Crystal Structure Report for Zhou21

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

Report Prepared for:

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Crystallographic Experimental Section

Data Collection

An irregular broken fragment (0.32 x 0.16 x 0.04mm) 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 P1(bar) based on systematic absences and intensity statistics. Patterson methods were used to locate the Pd and several C atoms. Repeated difference Fourier maps allowed recognition of all expected C, N, O, and S atoms. One CH_2Cl_2 molecule was found. 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. No anomalous bond lengths or thermal parameters were noted. All ORTEP diagrams have been drawn with 50% probability ellipsoids.

Equations of interest:

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

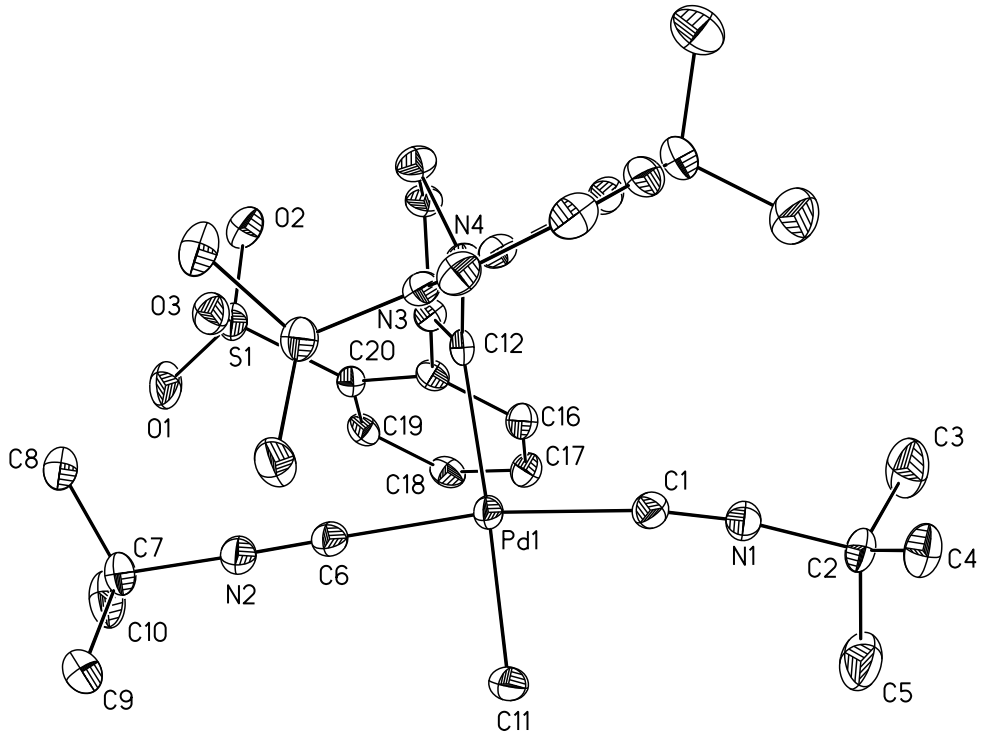
$wR2 = [\Sigma [w (F_o^2 - F_c^2)^2] / \Sigma [w (F_o^2)^2]]^{1/2}$ $\quad$ $GooF = S = [\Sigma [w (F_o^2 - F_c^2)^2] / (n-p)^{1/2}$

