# PAGES OF SUPPORTING INFORMATION FOR THE PAPER:

Synthesis and Characterization of Pt(II) and Pd(II) Complexes With Planar Aromatic Oximes.

Mikala Meadows, Lei Yang, Cody Turner, Mikhail Berezin, Sergiy Tyukhtenko

and Nikolay Gerasimchuk[*]

Actual photographs of powdery samples of Pt(II) naphtoquinone-oximes under x40 magnification.
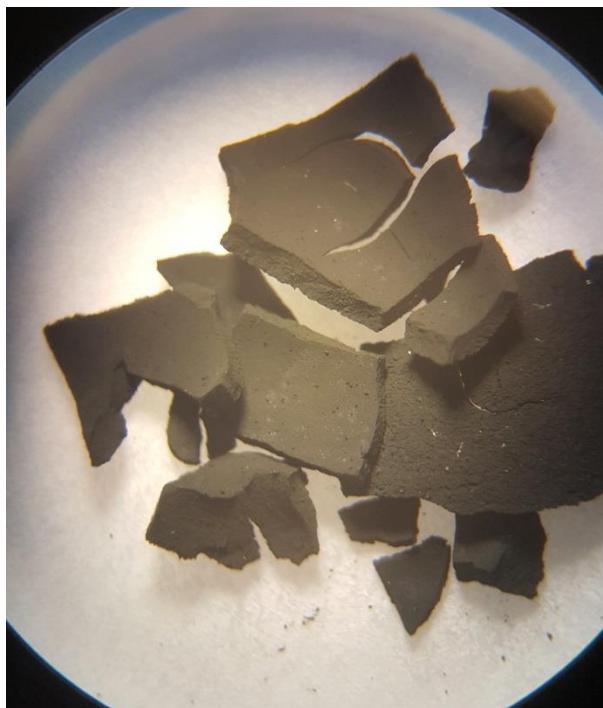

**PtL$^1_2$** = Pt(1NO-2O)$_2$

PtL$^2_2$ = Pt(2NO-1O)$_2$

1NO-2O = **L^1**

2NOH-1O = **L^2**
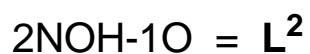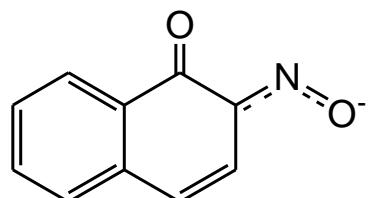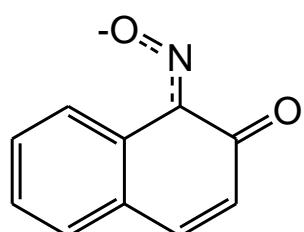
Actual photographs of powdery samples of Pd(II) naphtoquinone-oximes under x40 magnification.

PdL^1_2 = Pd(1NO-2O)$_2$ PdL^2_2 = Pd(2NO-1O)$_2$

1NO-2O = L^1 2NOH-1O = L^2
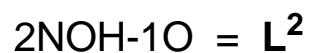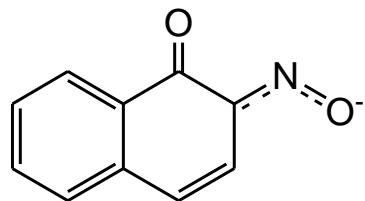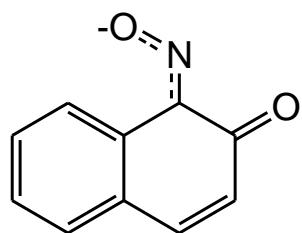
Analytical data for Pt complexes with ligands shown in yellow boxes.

ATLANTIC MICROLAB, INC.

Sample No. Pt(II) 1NO-2OH

SUBMITTER

Company / School Missouri State University

6180 Atlantic Blvd. Suite M
Norcross, GA 30071

Address 901 South National Avenue

Dept. Chemistry

www.atlanticmicrolab.com
PROFESSOR/SUPERVISOR: Dr. N. Gerasimchuk
PO# / CC#:

NAME Mikala Meadows
PHONE   DATE 1

Element	Theory	Found		Single ☑ Duplicate ☐
C	44.5300	44.35		Elements Present: C, H, N, O, Pt
H	2.2400	2.18		Analyze for: C, H, N
N	5.1900	5.18		Hygroscopic ☑ Explosive ☐ M.P. _____ B.P. _____
				To be dried: Yes ☐ No ☐ Temp. ____ Vac. ____ Time ____
				RUSH SERVICE ☐ Rush service guarantees analyses will be completed and results available by 5pm EST on the day the sample is received by 11am.
				Include Email Address or Fax # Below

Date Received NOV 0 9 2021   Date Completed NOV 1 0 2021
Remarks:

ATLANTIC MICROLAB, INC.

Sample No. Pt(II) 2NO-1OH

SUBMITTER

Company / School Missouri State University

6180 Atlantic Blvd. Suite M
Norcross, GA 30071

Address 901 South National Avenue

Dept. Chemistry

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PROFESSOR/SUPERVISOR: Dr. N. Gerasimchuk
PO# / CC#:

NAME Mikala Meadows
PHONE   DATE 11/9/21

Element	Theory	Found		Single ☑ Duplicate ☐
C	44.5300	44.89	45.02	Elements Present: C, H, N, O, Pt
H	2.2400	2.31	2.26	Analyze for: C, H, N
N	5.1900	4.78	4.81	Hygroscopic ☑ Explosive ☐ M.P. _____ B.P. _____
		NO CHARGE FOR DUPLICATES		To be dried: Yes ☐ No ☐ Temp. ____ Vac. ____ Time ____
				RUSH SERVICE ☐ Rush service guarantees analyses will be completed and results available by 5pm EST on the day the sample is received by 11am.
				Include Email Address or Fax # Below

Date Received NOV 0 9 2021   Date Completed NOV 1 0 2021
Remarks:

Example of analytical data for Pd complex with ligand shown in yellow box.

ATLANTIC MICROLAB, INC.

Sample No. Pd(II) 1NO-2OH

6180 Atlantic Blvd. Suite M
Norcross, GA 30071

www.atlanticmicrolab.com
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PO# / CC#:

SUBMITTER

Company / School Missouri State University
Address 901 South National Avenue
Dept.   Chemistry

NAME Mikala Meadows
PHONE   DATE 11/9/21

Element	Theory	Found	
C	53.2900	49.91	50.03
H	2.6800	2.80	2.70
N	6.2100	5.75	5.83
		NO CHARGE FOR DUPLICATES	

Single ☑   Duplicate ☐
Elements C, H, N, O, Pd
Present:
Analyze C, H, N
for:
Hygroscopic ☑   Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☐ No ☐
Temp. _____Vac. _____Time _____
RUSH SERVICE ☐ Rush service guarantees analyses will be
completed and results available by 5pm EST
on the day the sample is received by 11am.

Include Email Address or Fax # Below

Date Received   NOV 0 9 2021   Date Completed   NOV 1 0 2021
Remarks:

Herein average: C = 49.26%, H = 2.54%, N = 5.72%, Pd = 21.71% (by ICP method)

The best fit is for **PdL$^1_2$·2H$_2$O** calculated:

C = 49.35%, H = 3.31%, N = 5.75%, Pd = 21.86%.

The H-content is off by 0.77%, and the reason for such discrepancy is not clear.

Example of analytical data for Pd complex with ligand shown in yellow box.

ATLANTIC MICROLAB, INC.

SUBMITTER

Sample No. Pd(II) 2NO-1OH

Company / School Missouri State University

Address 901 South National Avenue

6180 Atlantic Blvd. Suite M
Norcross, GA 30071

Dept. Chemistry

www.atlanticmicrolab.com

PROFESSOR/SUPERVISOR: Dr. N. Gerasimchuk

NAME Mikala Meadows   DATE 11/9/21

PO# / CC#:

PHONE

Element	Theory	Found		Single ☑ Duplicate ☐
C	53.2900	49.88	49.74	Elements Present: C, H, N, O, Pd
H	2.6800	2.46	2.50	Analyze for: C, H, N
N	6.2100	5.17	5.17	Hygroscopic ☑ Explosive ☐ M.P. ___ B.P. ___
		NO CHARGE FOR DUPLICATES		To be dried: Yes ☐ No ☐ Temp. ___ Vac. ___ Time ___
				RUSH SERVICE ☐ Rush service guarantees analyses will be completed and results available by open EST on the day the sample is received by 11am.
				Include Email Address or Fax # Below

Date Received NOV 0 9 2021   Date Completed NOV 1 0 2021

Remarks:

Herein average: C = 49.81%, H = 2.48%, N = 5.17%.

The best fit is for **PdL$^1_2$·2H$_2$O** calculated:

C = 49.35%, H = 3.31%, N = 5.75%.

Photograph of actual crystals of **PtL$^2_2$** (as nitrobenzene solvate) grown in capillary during vapor diffusion by ether.

Videomicroscope face-indexing of a thin needle of **PtL$^2_2$**. Images were used for the crystal size determination.
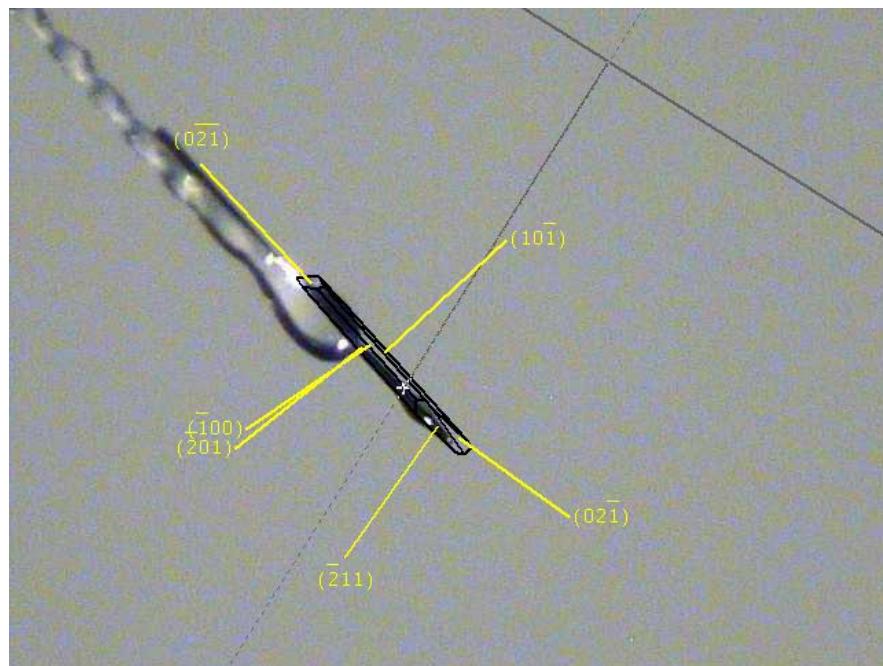
Twin Laws (transformation matrices for the first 4 domains) for crystal sample of **PtL$^2_2$**, *acetonitrile solvate*.

Transforms h1.1(1)->h1.2(2)

1.00053	0.00075	0.00462
-0.00030	0.99948	-0.00313
-0.01916	0.00437	0.99989

Transforms h1.1(1)->h1.3(3)

-0.63044	-0.49340	-0.14014
-1.15077	0.64935	-0.11580
0.78957	-0.04154	-0.90742

Transforms h1.1(1)->h1.4(4)

0.78613	0.21430	0.30329
-1.04753	0.53802	0.43076
-0.24473	-1.08173	0.42118

Transforms h1.2(2)->h1.3(3)

0.79152	0.21251	0.30033
-1.03844	0.53717	0.43728
-0.23690	-1.08395	0.41892

Transforms h1.2(2)->h1.4(4)

-0.63291	-0.49258	-0.13877
-1.15205	0.65103	-0.10846
0.77169	-0.03816	-0.91120

Transforms h1.3(3)->h1.4(4)

-0.85137	-0.32718	-0.16100
-0.18899	0.65113	-0.52861
1.17805	-0.80548	-0.54329

Twin Laws (transformation matrices) for crystal sample of **PtL$^2_2$**, *nitrobenzene solvate*.

During data processing there were 2,899 strong reflections selected from 1,454 frames with I > 20σ(I) from only four domains, among which 2,363 reflections were allocated to domain #1, then 1,238 reflections to domain #2, and 975 reflections to domain #3, then 360 reflections to domain #4. To determine the structure of PtL22 a total of 1,456 frames were collected and used for a successful solution. The total exposure time was 24.27 hours. The frames were integrated with the Bruker SAINT Software package using a narrow-frame algorithm. The integration of the data using a triclinic unit cell yielded a total of 3,891 reflections to a maximum θ angle of 25.50° (0.83 Å resolution), of which 3,891 were independent (average redundancy 1.000, completeness = 95.9%, Rint = 7.91%, Rsig = 11.75%) and 3,011 (77.38%) were greater than 2σ(F2). The final cell constants were obtained from the refinement of the XYZ-centroids of 2,257 reflections above 20 σ(I). The ratio of minimum to maximum apparent transmission was 0.722. The calculated minimum and maximum transmission coefficients (based on crystal size) were 0.1140 and 0.8200, while experimentally determined values were 0.4973 and 0.7454 respectively.

Transforms h1.1(1)->h1.2(2) with 8° rotation with respect to #1 main domain.

1.00420	-0.00118	-0.00815
-0.04217	0.98169	0.11175
0.06537	-0.14367	0.99762

 Transforms h1.1(1)->h1.3(3) with 4.3° rotation with respect to #1 main domain.

1.00012	0.00179	-0.00103
-0.03857	0.99108	0.07036
0.02211	-0.08802	1.00254

Transforms h1.1(1)->h1.4(4) with 93.4° rotation with respect to #1 main domain

0.94316	0.02297	-0.29755
-0.03817	-0.78823	-0.46256
-0.36626	0.62745	-0.84754

Transforms h1.2(2)->h1.3(3)

0.99567	0.00399	0.00665
0.00645	1.00346	-0.04182
-0.04060	0.05639	0.99828

Transforms h1.2(2)->h1.4(4)

|		
0.95725	-0.01767	-0.28846
-0.05003	-0.85687	-0.36810
-0.28435	0.50585	-0.90854

