78.7(3)
C(73)-C(74)-H(74)	120.0
C(75)-C(74)-H(74)	120.0
K(1)-C(74)-H(74)	120.0
C(76)-C(75)-C(74)	120.0
C(76)-C(75)-K(1)	74.8(2)
C(74)-C(75)-K(1)	77.2(3)
C(76)-C(75)-H(75)	120.0
C(74)-C(75)-H(75)	120.0
K(1)-C(75)-H(75)	120.0
C(75)-C(76)-C(71)	120.0
C(75)-C(76)-C(77)	120.3(13)
C(71)-C(76)-C(77)	119.7(13)

C(75)-C(76)-K(1)	80.9(3)
C(71)-C(76)-K(1)	73.6(2)
C(77)-C(76)-K(1)	114.0(8)
C(76)-C(77)-H(77A)	109.5
C(76)-C(77)-H(77B)	109.5
H(77A)-C(77)-H(77B)	109.5
C(76)-C(77)-H(77C)	109.5
H(77A)-C(77)-H(77C)	109.5
H(77B)-C(77)-H(77C)	109.5
C(79)-C(78)-C(83)	120.0
C(79)-C(78)-H(78)	120.0
C(83)-C(78)-H(78)	120.0
C(78)-C(79)-C(80)	120.0
C(78)-C(79)-H(79)	120.0
C(80)-C(79)-H(79)	120.0
C(81)-C(80)-C(79)	120.0
C(81)-C(80)-H(80)	120.0
C(79)-C(80)-H(80)	120.0
C(80)-C(81)-C(82)	120.0
C(80)-C(81)-H(81)	120.0
C(82)-C(81)-H(81)	120.0
C(83)-C(82)-C(81)	120.0
C(83)-C(82)-H(82)	120.0
C(81)-C(82)-H(82)	120.0
C(82)-C(83)-C(78)	120.0
C(82)-C(83)-C(84)	119.8(4)
C(78)-C(83)-C(84)	120.2(4)
C(83)-C(84)-H(84A)	109.5
C(83)-C(84)-H(84B)	109.5
H(84A)-C(84)-H(84B)	109.5

C(83)-C(84)-H(84C)	109.5
H(84A)-C(84)-H(84C)	109.5
H(84B)-C(84)-H(84C)	109.5
C(86)-C(85)-C(90)	120.0
C(86)-C(85)-H(85)	120.0
C(90)-C(85)-H(85)	120.0
C(85)-C(86)-C(87)	120.0
C(85)-C(86)-H(86)	120.0
C(87)-C(86)-H(86)	120.0
C(86)-C(87)-C(88)	120.0
C(86)-C(87)-H(87)	120.0
C(88)-C(87)-H(87)	120.0
C(89)-C(88)-C(87)	120.0
C(89)-C(88)-H(88)	120.0
C(87)-C(88)-H(88)	120.0
C(88)-C(89)-C(90)	120.0
C(88)-C(89)-H(89)	120.0
C(90)-C(89)-H(89)	120.0
C(89)-C(90)-C(85)	120.0
C(89)-C(90)-C(91)	120.2(4)
C(85)-C(90)-C(91)	119.8(4)
C(90)-C(91)-H(91A)	109.5
C(90)-C(91)-H(91B)	109.5
H(91A)-C(91)-H(91B)	109.5
C(90)-C(91)-H(91C)	109.5
H(91A)-C(91)-H(91C)	109.5
H(91B)-C(91)-H(91C)	109.5
N(4)-K(1)-N(2)	67.39(13)
N(4)-K(1)-C(7)	92.00(15)
N(2)-K(1)-C(7)	25.30(14)

N(4)-K(1)-N(3)	25.60(13)
N(2)-K(1)-N(3)	63.06(13)
C(7)-K(1)-N(3)	82.71(15)
N(4)-K(1)-C(72)	147.0(2)
N(2)-K(1)-C(72)	122.8(2)
C(7)-K(1)-C(72)	104.97(19)
N(3)-K(1)-C(72)	171.06(18)
N(4)-K(1)-C(64)	25.19(15)
N(2)-K(1)-C(64)	92.39(15)
C(7)-K(1)-C(64)	117.18(17)
N(3)-K(1)-C(64)	41.84(15)
C(72)-K(1)-C(64)	129.2(2)
N(4)-K(1)-C(71)	139.73(19)
N(2)-K(1)-C(71)	147.7(2)
C(7)-K(1)-C(71)	126.4(2)
N(3)-K(1)-C(71)	149.3(2)
C(72)-K(1)-C(71)	25.5
C(64)-K(1)-C(71)	115.2(2)
N(4)-K(1)-C(73)	124.3(3)
N(2)-K(1)-C(73)	110.38(18)
C(7)-K(1)-C(73)	102.0(2)
N(3)-K(1)-C(73)	149.7(3)
C(72)-K(1)-C(73)	25.18(6)
C(64)-K(1)-C(73)	113.9(3)
C(71)-K(1)-C(73)	44.28(7)
N(4)-K(1)-N(1)	65.00(13)
N(2)-K(1)-N(1)	24.65(13)
C(7)-K(1)-N(1)	41.77(15)
N(3)-K(1)-N(1)	72.32(14)
C(72)-K(1)-N(1)	110.3(3)

C(64)-K(1)-N(1)	86.37(15)
C(71)-K(1)-N(1)	134.8(2)
C(73)-K(1)-N(1)	91.16(19)
N(4)-K(1)-C(76)	114.80(19)
N(2)-K(1)-C(76)	159.8(2)
C(7)-K(1)-C(76)	149.09(19)
N(3)-K(1)-C(76)	128.06(17)
C(72)-K(1)-C(76)	44.12(7)
C(64)-K(1)-C(76)	90.3(2)
C(71)-K(1)-C(76)	24.9
C(73)-K(1)-C(76)	50.78(7)
N(1)-K(1)-C(76)	136.0(2)
N(4)-K(1)-C(16)#3	115.64(18)
N(2)-K(1)-C(16)#3	110.1(2)
C(7)-K(1)-C(16)#3	94.8(2)
N(3)-K(1)-C(16)#3	92.62(18)
C(72)-K(1)-C(16)#3	91.3(3)
C(64)-K(1)-C(16)#3	111.0(2)
C(71)-K(1)-C(16)#3	76.8(2)
C(73)-K(1)-C(16)#3	116.5(3)
N(1)-K(1)-C(16)#3	134.4(2)
C(76)-K(1)-C(16)#3	87.4(3)
N(4)-K(1)-C(74)	103.4(2)
N(2)-K(1)-C(74)	117.1(2)
C(7)-K(1)-C(74)	118.6(3)
N(3)-K(1)-C(74)	128.7(2)
C(72)-K(1)-C(74)	43.64(8)
C(64)-K(1)-C(74)	89.7(3)
C(71)-K(1)-C(74)	50.73(7)
C(73)-K(1)-C(74)	24.48(6)

N(1)-K(1)-C(74)	93.1(2)
C(76)-K(1)-C(74)	42.93(7)
C(16)#3-K(1)-C(74)	127.3(2)
N(8)-K(2)-C(49)	84.92(16)
N(8)-K(2)-N(5)	60.12(13)
C(49)-K(2)-N(5)	24.89(16)
N(8)-K(2)-C(35)	24.93(14)
C(49)-K(2)-C(35)	109.51(18)
N(5)-K(2)-C(35)	84.61(15)
N(8)-K(2)-N(7)	24.28(14)
C(49)-K(2)-N(7)	79.85(16)
N(5)-K(2)-N(7)	58.47(13)
C(35)-K(2)-N(7)	40.62(16)
N(8)-K(2)-C(26)#4	106.8(4)
C(49)-K(2)-C(26)#4	113.8(6)
N(5)-K(2)-C(26)#4	120.3(4)
C(35)-K(2)-C(26)#4	99.5(6)
N(7)-K(2)-C(26)#4	87.0(3)
N(8)-K(2)-C(27)#4	111.7(5)
C(49)-K(2)-C(27)#4	136.4(7)
N(5)-K(2)-C(27)#4	143.8(6)
C(35)-K(2)-C(27)#4	95.1(5)
N(7)-K(2)-C(27)#4	99.0(4)
C(26)#4-K(2)-C(27)#4	24.0(3)
N(8)-K(2)-C(69)#4	95.0(2)
C(49)-K(2)-C(69)#4	105.7(2)
N(5)-K(2)-C(69)#4	103.78(17)
C(35)-K(2)-C(69)#4	84.5(2)
N(7)-K(2)-C(69)#4	119.3(2)
C(26)#4-K(2)-C(69)#4	135.9(4)

C(27)#4-K(2)-C(69)#4	112.2(6)
N(8)-K(2)-C(25)#4	121.3(5)
C(49)-K(2)-C(25)#4	94.8(5)
N(5)-K(2)-C(25)#4	108.8(4)
C(35)-K(2)-C(25)#4	120.9(6)
N(7)-K(2)-C(25)#4	97.8(4)
C(26)#4-K(2)-C(25)#4	23.8(3)
C(27)#4-K(2)-C(25)#4	41.8(4)
C(69)#4-K(2)-C(25)#4	139.9(3)
N(8)-K(2)-C(28)#4	132.2(6)
C(49)-K(2)-C(28)#4	135.3(7)
N(5)-K(2)-C(28)#4	155.9(7)
C(35)-K(2)-C(28)#4	111.2(6)
N(7)-K(2)-C(28)#4	122.4(6)
C(26)#4-K(2)-C(28)#4	41.5(4)
C(27)#4-K(2)-C(28)#4	23.5(2)
C(69)#4-K(2)-C(28)#4	95.9(7)
C(25)#4-K(2)-C(28)#4	47.8(4)
N(8)-K(2)-C(48)	95.38(14)
C(49)-K(2)-C(48)	24.87(17)
N(5)-K(2)-C(48)	42.60(12)
C(35)-K(2)-C(48)	119.59(16)
N(7)-K(2)-C(48)	81.05(14)
C(26)#4-K(2)-C(48)	89.2(6)
C(27)#4-K(2)-C(48)	111.5(6)
C(69)#4-K(2)-C(48)	127.0(2)
C(25)#4-K(2)-C(48)	70.1(5)
C(28)#4-K(2)-C(48)	113.8(7)
N(8)-K(2)-C(24)#4	144.5(6)
C(49)-K(2)-C(24)#4	95.1(5)

N(5)-K(2)-C(24)#4	116.2(5)
C(35)-K(2)-C(24)#4	140.4(7)
N(7)-K(2)-C(24)#4	120.7(6)
C(26)#4-K(2)-C(24)#4	41.2(4)
C(27)#4-K(2)-C(24)#4	47.8(4)
C(69)#4-K(2)-C(24)#4	118.8(6)
C(25)#4-K(2)-C(24)#4	23.2(3)
C(28)#4-K(2)-C(24)#4	40.4(2)
C(48)-K(2)-C(24)#4	73.6(5)
C(8)-N(1)-N(2)	112.3(5)
C(8)-N(1)-Sm(1)	173.0(5)
N(2)-N(1)-Sm(1)	72.0(3)
C(8)-N(1)-K(1)	89.8(4)
N(2)-N(1)-K(1)	67.4(3)
Sm(1)-N(1)-K(1)	97.06(16)
C(7)-N(2)-N(1)	114.6(5)
C(7)-N(2)-Sm(1)	167.2(4)
N(1)-N(2)-Sm(1)	76.9(3)
C(7)-N(2)-K(1)	81.7(4)
N(1)-N(2)-K(1)	87.9(3)
Sm(1)-N(2)-K(1)	105.01(17)
C(63)-N(3)-N(4)	113.4(5)
C(63)-N(3)-Sm(1)	170.0(4)
N(4)-N(3)-Sm(1)	70.1(3)
C(63)-N(3)-K(1)	92.3(4)
N(4)-N(3)-K(1)	69.4(3)
Sm(1)-N(3)-K(1)	97.69(16)
C(64)-N(4)-N(3)	112.3(5)
C(64)-N(4)-Sm(1)	164.2(4)
N(3)-N(4)-Sm(1)	79.5(3)

C(64)-N(4)-K(1)	86.6(3)
N(3)-N(4)-K(1)	85.0(3)
Sm(1)-N(4)-K(1)	105.44(17)
C(49)-N(5)-N(6)	113.6(6)
C(49)-N(5)-Sm(1)	170.7(5)
N(6)-N(5)-Sm(1)	75.5(3)
C(49)-N(5)-K(2)	72.5(4)
N(6)-N(5)-K(2)	96.8(3)
Sm(1)-N(5)-K(2)	109.53(17)
C(50)-N(6)-N(5)	113.7(6)
C(50)-N(6)-Sm(1)	171.7(5)
N(5)-N(6)-Sm(1)	73.1(3)
C(36)-N(7)-N(8)	112.1(5)
C(36)-N(7)-Sm(1)	167.4(5)
N(8)-N(7)-Sm(1)	72.3(3)
C(36)-N(7)-K(2)	88.5(4)
N(8)-N(7)-K(2)	67.7(3)
Sm(1)-N(7)-K(2)	104.04(18)
C(35)-N(8)-N(7)	112.5(6)
C(35)-N(8)-Sm(1)	162.6(4)
N(7)-N(8)-Sm(1)	76.8(3)
C(35)-N(8)-K(2)	83.0(3)
N(7)-N(8)-K(2)	88.1(3)
Sm(1)-N(8)-K(2)	112.79(17)
C(22)-N(9)-N(10)	111.9(5)
C(22)-N(9)-Sm(1)	176.1(5)
N(10)-N(9)-Sm(1)	71.9(3)
C(21)-N(10)-N(9)	114.4(5)
C(21)-N(10)-Sm(1)	169.2(5)
N(9)-N(10)-Sm(1)	76.4(3)

C(7)-P(1)-C(8)	86.4(3)
C(7)-P(1)-K(1)	59.5(2)
C(8)-P(1)-K(1)	72.7(2)
C(22)-P(2)-C(21)	85.9(3)
C(36)-P(3)-C(35)	86.4(3)
C(36)-P(3)-K(2)	72.5(2)
C(35)-P(3)-K(2)	61.1(2)
C(49)-P(4)-C(50)	87.0(3)
C(49)-P(4)-K(2)	57.0(2)
C(50)-P(4)-K(2)	83.0(2)
C(64)-P(5)-C(63)	86.2(3)
C(64)-P(5)-K(1)	59.3(2)
C(63)-P(5)-K(1)	68.8(2)
N(10)-Sm(1)-N(2)	118.56(17)
N(10)-Sm(1)-N(5)	145.52(17)
N(2)-Sm(1)-N(5)	90.50(17)
N(10)-Sm(1)-N(9)	31.66(17)
N(2)-Sm(1)-N(9)	139.39(17)
N(5)-Sm(1)-N(9)	129.06(17)
N(10)-Sm(1)-N(4)	88.72(16)
N(2)-Sm(1)-N(4)	81.97(16)
N(5)-Sm(1)-N(4)	115.07(16)
N(9)-Sm(1)-N(4)	73.50(16)
N(10)-Sm(1)-N(6)	123.19(18)
N(2)-Sm(1)-N(6)	118.14(17)
N(5)-Sm(1)-N(6)	31.38(17)
N(9)-Sm(1)-N(6)	98.69(19)
N(4)-Sm(1)-N(6)	102.32(17)
N(10)-Sm(1)-N(8)	72.72(16)
N(2)-Sm(1)-N(8)	118.52(17)

N(5)-Sm(1)-N(8)	77.25(17)
N(9)-Sm(1)-N(8)	83.71(16)
N(4)-Sm(1)-N(8)	157.04(16)
N(6)-Sm(1)-N(8)	78.00(18)
N(10)-Sm(1)-N(1)	87.57(17)
N(2)-Sm(1)-N(1)	31.04(15)
N(5)-Sm(1)-N(1)	118.84(17)
N(9)-Sm(1)-N(1)	112.03(17)
N(4)-Sm(1)-N(1)	81.92(16)
N(6)-Sm(1)-N(1)	148.76(18)
N(8)-Sm(1)-N(1)	109.93(18)
N(10)-Sm(1)-N(7)	85.17(17)
N(2)-Sm(1)-N(7)	87.66(17)
N(5)-Sm(1)-N(7)	77.45(18)
N(9)-Sm(1)-N(7)	107.54(16)
N(4)-Sm(1)-N(7)	163.65(17)
N(6)-Sm(1)-N(7)	93.70(18)
N(8)-Sm(1)-N(7)	30.90(17)
N(1)-Sm(1)-N(7)	82.68(17)
N(10)-Sm(1)-N(3)	117.57(16)
N(2)-Sm(1)-N(3)	77.15(15)
N(5)-Sm(1)-N(3)	85.01(17)
N(9)-Sm(1)-N(3)	95.41(15)
N(4)-Sm(1)-N(3)	30.35(15)
N(6)-Sm(1)-N(3)	78.46(16)
N(8)-Sm(1)-N(3)	156.02(17)
N(1)-Sm(1)-N(3)	92.67(15)
N(7)-Sm(1)-N(3)	156.68(16)
N(10)-Sm(1)-K(1)	105.29(13)
N(2)-Sm(1)-K(1)	41.49(12)

N(5)-Sm(1)-K(1)	108.96(12)
N(9)-Sm(1)-K(1)	106.71(12)
N(4)-Sm(1)-K(1)	40.59(11)
N(6)-Sm(1)-K(1)	119.11(13)
N(8)-Sm(1)-K(1)	157.12(14)
N(1)-Sm(1)-K(1)	47.44(12)
N(7)-Sm(1)-K(1)	127.25(13)
N(3)-Sm(1)-K(1)	45.38(11)

Symmetry transformations used to generate equivalent atoms:

#1 $-x+3/2, -y+1, z-1/2$ #2 $-x+2, y+1/2, -z+1/2$

#3 $-x+3/2, -y+1, z+1/2$ #4 $-x+2, y-1/2, -z+1/2$

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 150429-1c.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
C(1)	67(5)	66(4)	63(4)	-9(4)	17(4)	-5(4)
C(2)	98(7)	91(6)	57(5)	20(4)	17(5)	-8(5)
C(3)	109(8)	101(7)	56(5)	21(5)	-1(5)	7(6)
C(4)	75(6)	102(6)	66(5)	14(4)	8(4)	9(5)
C(5)	70(5)	64(4)	56(4)	11(3)	13(3)	3(3)
C(6)	47(4)	54(4)	53(4)	-6(3)	15(3)	-4(3)
C(7)	44(3)	58(4)	53(3)	-8(3)	13(3)	-6(3)
C(8)	40(4)	73(4)	66(4)	-6(3)	7(3)	-1(3)
C(9)	49(3)	140(5)	110(5)	19(4)	-5(3)	14(3)
C(10)	60(3)	167(6)	130(5)	28(5)	-13(4)	4(4)
C(11)	72(4)	177(6)	144(5)	27(5)	-18(4)	8(4)
C(12)	82(4)	161(6)	138(5)	25(5)	-21(4)	20(4)
C(13)	85(4)	141(5)	124(5)	21(4)	-15(4)	20(4)
C(14)	67(4)	132(5)	114(5)	16(4)	-9(4)	16(4)
C(15)	94(6)	68(5)	72(5)	4(4)	-30(5)	8(4)
C(16)	73(6)	81(6)	98(6)	15(5)	-32(5)	8(4)
C(17)	81(6)	109(7)	118(7)	7(6)	-38(6)	-16(6)
C(18)	85(6)	75(5)	124(8)	23(6)	-25(6)	-6(4)
C(19)	76(5)	66(4)	68(4)	5(4)	-21(4)	-1(4)
C(20)	78(5)	51(4)	53(4)	-2(3)	-16(3)	7(3)