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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C8
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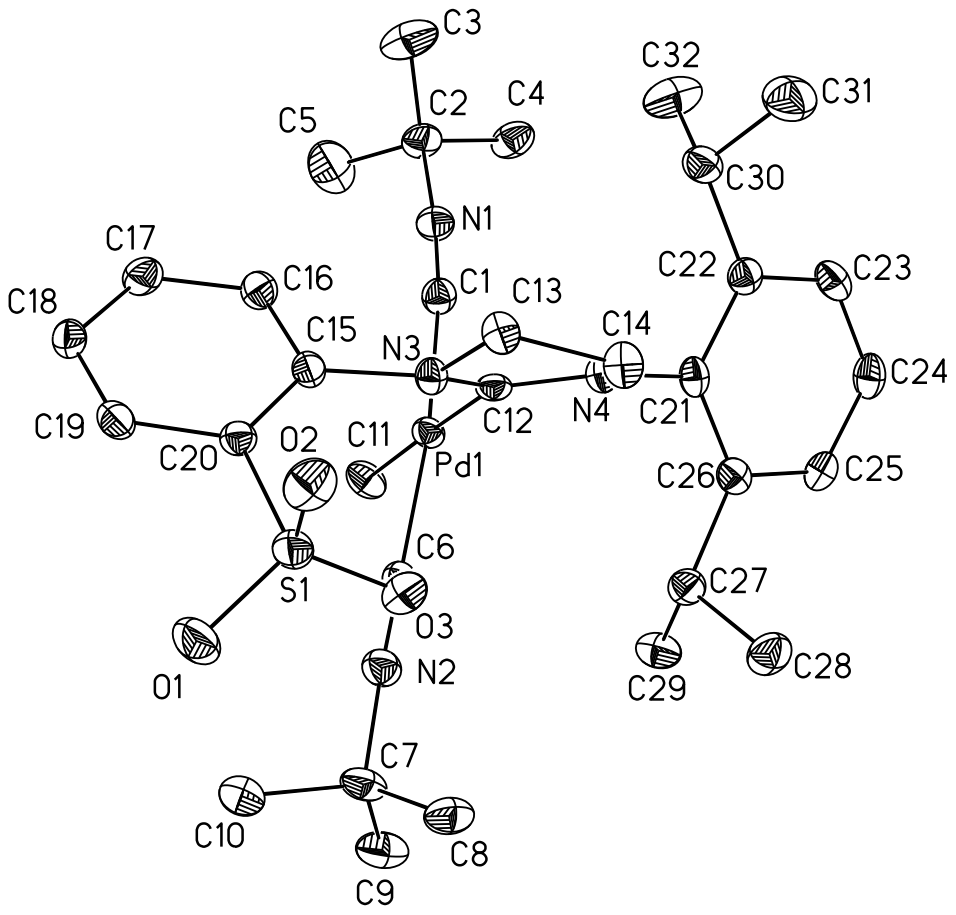
C2
C4
N2
C6
C10
C9
C11
C5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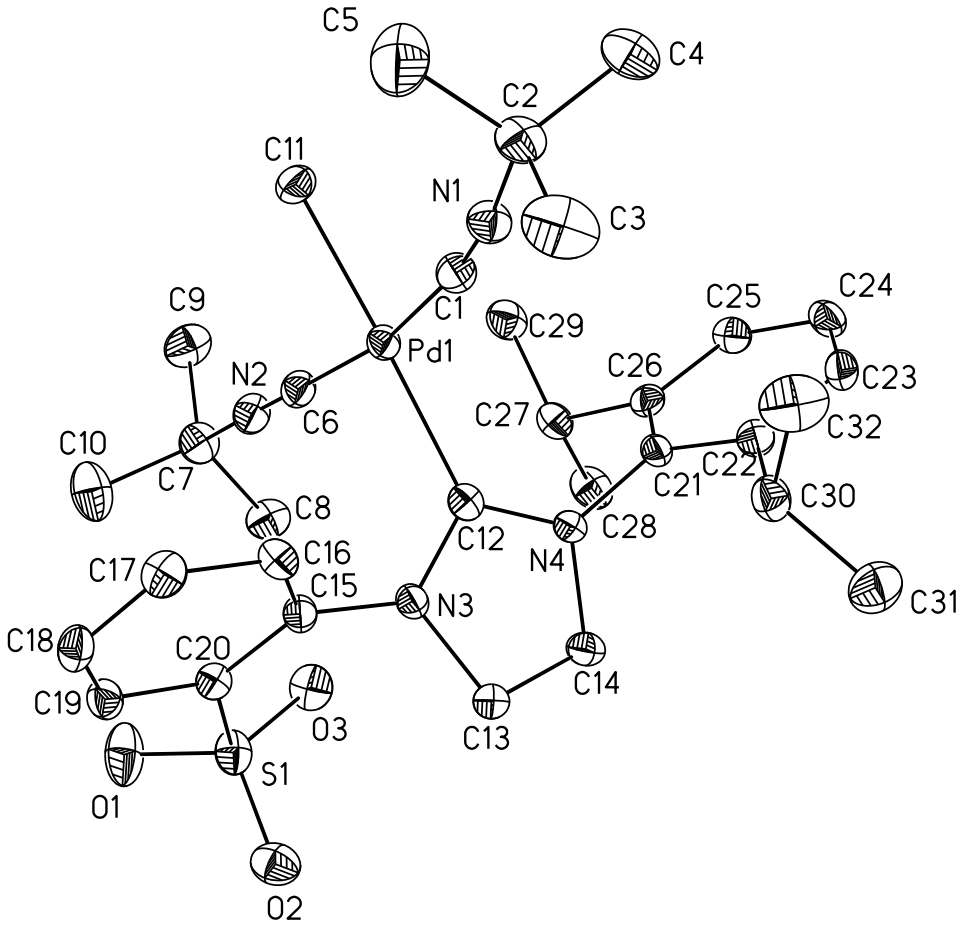
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C7
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C21
C8
C12
C28
C30
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C18
C20
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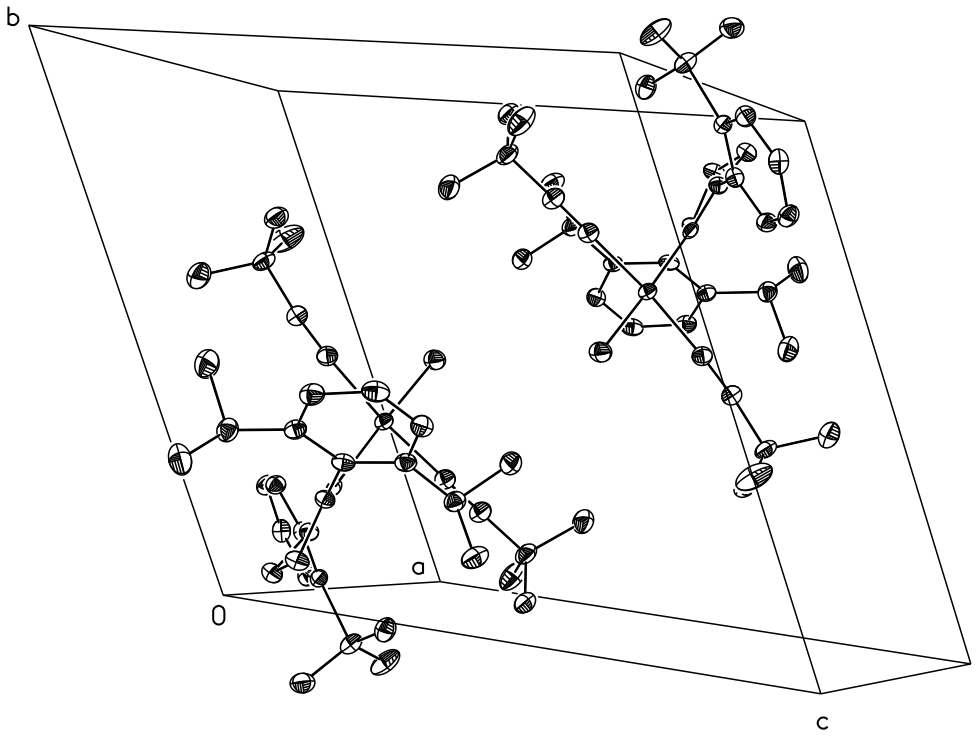
C13
S1
O1
O2


