dien_PtC7pyrene_7

測定日	14/10/20	測定者名	dien
化合物名	PtC7pyrene	構造	
略称(10字以内)	PtC7pyrene		
組成	C48H48N2O2Pt		
分子量	879.98		
使用溶媒	CHCl3-EtOAc		
結晶化方法	気相拡散法		
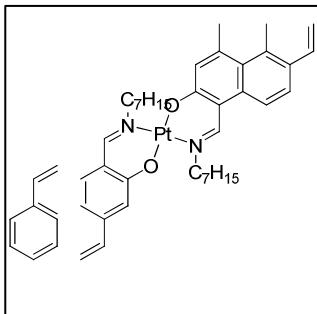
Crystal shape	plate	Note
Crystal color	red	
Crystal size	0.04 x 0.03 x 0.03	
Machine	rigaku, xtallab	
Mounting	cryoloop, palaton	
Temp	-100 C	
Exposure time	6	
Number of frame	width 0.5	

Crystal system	Monoclinic	Note
Space group	P21/c	1/2分子
Z	2	
a	4.8015(9)	
b	14.434(2)	
c	27.072(5)	
α	90	
β	93.043(7)	
γ	90	
V	1873.6(6)	
R factor	0.0500	

ORTEP 50% probability
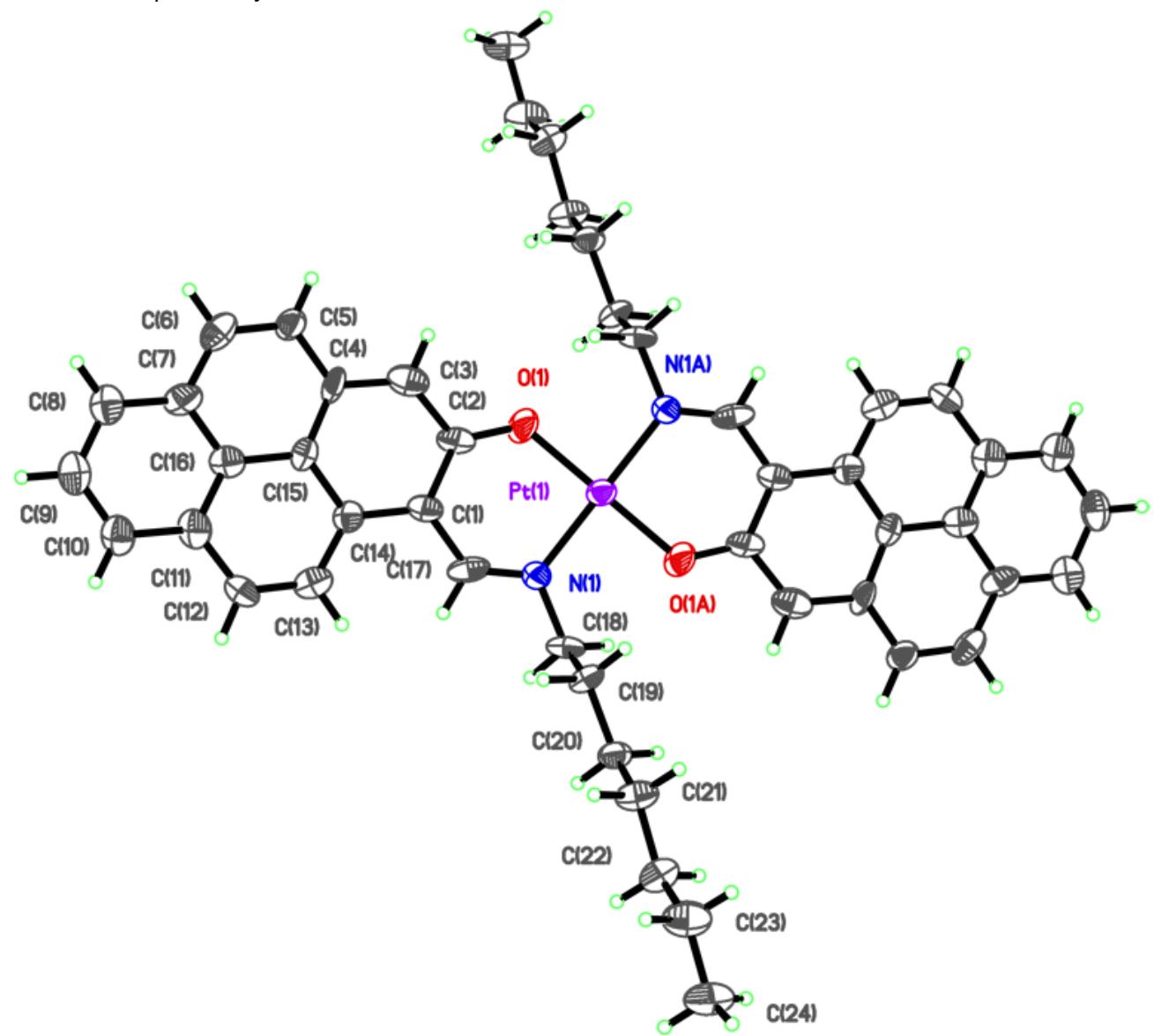
checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: P21c

```
Bond precision:    C-C = 0.0140 A          Wavelength=0.71075

Cell:              a=4.8015(9)      b=14.434(2)         c=27.072(5)
                   alpha=90         beta=93.043(7)      gamma=90
Temperature:       173 K

                   Calculated                   Reported
Volume             1873.6(6)                    1873.6(6)
Space group        P 21/c                       P 21/c
Hall group         -P 2ybc                      -P 2ybc
Moiety formula     C48 H48 N2 O2 Pt             ?
Sum formula        C48 H48 N2 O2 Pt             C48 H48 N2 O2 Pt
Mr                 879.96                       879.97
Dx,g cm-3          1.560                        1.560
Z                  2                            2
Mu (mm-1)          3.788                        3.788
F000               888.0                        888.0
F000'              884.94
h,k,lmax           6,18,35                      6,18,35
Nref               4324                         4308
Tmin,Tmax          0.873,0.893                  0.737,1.000
Tmin'              0.859

Correction method= EMPIRICAL

Data completeness= 0.996         Theta(max)= 27.524

R(reflections)= 0.0500( 2911)    wR2(reflections)= 0.2349( 4308)

S = 1.194                  Npar= 242
```

