Spin-Orbit TDDFT Electronic Structure of Diplatinum(II,II) Complexes

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SUPPLEMENTARY INFORMATION

Crystal and Structural Data

Table S1. Crystal data and structure refinement for CCDC 1049647.

Identification code	CCDC 1049647	
Empirical formula	C108 H98 As4 B8 F16 N6 O20 P8 Pt2	
Formula weight	3128.02	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 16.0077(5) Å	α= 90°
	b = 19.5713(7) Å	β= 96.5736(18)°
	c = 19.0271(6) Å	γ = 90°
Volume	5921.8(3) $Å^3$	
Z	2	
Density (calculated)	1.754 Mg/m^3	
Absorption coefficient	3.671 mm^{-1}	
F(000)	3080	
Crystal size	0.29 x 0.27 x 0.20 mm^3	
Theta range for data collection	1.889 to 41.858°.	
Index ranges	-29<=h<=30, -36<=k<=36, -35<=l<=35	
Reflections collected	327773	
Independent reflections	40315 [R(int) = 0.0464]	
Completeness to theta = 25.000°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.8739	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	40315 / 0 / 778	
Goodness-of-fit on F^2	1.005	
Final R indices [I>2sigma(I)]	R1 = 0.0245, wR2 = 0.0492	
R indices (all data)	R1 = 0.0403, wR2 = 0.0529	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.533 and -0.632 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$x 10^4) for CCDC 1049647. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	3452(2)	56809(2)	50764(2)	71(1)
P(1)	13345(2)	54439(2)	43339(2)	90(1)
P(2)	12899(2)	53438(2)	60099(2)	88(1)
P(3)	-6299(2)	59509(2)	58267(2)	88(1)
P(4)	-5871(2)	60491(2)	41467(2)	90(1)
F(1)	34232(5)	57683(4)	54438(4)	179(1)
F(2)	29260(5)	46770(4)	53256(4)	209(2)
F(3)	8548(6)	67927(4)	65830(4)	243(2)
F(4)	6305(5)	62705(4)	76152(4)	192(2)
F(5)	-3602(5)	73887(4)	51167(4)	183(1)
F(6)	-17866(5)	74762(4)	49486(4)	161(1)
F(7)	9193(5)	69661(4)	36740(5)	222(2)
F(8)	6955(5)	64096(4)	26194(4)	176(1)
O(1)	22560(5)	55584(4)	46442(4)	128(1)
O(2)	22205(5)	54931(4)	59364(4)	121(1)
O(3)	11434(6)	56226(4)	67435(4)	145(2)
O(4)	-2908(5)	60486(5)	66128(4)	171(2)
O(5)	-11988(6)	65633(4)	55951(5)	153(2)
O(6)	-11477(6)	66529(4)	43158(4)	148(2)
O(7)	-2168(5)	62108(5)	34529(4)	151(2)
O(8)	12385(6)	57998(5)	36079(4)	154(2)
O(9)	13197(6)	46421(4)	41267(5)	161(2)
O(10)	12781(5)	45260(4)	61117(4)	131(1)
B(1)	27168(8)	53599(7)	53421(7)	135(2)
B(2)	5955(8)	62071(7)	68956(6)	139(2)
B(3)	-11137(8)	70400(6)	49975(7)	116(2)
B(4)	6661(8)	63684(6)	33383(6)	122(2)
As(1)	37620(2)	79423(2)	38234(2)	109(1)
C(1)	38465(7)	89072(6)	37235(6)	124(2)
C(2)	40186(9)	92997(6)	43368(6)	170(2)

C(3)	40642(9)	100059(6)	42758(7)	190(2)
C(4)	39291(9)	103122(7)	36136(7)	202(2)
C(5)	37473(9)	99190(7)	30085(7)	220(2)
C(6)	37125(8)	92119(6)	30596(6)	168(2)
C(7)	34695(7)	75096(6)	29276(6)	127(2)
C(8)	26930(8)	71920(6)	27692(6)	160(2)
C(9)	25207(9)	68630(7)	21189(7)	200(2)
C(10)	31086(9)	68597(7)	16346(7)	195(2)
C(11)	38821(8)	71780(6)	17983(6)	173(2)
C(12)	40688(8)	75013(6)	24473(6)	150(2)
C(13)	48297(7)	75631(6)	41675(6)	137(2)
C(14)	48911(8)	68539(6)	42389(7)	172(2)
C(15)	56771(8)	65582(7)	44229(7)	206(2)
C(16)	63877(9)	69686(7)	45304(8)	229(2)
C(17)	63193(8)	76744(8)	44582(8)	240(3)
C(18)	55376(8)	79767(7)	42746(7)	192(2)
C(19)	29043(7)	77796(6)	44217(6)	129(2)
C(20)	21894(8)	81906(7)	43177(6)	170(2)
C(21)	15376(8)	80808(8)	47276(7)	199(2)
C(22)	16029(8)	75710(7)	52374(7)	193(2)
C(23)	23162(9)	71673(7)	53394(7)	198(2)
C(24)	29737(8)	72653(6)	49282(7)	174(2)
As(2)	53789(2)	51414(2)	19447(2)	108(1)
C(25)	45611(7)	53197(6)	11521(6)	134(2)
C(26)	47119(8)	58373(6)	6793(6)	165(2)
C(27)	41052(9)	59804(7)	1163(6)	203(2)
C(28)	33644(9)	56075(7)	231(7)	214(2)
C(29)	32185(9)	50912(7)	4949(7)	225(2)
C(30)	38151(8)	49475(7)	10686(7)	194(2)
C(31)	59075(7)	42764(6)	18600(6)	126(2)
C(32)	54000(8)	37134(6)	16576(6)	159(2)
C(33)	57733(8)	30851(6)	15624(7)	179(2)
C(34)	66427(9)	30211(7)	16661(7)	198(2)
C(35)	71438(9)	35768(7)	18869(8)	222(2)
C(36)	67789(8)	42089(6)	19872(7)	188(2)

