

## “Supporting Information”

### Potential Anticancer Activities and Catalytic Oxidation

### Efficiency of Platinum(IV) Complex

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**Keywords:** platinum(IV); Pyridine-2-carbaldehyde-oxime; anticancer agent; catalytic oxidation activity; luminescence

## **2.8. A general procedure for the oxidation of benzyl alcohols:**

### **2.8.1. Sonicated reactions:**

A mixture of benzyl alcohol derivatives (5 mmol) and 30 % aqueous hydrogen peroxide (7.5 mmol), the complex **1** catalyst (10 mol%) in a 25ml round bottom flask was sonicated using an Elma sonicator P30H instrument. All the reactions were carried out at 60-70 °C, which was maintained by adding or removing the water in an ultrasonic bath (the temperature inside the reaction vessel was 66-68°C). The sonochemical reactions were continued for a determined time until the starting material was no longer detectable by TLC. Water (5 mL) was added and the mixture was extracted with ethyl acetate (3 × 5 mL). The combined organic layers were dried over sodium sulfate and concentrated under reduced pressure to give pure aldehyde derivatives **2a-c**. The identity of the products was ascertained by comparison with an authentic sample and IR, <sup>1</sup>NMR & <sup>13</sup>C NMR.

### **2.8.2. Method A: Silent Reaction**

The reactions under silent conditions were performed on the same scale and conditions as described for sonicated reactions. The reaction was stirred and carried out at 60-70 °C, the reaction was continued for a determined time [until the starting material was no longer detectable by TLC]. After completion of the reaction, the products obtained were purified as described previously in sonicated reaction.

## **2.8. The synthesized compounds with their physical data**

### **4-Methoxybenzaldehyde (2a)**

Colorless liquid; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 9.77 (s, 1H), 7.77 (d, *J* = 8.0 Hz, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 3.83 (s, 3H); <sup>13</sup>CNMR (100 MHz, CDCl<sub>3</sub>): δ 190.11, 164.5, 131.9, 129.8, 114.3, 55.4.

### **4-Chlorobenzaldehyde (2b)**

White solid; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 9.79 (s, 1H), 8.00 (d, *J* = 8.0 Hz, 2H), 7.84 (d, *J* = 8.0 Hz, 2H); <sup>13</sup>CNMR (100 MHz, CDCl<sub>3</sub>): δ 190.9, 129.5, 128.9, 130.9, 131.5.

### **4-Bromobenzaldehyde (2c)**

Off white crystals; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 9.91 (s, 1H), 8.02 (d, *J* = 8.0 Hz, 2H), 7.81 (d, *J* = 8.0 Hz, 2H); <sup>13</sup>CNMR (100 MHz, CDCl<sub>3</sub>): δ 190.9, 129.8, 129.4, 131.9, 134.5.

**Table S1 Crystal data and structure refinement for complex 1**

Empirical formula	C <sub>14</sub> H <sub>10</sub> N <sub>6</sub> O <sub>2</sub> PtS <sub>2</sub>
CCDC	2096540
Formula weight	553.49
Temperature/K	120
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /n
a, b, c /Å	6.4862(2), 7.8537(2), 15.9544(5)
β/°	99.0950(10)
Volume/Å <sup>3</sup>	802.51(4)
Z	2
ρ <sub>calc</sub> /cm <sup>3</sup>	2.291
μ/mm <sup>-1</sup>	9.025
F(000)	524.0
Crystal size/mm <sup>3</sup>	0.217 × 0.064 × 0.06
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	7.326 to 120.324
Index ranges	-15 ≤ h ≤ 15, -19 ≤ k ≤ 19, -38 ≤ l ≤ 38
Reflections collected	207792
Independent reflections	12182 [R <sub>int</sub> = 0.0341, R <sub>sigma</sub> = 0.0125]
Data/restraints/parameters	12182/0/115
Goodness-of-fit on F <sup>2</sup>	1.110
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0153, wR <sub>2</sub> = 0.0332
Final R indexes [all data]	R <sub>1</sub> = 0.0220, wR <sub>2</sub> = 0.0360
Largest diff. peak/hole / e Å <sup>-3</sup>	2.88/-1.42

