Crystal Structure Report for Zhon11

$C_{35}H_{43}NO_6PPdS_2 + C_{14}H_{28}N_2O_4Li + CH_2Cl_2$

Report Prepared for:

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April, 2009

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Crystallographic Experimental Section

Data Collection

A thin plate (0.80 x 0.16 x 0.02 mm) was selected under a stereo-microscope while immersed in Fluorolube oil to avoid possible reaction with air. The crystal was removed from the oil using a tapered glass fiber that also served to hold the crystal for data collection. The crystal was mounted and centered on a Bruker SMART APEX system at 100 K. Rotation and still images showed the diffractions to be sharp. Frames separated in reciprocal space were obtained and provided an orientation matrix and initial cell parameters. Final cell parameters were obtained from the full data set.

A "full sphere" data set was obtained which samples approximately all of reciprocal space to a resolution of 0.75 Å using 0.3^{o} steps in ω using 10 second integration times for each frame. Data collection was made at 100 K. Integration of intensities and refinement of cell parameters were done using SAINT [1]. Absorption corrections were applied using SADABS [1] based on redundant diffractions.

Structure solution and refinement

The space group was determined as $P2_1/c$ based on systematic absences and intensity statistics. Direct methods were used to locate the Pd and many C atoms from the E-map. Repeated difference Fourier maps allowed recognition of all expected P, S, C, N, O and Li atoms. Following anisotropic refinement of all non-H atoms, ideal H-atom positions were calculated. Final refinement was anisotropic for all non-H atoms, and isotropic-riding for H atoms. CH_2Cl_2 solvent is present and refined to an occupancy of 0.78 although the C50 atom could not be refined isotropically. Carbon atoms C27 to C35 showed increasing positional disorder away from the attached atom C27. This disorder affected the entire molecule so all thermal parameters are large and the R value reflects this disorder. Bond lengths between carbon atoms C27 to C35 are poorly defined due to disorder. All ORTEP diagrams have been drawn with 50% probability ellipsoids.

Equations of interest:

$R_{int} = \Sigma \mid F_o^2 - \langle F_o^2 \rangle \mid / \Sigma \mid F_o^2 \mid$ $\quad$ $R1 = \Sigma \mid \mid F_o \mid - \mid F_c \mid \mid / \Sigma \mid F_o \mid$

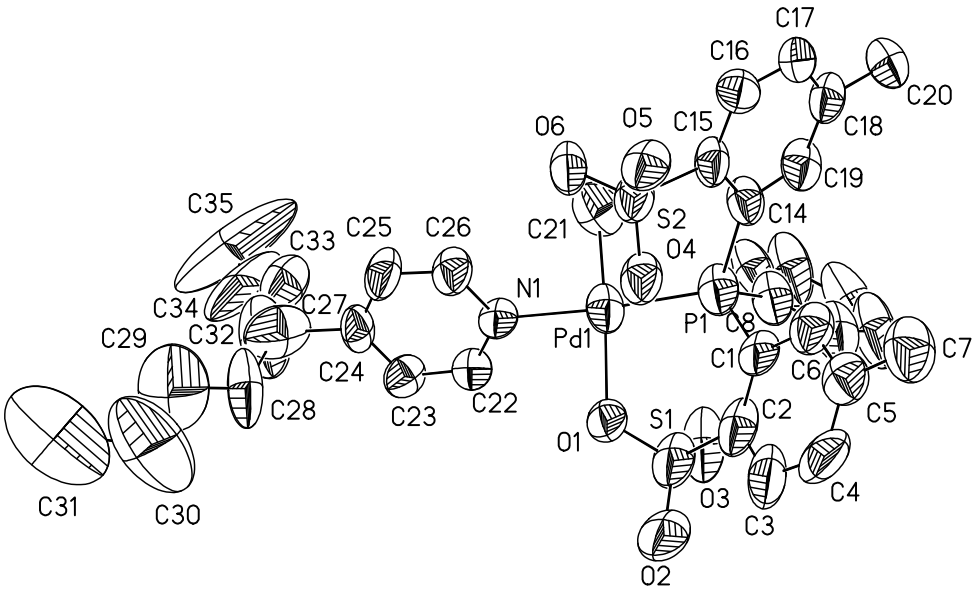
$wR2 = [\Sigma [w (F_o^2 - F_c^2)^2] / \Sigma [w (F_o^2)^2]]^{1/2}$ $\quad$ $GooF = S = [\Sigma [w (F_o^2 - F_c^2)^2] / (n-p)^{1/2}$

where: $w = q / \sigma^2 (F_o^2) + (aP)^2 + bP$; $\quad$ n = number of independent reflections;

q, a, b, P as defined in [1] $\quad$ p = number of parameters refined.

