Crystal Structure Report for Zhou19

$C_{32}H_{46}N_4O_3PdS + CH_2Cl_2$

Report Prepared for:

Xiaoyuan Zhou and Mr. Richard Jordan

March, 2010

Ian M. Steele (steele@geosci.uchicago.edu)
X-ray Laboratory, Searle B013, 773-834-5861
Department of Chemistry
The University of Chicago
5735 S. Ellis Ave.
Chicago, Il 60637

Crystallographic Experimental Section

Data Collection

An irregular broken fragment (0.12 x 0.12 x 0.08 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. There was considerable difficulty to find a crystal with sharp diffraction spots. Large crystal were always poor, and finally a small crystal was found which was good but not great. 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 0.84 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 P1(bar) based on systematic absences and intensity statistics. Direct methods were used to locate the Pd atom and some C atoms from the E-map. Repeated difference Fourier maps allowed recognition of all expected C, N, O and S atoms. CH_2Cl_2 solvent is present but shows considerable positional disorder; one Cl atom was spit into two with occupancies of 0.41 and 0.59. Two $C\text{-}C_3$ units of the main molecule which are close to the solvent also show considerable disorder, and it is most probable that this is due to interaction with the solvent. Final refinement was anisotropic for all non-H atoms and isotropic-riding for H atoms. No anomalous bond lengths or other thermal parameters were noted. All ORTEP diagrams have been drawn with 50% probability ellipsoids.

Equations of interest:

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

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

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

where: $w = q / \sigma^2 (F_o^2) + (aP)^2 + bP$;

q, a, b, P as defined in [1]

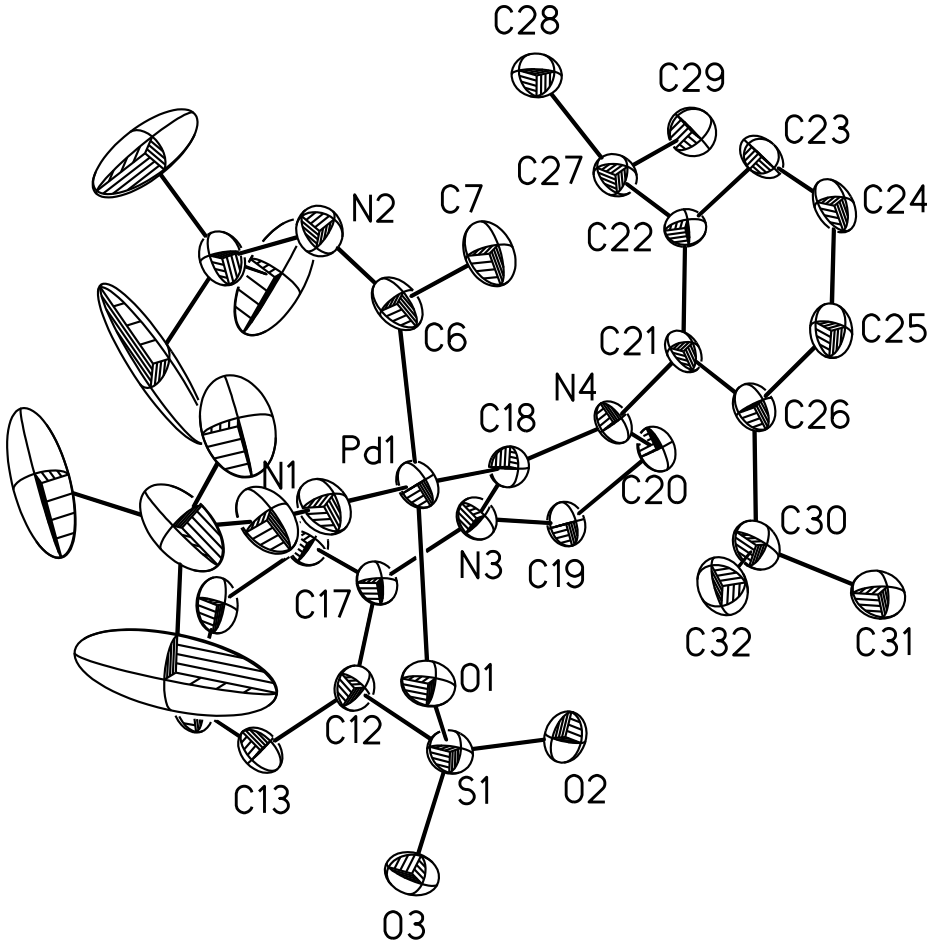
$GooF = S = [\Sigma [w (F_o^2 - F_c^2)^2] / (n-p)^{1/2}$