C(21)	72(4)	44(3)	44(3)	-1(3)	-6(3)	3(3)
C(22)	76(5)	38(3)	46(4)	3(3)	3(3)	1(3)
C(23)	77(5)	44(3)	59(4)	1(3)	15(3)	-2(3)
C(24)	101(6)	79(6)	74(5)	22(4)	24(5)	-14(5)
C(25)	124(9)	82(7)	106(7)	9(6)	42(7)	-25(6)
C(26)	80(6)	73(6)	158(10)	0(6)	35(7)	-22(5)
C(27)	86(6)	80(6)	102(6)	-6(5)	5(5)	-18(5)
C(28)	70(5)	65(5)	74(5)	-5(4)	6(4)	-5(4)
C(29)	106(4)	83(4)	69(3)	-3(3)	25(3)	22(3)
C(30)	116(5)	101(4)	83(4)	7(4)	30(4)	23(4)
C(31)	119(5)	110(5)	76(4)	6(4)	27(4)	34(4)
C(32)	116(5)	110(4)	67(3)	-3(4)	11(3)	39(4)
C(33)	106(4)	92(4)	59(3)	-5(3)	-1(3)	38(3)
C(34)	98(4)	72(4)	51(3)	-6(3)	5(3)	33(3)
C(35)	81(5)	45(3)	52(4)	-7(3)	-15(4)	20(4)
C(36)	73(5)	35(3)	70(4)	8(3)	-20(4)	-7(3)
C(37)	78(4)	75(4)	127(5)	34(4)	-30(4)	-33(3)
C(38)	89(4)	93(4)	136(5)	24(4)	-1(4)	-34(4)
C(39)	97(4)	110(5)	147(5)	24(4)	4(4)	-38(4)
C(40)	99(4)	115(5)	152(5)	35(4)	-4(4)	-40(4)
C(41)	98(4)	114(5)	156(5)	26(4)	-22(5)	-44(4)
C(42)	91(4)	101(4)	142(5)	26(4)	-32(4)	-40(4)
C(43)	112(8)	52(4)	87(6)	3(4)	29(5)	2(4)
C(44)	146(10)	65(5)	106(7)	6(6)	41(7)	3(6)
C(45)	231(17)	75(7)	108(9)	22(7)	66(11)	2(9)
C(46)	233(17)	102(9)	98(9)	41(7)	4(11)	10(11)
C(47)	171(11)	86(7)	89(7)	39(6)	-22(7)	13(7)
C(48)	121(7)	37(4)	67(5)	2(3)	0(5)	2(4)
C(49)	76(5)	59(4)	51(4)	-11(3)	-11(3)	23(4)
C(50)	51(4)	80(5)	57(4)	-19(3)	-8(3)	21(4)

C(51)	48(3)	136(5)	100(4)	-3(4)	8(4)	8(3)
C(52)	60(3)	127(5)	118(5)	8(4)	8(4)	7(4)
C(53)	74(4)	142(5)	132(5)	11(4)	14(4)	5(4)
C(54)	80(4)	166(6)	141(5)	13(5)	14(4)	-9(4)
C(55)	80(4)	183(6)	138(5)	12(5)	8(4)	-8(4)
C(56)	68(4)	169(5)	121(5)	6(5)	4(4)	-6(4)
C(57)	61(4)	73(5)	64(4)	3(4)	-13(3)	10(4)
C(58)	81(6)	96(6)	90(6)	16(5)	-18(5)	10(5)
C(59)	77(6)	124(9)	77(6)	28(6)	-24(4)	2(5)
C(60)	93(7)	127(8)	59(4)	2(5)	-31(5)	-11(7)
C(61)	64(5)	89(6)	65(5)	-5(4)	-6(4)	-6(4)
C(62)	41(3)	74(5)	47(3)	-4(3)	0(3)	-6(3)
C(63)	41(3)	57(4)	44(3)	-6(3)	-1(3)	-6(3)
C(64)	47(3)	42(3)	49(3)	-6(3)	5(2)	-7(3)
C(65)	53(3)	46(3)	52(3)	-4(3)	3(3)	0(3)
C(66)	82(5)	47(4)	64(4)	-8(3)	-15(4)	5(3)
C(67)	100(7)	66(5)	88(6)	-3(4)	-37(5)	13(5)
C(68)	104(7)	69(5)	81(6)	11(4)	-15(5)	12(5)
C(69)	120(8)	46(4)	116(7)	33(4)	8(6)	7(5)
C(70)	104(7)	47(4)	71(5)	1(3)	-13(4)	-17(4)
C(71)	133(10)	95(7)	96(7)	13(6)	61(7)	46(7)
C(72)	89(8)	83(7)	222(17)	14(8)	76(9)	12(6)
C(73)	167(15)	220(20)	131(12)	-41(14)	-36(11)	97(14)
C(74)	290(30)	230(20)	89(10)	-44(12)	-18(13)	170(20)
C(75)	234(19)	134(11)	76(7)	15(7)	62(10)	78(12)
C(76)	127(10)	62(6)	192(14)	-19(7)	66(10)	7(6)
C(77)	164(16)	109(11)	430(30)	-83(17)	-10(20)	-29(11)
C(78)	283(19)	142(11)	101(8)	19(7)	-8(11)	-60(12)
C(79)	282(19)	140(11)	103(9)	19(7)	-8(11)	-57(12)
C(80)	281(19)	137(11)	106(9)	21(7)	-8(11)	-56(12)

C(81)	283(19)	137(11)	108(8)	24(7)	-6(11)	-57(12)
C(82)	282(18)	141(10)	108(8)	23(7)	-6(10)	-59(11)
C(83)	281(19)	141(11)	103(8)	22(7)	-7(10)	-61(12)
C(84)	282(18)	141(10)	108(8)	23(7)	-6(10)	-59(11)
C(85)	163(12)	88(8)	283(18)	-32(11)	53(13)	-55(8)
C(86)	166(12)	95(8)	285(18)	-32(11)	55(13)	-52(9)
C(87)	167(12)	93(8)	284(18)	-36(11)	53(13)	-49(9)
C(88)	166(12)	86(8)	281(18)	-36(11)	55(13)	-53(8)
C(89)	165(12)	80(8)	281(17)	-38(10)	51(13)	-60(8)
C(90)	165(12)	82(8)	285(17)	-35(10)	48(13)	-60(8)
C(91)	169(13)	87(9)	289(18)	-33(11)	44(14)	-59(9)
K(1)	83(1)	66(1)	98(1)	-18(1)	35(1)	0(1)
K(2)	106(2)	75(1)	90(1)	-7(1)	-24(1)	8(1)
N(1)	42(3)	58(3)	53(3)	1(2)	0(2)	-3(2)
N(2)	35(2)	54(3)	47(2)	2(2)	1(2)	-6(2)
N(3)	41(3)	46(3)	52(3)	0(2)	7(2)	2(2)
N(4)	42(3)	45(3)	47(3)	-3(2)	-2(2)	2(2)
N(5)	52(3)	49(3)	45(3)	3(2)	-6(2)	7(2)
N(6)	46(3)	59(3)	62(4)	-6(3)	-7(2)	11(3)
N(7)	61(3)	51(3)	48(3)	-1(2)	-3(3)	-6(3)
N(8)	58(3)	45(3)	45(2)	-2(2)	1(3)	4(3)
N(9)	61(3)	37(3)	37(2)	3(2)	1(2)	-6(2)
N(10)	59(3)	45(3)	41(3)	2(2)	-4(2)	-1(2)
P(1)	43(1)	92(1)	70(1)	6(1)	16(1)	1(1)
P(2)	93(2)	64(1)	47(1)	18(1)	-7(1)	-2(1)
P(3)	110(2)	50(1)	70(1)	-10(1)	-27(1)	-8(1)
P(4)	81(2)	85(1)	84(1)	-5(1)	-18(1)	41(1)
P(5)	66(1)	50(1)	60(1)	-9(1)	-13(1)	-8(1)
Sm(1)	39(1)	36(1)	37(1)	2(1)	1(1)	0(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 150429-1c.

	x	y	z	U(eq)
H(1)	7001	3335	5478	78
H(2)	7577	2944	6322	98
H(3)	8876	3082	6466	106
H(4)	9596	3603	5768	97
H(5)	9007	3993	4898	76
H(10)	5410	4131	3529	143
H(11)	4543	4534	2840	157
H(12)	4903	5339	2213	152
H(13)	6132	5742	2274	140
H(14)	6999	5340	2963	125
H(15)	7002	5413	1261	93
H(16)	5927	5099	1053	101
H(17)	5519	4092	1193	123
H(18)	6213	3595	1933	113
H(19)	7412	3925	2172	84
H(24)	10377	5666	1068	102
H(25)	11568	6138	1112	125
H(26)	12164	6286	2037	124
H(27)	11569	5962	2918	107
H(28)	10378	5490	2874	84
H(29)	9940	3931	1865	104

H(30)	10861	4155	1136	120
H(31)	10902	3576	267	122
H(32)	10093	2767	129	117
H(33)	9201	2512	855	103
H(38)	7275	3104	3624	127
H(39)	6166	2791	4114	141
H(40)	5367	2069	3668	146
H(41)	5676	1659	2732	147
H(42)	6785	1971	2242	134
H(43)	8497	2776	4086	100
H(44)	7734	2146	4681	127
H(45)	8294	1447	5338	166
H(46)	9618	1377	5400	173
H(47)	10382	2006	4805	138
H(52)	10989	4143	2482	122
H(53)	12008	4663	2039	139
H(54)	13143	4720	2523	154
H(55)	13394	4068	3306	160
H(56)	12385	3447	3740	143
H(57)	10514	4060	4523	80
H(58)	11302	3593	5239	107
H(59)	11642	4125	6096	111
H(60)	11298	5134	6195	112
H(61)	10549	5613	5486	87
H(66)	8239	5685	2896	77
H(67)	7687	6394	2243	102
H(68)	7955	7440	2351	102
H(69)	8670	7747	3178	113
H(70)	9264	7061	3778	89
H(71)	7177	6425	5798	130

H(72)	6189	5802	5400	158
H(73)	5944	5797	4350	209
H(74)	6691	6416	3696	246
H(75)	7683	7041	4094	178
H(77A)	8654	7045	5021	350
H(77B)	8250	7051	5653	350
H(77C)	8075	7572	5182	350
H(78)	1951	3777	8699	210
H(79)	2898	4274	9249	210
H(80)	2569	5040	9933	209
H(81)	1294	5309	10066	211
H(82)	347	4812	9515	212
H(84A)	-44	4001	8887	265
H(84B)	545	3492	8695	265
H(84C)	439	4082	8296	265
H(85)	2928	3299	1989	214
H(86)	3986	2914	2498	219
H(87)	5065	2611	1964	217
H(88)	5086	2694	919	213
H(89)	4028	3079	410	210
H(91A)	2873	3649	439	272
H(91B)	2516	3845	1059	272
H(91C)	2317	3201	779	272

Table 6. Torsion angles [deg] for 150429-1c.

C(6)-C(1)-C(2)-C(3)	-0.2(13)
C(1)-C(2)-C(3)-C(4)	-0.3(15)
C(2)-C(3)-C(4)-C(5)	-0.1(15)
C(3)-C(4)-C(5)-C(6)	1.0(13)
C(4)-C(5)-C(6)-C(1)	-1.5(11)
C(4)-C(5)-C(6)-C(7)	178.7(7)
C(2)-C(1)-C(6)-C(5)	1.1(11)
C(2)-C(1)-C(6)-C(7)	-179.0(7)
C(5)-C(6)-C(7)-N(2)	20.9(10)
C(1)-C(6)-C(7)-N(2)	-159.0(6)
C(5)-C(6)-C(7)-P(1)	-156.6(6)
C(1)-C(6)-C(7)-P(1)	23.5(9)
C(5)-C(6)-C(7)-K(1)	-56.1(7)
C(1)-C(6)-C(7)-K(1)	124.0(6)
N(1)-C(8)-C(9)-C(10)	141.9(6)
P(1)-C(8)-C(9)-C(10)	-37.2(9)
K(1)-C(8)-C(9)-C(10)	-136.5(4)
N(1)-C(8)-C(9)-C(14)	-38.0(9)
P(1)-C(8)-C(9)-C(14)	142.9(5)
K(1)-C(8)-C(9)-C(14)	43.7(7)
C(14)-C(9)-C(10)-C(11)	0.0
C(8)-C(9)-C(10)-C(11)	-179.9(7)
C(9)-C(10)-C(11)-C(12)	0.0
C(10)-C(11)-C(12)-C(13)	0.0
C(11)-C(12)-C(13)-C(14)	0.0
C(12)-C(13)-C(14)-C(9)	0.0

C(10)-C(9)-C(14)-C(13)	0.0
C(8)-C(9)-C(14)-C(13)	179.9(7)
C(20)-C(15)-C(16)-C(17)	-0.7(15)
K(1)#1-C(15)-C(16)-C(17)	121.2(10)
C(20)-C(15)-C(16)-K(1)#1	-122.0(8)
C(15)-C(16)-C(17)-C(18)	1.0(16)
K(1)#1-C(16)-C(17)-C(18)	104.2(10)
C(16)-C(17)-C(18)-C(19)	-2.0(17)
C(17)-C(18)-C(19)-C(20)	2.6(15)
C(16)-C(15)-C(20)-C(19)	1.2(13)
K(1)#1-C(15)-C(20)-C(19)	-87.2(9)
C(16)-C(15)-C(20)-C(21)	177.0(8)
K(1)#1-C(15)-C(20)-C(21)	88.6(8)
C(18)-C(19)-C(20)-C(15)	-2.2(12)
C(18)-C(19)-C(20)-C(21)	-178.0(8)
C(15)-C(20)-C(21)-N(10)	165.0(7)
C(19)-C(20)-C(21)-N(10)	-19.4(10)
C(15)-C(20)-C(21)-P(2)	-14.9(10)
C(19)-C(20)-C(21)-P(2)	160.8(6)
N(9)-C(22)-C(23)-C(24)	155.6(5)
P(2)-C(22)-C(23)-C(24)	-27.0(7)
N(9)-C(22)-C(23)-C(28)	-25.1(8)
P(2)-C(22)-C(23)-C(28)	152.3(4)
N(9)-C(22)-C(23)-K(2)#2	-113.9(5)
P(2)-C(22)-C(23)-K(2)#2	63.4(6)
C(28)-C(23)-C(24)-C(25)	0.0
C(22)-C(23)-C(24)-C(25)	179.3(5)
K(2)#2-C(23)-C(24)-C(25)	64.9(2)
C(28)-C(23)-C(24)-K(2)#2	-64.9(2)
C(22)-C(23)-C(24)-K(2)#2	114.4(4)

C(23)-C(24)-C(25)-C(26)	0.0
K(2)#2-C(24)-C(25)-C(26)	67.9(2)
C(23)-C(24)-C(25)-K(2)#2	-67.9(2)
C(24)-C(25)-C(26)-C(27)	0.0
K(2)#2-C(25)-C(26)-C(27)	72.11(19)
C(24)-C(25)-C(26)-K(2)#2	-72.11(19)
C(25)-C(26)-C(27)-C(28)	0.0
K(2)#2-C(26)-C(27)-C(28)	73.1(2)
C(25)-C(26)-C(27)-K(2)#2	-73.1(2)
C(26)-C(27)-C(28)-C(23)	0.0
K(2)#2-C(27)-C(28)-C(23)	69.9(2)
C(26)-C(27)-C(28)-K(2)#2	-69.9(2)
C(24)-C(23)-C(28)-C(27)	0.0
C(22)-C(23)-C(28)-C(27)	-179.3(5)
K(2)#2-C(23)-C(28)-C(27)	-65.9(2)
C(24)-C(23)-C(28)-K(2)#2	65.9(2)
C(22)-C(23)-C(28)-K(2)#2	-113.4(5)
C(34)-C(29)-C(30)-C(31)	1.6(15)
C(29)-C(30)-C(31)-C(32)	-1.3(16)
C(30)-C(31)-C(32)-C(33)	0.2(16)
C(31)-C(32)-C(33)-C(34)	0.7(14)
C(30)-C(29)-C(34)-C(33)	-0.7(14)
C(30)-C(29)-C(34)-C(35)	180.0(8)
C(32)-C(33)-C(34)-C(29)	-0.5(13)
C(32)-C(33)-C(34)-C(35)	178.9(8)
C(29)-C(34)-C(35)-N(8)	-8.8(11)
C(33)-C(34)-C(35)-N(8)	171.8(7)
C(29)-C(34)-C(35)-P(3)	168.5(7)
C(33)-C(34)-C(35)-P(3)	-10.9(10)
C(29)-C(34)-C(35)-K(2)	-87.6(8)

C(33)-C(34)-C(35)-K(2)	93.0(7)
N(7)-C(36)-C(37)-C(38)	-0.2(8)
P(3)-C(36)-C(37)-C(38)	-176.1(4)
K(2)-C(36)-C(37)-C(38)	81.8(6)
N(7)-C(36)-C(37)-C(42)	178.9(5)
P(3)-C(36)-C(37)-C(42)	3.0(8)
K(2)-C(36)-C(37)-C(42)	-99.1(5)
C(42)-C(37)-C(38)-C(39)	0.0
C(36)-C(37)-C(38)-C(39)	179.1(6)
C(37)-C(38)-C(39)-C(40)	0.0
C(38)-C(39)-C(40)-C(41)	0.0
C(39)-C(40)-C(41)-C(42)	0.0
C(40)-C(41)-C(42)-C(37)	0.0
C(38)-C(37)-C(42)-C(41)	0.0
C(36)-C(37)-C(42)-C(41)	-179.1(6)
C(48)-C(43)-C(44)-C(45)	0.0
C(43)-C(44)-C(45)-C(46)	0.0
C(44)-C(45)-C(46)-C(47)	0.0
C(45)-C(46)-C(47)-C(48)	0.0
C(46)-C(47)-C(48)-C(43)	0.0
C(46)-C(47)-C(48)-C(49)	178.8(6)
C(46)-C(47)-C(48)-K(2)	-110.2(3)
C(44)-C(43)-C(48)-C(47)	0.0
C(44)-C(43)-C(48)-C(49)	-178.8(6)
C(44)-C(43)-C(48)-K(2)	123.1(3)
C(47)-C(48)-C(49)-N(5)	-169.7(5)
C(43)-C(48)-C(49)-N(5)	9.1(8)
K(2)-C(48)-C(49)-N(5)	83.5(6)
C(47)-C(48)-C(49)-P(4)	8.9(8)
C(43)-C(48)-C(49)-P(4)	-172.3(5)

K(2)-C(48)-C(49)-P(4)	-97.9(5)
C(47)-C(48)-C(49)-K(2)	106.8(4)
C(43)-C(48)-C(49)-K(2)	-74.4(5)
N(6)-C(50)-C(51)-C(56)	159.4(9)
P(4)-C(50)-C(51)-C(56)	-19.2(14)
N(6)-C(50)-C(51)-C(52)	-26.8(14)
P(4)-C(50)-C(51)-C(52)	154.6(8)
C(56)-C(51)-C(52)-C(53)	-7.4(18)
C(50)-C(51)-C(52)-C(53)	178.9(10)
C(51)-C(52)-C(53)-C(54)	-2.5(19)
C(52)-C(53)-C(54)-C(55)	9(2)
C(53)-C(54)-C(55)-C(56)	-6(2)
C(52)-C(51)-C(56)-C(55)	9.8(18)
C(50)-C(51)-C(56)-C(55)	-176.4(10)
C(54)-C(55)-C(56)-C(51)	-3(2)
C(62)-C(57)-C(58)-C(59)	2.4(13)
C(57)-C(58)-C(59)-C(60)	-2.8(15)
C(58)-C(59)-C(60)-C(61)	2.0(16)
C(59)-C(60)-C(61)-C(62)	-0.6(15)
C(58)-C(57)-C(62)-C(61)	-1.1(11)
C(58)-C(57)-C(62)-C(63)	179.0(7)
C(60)-C(61)-C(62)-C(57)	0.2(12)
C(60)-C(61)-C(62)-C(63)	-179.9(7)
C(57)-C(62)-C(63)-N(3)	21.2(10)
C(61)-C(62)-C(63)-N(3)	-158.8(6)
C(57)-C(62)-C(63)-P(5)	-157.0(6)
C(61)-C(62)-C(63)-P(5)	23.1(9)
C(57)-C(62)-C(63)-K(1)	98.3(7)
C(61)-C(62)-C(63)-K(1)	-81.7(7)
N(4)-C(64)-C(65)-C(66)	6.5(9)