The following ALERTS were generated. Each ALERT has the format
    test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
            a literature citation. This should be contained in the
            _exptl_absorpt_process_details field.
            Absorption correction given as empirical
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N1      -- C17      ..        5.2 su
PLAT234_ALERT_4_C Large Hirshfeld Difference C3      -- C4       ..       0.20 Ang.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............   0.0140 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H13    .. H17      ..       1.95 Ang.
```

Alert level G

```
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.      0.13 Report
PLAT333_ALERT_2_G Check Large Av C6-Ring C-C Dist. C1      -C14          1.43 Ang.
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   2 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

# PLATON version of 20/08/2014; check.def file version of 18/08/2014
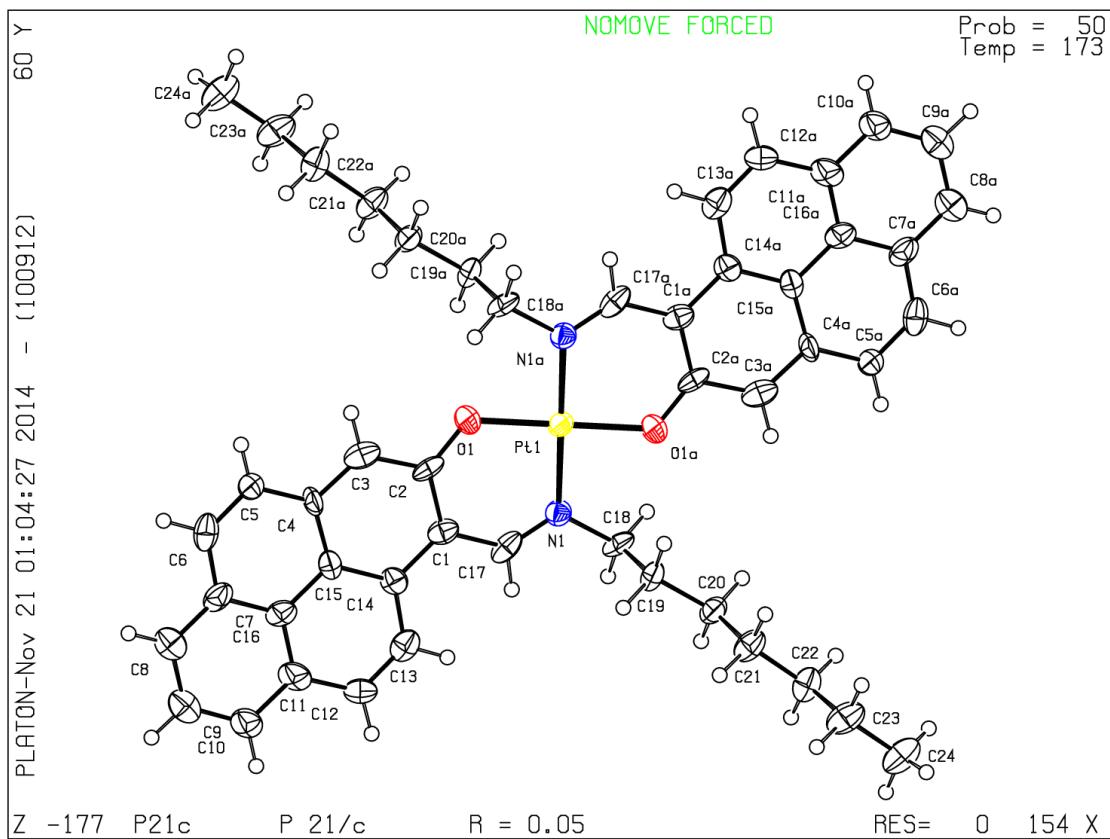
Table 7.   Crystal data and structure refinement for P21c.

Identification code	P21c
Empirical formula	C48 H48 N2 O2 Pt
Formula weight	879.97
Temperature	173(2) K
Wavelength	0.71075 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 4.8015(9) Å $\alpha = 90°$.
	b = 14.434(2) Å $\beta = 93.043(7)°$.
	c = 27.072(5) Å $\gamma = 90°$.
Volume	1873.6(6) Å^3
Z	2
Density (calculated)	1.560 Mg/m^3
Absorption coefficient	3.788 mm^{-1}
F(000)	888
Crystal size	0.040 x 0.030 x 0.030 mm^3
Theta range for data collection	3.014 to 27.524°.
Index ranges	-6<=h<=6, -18<=k<=18, -35<=l<=35
Reflections collected	17433
Independent reflections	4308 [R(int) = 0.0915]
Completeness to theta = 25.242°	99.8 %
Absorption correction	Empirical
Max. and min. transmission	1.000 and 0.737
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4308 / 0 / 242
Goodness-of-fit on F^2	1.194
Final R indices [I>2sigma(I)]	R1 = 0.0500, wR2 = 0.1435
R indices (all data)	R1 = 0.0881, wR2 = 0.2349
Extinction coefficient	n/a
Largest diff. peak and hole	2.299 and -2.736 e.Å^{-3}