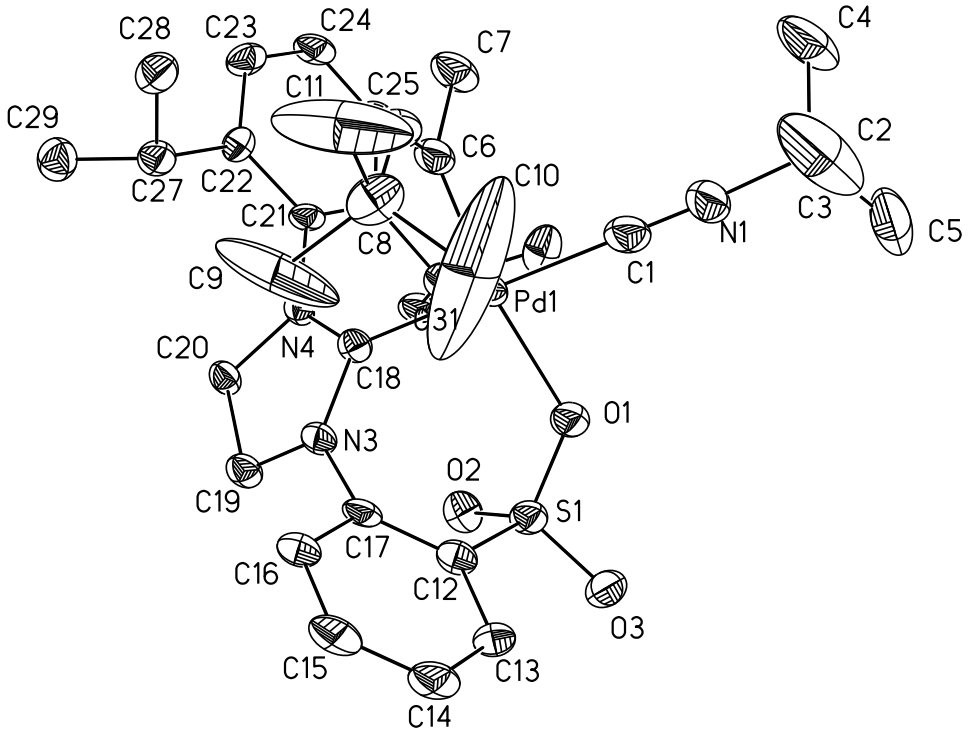
n = number of independent reflections;

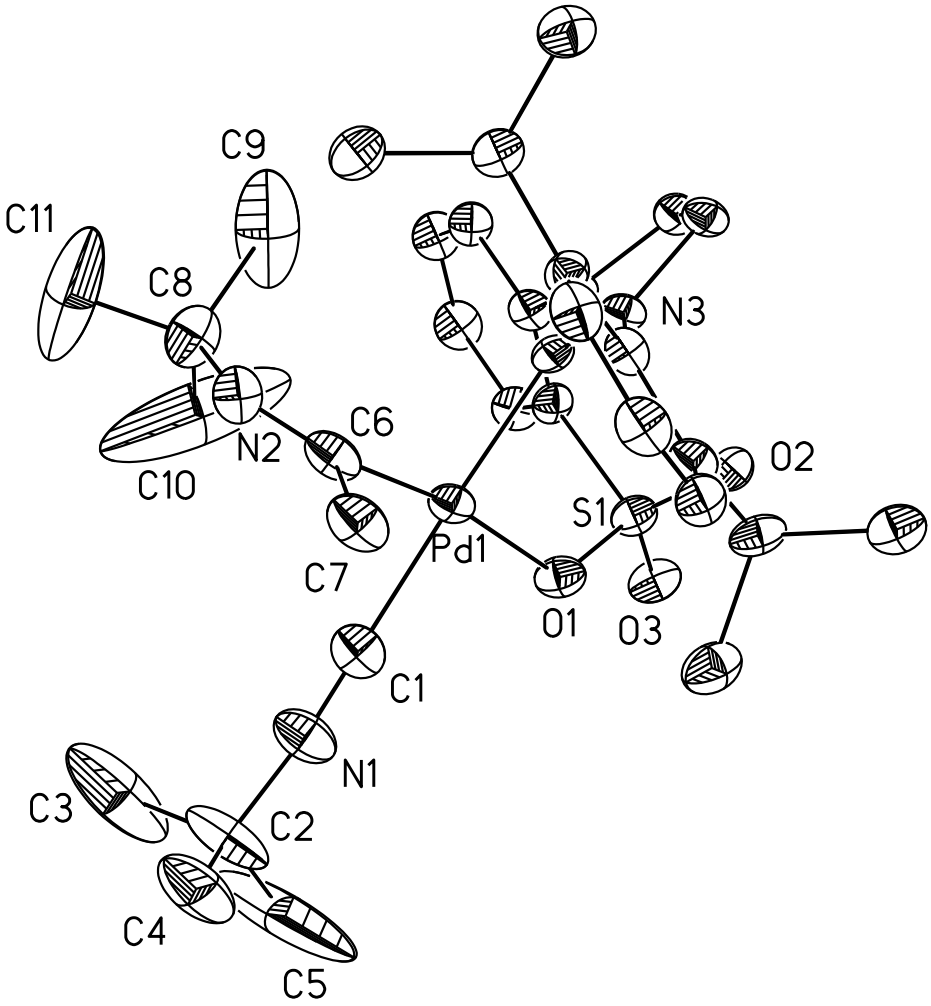
p = number of parameters refined.