References

[1] All software and sources of scattering factors are contained in the SHELXTL (version 5.1) program library (G. Sheldrick, Bruker Analytical X-ray Systems, Madison, WI).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O6
O5
C15
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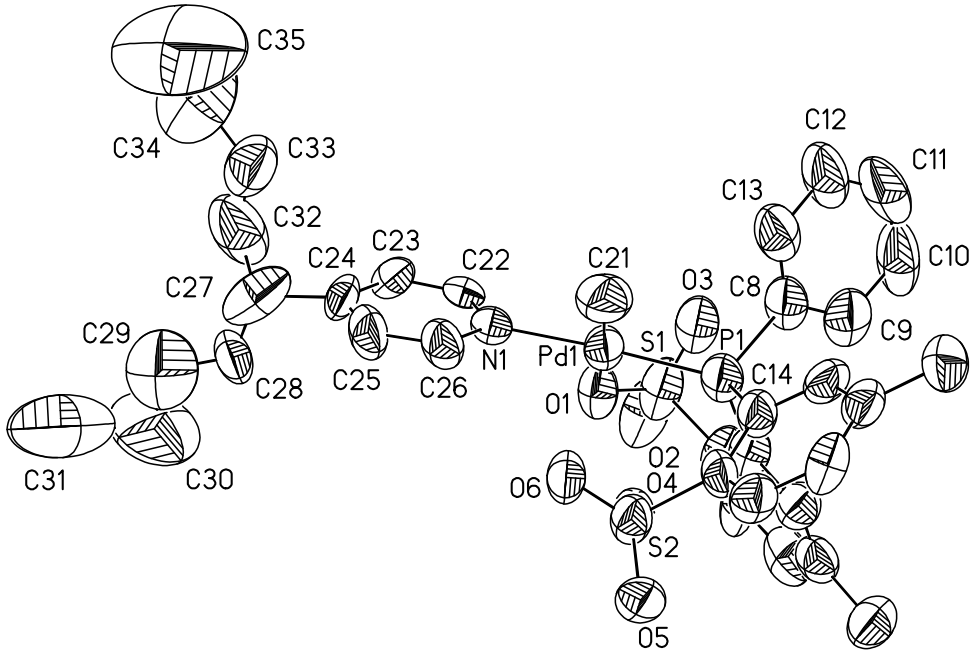
C19
C35
C33
C25
C26
C21
S2
C14
O4
C34
C27
N1
P1
C8
C29
C32
Pd1
C1
C6
C7
C24
C28
C23
C22
C2
C5
O1
S1
C31
C30
O3
C4
C3
O2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S1
P1
C9
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O1
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C31
C30
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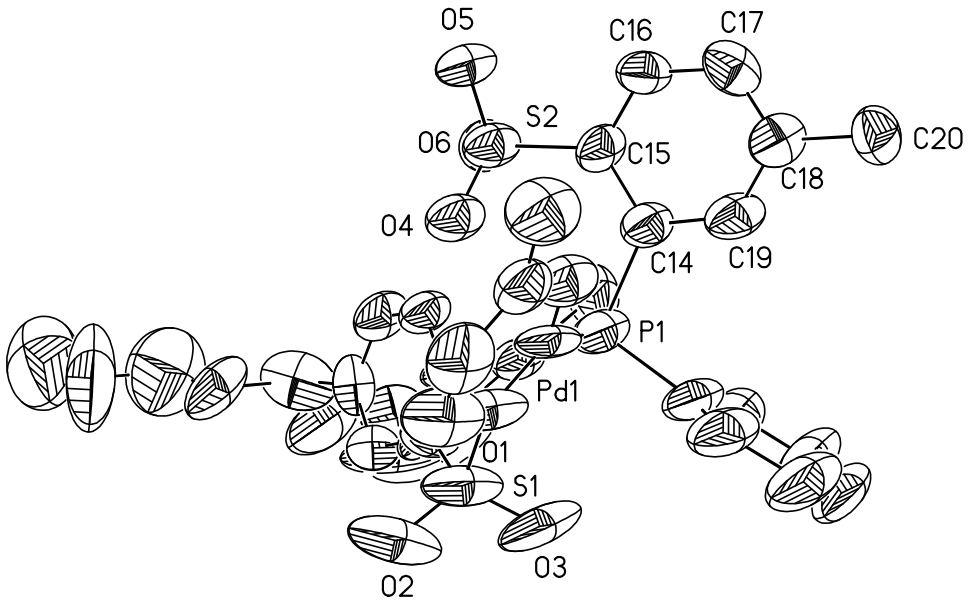
O4
S2
O5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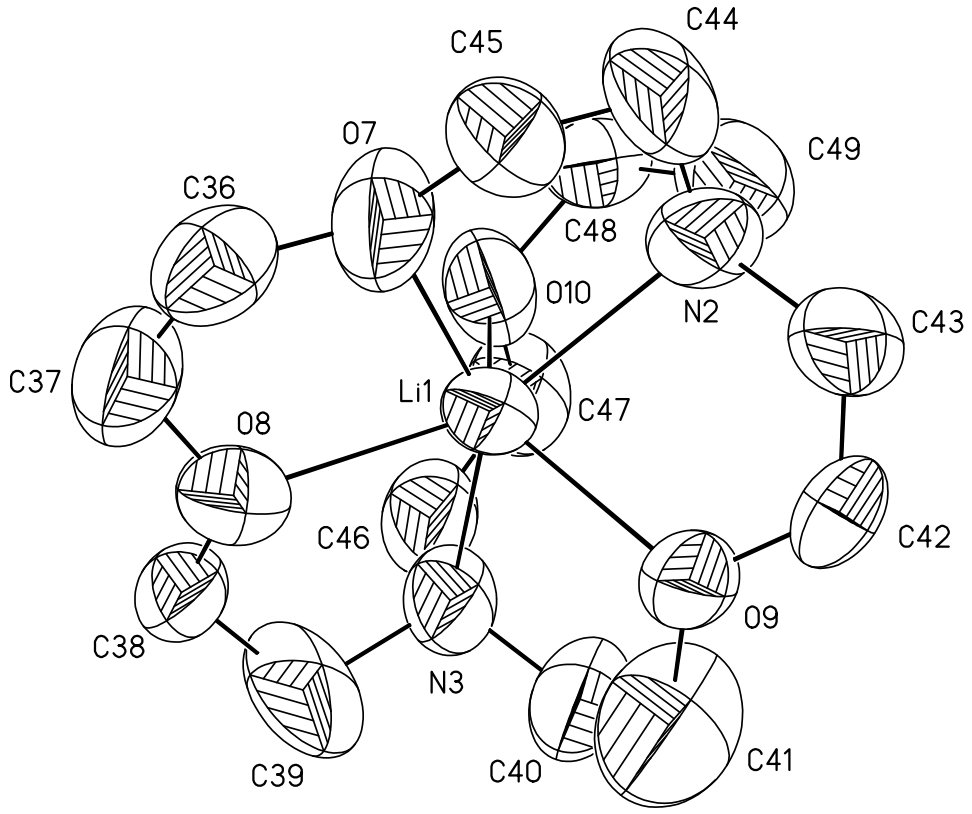
C20
C18
O4
C14
C19
P1
Pd1
O1
S1
O2
O3


C44
C45
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C49
C36
C48
O10
N2
C43
C37
Li1
C47
O8
C46
C42
O9
C38
N3
C39
C40
C41

Table 1. Crystal and structure refinement for Zhon11.

Identification Code	Zhon11	
Empirical formula	$C_{35}H_{43}NO_6PPdS_2 + C_{14}H_{28}N_2O_4Li + CH_2Cl_2$	
Formula weight	1137.21	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space Group	$P2_1/c$	
Unit cell dimensions	a = 10.704(5) Å	α = 90.0 °
	b = 34.391(15) Å	β = 90.933(7) °
	c = 14.836(6) Å	γ = 90.0 °
Volume	5461(4) $Å^3$	
Z	4	
Density (calculated)	1.383 Mg/m^3	
Absorption coefficient	0.576 mm^{-1}	
F(000)	2380	
Crystal size, color, habit	0.80 x 0.16 x 0.02 mm, clear, plate	
Theta range for data collection	1.81 – 25.37 °	
Index ranges	$-12 \le h \le 12$, $-41 \le k \le 41$, $-17 \le l \le 17$	
Reflections collected	51,645	
Independent reflections	(R_{int} = 0.0449)	
Reflections with $I > 4\sigma(F_o)$	9,883	
Flack parameter	3,212	
Absorption correction	SADABS based on redundant diffractions	
Max. and min. transmission	1.0, 0.670	
Refinement method	Full-matrix least squares on F^2	
Weighting scheme	$w = q\,[\sigma^2 (F_o^2) + (aP)^2 + bP]^{-1}$ where:	
	$P = (F_o^2 + 2F_c^2)/3$, a = 0.0833, b = 0.0, q =1	
Data / restraints / parameters	9883 / 0 / 636	
Goodness-of-fit on F^2	0.918	
Final R indices [I > 2 sigma(I)]	R1 =0.0868, wR2 = 0.1780	
R indices (all data)	R1 =0.2418, wR2 = 0.2595	
Largest diff. peak and hole	0.632, -0.717 $eÅ^{-3}$	