b
a
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c

Table 1. Crystal and structure refinement for Zhou21.

Identification Code	Zhou21	
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 = 10.437(3) Å	α = 107.881(5) ^{o}
	b = 13.551(4) Å	β = 90.359(6) ^{o}
	c = 14.524(5) Å	γ = 106.644(5) ^{o}
Volume	1863.0(11) $Å^3$	
Z	2	
Density (calculated)	1.351 Mg/m^3	
Absorption coefficient	0.734 mm^{-1}	
F(000)	788	
Crystal size, color, habit	0.32 x 0.16 x 0.04 mm, clear, irregular	
Theta range for data collection	1.66 – 28.30 ^{o}	
Index ranges	$-13 \le h \le 13$, $-17 \le k \le 18$, $-19 \le l \le 19$	
Reflections collected	22,477	
Independent reflections	8,886 (R_{int} = 0.0299)	
Reflections with $I > 4\sigma(F_o)$	7,469	
Absorption correction	SADABS based on redundant diffractions	
Max. and min. transmission	1.0, 0.807	
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 = 0.0364, b = 0.0, q =1	
Data / restraints / parameters	8886 / 0 / 408	
Goodness-of-fit on F^2	0.963	
Final R indices [I > 2 sigma(I)]	R1 = 0.0365, wR2 = 0.0802	
R indices (all data)	R1 = 0.0444, wR2 = 0.0821	
Largest diff. peak and hole	0.784, -0.588 $eÅ^{-3}$	