Table 8.   Atomic coordinates   (x 10^4) and equivalent   isotropic displacement parameters (Å^2x 10^3) for P21c.   U(eq) is defined as one third of   the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7152(19)	9188(6)	1109(3)	34(2)
C(2)	8270(20)	10032(5)	938(4)	32(2)
C(3)	10410(20)	10473(7)	1251(4)	43(2)
C(4)	11530(30)	10099(6)	1697(4)	36(2)
C(5)	13740(20)	10528(7)	1962(3)	39(2)
C(6)	14730(30)	10140(7)	2384(4)	42(3)
C(7)	13780(20)	9277(6)	2571(4)	41(2)
C(8)	14940(20)	8881(7)	3001(4)	42(2)
C(9)	13870(20)	8046(7)	3173(3)	43(2)
C(10)	11760(20)	7583(8)	2903(4)	43(2)
C(11)	10620(20)	7975(7)	2464(4)	41(2)
C(12)	8410(20)	7522(7)	2167(4)	38(2)
C(13)	7380(20)	7914(7)	1753(4)	39(2)
C(14)	8258(18)	8772(6)	1567(3)	32(2)
C(15)	10499(18)	9227(6)	1842(3)	30(2)
C(16)	11581(19)	8822(6)	2297(4)	35(2)
C(17)	4921(18)	8743(6)	834(4)	37(2)
C(18)	1480(20)	8318(6)	213(4)	38(2)
C(19)	2620(18)	7568(6)	-84(3)	32(2)
C(20)	337(19)	6895(6)	-276(4)	35(2)
C(21)	1320(20)	6096(6)	-568(4)	42(2)
C(22)	-880(20)	5381(8)	-721(4)	43(2)
C(23)	110(30)	4591(8)	-1041(5)	53(3)
C(24)	-2090(20)	3896(7)	-1187(5)	54(3)
N(1)	3695(15)	8951(5)	412(2)	31(2)
O(1)	7485(15)	10479(5)	535(2)	44(2)
Pt(1)	5000	10000	0	30(1)

Table 9.   Bond lengths [Å] and angles [°] for   P21c.

_____

C(1)-C(2)	1.418(11)
C(1)-C(17)	1.425(12)
C(1)-C(14)	1.453(12)
C(2)-O(1)	1.307(13)
C(2)-C(3)	1.446(16)
C(3)-C(4)	1.403(14)
C(3)-H(3)	0.9500
C(4)-C(5)	1.393(13)
C(4)-C(15)	1.417(13)
C(5)-C(6)	1.337(15)
C(5)-H(5)	0.9500
C(6)-C(7)	1.429(14)
C(6)-H(6)	0.9500
C(7)-C(8)	1.388(14)
C(7)-C(16)	1.419(13)
C(8)-C(9)	1.398(14)
C(8)-H(8)	0.9500
C(9)-C(10)	1.389(15)
C(9)-H(9)	0.9500
C(10)-C(11)	1.400(14)
C(10)-H(10)	0.9500
C(11)-C(16)	1.391(13)
C(11)-C(12)	1.452(15)
C(12)-C(13)	1.328(14)
C(12)-H(12)	0.9500
C(13)-C(14)	1.409(13)
C(13)-H(13)	0.9500
C(14)-C(15)	1.435(12)
C(15)-C(16)	1.434(12)
C(17)-N(1)	1.294(12)
C(17)-H(17)	0.9500

C(18)-C(19)	1.471(12)
C(18)-N(1)	1.482(11)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.534(11)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-C(21)	1.490(12)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-C(22)	1.519(13)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(23)	1.524(15)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(24)	1.497(15)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
N(1)-Pt(1)	2.000(7)
O(1)-Pt(1)	1.953(6)
Pt(1)-O(1)#1	1.953(6)
Pt(1)-N(1)#1	2.000(7)
C(2)-C(1)-C(17)	120.2(10)
C(2)-C(1)-C(14)	120.4(9)
C(17)-C(1)-C(14)	119.3(8)
O(1)-C(2)-C(1)	126.9(10)
O(1)-C(2)-C(3)	115.9(8)
C(1)-C(2)-C(3)	117.2(10)