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for Zhon11. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	SOF
C(1)	4860(13)	3967(3)	5276(7)	72(4)	
C(2)	3962(18)	3814(3)	5852(8)	91(5)	
C(3)	2858(19)	3994(4)	5933(9)	113(6)	
C(4)	2620(14)	4347(5)	5513(10)	101(5)	
C(5)	3512(15)	4498(4)	4933(8)	77(4)	
C(6)	4631(14)	4308(3)	4825(7)	78(4)	
C(7)	3252(13)	4878(3)	4412(9)	104(5)	
C(8)	7338(16)	3884(4)	6028(8)	88(4)	
C(9)	6996(16)	4204(4)	6519(8)	109(5)	
C(10)	7880(20)	4343(5)	7182(11)	158(10)	
C(11)	8980(20)	4156(6)	7309(12)	160(11)	
C(12)	9298(19)	3847(5)	6820(11)	145(8)	
C(13)	8467(17)	3721(4)	6198(9)	106(5)	
C(14)	6978(12)	3963(3)	4132(7)	69(3)	
C(15)	6580(11)	3901(3)	3218(7)	65(3)	
C(16)	7150(11)	4106(3)	2544(7)	68(3)	
C(17)	8094(12)	4374(3)	2732(9)	76(4)	
C(18)	8489(12)	4433(3)	3592(9)	71(4)	
C(19)	7942(12)	4230(3)	4260(8)	74(4)	
C(20)	9546(11)	4722(3)	3786(8)	82(4)	
C(21)	7809(10)	3050(3)	4409(9)	98(4)	
C(22)	5700(9)	2240(3)	5515(7)	55(3)	
C(23)	5576(10)	1850(3)	5407(8)	68(3)	
C(24)	5719(11)	1691(3)	4567(10)	71(4)	
C(25)	5996(12)	1945(4)	3878(8)	86(4)	
C(26)	6108(11)	2324(3)	4065(7)	76(4)	
C(27)	5440(19)	1264(5)	4261(14)	133(7)	
C(28)	3990(19)	1195(4)	4213(10)	129(7)	
C(29)	3620(30)	864(7)	3802(18)	235(11)	
C(30)	2240(20)	864(9)	3780(20)	279(18)	
C(31)	2080(20)	398(8)	3330(20)	297(17)	
C(32)	6120(30)	1039(6)	4751(12)	183(11)	
C(33)	7534(18)	1058(4)	4725(12)	121(6)	
C(34)	8200(30)	656(8)	5081(12)	251(17)	
C(35)	9130(40)	565(15)	4880(20)	480(40)	
C(36)	-1612(13)	2528(4)	1960(8)	86(4)	
C(37)	-1065(15)	2174(4)	2343(10)	112(5)	
C(38)	224(13)	1967(3)	3532(8)	86(4)	
C(39)	968(15)	2106(4)	4263(11)	136(6)	
C(40)	2050(20)	2681(4)	4760(10)	152(8)	
C(41)	1290(20)	2964(5)	4958(13)	190(10)	
C(42)	1089(15)	3519(4)	4035(9)	109(5)	
C(43)	714(14)	3665(3)	3164(9)	103(5)	
C(44)	17(19)	3453(4)	1692(12)	156(8)	
C(45)	-1129(12)	3194(4)	1743(9)	86(4)	
C(46)	2870(19)	2317(4)	3524(11)	127(6)	
C(47)	3337(15)	2596(4)	2932(11)	117(6)	
C(48)	2533(12)	3044(4)	1762(7)	83(4)	

C(49)	2142(17)	3405(4)	2114(11)	127(6)	
C(50)	3590(20)	4604(11)	1740(20)	290(20)	0.78
Cl(1)	4573(8)	4865(2)	1734(7)	244(5)	0.78
Cl(2)	2086(7)	4595(1)	1719(5)	161(3)	0.78
Li(1)	656(19)	2801(5)	3012(12)	71(6)	
N(1)	5954(8)	2484(2)	4862(5)	56(2)	
N(2)	829(12)	3401(3)	2427(7)	83(3)	
N(3)	1765(13)	2446(3)	4003(8)	90(4)	
O(1)	4368(7)	3071(2)	5778(4)	79(2)	
O(2)	3008(11)	3304(3)	6906(6)	130(4)	
O(3)	5219(11)	3434(2)	7011(5)	128(4)	
O(4)	4581(8)	3539(2)	3650(5)	79(2)	
O(5)	4834(7)	3756(2)	2117(4)	73(2)	
O(6)	6036(7)	3208(2)	2666(5)	76(2)	
O(7)	-677(10)	2822(3)	1927(6)	115(4)	
O(8)	-404(9)	2257(2)	3089(6)	86(3)	
O(9)	752(8)	3159(2)	4176(5)	78(2)	
O(10)	2251(9)	2711(2)	2296(6)	98(3)	
P(1)	6342(4)	3713(1)	5117(2)	77(1)	
Pd(1)	6136(1)	3080(1)	5052(1)	70(1)	
S(1)	4162(5)	3372(1)	6456(2)	105(2)	
S(2)	5399(3)	3566(1)	2896(2)	71(1)	

Table 3. Bond lengths [Å] and angles [°] for Zhon11.