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).


C28
C29
C23
C27
C24
N2
C7
C22
C6
C25
C21
N4
C26
C18
Pd1
N1
C20
C30
N3
C19
C17
C32
C31
O1
C12
S1
O2
C13
O3


C28
C23
C24
C7
C4
C11
C25
C29
C6
C2
C10
C27
C22
C21
C8
N1
C3
C5
C1
C9
Pd1
C31
N4
C20
C18
O1
N3
O2
C19
S1
C17
C16
C12
O3
C15
C13
C14


C9
C11
C8
N3
N2
C6
O2
C10
S1
Pd1
C7
O1
O3
C1
N1
C3
C2
C4
C5

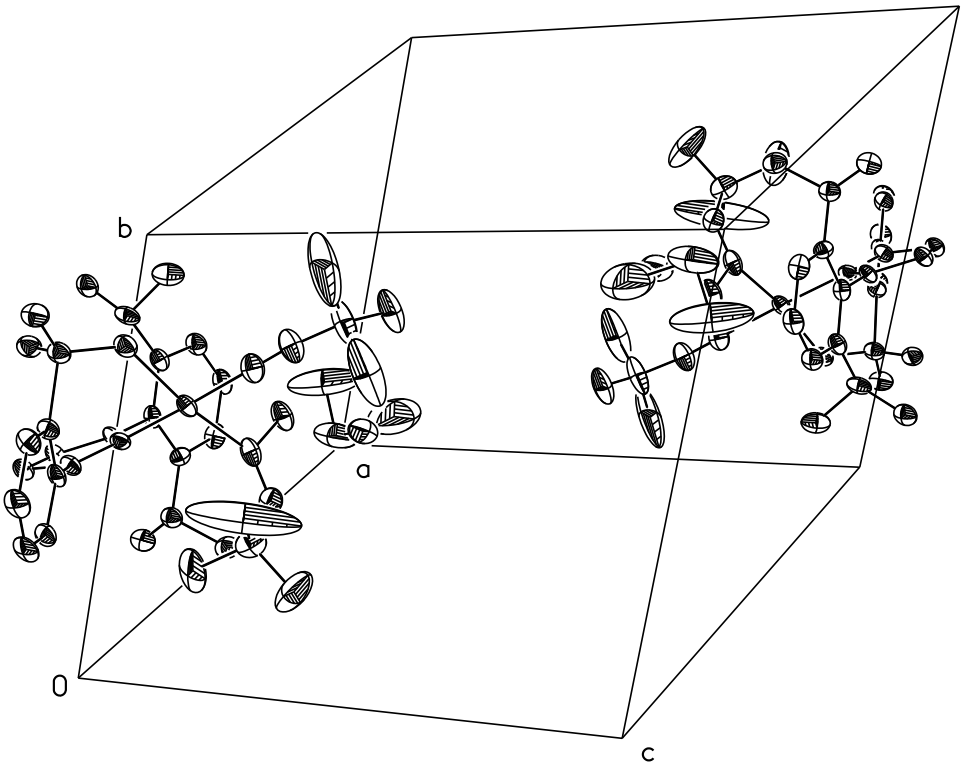

b
a
0
c

Table 1. Crystal and structure refinement for Zhou19.