C(37)	61966(7)	58490(6)	19989(6)	143(2)
C(38)	67867(8)	58709(6)	15129(7)	166(2)
C(39)	73460(8)	64138(7)	15345(7)	205(2)
C(40)	73001(10)	69348(8)	20255(8)	262(3)
C(41)	67084(10)	69135(8)	25010(8)	276(3)
C(42)	61537(9)	63682(7)	24960(7)	209(2)
C(43)	48279(7)	51329(6)	27786(6)	125(2)
C(44)	40547(8)	54562(6)	27939(7)	163(2)
C(45)	36601(8)	54190(7)	34063(7)	189(2)
C(46)	40391(8)	50652(7)	39915(7)	195(2)
C(47)	48139(8)	47559(7)	39761(6)	195(2)
C(48)	52185(7)	47858(7)	33661(6)	154(2)
N(1)	35069(8)	37583(7)	24141(7)	261(2)
C(49)	32328(9)	36785(7)	29340(8)	219(2)
C(50)	28757(12)	35701(10)	35976(9)	368(4)
N(3)	45746(14)	82768(9)	58435(8)	479(5)
C(53)	46622(12)	78113(9)	61896(8)	315(3)
C(54)	47490(20)	72136(15)	66387(16)	753(9)
N(2)	85004(10)	47027(10)	9218(8)	415(4)
C(51)	87788(9)	50124(9)	14003(8)	257(3)
C(52)	91247(10)	54102(8)	20114(7)	243(3)

Table S3. Bond lengths [Å] and angles [°] for CCDC 1049647.

Pt(1)-Pt(1)#1	2.88730(11)
Pt(1)-P(1)	2.2872(3)
Pt(1)-P(2)	2.2938(3)
Pt(1)-P(3)	2.2943(3)
Pt(1)-P(4)	2.2960(3)
P(1)-O(1)	1.5411(9)
P(1)-O(8)	1.5390(9)
P(1)-O(9)	1.6174(9)
P(2)-O(2)	1.5401(8)
P(2)-O(3)	1.5415(8)
P(2)-O(10)	1.6128(9)
P(3)-O(4)	1.5436(9)
P(3)-O(5)	1.5389(9)
P(3)-O(9)#1	1.6115(9)
P(4)-O(6)	1.5399(9)
P(4)-O(7)	1.5407(8)
P(4)-O(10)#1	1.6147(9)
F(1)-B(1)	1.3802(15)
F(2)-B(1)	1.3790(15)
F(3)-B(2)	1.3772(16)
F(4)-B(2)	1.3695(14)
F(5)-B(3)	1.3818(15)
F(6)-B(3)	1.3691(14)
F(7)-B(4)	1.3717(15)
F(8)-B(4)	1.3764(14)
O(1)-B(1)	1.4946(16)
O(2)-B(1)	1.4777(15)
O(3)-B(2)	1.4897(16)
O(4)-B(2)	1.4913(16)
O(5)-B(3)	1.4891(15)
O(6)-B(3)	1.4978(15)
O(7)-B(4)	1.4868(15)
O(8)-B(4)	1.4944(16)

O(9)-P(3)#1	1.6115(9)
O(10)-P(4)#1	1.6148(9)
As(1)-C(1)	1.9043(11)
As(1)-C(7)	1.9129(11)
As(1)-C(13)	1.9090(11)
As(1)-C(19)	1.9079(11)
C(1)-C(2)	1.3979(16)
C(1)-C(6)	1.3911(16)
C(2)-H(2)	0.9500
C(2)-C(3)	1.3897(17)
C(3)-H(3)	0.9500
C(3)-C(4)	1.3897(18)
C(4)-H(4)	0.9500
C(4)-C(5)	1.388(2)
C(5)-H(5)	0.9500
C(5)-C(6)	1.3890(18)
C(6)-H(6)	0.9500
C(7)-C(8)	1.3915(16)
C(7)-C(12)	1.3988(15)
C(8)-H(8)	0.9500
C(8)-C(9)	1.3942(17)
C(9)-H(9)	0.9500
C(9)-C(10)	1.3904(18)
C(10)-H(10)	0.9500
C(10)-C(11)	1.3893(19)
C(11)-H(11)	0.9500
C(11)-C(12)	1.3893(17)
C(12)-H(12)	0.9500
C(13)-C(14)	1.3970(17)
C(13)-C(18)	1.3886(17)
C(14)-H(14)	0.9500
C(14)-C(15)	1.3926(18)
C(15)-H(15)	0.9500
C(15)-C(16)	1.388(2)
C(16)-H(16)	0.9500