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The ASU in the structure of **PtL$^2_2$**, *acetonitrile solvate* showing several residual peaks of electron density close to heavy atom Pt. All shown 5 Q-peaks have no chemical meaning, distant at ~1 Å from and represent "ripples" of electron density most likely stemming from multidomain nature of the crystal selected for studies.
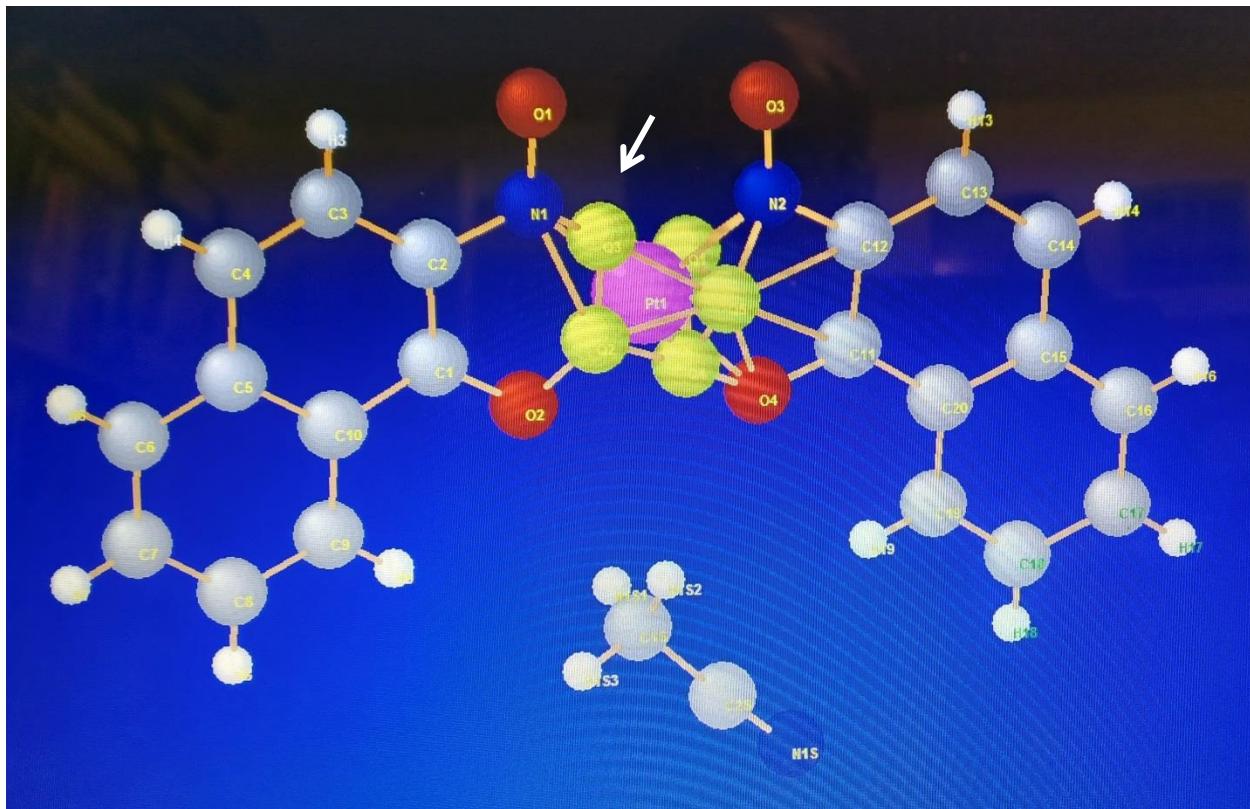
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The ASU in the structure of **PtL$^2_2$**, *nitrobenzene solvate* showing several residual peaks of electron density close to heavy atom Pt. All shown 6 Q-peaks have no chemical meaning, and located between metal center and closest donor atoms of N and O of the organic ligand. These peaks and represent "ripples" of elec tron density most likely stemming from multidomain (multicomponent?) nature of the crystal selected for studies.
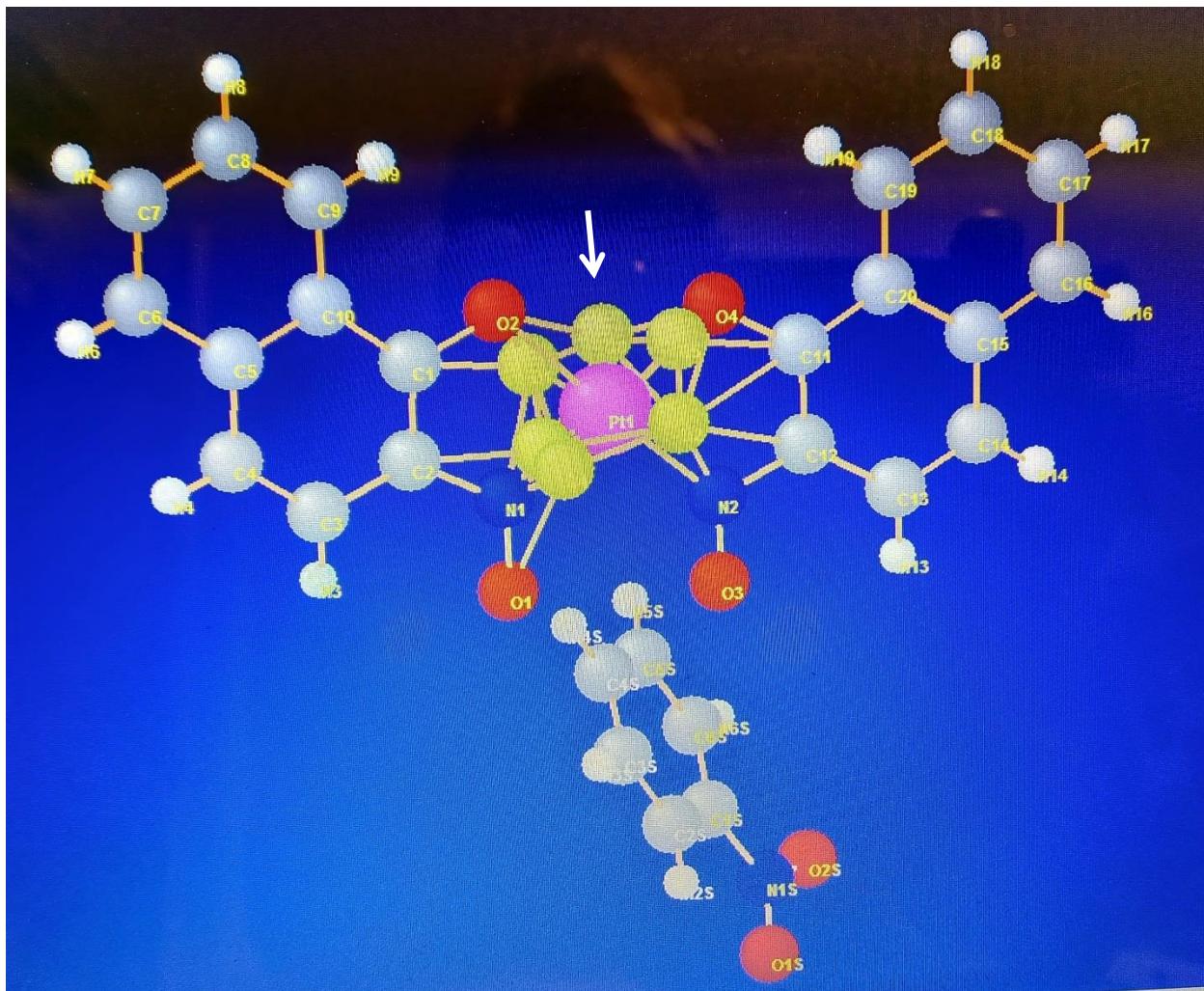
TG/DSC data for a powdery sample of pure ligand, **HL**[1]: **A** – panoramic view of both weight loss trace and heat flow; **B** – individual weight loss trace.

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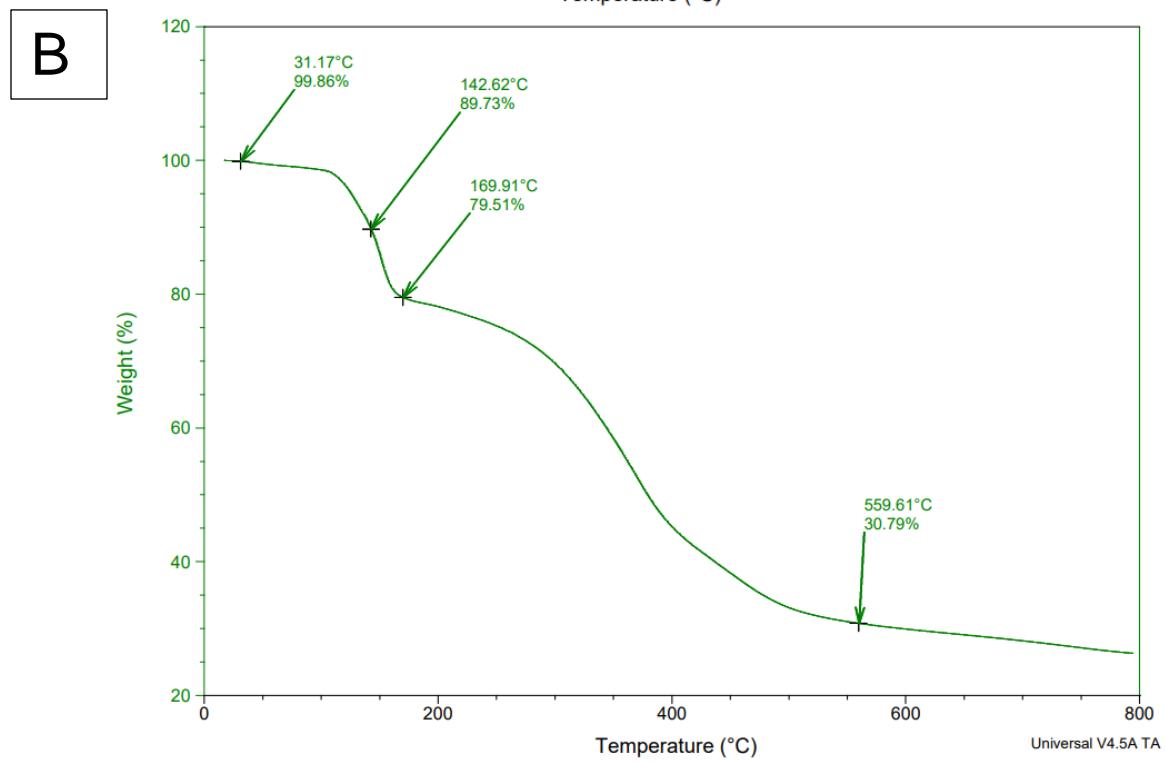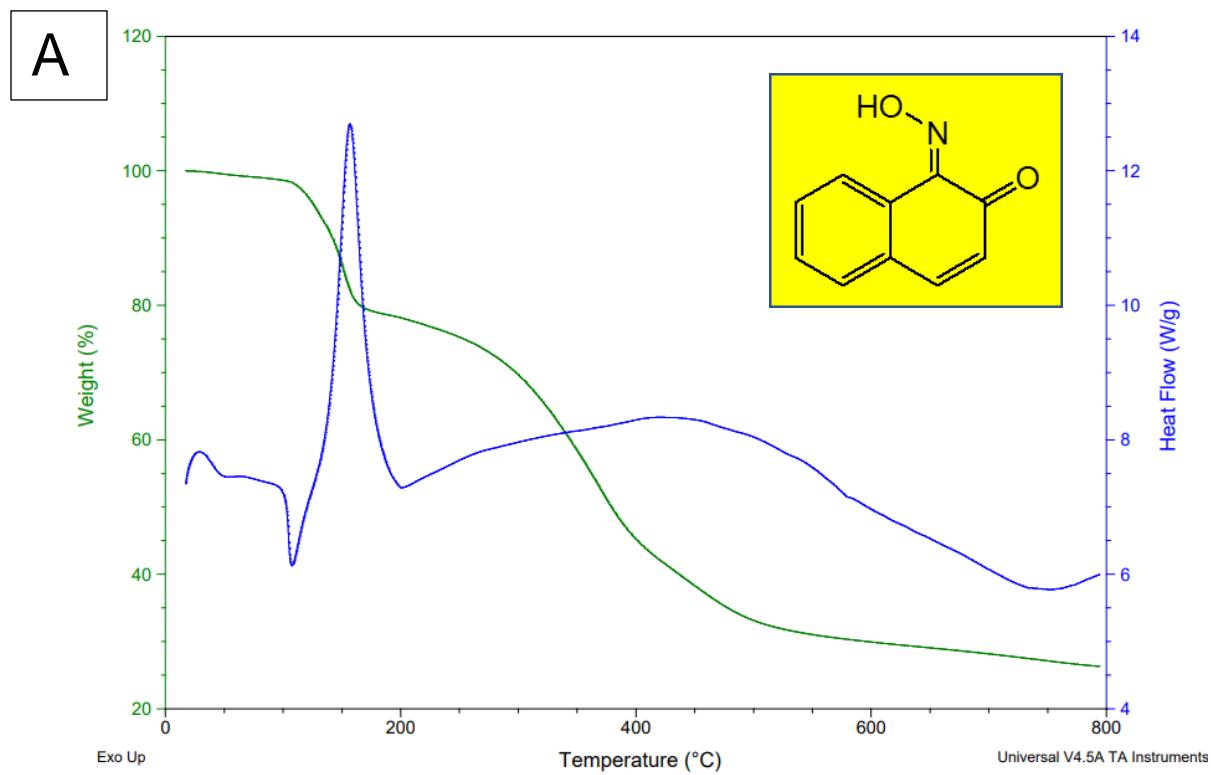
Details of the heat flow trace for **HL^1** showing a strong exothermic peak in the range before 500°C (**A**), and actual photograph under microscope crucible content after TG/DSC experiment showing the formation of a glassy carbon upon heating under an inert atmosphere (**B**).

A

156.23°C
12.68W/g
156.65°C

135.22°C
1109J/g

200.96°C
7.287W/g

108.47°C
6.150W/g

0   200   400

Exo Up   Temperature (°C)

B
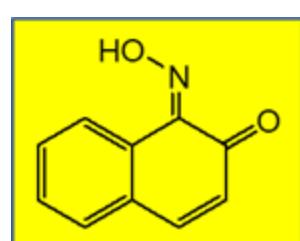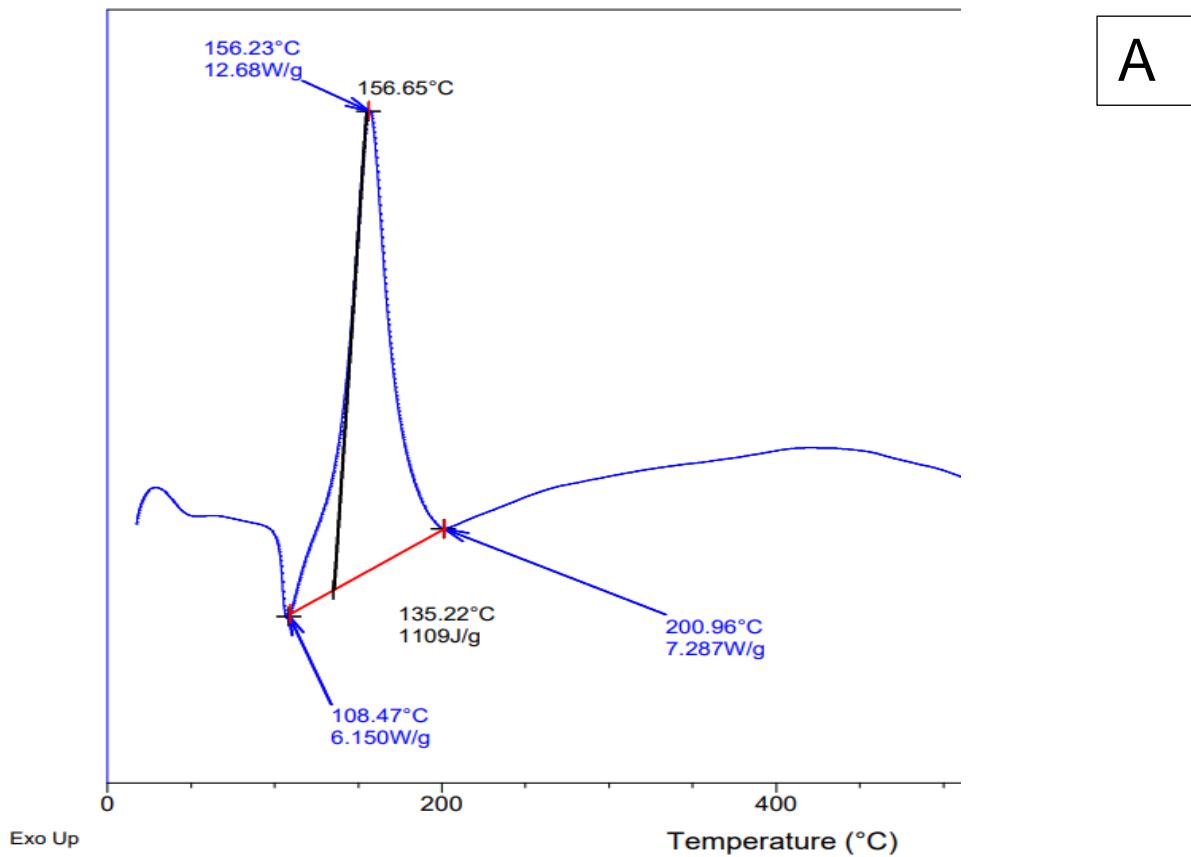
Sheets of glassy carbon

TG/DSC data for a powdery sample of pure ligand, **HL^2**: **A** – panoramic view of both weight loss trace and heat flow; **B** – individual weight loss trace.