Identification Code	Zhou19	
Empirical formula	$C_{32}H_{46}N_4O_3PdS + CH_2Cl_2$	
Formula weight	758.11	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space Group	P1(bar)	
Unit cell dimensions	a = 11.319(4) Å	α = 75.514(5) ^{o}
	b = 11.668(4) Å	β = 85.177(5) ^{o}
	c = 16.185(5) Å	γ = 63.834(5) ^{o}
Volume	1856.7(11) $Å^3$	
Z	2	
Density (calculated)	1.356 Mg/m^3	
Absorption coefficient	0.736 mm^{-1}	
F(000)	788	
Crystal size, color, habit	0.12 x 0.12 x 0.08 mm, clear, fragment	
Theta range for data collection	2.00 – 25.09 ^{o}	
Index ranges	$13 \leq h \leq 13$, $13 \leq k \leq 13$, $-19 \leq l \leq 19$	
Reflections collected	17,916	
Independent reflections	6,574 (R_{int} = 0.0372)	
Reflections with $I > 4\sigma(F_o)$	5,194	
Absorption correction	SADABS based on redundant diffractions	
Max. and min. transmission	1.0, 0.742	
Refinement method	Full-matrix least squares on F^2	
Weighting scheme	$w = q\,[\sigma^2 (F_o^2) + (aP)^2 + bP]^{-1}$ where:	
	$P = (F_o^2 + 2 F_c^2)/3$, a = 0.888, b = 0.0, q =1	
Data / restraints / parameters	6574 / 0 / 417	
Goodness-of-fit on F^2	1.019	
Final R indices [I > 2 sigma(I)]	R1 = 0.0621, wR2 = 0.1501	
R indices (all data)	R1 = 0.0801, wR2 = 0.1586	
Largest diff. peak and hole	1.359, -1.309 e$Å^{-3}$	

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for Zhou19. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	SOF
C(1)	2935(6)	1317(6)	6141(4)	34(1)	
C(2)	2597(7)	546(9)	4833(5)	62(2)	
C(3)	3128(10)	1243(15)	4070(6)	119(5)	
C(4)	1128(7)	1046(9)	4699(5)	64(2)	
C(5)	3392(15)	-889(12)	4969(10)	202(10)	
C(6)	1697(5)	3711(6)	6508(4)	31(1)	
C(7)	361(6)	3665(7)	6654(4)	37(2)	
C(8)	2873(6)	4923(6)	5682(4)	40(2)	
C(9)	3421(10)	5224(13)	6392(6)	122(5)	
C(10)	3901(18)	3797(14)	5410(14)	266(14)	
C(11)	2433(10)	6104(12)	4977(7)	134(6)	
C(12)	6464(5)	761(5)	7867(3)	25(1)	
C(13)	7705(5)	333(6)	7507(4)	29(1)	
C(14)	8277(6)	1207(6)	7226(4)	33(1)	
C(15)	7623(6)	2475(6)	7309(4)	33(1)	
C(16)	6381(5)	2919(6)	7671(3)	27(1)	
C(17)	5798(5)	2056(5)	7946(3)	23(1)	
C(18)	3402(5)	2651(5)	8125(3)	21(1)	
C(19)	4597(5)	2662(6)	9254(3)	25(1)	
C(20)	3145(5)	3144(5)	9475(3)	23(1)	
C(21)	1176(5)	3344(5)	8722(3)	21(1)	
C(22)	252(5)	4695(5)	8520(3)	23(1)	
C(23)	-1079(5)	4959(6)	8555(3)	28(1)	
C(24)	-1470(5)	3959(6)	8770(4)	29(1)	
C(25)	-561(5)	2665(6)	8959(3)	28(1)	
C(26)	798(5)	2314(5)	8949(3)	24(1)	
C(27)	664(5)	5800(5)	8295(4)	27(1)	
C(28)	52(6)	6736(6)	7422(4)	33(1)	
C(29)	273(6)	6577(6)	8984(4)	34(1)	
C(30)	1789(5)	869(5)	9202(4)	28(1)	
C(31)	1678(6)	293(6)	10139(4)	32(1)	
C(32)	1615(6)	78(6)	8630(4)	39(2)	
C(33)	5127(10)	2923(9)	1987(8)	95(4)	
Cl(1A)	4282(5)	3511(4)	2865(4)	84(2)	0.59
Cl(1B)	5610(30)	3144(13)	2859(8)	287(12)	0.41
Cl(2)	5779(4)	3805(3)	1279(4)	187(2)	
N(1)	2796(5)	925(6)	5590(3)	41(1)	
N(2)	1710(5)	4695(5)	5988(3)	33(1)	
N(3)	4577(4)	2536(4)	8373(3)	23(1)	
N(4)	2554(4)	3036(4)	8732(3)	20(1)	
O(1)	4709(4)	0(4)	7621(2)	30(1)	
O(2)	5317(4)	-266(4)	9090(2)	30(1)	
O(3)	6830(4)	-1669(4)	8214(3)	33(1)	
Pd(1)	3167(1)	1997(1)	7107(1)	23(1)	
S(1)	5784(1)	-398(1)	8251(1)	26(1)	

Table 3. Bond lengths [Å] and angles [°] for Zhou19.