P(5)-C(64)-C(65)-C(66)	-174.4(5)
K(1)-C(64)-C(65)-C(66)	-68.0(7)
N(4)-C(64)-C(65)-C(70)	-175.9(6)
P(5)-C(64)-C(65)-C(70)	3.2(9)
K(1)-C(64)-C(65)-C(70)	109.6(6)
C(70)-C(65)-C(66)-C(67)	2.3(12)
C(64)-C(65)-C(66)-C(67)	-180.0(7)
C(65)-C(66)-C(67)-C(68)	-3.2(14)
C(66)-C(67)-C(68)-C(69)	3.4(15)
C(67)-C(68)-C(69)-C(70)	-2.9(15)
C(67)-C(68)-C(69)-K(2)#2	85.9(9)
C(68)-C(69)-C(70)-C(65)	2.1(15)
K(2)#2-C(69)-C(70)-C(65)	-94.5(8)
C(68)-C(69)-C(70)-K(2)#2	96.5(10)
C(66)-C(65)-C(70)-C(69)	-1.8(12)
C(64)-C(65)-C(70)-C(69)	-179.5(8)
C(66)-C(65)-C(70)-K(2)#2	-78.5(7)
C(64)-C(65)-C(70)-K(2)#2	103.7(5)
C(76)-C(71)-C(72)-C(73)	0.0
K(1)-C(71)-C(72)-C(73)	-71.6(3)
C(76)-C(71)-C(72)-K(1)	71.6(3)
C(71)-C(72)-C(73)-C(74)	0.0
K(1)-C(72)-C(73)-C(74)	-70.2(3)
C(71)-C(72)-C(73)-K(1)	70.2(3)
C(72)-C(73)-C(74)-C(75)	0.0
K(1)-C(73)-C(74)-C(75)	-66.3(2)
C(72)-C(73)-C(74)-K(1)	66.3(2)
C(73)-C(74)-C(75)-C(76)	0.0
K(1)-C(74)-C(75)-C(76)	-63.8(2)
C(73)-C(74)-C(75)-K(1)	63.8(2)

C(74)-C(75)-C(76)-C(71)	0.0
K(1)-C(75)-C(76)-C(71)	-65.1(2)
C(74)-C(75)-C(76)-C(77)	177.6(10)
K(1)-C(75)-C(76)-C(77)	112.6(9)
C(74)-C(75)-C(76)-K(1)	65.1(2)
C(72)-C(71)-C(76)-C(75)	0.0
K(1)-C(71)-C(76)-C(75)	68.9(3)
C(72)-C(71)-C(76)-C(77)	-177.6(10)
K(1)-C(71)-C(76)-C(77)	-108.7(9)
C(72)-C(71)-C(76)-K(1)	-68.9(3)
C(83)-C(78)-C(79)-C(80)	0.0
C(78)-C(79)-C(80)-C(81)	0.0
C(79)-C(80)-C(81)-C(82)	0.0
C(80)-C(81)-C(82)-C(83)	0.0
C(81)-C(82)-C(83)-C(78)	0.0
C(81)-C(82)-C(83)-C(84)	179.9(3)
C(79)-C(78)-C(83)-C(82)	0.0
C(79)-C(78)-C(83)-C(84)	-179.9(3)
C(90)-C(85)-C(86)-C(87)	0.0
C(85)-C(86)-C(87)-C(88)	0.0
C(86)-C(87)-C(88)-C(89)	0.0
C(87)-C(88)-C(89)-C(90)	0.0
C(88)-C(89)-C(90)-C(85)	0.0
C(88)-C(89)-C(90)-C(91)	176.7(16)
C(86)-C(85)-C(90)-C(89)	0.0
C(86)-C(85)-C(90)-C(91)	-176.7(16)
N(2)-C(7)-K(1)-N(4)	-13.1(4)
C(6)-C(7)-K(1)-N(4)	105.2(4)
P(1)-C(7)-K(1)-N(4)	-126.7(2)
C(6)-C(7)-K(1)-N(2)	118.3(5)

P(1)-C(7)-K(1)-N(2)	-113.6(5)
N(2)-C(7)-K(1)-N(3)	-37.1(3)
C(6)-C(7)-K(1)-N(3)	81.3(4)
P(1)-C(7)-K(1)-N(3)	-150.6(2)
N(2)-C(7)-K(1)-C(72)	138.3(4)
C(6)-C(7)-K(1)-C(72)	-103.4(4)
P(1)-C(7)-K(1)-C(72)	24.7(4)
N(2)-C(7)-K(1)-C(64)	-12.5(4)
C(6)-C(7)-K(1)-C(64)	105.8(4)
P(1)-C(7)-K(1)-C(64)	-126.1(2)
N(2)-C(7)-K(1)-C(71)	153.8(3)
C(6)-C(7)-K(1)-C(71)	-87.9(4)
P(1)-C(7)-K(1)-C(71)	40.2(4)
N(2)-C(7)-K(1)-C(73)	112.6(4)
C(6)-C(7)-K(1)-C(73)	-129.1(4)
P(1)-C(7)-K(1)-C(73)	-1.0(4)
N(2)-C(7)-K(1)-N(1)	34.5(3)
C(6)-C(7)-K(1)-N(1)	152.8(5)
P(1)-C(7)-K(1)-N(1)	-79.1(3)
N(2)-C(7)-K(1)-C(76)	137.9(5)
C(6)-C(7)-K(1)-C(76)	-103.7(6)
P(1)-C(7)-K(1)-C(76)	24.4(6)
N(2)-C(7)-K(1)-C(16)#3	-129.1(4)
C(6)-C(7)-K(1)-C(16)#3	-10.7(4)
P(1)-C(7)-K(1)-C(16)#3	117.4(3)
N(2)-C(7)-K(1)-C(74)	93.3(4)
C(6)-C(7)-K(1)-C(74)	-148.3(4)
P(1)-C(7)-K(1)-C(74)	-20.2(3)
C(71)-C(72)-K(1)-N(4)	-91.4(7)
C(73)-C(72)-K(1)-N(4)	32.2(7)

C(71)-C(72)-K(1)-N(2)	169.8(4)
C(73)-C(72)-K(1)-N(2)	-66.6(4)
C(71)-C(72)-K(1)-C(7)	150.0(4)
C(73)-C(72)-K(1)-C(7)	-86.4(4)
C(71)-C(72)-K(1)-N(3)	-61(2)
C(73)-C(72)-K(1)-N(3)	62(2)
C(71)-C(72)-K(1)-C(64)	-64.0(6)
C(73)-C(72)-K(1)-C(64)	59.6(6)
C(71)-C(72)-K(1)-N(1)	-166.4(4)
C(73)-C(72)-K(1)-N(1)	-42.8(4)
C(73)-C(72)-K(1)-C(76)	93.37(10)
C(71)-C(72)-K(1)-C(16)#3	54.7(5)
C(73)-C(72)-K(1)-C(16)#3	178.3(5)
C(65)-C(64)-K(1)-N(4)	115.6(5)
P(5)-C(64)-K(1)-N(4)	-115.2(5)
N(4)-C(64)-K(1)-N(2)	-6.7(3)
C(65)-C(64)-K(1)-N(2)	108.9(4)
P(5)-C(64)-K(1)-N(2)	-122.0(2)
N(4)-C(64)-K(1)-C(7)	-1.4(4)
C(65)-C(64)-K(1)-C(7)	114.2(4)
P(5)-C(64)-K(1)-C(7)	-116.7(3)
N(4)-C(64)-K(1)-N(3)	36.7(3)
C(65)-C(64)-K(1)-N(3)	152.3(5)
P(5)-C(64)-K(1)-N(3)	-78.6(3)
N(4)-C(64)-K(1)-C(72)	-144.0(4)
C(65)-C(64)-K(1)-C(72)	-28.4(5)
P(5)-C(64)-K(1)-C(72)	100.8(4)
N(4)-C(64)-K(1)-C(71)	-169.2(3)
C(65)-C(64)-K(1)-C(71)	-53.6(4)
P(5)-C(64)-K(1)-C(71)	75.5(3)

N(4)-C(64)-K(1)-C(73)	-120.3(4)
C(65)-C(64)-K(1)-C(73)	-4.7(4)
P(5)-C(64)-K(1)-C(73)	124.4(3)
N(4)-C(64)-K(1)-N(1)	-30.7(3)
C(65)-C(64)-K(1)-N(1)	84.9(4)
P(5)-C(64)-K(1)-N(1)	-145.9(3)
N(4)-C(64)-K(1)-C(76)	-166.7(4)
C(65)-C(64)-K(1)-C(76)	-51.1(4)
P(5)-C(64)-K(1)-C(76)	78.0(3)
N(4)-C(64)-K(1)-C(16)#3	105.9(4)
C(65)-C(64)-K(1)-C(16)#3	-138.5(4)
P(5)-C(64)-K(1)-C(16)#3	-9.3(3)
N(4)-C(64)-K(1)-C(74)	-123.8(4)
C(65)-C(64)-K(1)-C(74)	-8.2(4)
P(5)-C(64)-K(1)-C(74)	120.9(3)
C(72)-C(71)-K(1)-N(4)	122.7(6)
C(76)-C(71)-K(1)-N(4)	-1.1(6)
C(72)-C(71)-K(1)-N(2)	-16.1(5)
C(76)-C(71)-K(1)-N(2)	-139.9(5)
C(72)-C(71)-K(1)-C(7)	-36.8(5)
C(76)-C(71)-K(1)-C(7)	-160.6(5)
C(72)-C(71)-K(1)-N(3)	164.5(6)
C(76)-C(71)-K(1)-N(3)	40.8(5)
C(72)-C(71)-K(1)-C(64)	129.7(5)
C(76)-C(71)-K(1)-C(64)	5.9(5)
C(76)-C(71)-K(1)-C(73)	-93.29(11)
C(72)-C(71)-K(1)-N(1)	18.2(6)
C(76)-C(71)-K(1)-N(1)	-105.6(6)
C(72)-C(71)-K(1)-C(16)#3	-123.0(5)
C(76)-C(71)-K(1)-C(16)#3	113.2(5)

C(72)-C(71)-K(1)-C(74)	62.79(10)
C(76)-C(71)-K(1)-C(74)	-61.00(10)
C(74)-C(73)-K(1)-N(4)	-34.9(4)
C(72)-C(73)-K(1)-N(4)	-159.4(4)
C(74)-C(73)-K(1)-N(2)	-110.8(4)
C(72)-C(73)-K(1)-N(2)	124.6(4)
C(74)-C(73)-K(1)-C(7)	-135.7(4)
C(72)-C(73)-K(1)-C(7)	99.7(4)
C(74)-C(73)-K(1)-N(3)	-39.6(4)
C(72)-C(73)-K(1)-N(3)	-164.2(4)
C(74)-C(73)-K(1)-C(64)	-8.5(5)
C(72)-C(73)-K(1)-C(64)	-133.0(5)
C(74)-C(73)-K(1)-C(71)	93.68(11)
C(74)-C(73)-K(1)-N(1)	-95.0(4)
C(72)-C(73)-K(1)-N(1)	140.4(4)
C(74)-C(73)-K(1)-C(76)	60.78(10)
C(72)-C(73)-K(1)-C(76)	-63.76(11)
C(74)-C(73)-K(1)-C(16)#3	122.7(5)
C(72)-C(73)-K(1)-C(16)#3	-1.9(5)
C(75)-C(76)-K(1)-N(4)	54.1(4)
C(71)-C(76)-K(1)-N(4)	179.2(4)
C(77)-C(76)-K(1)-N(4)	-65.1(12)
C(75)-C(76)-K(1)-N(2)	-37.6(8)
C(71)-C(76)-K(1)-N(2)	87.5(8)
C(77)-C(76)-K(1)-N(2)	-156.8(11)
C(75)-C(76)-K(1)-C(7)	-93.7(8)
C(71)-C(76)-K(1)-C(7)	31.4(8)
C(77)-C(76)-K(1)-C(7)	147.1(11)
C(75)-C(76)-K(1)-N(3)	80.0(4)
C(71)-C(76)-K(1)-N(3)	-154.9(4)

C(77)-C(76)-K(1)-N(3)	-39.2(12)
C(75)-C(76)-K(1)-C(64)	60.3(5)
C(71)-C(76)-K(1)-C(64)	-174.6(5)
C(77)-C(76)-K(1)-C(64)	-58.9(12)
C(77)-C(76)-K(1)-C(71)	115.7(14)
C(75)-C(76)-K(1)-C(73)	-60.96(11)
C(71)-C(76)-K(1)-C(73)	64.12(11)
C(77)-C(76)-K(1)-C(73)	179.8(14)
C(75)-C(76)-K(1)-N(1)	-24.8(6)
C(71)-C(76)-K(1)-N(1)	100.3(6)
C(77)-C(76)-K(1)-N(1)	-144.0(11)
C(75)-C(76)-K(1)-C(16)#3	171.3(5)
C(71)-C(76)-K(1)-C(16)#3	-63.7(5)
C(77)-C(76)-K(1)-C(16)#3	52.1(12)
C(71)-C(76)-K(1)-C(74)	96.19(12)
C(77)-C(76)-K(1)-C(74)	-148.1(14)
C(73)-C(74)-K(1)-N(4)	150.9(4)
C(75)-C(74)-K(1)-N(4)	-83.0(4)
C(73)-C(74)-K(1)-N(2)	79.7(3)
C(75)-C(74)-K(1)-N(2)	-154.2(3)
C(73)-C(74)-K(1)-C(7)	51.1(4)
C(75)-C(74)-K(1)-C(7)	177.1(4)
C(73)-C(74)-K(1)-N(3)	155.7(3)
C(75)-C(74)-K(1)-N(3)	-78.3(3)
C(75)-C(74)-K(1)-C(72)	95.52(13)
C(73)-C(74)-K(1)-C(64)	172.2(4)
C(75)-C(74)-K(1)-C(64)	-61.7(4)
C(73)-C(74)-K(1)-C(71)	-64.15(12)
C(75)-C(74)-K(1)-C(71)	61.89(12)
C(73)-C(74)-K(1)-N(1)	85.9(4)

C(75)-C(74)-K(1)-N(1)	-148.1(4)
C(73)-C(74)-K(1)-C(16)#3	-71.3(7)
C(75)-C(74)-K(1)-C(16)#3	54.7(6)
N(5)-C(49)-K(2)-N(8)	-4.8(4)
C(48)-C(49)-K(2)-N(8)	114.6(4)
P(4)-C(49)-K(2)-N(8)	-117.2(3)
C(48)-C(49)-K(2)-N(5)	119.4(6)
P(4)-C(49)-K(2)-N(5)	-112.4(6)
N(5)-C(49)-K(2)-C(35)	-0.6(5)
C(48)-C(49)-K(2)-C(35)	118.8(4)
P(4)-C(49)-K(2)-C(35)	-113.0(3)
N(5)-C(49)-K(2)-N(7)	-28.8(4)
C(48)-C(49)-K(2)-N(7)	90.6(4)
P(4)-C(49)-K(2)-N(7)	-141.2(3)
N(5)-C(49)-K(2)-C(26)#4	-110.9(6)
C(48)-C(49)-K(2)-C(26)#4	8.4(6)
P(4)-C(49)-K(2)-C(26)#4	136.6(5)
N(5)-C(49)-K(2)-C(27)#4	-121.2(7)
C(48)-C(49)-K(2)-C(27)#4	-1.9(8)
P(4)-C(49)-K(2)-C(27)#4	126.3(7)
N(5)-C(49)-K(2)-C(69)#4	89.0(5)
C(48)-C(49)-K(2)-C(69)#4	-151.6(4)
P(4)-C(49)-K(2)-C(69)#4	-23.4(4)
N(5)-C(49)-K(2)-C(25)#4	-125.9(6)
C(48)-C(49)-K(2)-C(25)#4	-6.5(6)
P(4)-C(49)-K(2)-C(25)#4	121.7(5)
N(5)-C(49)-K(2)-C(28)#4	-155.1(10)
C(48)-C(49)-K(2)-C(28)#4	-35.8(10)
P(4)-C(49)-K(2)-C(28)#4	92.4(10)
N(5)-C(49)-K(2)-C(48)	-119.4(6)

P(4)-C(49)-K(2)-C(48)	128.2(5)
N(5)-C(49)-K(2)-C(24)#4	-149.1(7)
C(48)-C(49)-K(2)-C(24)#4	-29.7(7)
P(4)-C(49)-K(2)-C(24)#4	98.4(7)
C(34)-C(35)-K(2)-N(8)	115.8(7)
P(3)-C(35)-K(2)-N(8)	-114.8(6)
N(8)-C(35)-K(2)-C(49)	-10.0(5)
C(34)-C(35)-K(2)-C(49)	105.8(5)
P(3)-C(35)-K(2)-C(49)	-124.8(3)
N(8)-C(35)-K(2)-N(5)	-10.2(4)
C(34)-C(35)-K(2)-N(5)	105.6(5)
P(3)-C(35)-K(2)-N(5)	-125.0(3)
N(8)-C(35)-K(2)-N(7)	35.6(4)
C(34)-C(35)-K(2)-N(7)	151.4(6)
P(3)-C(35)-K(2)-N(7)	-79.2(3)
N(8)-C(35)-K(2)-C(26)#4	109.6(6)
C(34)-C(35)-K(2)-C(26)#4	-134.6(6)
P(3)-C(35)-K(2)-C(26)#4	-5.2(5)
N(8)-C(35)-K(2)-C(27)#4	133.4(7)
C(34)-C(35)-K(2)-C(27)#4	-110.7(7)
P(3)-C(35)-K(2)-C(27)#4	18.6(6)
N(8)-C(35)-K(2)-C(69)#4	-114.7(5)
C(34)-C(35)-K(2)-C(69)#4	1.1(5)
P(3)-C(35)-K(2)-C(69)#4	130.5(3)
N(8)-C(35)-K(2)-C(25)#4	98.5(6)
C(34)-C(35)-K(2)-C(25)#4	-145.7(6)
P(3)-C(35)-K(2)-C(25)#4	-16.4(5)
N(8)-C(35)-K(2)-C(28)#4	151.1(8)
C(34)-C(35)-K(2)-C(28)#4	-93.1(9)
P(3)-C(35)-K(2)-C(28)#4	36.3(8)

N(8)-C(35)-K(2)-C(48)	15.1(5)
C(34)-C(35)-K(2)-C(48)	130.9(5)
P(3)-C(35)-K(2)-C(48)	-99.7(2)
N(8)-C(35)-K(2)-C(24)#4	115.3(8)
C(34)-C(35)-K(2)-C(24)#4	-128.9(8)
P(3)-C(35)-K(2)-C(24)#4	0.5(8)
C(47)-C(48)-K(2)-N(8)	-175.7(3)
C(43)-C(48)-K(2)-N(8)	58.8(3)
C(49)-C(48)-K(2)-N(8)	-65.5(4)
C(47)-C(48)-K(2)-C(49)	-110.2(5)
C(43)-C(48)-K(2)-C(49)	124.3(5)
C(47)-C(48)-K(2)-N(5)	-143.0(4)
C(43)-C(48)-K(2)-N(5)	91.4(3)
C(49)-C(48)-K(2)-N(5)	-32.8(4)
C(47)-C(48)-K(2)-C(35)	178.0(3)
C(43)-C(48)-K(2)-C(35)	52.4(3)
C(49)-C(48)-K(2)-C(35)	-71.8(4)
C(47)-C(48)-K(2)-N(7)	164.7(3)
C(43)-C(48)-K(2)-N(7)	39.1(3)
C(49)-C(48)-K(2)-N(7)	-85.2(4)
C(47)-C(48)-K(2)-C(26)#4	77.5(4)
C(43)-C(48)-K(2)-C(26)#4	-48.0(4)
C(49)-C(48)-K(2)-C(26)#4	-172.3(5)
C(47)-C(48)-K(2)-C(27)#4	68.4(5)
C(43)-C(48)-K(2)-C(27)#4	-57.1(5)
C(49)-C(48)-K(2)-C(27)#4	178.6(6)
C(47)-C(48)-K(2)-C(69)#4	-75.2(3)
C(43)-C(48)-K(2)-C(69)#4	159.2(3)
C(49)-C(48)-K(2)-C(69)#4	34.9(4)
C(47)-C(48)-K(2)-C(25)#4	62.9(6)