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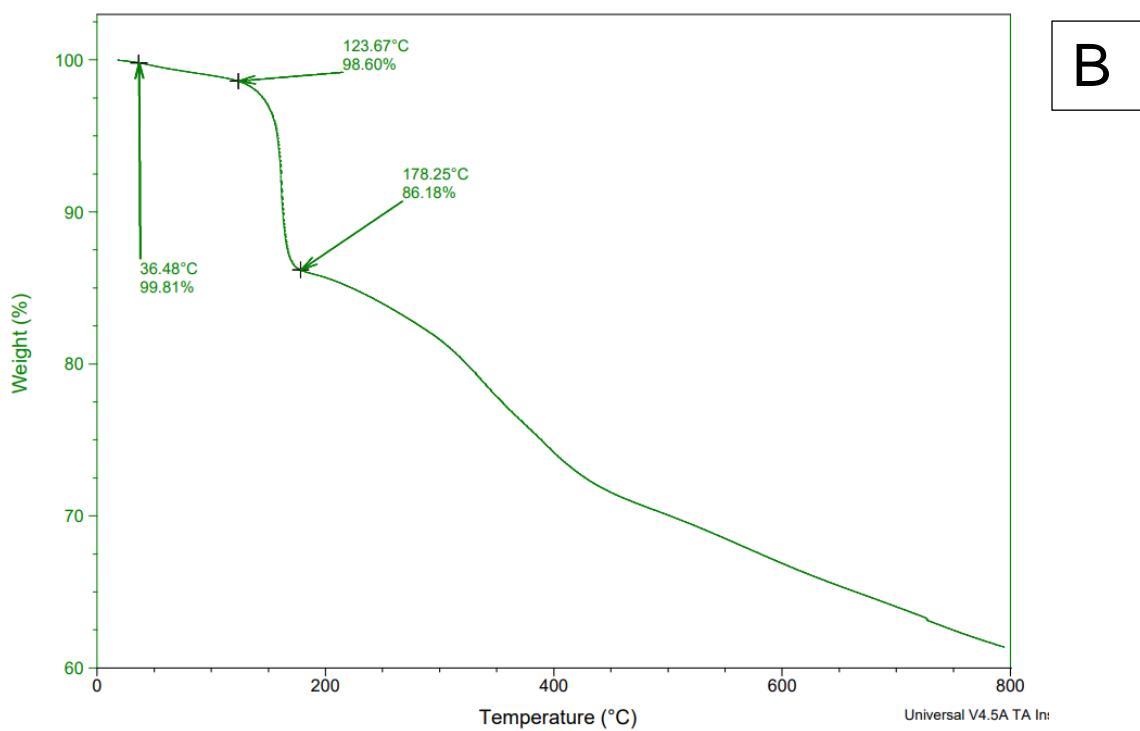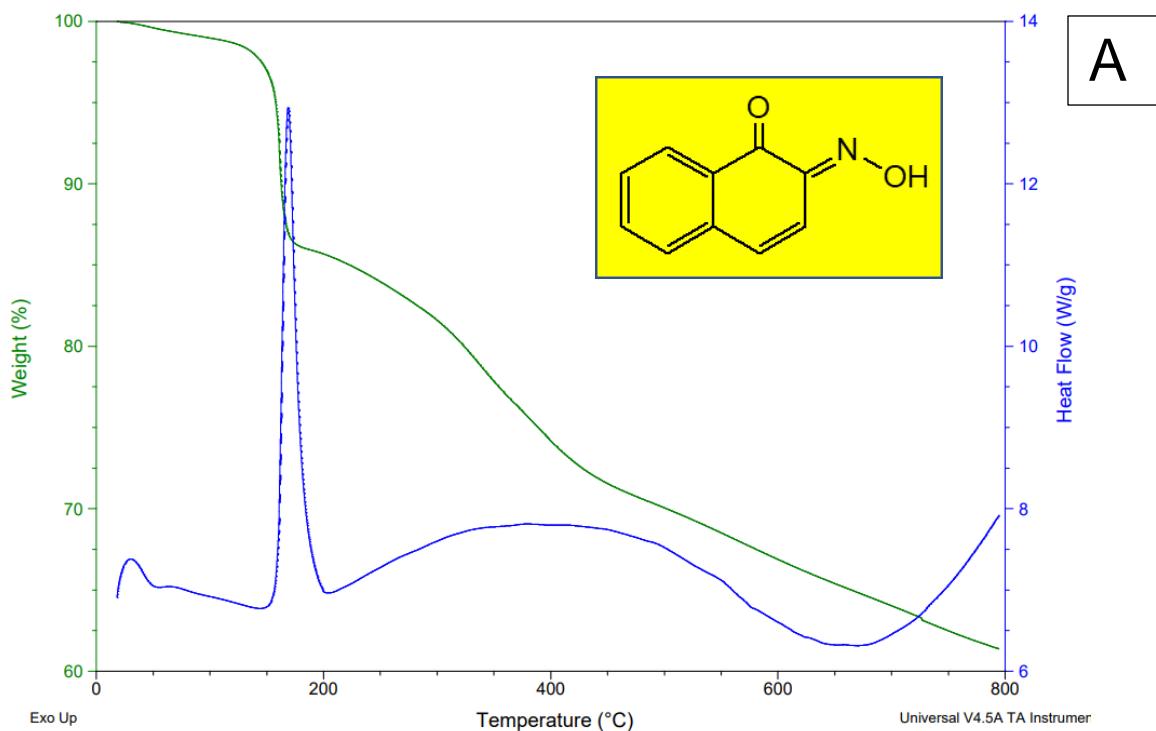
Details of the heat flow trace for **HL**^{2} showing a strong exothermic peak in the range before 500°C (**A**), and actual photograph under microscope crucible content after TG/DSC experiment showing the formation of a glassy carbon upon heating under an inert atmosphere (**B**).


Sheets of glassy carbon
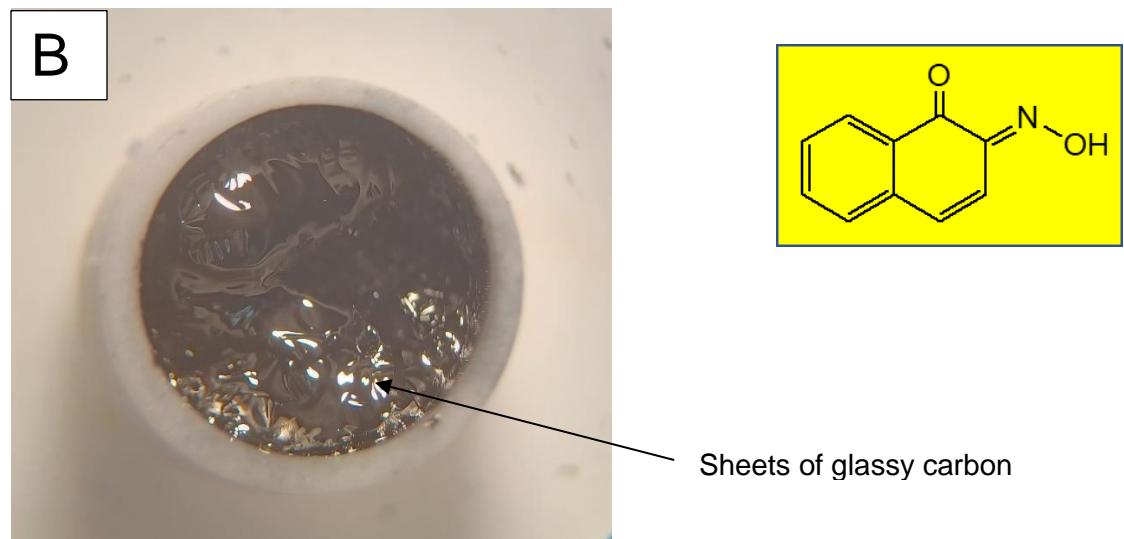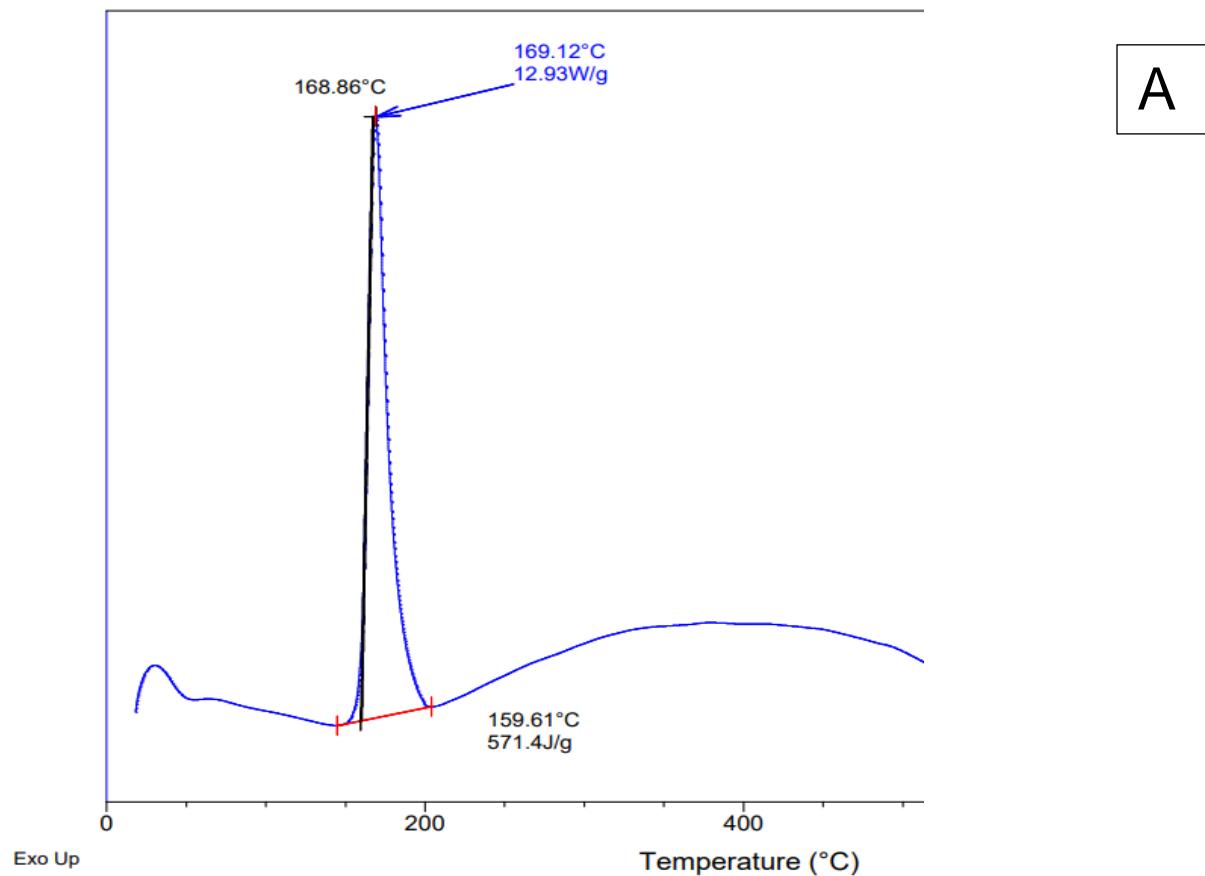
TG/DSC data for a sample of **PtL$^2_2$** showing: **A** - panoramic view of both traces, and **B** - integrated strong exothermic effect of compound's decomposition above 300°C (bottom panel).

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TG/DSC data for a sample of **PdL$^2_2$** showing: **A** - panoramic view of both traces, and **B** - integrated strong exothermic effect of compound's decomposition above 300°C (bottom panel).

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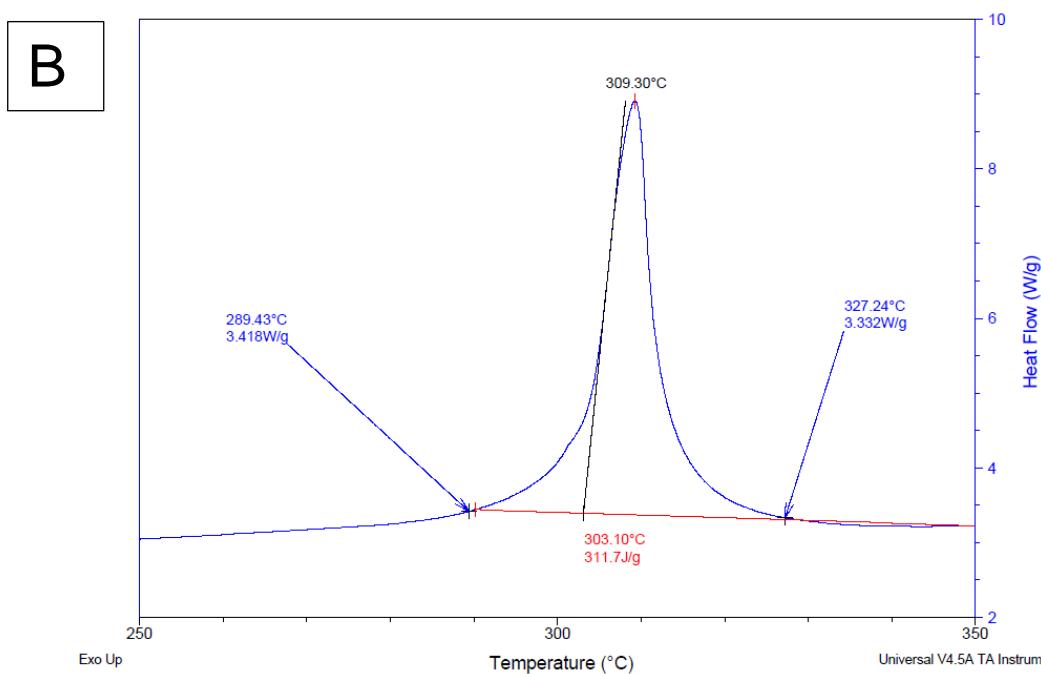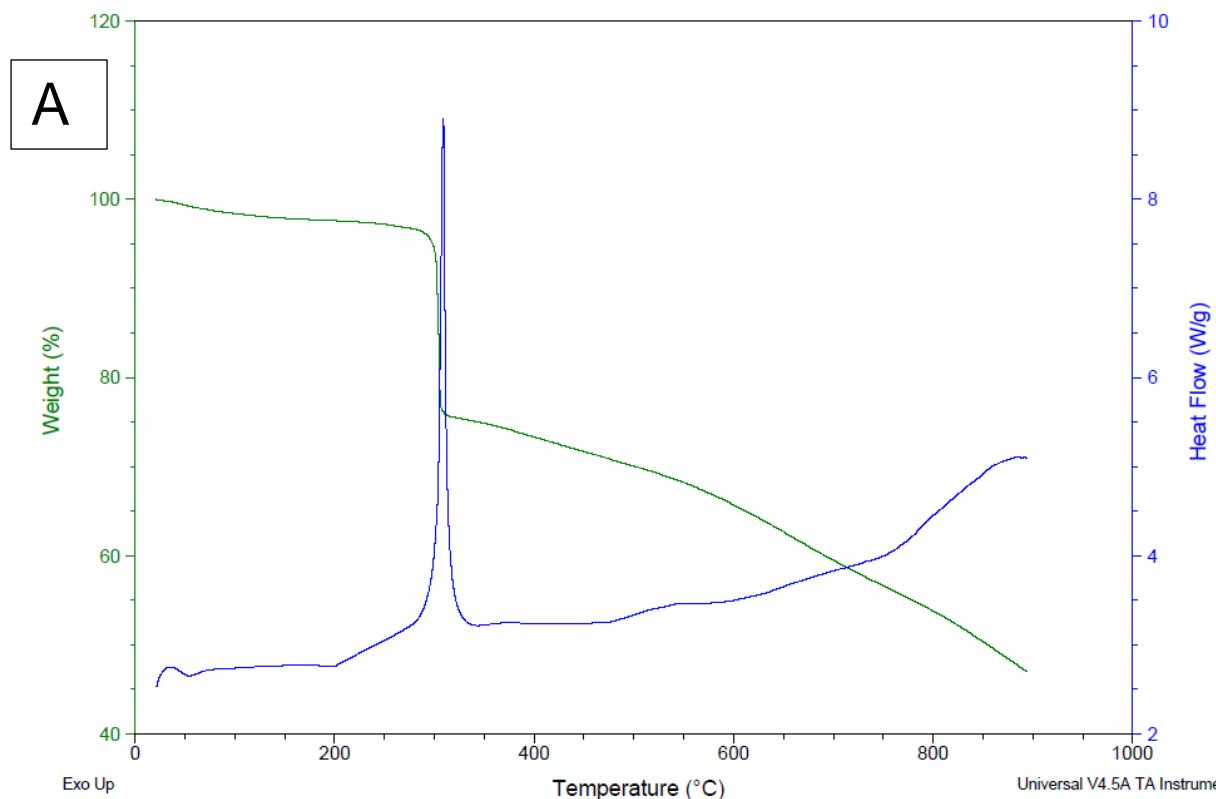
TG/DSC data for a sample of **PtL$^1_2$** showing traces of the weight loss (green line) and heat flow (blue line).
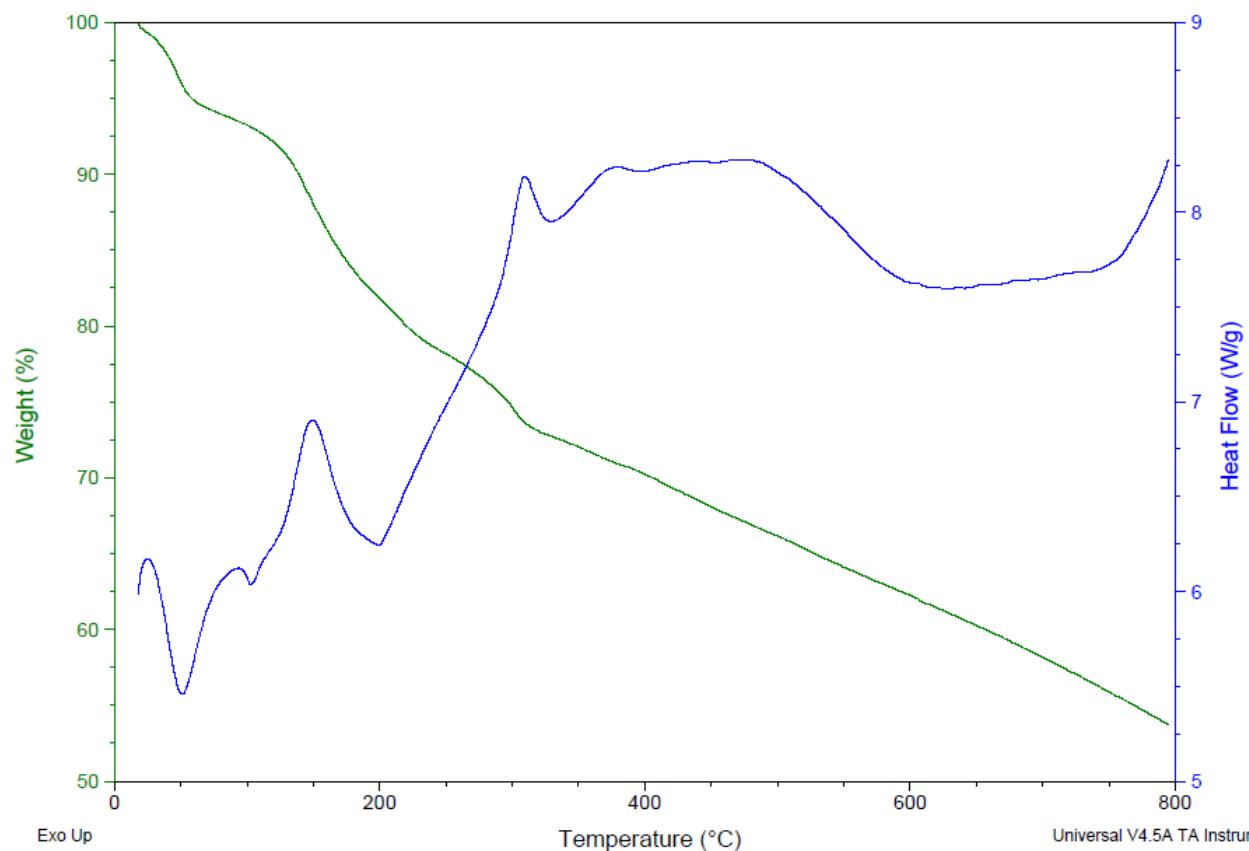
Exo Up — Temperature (°C) — Universal V4.5A TA Instrun

TG/DSC data for a sample of **PdL$^1_2$** showing traces of the weight loss (green line) and heat flow (blue line): **A** – panoramic view; **B** - integrated strong exothermic effect of compound's decomposition.