C(1)-N(1)	1.149(7)	C(18)-Pd(1)	2.061(5)
C(1)-Pd(1)	2.004(6)	C(19)-N(3)	1.473(7)
C(2)-N(1)	1.468(8)	C(19)-C(20)	1.527(7)
C(2)-C(5)	1.477(14)	C(20)-N(4)	1.482(6)
C(2)-C(4)	1.515(10)	C(21)-C(26)	1.403(8)
C(2)-C(3)	1.533(14)	C(21)-C(22)	1.425(7)
C(6)-N(2)	1.248(8)	C(21)-N(4)	1.439(6)
C(6)-C(7)	1.533(8)	C(22)-C(23)	1.398(8)
C(6)-Pd(1)	2.019(6)	C(22)-C(27)	1.510(8)
C(8)-C(10)	1.460(12)	C(23)-C(24)	1.380(8)
C(8)-C(11)	1.466(10)	C(24)-C(25)	1.373(8)
C(8)-N(2)	1.477(8)	C(25)-C(26)	1.406(7)
C(8)-C(9)	1.530(12)	C(26)-C(30)	1.528(8)
C(12)-C(17)	1.393(8)	C(27)-C(29)	1.527(8)
C(12)-C(13)	1.397(7)	C(27)-C(28)	1.547(8)
C(12)-S(1)	1.796(6)	C(30)-C(31)	1.516(8)
C(13)-C(14)	1.403(8)	C(30)-C(32)	1.538(8)
C(14)-C(15)	1.368(9)	C(33)-Cl(2)	1.689(11)
C(15)-C(16)	1.400(8)	C(33)-Cl(1A)	1.757(13)
C(16)-C(17)	1.400(8)	O(1)-S(1)	1.487(4)
C(17)-N(3)	1.433(7)	O(1)-Pd(1)	2.204(4)
C(18)-N(4)	1.330(6)	O(2)-S(1)	1.435(4)
C(18)-N(3)	1.361(7)	O(3)-S(1)	1.445(4)

N(1)-C(1)-Pd(1)	179.6(6)	C(22)-C(21)-N(4)	117.9(5)
N(1)-C(2)-C(5)	107.5(7)	C(23)-C(22)-C(21)	116.4(5)
N(1)-C(2)-C(4)	107.5(6)	C(23)-C(22)-C(27)	120.8(5)
C(5)-C(2)-C(4)	116.1(10)	C(21)-C(22)-C(27)	122.8(5)
N(1)-C(2)-C(3)	107.3(7)	C(24)-C(23)-C(22)	121.5(5)
C(5)-C(2)-C(3)	108.9(10)	C(25)-C(24)-C(23)	121.0(5)
C(4)-C(2)-C(3)	109.1(7)	C(24)-C(25)-C(26)	121.2(5)
N(2)-C(6)-C(7)	116.8(5)	C(21)-C(26)-C(25)	116.9(5)
N(2)-C(6)-Pd(1)	131.7(4)	C(21)-C(26)-C(30)	122.9(5)
C(7)-C(6)-Pd(1)	111.0(4)	C(25)-C(26)-C(30)	120.2(5)
C(10)-C(8)-C(11)	110.9(11)	C(22)-C(27)-C(29)	111.0(5)
C(10)-C(8)-N(2)	112.1(7)	C(22)-C(27)-C(28)	111.1(5)
C(11)-C(8)-N(2)	107.9(6)	C(29)-C(27)-C(28)	109.8(5)
C(10)-C(8)-C(9)	109.6(12)	C(31)-C(30)-C(26)	110.3(5)
C(11)-C(8)-C(9)	106.8(8)	C(31)-C(30)-C(32)	111.6(5)
N(2)-C(8)-C(9)	109.4(6)	C(26)-C(30)-C(32)	111.1(5)
C(17)-C(12)-C(13)	119.9(5)	Cl(2)-C(33)-Cl(1A)	120.2(6)
C(17)-C(12)-S(1)	121.4(4)	C(1)-N(1)-C(2)	174.6(7)
C(13)-C(12)-S(1)	118.7(4)	C(6)-N(2)-C(8)	127.3(5)
C(12)-C(13)-C(14)	119.9(5)	C(18)-N(3)-C(17)	126.6(4)
C(15)-C(14)-C(13)	120.1(5)	C(18)-N(3)-C(19)	113.4(4)
C(14)-C(15)-C(16)	120.8(6)	C(17)-N(3)-C(19)	118.7(4)
C(17)-C(16)-C(15)	119.5(5)	C(18)-N(4)-C(21)	126.5(4)
C(12)-C(17)-C(16)	119.9(5)	C(18)-N(4)-C(20)	114.0(4)
C(12)-C(17)-N(3)	123.0(5)	C(21)-N(4)-C(20)	119.5(4)
C(16)-C(17)-N(3)	116.8(5)	S(1)-O(1)-Pd(1)	127.4(2)
N(4)-C(18)-N(3)	107.1(4)	C(1)-Pd(1)-C(6)	84.8(2)
N(4)-C(18)-Pd(1)	128.3(4)	C(1)-Pd(1)-C(18)	178.3(2)
N(3)-C(18)-Pd(1)	123.7(4)	C(6)-Pd(1)-C(18)	96.3(2)
N(3)-C(19)-C(20)	102.1(4)	C(1)-Pd(1)-O(1)	86.8(2)
N(4)-C(20)-C(19)	102.5(4)	C(6)-Pd(1)-O(1)	171.49(18)
C(26)-C(21)-C(22)	123.0(5)	C(18)-Pd(1)-O(1)	92.15(18)
C(26)-C(21)-N(4)	119.0(5)	O(2)-S(1)-O(3)	115.1(2)