**Table S2. Selected bond lengths and angles for the platinum complex 1**

Atom	Atom	Length/Å	Atom	Atom	Atom	Angles/ °
S1	C1	1.6745(7)	S1	Pt1	S1 <sup>1</sup>	180.0
S1	Pt1	2.38012(19)	N2	Pt1	S1	87.589(17)
O1	N2	1.2678(8)	N2 <sup>1</sup>	Pt1	S1 <sup>1</sup>	87.589(17)
N1	C1	1.1613(10)	N2	Pt1	S1 <sup>1</sup>	92.410(17)
N2	C7	1.3124(9)	N2 <sup>1</sup>	Pt1	S1	92.411(17)
N2	Pt1	2.0767(5)	N2 <sup>1</sup>	Pt1	N2	180.00(2)
N3	C2	1.3406(8)	N3 <sup>1</sup>	Pt1	S1	87.597(17)
N3	C6	1.3619(8)	N3 <sup>1</sup>	Pt1	S1 <sup>1</sup>	92.403(17)
N3	Pt1	2.0414(5)	N3	Pt1	S1 <sup>1</sup>	87.596(17)
			N3	Pt1	S1	92.404(17)
			N3 <sup>1</sup>	Pt1	N2	100.76(2)
			N3	Pt1	N2	79.24(2)
			N3 <sup>1</sup>	Pt1	N2 <sup>1</sup>	79.24(2)
			N3	Pt1	N2 <sup>1</sup>	100.76(2)
			N3 <sup>1</sup>	Pt1	N3	180.00(3)

<sup>1</sup> = 1-X,1-Y,1-Z

**Table S3.** Hydrogen bond lengths (Å) and bond angles (deg.) in complex **1**

<b>D-H...A</b>	<b>d(D-H)</b>	<b>d(H...A)</b>	<b>d(D...A)</b>	<b>∠(DHA)</b>
C3–H3...N1	0.950	2.441	3.385	172.39
C7–H7...N1	0.950	2.721	3.499	139.62
C5 –H5...O1	0.950	2.362	3.141	138.85
C5 –H5...N1	0.950	2.866	3.639	139.26
C4 –H4...O1	0.950	3.068	3.483	108.51