C(43)-C(48)-K(2)-C(25)#4	-62.6(6)
C(49)-C(48)-K(2)-C(25)#4	173.1(7)
C(47)-C(48)-K(2)-C(28)#4	43.1(8)
C(43)-C(48)-K(2)-C(28)#4	-82.5(7)
C(49)-C(48)-K(2)-C(28)#4	153.3(8)
C(47)-C(48)-K(2)-C(24)#4	38.8(7)
C(43)-C(48)-K(2)-C(24)#4	-86.7(7)
C(49)-C(48)-K(2)-C(24)#4	149.0(8)
C(9)-C(8)-N(1)-N(2)	-179.1(6)
P(1)-C(8)-N(1)-N(2)	0.1(7)
K(1)-C(8)-N(1)-N(2)	65.4(4)
C(9)-C(8)-N(1)-Sm(1)	-52(4)
P(1)-C(8)-N(1)-Sm(1)	127(4)
K(1)-C(8)-N(1)-Sm(1)	-168(4)
C(9)-C(8)-N(1)-K(1)	115.5(6)
P(1)-C(8)-N(1)-K(1)	-65.4(4)
N(4)-K(1)-N(1)-C(8)	-155.7(4)
N(2)-K(1)-N(1)-C(8)	114.3(5)
C(7)-K(1)-N(1)-C(8)	78.9(4)
N(3)-K(1)-N(1)-C(8)	177.9(4)
C(72)-K(1)-N(1)-C(8)	-11.2(5)
C(64)-K(1)-N(1)-C(8)	-141.9(4)
C(71)-K(1)-N(1)-C(8)	-19.4(5)
C(73)-K(1)-N(1)-C(8)	-28.0(5)
C(76)-K(1)-N(1)-C(8)	-55.1(5)
C(16)#3-K(1)-N(1)-C(8)	102.1(5)
C(74)-K(1)-N(1)-C(8)	-52.4(5)
N(4)-K(1)-N(1)-N(2)	89.9(3)
C(7)-K(1)-N(1)-N(2)	-35.5(3)
N(3)-K(1)-N(1)-N(2)	63.6(3)

C(72)-K(1)-N(1)-N(2)	-125.5(3)
C(64)-K(1)-N(1)-N(2)	103.8(3)
C(71)-K(1)-N(1)-N(2)	-133.7(3)
C(73)-K(1)-N(1)-N(2)	-142.3(4)
C(76)-K(1)-N(1)-N(2)	-169.5(3)
C(16)#3-K(1)-N(1)-N(2)	-12.3(4)
C(74)-K(1)-N(1)-N(2)	-166.7(4)
N(4)-K(1)-N(1)-Sm(1)	22.77(14)
N(2)-K(1)-N(1)-Sm(1)	-67.2(3)
C(7)-K(1)-N(1)-Sm(1)	-102.7(3)
N(3)-K(1)-N(1)-Sm(1)	-3.62(14)
C(72)-K(1)-N(1)-Sm(1)	167.3(2)
C(64)-K(1)-N(1)-Sm(1)	36.62(17)
C(71)-K(1)-N(1)-Sm(1)	159.1(2)
C(73)-K(1)-N(1)-Sm(1)	150.5(3)
C(76)-K(1)-N(1)-Sm(1)	123.3(2)
C(16)#3-K(1)-N(1)-Sm(1)	-79.5(3)
C(74)-K(1)-N(1)-Sm(1)	126.1(3)
C(6)-C(7)-N(2)-N(1)	-177.8(5)
P(1)-C(7)-N(2)-N(1)	0.1(7)
K(1)-C(7)-N(2)-N(1)	-83.9(4)
C(6)-C(7)-N(2)-Sm(1)	29(2)
P(1)-C(7)-N(2)-Sm(1)	-153.3(16)
K(1)-C(7)-N(2)-Sm(1)	122.8(19)
C(6)-C(7)-N(2)-K(1)	-94.0(6)
P(1)-C(7)-N(2)-K(1)	83.9(4)
C(8)-N(1)-N(2)-C(7)	-0.1(8)
Sm(1)-N(1)-N(2)-C(7)	-174.2(5)
K(1)-N(1)-N(2)-C(7)	79.9(5)
C(8)-N(1)-N(2)-Sm(1)	174.1(5)

K(1)-N(1)-N(2)-Sm(1)	-105.94(13)
C(8)-N(1)-N(2)-K(1)	-80.0(5)
Sm(1)-N(1)-N(2)-K(1)	105.94(13)
N(4)-K(1)-N(2)-C(7)	165.7(4)
N(3)-K(1)-N(2)-C(7)	137.9(4)
C(72)-K(1)-N(2)-C(7)	-49.9(5)
C(64)-K(1)-N(2)-C(7)	168.9(4)
C(71)-K(1)-N(2)-C(7)	-41.7(5)
C(73)-K(1)-N(2)-C(7)	-74.5(5)
N(1)-K(1)-N(2)-C(7)	-115.2(5)
C(76)-K(1)-N(2)-C(7)	-93.6(6)
C(16)#3-K(1)-N(2)-C(7)	55.5(4)
C(74)-K(1)-N(2)-C(7)	-100.3(4)
N(4)-K(1)-N(2)-N(1)	-79.0(3)
C(7)-K(1)-N(2)-N(1)	115.2(5)
N(3)-K(1)-N(2)-N(1)	-106.9(3)
C(72)-K(1)-N(2)-N(1)	65.3(4)
C(64)-K(1)-N(2)-N(1)	-75.9(3)
C(71)-K(1)-N(2)-N(1)	73.5(4)
C(73)-K(1)-N(2)-N(1)	40.7(4)
C(76)-K(1)-N(2)-N(1)	21.6(7)
C(16)#3-K(1)-N(2)-N(1)	170.7(3)
C(74)-K(1)-N(2)-N(1)	14.9(4)
N(4)-K(1)-N(2)-Sm(1)	-3.18(14)
C(7)-K(1)-N(2)-Sm(1)	-168.9(4)
N(3)-K(1)-N(2)-Sm(1)	-31.03(15)
C(72)-K(1)-N(2)-Sm(1)	141.2(3)
C(64)-K(1)-N(2)-Sm(1)	-0.08(19)
C(71)-K(1)-N(2)-Sm(1)	149.3(3)
C(73)-K(1)-N(2)-Sm(1)	116.6(3)

N(1)-K(1)-N(2)-Sm(1)	75.9(3)
C(76)-K(1)-N(2)-Sm(1)	97.4(5)
C(16)#3-K(1)-N(2)-Sm(1)	-113.5(2)
C(74)-K(1)-N(2)-Sm(1)	90.8(3)
C(62)-C(63)-N(3)-N(4)	-178.8(5)
P(5)-C(63)-N(3)-N(4)	-0.5(7)
K(1)-C(63)-N(3)-N(4)	68.5(4)
C(62)-C(63)-N(3)-Sm(1)	-70(3)
P(5)-C(63)-N(3)-Sm(1)	108(2)
K(1)-C(63)-N(3)-Sm(1)	177(3)
C(62)-C(63)-N(3)-K(1)	112.7(5)
P(5)-C(63)-N(3)-K(1)	-69.0(4)
N(4)-K(1)-N(3)-C(63)	114.1(5)
N(2)-K(1)-N(3)-C(63)	-152.3(4)
C(7)-K(1)-N(3)-C(63)	-135.5(4)
C(72)-K(1)-N(3)-C(63)	74.8(18)
C(64)-K(1)-N(3)-C(63)	78.1(4)
C(71)-K(1)-N(3)-C(63)	27.3(6)
C(73)-K(1)-N(3)-C(63)	123.2(5)
N(1)-K(1)-N(3)-C(63)	-177.0(4)
C(76)-K(1)-N(3)-C(63)	47.8(5)
C(16)#3-K(1)-N(3)-C(63)	-41.0(4)
C(74)-K(1)-N(3)-C(63)	103.4(5)
N(2)-K(1)-N(3)-N(4)	93.6(3)
C(7)-K(1)-N(3)-N(4)	110.4(3)
C(72)-K(1)-N(3)-N(4)	-39.3(18)
C(64)-K(1)-N(3)-N(4)	-36.0(3)
C(71)-K(1)-N(3)-N(4)	-86.8(4)
C(73)-K(1)-N(3)-N(4)	9.1(5)
N(1)-K(1)-N(3)-N(4)	68.8(3)

C(76)-K(1)-N(3)-N(4)	-66.3(4)
C(16)#3-K(1)-N(3)-N(4)	-155.1(3)
C(74)-K(1)-N(3)-N(4)	-10.7(5)
N(4)-K(1)-N(3)-Sm(1)	-65.3(3)
N(2)-K(1)-N(3)-Sm(1)	28.26(14)
C(7)-K(1)-N(3)-Sm(1)	45.05(18)
C(72)-K(1)-N(3)-Sm(1)	-104.6(18)
C(64)-K(1)-N(3)-Sm(1)	-101.4(2)
C(71)-K(1)-N(3)-Sm(1)	-152.1(3)
C(73)-K(1)-N(3)-Sm(1)	-56.3(4)
N(1)-K(1)-N(3)-Sm(1)	3.50(14)
C(76)-K(1)-N(3)-Sm(1)	-131.7(3)
C(16)#3-K(1)-N(3)-Sm(1)	139.6(2)
C(74)-K(1)-N(3)-Sm(1)	-76.0(3)
C(65)-C(64)-N(4)-N(3)	178.3(5)
P(5)-C(64)-N(4)-N(3)	-0.9(6)
K(1)-C(64)-N(4)-N(3)	-83.2(4)
C(65)-C(64)-N(4)-Sm(1)	41.6(17)
P(5)-C(64)-N(4)-Sm(1)	-137.5(13)
K(1)-C(64)-N(4)-Sm(1)	140.2(15)
C(65)-C(64)-N(4)-K(1)	-98.6(5)
P(5)-C(64)-N(4)-K(1)	82.3(3)
C(63)-N(3)-N(4)-C(64)	0.9(7)
Sm(1)-N(3)-N(4)-C(64)	-169.0(5)
K(1)-N(3)-N(4)-C(64)	84.3(4)
C(63)-N(3)-N(4)-Sm(1)	169.9(5)
K(1)-N(3)-N(4)-Sm(1)	-106.73(13)
C(63)-N(3)-N(4)-K(1)	-83.4(5)
Sm(1)-N(3)-N(4)-K(1)	106.73(13)
N(2)-K(1)-N(4)-C(64)	172.7(4)

C(7)-K(1)-N(4)-C(64)	178.7(4)
N(3)-K(1)-N(4)-C(64)	-112.8(5)
C(72)-K(1)-N(4)-C(64)	56.8(6)
C(71)-K(1)-N(4)-C(64)	15.1(5)
C(73)-K(1)-N(4)-C(64)	72.8(4)
N(1)-K(1)-N(4)-C(64)	145.8(4)
C(76)-K(1)-N(4)-C(64)	14.6(4)
C(16)#3-K(1)-N(4)-C(64)	-85.0(4)
C(74)-K(1)-N(4)-C(64)	58.7(4)
N(2)-K(1)-N(4)-N(3)	-74.5(3)
C(7)-K(1)-N(4)-N(3)	-68.5(3)
C(72)-K(1)-N(4)-N(3)	169.6(5)
C(64)-K(1)-N(4)-N(3)	112.8(5)
C(71)-K(1)-N(4)-N(3)	127.9(4)
C(73)-K(1)-N(4)-N(3)	-174.5(3)
N(1)-K(1)-N(4)-N(3)	-101.4(3)
C(76)-K(1)-N(4)-N(3)	127.4(3)
C(16)#3-K(1)-N(4)-N(3)	27.8(4)
C(74)-K(1)-N(4)-N(3)	171.4(4)
N(2)-K(1)-N(4)-Sm(1)	3.14(14)
C(7)-K(1)-N(4)-Sm(1)	9.2(2)
N(3)-K(1)-N(4)-Sm(1)	77.7(3)
C(72)-K(1)-N(4)-Sm(1)	-112.7(4)
C(64)-K(1)-N(4)-Sm(1)	-169.6(4)
C(71)-K(1)-N(4)-Sm(1)	-154.4(3)
C(73)-K(1)-N(4)-Sm(1)	-96.8(3)
N(1)-K(1)-N(4)-Sm(1)	-23.71(15)
C(76)-K(1)-N(4)-Sm(1)	-154.9(2)
C(16)#3-K(1)-N(4)-Sm(1)	105.5(2)
C(74)-K(1)-N(4)-Sm(1)	-110.9(3)

C(48)-C(49)-N(5)-N(6)	-179.5(5)
P(4)-C(49)-N(5)-N(6)	1.6(7)
K(2)-C(49)-N(5)-N(6)	-89.8(5)
C(48)-C(49)-N(5)-Sm(1)	14(3)
P(4)-C(49)-N(5)-Sm(1)	-165(3)
K(2)-C(49)-N(5)-Sm(1)	104(3)
C(48)-C(49)-N(5)-K(2)	-89.7(6)
P(4)-C(49)-N(5)-K(2)	91.4(4)
N(8)-K(2)-N(5)-C(49)	174.5(5)
C(35)-K(2)-N(5)-C(49)	179.4(5)
N(7)-K(2)-N(5)-C(49)	146.2(5)
C(26)#4-K(2)-N(5)-C(49)	81.6(8)
C(27)#4-K(2)-N(5)-C(49)	88.1(10)
C(69)#4-K(2)-N(5)-C(49)	-97.6(5)
C(25)#4-K(2)-N(5)-C(49)	58.5(8)
C(28)#4-K(2)-N(5)-C(49)	46.5(16)
C(48)-K(2)-N(5)-C(49)	32.8(4)
C(24)#4-K(2)-N(5)-C(49)	34.7(9)
N(8)-K(2)-N(5)-N(6)	-72.9(3)
C(49)-K(2)-N(5)-N(6)	112.6(6)
C(35)-K(2)-N(5)-N(6)	-68.0(3)
N(7)-K(2)-N(5)-N(6)	-101.2(3)
C(26)#4-K(2)-N(5)-N(6)	-165.8(7)
C(27)#4-K(2)-N(5)-N(6)	-159.3(9)
C(69)#4-K(2)-N(5)-N(6)	15.0(4)
C(25)#4-K(2)-N(5)-N(6)	171.1(7)
C(28)#4-K(2)-N(5)-N(6)	159.2(16)
C(48)-K(2)-N(5)-N(6)	145.4(4)
C(24)#4-K(2)-N(5)-N(6)	147.3(8)
N(8)-K(2)-N(5)-Sm(1)	4.04(17)

C(49)-K(2)-N(5)-Sm(1)	-170.4(5)
C(35)-K(2)-N(5)-Sm(1)	9.0(2)
N(7)-K(2)-N(5)-Sm(1)	-24.21(16)
C(26)#4-K(2)-N(5)-Sm(1)	-88.9(7)
C(27)#4-K(2)-N(5)-Sm(1)	-82.3(9)
C(69)#4-K(2)-N(5)-Sm(1)	91.9(3)
C(25)#4-K(2)-N(5)-Sm(1)	-111.9(6)
C(28)#4-K(2)-N(5)-Sm(1)	-123.9(16)
C(48)-K(2)-N(5)-Sm(1)	-137.6(3)
C(24)#4-K(2)-N(5)-Sm(1)	-135.7(7)
C(51)-C(50)-N(6)-N(5)	-176.2(7)
P(4)-C(50)-N(6)-N(5)	2.5(7)
C(51)-C(50)-N(6)-Sm(1)	-31(4)
P(4)-C(50)-N(6)-Sm(1)	147(3)
C(49)-N(5)-N(6)-C(50)	-2.7(8)
Sm(1)-N(5)-N(6)-C(50)	175.1(5)
K(2)-N(5)-N(6)-C(50)	-76.5(5)
C(49)-N(5)-N(6)-Sm(1)	-177.7(5)
K(2)-N(5)-N(6)-Sm(1)	108.48(16)
C(37)-C(36)-N(7)-N(8)	-178.3(5)
P(3)-C(36)-N(7)-N(8)	-1.9(7)
K(2)-C(36)-N(7)-N(8)	65.1(4)
C(37)-C(36)-N(7)-Sm(1)	-70(2)
P(3)-C(36)-N(7)-Sm(1)	107(2)
K(2)-C(36)-N(7)-Sm(1)	174(2)
C(37)-C(36)-N(7)-K(2)	116.6(5)
P(3)-C(36)-N(7)-K(2)	-67.0(4)
N(8)-K(2)-N(7)-C(36)	114.7(5)
C(49)-K(2)-N(7)-C(36)	-145.0(4)
N(5)-K(2)-N(7)-C(36)	-158.8(4)

C(35)-K(2)-N(7)-C(36)	78.1(4)
C(26)#4-K(2)-N(7)-C(36)	-30.1(7)
C(27)#4-K(2)-N(7)-C(36)	-9.2(8)
C(69)#4-K(2)-N(7)-C(36)	112.6(4)
C(25)#4-K(2)-N(7)-C(36)	-51.5(7)
C(28)#4-K(2)-N(7)-C(36)	-7.2(9)
C(48)-K(2)-N(7)-C(36)	-119.8(4)
C(24)#4-K(2)-N(7)-C(36)	-55.0(8)
C(49)-K(2)-N(7)-N(8)	100.3(3)
N(5)-K(2)-N(7)-N(8)	86.5(3)
C(35)-K(2)-N(7)-N(8)	-36.6(3)
C(26)#4-K(2)-N(7)-N(8)	-144.9(7)
C(27)#4-K(2)-N(7)-N(8)	-124.0(7)
C(69)#4-K(2)-N(7)-N(8)	-2.1(4)
C(25)#4-K(2)-N(7)-N(8)	-166.2(6)
C(28)#4-K(2)-N(7)-N(8)	-121.9(8)
C(48)-K(2)-N(7)-N(8)	125.5(3)
C(24)#4-K(2)-N(7)-N(8)	-169.8(7)
N(8)-K(2)-N(7)-Sm(1)	-63.8(3)
C(49)-K(2)-N(7)-Sm(1)	36.4(2)
N(5)-K(2)-N(7)-Sm(1)	22.67(15)
C(35)-K(2)-N(7)-Sm(1)	-100.4(3)
C(26)#4-K(2)-N(7)-Sm(1)	151.3(6)
C(27)#4-K(2)-N(7)-Sm(1)	172.2(7)
C(69)#4-K(2)-N(7)-Sm(1)	-66.0(3)
C(25)#4-K(2)-N(7)-Sm(1)	130.0(6)
C(28)#4-K(2)-N(7)-Sm(1)	174.2(8)
C(48)-K(2)-N(7)-Sm(1)	61.63(17)
C(24)#4-K(2)-N(7)-Sm(1)	126.4(7)
C(34)-C(35)-N(8)-N(7)	174.8(6)

P(3)-C(35)-N(8)-N(7)	-2.8(7)
K(2)-C(35)-N(8)-N(7)	-85.0(4)
C(34)-C(35)-N(8)-Sm(1)	55(2)
P(3)-C(35)-N(8)-Sm(1)	-122.3(16)
K(2)-C(35)-N(8)-Sm(1)	155.6(17)
C(34)-C(35)-N(8)-K(2)	-100.2(6)
P(3)-C(35)-N(8)-K(2)	82.1(4)
C(36)-N(7)-N(8)-C(35)	3.0(7)
Sm(1)-N(7)-N(8)-C(35)	-164.5(5)
K(2)-N(7)-N(8)-C(35)	81.6(4)
C(36)-N(7)-N(8)-Sm(1)	167.5(5)
K(2)-N(7)-N(8)-Sm(1)	-113.96(15)
C(36)-N(7)-N(8)-K(2)	-78.6(5)
Sm(1)-N(7)-N(8)-K(2)	113.96(15)
C(49)-K(2)-N(8)-C(35)	170.6(5)
N(5)-K(2)-N(8)-C(35)	168.2(5)
N(7)-K(2)-N(8)-C(35)	-112.9(6)
C(26)#4-K(2)-N(8)-C(35)	-76.0(7)
C(27)#4-K(2)-N(8)-C(35)	-51.1(8)
C(69)#4-K(2)-N(8)-C(35)	65.2(5)
C(25)#4-K(2)-N(8)-C(35)	-96.9(8)
C(28)#4-K(2)-N(8)-C(35)	-37.5(10)
C(48)-K(2)-N(8)-C(35)	-166.8(4)
C(24)#4-K(2)-N(8)-C(35)	-97.7(10)
C(49)-K(2)-N(8)-N(7)	-76.5(3)
N(5)-K(2)-N(8)-N(7)	-78.8(3)
C(35)-K(2)-N(8)-N(7)	112.9(6)
C(26)#4-K(2)-N(8)-N(7)	36.9(7)
C(27)#4-K(2)-N(8)-N(7)	61.8(7)
C(69)#4-K(2)-N(8)-N(7)	178.1(3)