C(16)-C(17)	1.391(2)
C(17)-H(17)	0.9500
C(17)-C(18)	1.3920(18)
C(18)-H(18)	0.9500
C(19)-C(20)	1.3941(17)
C(19)-C(24)	1.3893(16)
C(20)-H(20)	0.9500
C(20)-C(21)	1.3891(17)
C(21)-H(21)	0.9500
C(21)-C(22)	1.3870(19)
C(22)-H(22)	0.9500
C(22)-C(23)	1.384(2)
C(23)-H(23)	0.9500
C(23)-C(24)	1.3948(17)
C(24)-H(24)	0.9500
As(2)-C(25)	1.9126(11)
As(2)-C(31)	1.9076(11)
As(2)-C(37)	1.9003(12)
As(2)-C(43)	1.9016(11)
C(25)-C(26)	1.3941(16)
C(25)-C(30)	1.3922(17)
C(26)-H(26)	0.9500
C(26)-C(27)	1.3896(18)
C(27)-H(27)	0.9500
C(27)-C(28)	1.386(2)
C(28)-H(28)	0.9500
C(28)-C(29)	1.389(2)
C(29)-H(29)	0.9500
C(29)-C(30)	1.3943(19)
C(30)-H(30)	0.9500
C(31)-C(32)	1.3967(16)
C(31)-C(36)	1.3944(17)
C(32)-H(32)	0.9500
C(32)-C(33)	1.3880(17)
C(33)-H(33)	0.9500

C(33)-C(34)	1.3886(19)
C(34)-H(34)	0.9500
C(34)-C(35)	1.3877(19)
C(35)-H(35)	0.9500
C(35)-C(36)	1.3906(18)
C(36)-H(36)	0.9500
C(37)-C(38)	1.3962(17)
C(37)-C(42)	1.3952(17)
C(38)-H(38)	0.9500
C(38)-C(39)	1.3870(18)
C(39)-H(39)	0.9500
C(39)-C(40)	1.390(2)
C(40)-H(40)	0.9500
C(40)-C(41)	1.383(2)
C(41)-H(41)	0.9500
C(41)-C(42)	1.3876(19)
C(42)-H(42)	0.9500
C(43)-C(44)	1.3933(16)
C(43)-C(48)	1.3935(16)
C(44)-H(44)	0.9500
C(44)-C(45)	1.3895(17)
C(45)-H(45)	0.9500
C(45)-C(46)	1.3902(19)
C(46)-H(46)	0.9500
C(46)-C(47)	1.3833(19)
C(47)-H(47)	0.9500
C(47)-C(48)	1.3936(16)
C(48)-H(48)	0.9500
N(1)-C(49)	1.1380(18)
C(49)-C(50)	1.460(2)
C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800
N(3)-C(53)	1.123(2)
C(53)-C(54)	1.446(3)

C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
N(2)-C(51)	1.141(2)
C(51)-C(52)	1.455(2)
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800

P(1)-Pt(1)-Pt(1)#1	91.993(7)
P(1)-Pt(1)-P(2)	88.756(10)
P(1)-Pt(1)-P(3)	178.272(10)
P(1)-Pt(1)-P(4)	91.304(10)
P(2)-Pt(1)-Pt(1)#1	91.336(7)
P(2)-Pt(1)-P(3)	91.121(10)
P(2)-Pt(1)-P(4)	178.400(10)
P(3)-Pt(1)-Pt(1)#1	89.734(7)
P(3)-Pt(1)-P(4)	88.771(10)
P(4)-Pt(1)-Pt(1)#1	90.260(7)
O(1)-P(1)-Pt(1)	115.71(3)
O(1)-P(1)-O(9)	102.78(5)
O(8)-P(1)-Pt(1)	117.23(4)
O(8)-P(1)-O(1)	105.72(5)
O(8)-P(1)-O(9)	102.90(5)
O(9)-P(1)-Pt(1)	110.82(3)
O(2)-P(2)-Pt(1)	115.72(3)
O(2)-P(2)-O(3)	105.31(5)
O(2)-P(2)-O(10)	102.94(5)
O(3)-P(2)-Pt(1)	116.38(3)
O(3)-P(2)-O(10)	103.74(5)
O(10)-P(2)-Pt(1)	111.27(3)
O(4)-P(3)-Pt(1)	116.27(3)
O(4)-P(3)-O(9)#1	101.72(5)
O(5)-P(3)-Pt(1)	115.07(3)
O(5)-P(3)-O(4)	108.18(5)

O(5)-P(3)-O(9)#1	100.94(5)
O(9)#1-P(3)-Pt(1)	112.81(3)
O(6)-P(4)-Pt(1)	115.01(3)
O(6)-P(4)-O(7)	108.18(5)
O(6)-P(4)-O(10)#1	101.73(5)
O(7)-P(4)-Pt(1)	116.40(4)
O(7)-P(4)-O(10)#1	101.52(5)
O(10)#1-P(4)-Pt(1)	112.22(3)
B(1)-O(1)-P(1)	130.99(7)
B(1)-O(2)-P(2)	130.27(8)
B(2)-O(3)-P(2)	126.99(8)
B(2)-O(4)-P(3)	126.15(7)
B(3)-O(5)-P(3)	127.14(7)
B(3)-O(6)-P(4)	127.22(7)
B(4)-O(7)-P(4)	129.32(8)
B(4)-O(8)-P(1)	129.75(7)
P(3)#1-O(9)-P(1)	132.56(5)
P(2)-O(10)-P(4)#1	132.24(6)
F(1)-B(1)-O(1)	106.69(9)
F(1)-B(1)-O(2)	107.11(10)
F(2)-B(1)-F(1)	111.55(10)
F(2)-B(1)-O(1)	109.16(10)
F(2)-B(1)-O(2)	109.98(10)
O(2)-B(1)-O(1)	112.33(9)
F(3)-B(2)-O(3)	109.99(10)
F(3)-B(2)-O(4)	109.79(10)
F(4)-B(2)-F(3)	112.12(10)
F(4)-B(2)-O(3)	107.83(10)
F(4)-B(2)-O(4)	107.94(10)
O(3)-B(2)-O(4)	109.10(10)
F(5)-B(3)-O(5)	109.79(10)
F(5)-B(3)-O(6)	109.65(9)
F(6)-B(3)-F(5)	111.62(10)
F(6)-B(3)-O(5)	107.61(9)
F(6)-B(3)-O(6)	107.83(9)