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for Zhou21. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	SOF
C(1)	2423(2)	4625(2)	2459(2)	21(1)	
C(2)	2461(3)	6251(2)	1832(2)	25(1)	
C(3)	1636(3)	5854(3)	855(2)	43(1)	
C(4)	1918(3)	7042(2)	2588(2)	30(1)	
C(5)	3938(3)	6750(3)	1762(3)	50(1)	
C(6)	3494(2)	2559(2)	3478(2)	21(1)	
C(7)	4383(3)	1297(2)	4199(2)	26(1)	
C(8)	3152(3)	462(2)	4357(2)	28(1)	
C(9)	5216(3)	2020(2)	5163(2)	33(1)	
C(10)	5233(3)	754(3)	3468(2)	39(1)	
C(11)	4621(2)	4761(2)	3577(2)	25(1)	
C(12)	1038(2)	2246(2)	2360(2)	16(1)	
C(13)	-378(2)	608(2)	1296(2)	20(1)	
C(14)	-1087(2)	971(2)	2191(2)	22(1)	
C(15)	2053(2)	1265(2)	997(2)	18(1)	
C(16)	2535(2)	2063(2)	555(2)	21(1)	
C(17)	3498(2)	1972(2)	-95(2)	23(1)	
C(18)	3965(2)	1070(2)	-329(2)	22(1)	
C(19)	3486(2)	284(2)	112(2)	21(1)	
C(20)	2541(2)	367(2)	786(2)	18(1)	
C(21)	-646(2)	2822(2)	3448(2)	18(1)	
C(22)	-1533(2)	3328(2)	3178(2)	20(1)	
C(23)	-2048(2)	3983(2)	3920(2)	24(1)	
C(24)	-1698(3)	4153(2)	4892(2)	24(1)	
C(25)	-836(2)	3639(2)	5136(2)	21(1)	
C(26)	-310(2)	2950(2)	4424(2)	19(1)	
C(27)	542(2)	2335(2)	4722(2)	22(1)	
C(28)	-339(3)	1450(2)	5106(2)	29(1)	
C(29)	1724(3)	3092(2)	5476(2)	28(1)	
C(30)	-1913(3)	3181(2)	2117(2)	24(1)	
C(31)	-3418(3)	2634(2)	1809(2)	38(1)	
C(32)	-1506(3)	4283(2)	1951(2)	42(1)	
C(33)	1429(3)	2028(2)	7929(2)	41(1)	
Cl(1)	2568(1)	1509(1)	7178(1)	40(1)	
Cl(2)	2026(1)	3444(1)	8430(1)	57(1)	
N(1)	2356(2)	5306(2)	2166(2)	23(1)	
N(2)	3901(2)	2005(2)	3780(2)	24(1)	
N(3)	1006(2)	1362(2)	1618(1)	17(1)	
N(4)	-187(2)	2092(2)	2679(1)	17(1)	
O(1)	3115(2)	-1140(2)	1289(2)	38(1)	
O(2)	847(2)	-1536(2)	562(1)	30(1)	
O(3)	1538(2)	-317(2)	2214(1)	28(1)	
Pd(1)	2807(1)	3524(1)	2961(1)	17(1)	
S(1)	1957(1)	-752(1)	1260(1)	23(1)	

Table 3. Bond lengths [Å] and angles [°] for Zhou21.