C(1)-C(6)	1.369(14)	C(34)-C(35)	1.09(4)
C(1)-C(2)	1.399(17)	C(36)-O(7)	1.424(14)
C(1)-P(1)	1.831(13)	C(36)-C(37)	1.464(15)
C(2)-C(3)	1.340(19)	C(37)-O(8)	1.334(13)
C(2)-S(1)	1.778(12)	C(38)-O(8)	1.365(12)
C(3)-C(4)	1.388(18)	C(38)-C(39)	1.417(16)
C(4)-C(5)	1.396(17)	C(39)-N(3)	1.504(16)
C(5)-C(6)	1.375(16)	C(40)-C(41)	1.31(2)
C(5)-C(7)	1.542(16)	C(40)-N(3)	1.413(15)
C(8)-C(13)	1.352(18)	C(41)-O(9)	1.452(16)
C(8)-C(9)	1.373(16)	C(42)-O(9)	1.309(13)
C(8)-P(1)	1.805(13)	C(42)-C(43)	1.436(15)
C(9)-C(10)	1.43(2)	C(43)-N(2)	1.429(14)
C(10)-C(11)	1.35(3)	C(44)-N(2)	1.394(15)
C(11)-C(12)	1.34(3)	C(44)-C(45)	1.520(18)
C(12)-C(13)	1.342(17)	C(45)-O(7)	1.391(13)
C(14)-C(19)	1.392(14)	C(46)-C(47)	1.400(18)
C(14)-C(15)	1.431(13)	C(46)-N(3)	1.459(18)
C(14)-P(1)	1.834(11)	C(47)-O(10)	1.537(15)
C(15)-C(16)	1.374(14)	C(48)-C(49)	1.413(15)
C(15)-S(2)	1.771(11)	C(48)-O(10)	1.428(13)
C(16)-C(17)	1.392(14)	C(49)-N(2)	1.487(16)
C(17)-C(18)	1.354(14)	C(50)-Cl(1)	1.38(2)
C(18)-C(19)	1.354(15)	C(50)-Cl(2)	1.61(2)
C(18)-C(20)	1.530(14)	Li(1)-O(10)	2.05(2)
C(21)-Pd(1)	2.045(12)	Li(1)-O(9)	2.121(19)
C(22)-N(1)	1.313(11)	Li(1)-O(7)	2.14(2)
C(22)-C(23)	1.357(13)	Li(1)-O(8)	2.19(2)
C(23)-C(24)	1.372(15)	Li(1)-N(3)	2.24(2)
C(24)-C(25)	1.381(15)	Li(1)-N(2)	2.25(2)
C(24)-C(27)	1.56(2)	N(1)-Pd(1)	2.077(8)
C(25)-C(26)	1.336(14)	O(1)-S(1)	1.462(7)
C(26)-N(1)	1.318(12)	O(1)-Pd(1)	2.192(8)
C(27)-C(32)	1.28(2)	O(2)-S(1)	1.432(10)
C(27)-C(28)	1.57(2)	O(3)-S(1)	1.405(10)
C(28)-C(29)	1.35(2)	O(4)-S(2)	1.435(8)
C(29)-C(30)	1.48(3)	O(5)-S(2)	1.451(7)
C(30)-C(31)	1.75(3)	O(6)-S(2)	1.450(7)
C(32)-C(33)	1.51(2)	P(1)-Pd(1)	2.192(3)
C(33)-C(34)	1.64(3)		

C(6)-C(1)-C(2)	120.1(13)	C(9)-C(8)-P(1)	120.0(13)
C(6)-C(1)-P(1)	119.6(11)	C(8)-C(9)-C(10)	116.9(16)
C(2)-C(1)-P(1)	120.3(10)	C(11)-C(10)-C(9)	120.1(19)
C(3)-C(2)-C(1)	119.8(13)	C(12)-C(11)-C(10)	122.0(19)
C(3)-C(2)-S(1)	116.6(14)	C(11)-C(12)-C(13)	117(2)
C(1)-C(2)-S(1)	123.5(13)	C(12)-C(13)-C(8)	125.2(17)
C(2)-C(3)-C(4)	121.3(16)	C(19)-C(14)-C(15)	115.8(10)
C(3)-C(4)-C(5)	118.6(15)	C(19)-C(14)-P(1)	118.9(9)
C(6)-C(5)-C(4)	120.1(13)	C(15)-C(14)-P(1)	125.3(9)
C(6)-C(5)-C(7)	119.7(14)	C(16)-C(15)-C(14)	119.0(10)
C(4)-C(5)-C(7)	120.3(15)	C(16)-C(15)-S(2)	117.4(8)
C(1)-C(6)-C(5)	119.9(13)	C(14)-C(15)-S(2)	123.5(9)
C(13)-C(8)-C(9)	118.5(13)	C(15)-C(16)-C(17)	121.5(11)
C(13)-C(8)-P(1)	121.4(12)	C(18)-C(17)-C(16)	120.2(12)

C(19)-C(18)-C(17)	118.7(12)	C(22)-N(1)-Pd(1)	123.4(7)
C(19)-C(18)-C(20)	121.7(11)	C(26)-N(1)-Pd(1)	121.5(7)
C(17)-C(18)-C(20)	119.6(12)	C(44)-N(2)-C(43)	117.1(12)
C(18)-C(19)-C(14)	124.7(11)	C(44)-N(2)-C(49)	109.6(13)
N(1)-C(22)-C(23)	124.4(10)	C(43)-N(2)-C(49)	109.0(12)
C(22)-C(23)-C(24)	119.4(11)	C(44)-N(2)-Li(1)	111.5(10)
C(23)-C(24)-C(25)	116.6(10)	C(43)-N(2)-Li(1)	106.2(8)
C(23)-C(24)-C(27)	128.0(13)	C(49)-N(2)-Li(1)	102.4(10)
C(25)-C(24)-C(27)	114.9(13)	C(40)-N(3)-C(46)	113.1(14)
C(26)-C(25)-C(24)	118.9(11)	C(40)-N(3)-C(39)	111.0(13)
N(1)-C(26)-C(25)	125.6(11)	C(46)-N(3)-C(39)	110.8(12)
C(32)-C(27)-C(24)	107.4(19)	C(40)-N(3)-Li(1)	108.6(9)
C(32)-C(27)-C(28)	119.1(19)	C(46)-N(3)-Li(1)	105.8(10)
C(24)-C(27)-C(28)	109.8(11)	C(39)-N(3)-Li(1)	107.2(10)
C(29)-C(28)-C(27)	115(2)	S(1)-O(1)-Pd(1)	118.0(5)
C(28)-C(29)-C(30)	107(3)	C(45)-O(7)-C(36)	114.6(10)
C(29)-C(30)-C(31)	96(3)	C(45)-O(7)-Li(1)	114.0(9)
C(27)-C(32)-C(33)	121(2)	C(36)-O(7)-Li(1)	114.3(9)
C(32)-C(33)-C(34)	112.4(19)	C(37)-O(8)-C(38)	119.5(10)
C(35)-C(34)-C(33)	123(4)	C(37)-O(8)-Li(1)	114.0(9)
O(7)-C(36)-C(37)	109.1(11)	C(38)-O(8)-Li(1)	113.4(9)
O(8)-C(37)-C(36)	110.3(11)	C(42)-O(9)-C(41)	117.1(12)
O(8)-C(38)-C(39)	112.9(11)	C(42)-O(9)-Li(1)	115.4(9)
C(38)-C(39)-N(3)	112.3(12)	C(41)-O(9)-Li(1)	113.4(10)
C(41)-C(40)-N(3)	118.4(17)	C(48)-O(10)-C(47)	112.5(10)
C(40)-C(41)-O(9)	114.0(16)	C(48)-O(10)-Li(1)	110.7(9)
O(9)-C(42)-C(43)	113.6(12)	C(47)-O(10)-Li(1)	110.4(10)
N(2)-C(43)-C(42)	116.2(10)	C(8)-P(1)-C(1)	104.5(7)
N(2)-C(44)-C(45)	112.2(12)	C(8)-P(1)-C(14)	102.8(6)
O(7)-C(45)-C(44)	105.7(11)	C(1)-P(1)-C(14)	102.3(5)
C(47)-C(46)-N(3)	113.3(14)	C(8)-P(1)-Pd(1)	114.5(5)
C(46)-C(47)-O(10)	106.7(13)	C(1)-P(1)-Pd(1)	113.2(4)
C(49)-C(48)-O(10)	115.7(11)	C(14)-P(1)-Pd(1)	117.9(4)
C(48)-C(49)-N(2)	113.2(13)	C(21)-Pd(1)-N(1)	88.2(4)
Cl(1)-C(50)-Cl(2)	140(3)	C(21)-Pd(1)-P(1)	88.9(4)
O(10)-Li(1)-O(9)	118.7(10)	N(1)-Pd(1)-P(1)	174.7(2)
O(10)-Li(1)-O(7)	99.6(8)	C(21)-Pd(1)-O(1)	176.0(4)
O(9)-Li(1)-O(7)	128.0(10)	N(1)-Pd(1)-O(1)	88.5(3)
O(10)-Li(1)-O(8)	109.6(9)	P(1)-Pd(1)-O(1)	94.5(2)
O(9)-Li(1)-O(8)	118.1(9)	O(3)-S(1)-O(2)	116.4(6)
O(7)-Li(1)-O(8)	74.3(7)	O(3)-S(1)-O(1)	112.5(6)
O(10)-Li(1)-N(3)	79.7(9)	O(2)-S(1)-O(1)	110.3(6)
O(9)-Li(1)-N(3)	76.3(7)	O(3)-S(1)-C(2)	104.7(6)
O(7)-Li(1)-N(3)	148.9(10)	O(2)-S(1)-C(2)	106.0(8)
O(8)-Li(1)-N(3)	76.7(7)	O(1)-S(1)-C(2)	106.0(5)
O(10)-Li(1)-N(2)	82.1(7)	O(4)-S(2)-O(6)	115.1(4)
O(9)-Li(1)-N(2)	77.2(7)	O(4)-S(2)-O(5)	113.5(5)
O(7)-Li(1)-N(2)	74.6(7)	O(6)-S(2)-O(5)	112.7(4)
O(8)-Li(1)-N(2)	148.2(11)	O(4)-S(2)-C(15)	105.9(5)
N(3)-Li(1)-N(2)	135.1(10)	O(6)-S(2)-C(15)	106.2(5)
C(22)-N(1)-C(26)	115.2(9)	O(5)-S(2)-C(15)	102.0(5)

