Reactivity of $(C_5Me_5)_3LaL_x$ Complexes: Synthesis of a Tris(pentamethylcyclopentadienyl) Complex with Two Additional Ligands, $(C_5Me_5)_3La(NCCMe_3)_2$

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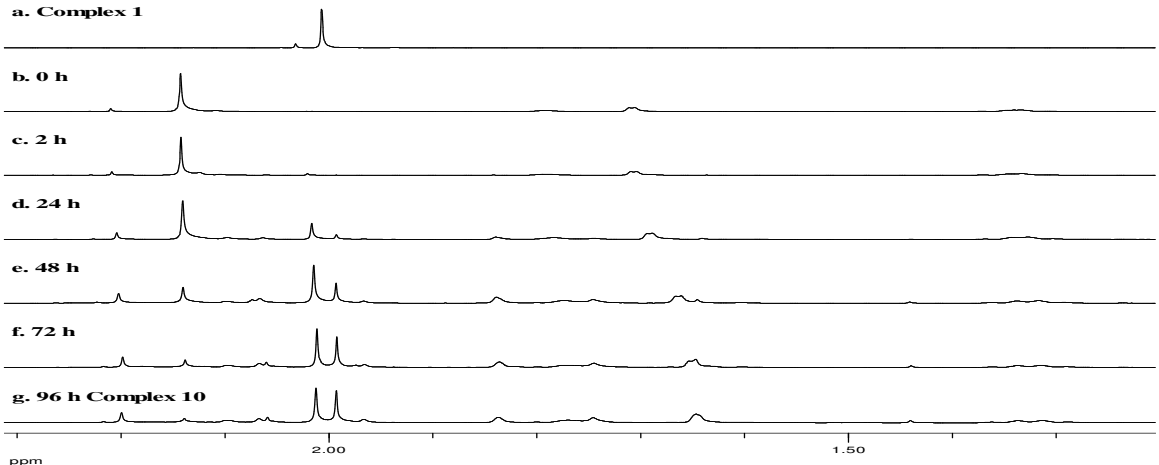

^{1}H NMR spectra of **1** with two equivalents of adamantyl azide after: (a) $(C_5Me_5)_3La$, **1**; (b) 0 h; (c) 2 h; (d) 24 h; (e) 48 h; (f) 72 h; (g) 96 h, $(C_5Me_5)_2La[\eta^2$-(N,N′)-$(C_5Me_5)NN'N''Ad](N_3Ad)$, **10**.

X-ray Data Collection, Structure Solution and Refinement for **4**.

A colorless crystal of approximate dimensions 0.07 x 0.18 x 0.27 mm was mounted on a glass fiber and transferred to a Bruker SMART1K diffractometer. The SMART[1] program package was used to determine the unit-cell parameters and for data collection (40 sec/frame scan time for a hemisphere of diffraction data). The raw frame data was processed using SAINT[2] and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program. The diffraction symmetry was 2/*m* and the systematic absences were consistent with the monoclinic space groups *Cc and C*2/*c*. It was later determined that the centrosymmetric space group *C*2/*c* was correct. The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. There were two molecules of toluene solvent present per formula unit. The molecule was located on a two-fold rotation axis. The tetraphenylborate anion and one of the toluene solvent molecules were also located on two-fold rotation axes. The remaining toluene molecule was disordered about an inversion center and included using multiple components, partial site-occupancy-factors, geometric restraints and equal (EADP)[4] isotropic thermal parameters. Hydrogen atoms associated with the disordered toluene were not included. At convergence, wR2 = 0.0968 and Goof = 1.048 for 456 variables refined against 8674 data (0.78Å), R1 = 0.0405 for those 6762 data with $I > 2.0\sigma(I)$.

Table 1. Crystal data and structure refinement for **4**.

Identification code	tjm5 (**4**)	
Empirical formula	$C_{80}\ H_{80}\ B\ La\ O_2\ P_2 \bullet 2(C_7H_8)$	
Formula weight	1469.37	
Temperature	143(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*C*2/*c*	
Unit cell dimensions	a = 13.4632(17) Å	α= 90°.
	b = 41.393(5) Å	β= 96.432(2)°.
	c = 14.2084(17) Å	γ = 90°.
Volume	7868.2(17) $Å^3$	
Z	4	
Density (calculated)	1.240 Mg/m^3	
Absorption coefficient	0.632 mm^{-1}	
F(000)	3072	
Crystal color	colorless	
Crystal size	0.27 x 0.18 x 0.07 mm^3	
Theta range for data collection	0.98 to 27.10°	

Index ranges	$-13 \leq h \leq 17$, $-45 \leq k \leq 52$, $-17 \leq l \leq 18$
Reflections collected	25169
Independent reflections	8674 [R(int) = 0.0516]
Completeness to theta = 27.10°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9571 and 0.8479
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8674 / 3 / 456
Goodness-of-fit on F^2	1.048
Final R indices [I>2sigma(I) = 6762 data]	R1 = 0.0405, wR2 = 0.0866
R indices (all data, 0.78Å)	R1 = 0.0644, wR2 = 0.0968
Largest diff. peak and hole	0.862 and -0.959 e.$Å^{-3}$

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

	x	y	z	U(eq)
La(1)	5000	5692(1)	7500	14(1)
P(1)	7023(1)	6356(1)	7992(1)	18(1)
O(1)	6210(2)	6103(1)	7966(1)	22(1)
B(1)	10000	6680(1)	12500	23(1)
C(1)	6063(2)	5288(1)	6356(2)	23(1)
C(2)	6110(2)	5597(1)	5926(2)	22(1)
C(3)	5136(2)	5681(1)	5528(2)	22(1)
C(4)	4488(2)	5427(1)	5705(2)	24(1)
C(5)	5061(2)	5179(1)	6203(2)	24(1)
C(6)	6951(3)	5106(1)	6831(2)	33(1)
C(7)	7052(2)	5778(1)	5764(2)	32(1)
C(8)	4860(3)	5971(1)	4912(2)	33(1)
C(9)	3394(3)	5404(1)	5358(2)	38(1)
C(10)	4666(3)	4845(1)	6349(2)	37(1)
C(11)	6872(2)	6673(1)	8826(2)	20(1)
C(12)	7037(2)	6600(1)	9799(2)	24(1)
C(13)	6913(2)	6837(1)	10459(2)	29(1)
C(14)	6628(2)	7144(1)	10165(2)	30(1)
C(15)	6459(3)	7220(1)	9210(2)	32(1)
C(16)	6587(2)	6985(1)	8542(2)	25(1)
C(17)	7006(2)	6543(1)	6851(2)	19(1)
C(18)	7873(2)	6626(1)	6463(2)	26(1)
C(19)	7820(3)	6769(1)	5578(2)	32(1)
C(20)	6895(3)	6835(1)	5083(2)	31(1)
C(21)	6029(3)	6760(1)	5464(2)	31(1)
C(22)	6075(2)	6612(1)	6351(2)	25(1)
C(23)	8219(2)	6175(1)	8337(2)	20(1)
C(24)	8322(2)	5843(1)	8220(2)	27(1)

C(25)	9224(3)	5693(1)	8529(3)	38(1)
C(26)	10010(3)	5872(1)	8951(3)	39(1)
C(27)	9917(2)	6200(1)	9072(2)	37(1)
C(28)	9025(2)	6352(1)	8768(2)	27(1)
C(29)	10194(2)	6918(1)	11620(2)	23(1)
C(30)	10959(2)	7153(1)	11747(2)	29(1)
C(31)	11150(3)	7367(1)	11040(2)	31(1)
C(32)	10581(3)	7360(1)	10165(2)	31(1)
C(33)	9824(3)	7135(1)	10016(2)	29(1)
C(34)	9635(2)	6920(1)	10724(2)	24(1)
C(35)	9045(2)	6432(1)	12257(2)	26(1)
C(36)	8246(3)	6405(1)	12798(3)	35(1)
C(37)	7512(3)	6167(1)	12630(3)	46(1)
C(38)	7559(3)	5946(1)	11901(3)	50(1)
C(39)	8330(3)	5965(1)	11348(3)	41(1)
C(40)	9065(3)	6202(1)	11531(2)	33(1)
C(41)	5000	7040(2)	12500	45(1)
C(42)	5887(3)	7216(1)	12589(2)	46(1)
C(43)	5881(4)	7550(1)	12588(2)	52(1)
C(44)	5000	7717(2)	12500	55(2)
C(45)	5000	6679(2)	12500	68(2)
C(46)	10428(7)	5217(2)	10735(6)	44(1)
C(47)	11021(8)	5091(3)	10039(6)	44(1)
C(48)	9412(8)	5124(2)	10662(7)	44(1)
C(49)	10920(13)	5456(4)	11432(12)	44(1)
C(50)	9205(7)	5017(2)	10288(7)	44(1)
C(51)	9715(14)	4848(4)	9550(12)	44(1)
C(52)	9559(14)	5182(4)	10945(12)	44(1)
C(53)	11152(14)	5129(5)	10364(13)	44(1)
C(54)	10683(7)	5325(2)	11189(6)	44(1)

Table 3. Bond lengths [Å] and angles [°] for **4**.

La(1)-Cnt	2.554
La(1)-O(1)	2.398(2)
La(1)-C(4)	2.791(3)
La(1)-C(5)	2.818(3)
La(1)-C(3)	2.829(3)
La(1)-C(1)	2.829(3)
La(1)-C(2)	2.852(3)
P(1)-O(1)	1.514(2)
P(1)-C(11)	1.794(3)
P(1)-C(17)	1.794(3)
P(1)-C(23)	1.795(3)
B(1)-C(29)	1.636(4)
B(1)-C(35)	1.650(4)
C(1)-C(5)	1.417(4)
C(1)-C(2)	1.423(4)
C(1)-C(6)	1.508(4)
C(2)-C(3)	1.411(4)
C(2)-C(7)	1.511(4)
C(3)-C(4)	1.410(4)
C(3)-C(8)	1.505(4)
C(4)-C(5)	1.422(4)
C(4)-C(9)	1.502(4)
C(5)-C(10)	1.505(4)
C(11)-C(16)	1.395(4)
C(11)-C(12)	1.408(4)
C(12)-C(13)	1.380(4)
C(13)-C(14)	1.378(5)
C(14)-C(15)	1.386(5)
C(15)-C(16)	1.382(4)
C(17)-C(18)	1.388(4)
C(17)-C(22)	1.398(4)
C(18)-C(19)	1.384(4)
C(19)-C(20)	1.386(5)
C(20)-C(21)	1.375(5)

C(21)-C(22)	1.397(4)
C(23)-C(24)	1.392(4)
C(23)-C(28)	1.394(4)
C(24)-C(25)	1.389(4)
C(25)-C(26)	1.373(5)
C(26)-C(27)	1.379(5)
C(27)-C(28)	1.381(5)
C(29)-C(34)	1.404(4)
C(29)-C(30)	1.412(4)
C(30)-C(31)	1.386(4)
C(31)-C(32)	1.387(5)
C(32)-C(33)	1.380(5)
C(33)-C(34)	1.388(4)
C(35)-C(36)	1.395(5)
C(35)-C(40)	1.406(4)
C(36)-C(37)	1.397(5)
C(37)-C(38)	1.389(6)
C(38)-C(39)	1.372(6)
C(39)-C(40)	1.396(5)
C(41)-C(42)	1.393(5)
C(41)-C(42)#1	1.393(5)
C(41)-C(45)	1.492(8)
C(42)-C(43)	1.384(6)
C(43)-C(44)	1.367(5)
C(44)-C(43)#1	1.367(6)
C(46)-C(48)	1.413(14)
C(46)-C(47)	1.438(14)
C(46)-C(49)	1.501(18)
C(47)-C(48)#2	1.412(11)
C(48)-C(47)#2	1.412(11)
C(50)-C(53)#2	1.164(18)
C(50)-C(52)	1.211(18)
C(50)-C(51)	1.49(2)
C(50)-C(51)#2	1.55(2)
C(51)-C(53)#2	1.19(3)
C(51)-C(52)#2	1.27(3)

C(51)-C(54)#2	1.332(18)
C(51)-C(50)#2	1.55(2)
C(51)-C(51)#2	1.89(3)
C(52)-C(51)#2	1.27(3)
C(52)-C(54)	1.62(2)
C(53)-C(50)#2	1.164(18)
C(53)-C(51)#2	1.19(3)
C(53)-C(54)	1.61(2)
C(54)-C(51)#2	1.332(18)

Cnt-La(1)-O(1)	110.0
Cnt-La(1)-O(1)#3	104.5
O(1)#3-La(1)-O(1)	89.50(10)
O(1)#3-La(1)-C(4)	86.34(8)
O(1)-La(1)-C(4)	128.49(8)
O(1)#3-La(1)-C(4)#3	128.50(8)
O(1)-La(1)-C(4)#3	86.34(8)
C(4)-La(1)-C(4)#3	133.68(13)
O(1)#3-La(1)-C(5)#3	130.31(8)
O(1)-La(1)-C(5)#3	115.00(8)
C(4)-La(1)-C(5)#3	106.22(9)
C(4)#3-La(1)-C(5)#3	29.36(9)
O(1)#3-La(1)-C(5)	115.00(8)
O(1)-La(1)-C(5)	130.31(8)
C(4)-La(1)-C(5)	29.36(9)
C(4)#3-La(1)-C(5)	106.22(9)
C(5)#3-La(1)-C(5)	82.31(13)
O(1)#3-La(1)-C(3)	81.63(8)
O(1)-La(1)-C(3)	99.61(8)
C(4)-La(1)-C(3)	29.05(9)
C(4)#3-La(1)-C(3)	149.58(9)
C(5)#3-La(1)-C(3)	130.28(9)
C(5)-La(1)-C(3)	48.00(9)
O(1)#3-La(1)-C(3)#3	99.61(8)
O(1)-La(1)-C(3)#3	81.63(8)
C(4)-La(1)-C(3)#3	149.58(9)

C(4)#3-La(1)-C(3)#3	29.06(9)
C(5)#3-La(1)-C(3)#3	47.99(9)
C(5)-La(1)-C(3)#3	130.28(9)
C(3)-La(1)-C(3)#3	178.27(13)
O(1)#3-La(1)-C(1)#3	101.91(8)
O(1)-La(1)-C(1)#3	129.21(8)
C(4)-La(1)-C(1)#3	101.76(9)
C(4)#3-La(1)-C(1)#3	48.07(9)
C(5)#3-La(1)-C(1)#3	29.06(9)
C(5)-La(1)-C(1)#3	89.14(9)
C(3)-La(1)-C(1)#3	130.81(9)
C(3)#3-La(1)-C(1)#3	47.83(9)
O(1)#3-La(1)-C(1)	129.21(8)
O(1)-La(1)-C(1)	101.91(8)
C(4)-La(1)-C(1)	48.07(9)
C(4)#3-La(1)-C(1)	101.76(9)
C(5)#3-La(1)-C(1)	89.14(9)
C(5)-La(1)-C(1)	29.06(9)
C(3)-La(1)-C(1)	47.83(9)
C(3)#3-La(1)-C(1)	130.81(9)
C(1)#3-La(1)-C(1)	107.63(13)
O(1)#3-La(1)-C(2)	106.24(8)
O(1)-La(1)-C(2)	85.10(8)
C(4)-La(1)-C(2)	47.72(9)
C(4)#3-La(1)-C(2)	124.41(9)
C(5)#3-La(1)-C(2)	117.78(9)
C(5)-La(1)-C(2)	47.77(9)
C(3)-La(1)-C(2)	28.76(8)
C(3)#3-La(1)-C(2)	150.75(9)
C(1)#3-La(1)-C(2)	135.49(9)
C(1)-La(1)-C(2)	29.00(8)
O(1)#3-La(1)-C(2)#3	85.10(8)
O(1)-La(1)-C(2)#3	106.24(8)
C(4)-La(1)-C(2)#3	124.41(9)
C(4)#3-La(1)-C(2)#3	47.72(9)
C(5)#3-La(1)-C(2)#3	47.77(9)

C(5)-La(1)-C(2)#3	117.78(9)
C(3)-La(1)-C(2)#3	150.75(9)
C(3)#3-La(1)-C(2)#3	28.76(8)
C(1)#3-La(1)-C(2)#3	29.00(8)
C(1)-La(1)-C(2)#3	135.48(9)
C(2)-La(1)-C(2)#3	164.27(12)
O(1)-P(1)-C(11)	112.73(13)
O(1)-P(1)-C(17)	109.95(12)
C(11)-P(1)-C(17)	106.95(14)
O(1)-P(1)-C(23)	109.89(13)
C(11)-P(1)-C(23)	106.83(14)
C(17)-P(1)-C(23)	110.40(14)
P(1)-O(1)-La(1)	164.96(13)
C(29)#4-B(1)-C(29)	105.8(3)
C(29)#4-B(1)-C(35)#4	113.69(15)
C(29)-B(1)-C(35)#4	110.30(16)
C(29)#4-B(1)-C(35)	110.31(16)
C(29)-B(1)-C(35)	113.69(15)
C(35)#4-B(1)-C(35)	103.2(3)
C(5)-C(1)-C(2)	107.9(3)
C(5)-C(1)-C(6)	127.1(3)
C(2)-C(1)-C(6)	124.9(3)
C(5)-C(1)-La(1)	75.03(17)
C(2)-C(1)-La(1)	76.41(17)
C(6)-C(1)-La(1)	117.68(19)
C(3)-C(2)-C(1)	108.0(3)
C(3)-C(2)-C(7)	125.1(3)
C(1)-C(2)-C(7)	126.0(3)
C(3)-C(2)-La(1)	74.68(16)
C(1)-C(2)-La(1)	74.59(17)
C(7)-C(2)-La(1)	125.04(19)
C(4)-C(3)-C(2)	108.1(3)
C(4)-C(3)-C(8)	125.6(3)
C(2)-C(3)-C(8)	125.9(3)
C(4)-C(3)-La(1)	73.99(16)
C(2)-C(3)-La(1)	76.56(16)

C(8)-C(3)-La(1)	121.7(2)
C(3)-C(4)-C(5)	108.4(3)
C(3)-C(4)-C(9)	126.3(3)
C(5)-C(4)-C(9)	125.1(3)
C(3)-C(4)-La(1)	76.96(16)
C(5)-C(4)-La(1)	76.37(16)
C(9)-C(4)-La(1)	117.2(2)
C(1)-C(5)-C(4)	107.5(3)
C(1)-C(5)-C(10)	128.1(3)
C(4)-C(5)-C(10)	123.4(3)
C(1)-C(5)-La(1)	75.91(16)
C(4)-C(5)-La(1)	74.27(16)
C(10)-C(5)-La(1)	124.4(2)
C(16)-C(11)-C(12)	119.3(3)
C(16)-C(11)-P(1)	122.2(2)
C(12)-C(11)-P(1)	118.5(2)
C(13)-C(12)-C(11)	119.9(3)
C(14)-C(13)-C(12)	119.9(3)
C(13)-C(14)-C(15)	121.0(3)
C(16)-C(15)-C(14)	119.6(3)
C(15)-C(16)-C(11)	120.2(3)
C(18)-C(17)-C(22)	119.6(3)
C(18)-C(17)-P(1)	122.5(2)
C(22)-C(17)-P(1)	117.8(2)
C(19)-C(18)-C(17)	120.3(3)
C(18)-C(19)-C(20)	119.8(3)
C(21)-C(20)-C(19)	120.7(3)
C(20)-C(21)-C(22)	119.9(3)
C(21)-C(22)-C(17)	119.6(3)
C(24)-C(23)-C(28)	119.2(3)
C(24)-C(23)-P(1)	118.7(2)
C(28)-C(23)-P(1)	122.0(2)
C(25)-C(24)-C(23)	119.9(3)
C(26)-C(25)-C(24)	120.1(4)
C(25)-C(26)-C(27)	120.7(3)
C(26)-C(27)-C(28)	119.8(3)

C(27)-C(28)-C(23)	120.4(3)
C(34)-C(29)-C(30)	115.0(3)
C(34)-C(29)-B(1)	125.4(3)
C(30)-C(29)-B(1)	119.6(2)
C(31)-C(30)-C(29)	122.7(3)
C(30)-C(31)-C(32)	120.5(3)
C(33)-C(32)-C(31)	118.4(3)
C(32)-C(33)-C(34)	121.0(3)
C(33)-C(34)-C(29)	122.5(3)
C(36)-C(35)-C(40)	115.4(3)
C(36)-C(35)-B(1)	124.5(3)
C(40)-C(35)-B(1)	119.7(3)
C(35)-C(36)-C(37)	122.5(4)
C(38)-C(37)-C(36)	120.1(4)
C(39)-C(38)-C(37)	119.3(4)
C(38)-C(39)-C(40)	120.0(4)
C(39)-C(40)-C(35)	122.8(4)
C(42)-C(41)-C(42)#1	116.9(6)
C(42)-C(41)-C(45)	121.5(3)
C(42)#1-C(41)-C(45)	121.5(3)
C(43)-C(42)-C(41)	121.2(4)
C(44)-C(43)-C(42)	120.8(5)
C(43)#1-C(44)-C(43)	119.1(6)
C(48)-C(46)-C(47)	117.2(8)
C(48)-C(46)-C(49)	125.6(10)
C(47)-C(46)-C(49)	117.0(10)
C(48)#2-C(47)-C(46)	119.7(9)
C(47)#2-C(48)-C(46)	123.0(9)
C(53)#2-C(50)-C(52)	177.1(12)
C(53)#2-C(50)-C(51)	51.5(12)
C(52)-C(50)-C(51)	129.4(14)
C(53)#2-C(50)-C(51)#2	127.0(14)
C(52)-C(50)-C(51)#2	53.1(12)
C(51)-C(50)-C(51)#2	77.0(11)
C(53)#2-C(51)-C(52)#2	153(2)
C(53)#2-C(51)-C(54)#2	79.1(14)

C(52)#2-C(51)-C(54)#2	77.2(13)
C(53)#2-C(51)-C(50)	49.9(12)
C(52)#2-C(51)-C(50)	151.4(17)
C(54)#2-C(51)-C(50)	129.1(15)
C(53)#2-C(51)-C(50)#2	150.4(18)
C(52)#2-C(51)-C(50)#2	49.6(11)
C(54)#2-C(51)-C(50)#2	126.8(15)
C(50)-C(51)-C(50)#2	103.0(11)
C(53)#2-C(51)-C(51)#2	101.8(19)
C(52)#2-C(51)-C(51)#2	99.2(18)
C(54)#2-C(51)-C(51)#2	170.3(18)
C(50)-C(51)-C(51)#2	52.9(10)
C(50)#2-C(51)-C(51)#2	50.1(9)
C(50)-C(52)-C(51)#2	77.3(13)
C(50)-C(52)-C(54)	130.3(15)
C(51)#2-C(52)-C(54)	53.1(11)
C(50)#2-C(53)-C(51)#2	78.6(14)
C(50)#2-C(53)-C(54)	132.9(15)
C(51)#2-C(53)-C(54)	54.3(12)
C(51)#2-C(54)-C(53)	46.6(11)
C(51)#2-C(54)-C(52)	49.7(11)
C(53)-C(54)-C(52)	95.3(11)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+5/2 #2 -x+2,-y+1,-z+2 #3 -x+1,y,-z+3/2

#4 -x+2,y,-z+5/2

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
La(1)	17(1)	13(1)	13(1)	0	2(1)	0
P(1)	18(1)	17(1)	19(1)	-1(1)	2(1)	-2(1)
O(1)	22(1)	21(1)	21(1)	0(1)	2(1)	-6(1)
B(1)	25(3)	21(3)	21(2)	0	-4(2)	0
C(1)	30(2)	22(2)	16(1)	-5(1)	6(1)	6(1)
C(2)	28(2)	21(2)	17(1)	-7(1)	8(1)	0(1)
C(3)	30(2)	21(2)	14(1)	-3(1)	5(1)	2(1)
C(4)	28(2)	29(2)	14(1)	-8(1)	4(1)	-2(1)
C(5)	36(2)	20(2)	17(2)	-7(1)	7(1)	-3(1)
C(6)	38(2)	34(2)	28(2)	-4(2)	6(2)	13(2)
C(7)	30(2)	38(2)	29(2)	-8(2)	14(2)	-6(1)
C(8)	45(2)	29(2)	25(2)	2(1)	3(2)	6(2)
C(9)	30(2)	54(2)	29(2)	-12(2)	-1(2)	-6(2)
C(10)	60(2)	26(2)	27(2)	-7(2)	17(2)	-11(2)
C(11)	19(2)	22(2)	20(2)	-5(1)	2(1)	-3(1)
C(12)	22(2)	25(2)	25(2)	-1(1)	0(1)	1(1)
C(13)	27(2)	40(2)	18(2)	-6(1)	1(1)	2(2)
C(14)	32(2)	29(2)	30(2)	-14(2)	7(2)	0(1)
C(15)	43(2)	19(2)	34(2)	-2(1)	10(2)	2(1)
C(16)	29(2)	22(2)	25(2)	-1(1)	5(1)	1(1)
C(17)	26(2)	13(1)	18(1)	-3(1)	2(1)	0(1)
C(18)	23(2)	26(2)	28(2)	0(1)	2(1)	-2(1)
C(19)	36(2)	31(2)	32(2)	5(2)	13(2)	-2(2)
C(20)	47(2)	23(2)	24(2)	6(1)	5(2)	4(2)
C(21)	36(2)	27(2)	27(2)	2(1)	-3(2)	7(1)
C(22)	26(2)	22(2)	27(2)	-1(1)	4(1)	0(1)
C(23)	19(2)	25(2)	16(1)	1(1)	2(1)	2(1)
C(24)	29(2)	23(2)	29(2)	2(1)	5(1)	4(1)
C(25)	37(2)	34(2)	45(2)	9(2)	13(2)	13(2)