C(1)-N(1)	1.146(3)	C(17)-C(18)	1.391(3)
C(1)-Pd(1)	1.981(3)	C(18)-C(19)	1.382(3)
C(2)-N(1)	1.481(3)	C(19)-C(20)	1.398(3)
C(2)-C(5)	1.513(4)	C(20)-S(1)	1.805(2)
C(2)-C(3)	1.515(4)	C(21)-C(26)	1.404(3)
C(2)-C(4)	1.519(4)	C(21)-C(22)	1.415(3)
C(6)-N(2)	1.149(3)	C(21)-N(4)	1.434(3)
C(6)-Pd(1)	1.980(2)	C(22)-C(23)	1.390(3)
C(7)-N(2)	1.475(3)	C(22)-C(30)	1.527(3)
C(7)-C(8)	1.521(4)	C(23)-C(24)	1.388(4)
C(7)-C(9)	1.527(4)	C(24)-C(25)	1.389(3)
C(7)-C(10)	1.537(4)	C(25)-C(26)	1.396(3)
C(11)-Pd(1)	2.106(2)	C(26)-C(27)	1.521(3)
C(12)-N(3)	1.334(3)	C(27)-C(29)	1.531(4)
C(12)-N(4)	1.344(3)	C(27)-C(28)	1.542(3)
C(12)-Pd(1)	2.096(2)	C(30)-C(32)	1.525(4)
C(13)-N(3)	1.484(3)	C(30)-C(31)	1.528(4)
C(13)-C(14)	1.519(3)	C(33)-Cl(2)	1.746(3)
C(14)-N(4)	1.484(3)	C(33)-Cl(1)	1.766(3)
C(15)-C(16)	1.398(3)	O(1)-S(1)	1.4546(19)
C(15)-C(20)	1.401(3)	O(2)-S(1)	1.455(2)
C(15)-N(3)	1.431(3)	O(3)-S(1)	1.4535(19)
C(16)-C(17)	1.388(3)		

N(1)-C(1)-Pd(1)	172.1(2)	C(23)-C(22)-C(30)	120.2(2)
N(1)-C(2)-C(5)	106.7(2)	C(21)-C(22)-C(30)	122.2(2)
N(1)-C(2)-C(3)	108.6(2)	C(24)-C(23)-C(22)	121.7(2)
C(5)-C(2)-C(3)	111.8(3)	C(23)-C(24)-C(25)	119.5(2)
N(1)-C(2)-C(4)	107.5(2)	C(24)-C(25)-C(26)	121.5(2)
C(5)-C(2)-C(4)	111.2(2)	C(25)-C(26)-C(21)	117.7(2)
C(3)-C(2)-C(4)	110.9(2)	C(25)-C(26)-C(27)	119.6(2)
N(2)-C(6)-Pd(1)	179.5(2)	C(21)-C(26)-C(27)	122.6(2)
N(2)-C(7)-C(8)	107.4(2)	C(26)-C(27)-C(29)	112.3(2)
N(2)-C(7)-C(9)	107.3(2)	C(26)-C(27)-C(28)	110.2(2)
C(8)-C(7)-C(9)	111.1(2)	C(29)-C(27)-C(28)	110.6(2)
N(2)-C(7)-C(10)	107.5(2)	C(32)-C(30)-C(22)	110.0(2)
C(8)-C(7)-C(10)	111.6(2)	C(32)-C(30)-C(31)	109.0(2)
C(9)-C(7)-C(10)	111.7(2)	C(22)-C(30)-C(31)	112.4(2)
N(3)-C(12)-N(4)	108.0(2)	Cl(2)-C(33)-Cl(1)	111.53(16)
N(3)-C(12)-Pd(1)	122.93(17)	C(1)-N(1)-C(2)	172.5(2)
N(4)-C(12)-Pd(1)	128.73(17)	C(6)-N(2)-C(7)	177.6(3)
N(3)-C(13)-C(14)	101.06(19)	C(12)-N(3)-C(15)	125.1(2)
N(4)-C(14)-C(13)	101.38(19)	C(12)-N(3)-C(13)	112.29(19)
C(16)-C(15)-C(20)	120.1(2)	C(15)-N(3)-C(13)	120.07(19)
C(16)-C(15)-N(3)	118.3(2)	C(12)-N(4)-C(21)	128.4(2)
C(20)-C(15)-N(3)	121.6(2)	C(12)-N(4)-C(14)	111.96(19)
C(17)-C(16)-C(15)	120.4(2)	C(21)-N(4)-C(14)	119.39(19)
C(16)-C(17)-C(18)	120.1(2)	C(6)-Pd(1)-C(1)	170.93(10)
C(19)-C(18)-C(17)	119.3(2)	C(6)-Pd(1)-C(12)	89.86(10)
C(18)-C(19)-C(20)	121.9(2)	C(1)-Pd(1)-C(12)	98.49(10)
C(19)-C(20)-C(15)	118.3(2)	C(6)-Pd(1)-C(11)	87.78(10)
C(19)-C(20)-S(1)	116.73(18)	C(1)-Pd(1)-C(11)	83.82(10)
C(15)-C(20)-S(1)	124.84(18)	C(12)-Pd(1)-C(11)	177.60(9)
C(26)-C(21)-C(22)	122.0(2)	O(3)-S(1)-O(1)	113.47(12)
C(26)-C(21)-N(4)	120.5(2)	O(3)-S(1)-O(2)	112.80(11)
C(22)-C(21)-N(4)	117.3(2)	O(1)-S(1)-O(2)	113.21(12)
C(23)-C(22)-C(21)	117.5(2)	O(3)-S(1)-C(20)	107.00(11)