C(4)-C(3)-C(2)	124.3(9)
C(4)-C(3)-H(3)	117.9
C(2)-C(3)-H(3)	117.9
C(5)-C(4)-C(3)	121.2(10)
C(5)-C(4)-C(15)	121.4(9)
C(3)-C(4)-C(15)	117.2(9)
C(6)-C(5)-C(4)	118.6(10)
C(6)-C(5)-H(5)	120.7
C(4)-C(5)-H(5)	120.7
C(5)-C(6)-C(7)	124.3(10)
C(5)-C(6)-H(6)	117.9
C(7)-C(6)-H(6)	117.9
C(8)-C(7)-C(16)	120.3(9)
C(8)-C(7)-C(6)	122.3(10)
C(16)-C(7)-C(6)	117.4(9)
C(7)-C(8)-C(9)	119.6(10)
C(7)-C(8)-H(8)	120.2
C(9)-C(8)-H(8)	120.2
C(10)-C(9)-C(8)	120.8(9)
C(10)-C(9)-H(9)	119.6
C(8)-C(9)-H(9)	119.6
C(9)-C(10)-C(11)	119.5(11)
C(9)-C(10)-H(10)	120.2
C(11)-C(10)-H(10)	120.2
C(16)-C(11)-C(10)	120.7(10)
C(16)-C(11)-C(12)	117.4(9)
C(10)-C(11)-C(12)	121.9(10)
C(13)-C(12)-C(11)	120.3(9)
C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(12)-C(13)-C(14)	124.8(9)
C(12)-C(13)-H(13)	117.6
C(14)-C(13)-H(13)	117.6

C(13)-C(14)-C(15)	116.6(8)
C(13)-C(14)-C(1)	124.4(8)
C(15)-C(14)-C(1)	118.9(8)
C(4)-C(15)-C(14)	121.8(8)
C(4)-C(15)-C(16)	119.0(8)
C(14)-C(15)-C(16)	119.1(8)
C(11)-C(16)-C(7)	119.1(9)
C(11)-C(16)-C(15)	121.8(9)
C(7)-C(16)-C(15)	119.1(9)
N(1)-C(17)-C(1)	130.7(9)
N(1)-C(17)-H(17)	114.7
C(1)-C(17)-H(17)	114.7
C(19)-C(18)-N(1)	111.8(8)
C(19)-C(18)-H(18A)	109.3
N(1)-C(18)-H(18A)	109.3
C(19)-C(18)-H(18B)	109.3
N(1)-C(18)-H(18B)	109.3
H(18A)-C(18)-H(18B)	107.9
C(18)-C(19)-C(20)	111.7(7)
C(18)-C(19)-H(19A)	109.3
C(20)-C(19)-H(19A)	109.3
C(18)-C(19)-H(19B)	109.3
C(20)-C(19)-H(19B)	109.3
H(19A)-C(19)-H(19B)	107.9
C(21)-C(20)-C(19)	115.4(8)
C(21)-C(20)-H(20A)	108.4
C(19)-C(20)-H(20A)	108.4
C(21)-C(20)-H(20B)	108.4
C(19)-C(20)-H(20B)	108.4
H(20A)-C(20)-H(20B)	107.5
C(20)-C(21)-C(22)	115.7(8)
C(20)-C(21)-H(21A)	108.3
C(22)-C(21)-H(21A)	108.3

C(20)-C(21)-H(21B)	108.3
C(22)-C(21)-H(21B)	108.3
H(21A)-C(21)-H(21B)	107.4
C(21)-C(22)-C(23)	115.4(9)
C(21)-C(22)-H(22A)	108.4
C(23)-C(22)-H(22A)	108.4
C(21)-C(22)-H(22B)	108.4
C(23)-C(22)-H(22B)	108.4
H(22A)-C(22)-H(22B)	107.5
C(24)-C(23)-C(22)	114.5(10)
C(24)-C(23)-H(23A)	108.6
C(22)-C(23)-H(23A)	108.6
C(24)-C(23)-H(23B)	108.6
C(22)-C(23)-H(23B)	108.6
H(23A)-C(23)-H(23B)	107.6
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(17)-N(1)-C(18)	117.6(8)
C(17)-N(1)-Pt(1)	121.8(6)
C(18)-N(1)-Pt(1)	120.3(6)
C(2)-O(1)-Pt(1)	125.6(6)
O(1)#1-Pt(1)-O(1)	180.0
O(1)#1-Pt(1)-N(1)	87.0(3)
O(1)-Pt(1)-N(1)	93.0(3)
O(1)#1-Pt(1)-N(1)#1	93.0(3)
O(1)-Pt(1)-N(1)#1	87.0(3)
N(1)-Pt(1)-N(1)#1	180.0(3)