C(26)	23(2)	58(3)	38(2)	14(2)	8(2)	12(2)
C(27)	22(2)	59(3)	28(2)	4(2)	1(1)	-6(2)
C(28)	25(2)	33(2)	23(2)	-3(1)	2(1)	-3(1)
C(29)	24(2)	20(2)	23(2)	-3(1)	0(1)	4(1)
C(30)	30(2)	30(2)	25(2)	-1(1)	-2(1)	-2(1)
C(31)	36(2)	20(2)	39(2)	0(2)	10(2)	-4(1)
C(32)	50(2)	20(2)	24(2)	1(1)	12(2)	2(2)
C(33)	44(2)	22(2)	20(2)	-4(1)	1(1)	8(2)
C(34)	27(2)	19(2)	25(2)	-1(1)	3(1)	2(1)
C(35)	30(2)	22(2)	22(2)	5(1)	-7(1)	2(1)
C(36)	31(2)	32(2)	39(2)	3(2)	0(2)	-5(2)
C(37)	33(2)	46(2)	59(3)	11(2)	-2(2)	-8(2)
C(38)	46(2)	32(2)	65(3)	10(2)	-24(2)	-15(2)
C(39)	50(2)	25(2)	43(2)	1(2)	-22(2)	-4(2)
C(40)	42(2)	24(2)	29(2)	2(1)	-9(2)	-1(2)
C(41)	59(4)	56(4)	22(3)	0	11(3)	0
C(42)	47(2)	69(3)	24(2)	0(2)	7(2)	3(2)
C(43)	68(3)	68(3)	20(2)	-1(2)	6(2)	-16(2)
C(44)	85(5)	55(4)	25(3)	0	4(3)	0
C(45)	83(5)	53(4)	69(5)	0	14(4)	0

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10 ^{3})
for **4**.

	x	y	z	U(eq)
H(6A)	7531	5143	6485	50
H(6B)	6797	4874	6833	50
H(6C)	7102	5182	7485	50
H(7A)	7343	5681	5228	48
H(7B)	7533	5763	6334	48
H(7C)	6891	6005	5626	48
H(8A)	4706	5901	4253	50
H(8B)	5422	6123	4958	50
H(8C)	4274	6077	5123	50
H(9A)	3310	5300	4735	57
H(9B)	3105	5621	5308	57
H(9C)	3053	5276	5806	57
H(10A)	4364	4758	5742	55
H(10B)	4161	4854	6795	55
H(10C)	5217	4704	6607	55
H(12A)	7233	6389	10001	29
H(13A)	7024	6789	11116	34
H(14A)	6545	7306	10623	36
H(15A)	6257	7431	9016	38
H(16A)	6481	7036	7887	30
H(18A)	8507	6584	6807	31
H(19A)	8415	6821	5310	39
H(20A)	6860	6932	4475	37
H(21A)	5399	6809	5124	37
H(22A)	5478	6559	6614	30
H(24A)	7778	5719	7930	32
H(25A)	9296	5467	8448	46

H(26A)	10624	5768	9162	47
H(27A)	10465	6322	9364	44
H(28A)	8961	6578	8853	33
H(30A)	11358	7164	12341	34
H(31A)	11676	7520	11157	38
H(32A)	10708	7507	9678	37
H(33A)	9426	7127	9421	35
H(34A)	9109	6767	10598	29
H(36A)	8200	6554	13300	42
H(37A)	6980	6156	13015	56
H(38A)	7062	5783	11785	60
H(39A)	8365	5817	10842	49
H(40A)	9600	6208	11149	39
H(42)	6508	7104	12652	55
H(43)	6496	7665	12650	62
H(44)	5000	7947	12500	66
H(45A)	5672	6601	12420	102
H(45B)	4525	6601	11978	102
H(45C)	4804	6601	13103	102

X-ray Data Collection, Structure Solution and Refinement for **7**.

A yellow crystal of approximate dimensions 0.11 x 0.21 x 0.22 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2[6] program package was used to determine the unit-cell parameters and for data collection (20 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[7] and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program. There were no systematic absences nor any diffraction symmetry other than the Friedel condition. The centrosymmetric triclinic space group $P\bar{1}$ was assigned and later determined to be correct. The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. The pentamethylcyclopentadienyl ring defined by atoms C(1)-C(10) was disordered and included using multiple components, partial site-occupancy-factors (0.55:0.45) and isotropic thermal parameters. At convergence, wR2 = 0.0756 and Goof = 1.045 for 317 variables refined against 7231 data (0.75Å), R1 = 0.0298 for those 6704 data with I > 2.0σ(I).

Table 1. Crystal data and structure refinement for **7**.

Identification code	tjm9 (**7**)	
Empirical formula	C_{31} H_{45} La S_2	
Formula weight	620.70	
Temperature	163(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 9.9376(6) Å	α= 74.1820(10)°.
	b = 11.3390(7) Å	β= 83.3800(10)°.
	c = 14.4297(9) Å	γ = 70.7040(10)°.
Volume	1475.95(16) Å^3	
Z	2	
Density (calculated)	1.397 Mg/m^3	
Absorption coefficient	1.606 mm^{-1}	
F(000)	640	
Crystal color	yellow	
Crystal size	0.22 x 0.21 x 0.11 mm^3	
Theta range for data collection	3.92 to 28.28°	
Index ranges	$-13 \le h \le 13$, $-15 \le k \le 15$, $-19 \le l \le 19$	
Reflections collected	17905	

Independent reflections	7231 [R(int) = 0.0182]
Completeness to theta = 28.28°	98.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8432 and 0.7190
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7231 / 0 / 317
Goodness-of-fit on F^2	1.045
Final R indices [I>2sigma(I) = 6704 data]	R1 = 0.0298, wR2 = 0.0739
R indices (all data, 0.75Å)	R1 = 0.0328, wR2 = 0.0756
Largest diff. peak and hole	1.387 and -0.568 e.$Å^{-3}$

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

	x	y	z	U(eq)
La(1)	1951(1)	-875(1)	2965(1)	23(1)
S(2)	446(1)	1593(1)	1671(1)	27(1)
S(1)	-207(1)	1124(1)	3775(1)	27(1)
C(1)	-119(5)	-1677(5)	2396(5)	25(1)
C(2)	127(6)	-2410(5)	3344(4)	27(1)
C(3)	1500(7)	-3291(5)	3380(4)	25(1)
C(4)	2155(6)	-3150(5)	2442(5)	24(1)
C(5)	1128(7)	-2115(6)	1836(4)	28(1)
C(6)	-1438(8)	-687(7)	1905(6)	56(2)
C(7)	-1069(8)	-2247(8)	4106(6)	58(2)
C(8)	2008(8)	-4344(7)	4282(5)	51(2)
C(9)	3497(7)	-4098(7)	2212(5)	48(1)
C(10)	1433(8)	-1661(7)	766(5)	48(1)
C(1B)	107(6)	-1633(5)	2040(5)	20(1)
C(2B)	-173(6)	-2053(6)	3023(5)	22(1)
C(3B)	1027(8)	-3056(6)	3442(4)	20(1)
C(4B)	2045(7)	-3261(6)	2696(5)	20(2)
C(5B)	1502(8)	-2350(7)	1804(4)	21(1)
C(6B)	-1024(9)	-653(8)	1347(6)	47(2)
C(7B)	-1513(10)	-1674(9)	3617(7)	57(2)
C(8B)	1277(9)	-3937(8)	4440(6)	45(2)
C(9B)	3426(7)	-4378(7)	2696(6)	37(1)
C(10B)	2120(9)	-2165(8)	803(5)	43(2)
C(11)	3838(3)	439(2)	3077(2)	26(1)
C(12)	4069(3)	-626(3)	3897(2)	29(1)
C(13)	4717(3)	-1767(3)	3582(2)	33(1)
C(14)	4895(3)	-1416(3)	2573(2)	35(1)
C(15)	4339(3)	-52(3)	2257(2)	31(1)

C(16)	3267(3)	1841(3)	3081(2)	34(1)
C(17)	3638(3)	-565(3)	4921(2)	41(1)
C(18)	5253(4)	-3106(3)	4246(3)	51(1)
C(19)	5713(4)	-2290(4)	1937(3)	62(1)
C(20)	4387(4)	726(4)	1233(2)	46(1)
C(21)	-516(2)	2045(2)	2630(2)	21(1)
C(22)	-1685(2)	3373(2)	2444(2)	22(1)
C(23)	-2500(3)	3643(2)	1540(2)	25(1)
C(24)	-2303(3)	4680(2)	902(2)	27(1)
C(25)	-1341(3)	5162(2)	1297(2)	25(1)
C(26)	-969(3)	4427(2)	2188(2)	24(1)
C(27)	-2740(3)	3537(3)	3299(2)	32(1)
C(28)	-3411(3)	2852(3)	1472(3)	39(1)
C(29)	-2961(4)	5333(3)	-68(2)	44(1)
C(30)	-921(3)	6320(3)	755(2)	37(1)
C(31)	-119(3)	4618(3)	2889(2)	35(1)

Table 3. Bond lengths [Å] and angles [°] for **7**.

La(1)-Cnt1	2.542
La(1)-Cnt2	2.512
La(1)-C(12)	2.752(3)
La(1)-C(13)	2.758(3)
La(1)-C(5)	2.760(6)
La(1)-C(1)	2.787(5)
La(1)-C(11)	2.794(2)
La(1)-C(3B)	2.804(5)
La(1)-C(14)	2.807(3)
La(1)-C(4B)	2.807(6)
La(1)-C(3)	2.814(5)
La(1)-C(15)	2.817(3)
La(1)-C(4)	2.819(5)
La(1)-C(2)	2.819(5)
La(1)-C(5B)	2.828(6)
La(1)-C(2B)	2.829(5)
La(1)-C(1B)	2.848(5)
La(1)-S(2)	2.9291(6)
La(1)-S(1)	2.9587(6)
S(2)-C(21)	1.688(2)
S(1)-C(21)	1.697(2)
C(1)-C(2)	1.394(7)
C(1)-C(5)	1.421(8)
C(1)-C(6)	1.512(9)
C(2)-C(3)	1.396(7)
C(2)-C(7)	1.524(9)
C(3)-C(4)	1.423(8)
C(3)-C(8)	1.511(8)
C(4)-C(5)	1.428(8)
C(4)-C(9)	1.481(9)
C(5)-C(10)	1.516(9)
C(1B)-C(2B)	1.395(8)
C(1B)-C(5B)	1.413(9)
C(1B)-C(6B)	1.526(9)

C(2B)-C(3B)	1.405(9)
C(2B)-C(7B)	1.502(10)
C(3B)-C(4B)	1.402(9)
C(3B)-C(8B)	1.506(9)
C(4B)-C(5B)	1.442(9)
C(4B)-C(9B)	1.530(9)
C(5B)-C(10B)	1.491(10)
C(11)-C(15)	1.415(4)
C(11)-C(12)	1.418(4)
C(11)-C(16)	1.502(3)
C(12)-C(13)	1.413(4)
C(12)-C(17)	1.503(4)
C(13)-C(14)	1.408(4)
C(13)-C(18)	1.515(4)
C(14)-C(15)	1.419(4)
C(14)-C(19)	1.509(4)
C(15)-C(20)	1.505(4)
C(21)-C(22)	1.544(3)
C(22)-C(23)	1.521(3)
C(22)-C(26)	1.528(3)
C(22)-C(27)	1.534(3)
C(23)-C(24)	1.337(4)
C(23)-C(28)	1.496(4)
C(24)-C(25)	1.476(4)
C(24)-C(29)	1.504(4)
C(25)-C(26)	1.344(3)
C(25)-C(30)	1.495(3)
C(26)-C(31)	1.490(4)

Cnt1-La(1)-S(1)	112.7
Cnt1-La(1)-S(2)	104.9
Cnt2-La(1)-S(1)	108.6
Cnt2-La(1)-S(2)	103.4
Cnt1-La(1)-Cnt2	137.5
C(12)-La(1)-C(13)	29.72(8)
C(12)-La(1)-C(5)	149.25(16)

C(13)-La(1)-C(5)	119.70(16)
C(12)-La(1)-C(1)	165.68(13)
C(13)-La(1)-C(1)	142.14(11)
C(5)-La(1)-C(1)	29.67(17)
C(12)-La(1)-C(11)	29.61(8)
C(13)-La(1)-C(11)	48.78(8)
C(5)-La(1)-C(11)	144.22(14)
C(1)-La(1)-C(11)	164.70(13)
C(12)-La(1)-C(3B)	124.23(14)
C(13)-La(1)-C(3B)	105.10(15)
C(5)-La(1)-C(3B)	48.33(16)
C(1)-La(1)-C(3B)	41.65(16)
C(11)-La(1)-C(3B)	152.93(14)
C(12)-La(1)-C(14)	48.50(9)
C(13)-La(1)-C(14)	29.29(9)
C(5)-La(1)-C(14)	103.49(15)
C(1)-La(1)-C(14)	132.87(13)
C(11)-La(1)-C(14)	48.33(8)
C(3B)-La(1)-C(14)	114.02(16)
C(12)-La(1)-C(4B)	121.74(14)
C(13)-La(1)-C(4B)	93.73(14)
C(5)-La(1)-C(4B)	34.05(19)
C(1)-La(1)-C(4B)	48.48(16)
C(11)-La(1)-C(4B)	138.87(14)
C(3B)-La(1)-C(4B)	28.94(19)
C(14)-La(1)-C(4B)	90.98(15)
C(12)-La(1)-C(3)	118.88(12)
C(13)-La(1)-C(3)	97.04(13)
C(5)-La(1)-C(3)	47.91(16)
C(1)-La(1)-C(3)	47.64(15)
C(11)-La(1)-C(3)	145.72(13)
C(3B)-La(1)-C(3)	9.59(13)
C(14)-La(1)-C(3)	104.44(14)
C(4B)-La(1)-C(3)	21.89(18)
C(12)-La(1)-C(15)	48.47(8)
C(13)-La(1)-C(15)	48.45(8)

C(5)-La(1)-C(15)	115.23(14)
C(1)-La(1)-C(15)	141.90(15)
C(11)-La(1)-C(15)	29.21(8)
C(3B)-La(1)-C(15)	142.33(16)
C(14)-La(1)-C(15)	29.23(8)
C(4B)-La(1)-C(15)	115.95(15)
C(3)-La(1)-C(15)	132.78(14)
C(12)-La(1)-C(4)	123.20(12)
C(13)-La(1)-C(4)	94.07(12)
C(5)-La(1)-C(4)	29.64(17)
C(1)-La(1)-C(4)	48.87(15)
C(11)-La(1)-C(4)	135.97(13)
C(3B)-La(1)-C(4)	35.75(18)
C(14)-La(1)-C(4)	87.65(13)
C(4B)-La(1)-C(4)	7.52(16)
C(3)-La(1)-C(4)	29.27(16)
C(15)-La(1)-C(4)	110.79(13)
C(12)-La(1)-C(2)	137.23(14)
C(13)-La(1)-C(2)	123.53(14)
C(5)-La(1)-C(2)	48.03(16)
C(1)-La(1)-C(2)	28.78(15)
C(11)-La(1)-C(2)	165.96(13)
C(3B)-La(1)-C(2)	19.38(16)
C(14)-La(1)-C(2)	132.80(13)
C(4B)-La(1)-C(2)	43.26(17)
C(3)-La(1)-C(2)	28.70(15)
C(15)-La(1)-C(2)	159.11(12)
C(4)-La(1)-C(2)	48.33(16)
C(12)-La(1)-C(5B)	141.45(16)
C(13)-La(1)-C(5B)	111.94(16)
C(5)-La(1)-C(5B)	7.80(17)
C(1)-La(1)-C(5B)	36.75(19)
C(11)-La(1)-C(5B)	139.18(15)
C(3B)-La(1)-C(5B)	48.78(17)
C(14)-La(1)-C(5B)	96.17(16)
C(4B)-La(1)-C(5B)	29.66(19)

C(3)-La(1)-C(5B)	46.62(16)
C(15)-La(1)-C(5B)	109.97(15)
C(4)-La(1)-C(5B)	24.05(18)
C(2)-La(1)-C(5B)	51.80(17)
C(12)-La(1)-C(2B)	148.26(16)
C(13)-La(1)-C(2B)	133.98(15)
C(5)-La(1)-C(2B)	42.49(17)
C(1)-La(1)-C(2B)	18.27(15)
C(11)-La(1)-C(2B)	172.89(12)
C(3B)-La(1)-C(2B)	28.88(18)
C(14)-La(1)-C(2B)	138.04(13)
C(4B)-La(1)-C(2B)	47.10(17)
C(3)-La(1)-C(2B)	37.31(17)
C(15)-La(1)-C(2B)	157.70(13)
C(4)-La(1)-C(2B)	50.56(16)
C(2)-La(1)-C(2B)	11.42(12)
C(5B)-La(1)-C(2B)	47.81(18)
C(12)-La(1)-C(1B)	168.90(12)
C(13)-La(1)-C(1B)	139.52(13)
C(5)-La(1)-C(1B)	21.15(17)
C(1)-La(1)-C(1B)	10.79(12)
C(11)-La(1)-C(1B)	156.01(14)
C(3B)-La(1)-C(1B)	47.60(16)
C(14)-La(1)-C(1B)	124.36(14)
C(4B)-La(1)-C(1B)	47.21(17)
C(3)-La(1)-C(1B)	51.74(15)
C(15)-La(1)-C(1B)	131.11(15)
C(4)-La(1)-C(1B)	45.73(15)
C(2)-La(1)-C(1B)	38.02(17)
C(5B)-La(1)-C(1B)	28.83(18)
C(2B)-La(1)-C(1B)	28.45(16)
C(12)-La(1)-S(2)	110.83(6)
C(13)-La(1)-S(2)	129.26(6)
C(5)-La(1)-S(2)	88.58(13)
C(1)-La(1)-S(2)	82.74(11)
C(11)-La(1)-S(2)	83.04(5)

C(3B)-La(1)-S(2)	124.03(13)
C(14)-La(1)-S(2)	109.01(7)
C(4B)-La(1)-S(2)	122.63(14)
C(3)-La(1)-S(2)	130.28(11)
C(15)-La(1)-S(2)	82.24(6)
C(4)-La(1)-S(2)	117.60(12)
C(2)-La(1)-S(2)	106.88(13)
C(5B)-La(1)-S(2)	93.56(14)
C(2B)-La(1)-S(2)	95.87(15)
C(1B)-La(1)-S(2)	78.94(11)
C(12)-La(1)-S(1)	90.37(6)
C(13)-La(1)-S(1)	119.28(6)
C(5)-La(1)-S(1)	120.28(15)
C(1)-La(1)-S(1)	92.64(11)
C(11)-La(1)-S(1)	85.27(5)
C(3B)-La(1)-S(1)	107.01(15)
C(14)-La(1)-S(1)	133.44(6)
C(4B)-La(1)-S(1)	134.24(14)
C(3)-La(1)-S(1)	116.05(13)
C(15)-La(1)-S(1)	109.74(6)
C(4)-La(1)-S(1)	138.62(12)
C(2)-La(1)-S(1)	90.98(11)
C(5B)-La(1)-S(1)	128.06(15)
C(2B)-La(1)-S(1)	88.08(11)
C(1B)-La(1)-S(1)	99.30(12)
S(2)-La(1)-S(1)	60.561(17)
C(21)-S(2)-La(1)	88.90(8)
C(21)-S(1)-La(1)	87.76(8)
C(2)-C(1)-C(5)	107.6(5)
C(2)-C(1)-C(6)	132.3(6)
C(5)-C(1)-C(6)	119.7(6)
C(2)-C(1)-La(1)	76.9(3)
C(5)-C(1)-La(1)	74.1(3)
C(6)-C(1)-La(1)	119.9(4)
C(1)-C(2)-C(3)	108.4(4)
C(1)-C(2)-C(7)	120.1(6)

C(3)-C(2)-C(7)	131.3(6)
C(1)-C(2)-La(1)	74.3(3)
C(3)-C(2)-La(1)	75.4(3)
C(7)-C(2)-La(1)	120.9(4)
C(2)-C(3)-C(4)	109.9(5)
C(2)-C(3)-C(8)	120.8(6)
C(4)-C(3)-C(8)	128.5(6)
C(2)-C(3)-La(1)	75.9(3)
C(4)-C(3)-La(1)	75.5(3)
C(8)-C(3)-La(1)	123.5(4)
C(3)-C(4)-C(5)	105.1(5)
C(3)-C(4)-C(9)	122.6(6)
C(5)-C(4)-C(9)	131.4(6)
C(3)-C(4)-La(1)	75.2(3)
C(5)-C(4)-La(1)	72.9(3)
C(9)-C(4)-La(1)	125.4(4)
C(1)-C(5)-C(4)	109.0(5)
C(1)-C(5)-C(10)	129.7(6)
C(4)-C(5)-C(10)	121.3(6)
C(1)-C(5)-La(1)	76.2(3)
C(4)-C(5)-La(1)	77.4(3)
C(10)-C(5)-La(1)	114.2(4)
C(2B)-C(1B)-C(5B)	109.5(5)
C(2B)-C(1B)-C(6B)	122.8(6)
C(5B)-C(1B)-C(6B)	127.4(6)
C(2B)-C(1B)-La(1)	75.1(3)
C(5B)-C(1B)-La(1)	74.8(3)
C(6B)-C(1B)-La(1)	122.0(4)
C(1B)-C(2B)-C(3B)	109.1(5)
C(1B)-C(2B)-C(7B)	130.6(7)
C(3B)-C(2B)-C(7B)	120.1(7)
C(1B)-C(2B)-La(1)	76.5(3)
C(3B)-C(2B)-La(1)	74.6(3)
C(7B)-C(2B)-La(1)	119.2(5)
C(4B)-C(3B)-C(2B)	106.7(5)
C(4B)-C(3B)-C(8B)	120.8(7)

C(2B)-C(3B)-C(8B)	132.1(7)
C(4B)-C(3B)-La(1)	75.6(3)
C(2B)-C(3B)-La(1)	76.6(3)
C(8B)-C(3B)-La(1)	118.9(4)
C(3B)-C(4B)-C(5B)	109.7(6)
C(3B)-C(4B)-C(9B)	129.2(7)
C(5B)-C(4B)-C(9B)	120.3(6)
C(3B)-C(4B)-La(1)	75.4(3)
C(5B)-C(4B)-La(1)	76.0(4)
C(9B)-C(4B)-La(1)	123.4(4)
C(1B)-C(5B)-C(4B)	105.0(6)
C(1B)-C(5B)-C(10B)	123.0(6)
C(4B)-C(5B)-C(10B)	131.9(7)
C(1B)-C(5B)-La(1)	76.4(3)
C(4B)-C(5B)-La(1)	74.4(3)
C(10B)-C(5B)-La(1)	117.4(4)
C(15)-C(11)-C(12)	107.7(2)
C(15)-C(11)-C(16)	125.8(2)
C(12)-C(11)-C(16)	126.4(2)
C(15)-C(11)-La(1)	76.26(14)
C(12)-C(11)-La(1)	73.54(14)
C(16)-C(11)-La(1)	119.63(16)
C(13)-C(12)-C(11)	108.2(2)
C(13)-C(12)-C(17)	125.6(3)
C(11)-C(12)-C(17)	126.2(3)
C(13)-C(12)-La(1)	75.38(15)
C(11)-C(12)-La(1)	76.85(14)
C(17)-C(12)-La(1)	111.87(17)
C(14)-C(13)-C(12)	108.1(2)
C(14)-C(13)-C(18)	127.1(3)
C(12)-C(13)-C(18)	124.5(3)
C(14)-C(13)-La(1)	77.26(16)
C(12)-C(13)-La(1)	74.89(14)
C(18)-C(13)-La(1)	118.92(19)
C(13)-C(14)-C(15)	108.1(2)
C(13)-C(14)-C(19)	126.8(3)