O(5)-B(3)-O(6)	110.29(9)
F(7)-B(4)-F(8)	111.78(10)
F(7)-B(4)-O(7)	110.11(10)
F(7)-B(4)-O(8)	109.77(10)
F(8)-B(4)-O(7)	107.40(9)
F(8)-B(4)-O(8)	107.17(9)
O(7)-B(4)-O(8)	110.55(9)
C(1)-As(1)-C(7)	111.28(5)
C(1)-As(1)-C(13)	110.41(5)
C(1)-As(1)-C(19)	106.81(5)
C(13)-As(1)-C(7)	104.58(5)
C(19)-As(1)-C(7)	109.77(5)
C(19)-As(1)-C(13)	114.06(5)
C(2)-C(1)-As(1)	118.10(8)
C(6)-C(1)-As(1)	120.69(9)
C(6)-C(1)-C(2)	121.18(11)
C(1)-C(2)-H(2)	120.5
C(3)-C(2)-C(1)	118.95(11)
C(3)-C(2)-H(2)	120.5
C(2)-C(3)-H(3)	120.0
C(2)-C(3)-C(4)	120.04(12)
C(4)-C(3)-H(3)	120.0
C(3)-C(4)-H(4)	119.7
C(5)-C(4)-C(3)	120.61(12)
C(5)-C(4)-H(4)	119.7
C(4)-C(5)-H(5)	120.0
C(4)-C(5)-C(6)	120.05(12)
C(6)-C(5)-H(5)	120.0
C(1)-C(6)-H(6)	120.4
C(5)-C(6)-C(1)	119.16(11)
C(5)-C(6)-H(6)	120.4
C(8)-C(7)-As(1)	120.81(8)
C(8)-C(7)-C(12)	121.05(11)
C(12)-C(7)-As(1)	118.10(9)
C(7)-C(8)-H(8)	120.7

C(7)-C(8)-C(9)	118.66(11)
C(9)-C(8)-H(8)	120.7
C(8)-C(9)-H(9)	119.7
C(10)-C(9)-C(8)	120.68(12)
C(10)-C(9)-H(9)	119.7
C(9)-C(10)-H(10)	119.9
C(11)-C(10)-C(9)	120.19(11)
C(11)-C(10)-H(10)	119.9
C(10)-C(11)-H(11)	120.0
C(12)-C(11)-C(10)	119.94(11)
C(12)-C(11)-H(11)	120.0
C(7)-C(12)-H(12)	120.3
C(11)-C(12)-C(7)	119.48(11)
C(11)-C(12)-H(12)	120.3
C(14)-C(13)-As(1)	118.03(9)
C(18)-C(13)-As(1)	120.48(9)
C(18)-C(13)-C(14)	121.18(11)
C(13)-C(14)-H(14)	120.4
C(15)-C(14)-C(13)	119.26(12)
C(15)-C(14)-H(14)	120.4
C(14)-C(15)-H(15)	120.1
C(16)-C(15)-C(14)	119.87(12)
C(16)-C(15)-H(15)	120.1
C(15)-C(16)-H(16)	119.8
C(15)-C(16)-C(17)	120.39(12)
C(17)-C(16)-H(16)	119.8
C(16)-C(17)-H(17)	119.8
C(16)-C(17)-C(18)	120.34(13)
C(18)-C(17)-H(17)	119.8
C(13)-C(18)-C(17)	118.95(12)
C(13)-C(18)-H(18)	120.5
C(17)-C(18)-H(18)	120.5
C(20)-C(19)-As(1)	117.01(8)
C(24)-C(19)-As(1)	121.93(9)
C(24)-C(19)-C(20)	121.04(11)

C(19)-C(20)-H(20)	120.4
C(21)-C(20)-C(19)	119.22(11)
C(21)-C(20)-H(20)	120.4
C(20)-C(21)-H(21)	119.9
C(22)-C(21)-C(20)	120.18(12)
C(22)-C(21)-H(21)	119.9
C(21)-C(22)-H(22)	119.9
C(23)-C(22)-C(21)	120.24(11)
C(23)-C(22)-H(22)	119.9
C(22)-C(23)-H(23)	119.8
C(22)-C(23)-C(24)	120.42(12)
C(24)-C(23)-H(23)	119.8
C(19)-C(24)-C(23)	118.89(12)
C(19)-C(24)-H(24)	120.6
C(23)-C(24)-H(24)	120.6
C(31)-As(2)-C(25)	111.44(5)
C(37)-As(2)-C(25)	108.35(5)
C(37)-As(2)-C(31)	109.99(5)
C(37)-As(2)-C(43)	110.09(5)
C(43)-As(2)-C(25)	108.57(5)
C(43)-As(2)-C(31)	108.38(5)
C(26)-C(25)-As(2)	119.21(9)
C(30)-C(25)-As(2)	119.69(9)
C(30)-C(25)-C(26)	121.07(11)
C(25)-C(26)-H(26)	120.4
C(27)-C(26)-C(25)	119.11(12)
C(27)-C(26)-H(26)	120.4
C(26)-C(27)-H(27)	119.8
C(28)-C(27)-C(26)	120.31(12)
C(28)-C(27)-H(27)	119.8
C(27)-C(28)-H(28)	119.8
C(27)-C(28)-C(29)	120.32(12)
C(29)-C(28)-H(28)	119.8
C(28)-C(29)-H(29)	119.9
C(28)-C(29)-C(30)	120.13(13)