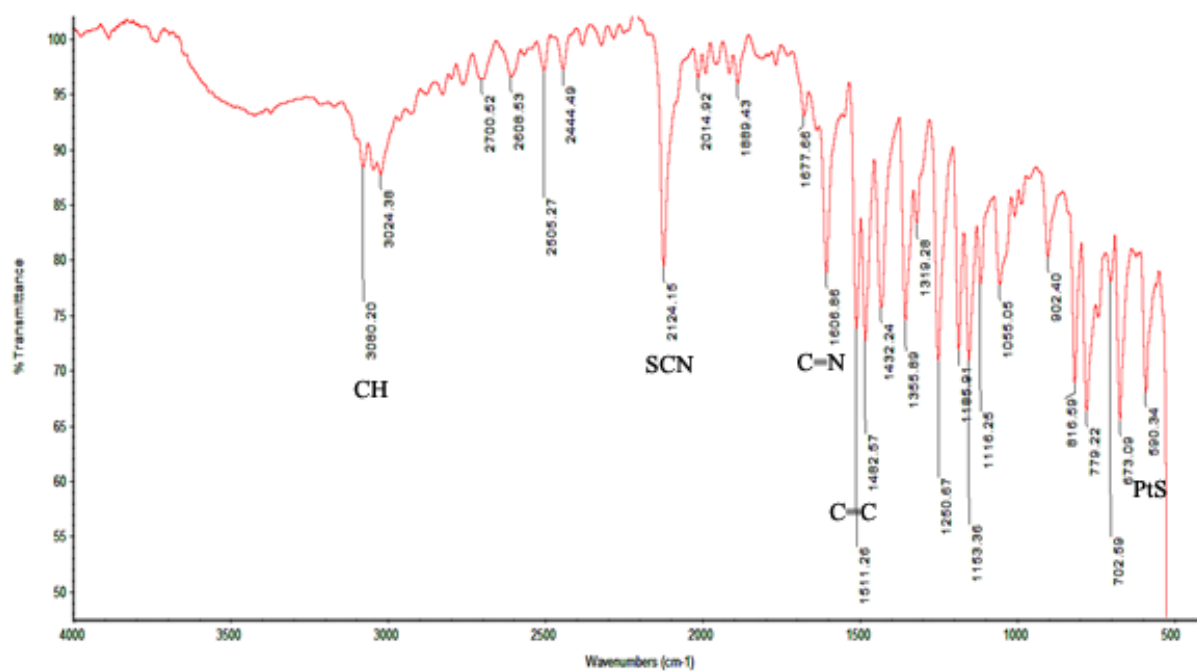


Fig.S1. IR spectrum of complex 1

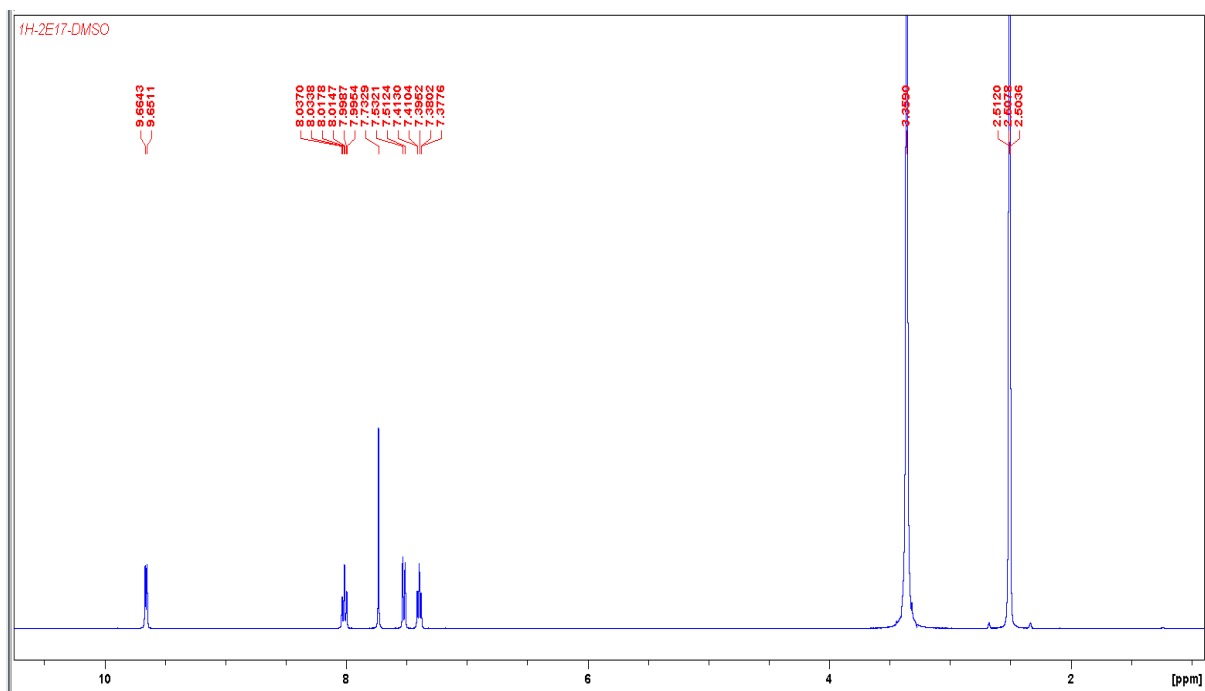
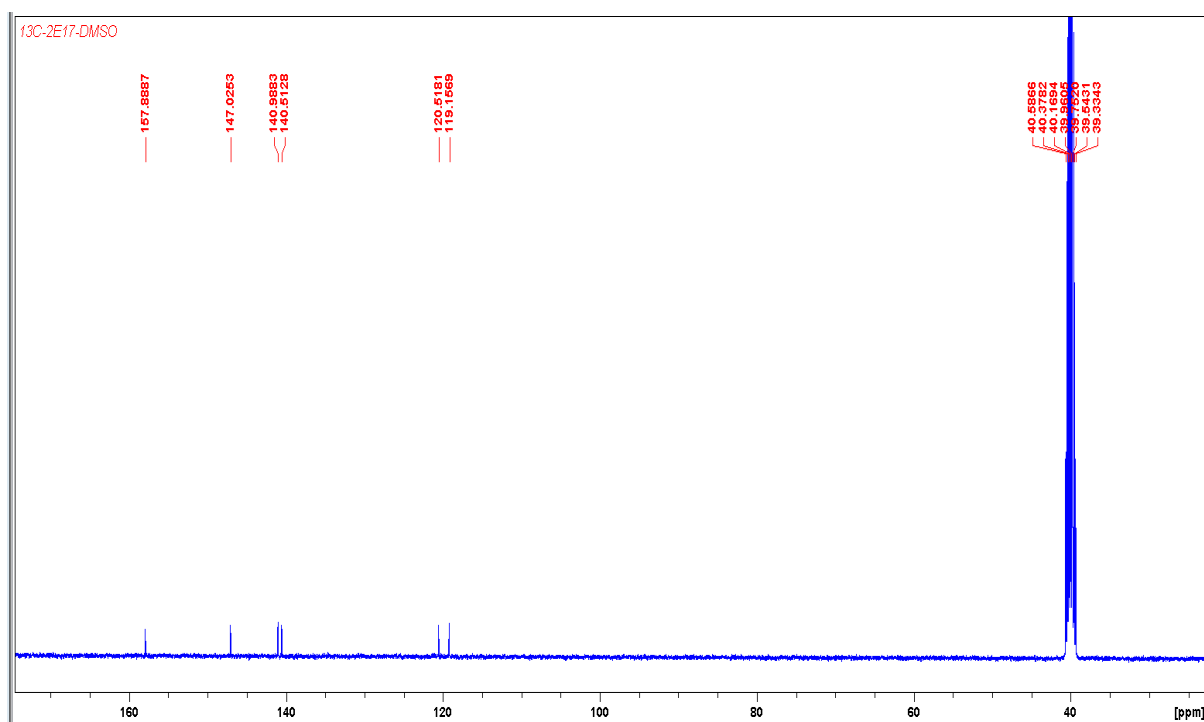
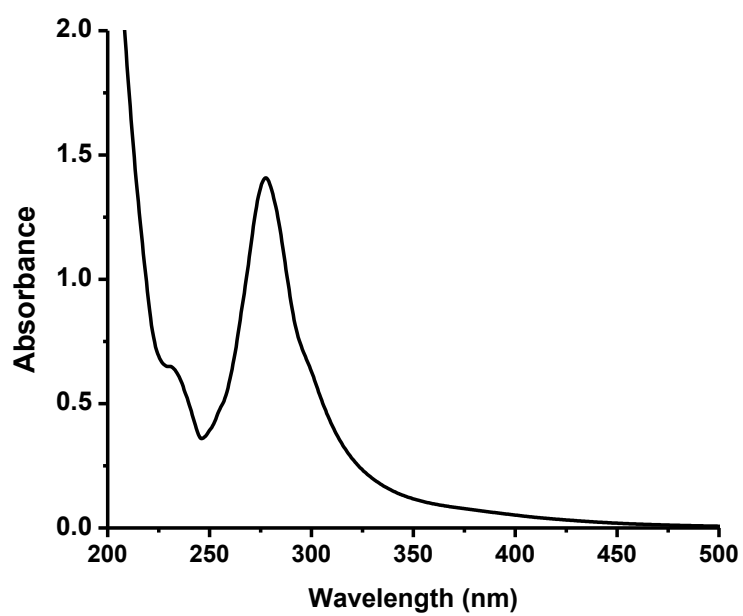


Figure S2. <sup>1</sup>H-NMR spectrum of complex 1



**Figure S3.** <sup>13</sup>C-NMR spectrum of complex **1**



**Figure S4.** UV absorption spectrum of the complex **1**

**Full cif file for complex 1:**

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(compiled 2020.11.12 svn.r5f609507 for OlexSys, GUI svn.r6272);  
\_shelx\_SHELXL\_version\_number '2018/3'  
loop\_  
\_audit\_author\_name  
\_audit\_author\_email  
\_audit\_author\_address  
'Davaasuren, B.' bambar.davaasuren@kaust.edu.sa  
;  
King Abdullah University of Science and Technology  
Core Labs  
KAUST  
Thuwal  
23955-6900  
Kingdom of Saudi Arabia;  
  