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for Zhon11. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+ ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	132(12)	61(8)	22(6)	-4(5)	8(7)	-1(8)
C(2)	182(17)	52(8)	38(7)	0(6)	-2(9)	16(10)
C(3)	210(20)	53(9)	78(10)	-15(8)	13(12)	-7(11)
C(4)	104(13)	110(13)	89(10)	-55(10)	15(10)	3(11)
C(5)	94(12)	78(9)	58(8)	-14(7)	-9(9)	-10(9)
C(6)	107(12)	67(9)	59(8)	-6(7)	-5(8)	6(8)
C(7)	136(13)	73(9)	103(10)	10(8)	-11(9)	7(9)
C(8)	153(15)	67(9)	42(7)	5(7)	-23(9)	-19(9)
C(9)	192(17)	75(9)	60(8)	18(8)	-26(10)	-17(10)
C(10)	310(30)	88(13)	74(11)	6(9)	-59(16)	-69(16)
C(11)	260(30)	132(18)	88(13)	50(12)	-105(16)	-101(18)
C(12)	240(20)	96(12)	95(12)	11(10)	-84(14)	-54(14)
C(13)	155(16)	79(10)	84(10)	25(8)	-38(11)	-43(11)
C(14)	103(10)	49(7)	53(7)	3(6)	-13(7)	-10(7)
C(15)	94(10)	46(6)	54(7)	-9(6)	-14(7)	-8(6)
C(16)	91(10)	60(7)	52(7)	8(6)	1(7)	-1(7)
C(17)	99(11)	44(7)	84(9)	-1(6)	22(8)	1(7)
C(18)	94(11)	46(7)	72(9)	-7(7)	-8(8)	13(7)
C(19)	111(11)	52(7)	59(8)	11(6)	-19(8)	11(7)
C(20)	88(10)	65(7)	95(9)	5(7)	-5(8)	-18(7)
C(21)	71(9)	96(10)	127(11)	13(9)	-13(8)	-3(8)
C(22)	54(8)	66(7)	45(6)	1(6)	-18(6)	1(6)
C(23)	79(9)	57(8)	67(8)	6(6)	2(7)	19(7)
C(24)	55(8)	38(7)	121(11)	-13(7)	2(8)	8(6)
C(25)	122(12)	70(9)	66(8)	-26(8)	-10(8)	-5(9)
C(26)	109(11)	70(8)	50(7)	-7(6)	-10(7)	-10(8)
C(27)	141(18)	120(15)	140(16)	29(13)	34(14)	63(14)
C(28)	200(20)	62(9)	120(13)	-10(9)	-81(14)	-23(12)
C(29)	240(30)	190(20)	270(30)	-20(20)	-20(30)	0(20)
C(30)	130(20)	300(40)	410(40)	20(30)	-80(30)	-80(30)
C(31)	200(30)	310(40)	380(40)	150(30)	-80(30)	-20(30)
C(32)	290(30)	130(17)	122(16)	23(12)	-90(20)	-60(20)
C(33)	152(16)	95(12)	115(13)	-15(10)	6(13)	30(12)
C(34)	450(60)	250(30)	51(11)	-25(14)	50(20)	110(30)
C(35)	370(60)	820(90)	230(40)	-210(50)	10(30)	350(60)
C(36)	91(11)	89(10)	78(9)	-9(8)	-18(8)	19(9)
C(37)	139(15)	81(10)	115(12)	-19(9)	-24(11)	-3(10)
C(38)	129(12)	62(8)	65(8)	2(7)	-24(8)	-9(9)
C(39)	171(17)	84(10)	152(15)	65(11)	-56(13)	-14(11)
C(40)	300(30)	65(10)	89(11)	8(9)	-88(14)	11(13)
C(41)	300(30)	111(14)	158(17)	8(14)	-87(18)	79(17)
C(42)	184(16)	70(9)	73(10)	-34(8)	30(10)	7(10)
C(43)	166(15)	63(8)	81(10)	6(8)	27(10)	30(9)
C(44)	250(20)	67(10)	147(15)	41(10)	-94(16)	-20(12)
C(45)	98(11)	72(9)	89(9)	10(7)	-4(8)	3(8)
C(46)	180(20)	85(12)	111(13)	3(10)	-55(14)	-14(13)
C(47)	138(15)	70(9)	140(14)	6(10)	-31(12)	33(10)
C(48)	91(10)	93(10)	63(8)	3(8)	2(7)	8(9)