O(1)-S(1)-C(20)	104.30(11)	O(2)-S(1)-C(20)	105.11(11)

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for Zhou21. 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(1)	20(1)	22(1)	8(1)	3(1)	6(1)
C(2)	31(2)	20(1)	29(2)	15(1)	4(1)	8(1)
C(3)	66(2)	39(2)	29(2)	17(2)	-1(2)	17(2)
C(4)	44(2)	25(2)	26(2)	12(1)	5(1)	13(1)
C(5)	42(2)	47(2)	80(3)	42(2)	22(2)	18(2)
C(6)	18(1)	21(1)	24(1)	8(1)	4(1)	5(1)
C(7)	28(2)	24(1)	33(2)	14(1)	0(1)	12(1)
C(8)	31(2)	25(2)	31(2)	15(1)	0(1)	7(1)
C(9)	31(2)	34(2)	37(2)	16(1)	-7(1)	8(1)
C(10)	44(2)	48(2)	43(2)	27(2)	14(2)	30(2)
C(11)	18(1)	22(1)	33(2)	8(1)	-2(1)	4(1)
C(12)	20(1)	16(1)	17(1)	9(1)	1(1)	8(1)
C(13)	18(1)	19(1)	21(1)	3(1)	2(1)	5(1)
C(14)	22(1)	17(1)	24(1)	3(1)	3(1)	4(1)
C(15)	16(1)	21(1)	17(1)	5(1)	2(1)	7(1)
C(16)	24(1)	19(1)	21(1)	6(1)	4(1)	9(1)
C(17)	24(1)	25(1)	24(1)	13(1)	5(1)	6(1)
C(18)	18(1)	31(2)	19(1)	9(1)	4(1)	8(1)
C(19)	20(1)	23(1)	22(1)	5(1)	1(1)	10(1)
C(20)	18(1)	18(1)	18(1)	7(1)	2(1)	6(1)
C(21)	16(1)	14(1)	22(1)	4(1)	6(1)	4(1)
C(22)	20(1)	18(1)	23(1)	9(1)	4(1)	5(1)
C(23)	18(1)	21(1)	32(2)	8(1)	3(1)	9(1)
C(24)	25(1)	19(1)	26(1)	4(1)	10(1)	7(1)
C(25)	24(1)	21(1)	18(1)	7(1)	6(1)	5(1)
C(26)	16(1)	16(1)	25(1)	7(1)	2(1)	3(1)
C(27)	25(1)	20(1)	21(1)	7(1)	4(1)	9(1)
C(28)	38(2)	25(2)	32(2)	15(1)	10(1)	13(1)
C(29)	31(2)	26(2)	27(2)	8(1)	-2(1)	13(1)
C(30)	25(1)	27(1)	25(1)	8(1)	2(1)	13(1)
C(31)	35(2)	44(2)	30(2)	7(1)	-6(1)	11(1)
C(32)	52(2)	41(2)	32(2)	19(2)	-4(2)	7(2)
C(33)	33(2)	44(2)	45(2)	16(2)	6(1)	7(2)
Cl(1)	41(1)	34(1)	46(1)	18(1)	10(1)	10(1)
Cl(2)	76(1)	39(1)	66(1)	20(1)	16(1)	29(1)
N(1)	25(1)	21(1)	24(1)	9(1)	2(1)	8(1)
N(2)	22(1)	24(1)	30(1)	13(1)	3(1)	7(1)
N(3)	17(1)	17(1)	18(1)	5(1)	4(1)	6(1)
N(4)	17(1)	15(1)	17(1)	3(1)	2(1)	5(1)
O(1)	33(1)	44(1)	58(1)	35(1)	18(1)	24(1)
O(2)	37(1)	22(1)	30(1)	10(1)	5(1)	6(1)
O(3)	30(1)	33(1)	24(1)	14(1)	5(1)	10(1)
Pd(1)	17(1)	16(1)	20(1)	7(1)	2(1)	6(1)
S(1)	24(1)	24(1)	28(1)	15(1)	7(1)	11(1)