O(2)-S(1)-O(1)	113.1(2)	O(3)-S(1)-C(12)	105.9(2)
O(3)-S(1)-O(1)	110.5(2)	O(1)-S(1)-C(12)	104.4(2)
O(2)-S(1)-C(12)	107.0(2)		

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for Zhou19. 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)	21(3)	43(4)	37(4)	-12(3)	1(3)	-12(3)
C(2)	36(4)	97(6)	64(5)	-57(5)	-4(4)	-18(4)
C(3)	70(7)	273(17)	72(7)	-99(9)	38(5)	-103(9)
C(4)	44(4)	117(7)	55(5)	-37(5)	0(4)	-47(5)
C(5)	180(14)	123(10)	251(17)	-144(12)	-155(13)	60(10)
C(6)	19(3)	43(4)	33(3)	-19(3)	1(2)	-11(3)
C(7)	24(3)	59(4)	37(4)	-18(3)	3(3)	-23(3)
C(8)	31(3)	42(4)	43(4)	-7(3)	13(3)	-16(3)
C(9)	102(8)	223(14)	78(7)	48(8)	-40(6)	-141(10)
C(10)	270(20)	171(14)	490(30)	-238(19)	340(20)	-187(15)
C(11)	74(7)	155(11)	138(10)	101(9)	-58(7)	-81(8)
C(12)	21(3)	29(3)	27(3)	-4(2)	2(2)	-16(3)
C(13)	17(3)	34(3)	36(3)	-13(3)	4(2)	-10(3)
C(14)	20(3)	49(4)	37(3)	-12(3)	8(3)	-21(3)
C(15)	24(3)	51(4)	37(3)	-8(3)	6(3)	-29(3)
C(16)	20(3)	33(3)	30(3)	-6(3)	0(2)	-15(3)
C(17)	14(3)	31(3)	28(3)	-7(2)	-1(2)	-13(2)
C(18)	20(3)	21(3)	27(3)	-4(2)	1(2)	-13(2)
C(19)	21(3)	31(3)	27(3)	-9(2)	3(2)	-16(2)
C(20)	21(3)	30(3)	26(3)	-12(2)	4(2)	-15(2)
C(21)	12(3)	30(3)	22(3)	-8(2)	2(2)	-8(2)
C(22)	24(3)	18(3)	24(3)	-4(2)	1(2)	-8(2)
C(23)	19(3)	32(3)	27(3)	-10(3)	4(2)	-4(2)
C(24)	15(3)	44(4)	31(3)	-12(3)	3(2)	-15(3)
C(25)	24(3)	38(3)	29(3)	-7(3)	3(2)	-19(3)
C(26)	19(3)	31(3)	25(3)	-11(2)	2(2)	-13(2)
C(27)	21(3)	27(3)	33(3)	-7(3)	2(2)	-11(2)
C(28)	29(3)	27(3)	39(4)	-6(3)	1(3)	-10(3)
C(29)	34(3)	33(3)	39(4)	-10(3)	4(3)	-17(3)
C(30)	20(3)	28(3)	43(4)	-12(3)	7(3)	-17(2)
C(31)	20(3)	33(3)	45(4)	-8(3)	-3(3)	-13(3)
C(32)	40(4)	34(4)	49(4)	-16(3)	17(3)	-20(3)
C(33)	64(6)	47(5)	182(12)	-29(6)	2(7)	-29(5)
Cl(1A)	92(3)	61(2)	109(4)	13(2)	-45(3)	-50(2)
Cl(1B)	630(40)	145(11)	156(11)	20(9)	-115(19)	-236(19)
Cl(2)	174(4)	55(2)	316(6)	-42(3)	119(4)	-55(2)
N(1)	28(3)	57(4)	43(3)	-26(3)	2(2)	-16(3)
N(2)	25(3)	39(3)	31(3)	-6(2)	2(2)	-13(2)
N(3)	18(2)	27(2)	28(3)	-8(2)	2(2)	-13(2)
N(4)	15(2)	25(2)	25(2)	-11(2)	4(2)	-12(2)
O(1)	23(2)	28(2)	40(2)	-9(2)	-2(2)	-12(2)
O(2)	35(2)	33(2)	29(2)	-6(2)	4(2)	-21(2)
O(3)	24(2)	26(2)	48(3)	-10(2)	3(2)	-10(2)
Pd(1)	17(1)	30(1)	27(1)	-11(1)	3(1)	-13(1)
S(1)	20(1)	26(1)	35(1)	-7(1)	2(1)	-12(1)