C(49)	170(19)	93(12)	118(13)	3(10)	47(13)	2(12)
C(50)	68(19)	480(60)	330(40)	190(40)	90(20)	-90(30)
Cl(1)	200(9)	104(5)	426(14)	76(7)	-17(9)	-8(5)
Cl(2)	217(7)	79(3)	186(6)	2(4)	-19(5)	-30(4)
Li(1)	83(15)	73(12)	57(12)	6(10)	8(11)	-17(11)
N(1)	80(7)	60(5)	27(5)	4(4)	-10(5)	1(5)
N(2)	101(9)	85(7)	64(7)	-5(6)	26(7)	13(7)
N(3)	126(11)	52(7)	93(9)	5(6)	-23(8)	13(7)
O(1)	121(7)	64(5)	52(4)	-7(4)	21(4)	-13(5)
O(2)	228(12)	88(7)	77(6)	10(5)	72(8)	7(7)
O(3)	262(13)	70(6)	51(5)	7(4)	-59(7)	-8(7)
O(4)	119(7)	63(5)	53(5)	-7(4)	-6(5)	-8(5)
O(5)	102(6)	74(5)	44(4)	1(4)	-8(4)	9(5)
O(6)	107(7)	47(4)	75(5)	-7(4)	-9(5)	-7(4)
O(7)	148(9)	64(6)	131(8)	-1(6)	-64(7)	-3(6)
O(8)	100(7)	87(6)	71(6)	13(5)	-5(5)	-6(5)
O(9)	108(7)	60(5)	65(5)	-6(4)	11(5)	13(5)
O(10)	108(8)	73(6)	115(7)	-3(6)	18(6)	-17(5)
P(1)	121(3)	62(2)	48(2)	2(2)	-17(2)	-8(2)
Pd(1)	109(1)	52(1)	50(1)	8(1)	-16(1)	-6(1)
S(1)	208(5)	65(2)	44(2)	0(2)	20(3)	-1(3)
S(2)	110(3)	54(2)	50(2)	-3(2)	-5(2)	-1(2)

Table 5. Hydrogen coordinates [x 10^4] and isotropic displacement parameters [$Å^2$ x 10^3] for Zhon11.

	x	y	z	U(eq)
H(3)	2227	3877	6285	135
H(4)	1865	4484	5619	121
H(6)	5243	4413	4438	93
H(7A)	2777	4820	3858	156
H(7B)	4046	5002	4258	156
H(7C)	2767	5055	4788	156
H(9)	6211	4327	6425	131
H(10)	7689	4566	7532	189
H(11)	9546	4249	7761	192
H(12)	10080	3721	6908	173
H(13)	8691	3501	5850	127
H(16)	6895	4063	1935	81
H(17)	8461	4515	2255	91
H(19)	8237	4272	4859	89
H(20A)	9611	4770	4436	124
H(20B)	9369	4967	3472	124
H(20C)	10336	4615	3573	124
H(21A)	8366	2870	4733	147
H(21B)	8191	3309	4395	147
H(21C)	7672	2957	3791	147
H(22)	5597	2344	6102	67
H(23)	5391	1689	5907	81
H(25)	6106	1852	3282	103
H(26)	6317	2491	3582	92
H(27)	5749	1240	3631	160
H(28A)	3668	1194	4835	154
H(28B)	3597	1417	3891	154
H(29A)	3944	636	4139	282
H(29B)	3949	854	3181	282
H(30A)	1884	1068	3382	335
H(30B)	1879	886	4391	335
H(31A)	2746	351	2898	446
H(31B)	1265	376	3014	446
H(31C)	2125	205	3812	446
H(32A)	5881	768	4598	219
H(32B)	5882	1082	5385	219
H(33A)	7829	1277	5106	145
H(33B)	7794	1110	4099	145
H(34A)	8207	668	5748	302
H(34B)	7622	441	4911	302
H(35A)	9241	620	4242	714
H(35B)	9225	285	4989	714
H(35C)	9756	707	5241	714
H(36A)	-1942	2475	1345	103
H(36B)	-2312	2617	2336	103
H(37A)	-1737	1988	2489	134
H(37B)	-515	2050	1896	134
H(38A)	767	1830	3101	103
H(38B)	-387	1776	3761	103

H(39A)	1513	1893	4486	164
H(39B)	416	2184	4761	164
H(40A)	2120	2508	5293	182
H(40B)	2893	2794	4669	182
H(41A)	1755	3158	5327	228
H(41B)	611	2859	5328	228
H(42A)	2010	3538	4096	130
H(42B)	722	3686	4505	130
H(43A)	-169	3748	3195	124
H(43B)	1219	3898	3034	124
H(44A)	466	3396	1129	188
H(44B)	-252	3728	1669	188
H(45A)	-1686	3282	2228	104
H(45B)	-1602	3197	1164	104
H(46A)	3532	2248	3971	152
H(46B)	2658	2079	3179	152
H(47A)	4036	2487	2584	140
H(47B)	3644	2826	3271	140
H(48A)	3449	3054	1680	99
H(48B)	2141	3010	1159	99
H(49A)	2226	3607	1643	152
H(49B)	2700	3477	2626	152
H(50A)	3795	4445	2275	351
H(50B)	3795	4434	1219	351

Table 6. Torsion angles [°] for Zhon11.