Table 5. Hydrogen coordinates [x 10^4] and isotropic displacement parameters [$Å^2$ x 10^3] for Zhou21.

	x	y	z	U(eq)
H(3A)	1964	5308	391	65
H(3B)	1720	6468	614	65
H(3C)	690	5529	927	65
H(4A)	965	6696	2623	45
H(4B)	2019	7696	2404	45
H(4C)	2420	7242	3224	45
H(5A)	4444	6963	2399	75
H(5B)	4058	7394	1558	75
H(5C)	4268	6217	1284	75
H(8A)	2630	835	4822	42
H(8B)	3438	-40	4614	42
H(8C)	2594	52	3736	42
H(9A)	5981	2569	5045	50
H(9B)	5547	1573	5466	50
H(9C)	4656	2382	5598	50
H(10A)	4671	308	2855	58
H(10B)	5589	291	3733	58
H(10C)	5980	1315	3348	58
H(11A)	5115	4532	4007	38
H(11B)	4425	5428	3952	38
H(11C)	5168	4899	3057	38
H(13A)	-398	-160	1144	24
H(13B)	-778	704	721	24
H(14A)	-2003	972	2013	27
H(14B)	-1140	504	2606	27
H(16)	2202	2671	700	25
H(17)	3839	2527	-380	28
H(18)	4606	995	-786	27
H(19)	3808	-331	-49	25
H(23)	-2655	4323	3757	28
H(24)	-2046	4619	5387	29
H(25)	-600	3758	5802	26
H(27)	917	1964	4129	26
H(28A)	-741	1792	5678	44
H(28B)	218	1053	5286	44
H(28C)	-1053	944	4598	44
H(29A)	2288	3634	5213	41
H(29B)	2258	2665	5631	41
H(29C)	1381	3462	6068	41
H(30)	-1412	2716	1697	29
H(31A)	-3923	3089	2204	57
H(31B)	-3685	1920	1905	57
H(31C)	-3610	2541	1121	57
H(32A)	-2024	4735	2332	63
H(32B)	-1688	4177	1259	63
H(32C)	-545	4644	2155	63
H(33A)	553	1817	7542	49
H(33B)	1285	1704	8460	49

Table 6. Torsion angles [°] for Zhou21.