C(25)#4-K(2)-N(8)-N(7)	16.0(7)
C(28)#4-K(2)-N(8)-N(7)	75.4(9)
C(48)-K(2)-N(8)-N(7)	-53.9(3)
C(24)#4-K(2)-N(8)-N(7)	15.2(10)
C(49)-K(2)-N(8)-Sm(1)	-1.7(2)
N(5)-K(2)-N(8)-Sm(1)	-4.08(17)
C(35)-K(2)-N(8)-Sm(1)	-172.3(6)
N(7)-K(2)-N(8)-Sm(1)	74.8(3)
C(26)#4-K(2)-N(8)-Sm(1)	111.7(6)
C(27)#4-K(2)-N(8)-Sm(1)	136.6(7)
C(69)#4-K(2)-N(8)-Sm(1)	-107.1(2)
C(25)#4-K(2)-N(8)-Sm(1)	90.8(7)
C(28)#4-K(2)-N(8)-Sm(1)	150.2(9)
C(48)-K(2)-N(8)-Sm(1)	20.9(2)
C(24)#4-K(2)-N(8)-Sm(1)	90.0(9)
C(23)-C(22)-N(9)-N(10)	176.4(5)
P(2)-C(22)-N(9)-N(10)	-1.2(7)
C(23)-C(22)-N(9)-Sm(1)	11(7)
P(2)-C(22)-N(9)-Sm(1)	-167(6)
C(20)-C(21)-N(10)-N(9)	178.3(5)
P(2)-C(21)-N(10)-N(9)	-1.9(7)
C(20)-C(21)-N(10)-Sm(1)	3(3)
P(2)-C(21)-N(10)-Sm(1)	-177(2)
C(22)-N(9)-N(10)-C(21)	2.0(7)
Sm(1)-N(9)-N(10)-C(21)	-179.0(5)
C(22)-N(9)-N(10)-Sm(1)	-179.0(5)
N(2)-C(7)-P(1)-C(8)	0.0(5)
C(6)-C(7)-P(1)-C(8)	177.7(6)
K(1)-C(7)-P(1)-C(8)	72.0(3)
N(2)-C(7)-P(1)-K(1)	-72.0(4)

C(6)-C(7)-P(1)-K(1)	105.7(6)
N(1)-C(8)-P(1)-C(7)	0.0(6)
C(9)-C(8)-P(1)-C(7)	179.1(7)
K(1)-C(8)-P(1)-C(7)	-59.1(2)
N(1)-C(8)-P(1)-K(1)	59.1(5)
C(9)-C(8)-P(1)-K(1)	-121.8(7)
N(4)-K(1)-P(1)-C(7)	57.9(3)
N(2)-K(1)-P(1)-C(7)	33.5(3)
N(3)-K(1)-P(1)-C(7)	30.8(3)
C(72)-K(1)-P(1)-C(7)	-155.6(3)
C(64)-K(1)-P(1)-C(7)	72.1(3)
C(71)-K(1)-P(1)-C(7)	-147.9(3)
C(73)-K(1)-P(1)-C(7)	179.0(4)
N(1)-K(1)-P(1)-C(7)	68.6(3)
C(76)-K(1)-P(1)-C(7)	-165.6(3)
C(16)#3-K(1)-P(1)-C(7)	-68.0(3)
C(74)-K(1)-P(1)-C(7)	162.3(3)
N(4)-K(1)-P(1)-C(8)	-38.3(3)
N(2)-K(1)-P(1)-C(8)	-62.7(3)
C(7)-K(1)-P(1)-C(8)	-96.2(3)
N(3)-K(1)-P(1)-C(8)	-65.4(3)
C(72)-K(1)-P(1)-C(8)	108.2(3)
C(64)-K(1)-P(1)-C(8)	-24.1(3)
C(71)-K(1)-P(1)-C(8)	116.0(3)
C(73)-K(1)-P(1)-C(8)	82.8(4)
N(1)-K(1)-P(1)-C(8)	-27.6(3)
C(76)-K(1)-P(1)-C(8)	98.2(3)
C(16)#3-K(1)-P(1)-C(8)	-164.2(3)
C(74)-K(1)-P(1)-C(8)	66.1(3)
N(9)-C(22)-P(2)-C(21)	0.2(5)

C(23)-C(22)-P(2)-C(21)	-177.3(6)
N(10)-C(21)-P(2)-C(22)	0.9(5)
C(20)-C(21)-P(2)-C(22)	-179.2(6)
N(7)-C(36)-P(3)-C(35)	0.3(5)
C(37)-C(36)-P(3)-C(35)	176.3(6)
K(2)-C(36)-P(3)-C(35)	-60.8(2)
N(7)-C(36)-P(3)-K(2)	61.1(5)
C(37)-C(36)-P(3)-K(2)	-122.9(6)
N(8)-C(35)-P(3)-C(36)	1.5(5)
C(34)-C(35)-P(3)-C(36)	-176.0(6)
K(2)-C(35)-P(3)-C(36)	72.0(3)
N(8)-C(35)-P(3)-K(2)	-70.5(4)
C(34)-C(35)-P(3)-K(2)	112.1(7)
N(8)-K(2)-P(3)-C(36)	-62.7(3)
C(49)-K(2)-P(3)-C(36)	-27.6(3)
N(5)-K(2)-P(3)-C(36)	-39.5(3)
C(35)-K(2)-P(3)-C(36)	-95.7(3)
N(7)-K(2)-P(3)-C(36)	-27.6(3)
C(26)#4-K(2)-P(3)-C(36)	78.9(5)
C(27)#4-K(2)-P(3)-C(36)	104.4(7)
C(69)#4-K(2)-P(3)-C(36)	-146.6(3)
C(25)#4-K(2)-P(3)-C(36)	70.3(4)
C(28)#4-K(2)-P(3)-C(36)	117.8(7)
C(48)-K(2)-P(3)-C(36)	1.5(3)
C(24)#4-K(2)-P(3)-C(36)	84.7(5)
N(8)-K(2)-P(3)-C(35)	32.9(3)
C(49)-K(2)-P(3)-C(35)	68.1(3)
N(5)-K(2)-P(3)-C(35)	56.2(3)
N(7)-K(2)-P(3)-C(35)	68.1(3)
C(26)#4-K(2)-P(3)-C(35)	174.6(5)

C(27)#4-K(2)-P(3)-C(35)	-159.9(7)
C(69)#4-K(2)-P(3)-C(35)	-51.0(3)
C(25)#4-K(2)-P(3)-C(35)	166.0(4)
C(28)#4-K(2)-P(3)-C(35)	-146.5(7)
C(48)-K(2)-P(3)-C(35)	97.2(3)
C(24)#4-K(2)-P(3)-C(35)	-179.7(5)
N(5)-C(49)-P(4)-C(50)	-0.2(5)
C(48)-C(49)-P(4)-C(50)	-178.9(6)
K(2)-C(49)-P(4)-C(50)	83.6(3)
N(5)-C(49)-P(4)-K(2)	-83.8(5)
C(48)-C(49)-P(4)-K(2)	97.5(6)
N(6)-C(50)-P(4)-C(49)	-1.3(5)
C(51)-C(50)-P(4)-C(49)	177.4(8)
N(6)-C(50)-P(4)-K(2)	55.8(5)
C(51)-C(50)-P(4)-K(2)	-125.5(7)
N(8)-K(2)-P(4)-C(49)	63.5(3)
N(5)-K(2)-P(4)-C(49)	34.0(3)
C(35)-K(2)-P(4)-C(49)	79.4(3)
N(7)-K(2)-P(4)-C(49)	39.2(3)
C(26)#4-K(2)-P(4)-C(49)	-58.3(4)
C(27)#4-K(2)-P(4)-C(49)	-89.1(10)
C(69)#4-K(2)-P(4)-C(49)	157.1(3)
C(25)#4-K(2)-P(4)-C(49)	-63.7(4)
C(28)#4-K(2)-P(4)-C(49)	-114.2(9)
C(48)-K(2)-P(4)-C(49)	-26.4(3)
C(24)#4-K(2)-P(4)-C(49)	-85.1(6)
N(8)-K(2)-P(4)-C(50)	-27.5(3)
C(49)-K(2)-P(4)-C(50)	-91.0(4)
N(5)-K(2)-P(4)-C(50)	-57.0(3)
C(35)-K(2)-P(4)-C(50)	-11.6(3)

N(7)-K(2)-P(4)-C(50)	-51.8(3)
C(26)#4-K(2)-P(4)-C(50)	-149.3(4)
C(27)#4-K(2)-P(4)-C(50)	179.9(10)
C(69)#4-K(2)-P(4)-C(50)	66.1(3)
C(25)#4-K(2)-P(4)-C(50)	-154.7(4)
C(28)#4-K(2)-P(4)-C(50)	154.8(9)
C(48)-K(2)-P(4)-C(50)	-117.4(3)
C(24)#4-K(2)-P(4)-C(50)	-176.1(6)
N(4)-C(64)-P(5)-C(63)	0.5(5)
C(65)-C(64)-P(5)-C(63)	-178.6(6)
K(1)-C(64)-P(5)-C(63)	67.6(2)
N(4)-C(64)-P(5)-K(1)	-67.0(4)
C(65)-C(64)-P(5)-K(1)	113.9(6)
N(3)-C(63)-P(5)-C(64)	0.0(5)
C(62)-C(63)-P(5)-C(64)	178.2(6)
K(1)-C(63)-P(5)-C(64)	-58.5(2)
N(3)-C(63)-P(5)-K(1)	58.4(4)
C(62)-C(63)-P(5)-K(1)	-123.3(6)
N(4)-K(1)-P(5)-C(64)	33.1(3)
N(2)-K(1)-P(5)-C(64)	62.3(3)
C(7)-K(1)-P(5)-C(64)	80.5(3)
N(3)-K(1)-P(5)-C(64)	69.9(3)
C(72)-K(1)-P(5)-C(64)	-102.9(4)
C(71)-K(1)-P(5)-C(64)	-114.6(3)
C(73)-K(1)-P(5)-C(64)	-70.9(4)
N(1)-K(1)-P(5)-C(64)	36.5(3)
C(76)-K(1)-P(5)-C(64)	-100.7(3)
C(16)#3-K(1)-P(5)-C(64)	171.2(3)
C(74)-K(1)-P(5)-C(64)	-62.1(3)
N(4)-K(1)-P(5)-C(63)	-65.4(3)

N(2)-K(1)-P(5)-C(63)	-36.2(2)
C(7)-K(1)-P(5)-C(63)	-18.0(3)
N(3)-K(1)-P(5)-C(63)	-28.6(3)
C(72)-K(1)-P(5)-C(63)	158.6(4)
C(64)-K(1)-P(5)-C(63)	-98.5(3)
C(71)-K(1)-P(5)-C(63)	146.9(3)
C(73)-K(1)-P(5)-C(63)	-169.4(3)
N(1)-K(1)-P(5)-C(63)	-62.0(2)
C(76)-K(1)-P(5)-C(63)	160.8(3)
C(16)#3-K(1)-P(5)-C(63)	72.7(3)
C(74)-K(1)-P(5)-C(63)	-160.6(3)
C(21)-N(10)-Sm(1)-N(2)	-45(2)
N(9)-N(10)-Sm(1)-N(2)	139.8(3)
C(21)-N(10)-Sm(1)-N(5)	99(2)
N(9)-N(10)-Sm(1)-N(5)	-76.1(4)
C(21)-N(10)-Sm(1)-N(9)	175(3)
C(21)-N(10)-Sm(1)-N(4)	-125(2)
N(9)-N(10)-Sm(1)-N(4)	59.7(3)
C(21)-N(10)-Sm(1)-N(6)	131(2)
N(9)-N(10)-Sm(1)-N(6)	-44.2(4)
C(21)-N(10)-Sm(1)-N(8)	69(2)
N(9)-N(10)-Sm(1)-N(8)	-106.6(3)
C(21)-N(10)-Sm(1)-N(1)	-43(2)
N(9)-N(10)-Sm(1)-N(1)	141.6(3)
C(21)-N(10)-Sm(1)-N(7)	40(2)
N(9)-N(10)-Sm(1)-N(7)	-135.5(3)
C(21)-N(10)-Sm(1)-N(3)	-135(2)
N(9)-N(10)-Sm(1)-N(3)	49.9(3)
C(21)-N(10)-Sm(1)-K(1)	-87(2)
N(9)-N(10)-Sm(1)-K(1)	97.2(3)

C(7)-N(2)-Sm(1)-N(10)	158.8(18)
N(1)-N(2)-Sm(1)-N(10)	3.5(4)
K(1)-N(2)-Sm(1)-N(10)	-80.7(2)
C(7)-N(2)-Sm(1)-N(5)	-1.9(19)
N(1)-N(2)-Sm(1)-N(5)	-157.1(3)
K(1)-N(2)-Sm(1)-N(5)	118.71(18)
C(7)-N(2)-Sm(1)-N(9)	-169.9(18)
N(1)-N(2)-Sm(1)-N(9)	34.9(4)
K(1)-N(2)-Sm(1)-N(9)	-49.3(3)
C(7)-N(2)-Sm(1)-N(4)	-117.1(19)
N(1)-N(2)-Sm(1)-N(4)	87.7(3)
K(1)-N(2)-Sm(1)-N(4)	3.46(16)
C(7)-N(2)-Sm(1)-N(6)	-17.4(19)
N(1)-N(2)-Sm(1)-N(6)	-172.6(3)
K(1)-N(2)-Sm(1)-N(6)	103.2(2)
C(7)-N(2)-Sm(1)-N(8)	73.9(19)
N(1)-N(2)-Sm(1)-N(8)	-81.3(3)
K(1)-N(2)-Sm(1)-N(8)	-165.55(16)
C(7)-N(2)-Sm(1)-N(1)	155(2)
K(1)-N(2)-Sm(1)-N(1)	-84.2(3)
C(7)-N(2)-Sm(1)-N(7)	75.5(19)
N(1)-N(2)-Sm(1)-N(7)	-79.7(3)
K(1)-N(2)-Sm(1)-N(7)	-163.87(18)
C(7)-N(2)-Sm(1)-N(3)	-86.6(19)
N(1)-N(2)-Sm(1)-N(3)	118.1(3)
K(1)-N(2)-Sm(1)-N(3)	33.95(16)
C(7)-N(2)-Sm(1)-K(1)	-120.6(19)
N(1)-N(2)-Sm(1)-K(1)	84.2(3)
C(49)-N(5)-Sm(1)-N(10)	-135(3)
N(6)-N(5)-Sm(1)-N(10)	58.0(5)

K(2)-N(5)-Sm(1)-N(10)	-34.2(4)
C(49)-N(5)-Sm(1)-N(2)	14(3)
N(6)-N(5)-Sm(1)-N(2)	-153.0(3)
K(2)-N(5)-Sm(1)-N(2)	114.83(19)
C(49)-N(5)-Sm(1)-N(9)	-176(3)
N(6)-N(5)-Sm(1)-N(9)	17.0(4)
K(2)-N(5)-Sm(1)-N(9)	-75.2(3)
C(49)-N(5)-Sm(1)-N(4)	95(3)
N(6)-N(5)-Sm(1)-N(4)	-71.7(3)
K(2)-N(5)-Sm(1)-N(4)	-163.80(16)
C(49)-N(5)-Sm(1)-N(6)	167(3)
K(2)-N(5)-Sm(1)-N(6)	-92.1(3)
C(49)-N(5)-Sm(1)-N(8)	-105(3)
N(6)-N(5)-Sm(1)-N(8)	87.8(3)
K(2)-N(5)-Sm(1)-N(8)	-4.35(18)
C(49)-N(5)-Sm(1)-N(1)	1(3)
N(6)-N(5)-Sm(1)-N(1)	-166.3(3)
K(2)-N(5)-Sm(1)-N(1)	101.6(2)
C(49)-N(5)-Sm(1)-N(7)	-74(3)
N(6)-N(5)-Sm(1)-N(7)	119.5(3)
K(2)-N(5)-Sm(1)-N(7)	27.34(18)
C(49)-N(5)-Sm(1)-N(3)	91(3)
N(6)-N(5)-Sm(1)-N(3)	-76.0(3)
K(2)-N(5)-Sm(1)-N(3)	-168.11(19)
C(49)-N(5)-Sm(1)-K(1)	52(3)
N(6)-N(5)-Sm(1)-K(1)	-115.1(3)
K(2)-N(5)-Sm(1)-K(1)	152.73(12)
C(22)-N(9)-Sm(1)-N(10)	166(7)
C(22)-N(9)-Sm(1)-N(2)	105(7)
N(10)-N(9)-Sm(1)-N(2)	-60.5(4)

C(22)-N(9)-Sm(1)-N(5)	-59(7)
N(10)-N(9)-Sm(1)-N(5)	135.0(3)
C(22)-N(9)-Sm(1)-N(4)	50(7)
N(10)-N(9)-Sm(1)-N(4)	-115.8(3)
C(22)-N(9)-Sm(1)-N(6)	-50(7)
N(10)-N(9)-Sm(1)-N(6)	143.8(3)
C(22)-N(9)-Sm(1)-N(8)	-127(7)
N(10)-N(9)-Sm(1)-N(8)	67.0(3)
C(22)-N(9)-Sm(1)-N(1)	124(7)
N(10)-N(9)-Sm(1)-N(1)	-42.0(3)
C(22)-N(9)-Sm(1)-N(7)	-147(7)
N(10)-N(9)-Sm(1)-N(7)	47.1(3)
C(22)-N(9)-Sm(1)-N(3)	29(7)
N(10)-N(9)-Sm(1)-N(3)	-137.1(3)
C(22)-N(9)-Sm(1)-K(1)	74(7)
N(10)-N(9)-Sm(1)-K(1)	-92.2(3)
C(64)-N(4)-Sm(1)-N(10)	-22.9(15)
N(3)-N(4)-Sm(1)-N(10)	-162.7(3)
K(1)-N(4)-Sm(1)-N(10)	115.56(19)
C(64)-N(4)-Sm(1)-N(2)	-142.0(15)
N(3)-N(4)-Sm(1)-N(2)	78.3(3)
K(1)-N(4)-Sm(1)-N(2)	-3.52(16)
C(64)-N(4)-Sm(1)-N(5)	131.2(14)
N(3)-N(4)-Sm(1)-N(5)	-8.5(3)
K(1)-N(4)-Sm(1)-N(5)	-90.3(2)
C(64)-N(4)-Sm(1)-N(9)	5.3(14)
N(3)-N(4)-Sm(1)-N(9)	-134.5(3)
K(1)-N(4)-Sm(1)-N(9)	143.8(2)
C(64)-N(4)-Sm(1)-N(6)	100.8(15)
N(3)-N(4)-Sm(1)-N(6)	-38.9(3)

K(1)-N(4)-Sm(1)-N(6)	-120.69(18)
C(64)-N(4)-Sm(1)-N(8)	12.6(17)
N(3)-N(4)-Sm(1)-N(8)	-127.2(4)
K(1)-N(4)-Sm(1)-N(8)	151.0(4)
C(64)-N(4)-Sm(1)-N(1)	-110.6(15)
N(3)-N(4)-Sm(1)-N(1)	109.6(3)
K(1)-N(4)-Sm(1)-N(1)	27.84(17)
C(64)-N(4)-Sm(1)-N(7)	-90.8(16)
N(3)-N(4)-Sm(1)-N(7)	129.4(6)
K(1)-N(4)-Sm(1)-N(7)	47.6(6)
C(64)-N(4)-Sm(1)-N(3)	139.8(16)
K(1)-N(4)-Sm(1)-N(3)	-81.8(3)
C(64)-N(4)-Sm(1)-K(1)	-138.5(15)
N(3)-N(4)-Sm(1)-K(1)	81.8(3)
C(50)-N(6)-Sm(1)-N(10)	68(3)
N(5)-N(6)-Sm(1)-N(10)	-145.0(3)
C(50)-N(6)-Sm(1)-N(2)	-116(3)
N(5)-N(6)-Sm(1)-N(2)	31.0(4)
C(50)-N(6)-Sm(1)-N(5)	-147(3)
C(50)-N(6)-Sm(1)-N(9)	47(3)
N(5)-N(6)-Sm(1)-N(9)	-166.8(3)
C(50)-N(6)-Sm(1)-N(4)	-28(3)
N(5)-N(6)-Sm(1)-N(4)	118.4(3)
C(50)-N(6)-Sm(1)-N(8)	128(3)
N(5)-N(6)-Sm(1)-N(8)	-85.1(3)
C(50)-N(6)-Sm(1)-N(1)	-123(3)
N(5)-N(6)-Sm(1)-N(1)	23.6(5)
C(50)-N(6)-Sm(1)-N(7)	155(3)
N(5)-N(6)-Sm(1)-N(7)	-58.4(3)
C(50)-N(6)-Sm(1)-N(3)	-47(3)