Table 5. Hydrogen coordinates [x 10^4] and isotropic displacement parameters [$Å^2$ x 10^3] for Zhou19.

	x	y	z	U(eq)
H(3A)	2692	2193	4026	179
H(3B)	2951	1064	3545	179
H(3C)	4079	919	4152	179
H(4A)	753	745	5229	96
H(4B)	968	707	4245	96
H(4C)	714	2009	4535	96
H(5A)	4310	-1114	5097	303
H(5B)	3346	-1161	4451	303
H(5C)	3047	-1344	5448	303
H(7A)	-345	4563	6539	55
H(7B)	327	3212	7247	55
H(7C)	248	3190	6269	55
H(9A)	4211	5344	6197	183
H(9B)	3647	4491	6898	183
H(9C)	2755	6029	6535	183
H(10A)	3675	3801	4838	399
H(10B)	3977	2983	5811	399
H(10C)	4743	3851	5398	399
H(11A)	1969	5997	4539	200
H(11B)	3198	6233	4730	200
H(11C)	1837	6870	5193	200
H(13)	8160	-549	7452	34
H(14)	9119	918	6979	40
H(15)	8017	3062	7118	40
H(16)	5937	3799	7730	32
H(19A)	4927	3309	9282	29
H(19B)	5146	1806	9640	29
H(20A)	3024	2579	10012	28
H(20B)	2760	4064	9531	28
H(23)	-1729	5846	8428	34
H(24)	-2383	4170	8787	35
H(25)	-855	1994	9099	34
H(27)	1644	5410	8254	32
H(28A)	385	6255	6972	49
H(28B)	291	7471	7306	49
H(28C)	-909	7075	7435	49
H(29A)	-687	6977	9028	52
H(29B)	578	7268	8834	52
H(29C)	679	5984	9533	52
H(30)	2693	823	9118	34
H(31A)	791	347	10241	48
H(31B)	1841	790	10486	48
H(31C)	2329	-628	10295	48
H(32A)	2300	-829	8778	59
H(32B)	1687	479	8030	59
H(32C)	746	81	8716	59
H(33A)	5854	2046	2215	114
H(33B)	4513	2788	1664	114

Table 6. Torsion angles [°] for Zhou19.