C(6)-C(1)-C(2)-C(3)	2.5(18)	C(42)-C(43)-N(2)-C(49)	-82.5(16)
P(1)-C(1)-C(2)-C(3)	-177.1(10)	C(42)-C(43)-N(2)-Li(1)	27.2(17)
C(6)-C(1)-C(2)-S(1)	179.2(9)	C(48)-C(49)-N(2)-C(44)	-81.9(15)
P(1)-C(1)-C(2)-S(1)	-0.4(14)	C(48)-C(49)-N(2)-C(43)	148.7(12)
C(1)-C(2)-C(3)-C(4)	-5(2)	C(48)-C(49)-N(2)-Li(1)	36.5(14)
S(1)-C(2)-C(3)-C(4)	177.9(9)	O(10)-Li(1)-N(2)-C(44)	101.2(12)
C(2)-C(3)-C(4)-C(5)	6(2)	O(9)-Li(1)-N(2)-C(44)	-137.0(12)
C(3)-C(4)-C(5)-C(6)	-3.6(18)	O(7)-Li(1)-N(2)-C(44)	-1.1(12)
C(3)-C(4)-C(5)-C(7)	176.5(11)	O(8)-Li(1)-N(2)-C(44)	-14(2)
C(2)-C(1)-C(6)-C(5)	-0.4(16)	N(3)-Li(1)-N(2)-C(44)	167.9(15)
P(1)-C(1)-C(6)-C(5)	179.2(8)	O(10)-Li(1)-N(2)-C(43)	-130.2(10)
C(4)-C(5)-C(6)-C(1)	1.0(17)	O(9)-Li(1)-N(2)-C(43)	-8.3(11)
C(7)-C(5)-C(6)-C(1)	-179.1(10)	O(7)-Li(1)-N(2)-C(43)	127.5(10)
C(13)-C(8)-C(9)-C(10)	0.2(19)	O(8)-Li(1)-N(2)-C(43)	115.0(19)
P(1)-C(8)-C(9)-C(10)	-174.9(10)	N(3)-Li(1)-N(2)-C(43)	-63.4(17)
C(8)-C(9)-C(10)-C(11)	-1(2)	O(10)-Li(1)-N(2)-C(49)	-15.9(10)
C(9)-C(10)-C(11)-C(12)	1(3)	O(9)-Li(1)-N(2)-C(49)	106.0(10)
C(10)-C(11)-C(12)-C(13)	-1(3)	O(7)-Li(1)-N(2)-C(49)	-118.2(10)
C(11)-C(12)-C(13)-C(8)	0(2)	O(8)-Li(1)-N(2)-C(49)	-130.7(19)
C(9)-C(8)-C(13)-C(12)	0(2)	N(3)-Li(1)-N(2)-C(49)	50.8(16)
P(1)-C(8)-C(13)-C(12)	175.3(11)	C(41)-C(40)-N(3)-C(46)	145.1(19)
C(19)-C(14)-C(15)-C(16)	-0.6(16)	C(41)-C(40)-N(3)-C(39)	-89.7(19)
P(1)-C(14)-C(15)-C(16)	-179.3(9)	C(41)-C(40)-N(3)-Li(1)	28(2)
C(19)-C(14)-C(15)-S(2)	178.3(8)	C(47)-C(46)-N(3)-C(40)	-81.6(15)
P(1)-C(14)-C(15)-S(2)	-0.3(15)	C(47)-C(46)-N(3)-C(39)	153.1(12)
C(14)-C(15)-C(16)-C(17)	-0.7(17)	C(47)-C(46)-N(3)-Li(1)	37.2(16)
S(2)-C(15)-C(16)-C(17)	-179.6(9)	C(38)-C(39)-N(3)-C(40)	154.2(14)
C(15)-C(16)-C(17)-C(18)	1.3(17)	C(38)-C(39)-N(3)-C(46)	-79.3(16)
C(16)-C(17)-C(18)-C(19)	-0.5(17)	C(38)-C(39)-N(3)-Li(1)	35.7(17)
C(16)-C(17)-C(18)-C(20)	178.7(10)	O(10)-Li(1)-N(3)-C(40)	114.2(13)
C(17)-C(18)-C(19)-C(14)	-0.8(18)	O(9)-Li(1)-N(3)-C(40)	-9.0(13)
C(20)-C(18)-C(19)-C(14)	-180.0(10)	O(7)-Li(1)-N(3)-C(40)	-154(2)
C(15)-C(14)-C(19)-C(18)	1.4(17)	O(8)-Li(1)-N(3)-C(40)	-132.7(13)
P(1)-C(14)-C(19)-C(18)	-179.9(9)	N(2)-Li(1)-N(3)-C(40)	46.5(19)
N(1)-C(22)-C(23)-C(24)	0.0(17)	O(10)-Li(1)-N(3)-C(46)	-7.6(10)
C(22)-C(23)-C(24)-C(25)	0.6(17)	O(9)-Li(1)-N(3)-C(46)	-130.7(10)
C(22)-C(23)-C(24)-C(27)	-170.8(13)	O(7)-Li(1)-N(3)-C(46)	84(2)
C(23)-C(24)-C(25)-C(26)	0.0(19)	O(8)-Li(1)-N(3)-C(46)	105.6(10)
C(27)-C(24)-C(25)-C(26)	172.6(13)	N(2)-Li(1)-N(3)-C(46)	-75.2(16)
C(24)-C(25)-C(26)-N(1)	-1(2)	O(10)-Li(1)-N(3)-C(39)	-125.8(11)
C(23)-C(24)-C(27)-C(32)	-59(2)	O(9)-Li(1)-N(3)-C(39)	111.1(11)
C(25)-C(24)-C(27)-C(32)	129.4(19)	O(7)-Li(1)-N(3)-C(39)	-34(3)
C(23)-C(24)-C(27)-C(28)	72(2)	O(8)-Li(1)-N(3)-C(39)	-12.7(11)
C(25)-C(24)-C(27)-C(28)	-99.7(16)	N(2)-Li(1)-N(3)-C(39)	166.5(13)
C(32)-C(27)-C(28)-C(29)	-67(3)	C(44)-C(45)-O(7)-C(36)	-177.1(11)
C(24)-C(27)-C(28)-C(29)	168.3(17)	C(44)-C(45)-O(7)-Li(1)	48.6(14)
C(27)-C(28)-C(29)-C(30)	-177(2)	C(37)-C(36)-O(7)-C(45)	-168.0(11)
C(28)-C(29)-C(30)-C(31)	-175(2)	C(37)-C(36)-O(7)-Li(1)	-33.9(14)
C(24)-C(27)-C(32)-C(33)	-63(3)	O(10)-Li(1)-O(7)-C(45)	-106.7(11)
C(28)-C(27)-C(32)-C(33)	171.7(16)	O(9)-Li(1)-O(7)-C(45)	31.9(16)
C(27)-C(32)-C(33)-C(34)	-158.4(19)	O(8)-Li(1)-O(7)-C(45)	145.5(10)
C(32)-C(33)-C(34)-C(35)	156(4)	N(3)-Li(1)-O(7)-C(45)	167.4(19)
O(7)-C(36)-C(37)-O(8)	47.3(16)	N(2)-Li(1)-O(7)-C(45)	-27.7(11)
O(8)-C(38)-C(39)-N(3)	-48.7(18)	O(10)-Li(1)-O(7)-C(36)	118.9(10)
N(3)-C(40)-C(41)-O(9)	-37(3)	O(9)-Li(1)-O(7)-C(36)	-102.5(13)
O(9)-C(42)-C(43)-N(2)	-40(2)	O(8)-Li(1)-O(7)-C(36)	11.1(10)
N(2)-C(44)-C(45)-O(7)	-49.0(17)	N(3)-Li(1)-O(7)-C(36)	33(2)
N(3)-C(46)-C(47)-O(10)	-55.0(16)	N(2)-Li(1)-O(7)-C(36)	-162.1(9)
O(10)-C(48)-C(49)-N(2)	-47.3(17)	C(36)-C(37)-O(8)-C(38)	-177.5(11)
C(23)-C(22)-N(1)-C(26)	-1.1(16)	C(36)-C(37)-O(8)-Li(1)	-38.7(16)
C(23)-C(22)-N(1)-Pd(1)	179.9(8)	C(39)-C(38)-O(8)-C(37)	174.8(13)
C(25)-C(26)-N(1)-C(22)	1.8(18)	C(39)-C(38)-O(8)-Li(1)	35.8(15)
C(25)-C(26)-N(1)-Pd(1)	-179.2(10)	O(10)-Li(1)-O(8)-C(37)	-79.0(13)
C(45)-C(44)-N(2)-C(43)	-95.8(15)	O(9)-Li(1)-O(8)-C(37)	140.9(12)
C(45)-C(44)-N(2)-C(49)	139.4(14)	O(7)-Li(1)-O(8)-C(37)	15.8(11)
C(45)-C(44)-N(2)-Li(1)	26.8(17)	N(3)-Li(1)-O(8)-C(37)	-152.8(10)
C(42)-C(43)-N(2)-C(44)	152.5(15)	N(2)-Li(1)-O(8)-C(37)	28(2)