\_audit\_contact\_author\_address ?  
\_audit\_contact\_author\_email ?  
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\_audit\_contact\_author\_phone ?  
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;  
Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H.  
(2009), J. Appl. Cryst. 42, 339-341.  
Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.  
Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.;  
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\_chemical\_formula\_weight        553.49

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loop\_

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\_atom\_type\_description

\_atom\_type\_scatter\_dispersion\_real

\_atom\_type\_scatter\_dispersion\_imag

\_atom\_type\_scatter\_source

'C' 'C' 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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'N' 'N' 0.0061 0.0033 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'O' 'O' 0.0106 0.0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Pt' 'Pt' -1.7033 8.3905

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'S' 'S' 0.1246 0.1234 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

\_shelx\_space\_group\_comment;

The symmetry employed for this shelxl refinement is uniquely defined

by the following loop, which should always be used as a source of

symmetry information in preference to the above space-group names.

They are only intended as comments.;

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\_space\_group\_IT\_number        14

\_space\_group\_name\_H-M\_alt      'P 1 21/n 1'

\_space\_group\_name\_Hall        '-P 2yn'

loop\_

\_space\_group\_symop\_operation\_xyz

'x, y, z'

'-x+1/2, y+1/2, -z+1/2'

'-x, -y, -z'

'x-1/2, -y-1/2, z-1/2'

\_cell\_length\_a                6.4862(2)

\_cell\_length\_b                7.8537(2)

\_cell\_length\_c                15.9544(5)

\_cell\_angle\_alpha             90

\_cell\_angle\_beta              99.0950(10)

\_cell\_angle\_gamma             90

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 \_exptl\_absorpt\_process\_details

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SADABS-2016/2 (Bruker,2016/2) was used for absorption correction.

wR2(int) was 0.0901 before and 0.0476 after correction.

The Ratio of minimum to maximum transmission is 0.4750.

The  $\lambda/2$  correction factor is Not present.

;

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_reflns_number_total	12182

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;

Reflections were merged by SHELXL according to the crystal class for the calculation of statistics and refinement.

\_reflns\_Friedel\_fraction is defined as the number of unique Friedel pairs measured divided by the number that would be possible theoretically, ignoring centric projections and systematic absences.

;

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\_computing\_data\_collection ?

\_computing\_data\_reduction ?

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\_computing\_publication\_material 'Olex2 1.3 (Dolomanov et al., 2009)'

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\_computing\_structure\_solution 'SHELXT 2018/2 (Sheldrick, 2018)'

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\_refine\_ls\_matrix\_type full

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\_refine\_ls\_number\_reflns 12182

\_refine\_ls\_number\_restraints 0

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\_refine\_ls\_R\_factor\_gt 0.0153

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\_refine\_ls\_shift/su\_max 0.002

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\_refine\_ls\_weighting\_details

'w=1/[σ<sup>2</sup>(F<sub>o</sub><sup>2</sup>)+(0.0127P)<sup>2</sup>+0.3756P] where P=(F<sub>o</sub><sup>2</sup>+2F<sub>c</sub><sup>2</sup>)/3'

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1. Fixed Uiso

At 1.2 times of:

All C(H) groups

2.a Aromatic/amide H refined with riding coordinates:

C2(H2), C3(H3), C4(H4), C5(H5), C7(H7)

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_atom_sites_solution_secondary   ?
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loop_
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_atom_site_adp_type
_atom_site_occupancy
_atom_site_site_symmetry_order
_atom_site_calc_flag
_atom_site_refinement_flags_posn
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_atom_site_refinement_flags_occupancy
_atom_site_disorder_assembly
_atom_site_disorder_group
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N1 N 0.32322(14) 0.94997(11) 0.38793(6) 0.02208(14) Uani 1 1 d . . . . .

N2 N 0.74948(9) 0.50254(7) 0.59917(3) 0.01031(6) Uani 1 1 d . . . . .

N3 N 0.38692(9) 0.65795(7) 0.58365(3) 0.00999(6) Uani 1 1 d . . . . .