C(30)-C(29)-H(29)	119.9
C(25)-C(30)-C(29)	119.05(12)
C(25)-C(30)-H(30)	120.5
C(29)-C(30)-H(30)	120.5
C(32)-C(31)-As(2)	118.29(9)
C(36)-C(31)-As(2)	120.93(9)
C(36)-C(31)-C(32)	120.78(11)
C(31)-C(32)-H(32)	120.3
C(33)-C(32)-C(31)	119.30(11)
C(33)-C(32)-H(32)	120.3
C(32)-C(33)-H(33)	120.0
C(32)-C(33)-C(34)	120.05(12)
C(34)-C(33)-H(33)	120.0
C(33)-C(34)-H(34)	119.8
C(35)-C(34)-C(33)	120.50(12)
C(35)-C(34)-H(34)	119.8
C(34)-C(35)-H(35)	120.0
C(34)-C(35)-C(36)	120.09(12)
C(36)-C(35)-H(35)	120.0
C(31)-C(36)-H(36)	120.4
C(35)-C(36)-C(31)	119.22(12)
C(35)-C(36)-H(36)	120.4
C(38)-C(37)-As(2)	120.03(9)
C(42)-C(37)-As(2)	118.72(9)
C(42)-C(37)-C(38)	121.08(11)
C(37)-C(38)-H(38)	120.4
C(39)-C(38)-C(37)	119.16(12)
C(39)-C(38)-H(38)	120.4
C(38)-C(39)-H(39)	120.1
C(38)-C(39)-C(40)	119.87(12)
C(40)-C(39)-H(39)	120.1
C(39)-C(40)-H(40)	119.7
C(41)-C(40)-C(39)	120.68(13)
C(41)-C(40)-H(40)	119.7
C(40)-C(41)-H(41)	119.9

C(40)-C(41)-C(42)	120.28(13)
C(42)-C(41)-H(41)	119.9
C(37)-C(42)-H(42)	120.5
C(41)-C(42)-C(37)	118.92(12)
C(41)-C(42)-H(42)	120.5
C(44)-C(43)-As(2)	120.76(9)
C(44)-C(43)-C(48)	121.51(10)
C(48)-C(43)-As(2)	117.72(8)
C(43)-C(44)-H(44)	120.5
C(45)-C(44)-C(43)	118.94(11)
C(45)-C(44)-H(44)	120.5
C(44)-C(45)-H(45)	120.0
C(44)-C(45)-C(46)	119.94(12)
C(46)-C(45)-H(45)	120.0
C(45)-C(46)-H(46)	119.6
C(47)-C(46)-C(45)	120.74(11)
C(47)-C(46)-H(46)	119.6
C(46)-C(47)-H(47)	119.9
C(46)-C(47)-C(48)	120.17(12)
C(48)-C(47)-H(47)	119.9
C(43)-C(48)-C(47)	118.68(11)
C(43)-C(48)-H(48)	120.7
C(47)-C(48)-H(48)	120.7
N(1)-C(49)-C(50)	179.38(17)
C(49)-C(50)-H(50A)	109.5
C(49)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
N(3)-C(53)-C(54)	178.3(2)
C(53)-C(54)-H(54A)	109.5
C(53)-C(54)-H(54B)	109.5
C(53)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54B)	109.5

H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
N(2)-C(51)-C(52)	179.38(19)
C(51)-C(52)-H(52A)	109.5
C(51)-C(52)-H(52B)	109.5
C(51)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5

Symmetry transformations used to generate equivalent atoms:

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

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for CCDC 1049647. 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}
Pt(1)	73(1)	67(1)	76(1)	1(1)	20(1)	5(1)
P(1)	89(1)	89(1)	97(1)	1(1)	34(1)	3(1)
P(2)	83(1)	94(1)	89(1)	1(1)	16(1)	3(1)
P(3)	89(1)	84(1)	94(1)	-6(1)	28(1)	8(1)
P(4)	95(1)	83(1)	92(1)	8(1)	14(1)	8(1)
F(1)	87(3)	244(4)	204(3)	42(3)	12(2)	-30(3)
F(2)	230(4)	151(3)	261(4)	42(3)	93(3)	76(3)
F(3)	338(5)	154(3)	236(4)	8(3)	24(3)	-55(3)
F(4)	206(4)	266(4)	99(3)	-53(3)	1(3)	49(3)
F(5)	132(3)	172(3)	242(3)	-5(3)	2(3)	-26(3)
F(6)	138(3)	132(3)	211(3)	0(2)	17(3)	62(2)
F(7)	242(4)	150(3)	277(4)	-65(3)	39(3)	-51(3)
F(8)	198(3)	224(4)	111(3)	51(3)	44(2)	-4(3)
O(1)	94(3)	164(4)	132(3)	9(3)	32(3)	-9(3)
O(2)	89(3)	146(3)	129(3)	6(3)	21(3)	-6(3)
O(3)	153(4)	185(4)	97(3)	-19(3)	11(3)	53(3)
O(4)	124(3)	282(5)	109(3)	-46(3)	20(3)	28(3)
O(5)	161(4)	140(3)	170(4)	39(3)	77(3)	66(3)
O(6)	173(4)	126(3)	137(3)	-10(3)	-16(3)	65(3)
O(7)	128(3)	214(4)	114(3)	49(3)	23(3)	-10(3)
O(8)	158(4)	197(4)	117(3)	41(3)	59(3)	44(3)
O(9)	161(4)	106(3)	238(4)	-43(3)	116(3)	-24(3)
O(10)	121(3)	99(3)	163(3)	25(3)	-20(3)	-12(3)
B(1)	94(4)	146(5)	168(5)	21(4)	30(4)	15(4)
B(2)	155(5)	153(5)	108(4)	-22(4)	11(4)	12(4)
B(3)	105(4)	95(4)	148(5)	3(4)	21(4)	21(4)
B(4)	134(5)	128(5)	109(4)	10(4)	30(4)	-13(4)
As(1)	103(1)	105(1)	119(1)	10(1)	13(1)	-1(1)
C(1)	121(4)	115(4)	138(4)	17(3)	18(3)	5(3)
C(2)	231(5)	134(4)	141(4)	11(4)	9(4)	6(4)