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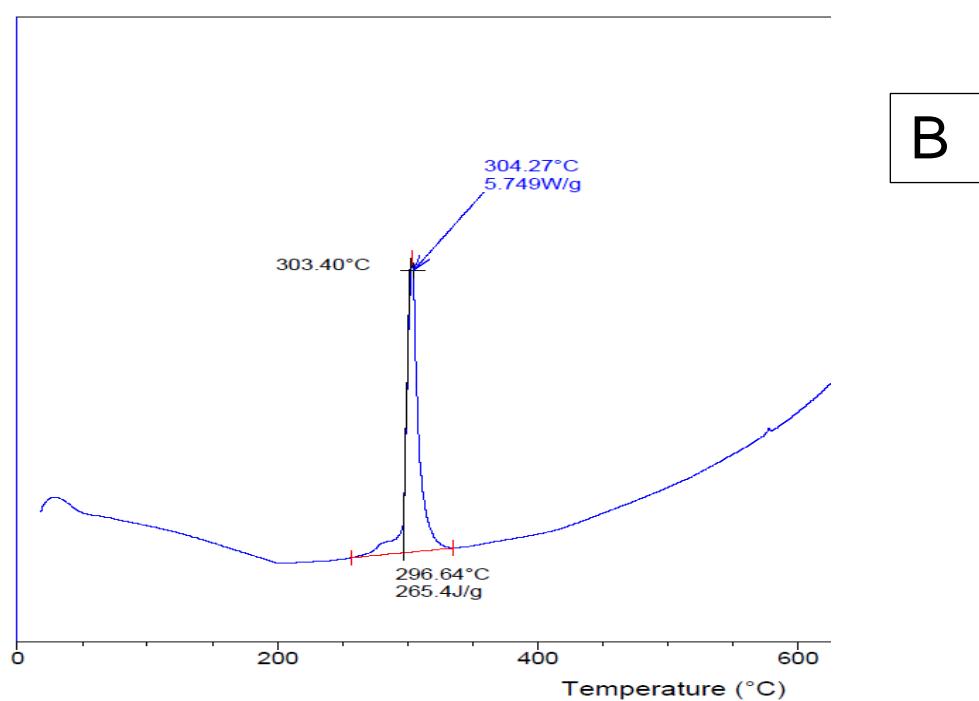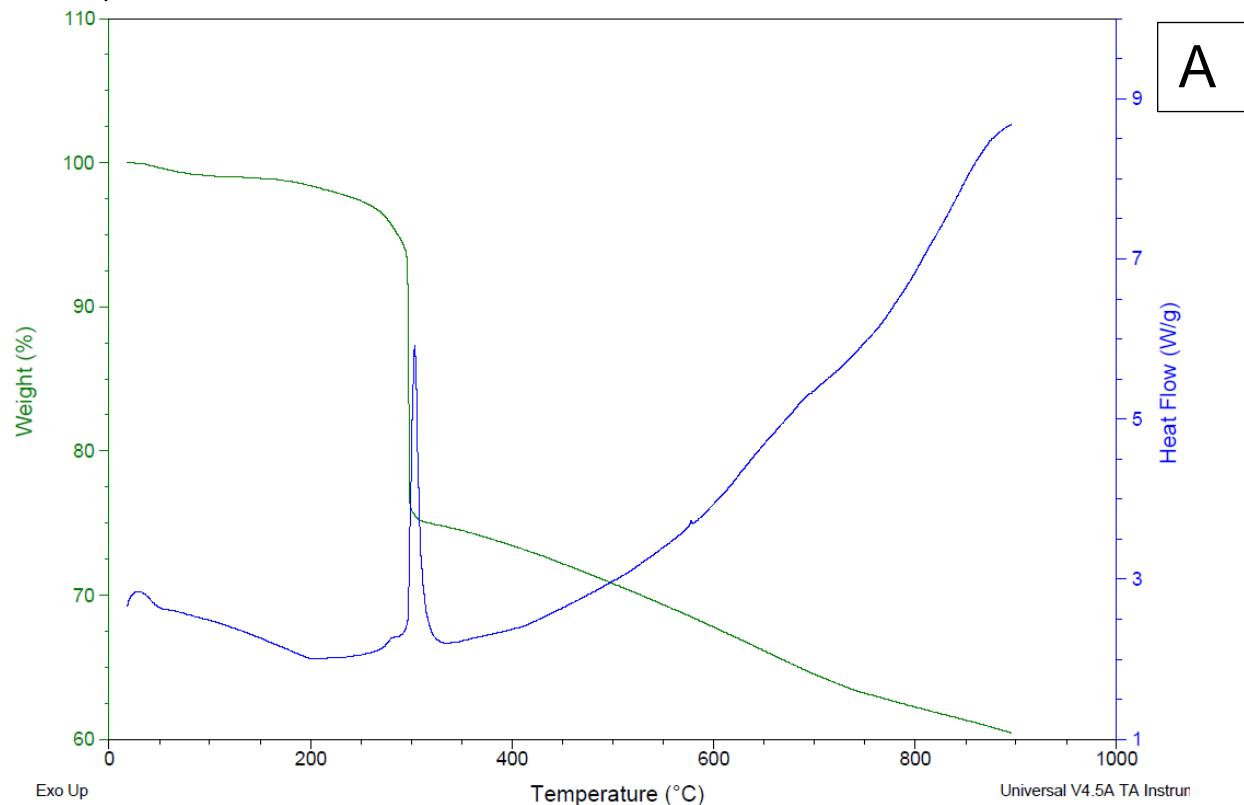
Photographs of alumina crucibles after thermal analysis experiments of synthesized Pt and Pd naphtoquinone-oximes. The formation of spongy metal residues as final products of decomposition is evident. They are not soluble in HCl and HNO_3, but dissolve in *aqua regia*.

Pd sponge

Pt sponge

_____

Geometry of square-planar environment of Pt center in **PtL$^2_2$,** CH$_3$CN-solvate: **A** – bonds, **B** – angles.
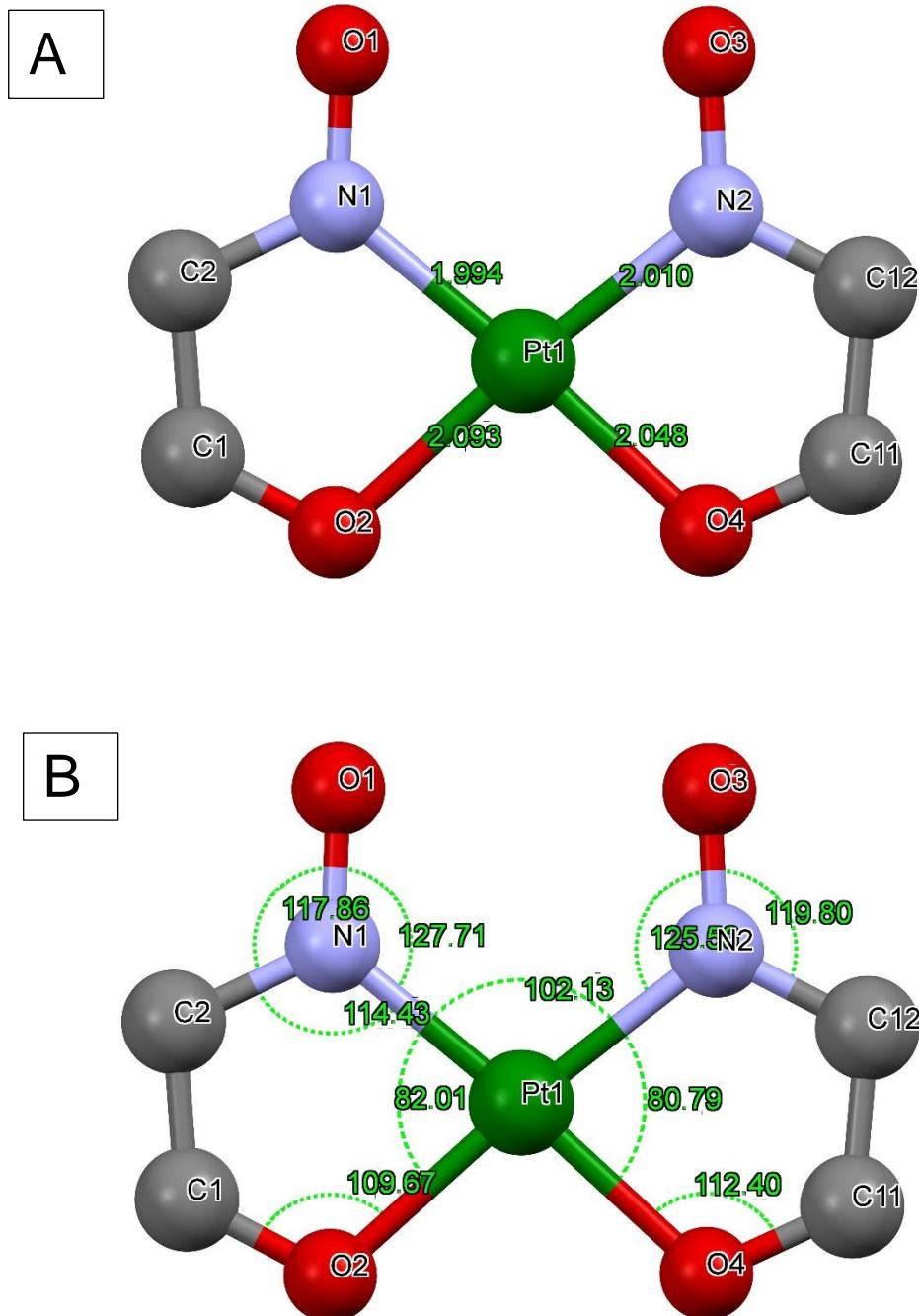
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The prospective view along a direction of the unit cell content in the structure of **PtL$^2_2$**, *acetonitrile solvate* showing solvent molecules in the unit cell indicated by arrows.
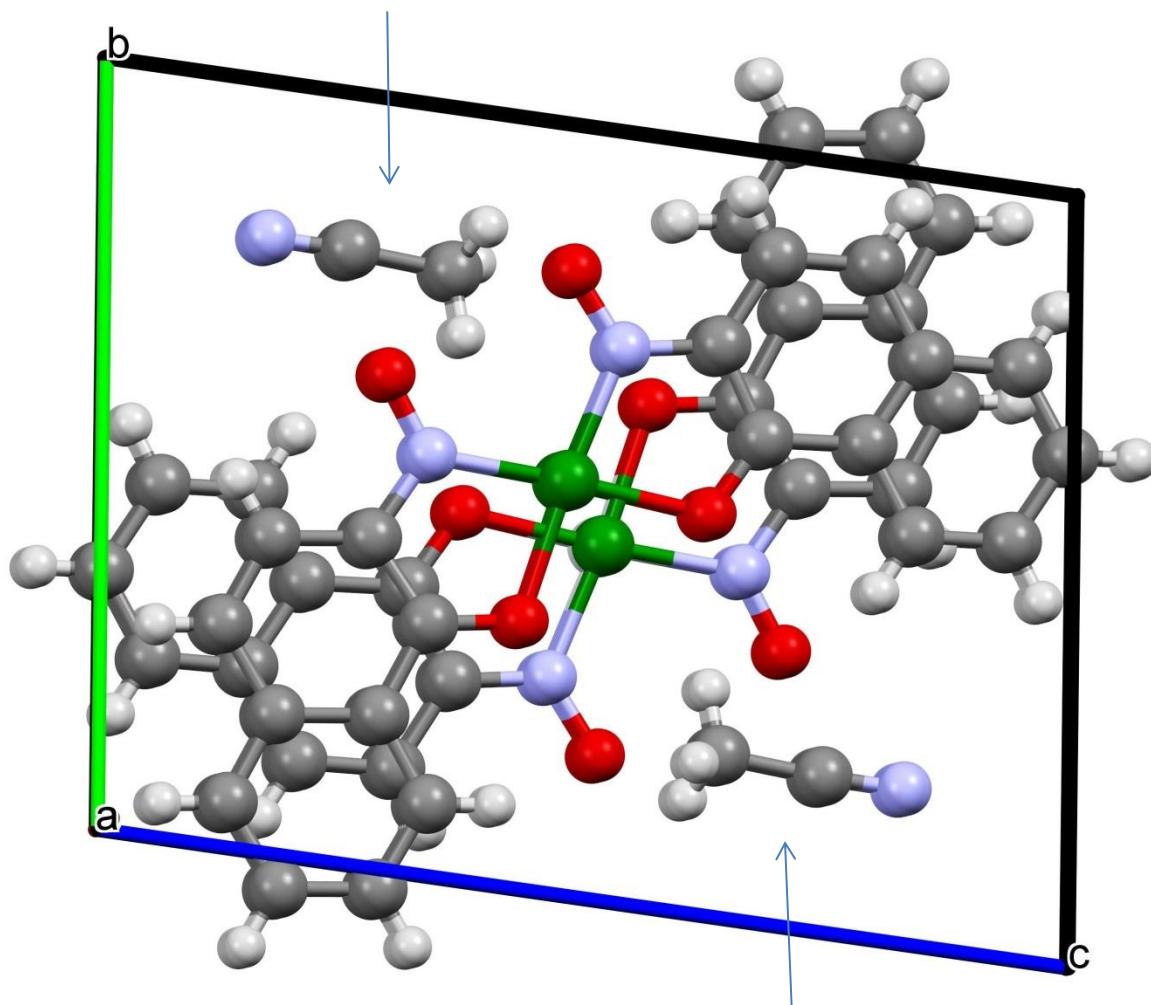
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Pruned view of several unit cells along c direction showing the geometry of "Pt-wires" in the structure of of **PtL$^2_2$**, *acetonitrile solvate*. Only metal centers are shown in their van-der-Waals size. The structure represents 1D-column built of dimers with metallophilic interactions in them and connected into a zigzag chain with ~145° angle.