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 H2 H 0.119237 0.732873 0.515287 0.016 Uiso 1 1 calc R U . . .  
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 C4 C 0.26025(15) 0.84557(11) 0.71223(5) 0.01745(12) Uani 1 1 d . . . . .  
 H4 H 0.214880 0.908895 0.756664 0.021 Uiso 1 1 calc R U . . .  
 C5 C 0.44889(13) 0.75956(10) 0.72671(5) 0.01495(10) Uani 1 1 d . . . . .  
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 C6 C 0.51253(11) 0.66835(8) 0.66041(4) 0.01100(8) Uani 1 1 d . . . . .  
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 N3 0.01042(15) 0.01086(16) 0.00890(15) -0.00082(12) 0.00216(12) 0.00259(12)  
 C1 0.0131(2) 0.0125(2) 0.0148(2) 0.00282(17) 0.00226(17) 0.00233(17)  
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 C6 0.0131(2) 0.01140(19) 0.00859(17) -0.00133(14) 0.00184(14) 0.00097(15)  
 C7 0.0124(2) 0.0154(2) 0.00890(18) -0.00124(16) -0.00029(15) 0.00174(17)  
 Pt1 0.00718(1) 0.00836(1) 0.00586(1) 0.00012(1) 0.00083(1) 0.00217(1)

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All esds (except the esd in the dihedral angle between two l.s. planes)  
 are estimated using the full covariance matrix. The cell esds are taken

into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.;

loop\_

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C3 H3 0.9500 . ?

C3 C4 1.3933(13) . ?

C4 H4 0.9500 . ?

C4 C5 1.3847(12) . ?

C5 H5 0.9500 . ?

C5 C6 1.3929(9) . ?

C6 C7 1.4345(10) . ?

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loop\_

\_geom\_angle\_atom\_site\_label\_1

\_geom\_angle\_atom\_site\_label\_2

\_geom\_angle\_atom\_site\_label\_3

\_geom\_angle

\_geom\_angle\_site\_symmetry\_1

\_geom\_angle\_site\_symmetry\_3

\_geom\_angle\_publ\_flag

C1 S1 Pt1 100.48(3) . . ?

O1 N2 C7 122.98(6) . . ?

O1 N2 Pt1 123.26(4) . . ?

C7 N2 Pt1 113.76(4) . . ?

C2 N3 C6 120.70(6) . . ?

C2 N3 Pt1 125.75(5) . . ?

C6 N3 Pt1 113.50(4) . . ?

N1 C1 S1 177.27(8) . . ?

N3 C2 H2 119.4 . . ?

N3 C2 C3 121.11(7) . . ?

C3 C2 H2 119.4 . . ?

C2 C3 H3 120.6 . . ?

C2 C3 C4 118.78(7) . . ?

C4 C3 H3 120.6 . . ?

C3 C4 H4 120.0 . . ?

C5 C4 C3 119.91(7) . . ?

C5 C4 H4 120.0 . . ?

C4 C5 H5 120.5 . . ?

C4 C5 C6 118.97(7) . . ?

C6 C5 H5 120.5 . . ?

N3 C6 C5 120.45(6) . . ?

N3 C6 C7 115.95(5) . . ?

C5 C6 C7 123.60(6) . . ?

N2 C7 C6 116.96(6) . . ?

N2 C7 H7 121.5 . . ?

C6 C7 H7 121.5 . . ?

S1 Pt1 S1 180.0 . 3\_666 ?

N2 Pt1 S1 87.589(17) 3\_666 3\_666 ?

N2 Pt1 S1 92.410(17) . 3\_666 ?

N2 Pt1 S1 87.589(17) . . ?

N2 Pt1 S1 92.411(17) 3\_666 . ?

N2 Pt1 N2 180.00(2) 3\_666 . ?

N3 Pt1 S1 92.403(17) 3\_666 3\_666 ?

N3 Pt1 S1 87.596(17) . 3\_666 ?

N3 Pt1 S1 87.597(17) 3\_666 . ?

N3 Pt1 S1 92.404(17) . . ?