C(3)	237(6)	138(5)	193(5)	-11(4)	15(4)	-2(4)
C(4)	232(6)	130(5)	244(6)	42(4)	33(5)	3(4)
C(5)	294(7)	170(5)	191(5)	71(4)	8(5)	-16(5)
C(6)	203(5)	165(5)	134(4)	19(4)	9(4)	-30(4)
C(7)	127(4)	124(4)	132(4)	4(3)	22(3)	-3(3)
C(8)	139(5)	172(5)	173(5)	-16(4)	32(4)	-23(4)
C(9)	193(5)	215(6)	187(5)	-51(4)	6(4)	-46(4)
C(10)	261(6)	168(5)	155(5)	-26(4)	23(4)	13(5)
C(11)	222(5)	153(5)	155(5)	10(4)	66(4)	16(4)
C(12)	147(5)	144(4)	168(5)	7(4)	49(4)	-11(4)
C(13)	121(4)	134(4)	151(4)	8(3)	-3(3)	13(3)
C(14)	153(5)	136(4)	221(5)	-11(4)	-10(4)	1(4)
C(15)	190(5)	160(5)	262(6)	13(4)	-1(5)	41(4)
C(16)	154(5)	233(6)	289(6)	23(5)	-24(5)	51(5)
C(17)	127(5)	227(6)	354(7)	23(5)	-23(5)	-14(4)
C(18)	142(5)	158(5)	268(6)	26(4)	-7(4)	-5(4)
C(19)	130(4)	121(4)	136(4)	-5(3)	21(3)	-16(3)
C(20)	154(5)	212(5)	145(4)	30(4)	27(4)	27(4)
C(21)	137(5)	301(6)	162(5)	-5(4)	30(4)	19(4)
C(22)	178(5)	245(6)	164(5)	-32(4)	50(4)	-76(4)
C(23)	252(6)	158(5)	196(5)	20(4)	84(5)	-43(4)
C(24)	200(5)	143(5)	186(5)	32(4)	56(4)	4(4)
As(2)	113(1)	102(1)	110(1)	6(1)	16(1)	-13(1)
C(25)	148(4)	126(4)	125(4)	8(3)	5(3)	0(4)
C(26)	199(5)	152(4)	145(4)	25(4)	29(4)	-4(4)
C(27)	289(6)	186(5)	131(4)	34(4)	14(4)	30(5)
C(28)	247(6)	222(6)	157(5)	-8(4)	-47(4)	49(5)
C(29)	196(6)	225(6)	235(6)	10(5)	-51(5)	-13(5)
C(30)	182(5)	185(5)	204(5)	45(4)	-26(4)	-42(4)
C(31)	143(4)	114(4)	123(4)	1(3)	26(3)	2(3)
C(32)	158(5)	141(4)	181(5)	-25(4)	33(4)	-14(4)
C(33)	220(5)	133(4)	185(5)	-27(4)	22(4)	-13(4)
C(34)	247(6)	150(5)	191(5)	-9(4)	2(4)	49(4)
C(35)	170(5)	181(5)	304(6)	-8(5)	-28(5)	35(4)
C(36)	149(5)	149(5)	254(6)	-3(4)	-23(4)	-2(4)

C(37)	138(4)	131(4)	160(4)	1(4)	18(4)	-30(4)
C(38)	154(5)	155(5)	192(5)	12(4)	39(4)	-21(4)
C(39)	161(5)	230(6)	224(5)	50(5)	25(4)	-51(4)
C(40)	263(7)	244(6)	276(6)	4(5)	15(5)	-130(5)
C(41)	330(8)	228(6)	274(7)	-82(5)	44(6)	-128(6)
C(42)	235(6)	193(5)	204(5)	-52(4)	51(5)	-61(5)
C(43)	128(4)	129(4)	123(4)	1(3)	29(3)	-13(3)
C(44)	161(5)	138(4)	193(5)	17(4)	35(4)	23(4)
C(45)	159(5)	178(5)	242(6)	-18(4)	76(4)	10(4)
C(46)	189(5)	234(6)	176(5)	-20(4)	74(4)	-17(4)
C(47)	192(5)	268(6)	129(4)	11(4)	37(4)	-3(5)
C(48)	133(4)	202(5)	128(4)	10(4)	22(4)	9(4)
N(1)	268(6)	267(6)	251(5)	-2(5)	38(5)	-65(5)
C(49)	184(5)	202(6)	277(6)	-28(5)	49(5)	-38(4)
C(50)	398(9)	393(9)	357(8)	-113(7)	238(7)	-145(7)
N(3)	832(14)	296(7)	278(7)	2(6)	-62(8)	-23(8)
C(53)	403(9)	297(8)	246(7)	-13(6)	38(6)	68(7)
C(54)	840(20)	628(17)	791(19)	428(15)	103(16)	198(15)
N(2)	342(8)	618(11)	283(7)	-76(7)	25(6)	-120(8)
C(51)	188(6)	377(8)	208(6)	32(5)	27(5)	-32(5)
C(52)	248(6)	266(7)	206(6)	34(5)	-12(5)	-38(5)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for CCDC 1049647.