_____

Symmetry transformations used to generate equivalent atoms:

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

Table 10.   Anisotropic displacement parameters   ($\text{Å}^2 \text{x } 10^3$) for P21c.   The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2\, a^{*2}U^{11} + ... \quad + 2\, h\, k\, a^*\, b^*\, U^{12}\,]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	28(4)	28(4)	45(5)	1(4)	8(4)	-2(4)
C(2)	39(6)	14(4)	46(6)	-12(3)	14(5)	1(3)
C(3)	43(6)	27(5)	59(6)	-2(5)	14(5)	2(4)
C(4)	41(6)	35(5)	30(5)	-3(3)	-20(4)	9(4)
C(5)	42(5)	29(5)	44(5)	1(4)	-14(4)	0(4)
C(6)	38(6)	52(6)	36(6)	-22(4)	1(5)	4(5)
C(7)	40(5)	24(4)	58(6)	-11(4)	-6(5)	5(4)
C(8)	34(5)	50(6)	42(5)	2(5)	4(4)	12(5)
C(9)	45(6)	53(6)	31(5)	0(4)	9(4)	16(5)
C(10)	51(6)	36(5)	43(6)	-1(4)	-1(5)	16(5)
C(11)	40(5)	35(5)	49(6)	3(4)	-1(4)	20(4)
C(12)	40(6)	32(5)	43(5)	9(4)	10(4)	-2(4)
C(13)	30(5)	35(5)	53(6)	-11(4)	1(4)	3(4)
C(14)	23(4)	33(5)	39(5)	2(4)	-2(3)	6(4)
C(15)	29(4)	35(5)	26(4)	-5(4)	-3(3)	7(4)
C(16)	32(5)	24(4)	48(5)	-3(4)	4(4)	8(4)
C(17)	20(4)	30(5)	61(6)	-15(4)	9(4)	-4(4)
C(18)	35(5)	22(4)	57(6)	-1(4)	5(4)	-11(4)
C(19)	25(4)	29(4)	41(5)	-12(4)	-4(4)	0(4)
C(20)	38(5)	28(4)	41(5)	-4(4)	0(4)	-7(4)
C(21)	30(5)	35(5)	61(6)	-10(5)	4(4)	-4(4)
C(22)	35(5)	45(6)	48(6)	-12(5)	1(4)	-3(5)
C(23)	55(7)	32(6)	74(8)	-12(6)	12(6)	5(5)
C(24)	46(6)	43(6)	74(8)	-15(6)	18(5)	-11(5)
N(1)	33(4)	31(4)	29(3)	0(3)	3(3)	-4(3)
O(1)	44(4)	38(4)	49(4)	5(3)	-23(3)	3(3)
Pt(1)	30(1)	24(1)	35(1)	-2(1)	-3(1)	-1(1)

Table 11. Hydrogen coordinates (x 10^4) and isotropic   displacement parameters (Å^{2}x 10 ^{3}) for P21c.

	x	y	z	U(eq)
H(3)	11111	11053	1148	51
H(5)	14529	11085	1845	47
H(6)	16150	10460	2573	50
H(8)	16459	9174	3178	50
H(9)	14595	7793	3477	51
H(10)	11097	7004	3015	52
H(12)	7704	6942	2269	46
H(13)	5952	7592	1568	47
H(17)	4217	8205	986	44
H(18A)	498	8046	490	46
H(18B)	103	8675	5	46
H(19A)	4043	7224	120	38
H(19B)	3546	7840	-369	38
H(20A)	-629	6651	11	43
H(20B)	-1052	7246	-484	43
H(21A)	2834	5780	-371	50
H(21B)	2135	6339	-871	50
H(22A)	-2440	5702	-904	51
H(22B)	-1628	5114	-419	51
H(23A)	851	4856	-1345	64
H(23B)	1667	4268	-859	64
H(24A)	-2670	3570	-892	81
H(24B)	-1345	3448	-1418	81
H(24C)	-3703	4213	-1347	81