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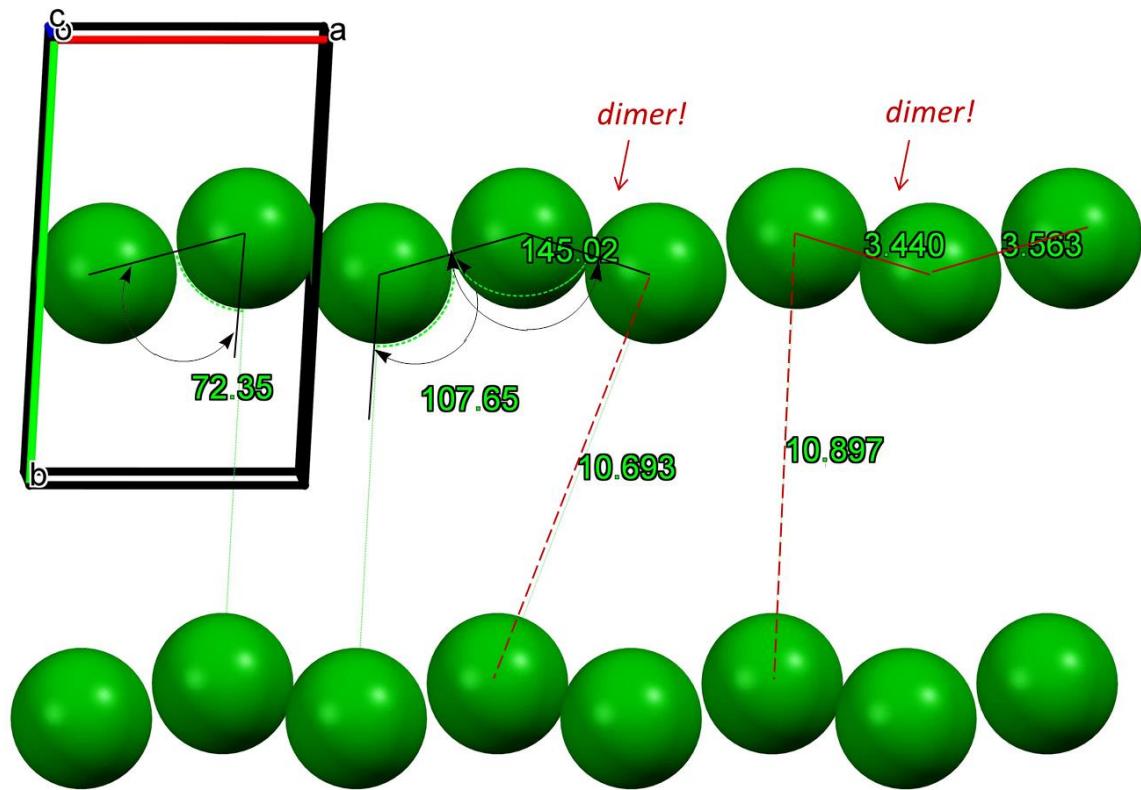
The ASU in the structure of **PtL²₂**, *acetonitrile solvate* showing: **A** - closest C-H---O contacts between oxygen atoms of the naphtol-groups in the metal complex and H-atoms in the solvent molecule, **B** - angles in these contacts. This specific solvent molecules insertion in this complex is *different* from such in the second complex with nitrobenzene.

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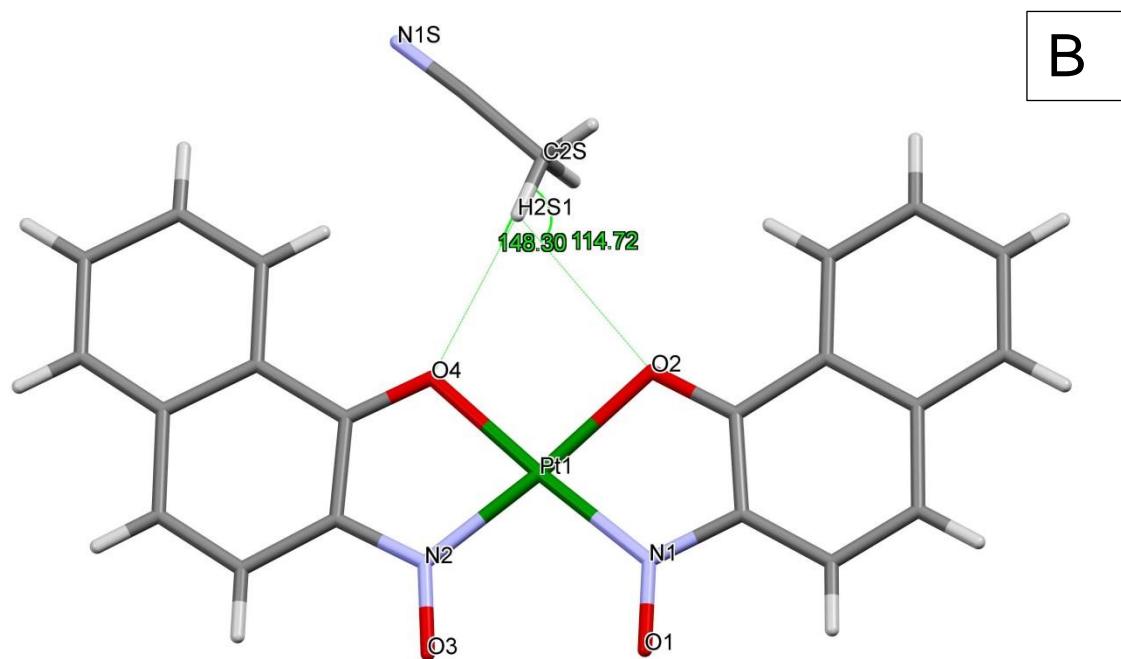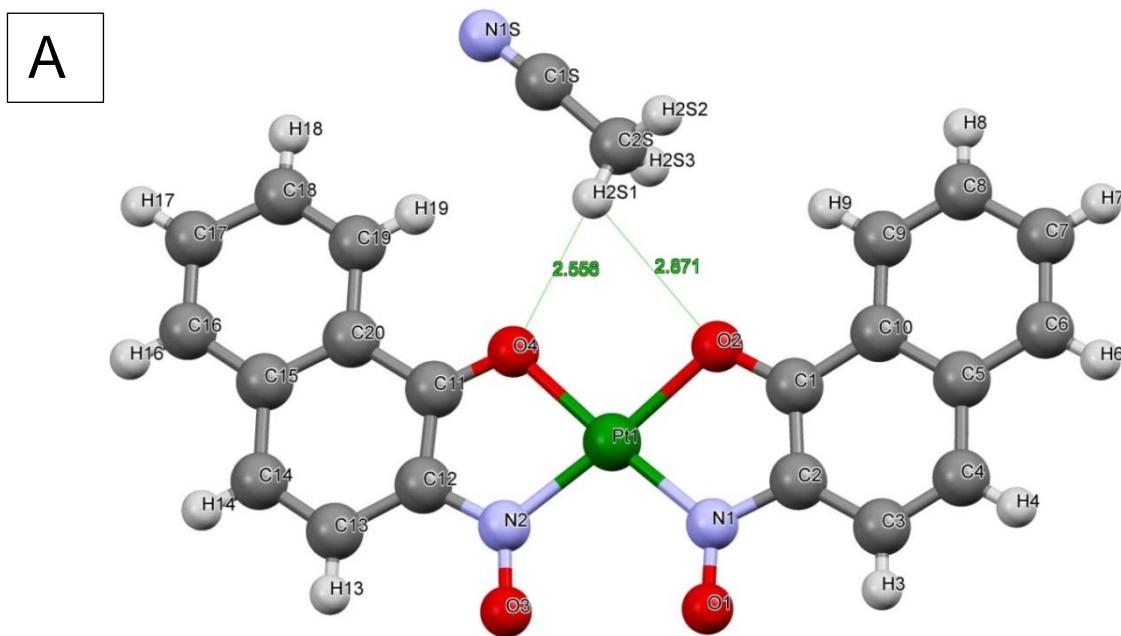
Geometry of square-planar environment of Pt center in **PtL$^2_2$,** $C_6H_5NO_2$-solvate: **A** – bonds, **B** – angles.
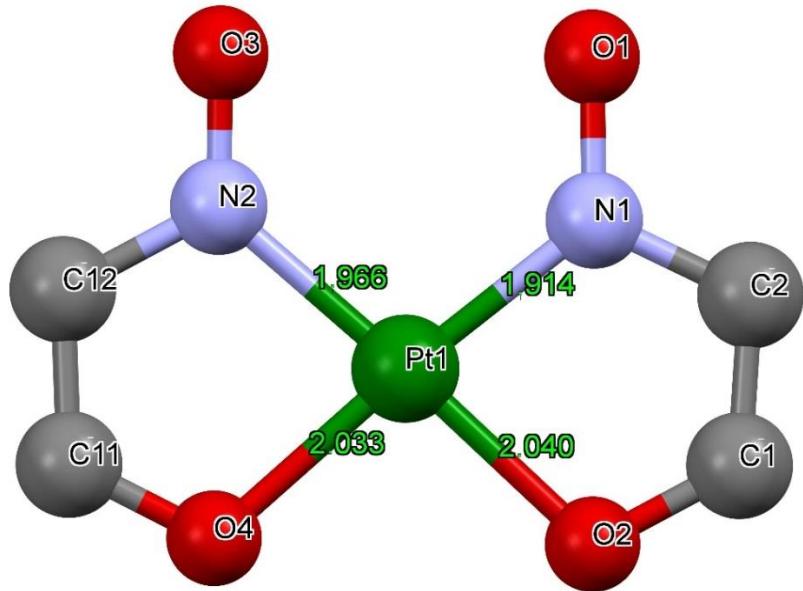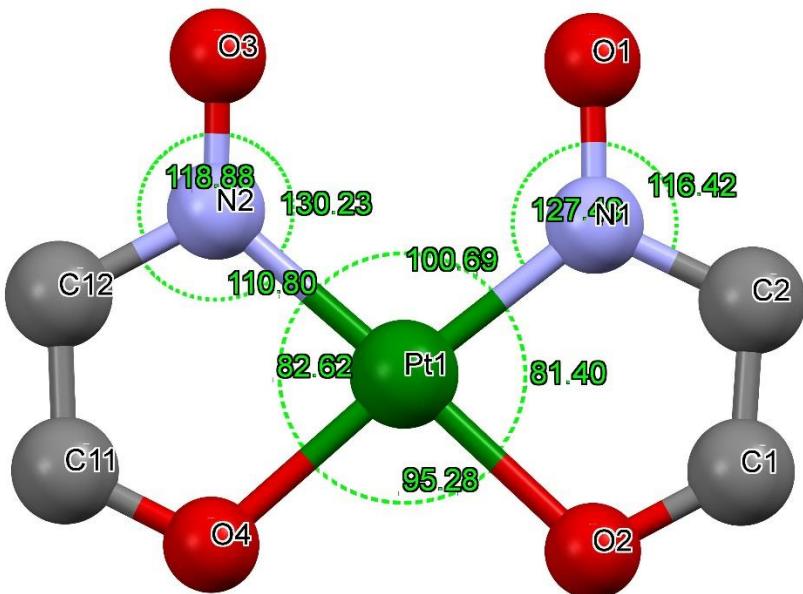
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The prospective view along a direction of the unit cell content in the structure of PtL$^2_2$, **nitrobenzene solvate** showing solvent molecules positioned in corners of the unit cell indicated by arrows.
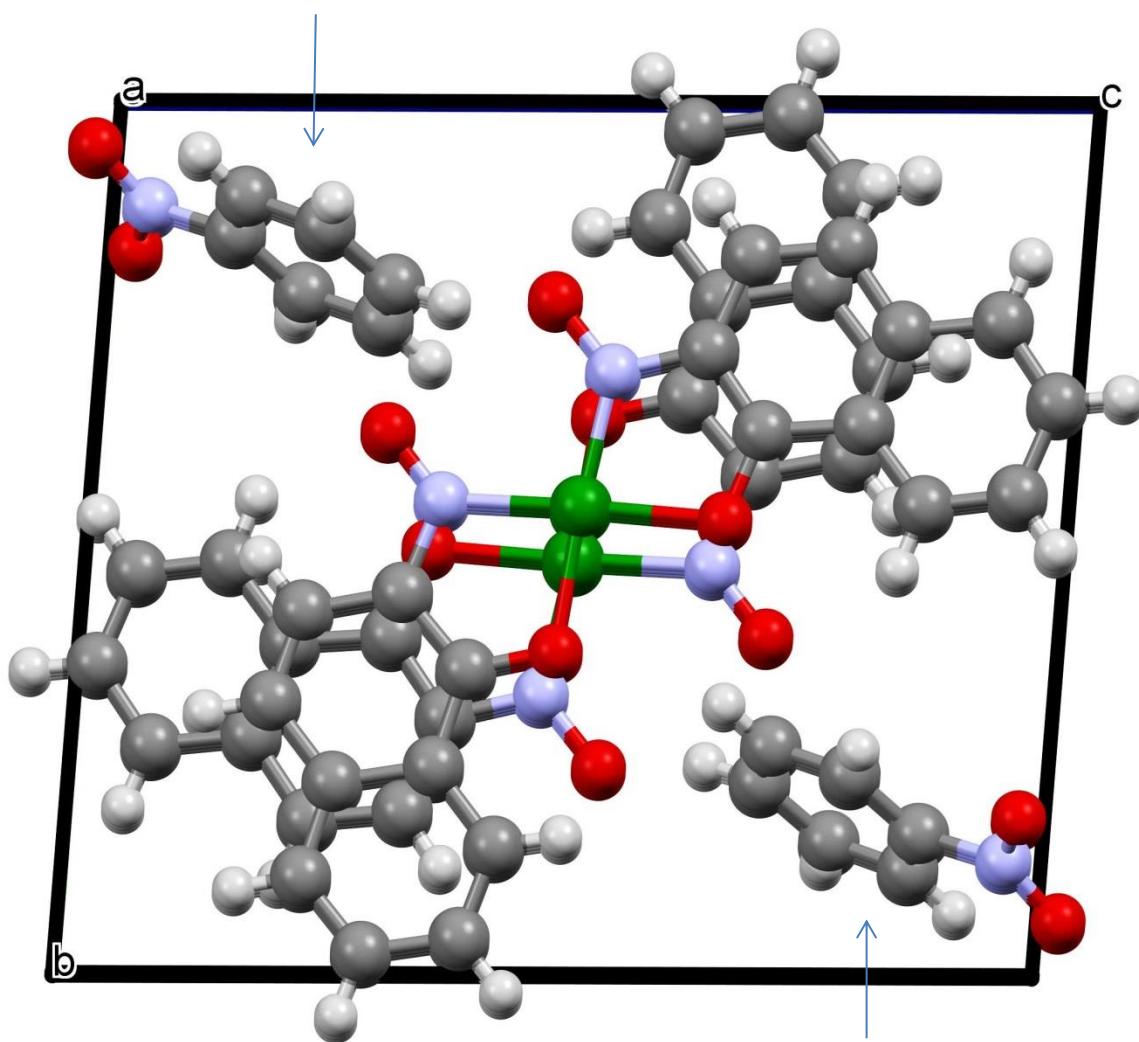
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Pruned view of several unit cells along c direction showing the geometry of "Pt-wires" in the structure of of PtL$^2_2$, **nitrobenzene solvate**. Only metal centers are shown in their van-der-Waals size. The structure represents 1D-column built of dimers with metallophilic interactions in them and connected into a zigzag chain with ~156° angle.

_____
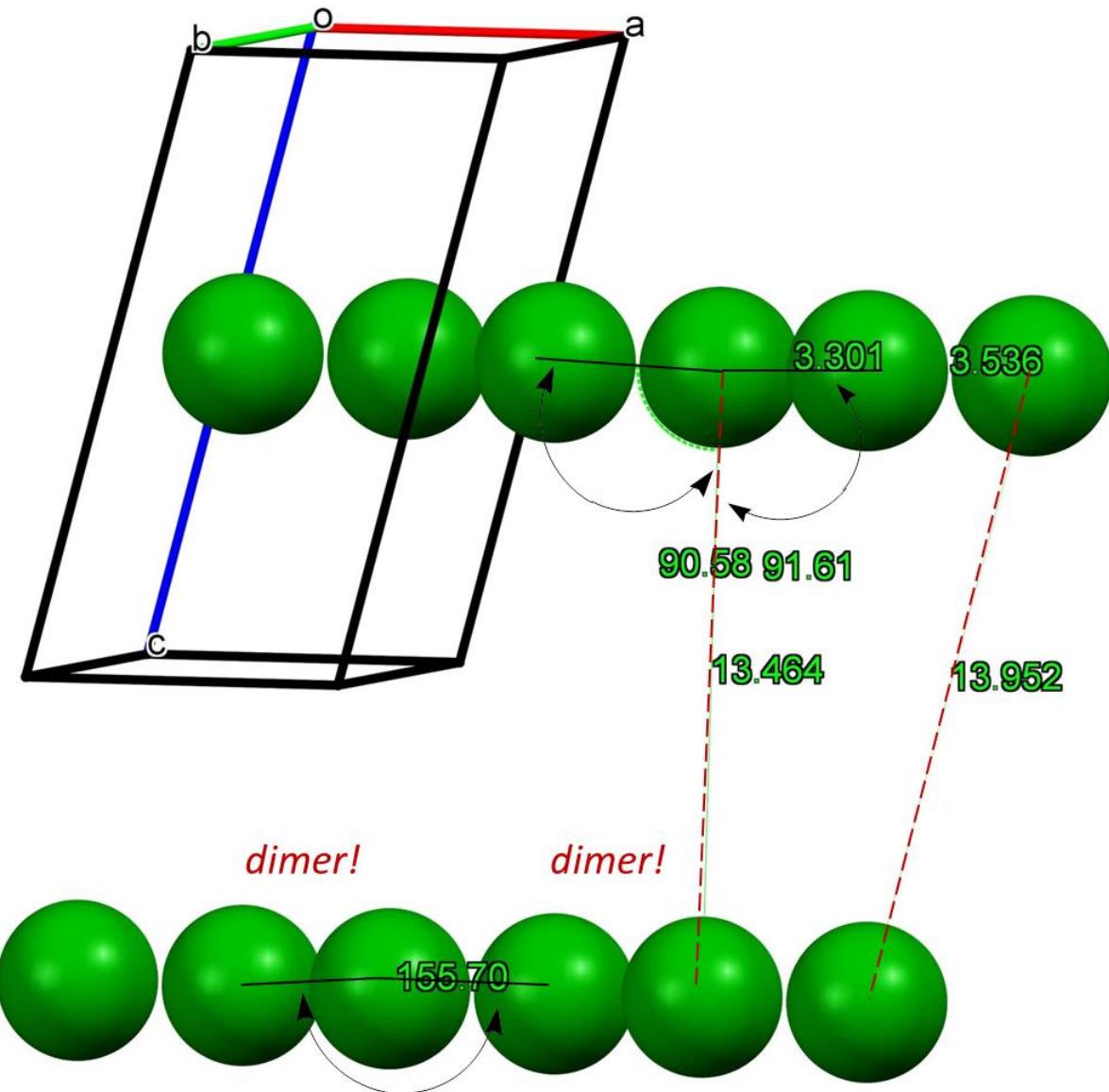
Further details of the structure of PtL$^2_2$, **_nitrobenzene solvate_** showing position of intercalating solvent molecule between two dimers: A – side view, B – top view.