N(5)-N(6)-Sm(1)-N(3)	99.4(3)
C(50)-N(6)-Sm(1)-K(1)	-68(3)
N(5)-N(6)-Sm(1)-K(1)	78.5(3)
C(35)-N(8)-Sm(1)-N(10)	13.9(17)
N(7)-N(8)-Sm(1)-N(10)	-110.4(4)
K(2)-N(8)-Sm(1)-N(10)	167.5(3)
C(35)-N(8)-Sm(1)-N(2)	127.5(17)
N(7)-N(8)-Sm(1)-N(2)	3.3(4)
K(2)-N(8)-Sm(1)-N(2)	-78.9(2)
C(35)-N(8)-Sm(1)-N(5)	-149.0(18)
N(7)-N(8)-Sm(1)-N(5)	86.8(3)
K(2)-N(8)-Sm(1)-N(5)	4.6(2)
C(35)-N(8)-Sm(1)-N(9)	-16.5(18)
N(7)-N(8)-Sm(1)-N(9)	-140.8(3)
K(2)-N(8)-Sm(1)-N(9)	137.1(2)
C(35)-N(8)-Sm(1)-N(4)	-24(2)
N(7)-N(8)-Sm(1)-N(4)	-147.8(4)
K(2)-N(8)-Sm(1)-N(4)	130.1(3)
C(35)-N(8)-Sm(1)-N(6)	-116.8(18)
N(7)-N(8)-Sm(1)-N(6)	118.9(3)
K(2)-N(8)-Sm(1)-N(6)	36.8(2)
C(35)-N(8)-Sm(1)-N(1)	94.7(18)
N(7)-N(8)-Sm(1)-N(1)	-29.6(4)
K(2)-N(8)-Sm(1)-N(1)	-111.7(2)
C(35)-N(8)-Sm(1)-N(7)	124.2(19)
K(2)-N(8)-Sm(1)-N(7)	-82.2(3)
C(35)-N(8)-Sm(1)-N(3)	-105.7(18)
N(7)-N(8)-Sm(1)-N(3)	130.1(4)
K(2)-N(8)-Sm(1)-N(3)	47.9(5)
C(35)-N(8)-Sm(1)-K(1)	102.3(17)

N(7)-N(8)-Sm(1)-K(1)	-21.9(5)
K(2)-N(8)-Sm(1)-K(1)	-104.1(3)
C(8)-N(1)-Sm(1)-N(10)	54(4)
N(2)-N(1)-Sm(1)-N(10)	-176.9(3)
K(1)-N(1)-Sm(1)-N(10)	-113.41(17)
C(8)-N(1)-Sm(1)-N(2)	-129(4)
K(1)-N(1)-Sm(1)-N(2)	63.5(3)
C(8)-N(1)-Sm(1)-N(5)	-103(4)
N(2)-N(1)-Sm(1)-N(5)	26.4(4)
K(1)-N(1)-Sm(1)-N(5)	89.87(19)
C(8)-N(1)-Sm(1)-N(9)	75(4)
N(2)-N(1)-Sm(1)-N(9)	-156.3(3)
K(1)-N(1)-Sm(1)-N(9)	-92.84(17)
C(8)-N(1)-Sm(1)-N(4)	143(4)
N(2)-N(1)-Sm(1)-N(4)	-87.8(3)
K(1)-N(1)-Sm(1)-N(4)	-24.36(15)
C(8)-N(1)-Sm(1)-N(6)	-116(4)
N(2)-N(1)-Sm(1)-N(6)	12.6(5)
K(1)-N(1)-Sm(1)-N(6)	76.1(3)
C(8)-N(1)-Sm(1)-N(8)	-17(4)
N(2)-N(1)-Sm(1)-N(8)	112.5(3)
K(1)-N(1)-Sm(1)-N(8)	175.96(14)
C(8)-N(1)-Sm(1)-N(7)	-31(4)
N(2)-N(1)-Sm(1)-N(7)	97.7(3)
K(1)-N(1)-Sm(1)-N(7)	161.15(17)
C(8)-N(1)-Sm(1)-N(3)	172(4)
N(2)-N(1)-Sm(1)-N(3)	-59.4(3)
K(1)-N(1)-Sm(1)-N(3)	4.10(16)
C(8)-N(1)-Sm(1)-K(1)	168(4)
N(2)-N(1)-Sm(1)-K(1)	-63.5(3)

C(36)-N(7)-Sm(1)-N(10)	-49(2)
N(8)-N(7)-Sm(1)-N(10)	63.9(3)
K(2)-N(7)-Sm(1)-N(10)	124.55(19)
C(36)-N(7)-Sm(1)-N(2)	70(2)
N(8)-N(7)-Sm(1)-N(2)	-177.1(3)
K(2)-N(7)-Sm(1)-N(2)	-116.53(17)
C(36)-N(7)-Sm(1)-N(5)	161(2)
N(8)-N(7)-Sm(1)-N(5)	-86.1(3)
K(2)-N(7)-Sm(1)-N(5)	-25.49(16)
C(36)-N(7)-Sm(1)-N(9)	-72(2)
N(8)-N(7)-Sm(1)-N(9)	41.3(4)
K(2)-N(7)-Sm(1)-N(9)	101.85(18)
C(36)-N(7)-Sm(1)-N(4)	19(3)
N(8)-N(7)-Sm(1)-N(4)	132.4(6)
K(2)-N(7)-Sm(1)-N(4)	-167.0(5)
C(36)-N(7)-Sm(1)-N(6)	-172(2)
N(8)-N(7)-Sm(1)-N(6)	-59.1(3)
K(2)-N(7)-Sm(1)-N(6)	1.52(19)
C(36)-N(7)-Sm(1)-N(8)	-113(2)
K(2)-N(7)-Sm(1)-N(8)	60.6(3)
C(36)-N(7)-Sm(1)-N(1)	39(2)
N(8)-N(7)-Sm(1)-N(1)	152.1(3)
K(2)-N(7)-Sm(1)-N(1)	-147.29(18)
C(36)-N(7)-Sm(1)-N(3)	119(2)
N(8)-N(7)-Sm(1)-N(3)	-128.2(4)
K(2)-N(7)-Sm(1)-N(3)	-67.6(5)
C(36)-N(7)-Sm(1)-K(1)	57(2)
N(8)-N(7)-Sm(1)-K(1)	169.5(3)
K(2)-N(7)-Sm(1)-K(1)	-129.90(12)
C(63)-N(3)-Sm(1)-N(10)	-93(3)

N(4)-N(3)-Sm(1)-N(10)	19.6(4)
K(1)-N(3)-Sm(1)-N(10)	84.4(2)
C(63)-N(3)-Sm(1)-N(2)	152(3)
N(4)-N(3)-Sm(1)-N(2)	-96.1(3)
K(1)-N(3)-Sm(1)-N(2)	-31.31(16)
C(63)-N(3)-Sm(1)-N(5)	60(3)
N(4)-N(3)-Sm(1)-N(5)	172.3(3)
K(1)-N(3)-Sm(1)-N(5)	-122.97(17)
C(63)-N(3)-Sm(1)-N(9)	-69(3)
N(4)-N(3)-Sm(1)-N(9)	43.4(3)
K(1)-N(3)-Sm(1)-N(9)	108.19(18)
C(63)-N(3)-Sm(1)-N(4)	-112(3)
K(1)-N(3)-Sm(1)-N(4)	64.8(3)
C(63)-N(3)-Sm(1)-N(6)	29(3)
N(4)-N(3)-Sm(1)-N(6)	141.2(3)
K(1)-N(3)-Sm(1)-N(6)	-154.01(19)
C(63)-N(3)-Sm(1)-N(8)	18(3)
N(4)-N(3)-Sm(1)-N(8)	130.1(4)
K(1)-N(3)-Sm(1)-N(8)	-165.1(3)
C(63)-N(3)-Sm(1)-N(1)	179(100)
N(4)-N(3)-Sm(1)-N(1)	-69.0(3)
K(1)-N(3)-Sm(1)-N(1)	-4.24(17)
C(63)-N(3)-Sm(1)-N(7)	101(3)
N(4)-N(3)-Sm(1)-N(7)	-146.7(4)
K(1)-N(3)-Sm(1)-N(7)	-81.9(4)
C(63)-N(3)-Sm(1)-K(1)	-177(3)
N(4)-N(3)-Sm(1)-K(1)	-64.8(3)
N(4)-K(1)-Sm(1)-N(10)	-69.2(2)
N(2)-K(1)-Sm(1)-N(10)	116.0(2)
C(7)-K(1)-Sm(1)-N(10)	121.6(2)

N(3)-K(1)-Sm(1)-N(10)	-113.9(2)
C(72)-K(1)-Sm(1)-N(10)	51.2(3)
C(64)-K(1)-Sm(1)-N(10)	-64.05(19)
C(71)-K(1)-Sm(1)-N(10)	9.2(7)
C(73)-K(1)-Sm(1)-N(10)	36.7(3)
N(1)-K(1)-Sm(1)-N(10)	71.9(2)
C(76)-K(1)-Sm(1)-N(10)	-28.5(3)
C(16)#3-K(1)-Sm(1)-N(10)	-162.0(2)
C(74)-K(1)-Sm(1)-N(10)	10.9(3)
N(4)-K(1)-Sm(1)-N(2)	174.7(2)
C(7)-K(1)-Sm(1)-N(2)	5.5(2)
N(3)-K(1)-Sm(1)-N(2)	130.1(2)
C(72)-K(1)-Sm(1)-N(2)	-64.9(3)
C(64)-K(1)-Sm(1)-N(2)	179.9(2)
C(71)-K(1)-Sm(1)-N(2)	-106.8(7)
C(73)-K(1)-Sm(1)-N(2)	-79.4(3)
N(1)-K(1)-Sm(1)-N(2)	-44.1(2)
C(76)-K(1)-Sm(1)-N(2)	-144.6(3)
C(16)#3-K(1)-Sm(1)-N(2)	82.0(3)
C(74)-K(1)-Sm(1)-N(2)	-105.1(4)
N(4)-K(1)-Sm(1)-N(5)	106.7(2)
N(2)-K(1)-Sm(1)-N(5)	-68.0(2)
C(7)-K(1)-Sm(1)-N(5)	-62.5(2)
N(3)-K(1)-Sm(1)-N(5)	62.1(2)
C(72)-K(1)-Sm(1)-N(5)	-132.9(3)
C(64)-K(1)-Sm(1)-N(5)	111.89(19)
C(71)-K(1)-Sm(1)-N(5)	-174.8(7)
C(73)-K(1)-Sm(1)-N(5)	-147.4(3)
N(1)-K(1)-Sm(1)-N(5)	-112.2(2)
C(76)-K(1)-Sm(1)-N(5)	147.4(3)

C(16)#3-K(1)-Sm(1)-N(5)	13.9(2)
C(74)-K(1)-Sm(1)-N(5)	-173.2(3)
N(4)-K(1)-Sm(1)-N(9)	-36.3(2)
N(2)-K(1)-Sm(1)-N(9)	149.0(2)
C(7)-K(1)-Sm(1)-N(9)	154.5(2)
N(3)-K(1)-Sm(1)-N(9)	-80.9(2)
C(72)-K(1)-Sm(1)-N(9)	84.1(3)
C(64)-K(1)-Sm(1)-N(9)	-31.11(19)
C(71)-K(1)-Sm(1)-N(9)	42.2(7)
C(73)-K(1)-Sm(1)-N(9)	69.6(3)
N(1)-K(1)-Sm(1)-N(9)	104.8(2)
C(76)-K(1)-Sm(1)-N(9)	4.4(3)
C(16)#3-K(1)-Sm(1)-N(9)	-129.1(2)
C(74)-K(1)-Sm(1)-N(9)	43.8(3)
N(2)-K(1)-Sm(1)-N(4)	-174.7(2)
C(7)-K(1)-Sm(1)-N(4)	-169.2(2)
N(3)-K(1)-Sm(1)-N(4)	-44.6(2)
C(72)-K(1)-Sm(1)-N(4)	120.4(3)
C(64)-K(1)-Sm(1)-N(4)	5.2(2)
C(71)-K(1)-Sm(1)-N(4)	78.5(7)
C(73)-K(1)-Sm(1)-N(4)	105.9(3)
N(1)-K(1)-Sm(1)-N(4)	141.1(2)
C(76)-K(1)-Sm(1)-N(4)	40.7(3)
C(16)#3-K(1)-Sm(1)-N(4)	-92.8(3)
C(74)-K(1)-Sm(1)-N(4)	80.1(4)
N(4)-K(1)-Sm(1)-N(6)	74.1(2)
N(2)-K(1)-Sm(1)-N(6)	-100.7(2)
C(7)-K(1)-Sm(1)-N(6)	-95.1(2)
N(3)-K(1)-Sm(1)-N(6)	29.4(2)
C(72)-K(1)-Sm(1)-N(6)	-165.5(3)

C(64)-K(1)-Sm(1)-N(6)	79.2(2)
C(71)-K(1)-Sm(1)-N(6)	152.5(7)
C(73)-K(1)-Sm(1)-N(6)	180.0(3)
N(1)-K(1)-Sm(1)-N(6)	-144.8(2)
C(76)-K(1)-Sm(1)-N(6)	114.8(3)
C(16)#3-K(1)-Sm(1)-N(6)	-18.7(3)
C(74)-K(1)-Sm(1)-N(6)	154.2(4)
N(4)-K(1)-Sm(1)-N(8)	-150.9(3)
N(2)-K(1)-Sm(1)-N(8)	34.3(3)
C(7)-K(1)-Sm(1)-N(8)	39.9(3)
N(3)-K(1)-Sm(1)-N(8)	164.4(3)
C(72)-K(1)-Sm(1)-N(8)	-30.5(4)
C(64)-K(1)-Sm(1)-N(8)	-145.8(3)
C(71)-K(1)-Sm(1)-N(8)	-72.5(7)
C(73)-K(1)-Sm(1)-N(8)	-45.0(4)
N(1)-K(1)-Sm(1)-N(8)	-9.8(3)
C(76)-K(1)-Sm(1)-N(8)	-110.2(4)
C(16)#3-K(1)-Sm(1)-N(8)	116.3(3)
C(74)-K(1)-Sm(1)-N(8)	-70.8(4)
N(4)-K(1)-Sm(1)-N(1)	-141.1(2)
N(2)-K(1)-Sm(1)-N(1)	44.1(2)
C(7)-K(1)-Sm(1)-N(1)	49.7(2)
N(3)-K(1)-Sm(1)-N(1)	174.2(2)
C(72)-K(1)-Sm(1)-N(1)	-20.7(3)
C(64)-K(1)-Sm(1)-N(1)	-136.0(2)
C(71)-K(1)-Sm(1)-N(1)	-62.7(7)
C(73)-K(1)-Sm(1)-N(1)	-35.2(3)
C(76)-K(1)-Sm(1)-N(1)	-100.4(3)
C(16)#3-K(1)-Sm(1)-N(1)	126.1(3)
C(74)-K(1)-Sm(1)-N(1)	-61.0(4)

N(4)-K(1)-Sm(1)-N(7)	-164.9(2)
N(2)-K(1)-Sm(1)-N(7)	20.4(2)
C(7)-K(1)-Sm(1)-N(7)	25.9(2)
N(3)-K(1)-Sm(1)-N(7)	150.5(2)
C(72)-K(1)-Sm(1)-N(7)	-44.5(3)
C(64)-K(1)-Sm(1)-N(7)	-159.7(2)
C(71)-K(1)-Sm(1)-N(7)	-86.4(7)
C(73)-K(1)-Sm(1)-N(7)	-58.9(3)
N(1)-K(1)-Sm(1)-N(7)	-23.7(2)
C(76)-K(1)-Sm(1)-N(7)	-124.2(3)
C(16)#3-K(1)-Sm(1)-N(7)	102.4(2)
C(74)-K(1)-Sm(1)-N(7)	-84.7(4)
N(4)-K(1)-Sm(1)-N(3)	44.6(2)
N(2)-K(1)-Sm(1)-N(3)	-130.1(2)
C(7)-K(1)-Sm(1)-N(3)	-124.6(2)
C(72)-K(1)-Sm(1)-N(3)	165.0(3)
C(64)-K(1)-Sm(1)-N(3)	49.8(2)
C(71)-K(1)-Sm(1)-N(3)	123.1(7)
C(73)-K(1)-Sm(1)-N(3)	150.5(3)
N(1)-K(1)-Sm(1)-N(3)	-174.2(2)
C(76)-K(1)-Sm(1)-N(3)	85.3(3)
C(16)#3-K(1)-Sm(1)-N(3)	-48.1(2)
C(74)-K(1)-Sm(1)-N(3)	124.8(4)

Symmetry transformations used to generate equivalent atoms:

#1 $-x+3/2, -y+1, z-1/2$ #2 $-x+2, y+1/2, -z+1/2$

#3 $-x+3/2, -y+1, z+1/2$ #4 $-x+2, y-1/2, -z+1/2$

4.10 Crystal structural analysis data for **12**

Table 1. Crystal data and structure refinement for **12**.

Identification code	exp_738
Empirical formula	C ₅₆ H ₁₀₄ Cl ₂ N ₈ O ₄ P ₄ Pr ₂
Formula weight	1430.07
Temperature	110(14) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 10.8923(10) Å alpha = 105.787(7) deg. b = 12.7350(12) Å beta = 104.523(7) deg. c = 14.5804(9) Å gamma = 108.687(8) deg.
Volume	1712.2(3) Å ³
Z, Calculated density	1, 1.387 Mg/m ³
Absorption coefficient	1.623 mm ⁻¹
F(000)	740
Crystal size	0.2100 x 0.0900 x 0.0600 mm
Theta range for data collection	2.95 to 25.12 deg.
Limiting indices	-12 ≤ h ≤ 13, -15 ≤ k ≤ 15, -12 ≤ l ≤ 17
Reflections collected / unique	12116 / 6107 [R(int) = 0.0599]
Completeness to theta = 25.12	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.87808
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6107 / 42 / 389
Goodness-of-fit on F ²	1.072
Final R indices [I > 2σ(I)]	R1 = 0.0782, wR2 = 0.1906
R indices (all data)	R1 = 0.1029, wR2 = 0.2146
Largest diff. peak and hole	3.180 and -1.477 e.Å ⁻³

Table 3. Bond lengths [Å] and angles [deg] for **12**.