C(15)-C(14)-C(19)	124.6(3)
C(13)-C(14)-La(1)	73.45(15)
C(15)-C(14)-La(1)	75.77(15)
C(19)-C(14)-La(1)	123.3(2)
C(11)-C(15)-C(14)	108.0(2)
C(11)-C(15)-C(20)	126.5(3)
C(14)-C(15)-C(20)	125.4(3)
C(11)-C(15)-La(1)	74.53(14)
C(14)-C(15)-La(1)	75.00(15)
C(20)-C(15)-La(1)	120.0(2)
C(22)-C(21)-S(2)	117.78(16)
C(22)-C(21)-S(1)	119.62(17)
S(2)-C(21)-S(1)	122.57(14)
C(23)-C(22)-C(26)	102.53(19)
C(23)-C(22)-C(27)	109.5(2)
C(26)-C(22)-C(27)	110.5(2)
C(23)-C(22)-C(21)	111.83(19)
C(26)-C(22)-C(21)	108.67(19)
C(27)-C(22)-C(21)	113.25(19)
C(24)-C(23)-C(28)	129.1(2)
C(24)-C(23)-C(22)	109.2(2)
C(28)-C(23)-C(22)	121.6(2)
C(23)-C(24)-C(25)	109.8(2)
C(23)-C(24)-C(29)	127.7(3)
C(25)-C(24)-C(29)	122.5(2)
C(26)-C(25)-C(24)	109.5(2)
C(26)-C(25)-C(30)	127.8(3)
C(24)-C(25)-C(30)	122.7(2)
C(25)-C(26)-C(31)	128.3(2)
C(25)-C(26)-C(22)	108.9(2)
C(31)-C(26)-C(22)	122.6(2)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **7**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
La(1)	19(1)	14(1)	35(1)	-6(1)	-3(1)	-4(1)
S(2)	28(1)	22(1)	25(1)	-5(1)	0(1)	-1(1)
S(1)	29(1)	21(1)	24(1)	-1(1)	0(1)	-2(1)
C(11)	21(1)	22(1)	37(1)	-8(1)	-1(1)	-9(1)
C(12)	22(1)	30(1)	36(1)	-5(1)	-4(1)	-11(1)
C(13)	19(1)	24(1)	54(2)	-5(1)	-5(1)	-5(1)
C(14)	22(1)	30(1)	56(2)	-20(1)	9(1)	-9(1)
C(15)	30(1)	29(1)	39(1)	-10(1)	6(1)	-16(1)
C(16)	30(1)	25(1)	51(2)	-11(1)	-2(1)	-11(1)
C(17)	39(2)	53(2)	36(2)	-5(1)	-1(1)	-24(1)
C(18)	37(2)	28(2)	81(3)	2(2)	-19(2)	-6(1)
C(19)	43(2)	55(2)	100(3)	-49(2)	33(2)	-20(2)
C(20)	56(2)	53(2)	37(2)	-11(1)	11(1)	-32(2)
C(21)	22(1)	15(1)	25(1)	-3(1)	-2(1)	-6(1)
C(22)	21(1)	17(1)	25(1)	-4(1)	-1(1)	-3(1)
C(23)	20(1)	21(1)	33(1)	-7(1)	-5(1)	-2(1)
C(24)	27(1)	21(1)	28(1)	-5(1)	-5(1)	1(1)
C(25)	25(1)	17(1)	30(1)	-6(1)	4(1)	-4(1)
C(26)	23(1)	17(1)	31(1)	-8(1)	0(1)	-5(1)
C(27)	29(1)	25(1)	32(1)	-4(1)	6(1)	-2(1)
C(28)	28(1)	32(1)	60(2)	-15(1)	-10(1)	-8(1)
C(29)	51(2)	34(2)	36(2)	-1(1)	-19(1)	1(1)
C(30)	43(2)	22(1)	43(2)	-5(1)	13(1)	-12(1)
C(31)	38(2)	27(1)	45(2)	-14(1)	-8(1)	-9(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10 ^{3})
for **7**.

	x	y	z	U(eq)
H(6A)	-1915	-1106	1597	84
H(6B)	-1163	-10	1416	84
H(6C)	-2089	-304	2384	84
H(7A)	-1796	-1407	3893	86
H(7B)	-681	-2295	4714	86
H(7C)	-1500	-2936	4202	86
H(8A)	1751	-3979	4844	76
H(8B)	3046	-4726	4239	76
H(8C)	1556	-5013	4350	76
H(9A)	4157	-4376	2741	72
H(9B)	3933	-3699	1617	72
H(9C)	3291	-4848	2123	72
H(10A)	947	-732	547	72
H(10B)	1085	-2122	412	72
H(10C)	2463	-1835	649	72
H(6B1)	-1311	-1092	942	71
H(6B2)	-632	8	937	71
H(6B3)	-1857	-245	1715	71
H(7B1)	-2143	-836	3276	85
H(7B2)	-1273	-1612	4239	85
H(7B3)	-2000	-2326	3726	85
H(8B1)	819	-4605	4517	67
H(8B2)	869	-3435	4918	67
H(8B3)	2304	-4346	4534	67
H(9B1)	3943	-4562	3284	55
H(9B2)	4022	-4142	2131	55
H(9B3)	3199	-5147	2672	55

H(10D)	1584	-2410	398	65
H(10E)	3121	-2706	811	65
H(10F)	2063	-1256	542	65
H(16A)	4064	2176	3062	51
H(16B)	2684	1935	3668	51
H(16C)	2682	2326	2516	51
H(17A)	4391	-1183	5351	62
H(17B)	2750	-782	5095	62
H(17C)	3490	308	4983	62
H(18A)	6005	-3139	4645	77
H(18B)	5637	-3740	3860	77
H(18C)	4463	-3304	4661	77
H(19A)	6700	-2275	1850	93
H(19B)	5266	-1990	1308	93
H(19C)	5704	-3174	2239	93
H(20A)	5321	860	1087	69
H(20B)	3640	1564	1151	69
H(20C)	4230	262	795	69
H(27A)	-3453	4394	3139	47
H(27B)	-2224	3448	3866	47
H(27C)	-3216	2874	3439	47
H(28A)	-3757	3105	815	58
H(28B)	-4226	2996	1926	58
H(28C)	-2847	1936	1630	58
H(29A)	-3524	4838	-205	66
H(29B)	-2206	5379	-564	66
H(29D)	-3582	6207	-66	66
H(30A)	-349	6518	1166	56
H(30D)	-1780	7059	569	56
H(30B)	-360	6141	176	56
H(31D)	473	5149	2542	53
H(31A)	495	3778	3240	53
H(31B)	-765	5053	3346	53

X-ray Data Collection, Structure Solution and Refinement for **8**.

A yellow crystal of approximate dimensions 0.09 x 0.11 x 0.17 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2[8] program package was used to determine the unit-cell parameters and for data collection (30 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[9] and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program. The diffraction symmetry was 2/*m* and the systematic absences were consistent with the monoclinic space group $P2_1/c$ that was later determined to be correct. The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. Least-squares analysis yielded wR2 = 0.1243 and Goof = 1.049 for 502 variables refined against 7704 data (0.85Å), R1 = 0.0503 for those 6003 data with $I > 2.0\sigma(I)$.

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

Identification code	tjm11 (**8**)	
Empirical formula	$C_{49}\ H_{60}\ La\ O\ P\ S_2$	
Formula weight	898.97	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.0956(19) Å	α= 90°.
	b = 12.0752(19) Å	β= 91.606(2)°.
	c = 31.142(5) Å	γ = 90°.
Volume	4546.7(12) $Å^3$	
Z	4	
Density (calculated)	1.313 Mg/m^3	
Absorption coefficient	1.100 mm^{-1}	
F(000)	1864	
Crystal color	yellow	
Crystal size	0.17 x 0.11 x 0.09 mm^3	
Theta range for data collection	4.09 to 24.71°.	
Index ranges	$-14 \le h \le 14$, $-14 \le k \le 14$, $-36 \le l \le 36$	
Reflections collected	39228	
Independent reflections	7704 [R(int) = 0.0752]	
Completeness to theta = 24.71°	99.4 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9123 and 0.8350
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7704 / 0 / 502
Goodness-of-fit on F^2	1.049
Final R indices [I>2sigma(I) = 6003 data]	R1 = 0.0503, wR2 = 0.1167
R indices (all data, 0.85Å)	R1 = 0.0684, wR2 = 0.1243
Largest diff. peak and hole	1.350 and -2.159 e.Å^{-3}

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

	x	y	z	U(eq)
La(1)	6543(1)	8373(1)	6158(1)	16(1)
P(1)	8427(1)	6572(1)	6963(1)	19(1)
O(1)	7631(3)	7264(3)	6692(1)	18(1)
S(1)	8077(1)	6977(1)	5630(1)	22(1)
S(2)	6818(1)	8805(1)	5219(1)	22(1)
C(1)	4737(4)	7153(5)	5766(2)	24(1)
C(2)	4267(4)	8131(5)	5920(2)	28(1)
C(3)	4313(5)	8137(6)	6371(2)	39(2)
C(4)	4808(5)	7149(7)	6496(2)	48(2)
C(5)	5080(5)	6501(5)	6127(3)	42(2)
C(6)	4766(6)	6788(7)	5300(2)	51(2)
C(7)	3751(6)	9026(6)	5635(3)	49(2)
C(8)	3693(6)	8952(8)	6655(3)	65(3)
C(9)	4905(7)	6749(10)	6965(3)	104(5)
C(10)	5518(6)	5346(6)	6109(4)	90(4)
C(11)	7884(4)	10354(4)	6195(2)	21(1)
C(12)	7813(4)	10012(4)	6630(2)	22(1)
C(13)	6709(5)	10176(4)	6752(2)	24(1)
C(14)	6106(5)	10655(5)	6403(2)	27(1)
C(15)	6826(5)	10747(4)	6055(2)	24(1)
C(16)	8914(5)	10420(5)	5936(2)	33(2)
C(17)	8753(5)	9722(5)	6934(2)	31(1)
C(18)	6306(6)	10034(6)	7207(2)	44(2)
C(19)	5014(5)	11250(6)	6411(3)	46(2)
C(20)	6564(6)	11338(5)	5634(2)	38(2)
C(21)	7803(4)	7830(4)	5206(2)	16(1)
C(22)	8508(4)	7692(4)	4799(2)	20(1)
C(23)	8233(4)	6592(5)	4575(2)	21(1)

C(24)	9183(5)	6030(4)	4519(2)	22(1)
C(25)	10123(4)	6637(5)	4723(2)	22(1)
C(26)	9744(4)	7560(4)	4904(2)	20(1)
C(27)	8335(4)	8648(4)	4475(2)	22(1)
C(28)	7082(5)	6309(5)	4428(2)	30(1)
C(29)	9318(5)	4955(5)	4286(2)	29(1)
C(30)	11299(5)	6216(5)	4711(2)	30(1)
C(31)	10374(5)	8404(5)	5162(2)	28(1)
C(32)	8070(4)	5118(4)	6961(2)	20(1)
C(33)	7984(4)	4599(4)	6559(2)	22(1)
C(34)	7716(5)	3491(5)	6537(2)	30(1)
C(35)	7565(5)	2884(5)	6904(2)	36(2)
C(36)	7665(7)	3391(5)	7301(2)	46(2)
C(37)	7914(6)	4508(5)	7334(2)	36(2)
C(38)	8451(4)	7042(4)	7514(2)	17(1)
C(39)	7445(5)	7211(5)	7717(2)	31(1)
C(40)	7429(5)	7605(5)	8139(2)	35(2)
C(41)	8414(5)	7820(5)	8360(2)	29(1)
C(42)	9407(5)	7647(5)	8164(2)	35(2)
C(43)	9440(5)	7259(5)	7744(2)	27(1)
C(44)	9830(4)	6602(5)	6772(2)	21(1)
C(45)	10143(5)	7395(4)	6479(2)	22(1)
C(46)	11218(5)	7424(5)	6335(2)	27(1)
C(47)	11983(5)	6650(5)	6485(2)	30(1)
C(48)	11663(5)	5854(5)	6778(2)	27(1)
C(49)	10592(4)	5826(5)	6919(2)	23(1)

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

La(1)-Cnt1	2.575
La(1)-Cnt2	2.627
La(1)-O(1)	2.483(3)
La(1)-C(4)	2.797(6)
La(1)-C(3)	2.811(6)
La(1)-C(2)	2.846(5)
La(1)-C(13)	2.861(5)
La(1)-C(5)	2.870(6)
La(1)-C(1)	2.878(5)
La(1)-C(12)	2.883(5)
La(1)-C(11)	2.890(5)
La(1)-C(15)	2.905(6)
La(1)-C(14)	2.912(6)
La(1)-S(2)	2.9982(14)
La(1)-S(1)	3.0263(14)
P(1)-O(1)	1.515(4)
P(1)-C(38)	1.807(5)
P(1)-C(32)	1.808(5)
P(1)-C(44)	1.814(5)
S(1)-C(21)	1.700(5)
S(2)-C(21)	1.675(5)
C(1)-C(2)	1.401(8)
C(1)-C(5)	1.424(8)
C(1)-C(6)	1.519(9)
C(2)-C(3)	1.405(9)
C(2)-C(7)	1.520(9)
C(3)-C(4)	1.386(10)
C(3)-C(8)	1.534(10)
C(4)-C(5)	1.434(11)
C(4)-C(9)	1.541(9)
C(5)-C(10)	1.494(10)
C(11)-C(15)	1.421(8)
C(11)-C(12)	1.421(7)
C(11)-C(16)	1.506(8)

C(12)-C(13)	1.414(8)
C(12)-C(17)	1.501(7)
C(13)-C(14)	1.414(8)
C(13)-C(18)	1.520(8)
C(14)-C(15)	1.413(8)
C(14)-C(19)	1.505(8)
C(15)-C(20)	1.519(8)
C(21)-C(22)	1.557(7)
C(22)-C(26)	1.529(7)
C(22)-C(23)	1.533(7)
C(22)-C(27)	1.543(7)
C(23)-C(24)	1.350(8)
C(23)-C(28)	1.492(8)
C(24)-C(25)	1.482(8)
C(24)-C(29)	1.498(8)
C(25)-C(26)	1.335(8)
C(25)-C(30)	1.512(7)
C(26)-C(31)	1.495(8)
C(32)-C(37)	1.394(8)
C(32)-C(33)	1.400(7)
C(33)-C(34)	1.378(8)
C(34)-C(35)	1.375(9)
C(35)-C(36)	1.381(9)
C(36)-C(37)	1.385(9)
C(38)-C(43)	1.401(7)
C(38)-C(39)	1.402(8)
C(39)-C(40)	1.396(8)
C(40)-C(41)	1.385(8)
C(41)-C(42)	1.379(9)
C(42)-C(43)	1.390(8)
C(44)-C(49)	1.383(8)
C(44)-C(45)	1.384(8)
C(45)-C(46)	1.388(8)
C(46)-C(47)	1.387(8)
C(47)-C(48)	1.386(8)
C(48)-C(49)	1.381(8)

Cnt1-La(1)-S(1)	107.2
Cnt1-La(1)-S(2)	100.2
Cnt1-La(1)-O(1)	103.4
Cnt2-La(1)-S(1)	122.0
Cnt2-La(1)-S(2)	95.4
Cnt2-La(1)-O(1)	100.5
Cnt1-La(1)-Cnt2	129.2
O(1)-La(1)-C(4)	81.48(17)
O(1)-La(1)-C(3)	106.31(17)
C(4)-La(1)-C(3)	28.6(2)
O(1)-La(1)-C(2)	127.54(14)
C(4)-La(1)-C(2)	46.61(18)
C(3)-La(1)-C(2)	28.75(18)
O(1)-La(1)-C(13)	87.19(14)
C(4)-La(1)-C(13)	101.4(2)
C(3)-La(1)-C(13)	88.53(18)
C(2)-La(1)-C(13)	107.22(17)
O(1)-La(1)-C(5)	84.94(15)
C(4)-La(1)-C(5)	29.3(2)
C(3)-La(1)-C(5)	48.2(2)
C(2)-La(1)-C(5)	47.13(17)
C(13)-La(1)-C(5)	130.7(2)
O(1)-La(1)-C(1)	112.89(14)
C(4)-La(1)-C(1)	47.14(17)
C(3)-La(1)-C(1)	47.60(18)
C(2)-La(1)-C(1)	28.32(16)
C(13)-La(1)-C(1)	134.58(16)
C(5)-La(1)-C(1)	28.70(17)
O(1)-La(1)-C(12)	76.35(14)
C(4)-La(1)-C(12)	124.44(19)
C(3)-La(1)-C(12)	116.76(17)
C(2)-La(1)-C(12)	134.50(16)
C(13)-La(1)-C(12)	28.49(15)
C(5)-La(1)-C(12)	151.21(19)
C(1)-La(1)-C(12)	162.71(16)

O(1)-La(1)-C(11)	97.68(14)
C(4)-La(1)-C(11)	148.0(2)
C(3)-La(1)-C(11)	128.00(18)
C(2)-La(1)-C(11)	129.26(16)
C(13)-La(1)-C(11)	46.80(15)
C(5)-La(1)-C(11)	176.04(17)
C(1)-La(1)-C(11)	149.22(16)
C(12)-La(1)-C(11)	28.50(15)
O(1)-La(1)-C(15)	122.93(14)
C(4)-La(1)-C(15)	130.9(2)
C(3)-La(1)-C(15)	104.05(19)
C(2)-La(1)-C(15)	100.88(16)
C(13)-La(1)-C(15)	46.67(16)
C(5)-La(1)-C(15)	147.96(16)
C(1)-La(1)-C(15)	123.31(16)
C(12)-La(1)-C(15)	46.83(15)
C(11)-La(1)-C(15)	28.38(15)
O(1)-La(1)-C(14)	115.53(14)
C(4)-La(1)-C(14)	104.9(2)
C(3)-La(1)-C(14)	81.45(18)
C(2)-La(1)-C(14)	89.08(16)
C(13)-La(1)-C(14)	28.35(16)
C(5)-La(1)-C(14)	129.59(18)
C(1)-La(1)-C(14)	117.02(16)
C(12)-La(1)-C(14)	46.73(16)
C(11)-La(1)-C(14)	46.55(15)
C(15)-La(1)-C(14)	28.12(16)
O(1)-La(1)-S(2)	132.51(9)
C(4)-La(1)-S(2)	124.33(13)
C(3)-La(1)-S(2)	112.44(15)
C(2)-La(1)-S(2)	84.09(13)
C(13)-La(1)-S(2)	119.42(11)
C(5)-La(1)-S(2)	100.96(16)
C(1)-La(1)-S(2)	77.28(11)
C(12)-La(1)-S(2)	107.82(11)
C(11)-La(1)-S(2)	79.49(11)

C(15)-La(1)-S(2)	72.85(11)
C(14)-La(1)-S(2)	96.77(12)
O(1)-La(1)-S(1)	75.04(9)
C(4)-La(1)-S(1)	112.8(2)
C(3)-La(1)-S(1)	132.75(14)
C(2)-La(1)-S(1)	113.87(13)
C(13)-La(1)-S(1)	137.97(12)
C(5)-La(1)-S(1)	85.99(16)
C(1)-La(1)-S(1)	87.39(12)
C(12)-La(1)-S(1)	109.49(11)
C(11)-La(1)-S(1)	97.54(11)
C(15)-La(1)-S(1)	114.49(12)
C(14)-La(1)-S(1)	142.06(12)
S(2)-La(1)-S(1)	58.71(4)
O(1)-P(1)-C(38)	110.5(2)
O(1)-P(1)-C(32)	112.7(2)
C(38)-P(1)-C(32)	107.8(2)
O(1)-P(1)-C(44)	113.1(2)
C(38)-P(1)-C(44)	108.4(2)
C(32)-P(1)-C(44)	104.1(2)
P(1)-O(1)-La(1)	171.0(2)
C(21)-S(1)-La(1)	88.54(18)
C(21)-S(2)-La(1)	89.95(18)
C(2)-C(1)-C(5)	108.0(6)
C(2)-C(1)-C(6)	126.2(6)
C(5)-C(1)-C(6)	125.5(6)
C(2)-C(1)-La(1)	74.6(3)
C(5)-C(1)-La(1)	75.4(3)
C(6)-C(1)-La(1)	121.0(4)
C(1)-C(2)-C(3)	109.9(5)
C(1)-C(2)-C(7)	124.3(6)
C(3)-C(2)-C(7)	125.7(6)
C(1)-C(2)-La(1)	77.1(3)
C(3)-C(2)-La(1)	74.2(3)
C(7)-C(2)-La(1)	117.2(4)
C(4)-C(3)-C(2)	106.3(6)

C(4)-C(3)-C(8)	127.2(7)
C(2)-C(3)-C(8)	125.1(7)
C(4)-C(3)-La(1)	75.1(4)
C(2)-C(3)-La(1)	77.0(3)
C(8)-C(3)-La(1)	124.0(4)
C(3)-C(4)-C(5)	110.6(5)
C(3)-C(4)-C(9)	123.8(8)
C(5)-C(4)-C(9)	125.1(9)
C(3)-C(4)-La(1)	76.2(4)
C(5)-C(4)-La(1)	78.2(3)
C(9)-C(4)-La(1)	119.0(4)
C(1)-C(5)-C(4)	105.2(6)
C(1)-C(5)-C(10)	125.5(8)
C(4)-C(5)-C(10)	129.0(8)
C(1)-C(5)-La(1)	75.9(3)
C(4)-C(5)-La(1)	72.5(3)
C(10)-C(5)-La(1)	121.2(4)
C(15)-C(11)-C(12)	108.1(5)
C(15)-C(11)-C(16)	124.8(5)
C(12)-C(11)-C(16)	126.8(5)
C(15)-C(11)-La(1)	76.4(3)
C(12)-C(11)-La(1)	75.5(3)
C(16)-C(11)-La(1)	119.6(3)
C(13)-C(12)-C(11)	107.4(5)
C(13)-C(12)-C(17)	124.6(5)
C(11)-C(12)-C(17)	127.3(5)
C(13)-C(12)-La(1)	74.9(3)
C(11)-C(12)-La(1)	76.0(3)
C(17)-C(12)-La(1)	123.0(4)
C(12)-C(13)-C(14)	108.7(5)
C(12)-C(13)-C(18)	124.4(5)
C(14)-C(13)-C(18)	126.2(6)
C(12)-C(13)-La(1)	76.6(3)
C(14)-C(13)-La(1)	77.8(3)
C(18)-C(13)-La(1)	119.9(4)
C(15)-C(14)-C(13)	107.8(5)

C(15)-C(14)-C(19)	122.4(6)
C(13)-C(14)-C(19)	128.1(6)
C(15)-C(14)-La(1)	75.7(3)
C(13)-C(14)-La(1)	73.8(3)
C(19)-C(14)-La(1)	128.5(4)
C(14)-C(15)-C(11)	108.0(5)
C(14)-C(15)-C(20)	125.5(5)
C(11)-C(15)-C(20)	125.8(5)
C(14)-C(15)-La(1)	76.2(3)
C(11)-C(15)-La(1)	75.2(3)
C(20)-C(15)-La(1)	122.4(4)
C(22)-C(21)-S(2)	120.1(4)
C(22)-C(21)-S(1)	117.9(4)
S(2)-C(21)-S(1)	122.1(3)
C(26)-C(22)-C(23)	101.9(4)
C(26)-C(22)-C(27)	109.4(4)
C(23)-C(22)-C(27)	109.0(4)
C(26)-C(22)-C(21)	113.1(4)
C(23)-C(22)-C(21)	110.3(4)
C(27)-C(22)-C(21)	112.6(4)
C(24)-C(23)-C(28)	129.5(5)
C(24)-C(23)-C(22)	108.6(5)
C(28)-C(23)-C(22)	121.8(5)
C(23)-C(24)-C(25)	110.0(5)
C(23)-C(24)-C(29)	127.1(5)
C(25)-C(24)-C(29)	122.9(5)
C(26)-C(25)-C(24)	109.0(5)
C(26)-C(25)-C(30)	128.7(5)
C(24)-C(25)-C(30)	122.3(5)
C(25)-C(26)-C(31)	128.3(5)
C(25)-C(26)-C(22)	110.0(5)
C(31)-C(26)-C(22)	121.7(5)
C(37)-C(32)-C(33)	120.0(5)
C(37)-C(32)-P(1)	123.2(4)
C(33)-C(32)-P(1)	116.8(4)
C(34)-C(33)-C(32)	119.4(5)