N3 Pt1 N2 100.76(2) 3\_666 . ?  
N3 Pt1 N2 100.76(2) . 3\_666 ?  
N3 Pt1 N2 79.24(2) . . ?  
N3 Pt1 N2 79.24(2) 3\_666 3\_666 ?  
N3 Pt1 N3 180.00(3) 3\_666 . ?

loop\_

\_geom\_hbond\_atom\_site\_label\_D  
\_geom\_hbond\_atom\_site\_label\_H  
\_geom\_hbond\_atom\_site\_label\_A  
\_geom\_hbond\_distance\_DH  
\_geom\_hbond\_distance\_HA  
\_geom\_hbond\_distance\_DA  
\_geom\_hbond\_angle\_DHA  
\_geom\_hbond\_site\_symmetry\_A  
\_geom\_hbond\_publ\_flag  
C2 H2 O1 0.95 2.17 2.9537(10) 139.4 3\_666 yes  
C3 H3 N1 0.95 2.44 3.3847(11) 172.4 3\_576 yes  
C5 H5 O1 0.95 2.36 3.1406(9) 138.8 2\_656 yes

loop\_

\_geom\_torsion\_atom\_site\_label\_1  
\_geom\_torsion\_atom\_site\_label\_2  
\_geom\_torsion\_atom\_site\_label\_3  
\_geom\_torsion\_atom\_site\_label\_4  
\_geom\_torsion  
\_geom\_torsion\_site\_symmetry\_1  
\_geom\_torsion\_site\_symmetry\_2  
\_geom\_torsion\_site\_symmetry\_3  
\_geom\_torsion\_site\_symmetry\_4  
\_geom\_torsion\_publ\_flag  
O1 N2 C7 C6 175.59(7) . . . . ?  
N3 C2 C3 C4 -2.01(13) . . . . ?  
N3 C6 C7 N2 -1.46(10) . . . . ?  
C2 N3 C6 C5 2.88(10) . . . . ?  
C2 N3 C6 C7 -175.82(7) . . . . ?  
C2 C3 C4 C5 2.01(13) . . . . ?  
C3 C4 C5 C6 0.34(13) . . . . ?

C4 C5 C6 N3 -2.81(11) . . . . ?  
 C4 C5 C6 C7 175.79(8) . . . . ?  
 C5 C6 C7 N2 179.89(7) . . . . ?  
 C6 N3 C2 C3 -0.43(11) . . . . ?  
 Pt1 N2 C7 C6 -4.47(8) . . . . ?  
 Pt1 N3 C2 C3 176.72(6) . . . . ?  
 Pt1 N3 C6 C5 -174.60(6) . . . . ?  
 Pt1 N3 C6 C7 6.70(8) . . . . ?  
 \_shelx\_res\_file;  
 TITL A3\_2\_mon\_a.res in P2(1)/n  
 a3\_2\_mon\_a.res  
 created by SHELXL-2018/3 at 12:20:02 on 14-Jul-2021  
 REM Old TITL A3\_2\_mon in P2(1)/n  
 REM SHELXT solution in P2(1)/n: R1 0.041, Rweak 0.001, Alpha 0.019  
 REM <I/s> 2.198 for 128 systematic absences, Orientation as input  
 REM Formula found by SHELXT: C16 O6 S2 Pt  
 CELL 0.71073 6.4862 7.8537 15.9544 90 99.095 90  
 ZERR 2 0.0002 0.0002 0.0005 0 0.001 0  
 LATT 1  
 SYMM 0.5-X,0.5+Y,0.5-Z  
 SFAC C H N O Pt S  
 UNIT 28 20 12 4 2 4  
 EQIV \$1 1-X,1-Y,1-Z  
 EQIV \$2 -X,2-Y,1-Z  
 EQIV \$3 1.5-X,0.5+Y,1.5-Z  
  
 L.S. 40  
 PLAN 10  
 SIZE 0.06 0.064 0.217  
 TEMP -153.13  
 CONF  
 HTAB C2 O1\_\$1  
 HTAB C3 N1\_\$2  
 HTAB C5 O1\_\$3  
 HTAB  
 BOND \$H  
 LIST 4