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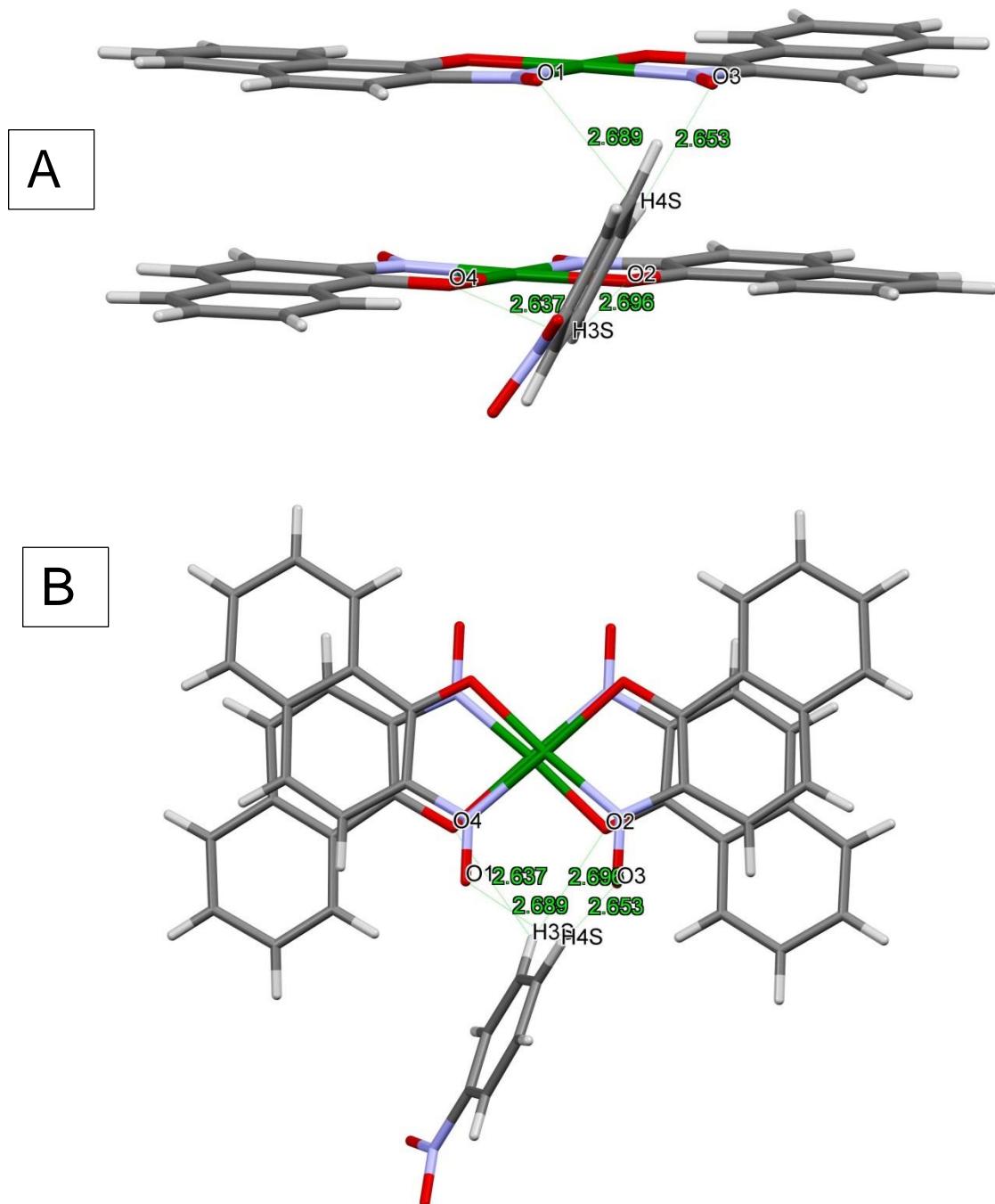
Details of the structure of PtL$^2_2$, **_nitrobenzene solvate_** showing bridging role of the solvent molecule located between 2 neighboring π-stacked units in the structure of 1D-column. Highlighted are the closest C-H---O contacts between oxygen atoms O1 and O3 of the nitroso-group and O2 and O4 oxygen atoms of the naphtol group (**A**), and respective angles (**B**).

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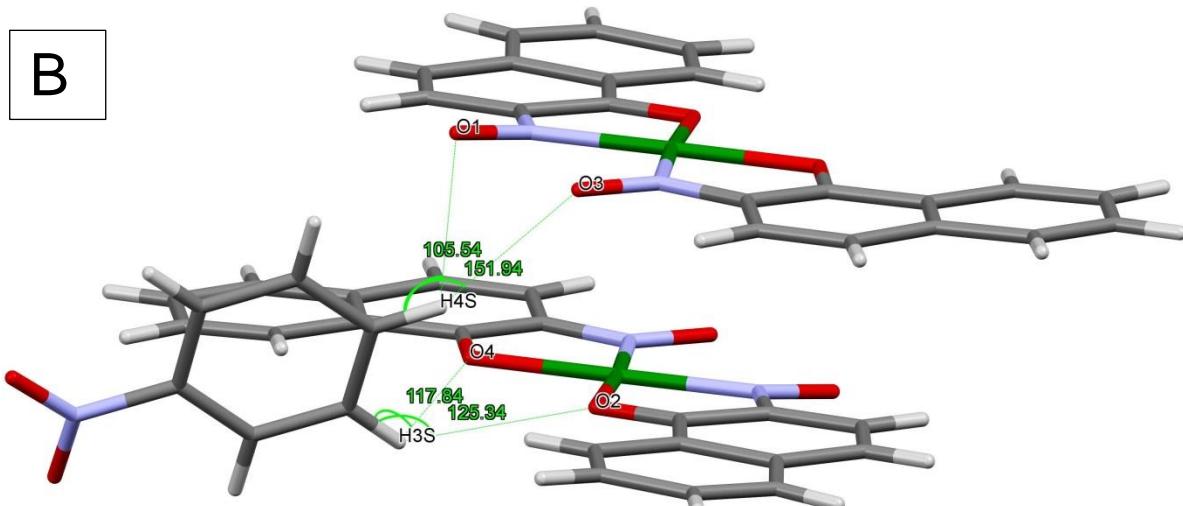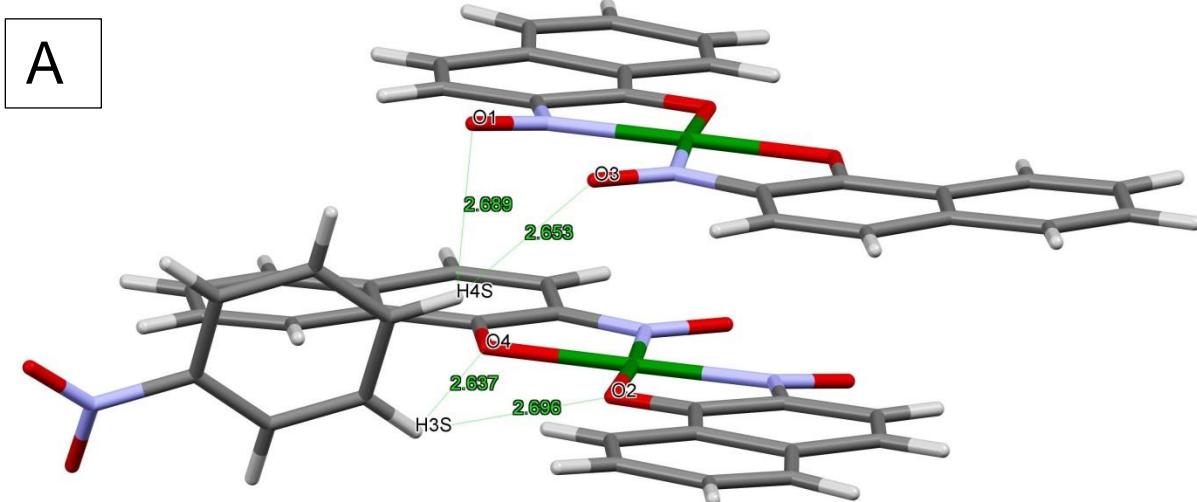
Fragment of the IR-spectrum of solid HL^1 in the fingerprint region. Weak ν(C-H) aromatic band is observed at 3065, 3020 cm^{-1}
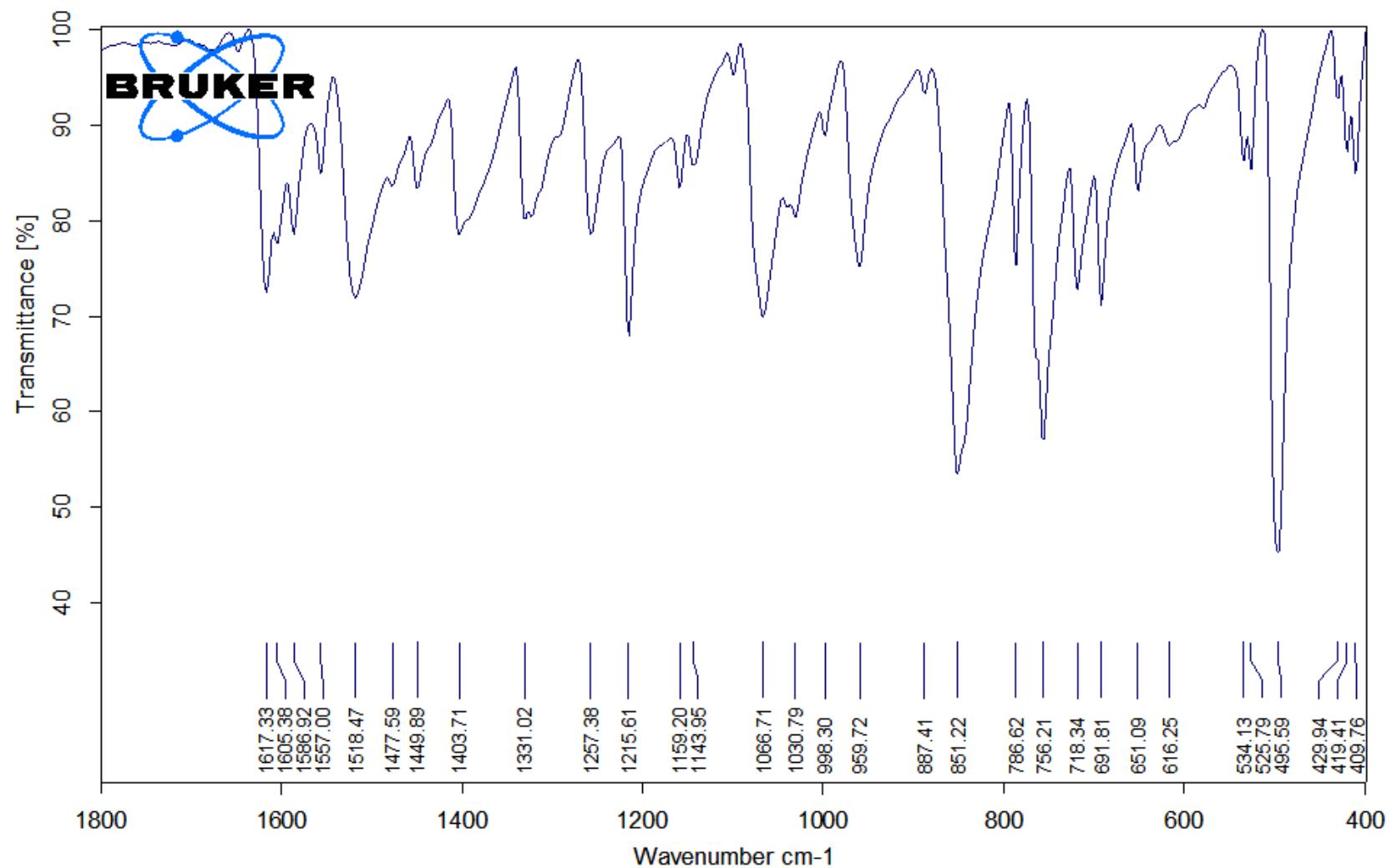
Fragment of the IR-spectrum of solid HL^2 in the fingerprint region. Weak ν(C-H) aromatic band is observed at 3085, 2973 cm^{-1}
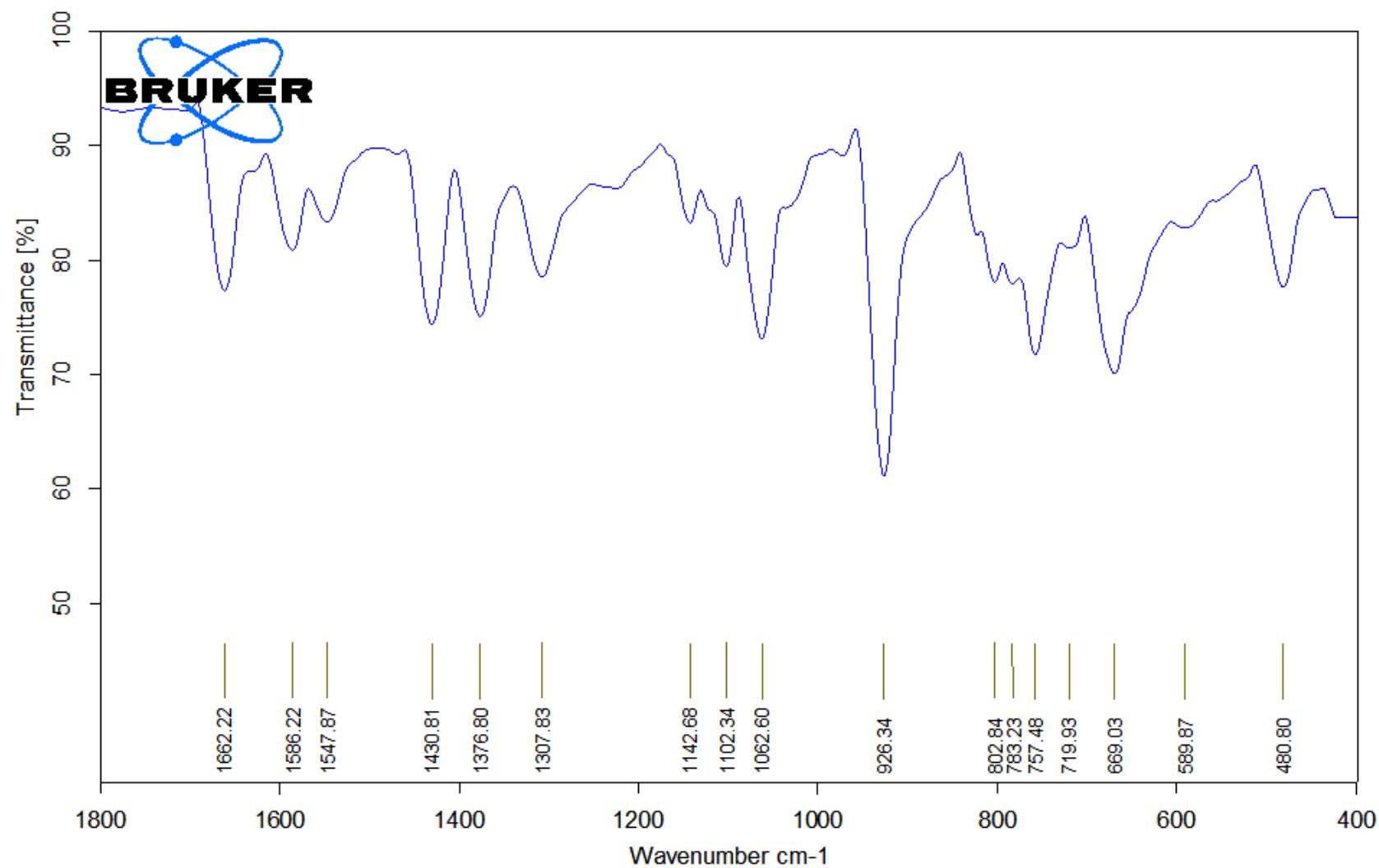
Fragment of the IR-spectrum of solid PdL$^1_2$ in the fingerprint region. Weak ν(C-H) aromatic band is observed at 3047 cm^{-1}