C(8)-C(7)	1.568(13)
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
Pr(1)-N(2)	2.442(8)
Pr(1)-N(3)	2.445(8)
Pr(1)-N(4)	2.447(7)
Pr(1)-N(1)	2.478(8)
Pr(1)-O(1)	2.494(7)
Pr(1)-O(2)	2.572(7)
Pr(1)-Cl(1)	2.879(3)
Pr(1)-Cl(1)#1	2.881(3)
Pr(2)-N(2)	2.080(10)
Pr(2)-N(4)	2.366(9)
Pr(2)-N(1)	2.380(10)
Pr(2)-Cl(1)	2.486(7)
Pr(2)-O(1)	2.584(9)
Pr(2)-N(3)	2.725(10)
Pr(2)-Cl(1)#1	3.282(7)
P(1)-C(15)	1.745(9)
P(1)-C(16)	1.763(10)
P(2)-C(5)	1.747(10)
P(2)-C(6)	1.759(10)
N(1)-C(6)	1.334(13)
N(1)-N(2)	1.379(11)
N(3)-C(16)	1.326(12)
N(3)-N(4)	1.373(11)

N(4)-C(15)	1.332(12)
N(2)-C(5)	1.346(12)
O(1)-C(28)	1.471(12)
O(1)-C(25)	1.489(12)
O(2)-C(24)	1.449(12)
O(2)-C(21)	1.457(13)
C(15)-C(12)	1.539(14)
C(7)-C(10)	1.498(15)
C(7)-C(6)	1.531(13)
C(7)-C(9)	1.544(14)
C(16)-C(17)	1.489(15)
C(14)-C(12)	1.535(15)
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(12)-C(11)	1.511(17)
C(12)-C(13)	1.528(16)
C(5)-C(1)	1.537(14)
C(28)-C(27)	1.511(17)
C(28)-H(28A)	0.9700
C(28)-H(28B)	0.9700
C(4)-C(1)	1.577(16)
C(4)-H(4A)	0.9600
C(4)-H(4B)	0.9600
C(4)-H(4C)	0.9600
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600

C(9)-H(9C)	0.9600
C(17)-C(18')	1.40(3)
C(17)-C(18)	1.43(3)
C(17)-C(20)	1.48(3)
C(17)-C(20')	1.58(3)
C(17)-C(19')	1.67(3)
C(17)-C(19)	1.70(3)
C(3)-C(1)	1.545(16)
C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600
C(3)-H(3C)	0.9600
C(1)-C(2)	1.443(17)
Cl(1)-Pr(1)#1	2.881(2)
Cl(1)-Pr(2)#1	3.282(7)
C(24)-C(23)	1.531(15)
C(24)-H(24A)	0.9700
C(24)-H(24B)	0.9700
C(23)-C(22)	1.464(18)
C(23)-H(23A)	0.9700
C(23)-H(23B)	0.9700
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(21)-C(22)	1.534(17)
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(2)-H(2A)	0.9600
C(2)-H(2B)	0.9600

C(2)-H(2C)	0.9600
C(26)-C(27)	1.50(2)
C(26)-C(25)	1.521(15)
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(18')-H(18D)	0.9600
C(18')-H(18E)	0.9600
C(18')-H(18F)	0.9600
C(19')-H(19D)	0.9600
C(19')-H(19E)	0.9600
C(19')-H(19F)	0.9600
C(20')-H(20D)	0.9600
C(20')-H(20E)	0.9600
C(20')-H(20F)	0.9600

C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
N(2)-Pr(1)-N(3)	115.8(3)
N(2)-Pr(1)-N(4)	94.3(3)
N(3)-Pr(1)-N(4)	32.6(3)
N(2)-Pr(1)-N(1)	32.5(3)
N(3)-Pr(1)-N(1)	88.7(3)
N(4)-Pr(1)-N(1)	79.2(3)
N(2)-Pr(1)-O(1)	77.9(3)
N(3)-Pr(1)-O(1)	161.8(3)
N(4)-Pr(1)-O(1)	165.1(3)
N(1)-Pr(1)-O(1)	99.5(2)
N(2)-Pr(1)-O(2)	100.8(2)
N(3)-Pr(1)-O(2)	91.7(3)
N(4)-Pr(1)-O(2)	121.1(3)
N(1)-Pr(1)-O(2)	84.2(3)
O(1)-Pr(1)-O(2)	73.1(3)
N(2)-Pr(1)-Cl(1)	95.92(19)
N(3)-Pr(1)-Cl(1)	105.14(19)
N(4)-Pr(1)-Cl(1)	84.00(18)
N(1)-Pr(1)-Cl(1)	122.3(2)
O(1)-Pr(1)-Cl(1)	84.27(18)
O(2)-Pr(1)-Cl(1)	148.12(18)
N(2)-Pr(1)-Cl(1)#1	157.0(2)
N(3)-Pr(1)-Cl(1)#1	86.96(19)

N(4)-Pr(1)-Cl(1)#1	104.43(19)
N(1)-Pr(1)-Cl(1)#1	164.5(2)
O(1)-Pr(1)-Cl(1)#1	80.79(17)
O(2)-Pr(1)-Cl(1)#1	81.03(17)
Cl(1)-Pr(1)-Cl(1)#1	73.25(9)
N(2)-Pr(2)-N(4)	107.3(4)
N(2)-Pr(2)-N(1)	35.2(3)
N(4)-Pr(2)-N(1)	82.9(3)
N(2)-Pr(2)-Cl(1)	120.2(4)
N(4)-Pr(2)-Cl(1)	95.0(3)
N(1)-Pr(2)-Cl(1)	149.5(4)
N(2)-Pr(2)-O(1)	82.7(3)
N(4)-Pr(2)-O(1)	163.5(4)
N(1)-Pr(2)-O(1)	99.6(3)
Cl(1)-Pr(2)-O(1)	91.0(3)
N(2)-Pr(2)-N(3)	118.4(4)
N(4)-Pr(2)-N(3)	30.2(3)
N(1)-Pr(2)-N(3)	84.5(3)
Cl(1)-Pr(2)-N(3)	108.7(3)
O(1)-Pr(2)-N(3)	133.4(4)
N(2)-Pr(2)-Cl(1)#1	152.6(4)
N(4)-Pr(2)-Cl(1)#1	95.3(3)
N(1)-Pr(2)-Cl(1)#1	138.8(4)
Cl(1)-Pr(2)-Cl(1)#1	71.62(17)
O(1)-Pr(2)-Cl(1)#1	72.0(2)
N(3)-Pr(2)-Cl(1)#1	74.9(2)
C(15)-P(1)-C(16)	87.0(5)
C(5)-P(2)-C(6)	86.7(5)
C(6)-N(1)-N(2)	112.0(8)
C(6)-N(1)-Pr(2)	158.4(8)

N(2)-N(1)-Pr(2)	60.4(5)
C(6)-N(1)-Pr(1)	168.5(7)
N(2)-N(1)-Pr(1)	72.3(5)
Pr(2)-N(1)-Pr(1)	15.66(18)
C(16)-N(3)-N(4)	112.6(8)
C(16)-N(3)-Pr(1)	173.6(7)
N(4)-N(3)-Pr(1)	73.8(4)
C(16)-N(3)-Pr(2)	172.8(7)
N(4)-N(3)-Pr(2)	60.3(4)
Pr(1)-N(3)-Pr(2)	13.52(15)
C(15)-N(4)-N(3)	113.6(7)
C(15)-N(4)-Pr(2)	156.9(7)
N(3)-N(4)-Pr(2)	89.5(5)
C(15)-N(4)-Pr(1)	172.8(7)
N(3)-N(4)-Pr(1)	73.6(5)
Pr(2)-N(4)-Pr(1)	15.86(18)
C(5)-N(2)-N(1)	113.1(8)
C(5)-N(2)-Pr(2)	152.9(7)
N(1)-N(2)-Pr(2)	84.4(5)
C(5)-N(2)-Pr(1)	167.2(7)
N(1)-N(2)-Pr(1)	75.2(5)
Pr(2)-N(2)-Pr(1)	14.3(2)
C(28)-O(1)-C(25)	109.0(7)
C(28)-O(1)-Pr(1)	122.7(5)
C(25)-O(1)-Pr(1)	127.4(6)
C(28)-O(1)-Pr(2)	123.1(6)
C(25)-O(1)-Pr(2)	121.4(6)
Pr(1)-O(1)-Pr(2)	15.00(16)
C(24)-O(2)-C(21)	109.0(8)
C(24)-O(2)-Pr(1)	126.4(6)

C(21)-O(2)-Pr(1)	123.5(6)
N(4)-C(15)-C(12)	119.3(8)
N(4)-C(15)-P(1)	113.4(7)
C(12)-C(15)-P(1)	127.4(8)
C(10)-C(7)-C(6)	112.4(8)
C(10)-C(7)-C(9)	109.3(9)
C(6)-C(7)-C(9)	107.3(8)
C(10)-C(7)-C(8)	107.7(9)
C(6)-C(7)-C(8)	112.5(9)
C(9)-C(7)-C(8)	107.5(8)
N(3)-C(16)-C(17)	119.8(9)
N(3)-C(16)-P(1)	113.5(7)
C(17)-C(16)-P(1)	126.7(8)
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
N(1)-C(6)-C(7)	119.9(9)
N(1)-C(6)-P(2)	114.4(7)
C(7)-C(6)-P(2)	125.6(7)
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(11)-C(12)-C(13)	111.1(12)
C(11)-C(12)-C(14)	110.8(9)

C(13)-C(12)-C(14)	107.8(10)
C(11)-C(12)-C(15)	109.1(9)
C(13)-C(12)-C(15)	108.2(9)
C(14)-C(12)-C(15)	109.9(9)
N(2)-C(5)-C(1)	122.8(9)
N(2)-C(5)-P(2)	113.6(7)
C(1)-C(5)-P(2)	123.5(7)
O(1)-C(28)-C(27)	104.3(9)
O(1)-C(28)-H(28A)	110.9
C(27)-C(28)-H(28A)	110.9
O(1)-C(28)-H(28B)	110.9
C(27)-C(28)-H(28B)	110.9
H(28A)-C(28)-H(28B)	108.9
C(1)-C(4)-H(4A)	109.5
C(1)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(1)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(18')-C(17)-C(18)	49.5(18)
C(18')-C(17)-C(20)	123.1(19)
C(18)-C(17)-C(20)	120(2)
C(18')-C(17)-C(16)	118.3(17)
C(18)-C(17)-C(16)	113.5(16)

C(20)-C(17)-C(16)	115.4(15)
C(18')-C(17)-C(20')	115(2)
C(18)-C(17)-C(20')	134.3(19)
C(20)-C(17)-C(20')	22.6(14)
C(16)-C(17)-C(20')	110.7(14)
C(18')-C(17)-C(19')	104.3(19)
C(18)-C(17)-C(19')	57.9(18)
C(20)-C(17)-C(19')	76.7(17)
C(16)-C(17)-C(19')	106.4(12)
C(20')-C(17)-C(19')	99.2(18)
C(18')-C(17)-C(19)	49.4(17)
C(18)-C(17)-C(19)	98.8(19)
C(20)-C(17)-C(19)	102.1(17)
C(16)-C(17)-C(19)	102.7(12)
C(20')-C(17)-C(19)	81.9(16)
C(19')-C(17)-C(19)	148.3(15)
C(1)-C(3)-H(3A)	109.5
C(1)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(1)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(1)-C(5)	110.8(11)
C(2)-C(1)-C(3)	112.8(10)
C(5)-C(1)-C(3)	110.0(9)
C(2)-C(1)-C(4)	107.2(10)
C(5)-C(1)-C(4)	108.1(8)
C(3)-C(1)-C(4)	107.7(11)
Pr(2)-Cl(1)-Pr(1)	11.62(16)
Pr(2)-Cl(1)-Pr(1)#1	118.36(19)

Pr(1)-Cl(1)-Pr(1)#1	106.75(9)
Pr(2)-Cl(1)-Pr(2)#1	108.38(17)
Pr(1)-Cl(1)-Pr(2)#1	96.77(13)
Pr(1)#1-Cl(1)-Pr(2)#1	9.99(11)
O(2)-C(24)-C(23)	104.6(8)
O(2)-C(24)-H(24A)	110.8
C(23)-C(24)-H(24A)	110.8
O(2)-C(24)-H(24B)	110.8
C(23)-C(24)-H(24B)	110.8
H(24A)-C(24)-H(24B)	108.9
C(22)-C(23)-C(24)	103.5(10)
C(22)-C(23)-H(23A)	111.1
C(24)-C(23)-H(23A)	111.1
C(22)-C(23)-H(23B)	111.1
C(24)-C(23)-H(23B)	111.1
H(23A)-C(23)-H(23B)	109.0
C(12)-C(11)-H(11A)	109.5
C(12)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(12)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(2)-C(21)-C(22)	105.4(9)
O(2)-C(21)-H(21A)	110.7
C(22)-C(21)-H(21A)	110.7
O(2)-C(21)-H(21B)	110.7
C(22)-C(21)-H(21B)	110.7
H(21A)-C(21)-H(21B)	108.8
C(23)-C(22)-C(21)	102.5(10)
C(23)-C(22)-H(22A)	111.3

C(21)-C(22)-H(22A)	111.3
C(23)-C(22)-H(22B)	111.3
C(21)-C(22)-H(22B)	111.3
H(22A)-C(22)-H(22B)	109.2
C(1)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(27)-C(26)-C(25)	105.6(11)
C(27)-C(26)-H(26A)	110.6
C(25)-C(26)-H(26A)	110.6
C(27)-C(26)-H(26B)	110.6
C(25)-C(26)-H(26B)	110.6
H(26A)-C(26)-H(26B)	108.8
O(1)-C(25)-C(26)	104.2(8)
O(1)-C(25)-H(25A)	110.9
C(26)-C(25)-H(25A)	110.9
O(1)-C(25)-H(25B)	110.9
C(26)-C(25)-H(25B)	110.9
H(25A)-C(25)-H(25B)	108.9
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(26)-C(27)-C(28)	102.3(12)
C(26)-C(27)-H(27A)	111.3

C(28)-C(27)-H(27A)	111.3
C(26)-C(27)-H(27B)	111.3
C(28)-C(27)-H(27B)	111.3
H(27A)-C(27)-H(27B)	109.2
C(17)-C(20)-H(20A)	109.5
C(17)-C(20)-H(20B)	109.5
C(17)-C(20)-H(20C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
C(17)-C(18')-H(18D)	109.5
C(17)-C(18')-H(18E)	109.5
H(18D)-C(18')-H(18E)	109.5
C(17)-C(18')-H(18F)	109.5
H(18D)-C(18')-H(18F)	109.5
H(18E)-C(18')-H(18F)	109.5
C(17)-C(19')-H(19D)	109.5
C(17)-C(19')-H(19E)	109.5
H(19D)-C(19')-H(19E)	109.5
C(17)-C(19')-H(19F)	109.5
H(19D)-C(19')-H(19F)	109.5
H(19E)-C(19')-H(19F)	109.5
C(17)-C(20')-H(20D)	109.5
C(17)-C(20')-H(20E)	109.5
H(20D)-C(20')-H(20E)	109.5
C(17)-C(20')-H(20F)	109.5
H(20D)-C(20')-H(20F)	109.5

H(20E)-C(20')-H(20F) 109.5

Symmetry transformations used to generate equivalent atoms:

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

Table 6. Torsion angles [deg] for **12**.

N(2)-Pr(2)-N(1)-C(6)	-75(2)
N(4)-Pr(2)-N(1)-C(6)	59(2)
Cl(1)-Pr(2)-N(1)-C(6)	-28(2)
O(1)-Pr(2)-N(1)-C(6)	-137.0(19)
N(3)-Pr(2)-N(1)-C(6)	89.9(19)
Cl(1)#1-Pr(2)-N(1)-C(6)	149.3(18)
N(4)-Pr(2)-N(1)-N(2)	134.2(6)
Cl(1)-Pr(2)-N(1)-N(2)	46.5(9)
O(1)-Pr(2)-N(1)-N(2)	-62.3(6)
N(3)-Pr(2)-N(1)-N(2)	164.5(6)
Cl(1)#1-Pr(2)-N(1)-N(2)	-136.0(6)
N(2)-Pr(2)-N(1)-Pr(1)	137.0(8)
N(4)-Pr(2)-N(1)-Pr(1)	-88.9(6)
Cl(1)-Pr(2)-N(1)-Pr(1)	-176.6(11)
O(1)-Pr(2)-N(1)-Pr(1)	74.7(6)
N(3)-Pr(2)-N(1)-Pr(1)	-58.5(5)
Cl(1)#1-Pr(2)-N(1)-Pr(1)	1.0(3)
N(2)-Pr(1)-N(1)-C(6)	-114(4)
N(3)-Pr(1)-N(1)-C(6)	34(4)
N(4)-Pr(1)-N(1)-C(6)	2(4)
O(1)-Pr(1)-N(1)-C(6)	-163(4)
O(2)-Pr(1)-N(1)-C(6)	126(4)
Cl(1)-Pr(1)-N(1)-C(6)	-73(4)
Cl(1)#1-Pr(1)-N(1)-C(6)	108(4)
N(3)-Pr(1)-N(1)-N(2)	147.5(5)
N(4)-Pr(1)-N(1)-N(2)	116.1(5)
O(1)-Pr(1)-N(1)-N(2)	-48.9(6)

O(2)-Pr(1)-N(1)-N(2)	-120.7(5)
Cl(1)-Pr(1)-N(1)-N(2)	40.3(6)
Cl(1)#1-Pr(1)-N(1)-N(2)	-138.7(6)
N(2)-Pr(1)-N(1)-Pr(2)	-38.5(7)
N(3)-Pr(1)-N(1)-Pr(2)	108.9(6)
N(4)-Pr(1)-N(1)-Pr(2)	77.5(6)
O(1)-Pr(1)-N(1)-Pr(2)	-87.4(6)
O(2)-Pr(1)-N(1)-Pr(2)	-159.2(6)
Cl(1)-Pr(1)-N(1)-Pr(2)	1.8(6)
Cl(1)#1-Pr(1)-N(1)-Pr(2)	-177.2(9)
N(2)-Pr(1)-N(3)-C(16)	130(6)
N(4)-Pr(1)-N(3)-C(16)	-177(6)
N(1)-Pr(1)-N(3)-C(16)	111(6)
O(1)-Pr(1)-N(3)-C(16)	-6(6)
O(2)-Pr(1)-N(3)-C(16)	27(6)
Cl(1)-Pr(1)-N(3)-C(16)	-125(6)
Cl(1)#1-Pr(1)-N(3)-C(16)	-54(6)
N(2)-Pr(1)-N(3)-N(4)	-53.1(5)
N(1)-Pr(1)-N(3)-N(4)	-71.8(5)
O(1)-Pr(1)-N(3)-N(4)	170.8(6)
O(2)-Pr(1)-N(3)-N(4)	-156.0(4)
Cl(1)-Pr(1)-N(3)-N(4)	51.4(4)
Cl(1)#1-Pr(1)-N(3)-N(4)	123.1(4)
N(2)-Pr(1)-N(3)-Pr(2)	-53.8(6)
N(4)-Pr(1)-N(3)-Pr(2)	-0.8(7)
N(1)-Pr(1)-N(3)-Pr(2)	-72.6(6)
O(1)-Pr(1)-N(3)-Pr(2)	170.0(10)
O(2)-Pr(1)-N(3)-Pr(2)	-156.7(6)
Cl(1)-Pr(1)-N(3)-Pr(2)	50.6(5)
Cl(1)#1-Pr(1)-N(3)-Pr(2)	122.3(5)

N(2)-Pr(2)-N(3)-C(16)	-80(5)
N(4)-Pr(2)-N(3)-C(16)	-4(5)
N(1)-Pr(2)-N(3)-C(16)	-90(5)
Cl(1)-Pr(2)-N(3)-C(16)	62(5)
O(1)-Pr(2)-N(3)-C(16)	172(5)
Cl(1)#1-Pr(2)-N(3)-C(16)	126(5)
N(2)-Pr(2)-N(3)-N(4)	-75.2(6)
N(1)-Pr(2)-N(3)-N(4)	-85.2(5)
Cl(1)-Pr(2)-N(3)-N(4)	66.6(5)
O(1)-Pr(2)-N(3)-N(4)	176.7(5)
Cl(1)#1-Pr(2)-N(3)-N(4)	130.8(5)
N(2)-Pr(2)-N(3)-Pr(1)	104.0(7)
N(4)-Pr(2)-N(3)-Pr(1)	179.2(8)
N(1)-Pr(2)-N(3)-Pr(1)	93.9(6)
Cl(1)-Pr(2)-N(3)-Pr(1)	-114.3(6)
O(1)-Pr(2)-N(3)-Pr(1)	-4.1(4)
Cl(1)#1-Pr(2)-N(3)-Pr(1)	-50.1(5)
C(16)-N(3)-N(4)-C(15)	-0.7(10)
Pr(1)-N(3)-N(4)-C(15)	179.6(7)
Pr(2)-N(3)-N(4)-C(15)	179.8(8)
C(16)-N(3)-N(4)-Pr(2)	179.4(7)
Pr(1)-N(3)-N(4)-Pr(2)	-0.21(19)
C(16)-N(3)-N(4)-Pr(1)	179.6(7)
Pr(2)-N(3)-N(4)-Pr(1)	0.21(19)
N(2)-Pr(2)-N(4)-C(15)	-62.6(16)
N(1)-Pr(2)-N(4)-C(15)	-88.3(16)
Cl(1)-Pr(2)-N(4)-C(15)	61.1(16)
O(1)-Pr(2)-N(4)-C(15)	171.9(14)
N(3)-Pr(2)-N(4)-C(15)	-179.6(18)
Cl(1)#1-Pr(2)-N(4)-C(15)	133.1(15)