	x	y	z	U(eq)
H(2)	4103	9087	4788	20
H(3)	4188	10279	4687	23
H(4)	3961	10795	3575	24
H(5)	3647	10134	2559	26
H(6)	3599	8940	2646	20
H(8)	2289	7199	3098	19
H(9)	1996	6639	2005	24
H(10)	2981	6639	1191	23
H(11)	4283	7175	1467	21
H(12)	4599	7715	2564	18
H(14)	4402	6576	4163	21
H(15)	5727	6077	4475	25
H(16)	6924	6766	4654	27
H(17)	6809	7951	4535	29
H(18)	5489	8458	4223	23
H(20)	2149	8542	3970	20
H(21)	1046	8356	4659	24
H(22)	1156	7499	5518	23
H(23)	2358	6821	5692	24
H(24)	3461	6985	4993	21
H(26)	5223	6089	741	20
H(27)	4198	6335	-206	24
H(28)	2955	5706	-365	26
H(29)	2711	4836	427	27
H(30)	3714	4601	1398	23
H(32)	4806	3760	1586	19
H(33)	5434	2699	1426	22
H(34)	6896	2594	1585	24
H(35)	7737	3525	1970	27
H(36)	7119	4590	2141	23

H(38)	6805	5518	1172	20
H(39)	7760	6430	1214	25
H(40)	7679	7309	2035	31
H(41)	6682	7274	2832	33
H(42)	5751	6349	2826	25
H(44)	3801	5698	2392	20
H(45)	3132	5635	3425	23
H(46)	3763	5035	4407	23
H(47)	5071	4523	4382	23
H(48)	5750	4574	3351	18
H(50A)	2379	3276	3513	55
H(50B)	2713	4011	3785	55
H(50C)	3295	3351	3941	55
H(54A)	4861	6813	6355	113
H(54B)	4228	7142	6854	113
H(54C)	5217	7281	7012	113
H(52A)	9365	5835	1851	36
H(52B)	9565	5145	2290	36
H(52C)	8677	5518	2305	36

Table S6. Torsion angles [°] for CCDC 1049647.

Pt(1)-P(1)-O(1)-B(1)	45.77(11)
Pt(1)-P(1)-O(8)-B(4)	10.47(12)
Pt(1)-P(1)-O(9)-P(3)#1	17.78(9)
Pt(1)-P(2)-O(2)-B(1)	-48.25(11)
Pt(1)-P(2)-O(3)-B(2)	-15.89(11)
Pt(1)-P(2)-O(10)-P(4)#1	-20.31(8)
Pt(1)-P(3)-O(4)-B(2)	21.07(11)
Pt(1)-P(3)-O(5)-B(3)	-8.12(11)
Pt(1)-P(4)-O(6)-B(3)	3.63(11)
Pt(1)-P(4)-O(7)-B(4)	-20.56(11)
P(1)-O(1)-B(1)-F(1)	-160.71(8)
P(1)-O(1)-B(1)-F(2)	78.62(12)
P(1)-O(1)-B(1)-O(2)	-43.64(15)
P(1)-O(8)-B(4)-F(7)	70.45(13)
P(1)-O(8)-B(4)-F(8)	-167.97(8)
P(1)-O(8)-B(4)-O(7)	-51.22(14)
P(2)-O(2)-B(1)-F(1)	161.73(8)
P(2)-O(2)-B(1)-F(2)	-76.89(13)
P(2)-O(2)-B(1)-O(1)	44.91(14)
P(2)-O(3)-B(2)-F(3)	-58.98(14)
P(2)-O(3)-B(2)-F(4)	178.48(8)
P(2)-O(3)-B(2)-O(4)	61.50(13)
P(3)-O(4)-B(2)-F(3)	55.96(13)
P(3)-O(4)-B(2)-F(4)	178.44(8)
P(3)-O(4)-B(2)-O(3)	-64.64(13)
P(3)-O(5)-B(3)-F(5)	-62.72(13)
P(3)-O(5)-B(3)-F(6)	175.60(8)
P(3)-O(5)-B(3)-O(6)	58.22(13)
P(4)-O(6)-B(3)-F(5)	65.68(12)
P(4)-O(6)-B(3)-F(6)	-172.59(8)
P(4)-O(6)-B(3)-O(5)	-55.34(13)
P(4)-O(7)-B(4)-F(7)	-63.90(13)
P(4)-O(7)-B(4)-F(8)	174.17(8)