MORE -1

fmap 2

acta

REM <olex2.extras>

REM <HklSrc "%.\A3\_2\_mon\_a.hkl">

REM </olex2.extras>

WGHT 0.012700 0.375600

FVAR 0.58255

S1 6 0.665495 0.728676 0.438731 11.00000 0.00979 0.01231 =  
0.01423 0.00274 0.00311 0.00171

O1 4 0.923339 0.431911 0.595022 11.00000 0.00946 0.01930 =  
0.01315 0.00093 0.00040 0.00499

N1 3 0.323218 0.949970 0.387927 11.00000 0.01809 0.01847 =  
0.02925 0.00713 0.00241 0.00680

N2 3 0.749480 0.502543 0.599165 11.00000 0.00977 0.01236 =  
0.00846 0.00071 0.00037 0.00224

N3 3 0.386925 0.657952 0.583651 11.00000 0.01042 0.01086 =  
0.00890 -0.00082 0.00216 0.00259

C1 1 0.461618 0.858564 0.410504 11.00000 0.01309 0.01246 =  
0.01480 0.00282 0.00226 0.00233

C2 1 0.204225 0.741089 0.569382 11.00000 0.01169 0.01438 =  
0.01420 -0.00081 0.00343 0.00416

AFIX 43

H2 2 0.119237 0.732873 0.515287 11.00000 -1.20000

AFIX 0

C3 1 0.137059 0.839101 0.632401 11.00000 0.01660 0.01610 =  
0.01886 -0.00263 0.00730 0.00525

AFIX 43

H3 2 0.009508 0.900553 0.621254 11.00000 -1.20000

AFIX 0

C4 1 0.260248 0.845567 0.712229 11.00000 0.02242 0.01553 =  
0.01633 -0.00364 0.00903 0.00303

AFIX 43

H4 2 0.214880 0.908895 0.756664 11.00000 -1.20000

AFIX 0

C5 1 0.448889 0.759563 0.726707 11.00000 0.02049 0.01430 =

```

0.01065 -0.00332 0.00426 0.00105
AFIX 43
H5 2 0.533591 0.762719 0.781007 11.00000 -1.20000
AFIX 0
C6 1 0.512526 0.668349 0.660415 11.00000 0.01306 0.01140 =
0.00859 -0.00133 0.00184 0.00097
C7 1 0.710583 0.584050 0.666761 11.00000 0.01238 0.01535 =
0.00890 -0.00124 -0.00029 0.00174
AFIX 43
H7 2 0.809108 0.587083 0.717578 11.00000 -1.20000
AFIX 0
PART 1
PT1 5 0.500000 0.500000 0.500000 10.50000 0.00718 0.00836 =
0.00586 0.00012 0.00083 0.00217
HKLF 4
REM A3_2_mon_a.res in P2(1)/n
REM wR2 = 0.0360, GooF = S = 1.110, Restrained GooF = 1.110 for all data
REM R1 = 0.0153 for 10035 Fo > 4sig(Fo) and 0.0220 for all 12182 data
REM 115 parameters refined using 0 restraints
END
WGHT 0.0127 0.3757
REM Instructions for potential hydrogen bonds
EQIV $4 x-1, y, z
HTAB C2 S1_$4
HTAB C2 O1_$1
HTAB C3 N1_$2
HTAB C5 O1_$3
REM Highest difference peak 2.875, deepest hole -1.419, 1-sigma level 0.140
Q1 1 0.4557 0.4615 0.4841 11.00000 0.05 2.87
Q2 1 0.5509 0.5073 0.4838 11.00000 0.05 2.45
Q3 1 0.4479 0.5186 0.4842 11.00000 0.05 2.36
Q4 1 0.4834 0.5189 0.4602 11.00000 0.05 1.36
Q5 1 0.4789 0.5733 0.5031 11.00000 0.05 1.35
Q6 1 0.4114 0.9206 0.4000 11.00000 0.05 0.86
Q7 1 0.6315 0.6174 0.6650 11.00000 0.05 0.75
Q8 1 0.1608 0.7602 0.5923 11.00000 0.05 0.61
Q9 1 0.6217 0.7244 0.4142 11.00000 0.05 0.58

```

Q10 1 0.4659 0.6851 0.6869 11.00000 0.05 0.58;

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