N(2)-Pr(2)-N(4)-N(3)	117.0(6)
N(1)-Pr(2)-N(4)-N(3)	91.4(5)
Cl(1)-Pr(2)-N(4)-N(3)	-119.2(5)
O(1)-Pr(2)-N(4)-N(3)	-8.5(14)
Cl(1)#1-Pr(2)-N(4)-N(3)	-47.3(5)
N(2)-Pr(2)-N(4)-Pr(1)	116.3(7)
N(1)-Pr(2)-N(4)-Pr(1)	90.6(6)
Cl(1)-Pr(2)-N(4)-Pr(1)	-119.9(6)
O(1)-Pr(2)-N(4)-Pr(1)	-9.2(9)
N(3)-Pr(2)-N(4)-Pr(1)	-0.7(7)
Cl(1)#1-Pr(2)-N(4)-Pr(1)	-48.0(4)
N(2)-Pr(1)-N(4)-C(15)	-44(5)
N(3)-Pr(1)-N(4)-C(15)	-177(5)
N(1)-Pr(1)-N(4)-C(15)	-73(5)
O(1)-Pr(1)-N(4)-C(15)	14(5)
O(2)-Pr(1)-N(4)-C(15)	-149(5)
Cl(1)-Pr(1)-N(4)-C(15)	52(5)
Cl(1)#1-Pr(1)-N(4)-C(15)	123(5)
N(2)-Pr(1)-N(4)-N(3)	133.8(5)
N(1)-Pr(1)-N(4)-N(3)	104.8(5)
O(1)-Pr(1)-N(4)-N(3)	-168.7(8)
O(2)-Pr(1)-N(4)-N(3)	28.4(5)
Cl(1)-Pr(1)-N(4)-N(3)	-130.7(4)
Cl(1)#1-Pr(1)-N(4)-N(3)	-59.7(4)
N(2)-Pr(1)-N(4)-Pr(2)	-47.0(6)
N(3)-Pr(1)-N(4)-Pr(2)	179.2(7)
N(1)-Pr(1)-N(4)-Pr(2)	-75.9(6)
O(1)-Pr(1)-N(4)-Pr(2)	10.5(10)
O(2)-Pr(1)-N(4)-Pr(2)	-152.4(6)
Cl(1)-Pr(1)-N(4)-Pr(2)	48.6(5)

Cl(1)#1-Pr(1)-N(4)-Pr(2)	119.5(5)
C(6)-N(1)-N(2)-C(5)	-1.0(12)
Pr(2)-N(1)-N(2)-C(5)	-158.5(9)
Pr(1)-N(1)-N(2)-C(5)	-169.6(8)
C(6)-N(1)-N(2)-Pr(2)	157.5(8)
Pr(1)-N(1)-N(2)-Pr(2)	-11.1(2)
C(6)-N(1)-N(2)-Pr(1)	168.6(8)
Pr(2)-N(1)-N(2)-Pr(1)	11.1(2)
N(4)-Pr(2)-N(2)-C(5)	84.0(16)
N(1)-Pr(2)-N(2)-C(5)	132.2(19)
Cl(1)-Pr(2)-N(2)-C(5)	-22.6(18)
O(1)-Pr(2)-N(2)-C(5)	-109.4(16)
N(3)-Pr(2)-N(2)-C(5)	114.7(16)
Cl(1)#1-Pr(2)-N(2)-C(5)	-131.8(15)
N(4)-Pr(2)-N(2)-N(1)	-48.2(6)
Cl(1)-Pr(2)-N(2)-N(1)	-154.8(5)
O(1)-Pr(2)-N(2)-N(1)	118.3(6)
N(3)-Pr(2)-N(2)-N(1)	-17.6(7)
Cl(1)#1-Pr(2)-N(2)-N(1)	95.9(9)
N(4)-Pr(2)-N(2)-Pr(1)	-97.3(8)
N(1)-Pr(2)-N(2)-Pr(1)	-49.0(9)
Cl(1)-Pr(2)-N(2)-Pr(1)	156.1(9)
O(1)-Pr(2)-N(2)-Pr(1)	69.3(7)
N(3)-Pr(2)-N(2)-Pr(1)	-66.6(7)
Cl(1)#1-Pr(2)-N(2)-Pr(1)	46.9(7)
N(3)-Pr(1)-N(2)-C(5)	95(3)
N(4)-Pr(1)-N(2)-C(5)	69(3)
N(1)-Pr(1)-N(2)-C(5)	132(3)
O(1)-Pr(1)-N(2)-C(5)	-98(3)
O(2)-Pr(1)-N(2)-C(5)	-168(3)

Cl(1)-Pr(1)-N(2)-C(5)	-15(3)
Cl(1)#1-Pr(1)-N(2)-C(5)	-75(3)
N(3)-Pr(1)-N(2)-N(1)	-36.7(6)
N(4)-Pr(1)-N(2)-N(1)	-62.3(5)
O(1)-Pr(1)-N(2)-N(1)	130.5(6)
O(2)-Pr(1)-N(2)-N(1)	60.6(5)
Cl(1)-Pr(1)-N(2)-N(1)	-146.6(5)
Cl(1)#1-Pr(1)-N(2)-N(1)	153.1(5)
N(3)-Pr(1)-N(2)-Pr(2)	92.3(7)
N(4)-Pr(1)-N(2)-Pr(2)	66.7(7)
N(1)-Pr(1)-N(2)-Pr(2)	129.0(9)
O(1)-Pr(1)-N(2)-Pr(2)	-100.5(7)
O(2)-Pr(1)-N(2)-Pr(2)	-170.4(7)
Cl(1)-Pr(1)-N(2)-Pr(2)	-17.7(7)
Cl(1)#1-Pr(1)-N(2)-Pr(2)	-77.9(9)
N(2)-Pr(1)-O(1)-C(28)	-47.4(9)
N(3)-Pr(1)-O(1)-C(28)	93.0(11)
N(4)-Pr(1)-O(1)-C(28)	-106.7(12)
N(1)-Pr(1)-O(1)-C(28)	-22.9(10)
O(2)-Pr(1)-O(1)-C(28)	58.0(9)
Cl(1)-Pr(1)-O(1)-C(28)	-144.7(9)
Cl(1)#1-Pr(1)-O(1)-C(28)	141.4(9)
N(2)-Pr(1)-O(1)-C(25)	120.6(10)
N(3)-Pr(1)-O(1)-C(25)	-99.0(12)
N(4)-Pr(1)-O(1)-C(25)	61.3(14)
N(1)-Pr(1)-O(1)-C(25)	145.1(10)
O(2)-Pr(1)-O(1)-C(25)	-134.0(10)
Cl(1)-Pr(1)-O(1)-C(25)	23.3(10)
Cl(1)#1-Pr(1)-O(1)-C(25)	-50.6(10)
N(2)-Pr(1)-O(1)-Pr(2)	49.1(5)

N(3)-Pr(1)-O(1)-Pr(2)	-170.5(9)
N(4)-Pr(1)-O(1)-Pr(2)	-10.2(10)
N(1)-Pr(1)-O(1)-Pr(2)	73.6(6)
O(2)-Pr(1)-O(1)-Pr(2)	154.6(5)
Cl(1)-Pr(1)-O(1)-Pr(2)	-48.2(5)
Cl(1)#1-Pr(1)-O(1)-Pr(2)	-122.1(5)
N(2)-Pr(2)-O(1)-C(28)	-25.6(10)
N(4)-Pr(2)-O(1)-C(28)	102.8(14)
N(1)-Pr(2)-O(1)-C(28)	5.4(10)
Cl(1)-Pr(2)-O(1)-C(28)	-145.9(9)
N(3)-Pr(2)-O(1)-C(28)	96.9(10)
Cl(1)#1-Pr(2)-O(1)-C(28)	143.8(9)
N(2)-Pr(2)-O(1)-C(25)	123.1(9)
N(4)-Pr(2)-O(1)-C(25)	-108.5(14)
N(1)-Pr(2)-O(1)-C(25)	154.1(9)
Cl(1)-Pr(2)-O(1)-C(25)	2.8(9)
N(3)-Pr(2)-O(1)-C(25)	-114.4(9)
Cl(1)#1-Pr(2)-O(1)-C(25)	-67.6(8)
N(2)-Pr(2)-O(1)-Pr(1)	-118.9(6)
N(4)-Pr(2)-O(1)-Pr(1)	9.5(9)
N(1)-Pr(2)-O(1)-Pr(1)	-87.9(6)
Cl(1)-Pr(2)-O(1)-Pr(1)	120.8(6)
N(3)-Pr(2)-O(1)-Pr(1)	3.7(3)
Cl(1)#1-Pr(2)-O(1)-Pr(1)	50.5(5)
N(2)-Pr(1)-O(2)-C(24)	-28.7(8)
N(3)-Pr(1)-O(2)-C(24)	88.0(8)
N(4)-Pr(1)-O(2)-C(24)	73.1(8)
N(1)-Pr(1)-O(2)-C(24)	-0.6(8)
O(1)-Pr(1)-O(2)-C(24)	-102.4(8)
Cl(1)-Pr(1)-O(2)-C(24)	-149.1(7)

Cl(1)#1-Pr(1)-O(2)-C(24)	174.6(8)
N(2)-Pr(1)-O(2)-C(21)	138.2(8)
N(3)-Pr(1)-O(2)-C(21)	-105.2(8)
N(4)-Pr(1)-O(2)-C(21)	-120.0(8)
N(1)-Pr(1)-O(2)-C(21)	166.3(8)
O(1)-Pr(1)-O(2)-C(21)	64.5(8)
Cl(1)-Pr(1)-O(2)-C(21)	17.7(9)
Cl(1)#1-Pr(1)-O(2)-C(21)	-18.5(8)
N(3)-N(4)-C(15)-C(12)	179.5(7)
Pr(2)-N(4)-C(15)-C(12)	-1(2)
Pr(1)-N(4)-C(15)-C(12)	-3(5)
N(3)-N(4)-C(15)-P(1)	0.2(9)
Pr(2)-N(4)-C(15)-P(1)	179.8(12)
Pr(1)-N(4)-C(15)-P(1)	177(4)
C(16)-P(1)-C(15)-N(4)	0.2(7)
C(16)-P(1)-C(15)-C(12)	-179.0(8)
N(4)-N(3)-C(16)-C(17)	178.8(9)
Pr(1)-N(3)-C(16)-C(17)	-5(6)
Pr(2)-N(3)-C(16)-C(17)	-177(5)
N(4)-N(3)-C(16)-P(1)	0.9(10)
Pr(1)-N(3)-C(16)-P(1)	178(5)
Pr(2)-N(3)-C(16)-P(1)	5(6)
C(15)-P(1)-C(16)-N(3)	-0.6(7)
C(15)-P(1)-C(16)-C(17)	-178.3(10)
N(2)-N(1)-C(6)-C(7)	-172.7(8)
Pr(2)-N(1)-C(6)-C(7)	-108.0(19)
Pr(1)-N(1)-C(6)-C(7)	-63(4)
N(2)-N(1)-C(6)-P(2)	3.4(11)
Pr(2)-N(1)-C(6)-P(2)	68(2)
Pr(1)-N(1)-C(6)-P(2)	113(3)

C(10)-C(7)-C(6)-N(1)	-35.0(13)
C(9)-C(7)-C(6)-N(1)	85.2(12)
C(8)-C(7)-C(6)-N(1)	-156.7(9)
C(10)-C(7)-C(6)-P(2)	149.3(8)
C(9)-C(7)-C(6)-P(2)	-90.5(10)
C(8)-C(7)-C(6)-P(2)	27.6(13)
C(5)-P(2)-C(6)-N(1)	-3.7(8)
C(5)-P(2)-C(6)-C(7)	172.2(9)
N(4)-C(15)-C(12)-C(11)	144.4(10)
P(1)-C(15)-C(12)-C(11)	-36.5(12)
N(4)-C(15)-C(12)-C(13)	-94.6(12)
P(1)-C(15)-C(12)-C(13)	84.5(12)
N(4)-C(15)-C(12)-C(14)	22.8(12)
P(1)-C(15)-C(12)-C(14)	-158.1(7)
N(1)-N(2)-C(5)-C(1)	-178.7(9)
Pr(2)-N(2)-C(5)-C(1)	54(2)
Pr(1)-N(2)-C(5)-C(1)	53(4)
N(1)-N(2)-C(5)-P(2)	-1.9(11)
Pr(2)-N(2)-C(5)-P(2)	-128.7(13)
Pr(1)-N(2)-C(5)-P(2)	-130(3)
C(6)-P(2)-C(5)-N(2)	3.1(8)
C(6)-P(2)-C(5)-C(1)	179.9(10)
C(25)-O(1)-C(28)-C(27)	23.9(15)
Pr(1)-O(1)-C(28)-C(27)	-166.1(9)
Pr(2)-O(1)-C(28)-C(27)	176.0(9)
N(3)-C(16)-C(17)-C(18')	22(2)
P(1)-C(16)-C(17)-C(18')	-160.6(18)
N(3)-C(16)-C(17)-C(18)	-33(2)
P(1)-C(16)-C(17)-C(18)	144.1(19)
N(3)-C(16)-C(17)-C(20)	-177.7(17)

P(1)-C(16)-C(17)-C(20)	0(2)
N(3)-C(16)-C(17)-C(20')	158.3(16)
P(1)-C(16)-C(17)-C(20')	-24.2(19)
N(3)-C(16)-C(17)-C(19')	-94.9(15)
P(1)-C(16)-C(17)-C(19')	82.6(14)
N(3)-C(16)-C(17)-C(19)	72.2(14)
P(1)-C(16)-C(17)-C(19)	-110.2(12)
N(2)-C(5)-C(1)-C(2)	-132.9(11)
P(2)-C(5)-C(1)-C(2)	50.5(12)
N(2)-C(5)-C(1)-C(3)	101.6(12)
P(2)-C(5)-C(1)-C(3)	-74.9(13)
N(2)-C(5)-C(1)-C(4)	-15.8(15)
P(2)-C(5)-C(1)-C(4)	167.7(9)
N(2)-Pr(2)-Cl(1)-Pr(1)	-155.1(10)
N(4)-Pr(2)-Cl(1)-Pr(1)	91.6(7)
N(1)-Pr(2)-Cl(1)-Pr(1)	176.0(13)
O(1)-Pr(2)-Cl(1)-Pr(1)	-73.0(7)
N(3)-Pr(2)-Cl(1)-Pr(1)	64.0(6)
Cl(1)#1-Pr(2)-Cl(1)-Pr(1)	-2.3(6)
N(2)-Pr(2)-Cl(1)-Pr(1)#1	-152.3(4)
N(4)-Pr(2)-Cl(1)-Pr(1)#1	94.4(3)
N(1)-Pr(2)-Cl(1)-Pr(1)#1	178.8(6)
O(1)-Pr(2)-Cl(1)-Pr(1)#1	-70.2(3)
N(3)-Pr(2)-Cl(1)-Pr(1)#1	66.8(3)
Cl(1)#1-Pr(2)-Cl(1)-Pr(1)#1	0.52(14)
N(2)-Pr(2)-Cl(1)-Pr(2)#1	-152.8(4)
N(4)-Pr(2)-Cl(1)-Pr(2)#1	93.9(3)
N(1)-Pr(2)-Cl(1)-Pr(2)#1	178.3(7)
O(1)-Pr(2)-Cl(1)-Pr(2)#1	-70.7(2)
N(3)-Pr(2)-Cl(1)-Pr(2)#1	66.3(3)

Cl(1)#1-Pr(2)-Cl(1)-Pr(2)#1	0.0
N(2)-Pr(1)-Cl(1)-Pr(2)	18.2(7)
N(3)-Pr(1)-Cl(1)-Pr(2)	-100.6(7)
N(4)-Pr(1)-Cl(1)-Pr(2)	-75.5(7)
N(1)-Pr(1)-Cl(1)-Pr(2)	-2.3(7)
O(1)-Pr(1)-Cl(1)-Pr(2)	95.3(7)
O(2)-Pr(1)-Cl(1)-Pr(2)	139.8(8)
Cl(1)#1-Pr(1)-Cl(1)-Pr(2)	177.4(7)
N(2)-Pr(1)-Cl(1)-Pr(1)#1	-159.2(2)
N(3)-Pr(1)-Cl(1)-Pr(1)#1	82.0(2)
N(4)-Pr(1)-Cl(1)-Pr(1)#1	107.05(19)
N(1)-Pr(1)-Cl(1)-Pr(1)#1	-179.7(2)
O(1)-Pr(1)-Cl(1)-Pr(1)#1	-82.09(19)
O(2)-Pr(1)-Cl(1)-Pr(1)#1	-37.6(3)
Cl(1)#1-Pr(1)-Cl(1)-Pr(1)#1	0.0
N(2)-Pr(1)-Cl(1)-Pr(2)#1	-159.6(2)
N(3)-Pr(1)-Cl(1)-Pr(2)#1	81.6(2)
N(4)-Pr(1)-Cl(1)-Pr(2)#1	106.7(2)
N(1)-Pr(1)-Cl(1)-Pr(2)#1	179.9(2)
O(1)-Pr(1)-Cl(1)-Pr(2)#1	-82.5(2)
O(2)-Pr(1)-Cl(1)-Pr(2)#1	-38.0(3)
Cl(1)#1-Pr(1)-Cl(1)-Pr(2)#1	-0.40(11)
C(21)-O(2)-C(24)-C(23)	-14.0(12)
Pr(1)-O(2)-C(24)-C(23)	154.4(7)
O(2)-C(24)-C(23)-C(22)	33.4(12)
C(24)-O(2)-C(21)-C(22)	-9.6(12)
Pr(1)-O(2)-C(21)-C(22)	-178.5(7)
C(24)-C(23)-C(22)-C(21)	-38.4(13)
O(2)-C(21)-C(22)-C(23)	30.4(13)
C(28)-O(1)-C(25)-C(26)	-1.4(16)

Pr(1)-O(1)-C(25)-C(26)	-170.7(10)
Pr(2)-O(1)-C(25)-C(26)	-154.0(10)
C(27)-C(26)-C(25)-O(1)	-22.0(18)
C(25)-C(26)-C(27)-C(28)	36.3(18)
O(1)-C(28)-C(27)-C(26)	-36.8(16)

Symmetry transformations used to generate equivalent atoms:

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

5. Magnetic susceptibility data of complex **11**

Magnetic susceptibility measurements of **11** as polycrystalline samples were carried out on a Quantum Design SQUID MPMSXL-7 magnetometer.

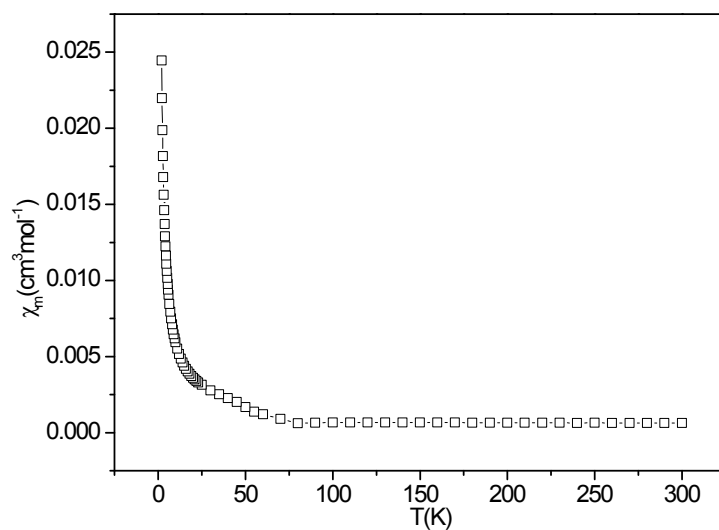


Fig. 4 χ_m vs T plots of complex **11** over the range of 2–300 K.

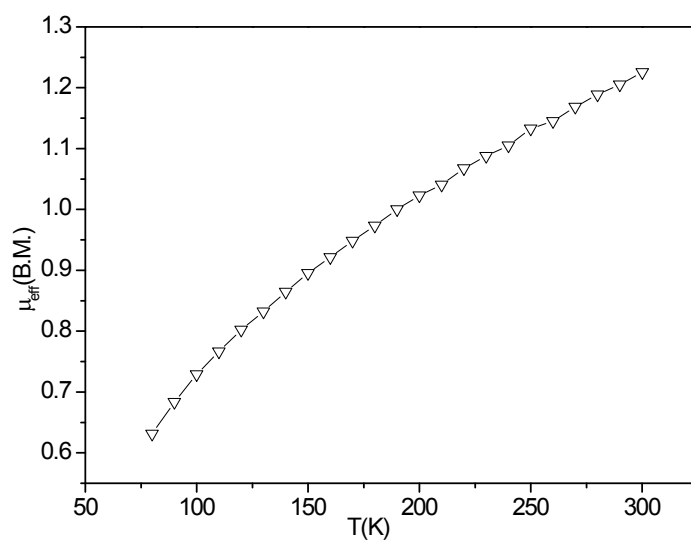


Fig. 5 μ_{eff} vs T plots of complex **11** over the range of 80–300 K.