O(10)-Li(1)-O(8)-C(38)	62.3(12)	C(2)-C(1)-P(1)-C(14)	167.0(9)
O(9)-Li(1)-O(8)-C(38)	-77.8(13)	C(6)-C(1)-P(1)-Pd(1)	-140.5(8)
O(7)-Li(1)-O(8)-C(38)	157.1(9)	C(2)-C(1)-P(1)-Pd(1)	39.1(10)
N(3)-Li(1)-O(8)-C(38)	-11.5(10)	C(19)-C(14)-P(1)-C(8)	-4.2(11)
N(2)-Li(1)-O(8)-C(38)	169.7(17)	C(15)-C(14)-P(1)-C(8)	174.4(11)
C(43)-C(42)-O(9)-C(41)	168.3(14)	C(19)-C(14)-P(1)-C(1)	104.0(10)
C(43)-C(42)-O(9)-Li(1)	30.9(17)	C(15)-C(14)-P(1)-C(1)	-77.4(10)
C(40)-C(41)-O(9)-C(42)	-112.5(19)	C(19)-C(14)-P(1)-Pd(1)	-131.2(8)
C(40)-C(41)-O(9)-Li(1)	26(2)	C(15)-C(14)-P(1)-Pd(1)	47.5(11)
O(10)-Li(1)-O(9)-C(42)	61.3(15)	C(22)-N(1)-Pd(1)-C(21)	128.8(9)
O(7)-Li(1)-O(9)-C(42)	-70.7(16)	C(26)-N(1)-Pd(1)-C(21)	-50.1(9)
O(8)-Li(1)-O(9)-C(42)	-162.2(11)	C(22)-N(1)-Pd(1)-P(1)	-174(2)
N(3)-Li(1)-O(9)-C(42)	131.2(11)	C(26)-N(1)-Pd(1)-P(1)	7(4)
N(2)-Li(1)-O(9)-C(42)	-12.2(12)	C(22)-N(1)-Pd(1)-O(1)	-49.1(8)
O(10)-Li(1)-O(9)-C(41)	-77.7(15)	C(26)-N(1)-Pd(1)-O(1)	132.0(9)
O(7)-Li(1)-O(9)-C(41)	150.3(14)	C(8)-P(1)-Pd(1)-C(21)	-81.3(7)
O(8)-Li(1)-O(9)-C(41)	58.7(16)	C(1)-P(1)-Pd(1)-C(21)	159.1(5)
N(3)-Li(1)-O(9)-C(41)	-7.8(13)	C(14)-P(1)-Pd(1)-C(21)	39.8(6)
N(2)-Li(1)-O(9)-C(41)	-151.2(12)	C(8)-P(1)-Pd(1)-N(1)	-139(3)
C(49)-C(48)-O(10)-C(47)	-94.1(14)	C(1)-P(1)-Pd(1)-N(1)	102(3)
C(49)-C(48)-O(10)-Li(1)	29.9(15)	C(14)-P(1)-Pd(1)-N(1)	-18(3)
C(46)-C(47)-O(10)-C(48)	169.4(12)	C(8)-P(1)-Pd(1)-O(1)	96.8(6)
C(46)-C(47)-O(10)-Li(1)	45.3(14)	C(1)-P(1)-Pd(1)-O(1)	-22.8(4)
O(9)-Li(1)-O(10)-C(48)	-76.6(12)	C(14)-P(1)-Pd(1)-O(1)	-142.1(5)
O(7)-Li(1)-O(10)-C(48)	67.0(10)	S(1)-O(1)-Pd(1)-C(21)	120(6)
O(8)-Li(1)-O(10)-C(48)	143.6(9)	S(1)-O(1)-Pd(1)-N(1)	153.3(5)
N(3)-Li(1)-O(10)-C(48)	-144.6(8)	S(1)-O(1)-Pd(1)-P(1)	-31.0(5)
N(2)-Li(1)-O(10)-C(48)	-5.8(10)	Pd(1)-O(1)-S(1)-O(3)	-43.9(6)
O(9)-Li(1)-O(10)-C(47)	48.6(13)	Pd(1)-O(1)-S(1)-O(2)	-175.7(5)
O(7)-Li(1)-O(10)-C(47)	-167.8(8)	Pd(1)-O(1)-S(1)-C(2)	69.9(8)
O(8)-Li(1)-O(10)-C(47)	-91.2(10)	C(3)-C(2)-S(1)-O(3)	-122.6(12)
N(3)-Li(1)-O(10)-C(47)	-19.4(9)	C(1)-C(2)-S(1)-O(3)	60.7(11)
N(2)-Li(1)-O(10)-C(47)	119.4(8)	C(3)-C(2)-S(1)-O(2)	1.0(12)
C(13)-C(8)-P(1)-C(1)	171.4(11)	C(1)-C(2)-S(1)-O(2)	-175.7(10)
C(9)-C(8)-P(1)-C(1)	-13.6(12)	C(3)-C(2)-S(1)-O(1)	118.3(11)
C(13)-C(8)-P(1)-C(14)	-82.1(12)	C(1)-C(2)-S(1)-O(1)	-58.5(12)
C(9)-C(8)-P(1)-C(14)	92.9(11)	C(16)-C(15)-S(2)-O(4)	-152.6(9)
C(13)-C(8)-P(1)-Pd(1)	47.1(13)	C(14)-C(15)-S(2)-O(4)	28.4(11)
C(9)-C(8)-P(1)-Pd(1)	-137.9(9)	C(16)-C(15)-S(2)-O(6)	84.6(9)
C(6)-C(1)-P(1)-C(8)	94.3(9)	C(14)-C(15)-S(2)-O(6)	-94.4(10)
C(2)-C(1)-P(1)-C(8)	-86.1(10)	C(16)-C(15)-S(2)-O(5)	-33.7(10)
C(6)-C(1)-P(1)-C(14)	-12.6(10)	C(14)-C(15)-S(2)-O(5)	147.4(9)