C(35)-C(34)-C(33)	120.8(6)
C(34)-C(35)-C(36)	119.9(6)
C(35)-C(36)-C(37)	120.8(6)
C(36)-C(37)-C(32)	119.1(6)
C(43)-C(38)-C(39)	118.8(5)
C(43)-C(38)-P(1)	122.3(4)
C(39)-C(38)-P(1)	118.9(4)
C(40)-C(39)-C(38)	120.6(5)
C(41)-C(40)-C(39)	119.8(6)
C(42)-C(41)-C(40)	119.9(6)
C(41)-C(42)-C(43)	121.1(6)
C(42)-C(43)-C(38)	119.8(5)
C(49)-C(44)-C(45)	119.7(5)
C(49)-C(44)-P(1)	119.9(4)
C(45)-C(44)-P(1)	120.4(4)
C(44)-C(45)-C(46)	120.5(5)
C(47)-C(46)-C(45)	119.7(5)
C(48)-C(47)-C(46)	119.6(5)
C(49)-C(48)-C(47)	120.5(5)
C(48)-C(49)-C(44)	120.0(5)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **8**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
La(1)	14(1)	18(1)	14(1)	1(1)	-1(1)	-1(1)
P(1)	22(1)	18(1)	16(1)	1(1)	-2(1)	-3(1)
O(1)	20(2)	19(2)	16(2)	2(2)	-5(2)	0(2)
S(1)	29(1)	20(1)	17(1)	3(1)	2(1)	7(1)
S(2)	24(1)	25(1)	18(1)	2(1)	0(1)	8(1)
C(1)	20(3)	24(3)	29(3)	4(2)	-1(2)	-6(2)
C(2)	15(3)	29(3)	38(4)	3(3)	1(2)	-1(2)
C(3)	25(3)	54(5)	38(4)	-10(3)	6(3)	-10(3)
C(4)	30(4)	93(6)	19(3)	20(4)	-15(3)	-36(4)
C(5)	17(3)	29(4)	79(6)	26(4)	-20(3)	-8(3)
C(6)	37(4)	59(5)	58(5)	-21(4)	2(3)	-18(4)
C(7)	36(4)	34(4)	75(6)	4(4)	-13(4)	5(3)
C(8)	42(4)	94(7)	58(5)	-33(5)	19(4)	-24(4)
C(9)	61(5)	203(12)	48(5)	80(7)	-30(4)	-82(7)
C(10)	39(5)	36(5)	191(11)	40(6)	-46(6)	-15(4)
C(11)	23(3)	11(3)	28(3)	-3(2)	3(2)	-2(2)
C(12)	28(3)	15(3)	22(3)	1(2)	-1(2)	-3(2)
C(13)	34(3)	13(3)	24(3)	-2(2)	5(2)	-6(2)
C(14)	23(3)	24(3)	35(4)	-7(3)	1(3)	3(2)
C(15)	34(3)	16(3)	24(3)	0(2)	-2(2)	2(2)
C(16)	38(4)	25(3)	37(4)	-5(3)	7(3)	-8(3)
C(17)	37(3)	15(3)	39(4)	-3(3)	-19(3)	-3(3)
C(18)	63(5)	45(4)	24(4)	-15(3)	12(3)	-14(4)
C(19)	34(4)	36(4)	70(5)	-15(4)	6(3)	10(3)
C(20)	61(4)	19(3)	32(4)	4(3)	-11(3)	3(3)
C(21)	17(3)	18(3)	12(3)	-6(2)	-2(2)	-7(2)
C(22)	19(3)	20(3)	20(3)	1(2)	1(2)	0(2)
C(23)	29(3)	26(3)	8(3)	1(2)	0(2)	-4(3)
C(24)	31(3)	18(3)	17(3)	2(2)	0(2)	3(2)

C(25)	25(3)	25(3)	15(3)	5(2)	5(2)	6(2)
C(26)	18(3)	24(3)	19(3)	4(2)	2(2)	-1(2)
C(27)	23(3)	21(3)	23(3)	4(2)	1(2)	3(2)
C(28)	32(3)	32(3)	25(3)	-6(3)	-1(3)	-6(3)
C(29)	45(4)	28(3)	15(3)	-4(2)	3(3)	2(3)
C(30)	28(3)	29(3)	31(3)	3(3)	3(3)	7(3)
C(31)	25(3)	35(3)	24(3)	-6(3)	2(2)	-5(3)
C(32)	18(3)	20(3)	21(3)	3(2)	0(2)	-4(2)
C(33)	22(3)	23(3)	20(3)	-2(2)	-1(2)	0(2)
C(34)	28(3)	23(3)	37(4)	-4(3)	-2(3)	4(3)
C(35)	50(4)	17(3)	42(4)	-7(3)	12(3)	-5(3)
C(36)	80(5)	20(3)	39(4)	8(3)	21(4)	-8(3)
C(37)	57(4)	28(4)	23(3)	2(3)	14(3)	-5(3)
C(38)	23(3)	10(2)	17(3)	2(2)	-7(2)	-2(2)
C(39)	28(3)	40(4)	24(3)	-9(3)	2(3)	-12(3)
C(40)	34(3)	43(4)	28(3)	-9(3)	6(3)	-19(3)
C(41)	45(4)	25(3)	17(3)	0(2)	1(3)	-6(3)
C(42)	38(4)	39(4)	27(3)	-7(3)	-13(3)	4(3)
C(43)	26(3)	28(3)	26(3)	-9(3)	-8(2)	4(3)
C(44)	22(3)	24(3)	18(3)	-2(2)	0(2)	-3(2)
C(45)	25(3)	13(3)	27(3)	-3(2)	-2(2)	-3(2)
C(46)	28(3)	27(3)	26(3)	2(3)	0(3)	-9(3)
C(47)	18(3)	40(4)	32(3)	-15(3)	0(2)	-7(3)
C(48)	22(3)	29(3)	29(3)	-10(3)	-8(2)	5(2)
C(49)	25(3)	24(3)	18(3)	-4(2)	-7(2)	1(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10 ^{3})
for **8**.

	x	y	z	U(eq)
H(6A)	4113	6334	5231	77
H(6B)	5436	6353	5255	77
H(6C)	4766	7442	5114	77
H(7A)	4329	9387	5471	73
H(7B)	3388	9576	5814	73
H(7C)	3204	8690	5437	73
H(8A)	2981	8632	6731	97
H(8B)	3567	9647	6499	97
H(8C)	4136	9100	6918	97
H(9A)	5245	7331	7144	157
H(9B)	5365	6081	6981	157
H(9C)	4167	6581	7070	157
H(10A)	4908	4832	6045	135
H(10B)	5870	5153	6386	135
H(10C)	6063	5294	5883	135
H(16A)	9152	11194	5916	49
H(16B)	8759	10129	5646	49
H(16C)	9502	9981	6076	49
H(17A)	8932	10362	7116	46
H(17B)	9402	9518	6770	46
H(17C)	8538	9097	7114	46
H(18A)	6451	9274	7304	66
H(18B)	5510	10182	7211	66
H(18C)	6699	10554	7398	66
H(19A)	4631	11054	6674	69
H(19B)	4558	11033	6160	69
H(19C)	5140	12052	6405	69

H(20A)	5856	11069	5514	56
H(20B)	7151	11190	5431	56
H(20C)	6515	12137	5686	56
H(27A)	8518	9353	4615	33
H(27B)	7560	8660	4374	33
H(27C)	8815	8537	4230	33
H(28A)	7095	5649	4245	45
H(28B)	6764	6931	4264	45
H(28C)	6631	6163	4678	45
H(29A)	8591	4618	4232	44
H(29B)	9779	4453	4462	44
H(29C)	9675	5090	4012	44
H(30A)	11782	6698	4887	44
H(30B)	11545	6218	4414	44
H(30C)	11332	5460	4825	44
H(31A)	10064	8457	5449	42
H(31B)	10319	9125	5019	42
H(31C)	11153	8182	5189	42
H(33)	8110	5006	6304	26
H(34)	7634	3142	6264	35
H(35)	7391	2118	6885	44
H(36)	7563	2969	7554	55
H(37)	7977	4854	7608	43
H(39)	6769	7056	7567	37
H(40)	6743	7726	8273	42
H(41)	8407	8085	8647	35
H(42)	10080	7796	8317	42
H(43)	10130	7142	7613	32
H(45)	9619	7924	6376	26
H(46)	11429	7970	6133	33
H(47)	12721	6667	6389	36
H(48)	12185	5322	6881	32
H(49)	10378	5275	7118	27

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

C(38)-P(1)-O(1)-La(1)	142.0(14)
C(32)-P(1)-O(1)-La(1)	-97.3(14)
C(44)-P(1)-O(1)-La(1)	20.3(15)
C(4)-La(1)-O(1)-P(1)	139.2(14)
C(3)-La(1)-O(1)-P(1)	153.5(14)
C(2)-La(1)-O(1)-P(1)	131.5(14)
C(13)-La(1)-O(1)-P(1)	-118.8(14)
C(5)-La(1)-O(1)-P(1)	109.9(14)
C(1)-La(1)-O(1)-P(1)	103.2(14)
C(12)-La(1)-O(1)-P(1)	-92.2(14)
C(11)-La(1)-O(1)-P(1)	-73.1(14)
C(15)-La(1)-O(1)-P(1)	-87.1(14)
C(14)-La(1)-O(1)-P(1)	-118.3(14)
S(2)-La(1)-O(1)-P(1)	9.6(15)
S(1)-La(1)-O(1)-P(1)	22.7(14)
O(1)-La(1)-S(1)-C(21)	-164.01(19)
C(4)-La(1)-S(1)-C(21)	122.2(2)
C(3)-La(1)-S(1)-C(21)	97.4(3)
C(2)-La(1)-S(1)-C(21)	71.1(2)
C(13)-La(1)-S(1)-C(21)	-95.9(2)
C(5)-La(1)-S(1)-C(21)	110.2(2)
C(1)-La(1)-S(1)-C(21)	81.5(2)
C(12)-La(1)-S(1)-C(21)	-94.7(2)
C(11)-La(1)-S(1)-C(21)	-68.0(2)
C(15)-La(1)-S(1)-C(21)	-44.2(2)
C(14)-La(1)-S(1)-C(21)	-51.5(3)
S(2)-La(1)-S(1)-C(21)	4.76(17)
O(1)-La(1)-S(2)-C(21)	9.9(2)
C(4)-La(1)-S(2)-C(21)	-102.6(3)
C(3)-La(1)-S(2)-C(21)	-132.3(2)
C(2)-La(1)-S(2)-C(21)	-127.5(2)
C(13)-La(1)-S(2)-C(21)	126.1(2)
C(5)-La(1)-S(2)-C(21)	-83.2(2)
C(1)-La(1)-S(2)-C(21)	-99.6(2)

C(12)-La(1)-S(2)-C(21)	97.6(2)
C(11)-La(1)-S(2)-C(21)	100.8(2)
C(15)-La(1)-S(2)-C(21)	129.2(2)
C(14)-La(1)-S(2)-C(21)	144.2(2)
S(1)-La(1)-S(2)-C(21)	-4.83(17)
O(1)-La(1)-C(1)-C(2)	127.6(3)
C(4)-La(1)-C(1)-C(2)	75.3(4)
C(3)-La(1)-C(1)-C(2)	36.1(4)
C(13)-La(1)-C(1)-C(2)	17.7(4)
C(5)-La(1)-C(1)-C(2)	113.8(5)
C(12)-La(1)-C(1)-C(2)	8.0(7)
C(11)-La(1)-C(1)-C(2)	-59.4(5)
C(15)-La(1)-C(1)-C(2)	-42.0(4)
C(14)-La(1)-C(1)-C(2)	-10.1(4)
S(2)-La(1)-C(1)-C(2)	-101.3(3)
S(1)-La(1)-C(1)-C(2)	-159.8(3)
O(1)-La(1)-C(1)-C(5)	13.9(4)
C(4)-La(1)-C(1)-C(5)	-38.5(4)
C(3)-La(1)-C(1)-C(5)	-77.7(4)
C(2)-La(1)-C(1)-C(5)	-113.8(5)
C(13)-La(1)-C(1)-C(5)	-96.1(4)
C(12)-La(1)-C(1)-C(5)	-105.8(6)
C(11)-La(1)-C(1)-C(5)	-173.2(4)
C(15)-La(1)-C(1)-C(5)	-155.8(4)
C(14)-La(1)-C(1)-C(5)	-123.9(4)
S(2)-La(1)-C(1)-C(5)	144.9(4)
S(1)-La(1)-C(1)-C(5)	86.4(4)
O(1)-La(1)-C(1)-C(6)	-109.0(5)
C(4)-La(1)-C(1)-C(6)	-161.3(6)
C(3)-La(1)-C(1)-C(6)	159.4(6)
C(2)-La(1)-C(1)-C(6)	123.3(7)
C(13)-La(1)-C(1)-C(6)	141.0(5)
C(5)-La(1)-C(1)-C(6)	-122.9(7)
C(12)-La(1)-C(1)-C(6)	131.3(6)
C(11)-La(1)-C(1)-C(6)	63.9(6)
C(15)-La(1)-C(1)-C(6)	81.4(5)

C(14)-La(1)-C(1)-C(6)	113.2(5)
S(2)-La(1)-C(1)-C(6)	22.0(5)
S(1)-La(1)-C(1)-C(6)	-36.5(5)
C(5)-C(1)-C(2)-C(3)	0.9(6)
C(6)-C(1)-C(2)-C(3)	174.8(6)
La(1)-C(1)-C(2)-C(3)	-67.7(4)
C(5)-C(1)-C(2)-C(7)	-177.1(5)
C(6)-C(1)-C(2)-C(7)	-3.1(9)
La(1)-C(1)-C(2)-C(7)	114.3(6)
C(5)-C(1)-C(2)-La(1)	68.6(4)
C(6)-C(1)-C(2)-La(1)	-117.4(6)
O(1)-La(1)-C(2)-C(1)	-66.9(4)
C(4)-La(1)-C(2)-C(1)	-77.4(4)
C(3)-La(1)-C(2)-C(1)	-115.3(5)
C(13)-La(1)-C(2)-C(1)	-166.9(3)
C(5)-La(1)-C(2)-C(1)	-36.8(4)
C(12)-La(1)-C(2)-C(1)	-176.7(3)
C(11)-La(1)-C(2)-C(1)	145.3(3)
C(15)-La(1)-C(2)-C(1)	145.3(3)
C(14)-La(1)-C(2)-C(1)	171.0(3)
S(2)-La(1)-C(2)-C(1)	74.1(3)
S(1)-La(1)-C(2)-C(1)	22.2(4)
O(1)-La(1)-C(2)-C(3)	48.4(4)
C(4)-La(1)-C(2)-C(3)	37.9(4)
C(13)-La(1)-C(2)-C(3)	-51.6(4)
C(5)-La(1)-C(2)-C(3)	78.5(4)
C(1)-La(1)-C(2)-C(3)	115.3(5)
C(12)-La(1)-C(2)-C(3)	-61.4(4)
C(11)-La(1)-C(2)-C(3)	-99.4(4)
C(15)-La(1)-C(2)-C(3)	-99.4(4)
C(14)-La(1)-C(2)-C(3)	-73.7(4)
S(2)-La(1)-C(2)-C(3)	-170.6(4)
S(1)-La(1)-C(2)-C(3)	137.5(4)
O(1)-La(1)-C(2)-C(7)	170.9(4)
C(4)-La(1)-C(2)-C(7)	160.4(6)
C(3)-La(1)-C(2)-C(7)	122.5(7)

C(13)-La(1)-C(2)-C(7)	70.9(5)
C(5)-La(1)-C(2)-C(7)	-159.0(6)
C(1)-La(1)-C(2)-C(7)	-122.2(6)
C(12)-La(1)-C(2)-C(7)	61.1(5)
C(11)-La(1)-C(2)-C(7)	23.1(6)
C(15)-La(1)-C(2)-C(7)	23.1(5)
C(14)-La(1)-C(2)-C(7)	48.8(5)
S(2)-La(1)-C(2)-C(7)	-48.1(5)
S(1)-La(1)-C(2)-C(7)	-100.1(5)
C(1)-C(2)-C(3)-C(4)	-0.4(7)
C(7)-C(2)-C(3)-C(4)	177.5(6)
La(1)-C(2)-C(3)-C(4)	-70.0(4)
C(1)-C(2)-C(3)-C(8)	-167.8(6)
C(7)-C(2)-C(3)-C(8)	10.1(10)
La(1)-C(2)-C(3)-C(8)	122.6(6)
C(1)-C(2)-C(3)-La(1)	69.6(4)
C(7)-C(2)-C(3)-La(1)	-112.5(6)
O(1)-La(1)-C(3)-C(4)	-30.8(4)
C(2)-La(1)-C(3)-C(4)	111.1(6)
C(13)-La(1)-C(3)-C(4)	-117.4(4)
C(5)-La(1)-C(3)-C(4)	36.5(4)
C(1)-La(1)-C(3)-C(4)	75.6(4)
C(12)-La(1)-C(3)-C(4)	-113.5(4)
C(11)-La(1)-C(3)-C(4)	-144.7(4)
C(15)-La(1)-C(3)-C(4)	-161.9(4)
C(14)-La(1)-C(3)-C(4)	-145.0(4)
S(2)-La(1)-C(3)-C(4)	121.1(4)
S(1)-La(1)-C(3)-C(4)	53.7(5)
O(1)-La(1)-C(3)-C(2)	-141.9(4)
C(4)-La(1)-C(3)-C(2)	-111.1(6)
C(13)-La(1)-C(3)-C(2)	131.5(4)
C(5)-La(1)-C(3)-C(2)	-74.5(4)
C(1)-La(1)-C(3)-C(2)	-35.5(3)
C(12)-La(1)-C(3)-C(2)	135.5(3)
C(11)-La(1)-C(3)-C(2)	104.2(4)
C(15)-La(1)-C(3)-C(2)	87.0(4)

C(14)-La(1)-C(3)-C(2)	103.9(4)
S(2)-La(1)-C(3)-C(2)	10.1(4)
S(1)-La(1)-C(3)-C(2)	-57.4(5)
O(1)-La(1)-C(3)-C(8)	94.4(6)
C(4)-La(1)-C(3)-C(8)	125.2(8)
C(2)-La(1)-C(3)-C(8)	-123.7(8)
C(13)-La(1)-C(3)-C(8)	7.7(6)
C(5)-La(1)-C(3)-C(8)	161.7(8)
C(1)-La(1)-C(3)-C(8)	-159.3(7)
C(12)-La(1)-C(3)-C(8)	11.7(7)
C(11)-La(1)-C(3)-C(8)	-19.5(7)
C(15)-La(1)-C(3)-C(8)	-36.7(7)
C(14)-La(1)-C(3)-C(8)	-19.8(6)
S(2)-La(1)-C(3)-C(8)	-113.7(6)
S(1)-La(1)-C(3)-C(8)	178.9(5)
C(2)-C(3)-C(4)-C(5)	-0.2(7)
C(8)-C(3)-C(4)-C(5)	166.8(6)
La(1)-C(3)-C(4)-C(5)	-71.5(4)
C(2)-C(3)-C(4)-C(9)	-172.8(6)
C(8)-C(3)-C(4)-C(9)	-5.8(10)
La(1)-C(3)-C(4)-C(9)	115.9(6)
C(2)-C(3)-C(4)-La(1)	71.3(4)
C(8)-C(3)-C(4)-La(1)	-121.7(7)
O(1)-La(1)-C(4)-C(3)	150.2(4)
C(2)-La(1)-C(4)-C(3)	-38.1(4)
C(13)-La(1)-C(4)-C(3)	64.8(4)
C(5)-La(1)-C(4)-C(3)	-114.9(5)
C(1)-La(1)-C(4)-C(3)	-77.3(4)
C(12)-La(1)-C(4)-C(3)	83.3(4)
C(11)-La(1)-C(4)-C(3)	59.3(5)
C(15)-La(1)-C(4)-C(3)	23.5(5)
C(14)-La(1)-C(4)-C(3)	35.9(4)
S(2)-La(1)-C(4)-C(3)	-73.3(5)
S(1)-La(1)-C(4)-C(3)	-140.1(4)
O(1)-La(1)-C(4)-C(5)	-94.9(4)
C(3)-La(1)-C(4)-C(5)	114.9(5)

C(2)-La(1)-C(4)-C(5)	76.8(4)
C(13)-La(1)-C(4)-C(5)	179.8(4)
C(1)-La(1)-C(4)-C(5)	37.6(3)
C(12)-La(1)-C(4)-C(5)	-161.8(3)
C(11)-La(1)-C(4)-C(5)	174.3(3)
C(15)-La(1)-C(4)-C(5)	138.5(4)
C(14)-La(1)-C(4)-C(5)	150.9(4)
S(2)-La(1)-C(4)-C(5)	41.6(5)
S(1)-La(1)-C(4)-C(5)	-25.1(4)
O(1)-La(1)-C(4)-C(9)	28.9(8)
C(3)-La(1)-C(4)-C(9)	-121.3(10)
C(2)-La(1)-C(4)-C(9)	-159.4(9)
C(13)-La(1)-C(4)-C(9)	-56.4(8)
C(5)-La(1)-C(4)-C(9)	123.8(10)
C(1)-La(1)-C(4)-C(9)	161.4(9)
C(12)-La(1)-C(4)-C(9)	-38.0(9)
C(11)-La(1)-C(4)-C(9)	-61.9(9)
C(15)-La(1)-C(4)-C(9)	-97.8(8)
C(14)-La(1)-C(4)-C(9)	-85.4(8)
S(2)-La(1)-C(4)-C(9)	165.4(7)
S(1)-La(1)-C(4)-C(9)	98.7(8)
C(2)-C(1)-C(5)-C(4)	-0.9(6)
C(6)-C(1)-C(5)-C(4)	-174.9(5)
La(1)-C(1)-C(5)-C(4)	67.1(4)
C(2)-C(1)-C(5)-C(10)	173.4(6)
C(6)-C(1)-C(5)-C(10)	-0.6(9)
La(1)-C(1)-C(5)-C(10)	-118.5(6)
C(2)-C(1)-C(5)-La(1)	-68.1(4)
C(6)-C(1)-C(5)-La(1)	117.9(5)
C(3)-C(4)-C(5)-C(1)	0.7(7)
C(9)-C(4)-C(5)-C(1)	173.2(6)
La(1)-C(4)-C(5)-C(1)	-69.6(4)
C(3)-C(4)-C(5)-C(10)	-173.4(6)
C(9)-C(4)-C(5)-C(10)	-0.9(10)
La(1)-C(4)-C(5)-C(10)	116.4(6)
C(3)-C(4)-C(5)-La(1)	70.2(5)

C(9)-C(4)-C(5)-La(1)	-117.3(6)
O(1)-La(1)-C(5)-C(1)	-167.2(4)
C(4)-La(1)-C(5)-C(1)	111.2(5)
C(3)-La(1)-C(5)-C(1)	75.6(4)
C(2)-La(1)-C(5)-C(1)	36.3(3)
C(13)-La(1)-C(5)-C(1)	110.9(4)
C(12)-La(1)-C(5)-C(1)	143.6(4)
C(11)-La(1)-C(5)-C(1)	61(3)
C(15)-La(1)-C(5)-C(1)	40.3(6)
C(14)-La(1)-C(5)-C(1)	73.6(5)
S(2)-La(1)-C(5)-C(1)	-34.8(4)
S(1)-La(1)-C(5)-C(1)	-91.9(4)
O(1)-La(1)-C(5)-C(4)	81.6(4)
C(3)-La(1)-C(5)-C(4)	-35.6(4)
C(2)-La(1)-C(5)-C(4)	-74.9(4)
C(13)-La(1)-C(5)-C(4)	-0.3(5)
C(1)-La(1)-C(5)-C(4)	-111.2(5)
C(12)-La(1)-C(5)-C(4)	32.4(6)
C(11)-La(1)-C(5)-C(4)	-50(3)
C(15)-La(1)-C(5)-C(4)	-70.9(6)
C(14)-La(1)-C(5)-C(4)	-37.6(5)
S(2)-La(1)-C(5)-C(4)	-146.0(4)
S(1)-La(1)-C(5)-C(4)	156.9(4)
O(1)-La(1)-C(5)-C(10)	-43.9(7)
C(4)-La(1)-C(5)-C(10)	-125.5(9)
C(3)-La(1)-C(5)-C(10)	-161.2(8)
C(2)-La(1)-C(5)-C(10)	159.6(8)
C(13)-La(1)-C(5)-C(10)	-125.8(7)
C(1)-La(1)-C(5)-C(10)	123.3(9)
C(12)-La(1)-C(5)-C(10)	-93.1(8)
C(11)-La(1)-C(5)-C(10)	-175(2)
C(15)-La(1)-C(5)-C(10)	163.6(6)
C(14)-La(1)-C(5)-C(10)	-163.1(7)
S(2)-La(1)-C(5)-C(10)	88.4(7)
S(1)-La(1)-C(5)-C(10)	31.4(7)
O(1)-La(1)-C(11)-C(15)	-154.8(3)