N(3)-C(13)-C(14)-N(4)	21.6(2)	C(9)-C(7)-N(2)-C(6)	-74(6)
C(20)-C(15)-C(16)-C(17)	0.0(4)	C(10)-C(7)-N(2)-C(6)	166(6)
N(3)-C(15)-C(16)-C(17)	-176.5(2)	N(4)-C(12)-N(3)-C(15)	171.2(2)
C(15)-C(16)-C(17)-C(18)	1.6(4)	Pd(1)-C(12)-N(3)-C(15)	-15.0(3)
C(16)-C(17)-C(18)-C(19)	-1.7(4)	N(4)-C(12)-N(3)-C(13)	9.3(3)
C(17)-C(18)-C(19)-C(20)	0.1(4)	Pd(1)-C(12)-N(3)-C(13)	-176.98(15)
C(18)-C(19)-C(20)-C(15)	1.5(4)	C(16)-C(15)-N(3)-C(12)	-52.4(3)
C(18)-C(19)-C(20)-S(1)	177.41(19)	C(20)-C(15)-N(3)-C(12)	131.2(3)
C(16)-C(15)-C(20)-C(19)	-1.5(4)	C(16)-C(15)-N(3)-C(13)	108.3(3)
N(3)-C(15)-C(20)-C(19)	174.8(2)	C(20)-C(15)-N(3)-C(13)	-68.1(3)
C(16)-C(15)-C(20)-S(1)	-177.10(19)	C(14)-C(13)-N(3)-C(12)	-20.3(2)
N(3)-C(15)-C(20)-S(1)	-0.8(3)	C(14)-C(13)-N(3)-C(15)	176.7(2)
C(26)-C(21)-C(22)-C(23)	1.3(4)	N(3)-C(12)-N(4)-C(21)	-178.6(2)
N(4)-C(21)-C(22)-C(23)	176.1(2)	Pd(1)-C(12)-N(4)-C(21)	8.2(3)
C(26)-C(21)-C(22)-C(30)	-179.4(2)	N(3)-C(12)-N(4)-C(14)	6.7(3)
N(4)-C(21)-C(22)-C(30)	-4.6(3)	Pd(1)-C(12)-N(4)-C(14)	-166.56(16)
C(21)-C(22)-C(23)-C(24)	0.9(4)	C(26)-C(21)-N(4)-C(12)	-78.1(3)
C(30)-C(22)-C(23)-C(24)	-178.5(2)	C(22)-C(21)-N(4)-C(12)	107.0(3)
C(22)-C(23)-C(24)-C(25)	-1.5(4)	C(26)-C(21)-N(4)-C(14)	96.3(3)
C(23)-C(24)-C(25)-C(26)	0.0(4)	C(22)-C(21)-N(4)-C(14)	-78.6(3)
C(24)-C(25)-C(26)-C(21)	2.0(4)	C(13)-C(14)-N(4)-C(12)	-18.8(3)
C(24)-C(25)-C(26)-C(27)	-175.2(2)	C(13)-C(14)-N(4)-C(21)	166.0(2)
C(22)-C(21)-C(26)-C(25)	-2.7(4)	N(2)-C(6)-Pd(1)-C(1)	16(28)
N(4)-C(21)-C(26)-C(25)	-177.3(2)	N(2)-C(6)-Pd(1)-C(12)	173(100)
C(22)-C(21)-C(26)-C(27)	174.5(2)	N(2)-C(6)-Pd(1)-C(11)	-6(27)
N(4)-C(21)-C(26)-C(27)	-0.2(3)	N(1)-C(1)-Pd(1)-C(6)	8(2)
C(25)-C(26)-C(27)-C(29)	-54.4(3)	N(1)-C(1)-Pd(1)-C(12)	-148.6(17)
C(21)-C(26)-C(27)-C(29)	128.5(2)	N(1)-C(1)-Pd(1)-C(11)	30.8(17)
C(25)-C(26)-C(27)-C(28)	69.4(3)	N(3)-C(12)-Pd(1)-C(6)	-68.55(19)
C(21)-C(26)-C(27)-C(28)	-107.7(3)	N(4)-C(12)-Pd(1)-C(6)	103.8(2)
C(23)-C(22)-C(30)-C(32)	58.8(3)	N(3)-C(12)-Pd(1)-C(1)	107.92(19)
C(21)-C(22)-C(30)-C(32)	-120.6(3)	N(4)-C(12)-Pd(1)-C(1)	-79.7(2)
C(23)-C(22)-C(30)-C(31)	-62.9(3)	N(3)-C(12)-Pd(1)-C(11)	-57(2)
C(21)-C(22)-C(30)-C(31)	117.8(3)	N(4)-C(12)-Pd(1)-C(11)	116(2)
Pd(1)-C(1)-N(1)-C(2)	-18(3)	C(19)-C(20)-S(1)-O(3)	153.65(19)
C(5)-C(2)-N(1)-C(1)	19(2)	C(15)-C(20)-S(1)-O(3)	-30.7(2)
C(3)-C(2)-N(1)-C(1)	139.4(19)	C(19)-C(20)-S(1)-O(1)	33.1(2)
C(4)-C(2)-N(1)-C(1)	-100.6(19)	C(15)-C(20)-S(1)-O(1)	-151.2(2)
Pd(1)-C(6)-N(2)-C(7)	114(26)	C(19)-C(20)-S(1)-O(2)	-86.2(2)
C(8)-C(7)-N(2)-C(6)	46(6)	C(15)-C(20)-S(1)-O(2)	89.4(2)