P(4)-O(7)-B(4)-O(8)	57.56(13)
O(1)-P(1)-O(8)-B(4)	-120.20(10)
O(1)-P(1)-O(9)-P(3)#1	141.98(8)
O(2)-P(2)-O(3)-B(2)	113.75(10)
O(2)-P(2)-O(10)-P(4)#1	-144.86(7)
O(3)-P(2)-O(2)-B(1)	-178.27(10)
O(3)-P(2)-O(10)-P(4)#1	105.56(8)
O(4)-P(3)-O(5)-B(3)	123.79(10)
O(5)-P(3)-O(4)-B(2)	-110.19(10)
O(6)-P(4)-O(7)-B(4)	110.73(10)
O(7)-P(4)-O(6)-B(3)	-128.41(9)
O(8)-P(1)-O(1)-B(1)	177.31(10)
O(8)-P(1)-O(9)-P(3)#1	-108.32(9)
O(9)-P(1)-O(1)-B(1)	-75.14(10)
O(9)-P(1)-O(8)-B(4)	132.33(10)
O(9)#1-P(3)-O(4)-B(2)	144.02(10)
O(9)#1-P(3)-O(5)-B(3)	-129.88(10)
O(10)-P(2)-O(2)-B(1)	73.33(10)
O(10)-P(2)-O(3)-B(2)	-138.44(10)
O(10)#1-P(4)-O(6)-B(3)	125.16(9)
O(10)#1-P(4)-O(7)-B(4)	-142.70(10)
As(1)-C(1)-C(2)-C(3)	-178.59(10)
As(1)-C(1)-C(6)-C(5)	177.55(10)
As(1)-C(7)-C(8)-C(9)	-177.77(10)
As(1)-C(7)-C(12)-C(11)	178.61(9)
As(1)-C(13)-C(14)-C(15)	173.85(10)
As(1)-C(13)-C(18)-C(17)	-173.69(11)
As(1)-C(19)-C(20)-C(21)	178.37(10)
As(1)-C(19)-C(24)-C(23)	-178.92(10)
C(1)-C(2)-C(3)-C(4)	0.8(2)
C(2)-C(1)-C(6)-C(5)	-0.29(19)
C(2)-C(3)-C(4)-C(5)	0.1(2)
C(3)-C(4)-C(5)-C(6)	-1.1(2)
C(4)-C(5)-C(6)-C(1)	1.2(2)
C(6)-C(1)-C(2)-C(3)	-0.70(19)

C(7)-C(8)-C(9)-C(10)	-0.8(2)
C(8)-C(7)-C(12)-C(11)	0.80(18)
C(8)-C(9)-C(10)-C(11)	0.9(2)
C(9)-C(10)-C(11)-C(12)	-0.07(19)
C(10)-C(11)-C(12)-C(7)	-0.75(18)
C(12)-C(7)-C(8)-C(9)	-0.02(18)
C(13)-C(14)-C(15)-C(16)	-0.2(2)
C(14)-C(13)-C(18)-C(17)	-0.2(2)
C(14)-C(15)-C(16)-C(17)	0.3(2)
C(15)-C(16)-C(17)-C(18)	-0.3(2)
C(16)-C(17)-C(18)-C(13)	0.2(2)
C(18)-C(13)-C(14)-C(15)	0.21(19)
C(19)-C(20)-C(21)-C(22)	0.5(2)
C(20)-C(19)-C(24)-C(23)	-0.51(19)
C(20)-C(21)-C(22)-C(23)	-0.2(2)
C(21)-C(22)-C(23)-C(24)	-0.4(2)
C(22)-C(23)-C(24)-C(19)	0.79(19)
C(24)-C(19)-C(20)-C(21)	-0.11(19)
As(2)-C(25)-C(26)-C(27)	-177.99(9)
As(2)-C(25)-C(30)-C(29)	178.91(11)
As(2)-C(31)-C(32)-C(33)	177.20(9)
As(2)-C(31)-C(36)-C(35)	-176.93(10)
As(2)-C(37)-C(38)-C(39)	176.16(10)
As(2)-C(37)-C(42)-C(41)	-175.05(12)
As(2)-C(43)-C(44)-C(45)	177.92(9)
As(2)-C(43)-C(48)-C(47)	-178.13(10)
C(25)-C(26)-C(27)-C(28)	-0.71(19)
C(26)-C(25)-C(30)-C(29)	1.0(2)
C(26)-C(27)-C(28)-C(29)	0.6(2)
C(27)-C(28)-C(29)-C(30)	0.4(2)
C(28)-C(29)-C(30)-C(25)	-1.2(2)
C(30)-C(25)-C(26)-C(27)	-0.08(18)
C(31)-C(32)-C(33)-C(34)	-0.19(18)
C(32)-C(31)-C(36)-C(35)	2.19(19)
C(32)-C(33)-C(34)-C(35)	2.1(2)

C(33)-C(34)-C(35)-C(36)	-1.8(2)
C(34)-C(35)-C(36)-C(31)	-0.3(2)
C(36)-C(31)-C(32)-C(33)	-1.94(18)
C(37)-C(38)-C(39)-C(40)	-1.5(2)
C(38)-C(37)-C(42)-C(41)	0.2(2)
C(38)-C(39)-C(40)-C(41)	0.9(2)
C(39)-C(40)-C(41)-C(42)	0.3(3)
C(40)-C(41)-C(42)-C(37)	-0.8(2)
C(42)-C(37)-C(38)-C(39)	1.00(19)
C(43)-C(44)-C(45)-C(46)	0.23(19)
C(44)-C(43)-C(48)-C(47)	1.02(18)
C(44)-C(45)-C(46)-C(47)	0.9(2)
C(45)-C(46)-C(47)-C(48)	-1.1(2)
C(46)-C(47)-C(48)-C(43)	0.1(2)
C(48)-C(43)-C(44)-C(45)	-1.21(18)

Symmetry transformations used to generate equivalent atoms:

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

Table S7. Hydrogen bonds for CCDC 1049647 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(2)-H(2)...N(3)	0.95	2.60	3.526(2)	164.5
C(8)-H(8)...F(7)	0.95	2.60	3.5128(14)	161.0
C(12)-H(12)...F(4)#2	0.95	2.58	3.4563(14)	154.1
C(24)-H(24)...F(1)	0.95	2.53	3.1468(15)	122.4
C(30)-H(30)...N(1)	0.95	2.59	3.5361(18)	173.1
C(48)-H(48)...F(1)#3	0.95	2.60	3.1470(14)	116.9
C(52)-H(52A)...N(3)#2	0.98	2.64	3.525(2)	150.7

Symmetry transformations used to generate equivalent atoms:

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