C(4)-La(1)-C(11)-C(15)	-68.6(5)
C(3)-La(1)-C(11)-C(15)	-37.1(4)
C(2)-La(1)-C(11)-C(15)	0.0(4)
C(13)-La(1)-C(11)-C(15)	-76.0(3)
C(5)-La(1)-C(11)-C(15)	-24(3)
C(1)-La(1)-C(11)-C(15)	31.8(5)
C(12)-La(1)-C(11)-C(15)	-113.1(5)
C(14)-La(1)-C(11)-C(15)	-36.6(3)
S(2)-La(1)-C(11)-C(15)	73.3(3)
S(1)-La(1)-C(11)-C(15)	129.4(3)
O(1)-La(1)-C(11)-C(12)	-41.7(3)
C(4)-La(1)-C(11)-C(12)	44.5(5)
C(3)-La(1)-C(11)-C(12)	76.0(4)
C(2)-La(1)-C(11)-C(12)	113.1(3)
C(13)-La(1)-C(11)-C(12)	37.1(3)
C(5)-La(1)-C(11)-C(12)	90(3)
C(1)-La(1)-C(11)-C(12)	144.9(3)
C(15)-La(1)-C(11)-C(12)	113.1(5)
C(14)-La(1)-C(11)-C(12)	76.5(3)
S(2)-La(1)-C(11)-C(12)	-173.6(3)
S(1)-La(1)-C(11)-C(12)	-117.5(3)
O(1)-La(1)-C(11)-C(16)	82.7(4)
C(4)-La(1)-C(11)-C(16)	168.9(4)
C(3)-La(1)-C(11)-C(16)	-159.6(4)
C(2)-La(1)-C(11)-C(16)	-122.6(4)
C(13)-La(1)-C(11)-C(16)	161.5(5)
C(5)-La(1)-C(11)-C(16)	-146(3)
C(1)-La(1)-C(11)-C(16)	-90.8(5)
C(12)-La(1)-C(11)-C(16)	124.3(6)
C(15)-La(1)-C(11)-C(16)	-122.6(6)
C(14)-La(1)-C(11)-C(16)	-159.2(5)
S(2)-La(1)-C(11)-C(16)	-49.3(4)
S(1)-La(1)-C(11)-C(16)	6.9(4)
C(15)-C(11)-C(12)-C(13)	1.2(6)
C(16)-C(11)-C(12)-C(13)	174.7(5)
La(1)-C(11)-C(12)-C(13)	-69.0(4)

C(15)-C(11)-C(12)-C(17)	-168.8(5)
C(16)-C(11)-C(12)-C(17)	4.7(9)
La(1)-C(11)-C(12)-C(17)	121.1(5)
C(15)-C(11)-C(12)-La(1)	70.1(4)
C(16)-C(11)-C(12)-La(1)	-116.4(5)
O(1)-La(1)-C(12)-C(13)	-110.0(3)
C(4)-La(1)-C(12)-C(13)	-40.5(4)
C(3)-La(1)-C(12)-C(13)	-8.4(4)
C(2)-La(1)-C(12)-C(13)	19.9(4)
C(5)-La(1)-C(12)-C(13)	-59.1(5)
C(1)-La(1)-C(12)-C(13)	14.6(7)
C(11)-La(1)-C(12)-C(13)	112.7(5)
C(15)-La(1)-C(12)-C(13)	75.9(3)
C(14)-La(1)-C(12)-C(13)	36.9(3)
S(2)-La(1)-C(12)-C(13)	119.3(3)
S(1)-La(1)-C(12)-C(13)	-178.4(3)
O(1)-La(1)-C(12)-C(11)	137.3(3)
C(4)-La(1)-C(12)-C(11)	-153.2(3)
C(3)-La(1)-C(12)-C(11)	-121.1(3)
C(2)-La(1)-C(12)-C(11)	-92.8(4)
C(13)-La(1)-C(12)-C(11)	-112.7(5)
C(5)-La(1)-C(12)-C(11)	-171.8(3)
C(1)-La(1)-C(12)-C(11)	-98.1(6)
C(15)-La(1)-C(12)-C(11)	-36.8(3)
C(14)-La(1)-C(12)-C(11)	-75.8(3)
S(2)-La(1)-C(12)-C(11)	6.6(3)
S(1)-La(1)-C(12)-C(11)	68.9(3)
O(1)-La(1)-C(12)-C(17)	11.7(4)
C(4)-La(1)-C(12)-C(17)	81.1(5)
C(3)-La(1)-C(12)-C(17)	113.3(5)
C(2)-La(1)-C(12)-C(17)	141.5(4)
C(13)-La(1)-C(12)-C(17)	121.7(6)
C(5)-La(1)-C(12)-C(17)	62.6(6)
C(1)-La(1)-C(12)-C(17)	136.3(5)
C(11)-La(1)-C(12)-C(17)	-125.6(6)
C(15)-La(1)-C(12)-C(17)	-162.4(5)

C(14)-La(1)-C(12)-C(17)	158.6(5)
S(2)-La(1)-C(12)-C(17)	-119.0(4)
S(1)-La(1)-C(12)-C(17)	-56.7(5)
C(11)-C(12)-C(13)-C(14)	-2.2(6)
C(17)-C(12)-C(13)-C(14)	168.0(5)
La(1)-C(12)-C(13)-C(14)	-72.0(4)
C(11)-C(12)-C(13)-C(18)	-173.0(5)
C(17)-C(12)-C(13)-C(18)	-2.7(9)
La(1)-C(12)-C(13)-C(18)	117.3(5)
C(11)-C(12)-C(13)-La(1)	69.7(4)
C(17)-C(12)-C(13)-La(1)	-120.0(5)
O(1)-La(1)-C(13)-C(12)	66.1(3)
C(4)-La(1)-C(13)-C(12)	146.8(3)
C(3)-La(1)-C(13)-C(12)	172.5(3)
C(2)-La(1)-C(13)-C(12)	-165.3(3)
C(5)-La(1)-C(13)-C(12)	147.0(3)
C(1)-La(1)-C(13)-C(12)	-174.0(3)
C(11)-La(1)-C(13)-C(12)	-37.1(3)
C(15)-La(1)-C(13)-C(12)	-76.5(3)
C(14)-La(1)-C(13)-C(12)	-112.9(5)
S(2)-La(1)-C(13)-C(12)	-72.4(3)
S(1)-La(1)-C(13)-C(12)	2.2(4)
O(1)-La(1)-C(13)-C(14)	179.0(3)
C(4)-La(1)-C(13)-C(14)	-100.3(3)
C(3)-La(1)-C(13)-C(14)	-74.6(4)
C(2)-La(1)-C(13)-C(14)	-52.4(4)
C(5)-La(1)-C(13)-C(14)	-100.1(4)
C(1)-La(1)-C(13)-C(14)	-61.1(4)
C(12)-La(1)-C(13)-C(14)	112.9(5)
C(11)-La(1)-C(13)-C(14)	75.7(3)
C(15)-La(1)-C(13)-C(14)	36.4(3)
S(2)-La(1)-C(13)-C(14)	40.5(4)
S(1)-La(1)-C(13)-C(14)	115.1(3)
O(1)-La(1)-C(13)-C(18)	-56.1(5)
C(4)-La(1)-C(13)-C(18)	24.6(5)
C(3)-La(1)-C(13)-C(18)	50.3(5)

C(2)-La(1)-C(13)-C(18)	72.5(5)
C(5)-La(1)-C(13)-C(18)	24.8(6)
C(1)-La(1)-C(13)-C(18)	63.8(5)
C(12)-La(1)-C(13)-C(18)	-122.2(6)
C(11)-La(1)-C(13)-C(18)	-159.4(6)
C(15)-La(1)-C(13)-C(18)	161.3(6)
C(14)-La(1)-C(13)-C(18)	124.9(6)
S(2)-La(1)-C(13)-C(18)	165.4(4)
S(1)-La(1)-C(13)-C(18)	-120.0(4)
C(12)-C(13)-C(14)-C(15)	2.5(6)
C(18)-C(13)-C(14)-C(15)	173.0(5)
La(1)-C(13)-C(14)-C(15)	-68.7(4)
C(12)-C(13)-C(14)-C(19)	-162.3(6)
C(18)-C(13)-C(14)-C(19)	8.3(10)
La(1)-C(13)-C(14)-C(19)	126.6(6)
C(12)-C(13)-C(14)-La(1)	71.1(4)
C(18)-C(13)-C(14)-La(1)	-118.3(6)
O(1)-La(1)-C(14)-C(15)	112.6(3)
C(4)-La(1)-C(14)-C(15)	-159.8(3)
C(3)-La(1)-C(14)-C(15)	-143.3(4)
C(2)-La(1)-C(14)-C(15)	-115.5(3)
C(13)-La(1)-C(14)-C(15)	113.7(5)
C(5)-La(1)-C(14)-C(15)	-141.8(3)
C(1)-La(1)-C(14)-C(15)	-110.7(3)
C(12)-La(1)-C(14)-C(15)	76.6(4)
C(11)-La(1)-C(14)-C(15)	37.0(3)
S(2)-La(1)-C(14)-C(15)	-31.6(3)
S(1)-La(1)-C(14)-C(15)	14.1(4)
O(1)-La(1)-C(14)-C(13)	-1.1(4)
C(4)-La(1)-C(14)-C(13)	86.4(3)
C(3)-La(1)-C(14)-C(13)	103.0(4)
C(2)-La(1)-C(14)-C(13)	130.8(3)
C(5)-La(1)-C(14)-C(13)	104.4(4)
C(1)-La(1)-C(14)-C(13)	135.6(3)
C(12)-La(1)-C(14)-C(13)	-37.1(3)
C(11)-La(1)-C(14)-C(13)	-76.7(3)

C(15)-La(1)-C(14)-C(13)	-113.7(5)
S(2)-La(1)-C(14)-C(13)	-145.3(3)
S(1)-La(1)-C(14)-C(13)	-99.6(3)
O(1)-La(1)-C(14)-C(19)	-127.2(5)
C(4)-La(1)-C(14)-C(19)	-39.7(6)
C(3)-La(1)-C(14)-C(19)	-23.2(6)
C(2)-La(1)-C(14)-C(19)	4.7(6)
C(13)-La(1)-C(14)-C(19)	-126.1(7)
C(5)-La(1)-C(14)-C(19)	-21.7(7)
C(1)-La(1)-C(14)-C(19)	9.5(6)
C(12)-La(1)-C(14)-C(19)	-163.2(7)
C(11)-La(1)-C(14)-C(19)	157.2(7)
C(15)-La(1)-C(14)-C(19)	120.2(7)
S(2)-La(1)-C(14)-C(19)	88.6(6)
S(1)-La(1)-C(14)-C(19)	134.3(5)
C(13)-C(14)-C(15)-C(11)	-1.7(6)
C(19)-C(14)-C(15)-C(11)	164.1(5)
La(1)-C(14)-C(15)-C(11)	-69.1(4)
C(13)-C(14)-C(15)-C(20)	-172.4(5)
C(19)-C(14)-C(15)-C(20)	-6.6(9)
La(1)-C(14)-C(15)-C(20)	120.2(6)
C(13)-C(14)-C(15)-La(1)	67.4(4)
C(19)-C(14)-C(15)-La(1)	-126.8(6)
C(12)-C(11)-C(15)-C(14)	0.3(6)
C(16)-C(11)-C(15)-C(14)	-173.3(5)
La(1)-C(11)-C(15)-C(14)	69.8(4)
C(12)-C(11)-C(15)-C(20)	171.0(5)
C(16)-C(11)-C(15)-C(20)	-2.7(9)
La(1)-C(11)-C(15)-C(20)	-119.6(5)
C(12)-C(11)-C(15)-La(1)	-69.5(4)
C(16)-C(11)-C(15)-La(1)	116.8(5)
O(1)-La(1)-C(15)-C(14)	-83.0(4)
C(4)-La(1)-C(15)-C(14)	26.1(4)
C(3)-La(1)-C(15)-C(14)	37.5(4)
C(2)-La(1)-C(15)-C(14)	66.8(4)
C(13)-La(1)-C(15)-C(14)	-36.7(3)

C(5)-La(1)-C(15)-C(14)	63.8(5)
C(1)-La(1)-C(15)-C(14)	85.6(4)
C(12)-La(1)-C(15)-C(14)	-76.2(4)
C(11)-La(1)-C(15)-C(14)	-113.2(5)
S(2)-La(1)-C(15)-C(14)	147.0(3)
S(1)-La(1)-C(15)-C(14)	-170.5(3)
O(1)-La(1)-C(15)-C(11)	30.2(4)
C(4)-La(1)-C(15)-C(11)	139.3(3)
C(3)-La(1)-C(15)-C(11)	150.7(3)
C(2)-La(1)-C(15)-C(11)	180.0(3)
C(13)-La(1)-C(15)-C(11)	76.5(3)
C(5)-La(1)-C(15)-C(11)	177.0(4)
C(1)-La(1)-C(15)-C(11)	-161.2(3)
C(12)-La(1)-C(15)-C(11)	37.0(3)
C(14)-La(1)-C(15)-C(11)	113.2(5)
S(2)-La(1)-C(15)-C(11)	-99.8(3)
S(1)-La(1)-C(15)-C(11)	-57.3(3)
O(1)-La(1)-C(15)-C(20)	153.5(4)
C(4)-La(1)-C(15)-C(20)	-97.4(5)
C(3)-La(1)-C(15)-C(20)	-86.0(5)
C(2)-La(1)-C(15)-C(20)	-56.7(5)
C(13)-La(1)-C(15)-C(20)	-160.2(6)
C(5)-La(1)-C(15)-C(20)	-59.7(6)
C(1)-La(1)-C(15)-C(20)	-37.9(5)
C(12)-La(1)-C(15)-C(20)	160.3(6)
C(11)-La(1)-C(15)-C(20)	123.3(6)
C(14)-La(1)-C(15)-C(20)	-123.5(6)
S(2)-La(1)-C(15)-C(20)	23.5(4)
S(1)-La(1)-C(15)-C(20)	66.0(5)
La(1)-S(2)-C(21)-C(22)	-170.7(4)
La(1)-S(2)-C(21)-S(1)	8.7(3)
La(1)-S(1)-C(21)-C(22)	170.8(4)
La(1)-S(1)-C(21)-S(2)	-8.6(3)
S(2)-C(21)-C(22)-C(26)	135.0(4)
S(1)-C(21)-C(22)-C(26)	-44.5(6)
S(2)-C(21)-C(22)-C(23)	-111.7(4)

S(1)-C(21)-C(22)-C(23)	68.9(5)
S(2)-C(21)-C(22)-C(27)	10.4(6)
S(1)-C(21)-C(22)-C(27)	-169.1(4)
C(26)-C(22)-C(23)-C(24)	-6.8(5)
C(27)-C(22)-C(23)-C(24)	108.8(5)
C(21)-C(22)-C(23)-C(24)	-127.1(5)
C(26)-C(22)-C(23)-C(28)	177.2(5)
C(27)-C(22)-C(23)-C(28)	-67.3(6)
C(21)-C(22)-C(23)-C(28)	56.8(6)
C(28)-C(23)-C(24)-C(25)	-179.9(5)
C(22)-C(23)-C(24)-C(25)	4.4(6)
C(28)-C(23)-C(24)-C(29)	0.4(9)
C(22)-C(23)-C(24)-C(29)	-175.3(5)
C(23)-C(24)-C(25)-C(26)	0.2(6)
C(29)-C(24)-C(25)-C(26)	180.0(5)
C(23)-C(24)-C(25)-C(30)	-179.6(5)
C(29)-C(24)-C(25)-C(30)	0.2(8)
C(24)-C(25)-C(26)-C(31)	176.9(5)
C(30)-C(25)-C(26)-C(31)	-3.3(9)
C(24)-C(25)-C(26)-C(22)	-4.8(6)
C(30)-C(25)-C(26)-C(22)	175.0(5)
C(23)-C(22)-C(26)-C(25)	7.0(6)
C(27)-C(22)-C(26)-C(25)	-108.2(5)
C(21)-C(22)-C(26)-C(25)	125.4(5)
C(23)-C(22)-C(26)-C(31)	-174.6(5)
C(27)-C(22)-C(26)-C(31)	70.1(6)
C(21)-C(22)-C(26)-C(31)	-56.2(6)
O(1)-P(1)-C(32)-C(37)	-125.4(5)
C(38)-P(1)-C(32)-C(37)	-3.2(6)
C(44)-P(1)-C(32)-C(37)	111.7(5)
O(1)-P(1)-C(32)-C(33)	56.5(5)
C(38)-P(1)-C(32)-C(33)	178.7(4)
C(44)-P(1)-C(32)-C(33)	-66.4(4)
C(37)-C(32)-C(33)-C(34)	1.8(8)
P(1)-C(32)-C(33)-C(34)	179.9(4)
C(32)-C(33)-C(34)-C(35)	-2.0(8)

C(33)-C(34)-C(35)-C(36)	1.0(10)
C(34)-C(35)-C(36)-C(37)	0.2(11)
C(35)-C(36)-C(37)-C(32)	-0.4(11)
C(33)-C(32)-C(37)-C(36)	-0.5(9)
P(1)-C(32)-C(37)-C(36)	-178.6(5)
O(1)-P(1)-C(38)-C(43)	-130.5(4)
C(32)-P(1)-C(38)-C(43)	105.9(5)
C(44)-P(1)-C(38)-C(43)	-6.1(5)
O(1)-P(1)-C(38)-C(39)	48.5(5)
C(32)-P(1)-C(38)-C(39)	-75.1(5)
C(44)-P(1)-C(38)-C(39)	172.9(4)
C(43)-C(38)-C(39)-C(40)	1.0(9)
P(1)-C(38)-C(39)-C(40)	-178.1(5)
C(38)-C(39)-C(40)-C(41)	-0.7(10)
C(39)-C(40)-C(41)-C(42)	0.2(9)
C(40)-C(41)-C(42)-C(43)	0.0(9)
C(41)-C(42)-C(43)-C(38)	0.2(9)
C(39)-C(38)-C(43)-C(42)	-0.7(8)
P(1)-C(38)-C(43)-C(42)	178.3(5)
O(1)-P(1)-C(44)-C(49)	-165.0(4)
C(38)-P(1)-C(44)-C(49)	72.2(5)
C(32)-P(1)-C(44)-C(49)	-42.4(5)
O(1)-P(1)-C(44)-C(45)	14.8(5)
C(38)-P(1)-C(44)-C(45)	-108.0(5)
C(32)-P(1)-C(44)-C(45)	137.4(4)
C(49)-C(44)-C(45)-C(46)	-0.6(8)
P(1)-C(44)-C(45)-C(46)	179.6(4)
C(44)-C(45)-C(46)-C(47)	0.0(8)
C(45)-C(46)-C(47)-C(48)	0.3(8)
C(46)-C(47)-C(48)-C(49)	-0.1(8)
C(47)-C(48)-C(49)-C(44)	-0.4(8)
C(45)-C(44)-C(49)-C(48)	0.8(8)
P(1)-C(44)-C(49)-C(48)	-179.4(4)

X-ray Data Collection, Structure Solution and Refinement for **9**.

A colorless crystal of approximate dimensions 0.29 x 0.31 x 0.38 mm was mounted on a glass fiber and transferred to a Bruker SMART1K diffractometer. The SMART[1] program package was used to determine the unit-cell parameters and for data collection (25 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[2] and SADABS[10] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program. The systematic absences were consistent with the trigonal space groups space groups $P3$ and $P\bar{3}$. It was later determined that the centrosymmetric space group $P\bar{3}$ was correct. The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were located from a difference-Fourier map and refined (x,y,z and U_{iso}). At convergence, wR2 = 0.0763 and GOF = 1.098 for 463 variables refined against 7086 data (0.76Å), R1 = 0.0289 for those 6351 data with $I > 2.0\sigma(I)$.

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

Identification code	tjm2 (**9**)	
Empirical formula	C_{26} H_{48} La N Si_2	
Formula weight	569.74	
Temperature	155(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	$P\bar{3}$	
Unit cell dimensions	a = 17.7905(10) Å	α= 90°.
	b = 17.7905(10) Å	β= 90°.
	c = 15.6247(17) Å	γ = 120°.
Volume	4282.7(6) $Å^3$	
Z	6	
Density (calculated)	1.325 Mg/m^3	
Absorption coefficient	1.593 mm^{-1}	
F(000)	1776	
Crystal color	colorless	
Crystal size	0.38 x 0.31 x 0.29 mm^3	
Theta range for data collection	1.30 to 28.29°	
Index ranges	$-23 \le h \le 23$, $-23 \le k \le 23$, $-20 \le l \le 20$	
Reflections collected	47466	
Independent reflections	7086 [R(int) = 0.0288]	
Completeness to theta = 28.29°	99.6 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.6552 and 0.5828
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7086 / 0 / 463
Goodness-of-fit on F^2	1.098
Final R indices [I>2sigma(I) = 6351 data]	R1 = 0.0289, wR2 = 0.0718
R indices (all data, 0.76Å)	R1 = 0.0340, wR2 = 0.0763
Largest diff. peak and hole	3.995 and -0.510 e.$Å^{-3}$

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

	x	y	z	U(eq)
La(1)	3367(1)	403(1)	2503(1)	13(1)
Si(1)	2712(1)	-1554(1)	3570(1)	21(1)
Si(2)	2567(1)	-1591(1)	1593(1)	21(1)
N(1)	2813(1)	-1128(1)	2577(1)	19(1)
C(1)	5086(1)	957(1)	3067(1)	19(1)
C(2)	5058(1)	1740(1)	3018(1)	20(1)
C(3)	5016(1)	1921(1)	2147(2)	20(1)
C(4)	5004(1)	1246(1)	1654(1)	19(1)
C(5)	5057(1)	656(1)	2226(1)	19(1)
C(6)	5277(2)	597(2)	3857(2)	34(1)
C(7)	5167(2)	2320(2)	3769(2)	34(1)
C(8)	5138(2)	2754(2)	1771(2)	35(1)
C(9)	5095(2)	1272(2)	696(2)	36(1)
C(10)	5164(2)	-104(2)	1980(2)	34(1)
C(11)	2238(1)	875(1)	3301(1)	18(1)
C(12)	2718(1)	1551(1)	2706(1)	18(1)
C(13)	2452(1)	1210(2)	1872(1)	21(1)
C(14)	1789(1)	325(2)	1954(1)	21(1)
C(15)	1657(1)	121(1)	2836(1)	19(1)
C(16)	2253(2)	998(2)	4253(2)	28(1)
C(17)	3303(2)	2486(2)	2945(2)	29(1)
C(18)	2738(2)	1710(2)	1048(2)	34(1)
C(19)	1215(2)	-239(2)	1245(2)	36(1)
C(20)	949(2)	-718(2)	3198(2)	30(1)
C(21)	2977(2)	-632(2)	4336(2)	26(1)
C(22)	1593(2)	-2464(2)	3833(2)	32(1)
C(23)	3472(2)	-1973(2)	3791(2)	35(1)
C(24)	2995(2)	-656(2)	811(2)	26(1)

C(25)	1375(2)	-2314(2)	1403(2)	32(1)
C(26)	3099(2)	-2232(2)	1307(2)	42(1)

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

La(1)-Cnt1	2.589
La(1)-Cnt2	2.577
La(1)-N(1)	2.3917(17)
La(1)-C(12)	2.822(2)
La(1)-C(11)	2.825(2)
La(1)-C(13)	2.833(2)
La(1)-C(5)	2.841(2)
La(1)-C(1)	2.844(2)
La(1)-C(4)	2.850(2)
La(1)-C(2)	2.863(2)
La(1)-C(14)	2.872(2)
La(1)-C(15)	2.873(2)
La(1)-C(3)	2.878(2)
La(1)-C(24)	3.120(2)
La(1)-Si(2)	3.4028(6)
Si(1)-N(1)	1.6963(19)
Si(1)-C(23)	1.874(3)
Si(1)-C(22)	1.878(3)
Si(1)-C(21)	1.891(3)
Si(2)-N(1)	1.6943(19)
Si(2)-C(26)	1.864(3)
Si(2)-C(25)	1.875(3)
Si(2)-C(24)	1.890(3)
C(1)-C(5)	1.411(3)
C(1)-C(2)	1.420(3)
C(1)-C(6)	1.505(3)
C(2)-C(3)	1.408(3)
C(2)-C(7)	1.510(3)
C(3)-C(4)	1.418(3)
C(3)-C(8)	1.507(3)
C(4)-C(5)	1.417(3)
C(4)-C(9)	1.504(3)
C(5)-C(10)	1.506(3)
C(11)-C(15)	1.417(3)

C(11)-C(12)	1.418(3)
C(11)-C(16)	1.503(3)
C(12)-C(13)	1.415(3)
C(12)-C(17)	1.504(3)
C(13)-C(14)	1.424(3)
C(13)-C(18)	1.502(3)
C(14)-C(15)	1.415(3)
C(14)-C(19)	1.501(3)
C(15)-C(20)	1.501(3)

Cnt1-La(1)-N(1)	113.5
Cnt2-La(1)-N(1)	113.3
Cnt1-La(1)-Cnt2	133.2
N(1)-La(1)-C(12)	137.24(6)
N(1)-La(1)-C(11)	111.61(6)
C(12)-La(1)-C(11)	29.08(6)
N(1)-La(1)-C(13)	125.45(6)
C(12)-La(1)-C(13)	28.99(6)
C(11)-La(1)-C(13)	47.81(6)
N(1)-La(1)-C(5)	89.33(6)
C(12)-La(1)-C(5)	133.32(6)
C(11)-La(1)-C(5)	150.88(6)
C(13)-La(1)-C(5)	134.21(6)
N(1)-La(1)-C(1)	98.01(6)
C(12)-La(1)-C(1)	118.22(6)
C(11)-La(1)-C(1)	124.18(6)
C(13)-La(1)-C(1)	136.33(6)
C(5)-La(1)-C(1)	28.74(6)
N(1)-La(1)-C(4)	110.63(6)
C(12)-La(1)-C(4)	110.59(6)
C(11)-La(1)-C(4)	137.75(6)
C(13)-La(1)-C(4)	105.43(6)
C(5)-La(1)-C(4)	28.84(6)
C(1)-La(1)-C(4)	47.39(6)
N(1)-La(1)-C(2)	126.59(6)
C(12)-La(1)-C(2)	90.44(6)