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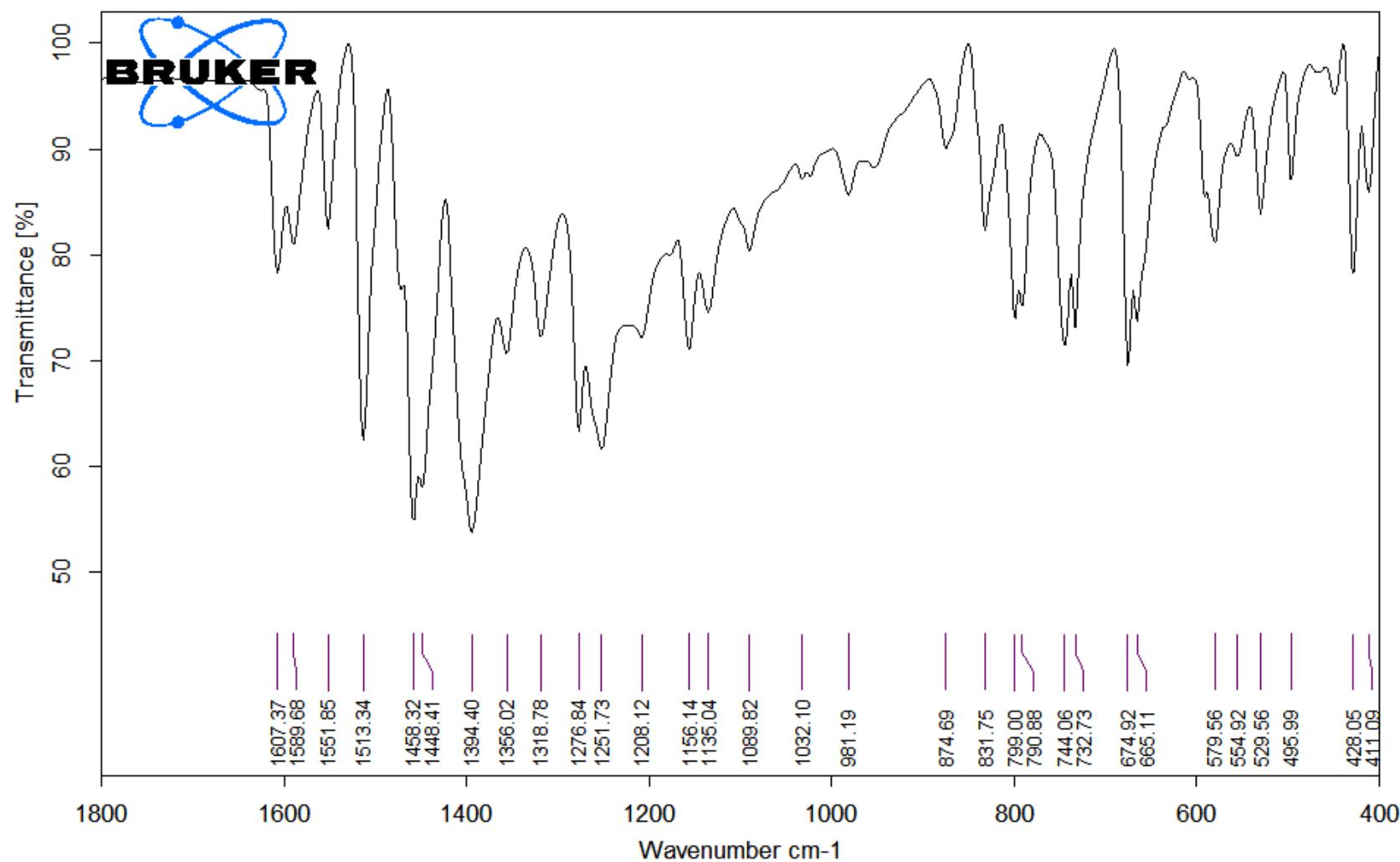
Fragment of the IR-spectrum of solid PdL^2_2 in the fingerprint region. Weak ν(C-H) aromatic band is observed at 3058 cm^{-1}
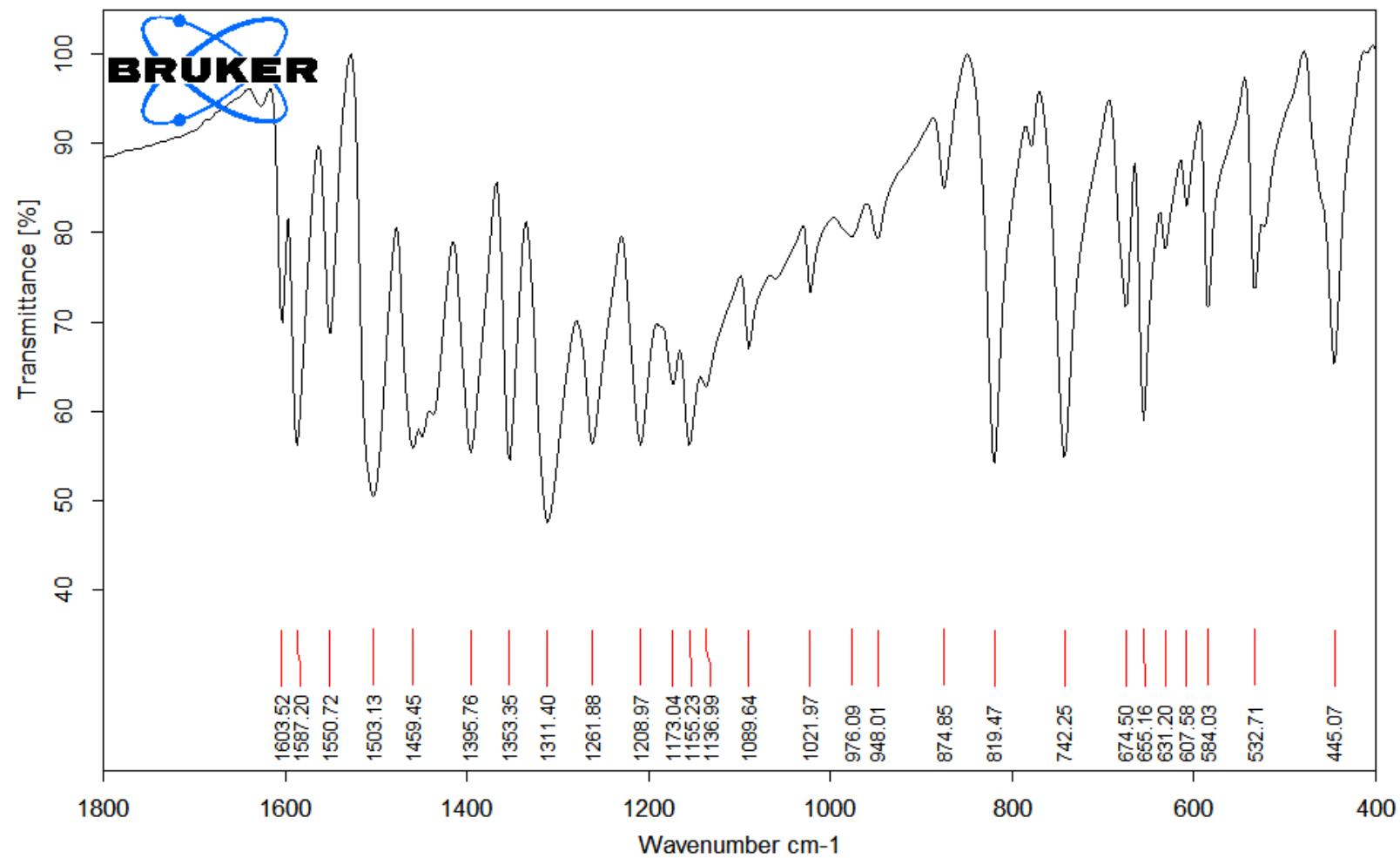
Fragment of the IR-spectrum of solid PtL^1_2 in the fingerprint region. Weak ν(C-H) aromatic band is observed at 3057 cm^{-1}
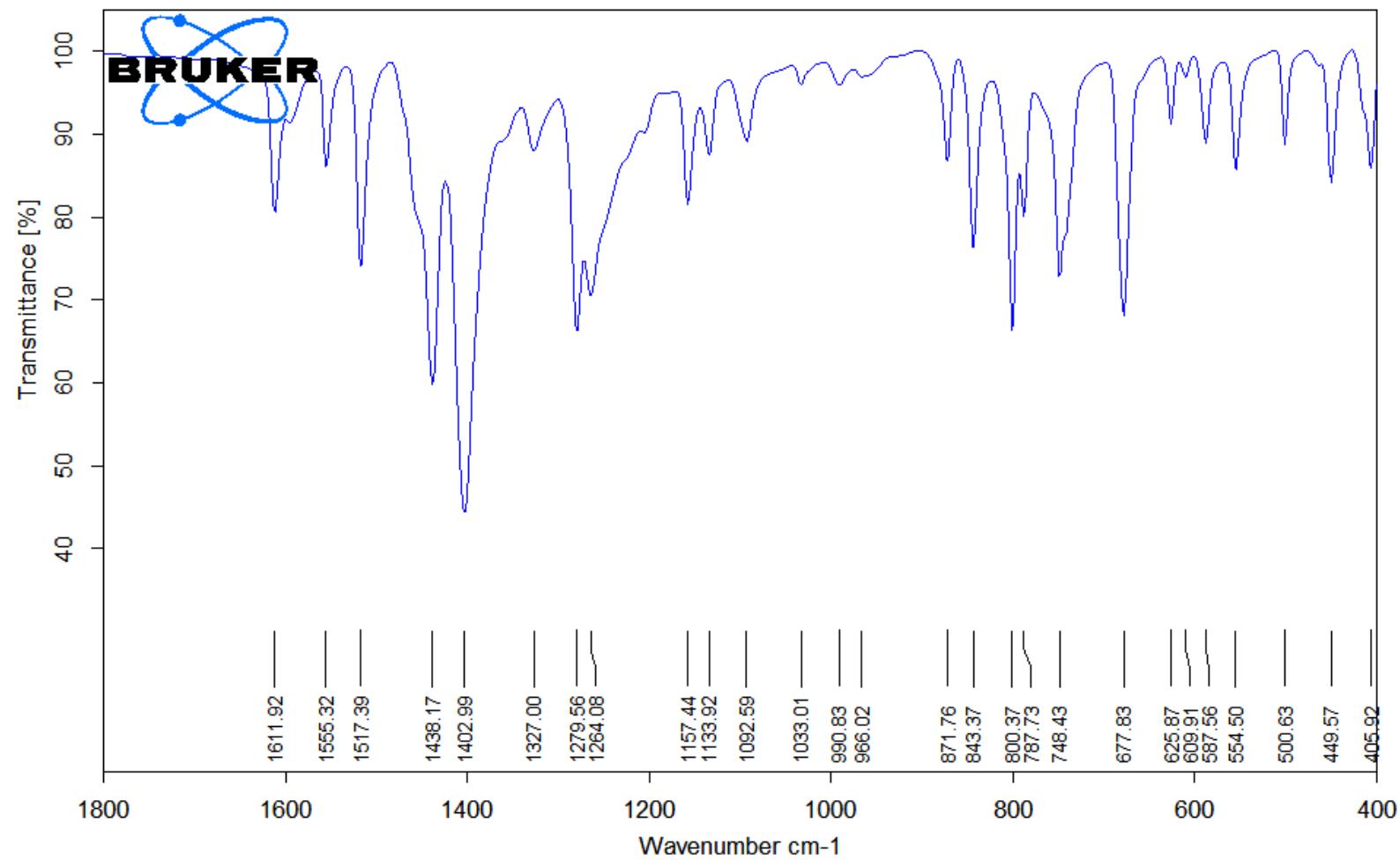
_____

Fragment of the IR-spectrum of solid PtL^1_2 in the fingerprint region. Weak ν(C-H) aromatic band is observed at 3065 cm^{-1}
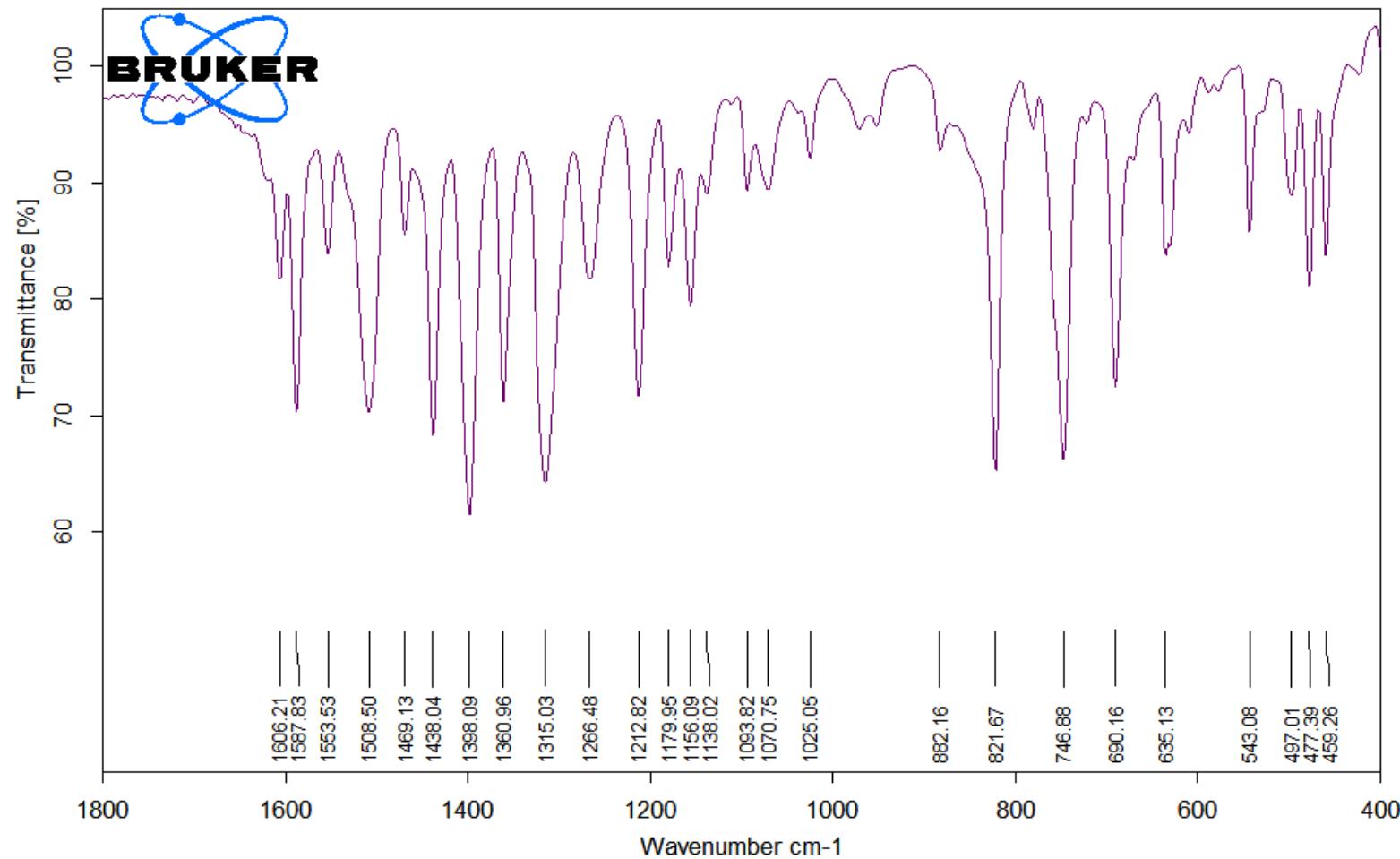
Spectra of diffuse reflectance (recorded in absorbance mode) of solid powders of Pt(II) naphtolo-oximes at 296 K in the range of 350-850 nm.