C(17)-C(12)-C(13)-C(14)	0.1(8)	N(4)-C(18)-N(3)-C(19)	8.8(6)
S(1)-C(12)-C(13)-C(14)	-178.0(4)	Pd(1)-C(18)-N(3)-C(19)	-161.1(4)
C(12)-C(13)-C(14)-C(15)	0.3(9)	C(12)-C(17)-N(3)-C(18)	-65.5(7)
C(13)-C(14)-C(15)-C(16)	-0.1(9)	C(16)-C(17)-N(3)-C(18)	120.4(6)
C(14)-C(15)-C(16)-C(17)	-0.5(9)	C(12)-C(17)-N(3)-C(19)	100.2(6)
C(13)-C(12)-C(17)-C(16)	-0.7(8)	C(16)-C(17)-N(3)-C(19)	-73.8(6)
S(1)-C(12)-C(17)-C(16)	177.4(4)	C(20)-C(19)-N(3)-C(18)	-10.5(6)
C(13)-C(12)-C(17)-N(3)	-174.5(5)	C(20)-C(19)-N(3)-C(17)	-178.1(4)
S(1)-C(12)-C(17)-N(3)	3.5(7)	N(3)-C(18)-N(4)-C(21)	176.8(5)
C(15)-C(16)-C(17)-C(12)	0.9(8)	Pd(1)-C(18)-N(4)-C(21)	-13.9(8)
C(15)-C(16)-C(17)-N(3)	175.1(5)	N(3)-C(18)-N(4)-C(20)	-3.1(6)
N(3)-C(19)-C(20)-N(4)	7.7(5)	Pd(1)-C(18)-N(4)-C(20)	166.2(4)
C(26)-C(21)-C(22)-C(23)	-0.3(8)	C(26)-C(21)-N(4)-C(18)	81.1(7)
N(4)-C(21)-C(22)-C(23)	-177.1(5)	C(22)-C(21)-N(4)-C(18)	-101.9(6)
C(26)-C(21)-C(22)-C(27)	178.6(5)	C(26)-C(21)-N(4)-C(20)	-99.0(6)
N(4)-C(21)-C(22)-C(27)	1.8(7)	C(22)-C(21)-N(4)-C(20)	77.9(6)
C(21)-C(22)-C(23)-C(24)	-0.3(8)	C(19)-C(20)-N(4)-C(18)	-3.3(6)
C(27)-C(22)-C(23)-C(24)	-179.2(5)	C(19)-C(20)-N(4)-C(21)	176.8(4)
C(22)-C(23)-C(24)-C(25)	0.1(9)	N(1)-C(1)-Pd(1)-C(6)	-85(98)
C(23)-C(24)-C(25)-C(26)	0.7(9)	N(1)-C(1)-Pd(1)-C(18)	44(100)
C(22)-C(21)-C(26)-C(25)	1.0(8)	N(1)-C(1)-Pd(1)-O(1)	94(98)
N(4)-C(21)-C(26)-C(25)	177.8(5)	N(2)-C(6)-Pd(1)-C(1)	-94.8(6)
C(22)-C(21)-C(26)-C(30)	-177.3(5)	C(7)-C(6)-Pd(1)-C(1)	76.4(4)
N(4)-C(21)-C(26)-C(30)	-0.5(8)	N(2)-C(6)-Pd(1)-C(18)	86.5(6)
C(24)-C(25)-C(26)-C(21)	-1.2(8)	C(7)-C(6)-Pd(1)-C(18)	-102.3(4)
C(24)-C(25)-C(26)-C(30)	177.2(5)	N(2)-C(6)-Pd(1)-O(1)	-102.6(14)
C(23)-C(22)-C(27)-C(29)	66.1(7)	C(7)-C(6)-Pd(1)-O(1)	68.6(15)
C(21)-C(22)-C(27)-C(29)	-112.7(6)	N(4)-C(18)-Pd(1)-C(1)	-63(8)
C(23)-C(22)-C(27)-C(28)	-56.3(7)	N(3)-C(18)-Pd(1)-C(1)	104(8)
C(21)-C(22)-C(27)-C(28)	124.9(5)	N(4)-C(18)-Pd(1)-C(6)	65.4(5)
C(21)-C(26)-C(30)-C(31)	112.3(6)	N(3)-C(18)-Pd(1)-C(6)	-126.9(5)
C(25)-C(26)-C(30)-C(31)	-66.0(6)	N(4)-C(18)-Pd(1)-O(1)	-113.2(5)
C(21)-C(26)-C(30)-C(32)	-123.3(6)	N(3)-C(18)-Pd(1)-O(1)	54.5(4)
C(25)-C(26)-C(30)-C(32)	58.4(7)	S(1)-O(1)-Pd(1)-C(1)	160.1(3)
Pd(1)-C(1)-N(1)-C(2)	123(95)	S(1)-O(1)-Pd(1)-C(6)	167.9(13)
C(5)-C(2)-N(1)-C(1)	150(6)	S(1)-O(1)-Pd(1)-C(18)	-21.1(3)
C(4)-C(2)-N(1)-C(1)	-84(7)	Pd(1)-O(1)-S(1)-O(2)	68.7(3)
C(3)-C(2)-N(1)-C(1)	33(7)	Pd(1)-O(1)-S(1)-O(3)	-160.7(3)
C(7)-C(6)-N(2)-C(8)	-174.4(5)	Pd(1)-O(1)-S(1)-C(12)	-47.3(3)
Pd(1)-C(6)-N(2)-C(8)	-3.7(10)	C(17)-C(12)-S(1)-O(2)	-46.1(5)
C(10)-C(8)-N(2)-C(6)	48.5(14)	C(13)-C(12)-S(1)-O(2)	131.9(4)
C(11)-C(8)-N(2)-C(6)	170.8(8)	C(17)-C(12)-S(1)-O(3)	-169.3(4)
C(9)-C(8)-N(2)-C(6)	-73.4(9)	C(13)-C(12)-S(1)-O(3)	8.7(5)
N(4)-C(18)-N(3)-C(17)	175.2(5)	C(17)-C(12)-S(1)-O(1)	74.0(5)
Pd(1)-C(18)-N(3)-C(17)	5.3(7)	C(13)-C(12)-S(1)-O(1)	-107.9(5)