C(11)-La(1)-C(2)	103.73(6)
C(13)-La(1)-C(2)	107.95(6)
C(5)-La(1)-C(2)	47.35(6)
C(1)-La(1)-C(2)	28.82(6)
C(4)-La(1)-C(2)	47.22(6)
N(1)-La(1)-C(14)	97.08(6)
C(12)-La(1)-C(14)	47.50(6)
C(11)-La(1)-C(14)	47.37(6)
C(13)-La(1)-C(14)	28.91(6)
C(5)-La(1)-C(14)	153.28(6)
C(1)-La(1)-C(14)	164.85(6)
C(4)-La(1)-C(14)	127.09(6)
C(2)-La(1)-C(14)	136.03(6)
N(1)-La(1)-C(15)	89.73(6)
C(12)-La(1)-C(15)	47.55(6)
C(11)-La(1)-C(15)	28.78(6)
C(13)-La(1)-C(15)	47.51(6)
C(5)-La(1)-C(15)	178.14(6)
C(1)-La(1)-C(15)	150.00(6)
C(4)-La(1)-C(15)	152.92(6)
C(2)-La(1)-C(15)	132.48(6)
C(14)-La(1)-C(15)	28.51(6)
N(1)-La(1)-C(3)	136.39(6)
C(12)-La(1)-C(3)	86.37(6)
C(11)-La(1)-C(3)	110.42(6)
C(13)-La(1)-C(3)	91.81(6)
C(5)-La(1)-C(3)	47.22(6)
C(1)-La(1)-C(3)	47.13(6)
C(4)-La(1)-C(3)	28.65(6)
C(2)-La(1)-C(3)	28.40(6)
C(14)-La(1)-C(3)	120.04(6)
C(15)-La(1)-C(3)	133.81(6)
N(1)-La(1)-C(24)	60.72(6)
C(12)-La(1)-C(24)	119.46(6)
C(11)-La(1)-C(24)	125.83(6)
C(13)-La(1)-C(24)	90.48(7)

C(5)-La(1)-C(24)	81.63(6)
C(1)-La(1)-C(24)	109.79(7)
C(4)-La(1)-C(24)	77.02(6)
C(2)-La(1)-C(24)	123.85(6)
C(14)-La(1)-C(24)	79.07(6)
C(15)-La(1)-C(24)	99.30(6)
C(3)-La(1)-C(24)	102.21(6)
N(1)-La(1)-Si(2)	27.57(4)
C(12)-La(1)-Si(2)	133.78(4)
C(11)-La(1)-Si(2)	120.35(4)
C(13)-La(1)-Si(2)	109.62(5)
C(5)-La(1)-Si(2)	87.65(4)
C(1)-La(1)-Si(2)	107.92(5)
C(4)-La(1)-Si(2)	97.97(5)
C(2)-La(1)-Si(2)	134.53(4)
C(14)-La(1)-Si(2)	86.30(4)
C(15)-La(1)-Si(2)	92.25(4)
C(3)-La(1)-Si(2)	126.58(5)
C(24)-La(1)-Si(2)	33.34(5)
N(1)-Si(1)-C(23)	114.17(12)
N(1)-Si(1)-C(22)	114.53(11)
C(23)-Si(1)-C(22)	106.37(13)
N(1)-Si(1)-C(21)	105.49(10)
C(23)-Si(1)-C(21)	108.16(13)
C(22)-Si(1)-C(21)	107.83(13)
N(1)-Si(1)-La(1)	37.85(6)
C(23)-Si(1)-La(1)	122.47(9)
C(22)-Si(1)-La(1)	130.15(9)
C(21)-Si(1)-La(1)	67.85(8)
N(1)-Si(2)-C(26)	115.30(13)
N(1)-Si(2)-C(25)	113.95(12)
C(26)-Si(2)-C(25)	106.76(14)
N(1)-Si(2)-C(24)	105.48(10)
C(26)-Si(2)-C(24)	106.24(15)
C(25)-Si(2)-C(24)	108.70(12)
N(1)-Si(2)-La(1)	40.79(6)

C(26)-Si(2)-La(1)	131.48(10)
C(25)-Si(2)-La(1)	121.43(9)
C(24)-Si(2)-La(1)	65.09(8)
Si(2)-N(1)-Si(1)	131.99(11)
Si(2)-N(1)-La(1)	111.64(9)
Si(1)-N(1)-La(1)	116.34(9)
C(5)-C(1)-C(2)	108.00(19)
C(5)-C(1)-C(6)	125.1(2)
C(2)-C(1)-C(6)	126.0(2)
C(5)-C(1)-La(1)	75.53(11)
C(2)-C(1)-La(1)	76.34(12)
C(6)-C(1)-La(1)	122.58(15)
C(3)-C(2)-C(1)	107.98(19)
C(3)-C(2)-C(7)	126.7(2)
C(1)-C(2)-C(7)	124.9(2)
C(3)-C(2)-La(1)	76.41(12)
C(1)-C(2)-La(1)	74.84(12)
C(7)-C(2)-La(1)	120.56(15)
C(2)-C(3)-C(4)	108.14(19)
C(2)-C(3)-C(8)	127.2(2)
C(4)-C(3)-C(8)	123.7(2)
C(2)-C(3)-La(1)	75.20(12)
C(4)-C(3)-La(1)	74.58(12)
C(8)-C(3)-La(1)	125.22(15)
C(5)-C(4)-C(3)	107.83(19)
C(5)-C(4)-C(9)	127.2(2)
C(3)-C(4)-C(9)	124.0(2)
C(5)-C(4)-La(1)	75.23(11)
C(3)-C(4)-La(1)	76.77(12)
C(9)-C(4)-La(1)	123.10(15)
C(1)-C(5)-C(4)	108.03(18)
C(1)-C(5)-C(10)	125.5(2)
C(4)-C(5)-C(10)	126.1(2)
C(1)-C(5)-La(1)	75.73(11)
C(4)-C(5)-La(1)	75.93(12)
C(10)-C(5)-La(1)	119.73(14)

C(15)-C(11)-C(12)	108.20(18)
C(15)-C(11)-C(16)	126.6(2)
C(12)-C(11)-C(16)	124.5(2)
C(15)-C(11)-La(1)	77.48(12)
C(12)-C(11)-La(1)	75.35(11)
C(16)-C(11)-La(1)	121.09(15)
C(13)-C(12)-C(11)	108.02(18)
C(13)-C(12)-C(17)	126.9(2)
C(11)-C(12)-C(17)	124.5(2)
C(13)-C(12)-La(1)	75.93(12)
C(11)-C(12)-La(1)	75.57(11)
C(17)-C(12)-La(1)	121.47(15)
C(12)-C(13)-C(14)	107.77(18)
C(12)-C(13)-C(18)	126.4(2)
C(14)-C(13)-C(18)	125.5(2)
C(12)-C(13)-La(1)	75.08(12)
C(14)-C(13)-La(1)	77.09(12)
C(18)-C(13)-La(1)	119.22(15)
C(15)-C(14)-C(13)	108.10(19)
C(15)-C(14)-C(19)	125.3(2)
C(13)-C(14)-C(19)	125.6(2)
C(15)-C(14)-La(1)	75.75(12)
C(13)-C(14)-La(1)	74.00(12)
C(19)-C(14)-La(1)	125.06(15)
C(14)-C(15)-C(11)	107.88(19)
C(14)-C(15)-C(20)	124.8(2)
C(11)-C(15)-C(20)	127.0(2)
C(14)-C(15)-La(1)	75.74(12)
C(11)-C(15)-La(1)	73.74(11)
C(20)-C(15)-La(1)	122.06(15)
Si(2)-C(24)-La(1)	81.58(8)

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
La(1)	11(1)	11(1)	18(1)	0(1)	0(1)	5(1)
Si(1)	17(1)	16(1)	27(1)	5(1)	-1(1)	8(1)
Si(2)	19(1)	15(1)	28(1)	-6(1)	-2(1)	7(1)
N(1)	17(1)	13(1)	25(1)	0(1)	-1(1)	7(1)
C(1)	11(1)	18(1)	25(1)	3(1)	-2(1)	4(1)
C(2)	13(1)	16(1)	27(1)	-4(1)	1(1)	5(1)
C(3)	13(1)	14(1)	31(1)	2(1)	1(1)	4(1)
C(4)	11(1)	21(1)	21(1)	1(1)	2(1)	5(1)
C(5)	10(1)	16(1)	30(1)	-3(1)	-1(1)	5(1)
C(6)	19(1)	37(1)	37(1)	13(1)	-6(1)	7(1)
C(7)	26(1)	32(1)	38(1)	-16(1)	-1(1)	10(1)
C(8)	26(1)	21(1)	56(2)	14(1)	5(1)	10(1)
C(9)	23(1)	43(2)	25(1)	0(1)	2(1)	5(1)
C(10)	20(1)	24(1)	61(2)	-13(1)	-4(1)	13(1)
C(11)	17(1)	20(1)	20(1)	0(1)	3(1)	12(1)
C(12)	17(1)	16(1)	25(1)	1(1)	1(1)	11(1)
C(13)	23(1)	25(1)	21(1)	5(1)	3(1)	17(1)
C(14)	18(1)	26(1)	23(1)	-4(1)	-4(1)	15(1)
C(15)	13(1)	18(1)	26(1)	2(1)	2(1)	9(1)
C(16)	36(1)	34(1)	22(1)	-2(1)	2(1)	22(1)
C(17)	26(1)	17(1)	47(2)	-1(1)	1(1)	12(1)
C(18)	42(2)	45(2)	27(1)	15(1)	10(1)	31(1)
C(19)	34(1)	46(2)	37(2)	-20(1)	-17(1)	28(1)
C(20)	17(1)	25(1)	46(2)	6(1)	6(1)	8(1)
C(21)	24(1)	31(1)	23(1)	0(1)	-1(1)	13(1)
C(22)	23(1)	26(1)	40(1)	11(1)	1(1)	6(1)
C(23)	28(1)	27(1)	52(2)	10(1)	-3(1)	16(1)
C(24)	22(1)	28(1)	22(1)	-3(1)	-2(1)	7(1)
C(25)	23(1)	23(1)	41(2)	-6(1)	-3(1)	4(1)

C(26)	38(2)	30(1)	62(2)	-17(1)	-4(1)	21(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10 ^{3})
for **9**.

	x	y	z	U(eq)
H(6A)	5840(30)	830(30)	3940(30)	64(12)
H(6B)	5120(20)	750(20)	4340(20)	50(10)
H(6C)	4960(20)	-60(30)	3860(20)	52(10)
H(7A)	4670(20)	2150(20)	4060(20)	42(9)
H(7B)	5620(30)	2360(30)	4170(20)	62(11)
H(7C)	5340(30)	2880(30)	3630(30)	67(12)
H(8A)	5130(30)	3100(30)	2160(30)	62(12)
H(8B)	4680(30)	2720(30)	1390(30)	65(12)
H(8C)	5700(40)	3040(40)	1470(40)	120(20)
H(9A)	4650(30)	1320(30)	400(30)	67(12)
H(9B)	5630(20)	1720(20)	550(20)	46(9)
H(9C)	5070(20)	770(20)	470(20)	52(10)
H(10A)	5740(20)	40(20)	1960(20)	42(9)
H(10B)	4960(30)	-260(30)	1410(30)	58(11)
H(10C)	4840(30)	-550(30)	2270(30)	67(13)
H(16A)	2100(20)	1410(20)	4400(20)	46(9)
H(16B)	2790(20)	1170(20)	4500(20)	42(9)
H(16C)	1790(20)	460(20)	4530(20)	51(10)
H(17A)	3660(30)	2560(30)	3300(30)	74(14)
H(17B)	2970(30)	2730(30)	3130(30)	77(14)
H(17C)	3550(30)	2820(30)	2460(30)	85(14)
H(18A)	2270(20)	1760(20)	730(20)	51(10)
H(18B)	2960(30)	1490(30)	670(30)	63(12)
H(18C)	3130(30)	2320(30)	1170(30)	68(12)
H(19A)	1490(30)	0(30)	730(30)	63(12)
H(19B)	680(40)	-280(40)	1190(30)	106(18)
H(19C)	1200(30)	-750(30)	1170(30)	81(14)

H(20A)	1070(20)	-790(20)	3800(20)	40(9)
H(20B)	400(30)	-800(30)	3100(20)	63(11)
H(20C)	910(20)	-1220(20)	2910(20)	51(10)
H(21A)	3600(20)	-110(20)	4260(20)	43(10)
H(21B)	2520(30)	-450(20)	4290(20)	59(11)
H(21C)	2970(20)	-780(20)	4880(30)	56(11)
H(22A)	1150(20)	-2330(20)	3780(20)	42(9)
H(22B)	1410(20)	-2930(20)	3410(20)	46(9)
H(22C)	1590(20)	-2700(20)	4380(20)	53(10)
H(23A)	4050(20)	-1590(20)	3709(19)	32(8)
H(23B)	3350(30)	-2470(30)	3400(30)	68(12)
H(23C)	3440(30)	-2160(30)	4350(30)	57(11)
H(24A)	3620(20)	-270(20)	920(20)	48(10)
H(24B)	2700(20)	-320(20)	820(20)	48(10)
H(24C)	2920(20)	-870(20)	240(20)	54(10)
H(25A)	1170(30)	-2400(30)	790(30)	69(12)
H(25B)	1190(20)	-2860(20)	1670(20)	50(10)
H(25C)	1090(20)	-2090(30)	1630(20)	54(11)
H(26A)	3720(30)	-1940(30)	1350(30)	77(14)
H(26B)	2950(40)	-2520(40)	750(30)	104(17)
H(26C)	2930(30)	-2720(30)	1650(20)	58(11)

X-ray Data Collection, Structure Solution and Refinement for **10**.

A colorless crystal of approximate dimensions 0.14 x 0.23 x 0.27 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2[8] program package was used to determine the unit-cell parameters and for data collection (20 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[9] and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program. There were no systematic absences nor any diffraction symmetry other than the Friedel condition. The centrosymmetric triclinic space group $P\bar{1}$ was assigned and later determined to be correct. The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. There was one molecule of toluene solvent present per formula-unit. At convergence, wR2 = 0.0843 and Goof = 1.044 for 593 variables refined against 12691 data, R1 = 0.0315 for those 11232 data with $I > 2.0\sigma(I)$.

Table 1. Crystal data and structure refinement for **10**.

Identification code	tjm10 (**10**)	
Empirical formula	$C_{50}\ H_{75}\ La\ N_6 \bullet (C_7H_8)$	
Formula weight	991.20	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 13.2291(8) Å	α= 76.5550(10)°.
	b = 14.6728(9) Å	β= 76.0620(10)°.
	c = 15.5581(10) Å	γ = 63.4860(10)°.
Volume	2595.5(3) $Å^3$	
Z	2	
Density (calculated)	1.268 Mg/m^3	
Absorption coefficient	0.865 mm^{-1}	
F(000)	1048	
Crystal color	colourless	
Crystal size	0.27 x 0.23 x 0.14 mm^3	
Theta range for data collection	4.17 to 28.27°	
Index ranges	$-17 \le h \le 17$, $-19 \le k \le 19$, $-20 \le l \le 20$	
Reflections collected	31532	
Independent reflections	12691 [R(int) = 0.0216]	
Completeness to theta = 28.27°	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8885 and 0.8000	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12691 / 0 / 593	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I) = 11232 data]	R1 = 0.0315, wR2 = 0.0794	
R indices (all data, 0.75Å)	R1 = 0.0390, wR2 = 0.0843	
Largest diff. peak and hole	1.732 and -0.532 $e.Å^{-3}$	

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

	x	y	z	U(eq)
La(1)	8262(1)	7913(1)	-2579(1)	19(1)
N(1)	7151(2)	7153(1)	-3027(1)	20(1)
N(2)	7610(1)	7523(1)	-3810(1)	19(1)
N(3)	7419(2)	7422(1)	-4538(1)	20(1)
N(4)	7395(2)	7150(2)	-1003(1)	33(1)
N(5)	7025(2)	6677(2)	-445(1)	37(1)
N(6)	6665(3)	6085(2)	76(2)	52(1)
C(1)	6559(2)	9936(2)	-2955(2)	25(1)
C(2)	7574(2)	10085(2)	-3043(2)	23(1)
C(3)	7865(2)	9871(2)	-2177(2)	26(1)
C(4)	7049(2)	9576(2)	-1561(2)	27(1)
C(5)	6241(2)	9618(2)	-2040(2)	26(1)
C(6)	5883(2)	10189(2)	-3699(2)	30(1)
C(7)	8148(2)	10534(2)	-3882(2)	31(1)
C(8)	8715(2)	10145(2)	-1929(2)	38(1)
C(9)	6975(3)	9396(2)	-556(2)	39(1)
C(10)	5167(2)	9447(2)	-1633(2)	35(1)
C(11)	10364(2)	6270(2)	-3088(2)	28(1)
C(12)	10676(2)	7096(2)	-3187(2)	31(1)
C(13)	10587(2)	7310(2)	-2326(2)	34(1)
C(14)	10186(2)	6636(2)	-1689(2)	32(1)
C(15)	10058(2)	5987(2)	-2169(2)	29(1)
C(16)	10457(2)	5712(2)	-3822(2)	44(1)
C(17)	11187(2)	7583(3)	-4044(2)	53(1)
C(18)	11095(3)	7958(3)	-2119(3)	62(1)
C(19)	10065(3)	6536(3)	-687(2)	54(1)
C(20)	9736(3)	5097(2)	-1744(2)	43(1)
C(21)	6423(2)	6631(2)	-3036(1)	20(1)

C(22)	7004(2)	5657(2)	-3479(1)	21(1)
C(23)	6342(2)	5690(2)	-4026(1)	21(1)
C(24)	5340(2)	6683(2)	-4053(1)	23(1)
C(25)	5390(2)	7259(2)	-3522(2)	24(1)
C(26)	5994(2)	6344(2)	-2047(2)	29(1)
C(27)	8089(2)	4796(2)	-3239(2)	33(1)
C(28)	6559(2)	4864(2)	-4554(2)	29(1)
C(29)	4450(2)	6970(2)	-4625(2)	34(1)
C(30)	4571(2)	8319(2)	-3348(2)	37(1)
C(31)	7988(2)	7870(2)	-5346(1)	19(1)
C(32)	8766(2)	6994(2)	-5901(1)	21(1)
C(33)	9312(2)	7414(2)	-6798(1)	24(1)
C(34)	8367(2)	8213(2)	-7330(2)	27(1)
C(35)	7583(2)	9092(2)	-6783(2)	25(1)
C(36)	8289(2)	9603(2)	-6605(2)	28(1)
C(37)	9233(2)	8813(2)	-6080(2)	25(1)
C(38)	8693(2)	8387(2)	-5180(1)	22(1)
C(39)	7048(2)	8663(2)	-5887(1)	22(1)
C(40)	10021(2)	7923(2)	-6619(2)	27(1)
C(41)	6208(2)	6320(2)	1025(2)	31(1)
C(42)	5759(3)	5499(2)	1493(2)	35(1)
C(43)	5289(3)	5673(2)	2473(2)	44(1)
C(44)	4329(3)	6739(3)	2506(2)	52(1)
C(45)	4778(3)	7561(2)	2025(2)	42(1)
C(46)	5737(3)	7450(2)	2472(2)	40(1)
C(47)	6709(3)	6380(2)	2453(2)	40(1)
C(48)	7175(2)	6208(2)	1471(2)	37(1)
C(49)	5253(2)	7385(2)	1044(2)	38(1)
C(50)	6251(3)	5567(2)	2920(2)	49(1)
C(51)	7910(3)	11602(2)	273(2)	40(1)
C(52)	6903(3)	12345(3)	538(2)	55(1)
C(53)	6604(4)	13341(3)	163(3)	66(1)
C(54)	7325(4)	13618(3)	-497(3)	64(1)
C(55)	8386(4)	12876(4)	-807(2)	68(1)
C(56)	8685(3)	11847(3)	-411(2)	49(1)
C(57)	8245(4)	10497(3)	719(3)	65(1)

Table 3. Bond lengths [Å] and angles [°] for **10**.

La(1)-Cnt1	2.583
La(1)-Cnt2	2.586
La(1)-N(1)	2.4916(17)
La(1)-N(2)	2.5460(17)
La(1)-N(4)	2.664(2)
La(1)-C(15)	2.817(2)
La(1)-C(11)	2.831(2)
La(1)-C(5)	2.834(2)
La(1)-C(1)	2.843(2)
La(1)-C(4)	2.848(2)
La(1)-C(14)	2.854(2)
La(1)-C(2)	2.857(2)
La(1)-C(12)	2.862(2)
La(1)-C(3)	2.872(2)
La(1)-C(13)	2.897(2)
N(1)-N(2)	1.333(2)
N(1)-C(21)	1.478(2)
N(2)-N(3)	1.272(2)
N(3)-C(31)	1.476(3)
N(4)-N(5)	1.136(3)
N(5)-N(6)	1.223(3)
N(6)-C(41)	1.511(3)
C(1)-C(5)	1.414(3)
C(1)-C(2)	1.425(3)
C(1)-C(6)	1.510(3)
C(2)-C(3)	1.417(3)
C(2)-C(7)	1.511(3)
C(3)-C(4)	1.413(3)
C(3)-C(8)	1.503(3)
C(4)-C(5)	1.416(3)
C(4)-C(9)	1.509(3)
C(5)-C(10)	1.515(3)
C(11)-C(15)	1.405(4)
C(11)-C(12)	1.413(3)

C(11)-C(16)	1.504(3)
C(12)-C(13)	1.412(4)
C(12)-C(17)	1.517(4)
C(13)-C(14)	1.414(4)
C(13)-C(18)	1.508(3)
C(14)-C(15)	1.425(3)
C(14)-C(19)	1.506(4)
C(15)-C(20)	1.512(3)
C(21)-C(22)	1.526(3)
C(21)-C(25)	1.529(3)
C(21)-C(26)	1.535(3)
C(22)-C(23)	1.341(3)
C(22)-C(27)	1.488(3)
C(23)-C(24)	1.468(3)
C(23)-C(28)	1.505(3)
C(24)-C(25)	1.341(3)
C(24)-C(29)	1.498(3)
C(25)-C(30)	1.490(3)
C(31)-C(38)	1.535(3)
C(31)-C(32)	1.537(3)
C(31)-C(39)	1.538(3)
C(32)-C(33)	1.536(3)
C(33)-C(40)	1.537(3)
C(33)-C(34)	1.537(3)
C(34)-C(35)	1.535(3)
C(35)-C(39)	1.534(3)
C(35)-C(36)	1.535(3)
C(36)-C(37)	1.526(3)
C(37)-C(40)	1.538(3)
C(37)-C(38)	1.540(3)
C(41)-C(49)	1.509(4)
C(41)-C(48)	1.527(4)
C(41)-C(42)	1.535(3)
C(42)-C(43)	1.536(3)
C(43)-C(44)	1.515(5)
C(43)-C(50)	1.526(5)

C(44)-C(45)	1.541(4)
C(45)-C(46)	1.518(4)
C(45)-C(49)	1.539(4)
C(46)-C(47)	1.523(4)
C(47)-C(50)	1.532(4)
C(47)-C(48)	1.538(4)
C(51)-C(52)	1.335(5)
C(51)-C(56)	1.393(4)
C(51)-C(57)	1.512(4)
C(52)-C(53)	1.354(5)
C(53)-C(54)	1.345(6)
C(54)-C(55)	1.393(6)
C(55)-C(56)	1.403(5)

Cnt1-La(1)-N(1)	112.5
Cnt1-La(1)-N(2)	109.4
Cnt1-La(1)-N(4)	95.1
Cnt2-La(1)-N(1)	113.7
Cnt2-La(1)-N(2)	108.9
Cnt2-La(1)-N(4)	96.2
Cnt1-La(1)-Cnt2	133.8
N(1)-La(1)-N(2)	30.67(5)
N(1)-La(1)-N(4)	77.81(6)
N(2)-La(1)-N(4)	108.48(6)
N(1)-La(1)-C(15)	93.61(6)
N(2)-La(1)-C(15)	99.84(6)
N(4)-La(1)-C(15)	76.82(7)
N(1)-La(1)-C(11)	91.90(6)
N(2)-La(1)-C(11)	83.79(6)
N(4)-La(1)-C(11)	104.55(7)
C(15)-La(1)-C(11)	28.81(7)
N(1)-La(1)-C(5)	91.87(6)
N(2)-La(1)-C(5)	99.41(6)
N(4)-La(1)-C(5)	76.41(7)
C(15)-La(1)-C(5)	150.84(7)
C(11)-La(1)-C(5)	176.23(6)