PtL$^1_2$
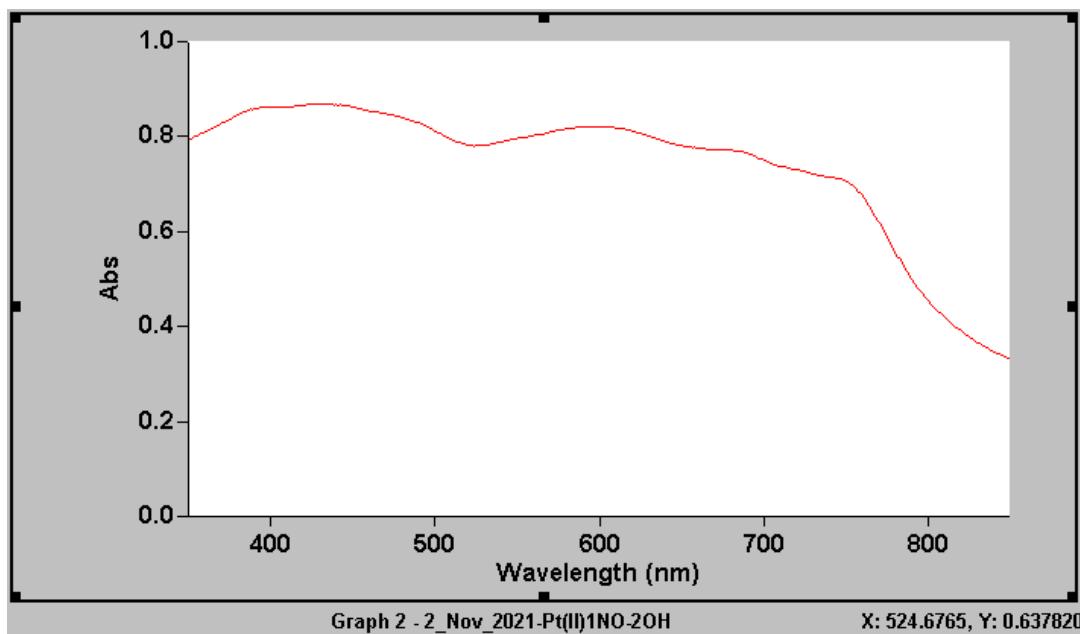
PtL$^2_2$
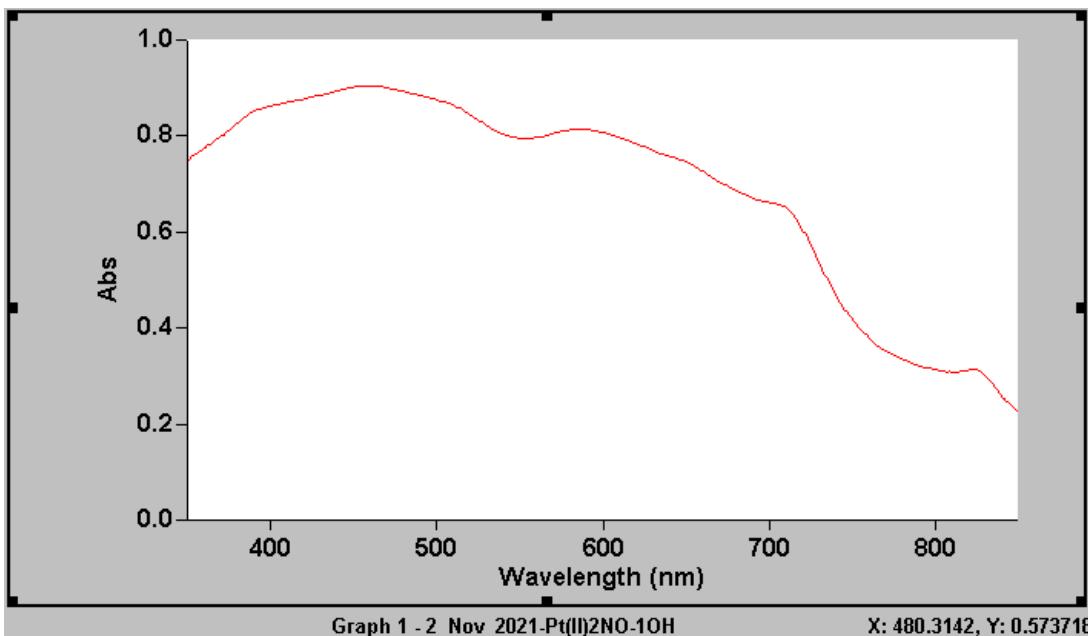
Two-dimensional fingerprint plot of complex **PtL^2$_2$·CH$_3$CN** showing the contribution of π–π stacking interaction to the total surface area.

_____

Two-dimensional fingerprint plot of complex **PtL$^2_2$·C$_6$H$_5$NO$_2$** showing the contribution of $\pi-\pi$ stacking interaction to the total surface area.

_____
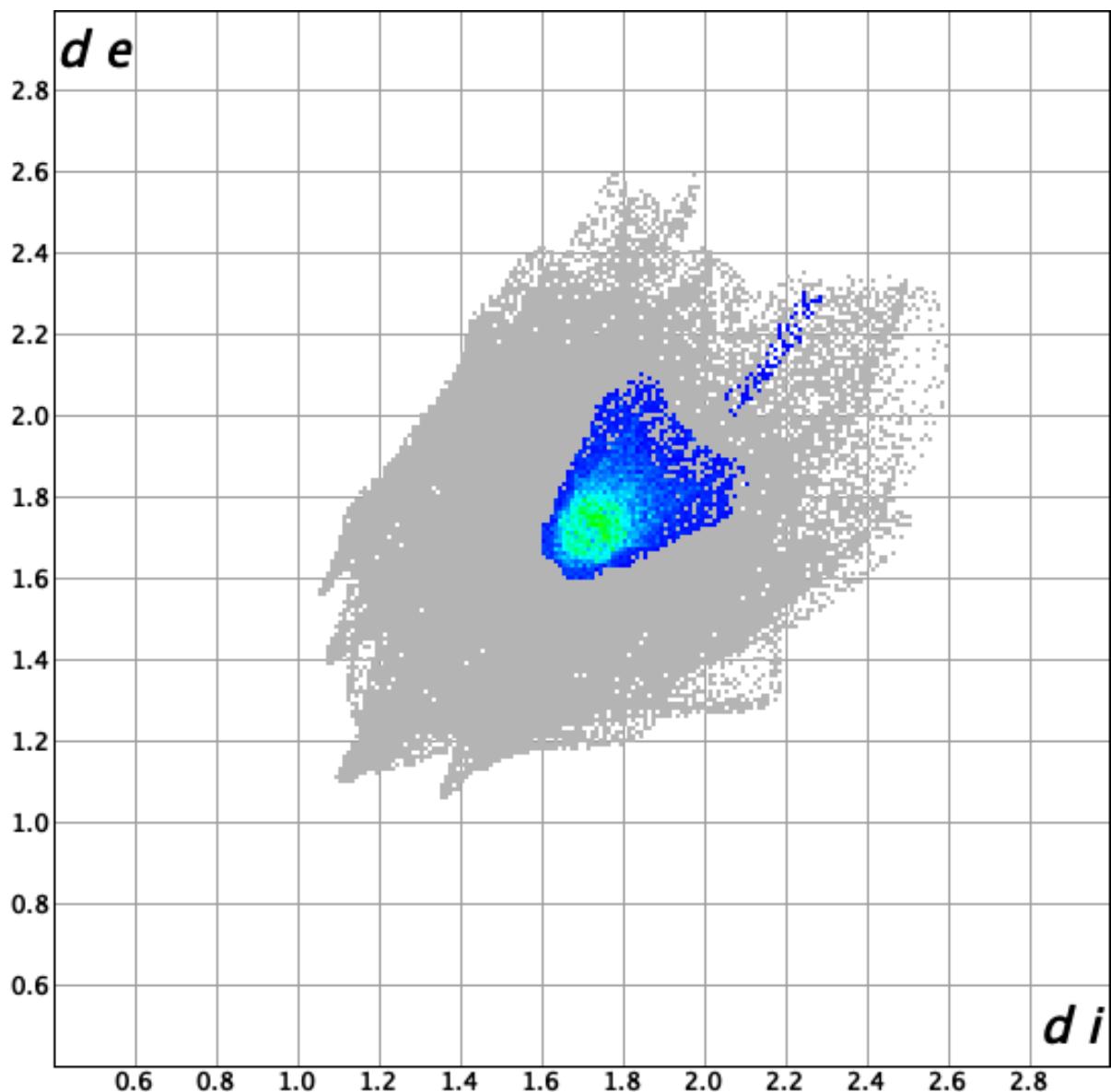
CHECK CIF reports for crystal structures in this paper.

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) Pt-2NO-1OH_acetonitrile

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: Pt-2NO-1OH_acetonitrile

```
Bond precision:  C-C = 0.0203 A          Wavelength=0.71073
Cell:         a=6.679(8)        b=10.897(13)    c=13.866(17)
              alpha=97.279(14) beta=93.082(16) gamma=92.877(14)
Temperature: 120 K
                   Calculated              Reported
Volume         998(2)                  998(2)
Space group    P -1                    P -1
Hall group     -P 1                    -P 1
Moiety formula C20 H12 N2 O4 Pt, C2 H3 C20 H12 N2 O4 Pt, C2 H3
               N                       N
Sum formula    C22 H15 N3 O4 Pt        C22 H15 N3 O4 Pt
Mr             580.45                  580.46
Dx,g cm-3      1.932                   1.932
Z              2                       2
Mu (mm-1)      7.064                   7.065
F000           556.0                   556.0
F000'          552.96
h,k,lmax       7,12,16                 7,13,17
Nref           3505                    3232
Tmin,Tmax      0.495,0.815             0.460,0.745
Tmin'          0.284
Correction method= # Reported T Limits:
Tmin=0.460 Tmax=0.745 AbsCorr = MULTI-SCAN
Data completeness= 0.922 Theta(max)= 24.999
                                       wR2(reflections)=
R(reflections)= 0.0586( 1881)          0.1250( 3232)

S = 0.752          Npar= 272
```

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 B

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ....   0.0203 Ang.
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L=   0.595   272 Report
PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on   Pt1   1.70 eA-3

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
          outside the range 0.80 <> 2.00
          Goodness of fit given =   0.752
PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full   ! Check
PLAT148_ALERT_3_C s.u. on the   a   - Axis is (Too) Large ....   0.008 Ang.
And 2 other PLAT148 Alerts
More ...
PLAT213_ALERT_2_C Atom C19   has ADP max/min Ratio .....   3.2 prolat
PLAT234_ALERT_4_C Large Hirshfeld Difference C7   --C8   .   0.17 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   3.528 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.09Ang From Pt1   2.33 eA-3
And 2 other PLAT971 Alerts
More ...
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.06Ang From Pt1   -1.56 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.78Ang From O4   .   0.99 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2S2   .   -0.35 eA-3

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...   11 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records   2 Report
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C1   -C10   .   1.45 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C11   -C20   .   1.45 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   3 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Pt1   (II)   .   2.06 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   66 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .   Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still   30% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File   13 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ....   1.0 Low
PLAT954_ALERT_1_G Reported (CIF) and Actual (FCF) Kmax Differ by .   1 Units
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by .   1 Units
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities ....   Please Check
PLAT963_ALERT_2_G Both SHELXL WEIGHT Parameter Values Zero ....   Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..   50.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   1 Info

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

  4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

15 ALERT type 2 Indicator that the structure model may be wrong or deficient
 9 ALERT type 3 Indicator that the structure quality may be low
 3 ALERT type 4 Improvement, methodology, query or suggestion
 3 ALERT type 5 Informative message, check

PLATON version of 18/05/2022; check.def file version of 17/05/2022

Datablock Pt-2NO-1OH_acetonitrile - ellipsoid plot
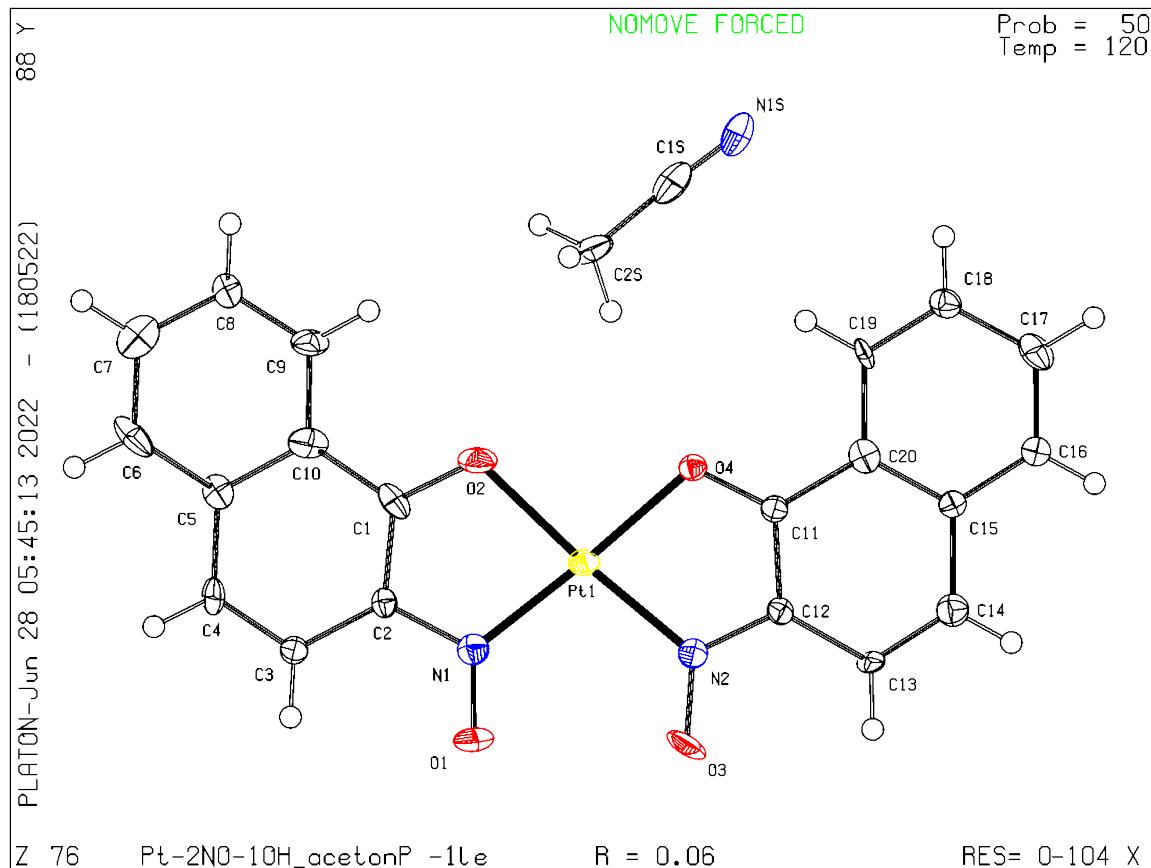
checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) R1-Pt-2NO1OH_nitrobenzene

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: R1-Pt-2NO1OH_nitrobenzene

Bond precision: C-C = 0.0150 A   Wavelength=0.71073

Cell: a=6.707(2)   b=12.203(4)   c=14.016(5)
              alpha=92.739(5) beta=103.808(5) gamma=96.875(5)

Temperature: 100 K

	Calculated	Reported
Volume	1102.5(6)	1102.5(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C20 H12 N2 O4 Pt, C6 H5 N O2	C20 H12 N2 O4 Pt, C6 H5 N O2
Sum formula	C26 H17 N3 O6 Pt	C26 H17 N3 O6 Pt
Mr	662.51	662.52
Dx,g cm-3	1.996	1.996
Z	2	2
Mu (mm-1)	6.415	6.413
F000	640.0	637.1
F000'	636.98	
h,k,lmax	8,15,17	8,15,17
Nref	4608	4553
Tmin,Tmax	0.191,0.764	0.722,1.000
Tmin'	0.067	

Correction method= # Reported T Limits:
Tmin=0.722 Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 0.988 Theta(max)= 26.550

R(reflections)= 0.0572(3824)   wR2(reflections)= 0.1515(4553)

S = 0.973   Npar= 323

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 A
PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.88Ang From O4   5.73 eA-3
And 4 other PLAT971 Alerts

More ...
PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.90Ang From Pt1   -3.99 eA-3
PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.86Ang From Pt1   -3.63 eA-3

🔴Alert level B

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.10Ang From N1   2.89 eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.20Ang From O4   2.77 eA-3
PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.90Ang From Pt1   -2.99 eA-3
And 2 other PLAT972 Alerts
More ...

🟡Alert level C

PLAT213_ALERT_2_C Atom C5   has ADP max/min Ratio .....   3.2 oblate
PLAT222_ALERT_3_C NonSolvent Resd 1 H   Uiso(max)/Uiso(min) Range   5.0 Ratio
PLAT245_ALERT_2_C U(iso) H16   Smaller than U(eq) C16   by   0.016 Ang**2
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....   2.1 Note
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.01496 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   2 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.36Ang From O4   2.49 eA-3
And 5 other PLAT971 Alerts
More ...
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.94Ang From Pt1   -1.95 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.10Ang From O4   -1.83 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.99Ang From N1   .   -1.19 eA-3

⚪Alert level G

PLAT012_ALERT_1_G No   _shelx_res_checksum Found in CIF ......   Please Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)   0.005 Degree
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.   4 Note
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   5 Report
PLAT769_ALERT_4_G CIF Embedded explicitly supplied scattering data   Please Note
PLAT794_ALERT_5_G Tentative Bond Valency for Pt1   (II)   .   2.42 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .   Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).   1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   54 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File   7 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ....   2.9 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged   Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   1 Info
PLAT982_ALERT_1_G The Pt-f'=   -1.6379 Deviates from IT-value =   -1.7033 Check
PLAT983_ALERT_1_G The Pt-f"=   8.5789 Deviates from IT-Value =   8.3905 Check

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

PLATON version of 28/11/2022; check.def file version of 28/11/2022

Datablock R1-Pt-2NO1OH_nitrobenzene - ellipsoid plot