N(1)-La(1)-C(1)	91.32(6)
N(2)-La(1)-C(1)	84.34(6)
N(4)-La(1)-C(1)	104.46(7)
C(15)-La(1)-C(1)	175.06(6)
C(11)-La(1)-C(1)	150.84(7)
C(5)-La(1)-C(1)	28.84(7)
N(1)-La(1)-C(4)	118.35(6)
N(2)-La(1)-C(4)	127.98(6)
N(4)-La(1)-C(4)	73.63(7)
C(15)-La(1)-C(4)	129.49(7)
C(11)-La(1)-C(4)	147.66(7)
C(5)-La(1)-C(4)	28.87(7)
C(1)-La(1)-C(4)	47.46(7)
N(1)-La(1)-C(14)	120.65(7)
N(2)-La(1)-C(14)	128.41(6)
N(4)-La(1)-C(14)	75.11(7)
C(15)-La(1)-C(14)	29.09(7)
C(11)-La(1)-C(14)	47.63(7)
C(5)-La(1)-C(14)	129.93(7)
C(1)-La(1)-C(14)	146.30(7)
C(4)-La(1)-C(14)	102.90(7)
N(1)-La(1)-C(2)	117.39(6)
N(2)-La(1)-C(2)	101.13(6)
N(4)-La(1)-C(2)	120.01(6)
C(15)-La(1)-C(2)	146.43(6)
C(11)-La(1)-C(2)	129.99(7)
C(5)-La(1)-C(2)	47.59(6)
C(1)-La(1)-C(2)	28.96(6)
C(4)-La(1)-C(2)	47.37(6)
C(14)-La(1)-C(2)	121.93(7)
N(1)-La(1)-C(12)	117.21(7)
N(2)-La(1)-C(12)	99.70(7)
N(4)-La(1)-C(12)	120.88(7)
C(15)-La(1)-C(12)	47.29(7)
C(11)-La(1)-C(12)	28.72(7)
C(5)-La(1)-C(12)	147.82(7)

C(1)-La(1)-C(12)	129.64(7)
C(4)-La(1)-C(12)	124.39(7)
C(14)-La(1)-C(12)	47.22(7)
C(2)-La(1)-C(12)	103.15(6)
N(1)-La(1)-C(3)	137.25(6)
N(2)-La(1)-C(3)	129.08(6)
N(4)-La(1)-C(3)	99.77(6)
C(15)-La(1)-C(3)	127.85(7)
C(11)-La(1)-C(3)	128.95(7)
C(5)-La(1)-C(3)	47.36(6)
C(1)-La(1)-C(3)	47.35(6)
C(4)-La(1)-C(3)	28.61(6)
C(14)-La(1)-C(3)	99.05(7)
C(2)-La(1)-C(3)	28.64(6)
C(12)-La(1)-C(3)	100.81(7)
N(1)-La(1)-C(13)	138.09(6)
N(2)-La(1)-C(13)	127.63(7)
N(4)-La(1)-C(13)	101.62(7)
C(15)-La(1)-C(13)	47.14(7)
C(11)-La(1)-C(13)	47.08(7)
C(5)-La(1)-C(13)	129.22(7)
C(1)-La(1)-C(13)	128.06(6)
C(4)-La(1)-C(13)	100.94(7)
C(14)-La(1)-C(13)	28.47(7)
C(2)-La(1)-C(13)	99.38(6)
C(12)-La(1)-C(13)	28.38(8)
C(3)-La(1)-C(13)	84.56(7)
N(2)-N(1)-C(21)	118.14(16)
N(2)-N(1)-La(1)	76.92(10)
C(21)-N(1)-La(1)	164.94(13)
N(3)-N(2)-N(1)	120.15(17)
N(3)-N(2)-La(1)	167.43(14)
N(1)-N(2)-La(1)	72.41(10)
N(2)-N(3)-C(31)	113.74(16)
N(5)-N(4)-La(1)	164.32(18)
N(4)-N(5)-N(6)	171.7(2)

N(5)-N(6)-C(41)	116.6(2)
C(5)-C(1)-C(2)	107.96(19)
C(5)-C(1)-C(6)	126.5(2)
C(2)-C(1)-C(6)	125.2(2)
C(5)-C(1)-La(1)	75.21(13)
C(2)-C(1)-La(1)	76.06(12)
C(6)-C(1)-La(1)	119.88(14)
C(3)-C(2)-C(1)	107.69(19)
C(3)-C(2)-C(7)	125.4(2)
C(1)-C(2)-C(7)	126.4(2)
C(3)-C(2)-La(1)	76.27(13)
C(1)-C(2)-La(1)	74.99(12)
C(7)-C(2)-La(1)	121.24(15)
C(4)-C(3)-C(2)	108.14(19)
C(4)-C(3)-C(8)	125.0(2)
C(2)-C(3)-C(8)	125.4(2)
C(4)-C(3)-La(1)	74.75(12)
C(2)-C(3)-La(1)	75.09(12)
C(8)-C(3)-La(1)	126.88(17)
C(3)-C(4)-C(5)	108.2(2)
C(3)-C(4)-C(9)	124.9(2)
C(5)-C(4)-C(9)	126.4(2)
C(3)-C(4)-La(1)	76.64(13)
C(5)-C(4)-La(1)	75.01(12)
C(9)-C(4)-La(1)	121.09(16)
C(1)-C(5)-C(4)	108.05(19)
C(1)-C(5)-C(10)	125.9(2)
C(4)-C(5)-C(10)	125.9(2)
C(1)-C(5)-La(1)	75.95(12)
C(4)-C(5)-La(1)	76.12(13)
C(10)-C(5)-La(1)	118.36(15)
C(15)-C(11)-C(12)	107.9(2)
C(15)-C(11)-C(16)	125.5(2)
C(12)-C(11)-C(16)	126.4(2)
C(15)-C(11)-La(1)	75.03(13)
C(12)-C(11)-La(1)	76.82(13)

C(16)-C(11)-La(1)	119.16(15)
C(13)-C(12)-C(11)	108.3(2)
C(13)-C(12)-C(17)	124.2(3)
C(11)-C(12)-C(17)	127.0(3)
C(13)-C(12)-La(1)	77.20(14)
C(11)-C(12)-La(1)	74.45(13)
C(17)-C(12)-La(1)	121.31(16)
C(12)-C(13)-C(14)	108.2(2)
C(12)-C(13)-C(18)	125.0(3)
C(14)-C(13)-C(18)	125.4(3)
C(12)-C(13)-La(1)	74.42(13)
C(14)-C(13)-La(1)	74.06(13)
C(18)-C(13)-La(1)	128.40(18)
C(13)-C(14)-C(15)	107.3(2)
C(13)-C(14)-C(19)	125.9(2)
C(15)-C(14)-C(19)	126.4(3)
C(13)-C(14)-La(1)	77.48(14)
C(15)-C(14)-La(1)	74.04(13)
C(19)-C(14)-La(1)	120.29(19)
C(11)-C(15)-C(14)	108.4(2)
C(11)-C(15)-C(20)	126.6(2)
C(14)-C(15)-C(20)	124.9(2)
C(11)-C(15)-La(1)	76.16(13)
C(14)-C(15)-La(1)	76.87(14)
C(20)-C(15)-La(1)	117.08(16)
N(1)-C(21)-C(22)	116.25(17)
N(1)-C(21)-C(25)	116.45(17)
C(22)-C(21)-C(25)	101.55(17)
N(1)-C(21)-C(26)	105.16(16)
C(22)-C(21)-C(26)	108.46(17)
C(25)-C(21)-C(26)	108.71(18)
C(23)-C(22)-C(27)	128.1(2)
C(23)-C(22)-C(21)	109.45(18)
C(27)-C(22)-C(21)	122.25(19)
C(22)-C(23)-C(24)	109.62(18)
C(22)-C(23)-C(28)	127.0(2)

C(24)-C(23)-C(28)	123.40(19)
C(25)-C(24)-C(23)	109.55(19)
C(25)-C(24)-C(29)	127.8(2)
C(23)-C(24)-C(29)	122.6(2)
C(24)-C(25)-C(30)	128.6(2)
C(24)-C(25)-C(21)	109.39(19)
C(30)-C(25)-C(21)	121.9(2)
N(3)-C(31)-C(38)	115.76(17)
N(3)-C(31)-C(32)	106.97(16)
C(38)-C(31)-C(32)	109.47(16)
N(3)-C(31)-C(39)	107.13(16)
C(38)-C(31)-C(39)	109.18(17)
C(32)-C(31)-C(39)	108.06(17)
C(33)-C(32)-C(31)	110.39(17)
C(32)-C(33)-C(40)	109.26(18)
C(32)-C(33)-C(34)	109.39(18)
C(40)-C(33)-C(34)	109.58(18)
C(35)-C(34)-C(33)	109.21(18)
C(39)-C(35)-C(36)	109.31(18)
C(39)-C(35)-C(34)	109.63(17)
C(36)-C(35)-C(34)	109.32(19)
C(37)-C(36)-C(35)	109.77(18)
C(36)-C(37)-C(40)	109.77(19)
C(36)-C(37)-C(38)	109.44(18)
C(40)-C(37)-C(38)	109.32(17)
C(31)-C(38)-C(37)	109.79(17)
C(35)-C(39)-C(31)	110.27(17)
C(33)-C(40)-C(37)	109.31(18)
C(49)-C(41)-N(6)	110.9(2)
C(49)-C(41)-C(48)	110.8(2)
N(6)-C(41)-C(48)	110.0(2)
C(49)-C(41)-C(42)	110.6(2)
N(6)-C(41)-C(42)	104.52(19)
C(48)-C(41)-C(42)	109.9(2)
C(43)-C(42)-C(41)	108.0(2)
C(44)-C(43)-C(50)	110.1(2)

C(44)-C(43)-C(42)	109.3(3)
C(50)-C(43)-C(42)	109.1(2)
C(43)-C(44)-C(45)	110.1(2)
C(46)-C(45)-C(49)	109.0(2)
C(46)-C(45)-C(44)	109.3(3)
C(49)-C(45)-C(44)	108.6(2)
C(45)-C(46)-C(47)	111.2(2)
C(46)-C(47)-C(50)	109.7(3)
C(46)-C(47)-C(48)	108.4(2)
C(50)-C(47)-C(48)	108.1(2)
C(41)-C(48)-C(47)	109.1(2)
C(41)-C(49)-C(45)	108.8(2)
C(43)-C(50)-C(47)	110.4(2)
C(52)-C(51)-C(56)	119.6(3)
C(52)-C(51)-C(57)	121.3(3)
C(56)-C(51)-C(57)	119.0(3)
C(51)-C(52)-C(53)	122.0(3)
C(54)-C(53)-C(52)	120.6(4)
C(53)-C(54)-C(55)	120.1(3)
C(54)-C(55)-C(56)	118.7(3)
C(51)-C(56)-C(55)	119.0(3)

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
La(1)	22(1)	22(1)	17(1)	-2(1)	-3(1)	-13(1)
N(1)	22(1)	24(1)	20(1)	-3(1)	-1(1)	-15(1)
N(2)	19(1)	19(1)	20(1)	-3(1)	-2(1)	-9(1)
N(3)	20(1)	22(1)	21(1)	-3(1)	-2(1)	-11(1)
N(4)	49(1)	38(1)	20(1)	-4(1)	1(1)	-28(1)
N(5)	59(2)	40(1)	21(1)	-7(1)	-1(1)	-31(1)
N(6)	98(2)	50(1)	24(1)	-7(1)	8(1)	-54(2)
C(1)	23(1)	20(1)	36(1)	-10(1)	-6(1)	-9(1)
C(2)	24(1)	22(1)	26(1)	-6(1)	-1(1)	-12(1)
C(3)	30(1)	26(1)	29(1)	-8(1)	-4(1)	-16(1)
C(4)	35(1)	27(1)	24(1)	-10(1)	0(1)	-17(1)
C(5)	26(1)	26(1)	31(1)	-13(1)	4(1)	-14(1)
C(6)	28(1)	30(1)	35(1)	-10(1)	-6(1)	-9(1)
C(7)	37(1)	29(1)	31(1)	-3(1)	-1(1)	-21(1)
C(8)	42(2)	41(1)	44(2)	-12(1)	-9(1)	-26(1)
C(9)	56(2)	44(2)	25(1)	-12(1)	0(1)	-28(1)
C(10)	31(1)	38(1)	40(1)	-17(1)	10(1)	-20(1)
C(11)	21(1)	26(1)	36(1)	-5(1)	-11(1)	-5(1)
C(12)	21(1)	30(1)	39(1)	2(1)	-7(1)	-10(1)
C(13)	28(1)	28(1)	52(2)	-5(1)	-17(1)	-12(1)
C(14)	34(1)	35(1)	31(1)	-2(1)	-17(1)	-13(1)
C(15)	26(1)	23(1)	42(1)	2(1)	-15(1)	-11(1)
C(16)	33(1)	44(2)	48(2)	-22(1)	-13(1)	2(1)
C(17)	24(1)	62(2)	59(2)	17(2)	-4(1)	-20(1)
C(18)	44(2)	44(2)	118(3)	-18(2)	-34(2)	-22(1)
C(19)	56(2)	69(2)	36(2)	-7(1)	-25(1)	-18(2)
C(20)	42(2)	31(1)	60(2)	13(1)	-24(1)	-20(1)
C(21)	20(1)	22(1)	22(1)	-4(1)	-1(1)	-12(1)
C(22)	22(1)	21(1)	22(1)	-4(1)	0(1)	-13(1)

C(23)	22(1)	23(1)	21(1)	-4(1)	1(1)	-14(1)
C(24)	21(1)	27(1)	25(1)	-2(1)	-3(1)	-15(1)
C(25)	18(1)	23(1)	31(1)	-4(1)	-1(1)	-11(1)
C(26)	37(1)	37(1)	23(1)	-6(1)	2(1)	-26(1)
C(27)	28(1)	25(1)	44(1)	-5(1)	-10(1)	-8(1)
C(28)	31(1)	33(1)	29(1)	-12(1)	2(1)	-18(1)
C(29)	29(1)	39(1)	41(1)	-4(1)	-13(1)	-16(1)
C(30)	27(1)	25(1)	59(2)	-13(1)	-8(1)	-8(1)
C(31)	19(1)	20(1)	19(1)	-2(1)	-2(1)	-11(1)
C(32)	23(1)	20(1)	21(1)	-4(1)	-2(1)	-11(1)
C(33)	25(1)	24(1)	22(1)	-5(1)	1(1)	-11(1)
C(34)	32(1)	28(1)	22(1)	-1(1)	-2(1)	-16(1)
C(35)	25(1)	23(1)	26(1)	2(1)	-5(1)	-10(1)
C(36)	29(1)	22(1)	31(1)	1(1)	-1(1)	-15(1)
C(37)	26(1)	25(1)	29(1)	-3(1)	0(1)	-16(1)
C(38)	21(1)	23(1)	26(1)	-5(1)	-2(1)	-12(1)
C(39)	21(1)	21(1)	24(1)	-1(1)	-4(1)	-10(1)
C(40)	24(1)	31(1)	28(1)	-4(1)	1(1)	-15(1)
C(41)	49(1)	36(1)	17(1)	-5(1)	1(1)	-30(1)
C(42)	55(2)	35(1)	27(1)	-4(1)	-3(1)	-30(1)
C(43)	73(2)	50(2)	24(1)	-7(1)	10(1)	-48(2)
C(44)	55(2)	59(2)	49(2)	-15(2)	15(1)	-37(2)
C(45)	40(2)	34(1)	50(2)	-12(1)	4(1)	-16(1)
C(46)	62(2)	40(1)	26(1)	-7(1)	-3(1)	-30(1)
C(47)	59(2)	42(2)	32(1)	-2(1)	-16(1)	-29(1)
C(48)	37(1)	35(1)	44(2)	-5(1)	-7(1)	-19(1)
C(49)	46(2)	35(1)	38(1)	4(1)	-15(1)	-23(1)
C(50)	85(2)	43(2)	25(1)	3(1)	-15(1)	-32(2)
C(51)	49(2)	51(2)	31(1)	-1(1)	-15(1)	-29(1)
C(52)	43(2)	86(3)	36(2)	-9(2)	-10(1)	-23(2)
C(53)	72(2)	67(2)	53(2)	-18(2)	-23(2)	-12(2)
C(54)	100(3)	42(2)	58(2)	-1(2)	-35(2)	-27(2)
C(55)	98(3)	100(3)	33(2)	2(2)	-6(2)	-74(3)
C(56)	49(2)	65(2)	38(2)	-18(1)	1(1)	-26(2)
C(57)	97(3)	63(2)	56(2)	9(2)	-37(2)	-47(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10 ^{3})
for **10**.

	x	y	z	U(eq)
H(6A)	5942	10785	-4114	46
H(6B)	5079	10349	-3445	46
H(6C)	6191	9596	-4021	46
H(7A)	8066	11209	-3807	46
H(7B)	7788	10609	-4392	46
H(7C)	8962	10073	-3993	46
H(8A)	8328	10841	-1767	57
H(8B)	9324	10119	-2440	57
H(8C)	9046	9654	-1420	57
H(9A)	6750	10049	-344	59
H(9B)	7722	8905	-393	59
H(9C)	6404	9117	-279	59
H(10A)	4504	10034	-1853	53
H(10B)	5065	9380	-979	53
H(10C)	5236	8816	-1802	53
H(16A)	10764	4970	-3615	66
H(16B)	10970	5862	-4348	66
H(16C)	9698	5943	-3980	66
H(17A)	11980	7427	-4013	79
H(17B)	10741	8330	-4120	79
H(17C)	11170	7306	-4554	79
H(18A)	11917	7554	-2118	93
H(18B)	10725	8174	-1530	93
H(18C)	10971	8567	-2576	93
H(19A)	10821	6145	-504	81
H(19B)	9574	6176	-399	81
H(19C)	9723	7223	-508	81

H(20A)	10212	4509	-2069	65
H(20B)	8929	5302	-1768	65
H(20C)	9859	4902	-1118	65
H(26A)	5561	6970	-1765	44
H(26B)	6650	5885	-1741	44
H(26C)	5499	5995	-2004	44
H(27A)	8441	4353	-3708	49
H(27B)	7925	4394	-2669	49
H(27C)	8614	5076	-3181	49
H(28A)	7171	4220	-4338	44
H(28B)	6790	5073	-5189	44
H(28C)	5859	4760	-4479	44
H(29A)	3834	7643	-4516	51
H(29B)	4136	6451	-4477	51
H(29C)	4797	7004	-5257	51
H(30A)	4134	8672	-3844	55
H(30B)	4995	8701	-3294	55
H(30C)	4046	8283	-2790	55
H(32A)	9373	6468	-5563	25
H(32B)	8311	6663	-6013	25
H(33A)	9821	6835	-7149	29
H(34A)	8713	8487	-7908	32
H(34B)	7916	7885	-7454	32
H(35A)	6964	9613	-7125	30
H(36A)	8632	9887	-7180	33
H(36B)	7786	10178	-6260	33
H(37A)	9691	9149	-5967	30
H(38A)	9303	7881	-4833	26
H(38B)	8194	8955	-4826	26
H(39A)	6591	8334	-5998	26
H(39B)	6530	9233	-5540	26
H(40A)	10384	8188	-7193	33
H(40B)	10633	7409	-6278	33
H(42A)	5147	5557	1195	42
H(42B)	6385	4803	1463	42
H(43A)	4990	5146	2792	52

H(44A)	4009	6848	3136	63
H(44B)	3709	6803	2213	63
H(45A)	4145	8265	2052	51
H(46A)	5434	7576	3100	48
H(46B)	6034	7972	2159	48
H(47A)	7329	6318	2754	48
H(48A)	7486	6718	1153	44
H(48B)	7801	5511	1442	44
H(49A)	4638	7450	744	45
H(49B)	5545	7907	722	45
H(50A)	6879	4871	2890	58
H(50B)	5962	5652	3558	58
H(52A)	6379	12169	1004	66
H(53A)	5879	13850	369	79
H(54A)	7110	14320	-753	77
H(55A)	8897	13064	-1277	81
H(56A)	9405	11326	-607	58
H(57A)	7564	10412	1074	98
H(57B)	8803	10325	1112	98
H(57C)	8585	10039	261	98

X-ray Data Collection, Structure Solution and Refinement for **11**.

A colorless crystal of approximate dimensions 0.22 x 0.24 x 0.34 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2[8] program package was used to determine the unit-cell parameters and for data collection (10 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[9] and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program. The diffraction symmetry was 2/*m* and the systematic absences were consistent with the centrosymmetric monoclinic space group $P2_1/c$ that was later determined to be correct. The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. There was one molecule of benzene solvent present per formula unit. At convergence, wR2 = 0.0527 and Goof = 1.072 for 463 variables refined against 13025 data (0.70 Å), R1 = 0.0200 for those 11592 data with $I > 2.0\sigma(I)$.

Table 1.Crystal data and structure refinement for **11**.

Identification code	tjm8 (**11**)	
Empirical formula	$C_{40}\ H_{63}\ La\ N_2 \bullet C_6H_6$	
Formula weight	788.94	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 19.1633(6) Å	α = 90°.
	b = 17.5365(5) Å	β = 101.8600(10)°.
	c = 12.9886(4) Å	γ = 90°.
Volume	4271.7(2) $Å^3$	
Z	4	
Density (calculated)	1.227 Mg/m^3	
Absorption coefficient	1.031 mm^{-1}	
F(000)	1664	
Crystal color	colorless	
Crystal size	0.34 x 0.24 x 0.22 mm^3	
Theta range for data collection	1.98 to 30.51°	
Index ranges	$-27 \le h \le 27$, $-25 \le k \le 25$, $-18 \le l \le 18$	
Reflections collected	67787	
Independent reflections	13025 [R(int) = 0.0227]	
Completeness to theta = 30.51°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8049 and 0.7207	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13025 / 0 / 463	
Goodness-of-fit on F^2	1.072	
Final R indices [I>2sigma(I) = 11592 data]	R1 = 0.0200, wR2 = 0.0484	
R indices (all data, 0.70 Å)	R1 = 0.0257, wR2 = 0.0527	
Largest diff. peak and hole	0.757 and -0.354 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for **11**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
La(1)	2247(1)	69(1)	3360(1)	11(1)
N(1)	3191(1)	1217(1)	3636(1)	19(1)
N(2)	1307(1)	-1063(1)	3128(1)	17(1)
C(1)	3399(1)	-164(1)	2146(1)	25(1)
C(2)	2760(1)	-31(1)	1408(1)	23(1)
C(3)	2317(1)	-677(1)	1405(1)	20(1)
C(4)	2695(1)	-1213(1)	2130(1)	20(1)
C(5)	3367(1)	-897(1)	2570(1)	23(1)
C(6)	4063(1)	316(1)	2246(2)	47(1)
C(7)	2667(1)	587(1)	581(2)	42(1)
C(8)	1636(1)	-864(1)	638(1)	35(1)
C(9)	2492(1)	-2032(1)	2247(2)	34(1)
C(10)	4024(1)	-1323(1)	3114(1)	44(1)
C(11)	1421(1)	1421(1)	3458(1)	15(1)
C(12)	1581(1)	1527(1)	2446(1)	16(1)
C(13)	1152(1)	1013(1)	1741(1)	18(1)
C(14)	747(1)	576(1)	2320(1)	18(1)
C(15)	903(1)	830(1)	3379(1)	16(1)
C(16)	1668(1)	1943(1)	4380(1)	22(1)
C(17)	2011(1)	2174(1)	2133(1)	22(1)
C(18)	983(1)	1071(1)	560(1)	31(1)
C(19)	139(1)	58(1)	1843(1)	28(1)
C(20)	484(1)	591(1)	4184(1)	24(1)
C(21)	3264(1)	-201(1)	5315(1)	19(1)
C(22)	2869(1)	389(1)	5678(1)	18(1)
C(23)	2197(1)	93(1)	5759(1)	17(1)
C(24)	2168(1)	-678(1)	5429(1)	17(1)
C(25)	2833(1)	-867(1)	5170(1)	18(1)

C(26)	4047(1)	-136(1)	5302(1)	28(1)
C(27)	3177(1)	1124(1)	6171(1)	26(1)
C(28)	1711(1)	441(1)	6410(1)	25(1)
C(29)	1603(1)	-1236(1)	5582(1)	24(1)
C(30)	3077(1)	-1668(1)	5038(1)	29(1)
C(31)	3589(1)	1713(1)	3761(1)	18(1)
C(32)	4103(1)	2356(1)	3930(1)	22(1)
C(33)	4366(1)	2484(1)	2904(1)	34(1)
C(34)	4724(1)	2135(1)	4827(2)	34(1)
C(35)	3719(1)	3064(1)	4219(2)	32(1)
C(36)	917(1)	-1564(1)	2987(1)	17(1)
C(37)	410(1)	-2212(1)	2792(1)	22(1)
C(38)	241(1)	-2381(1)	1611(1)	35(1)
C(39)	764(1)	-2913(1)	3387(2)	41(1)
C(40)	-255(1)	-1993(1)	3189(2)	60(1)
C(41)	4454(1)	9231(2)	9196(2)	72(1)
C(42)	4052(1)	9313(2)	8192(2)	67(1)
C(43)	3340(1)	9151(1)	7986(1)	41(1)
C(44)	3033(1)	8888(1)	8786(2)	41(1)
C(45)	3439(1)	8796(1)	9792(1)	36(1)
C(46)	4145(1)	8975(1)	9993(1)	41(1)

Table 3. Bond lengths [Å] and angles [°] for **11**.

La(1)-Cnt1	2.715
La(1)-Cnt2	2.734
La(1)-Cnt3	2.752
La(1)-N(2)	2.6561(11)
La(1)-N(1)	2.6811(11)
La(1)-C(11)	2.8693(12)
La(1)-C(3)	2.8836(13)
La(1)-C(25)	2.8979(12)
La(1)-C(21)	2.9048(13)
La(1)-C(15)	2.9054(12)
La(1)-C(2)	2.9066(14)
La(1)-C(4)	2.9845(13)
La(1)-C(12)	2.9917(12)
La(1)-C(1)	2.9928(14)
La(1)-C(24)	3.0219(12)
La(1)-C(14)	3.0462(12)
La(1)-C(22)	3.0541(13)
La(1)-C(5)	3.0715(13)
La(1)-C(13)	3.1224(12)
La(1)-C(23)	3.1378(13)
N(1)-C(31)	1.1451(17)
N(2)-C(36)	1.1434(17)
C(1)-C(5)	1.405(2)
C(1)-C(2)	1.411(2)
C(1)-C(6)	1.509(2)
C(2)-C(3)	1.4151(19)
C(2)-C(7)	1.510(2)
C(3)-C(4)	1.4194(19)
C(3)-C(8)	1.506(2)
C(4)-C(5)	1.411(2)
C(4)-C(9)	1.504(2)
C(5)-C(10)	1.508(2)
C(11)-C(12)	1.4227(18)
C(11)-C(15)	1.4246(17)

C(11)-C(16)	1.5037(18)
C(12)-C(13)	1.4193(17)
C(12)-C(17)	1.5060(18)
C(13)-C(14)	1.4125(19)
C(13)-C(18)	1.5045(19)
C(14)-C(15)	1.4181(18)
C(14)-C(19)	1.5059(18)
C(15)-C(20)	1.5034(19)
C(21)-C(22)	1.4188(19)
C(21)-C(25)	1.4220(19)
C(21)-C(26)	1.5072(19)
C(22)-C(23)	1.4116(18)
C(22)-C(27)	1.5059(19)
C(23)-C(24)	1.4150(17)
C(23)-C(28)	1.5087(18)
C(24)-C(25)	1.4225(18)
C(24)-C(29)	1.5021(18)
C(25)-C(30)	1.5007(19)
C(31)-C(32)	1.4839(18)
C(32)-C(35)	1.528(2)
C(32)-C(33)	1.536(2)
C(32)-C(34)	1.536(2)
C(36)-C(37)	1.4830(18)
C(37)-C(40)	1.520(2)
C(37)-C(38)	1.530(2)
C(37)-C(39)	1.533(2)
C(41)-C(46)	1.370(3)
C(41)-C(42)	1.380(3)
C(42)-C(43)	1.366(3)
C(43)-C(44)	1.374(3)
C(44)-C(45)	1.386(3)
C(45)-C(46)	1.361(3)

Cnt1-La(1)-N(1)	91.0
Cnt2-La(1)-N(1)	90.4
Cnt3-La(1)-N(1)	88.3

Cnt1-La(1)-N(2)	90.1
Cnt2-La(1)-N(2)	89.5
Cnt3-La(1)-N(2)	90.7
Cnt1-La(1)-Cnt2	118.9
Cnt1-La(1)-Cnt3	120.7
Cnt2-La(1)-Cnt3	120.4
N(2)-La(1)-N(1)	178.77(3)
N(2)-La(1)-C(11)	104.78(3)
N(1)-La(1)-C(11)	74.76(3)
N(2)-La(1)-C(3)	73.39(4)
N(1)-La(1)-C(3)	107.83(4)
C(11)-La(1)-C(3)	122.70(4)
N(2)-La(1)-C(25)	78.99(4)
N(1)-La(1)-C(25)	100.30(4)
C(11)-La(1)-C(25)	123.87(4)
C(3)-La(1)-C(25)	112.15(4)
N(2)-La(1)-C(21)	107.17(4)
N(1)-La(1)-C(21)	72.07(4)
C(11)-La(1)-C(21)	111.90(4)
C(3)-La(1)-C(21)	123.48(4)
C(25)-La(1)-C(21)	28.37(4)
N(2)-La(1)-C(15)	76.24(3)
N(1)-La(1)-C(15)	103.26(3)
C(11)-La(1)-C(15)	28.56(3)
C(3)-La(1)-C(15)	114.68(4)
C(25)-La(1)-C(15)	116.70(4)
C(21)-La(1)-C(15)	120.28(4)
N(2)-La(1)-C(2)	101.48(4)
N(1)-La(1)-C(2)	79.75(4)
C(11)-La(1)-C(2)	112.20(4)
C(3)-La(1)-C(2)	28.29(4)
C(25)-La(1)-C(2)	121.95(4)
C(21)-La(1)-C(2)	117.77(4)
C(15)-La(1)-C(2)	119.66(4)
N(2)-La(1)-C(4)	68.83(4)
N(1)-La(1)-C(4)	112.15(4)

C(11)-La(1)-C(4)	150.31(4)
C(3)-La(1)-C(4)	27.93(4)
C(25)-La(1)-C(4)	84.34(4)
C(21)-La(1)-C(4)	97.48(4)
C(15)-La(1)-C(4)	134.69(4)
C(2)-La(1)-C(4)	45.71(4)
N(2)-La(1)-C(12)	111.67(3)
N(1)-La(1)-C(12)	68.46(3)
C(11)-La(1)-C(12)	28.00(3)
C(3)-La(1)-C(12)	97.56(4)
C(25)-La(1)-C(12)	150.29(4)
C(21)-La(1)-C(12)	129.87(4)
C(15)-La(1)-C(12)	45.92(3)
C(2)-La(1)-C(12)	84.21(4)
C(4)-La(1)-C(12)	125.28(4)
N(2)-La(1)-C(1)	113.25(4)
N(1)-La(1)-C(1)	67.81(4)
C(11)-La(1)-C(1)	127.60(4)
C(3)-La(1)-C(1)	45.70(4)
C(25)-La(1)-C(1)	98.36(4)
C(21)-La(1)-C(1)	90.17(4)
C(15)-La(1)-C(1)	144.94(4)
C(2)-La(1)-C(1)	27.62(4)
C(4)-La(1)-C(1)	44.84(4)
C(12)-La(1)-C(1)	102.05(4)
N(2)-La(1)-C(24)	67.67(3)
N(1)-La(1)-C(24)	111.24(3)
C(11)-La(1)-C(24)	100.91(4)
C(3)-La(1)-C(24)	127.34(4)
C(25)-La(1)-C(24)	27.71(3)
C(21)-La(1)-C(24)	45.50(4)
C(15)-La(1)-C(24)	89.12(4)
C(2)-La(1)-C(24)	146.87(4)
C(4)-La(1)-C(24)	102.83(4)
C(12)-La(1)-C(24)	128.89(3)
C(1)-La(1)-C(24)	125.92(4)

N(2)-La(1)-C(14)	67.13(3)
N(1)-La(1)-C(14)	112.94(3)
C(11)-La(1)-C(14)	45.54(3)
C(3)-La(1)-C(14)	87.26(4)
C(25)-La(1)-C(14)	134.24(4)
C(21)-La(1)-C(14)	146.89(4)
C(15)-La(1)-C(14)	27.44(4)
C(2)-La(1)-C(14)	95.08(4)
C(4)-La(1)-C(14)	109.34(4)
C(12)-La(1)-C(14)	44.60(3)
C(1)-La(1)-C(14)	122.50(4)
C(24)-La(1)-C(14)	107.78(4)
N(2)-La(1)-C(22)	111.54(3)
N(1)-La(1)-C(22)	67.32(3)
C(11)-La(1)-C(22)	84.91(4)
C(3)-La(1)-C(22)	150.71(4)
C(25)-La(1)-C(22)	45.30(4)
C(21)-La(1)-C(22)	27.40(4)
C(15)-La(1)-C(22)	94.25(4)
C(2)-La(1)-C(22)	137.53(4)
C(4)-La(1)-C(22)	124.70(4)
C(12)-La(1)-C(22)	106.41(4)
C(1)-La(1)-C(22)	111.34(4)
C(24)-La(1)-C(22)	44.21(3)
C(14)-La(1)-C(22)	121.67(4)
N(2)-La(1)-C(5)	93.09(4)
N(1)-La(1)-C(5)	87.72(4)
C(11)-La(1)-C(5)	154.28(4)
C(3)-La(1)-C(5)	45.06(4)
C(25)-La(1)-C(5)	77.16(4)
C(21)-La(1)-C(5)	79.20(4)
C(15)-La(1)-C(5)	159.67(4)
C(2)-La(1)-C(5)	44.80(4)
C(4)-La(1)-C(5)	26.90(4)
C(12)-La(1)-C(5)	127.55(4)
C(1)-La(1)-C(5)	26.75(4)

C(24)-La(1)-C(5)	102.96(4)
C(14)-La(1)-C(5)	132.31(4)
C(22)-La(1)-C(5)	105.83(4)
N(2)-La(1)-C(13)	88.48(3)
N(1)-La(1)-C(13)	91.93(3)
C(11)-La(1)-C(13)	44.86(3)
C(3)-La(1)-C(13)	78.12(4)
C(25)-La(1)-C(13)	160.25(4)
C(21)-La(1)-C(13)	155.83(4)
C(15)-La(1)-C(13)	44.61(4)
C(2)-La(1)-C(13)	75.29(4)
C(4)-La(1)-C(13)	105.45(4)
C(12)-La(1)-C(13)	26.73(3)
C(1)-La(1)-C(13)	100.62(4)
C(24)-La(1)-C(13)	132.76(4)
C(14)-La(1)-C(13)	26.44(4)
C(22)-La(1)-C(13)	129.68(3)
C(5)-La(1)-C(13)	119.12(4)
N(2)-La(1)-C(23)	87.95(3)
N(1)-La(1)-C(23)	90.84(3)
C(11)-La(1)-C(23)	79.33(3)
C(3)-La(1)-C(23)	153.75(4)
C(25)-La(1)-C(23)	44.56(3)
C(21)-La(1)-C(23)	44.42(4)
C(15)-La(1)-C(23)	77.14(3)
C(2)-La(1)-C(23)	162.14(4)
C(4)-La(1)-C(23)	127.76(4)
C(12)-La(1)-C(23)	106.57(3)
C(1)-La(1)-C(23)	134.52(4)
C(24)-La(1)-C(23)	26.47(3)
C(14)-La(1)-C(23)	102.59(4)
C(22)-La(1)-C(23)	26.31(3)
C(5)-La(1)-C(23)	120.33(4)
C(13)-La(1)-C(23)	120.55(3)
C(31)-N(1)-La(1)	179.06(11)
C(36)-N(2)-La(1)	176.47(11)

C(5)-C(1)-C(2)	108.38(12)
C(5)-C(1)-C(6)	125.54(16)
C(2)-C(1)-C(6)	124.39(16)
C(5)-C(1)-La(1)	79.75(8)
C(2)-C(1)-La(1)	72.79(8)
C(6)-C(1)-La(1)	125.40(10)
C(1)-C(2)-C(3)	107.86(12)
C(1)-C(2)-C(7)	124.13(15)
C(3)-C(2)-C(7)	126.07(15)
C(1)-C(2)-La(1)	79.59(8)
C(3)-C(2)-La(1)	74.95(8)
C(7)-C(2)-La(1)	124.40(10)
C(2)-C(3)-C(4)	107.72(12)
C(2)-C(3)-C(8)	127.88(14)
C(4)-C(3)-C(8)	123.29(13)
C(2)-C(3)-La(1)	76.76(8)
C(4)-C(3)-La(1)	79.99(7)
C(8)-C(3)-La(1)	119.38(10)
C(5)-C(4)-C(3)	107.87(12)
C(5)-C(4)-C(9)	124.60(14)
C(3)-C(4)-C(9)	126.35(14)
C(5)-C(4)-La(1)	79.98(8)
C(3)-C(4)-La(1)	72.08(7)
C(9)-C(4)-La(1)	123.83(9)
C(1)-C(5)-C(4)	108.11(13)
C(1)-C(5)-C(10)	122.44(15)
C(4)-C(5)-C(10)	126.88(15)
C(1)-C(5)-La(1)	73.50(8)
C(4)-C(5)-La(1)	73.11(7)
C(10)-C(5)-La(1)	133.59(10)
C(12)-C(11)-C(15)	107.86(11)
C(12)-C(11)-C(16)	124.36(11)
C(15)-C(11)-C(16)	127.00(12)
C(12)-C(11)-La(1)	80.79(7)
C(15)-C(11)-La(1)	77.13(7)
C(16)-C(11)-La(1)	116.87(8)

C(13)-C(12)-C(11)	107.91(11)
C(13)-C(12)-C(17)	125.48(12)
C(11)-C(12)-C(17)	125.51(12)
C(13)-C(12)-La(1)	81.77(7)
C(11)-C(12)-La(1)	71.21(7)
C(17)-C(12)-La(1)	122.54(8)
C(14)-C(13)-C(12)	108.07(11)
C(14)-C(13)-C(18)	123.54(13)
C(12)-C(13)-C(18)	126.09(13)
C(14)-C(13)-La(1)	73.77(7)
C(12)-C(13)-La(1)	71.49(7)
C(18)-C(13)-La(1)	134.13(9)
C(13)-C(14)-C(15)	108.44(11)
C(13)-C(14)-C(19)	124.87(13)
C(15)-C(14)-C(19)	125.39(13)
C(13)-C(14)-La(1)	79.79(7)
C(15)-C(14)-La(1)	70.74(7)
C(19)-C(14)-La(1)	125.92(8)
C(14)-C(15)-C(11)	107.69(11)
C(14)-C(15)-C(20)	123.47(12)
C(11)-C(15)-C(20)	128.02(12)
C(14)-C(15)-La(1)	81.82(7)
C(11)-C(15)-La(1)	74.32(7)
C(20)-C(15)-La(1)	118.65(8)
C(22)-C(21)-C(25)	107.88(11)
C(22)-C(21)-C(26)	123.34(13)
C(25)-C(21)-C(26)	127.83(13)
C(22)-C(21)-La(1)	82.17(7)
C(25)-C(21)-La(1)	75.54(7)
C(26)-C(21)-La(1)	117.96(9)
C(23)-C(22)-C(21)	108.32(11)
C(23)-C(22)-C(27)	124.60(12)
C(21)-C(22)-C(27)	125.13(12)
C(23)-C(22)-La(1)	80.16(7)
C(21)-C(22)-La(1)	70.43(7)
C(27)-C(22)-La(1)	128.04(9)

C(22)-C(23)-C(24)	107.99(11)
C(22)-C(23)-C(28)	124.75(12)
C(24)-C(23)-C(28)	124.38(12)
C(22)-C(23)-La(1)	73.53(7)
C(24)-C(23)-La(1)	72.19(7)
C(28)-C(23)-La(1)	135.23(9)
C(23)-C(24)-C(25)	108.24(11)
C(23)-C(24)-C(29)	124.53(12)
C(25)-C(24)-C(29)	125.73(12)
C(23)-C(24)-La(1)	81.34(7)
C(25)-C(24)-La(1)	71.29(7)
C(29)-C(24)-La(1)	124.70(8)
C(21)-C(25)-C(24)	107.55(11)
C(21)-C(25)-C(30)	126.68(13)
C(24)-C(25)-C(30)	124.14(13)
C(21)-C(25)-La(1)	76.08(7)
C(24)-C(25)-La(1)	81.00(7)
C(30)-C(25)-La(1)	120.99(9)
N(1)-C(31)-C(32)	179.64(16)
C(31)-C(32)-C(35)	108.43(12)
C(31)-C(32)-C(33)	108.05(12)
C(35)-C(32)-C(33)	110.79(13)
C(31)-C(32)-C(34)	107.91(11)
C(35)-C(32)-C(34)	110.87(13)
C(33)-C(32)-C(34)	110.69(13)
N(2)-C(36)-C(37)	179.43(15)
C(36)-C(37)-C(40)	108.35(12)
C(36)-C(37)-C(38)	108.35(12)
C(40)-C(37)-C(38)	111.70(16)
C(36)-C(37)-C(39)	108.77(12)
C(40)-C(37)-C(39)	110.31(16)
C(38)-C(37)-C(39)	109.28(13)
C(46)-C(41)-C(42)	120.3(2)
C(43)-C(42)-C(41)	120.34(19)
C(42)-C(43)-C(44)	119.16(17)
C(43)-C(44)-C(45)	120.51(17)

C(46)-C(45)-C(44)	119.80(16)
C(45)-C(46)-C(41)	119.91(18)

Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
La(1)	11(1)	10(1)	12(1)	0(1)	2(1)	0(1)
N(1)	18(1)	18(1)	20(1)	1(1)	4(1)	0(1)
N(2)	17(1)	15(1)	19(1)	0(1)	3(1)	0(1)
C(1)	22(1)	30(1)	26(1)	-11(1)	14(1)	-7(1)
C(2)	33(1)	19(1)	21(1)	1(1)	15(1)	1(1)
C(3)	22(1)	22(1)	16(1)	-4(1)	4(1)	2(1)
C(4)	26(1)	16(1)	21(1)	-3(1)	11(1)	1(1)
C(5)	21(1)	32(1)	19(1)	-3(1)	7(1)	8(1)
C(6)	34(1)	56(1)	60(1)	-31(1)	32(1)	-22(1)
C(7)	65(1)	28(1)	41(1)	13(1)	31(1)	9(1)
C(8)	32(1)	44(1)	24(1)	-11(1)	-3(1)	2(1)
C(9)	47(1)	17(1)	44(1)	-3(1)	23(1)	2(1)
C(10)	33(1)	67(1)	32(1)	-1(1)	9(1)	27(1)
C(11)	15(1)	12(1)	18(1)	0(1)	2(1)	2(1)
C(12)	16(1)	12(1)	19(1)	3(1)	1(1)	2(1)
C(13)	20(1)	16(1)	16(1)	1(1)	-3(1)	3(1)
C(14)	14(1)	14(1)	24(1)	0(1)	-3(1)	1(1)
C(15)	12(1)	15(1)	22(1)	2(1)	3(1)	2(1)
C(16)	24(1)	17(1)	23(1)	-5(1)	2(1)	2(1)
C(17)	20(1)	18(1)	26(1)	6(1)	3(1)	-1(1)
C(18)	37(1)	33(1)	18(1)	2(1)	-5(1)	9(1)
C(19)	18(1)	17(1)	42(1)	-3(1)	-8(1)	0(1)
C(20)	17(1)	25(1)	33(1)	5(1)	10(1)	2(1)
C(21)	15(1)	26(1)	15(1)	3(1)	2(1)	3(1)
C(22)	19(1)	21(1)	15(1)	-1(1)	2(1)	-1(1)
C(23)	17(1)	19(1)	15(1)	0(1)	4(1)	2(1)
C(24)	18(1)	18(1)	15(1)	2(1)	3(1)	0(1)
C(25)	21(1)	18(1)	14(1)	3(1)	4(1)	5(1)
C(26)	16(1)	44(1)	25(1)	6(1)	4(1)	4(1)

C(27)	30(1)	27(1)	20(1)	-5(1)	3(1)	-9(1)
C(28)	27(1)	28(1)	24(1)	-2(1)	11(1)	5(1)
C(29)	27(1)	23(1)	21(1)	4(1)	6(1)	-5(1)
C(30)	41(1)	22(1)	28(1)	7(1)	16(1)	12(1)
C(31)	17(1)	18(1)	20(1)	2(1)	3(1)	2(1)
C(32)	16(1)	18(1)	30(1)	4(1)	1(1)	-3(1)
C(33)	33(1)	31(1)	41(1)	6(1)	14(1)	-10(1)
C(34)	22(1)	31(1)	43(1)	8(1)	-9(1)	-5(1)
C(35)	27(1)	19(1)	47(1)	-4(1)	2(1)	-2(1)
C(36)	18(1)	16(1)	18(1)	0(1)	4(1)	0(1)
C(37)	22(1)	16(1)	28(1)	-2(1)	5(1)	-6(1)
C(38)	41(1)	28(1)	30(1)	1(1)	-8(1)	-15(1)
C(39)	54(1)	21(1)	40(1)	10(1)	-7(1)	-13(1)
C(40)	39(1)	42(1)	112(2)	-30(1)	44(1)	-23(1)
C(41)	28(1)	117(2)	65(2)	45(2)	-1(1)	-4(1)
C(42)	38(1)	115(2)	50(1)	50(1)	15(1)	4(1)
C(43)	40(1)	58(1)	23(1)	4(1)	2(1)	9(1)
C(44)	31(1)	46(1)	46(1)	-11(1)	11(1)	-10(1)
C(45)	55(1)	30(1)	32(1)	3(1)	28(1)	6(1)
C(46)	46(1)	47(1)	27(1)	8(1)	0(1)	14(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10 ^{3})
for **11**.

	x	y	z	U(eq)
H(6A)	4308	339	2985	71
H(6B)	3932	832	1988	71
H(6C)	4380	88	1827	71
H(7A)	2675	1087	920	63
H(7B)	2210	517	89	63
H(7C)	3056	557	197	63
H(8A)	1228	-744	956	52
H(8B)	1630	-1408	462	52
H(8C)	1608	-561	-4	52
H(9A)	2917	-2355	2318	51
H(9B)	2140	-2189	1624	51
H(9C)	2286	-2087	2875	51
H(10A)	4376	-1325	2664	65
H(10B)	3895	-1849	3250	65
H(10C)	4227	-1071	3782	65
H(16A)	2187	1910	4603	32
H(16B)	1445	1791	4963	32
H(16C)	1532	2469	4175	32
H(17A)	2458	1975	1987	32
H(17B)	2116	2545	2708	32
H(17C)	1738	2422	1501	32
H(18A)	990	561	255	46
H(18B)	1340	1393	330	46
H(18C)	510	1298	328	46
H(19A)	-248	362	1426	42
H(19B)	-36	-207	2404	42
H(19C)	305	-317	1387	42

H(20A)	-27	652	3892	36
H(20B)	620	909	4813	36
H(20C)	585	55	4372	36
H(26A)	4104	52	4614	42
H(26B)	4271	-639	5434	42
H(26C)	4273	220	5851	42
H(27A)	2798	1431	6367	40
H(27B)	3394	1408	5667	40
H(27C)	3542	1012	6801	40
H(28A)	1916	364	7158	38
H(28B)	1242	196	6233	38
H(28C)	1660	988	6261	38
H(29A)	1652	-1343	6334	35
H(29B)	1658	-1710	5207	35
H(29C)	1131	-1017	5305	35
H(30A)	3521	-1656	4775	43
H(30B)	2710	-1939	4533	43
H(30C)	3159	-1931	5717	43
H(33A)	4631	2034	2752	51
H(33B)	4680	2931	2980	51
H(33C)	3957	2569	2325	51
H(34A)	4543	2036	5467	51
H(34B)	5071	2553	4957	51
H(34C)	4956	1674	4631	51
H(35A)	3313	3182	3648	48
H(35B)	4050	3496	4326	48
H(35C)	3548	2967	4868	48
H(38A)	31	-1928	1227	53
H(38B)	-97	-2806	1467	53
H(38C)	681	-2517	1382	53
H(39A)	1200	-3038	3139	61
H(39B)	434	-3346	3259	61
H(39C)	883	-2802	4142	61
H(40A)	-123	-1854	3935	90
H(40B)	-586	-2426	3105	90
H(40C)	-487	-1557	2784	90

H(41)	4948	9353	9336	86
H(42)	4271	9483	7640	80
H(43)	3060	9219	7298	49
H(44)	2539	8768	8648	49
H(45)	3225	8609	10340	43
H(46)	4423	8921	10684	49

Definitions:

$wR2 = [\Sigma[w(F_o^2-F_c^2)^2] / \Sigma[w(F_o^2)^2]]^{1/2}$

$R1 = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$

$Goof = S = [\Sigma[w(F_o^2-F_c^2)^2] / (n-p)]^{1/2}$ where n is the number of reflections and p is the total number of parameters refined.

[1] SMART Software Users Guide, Version 5.1, Bruker Analytical X-Ray Systems, Inc.; Madison,WI 1999.

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