Supplementary data for the article:

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Supplementary Material

Synthesis, structural and DFT analysis of a binuclear nickel(II) complex with the 1,4-bis-{2-[2-(diphenylphosphino)benzylidene]}phthalazinyl hydrazone ligand

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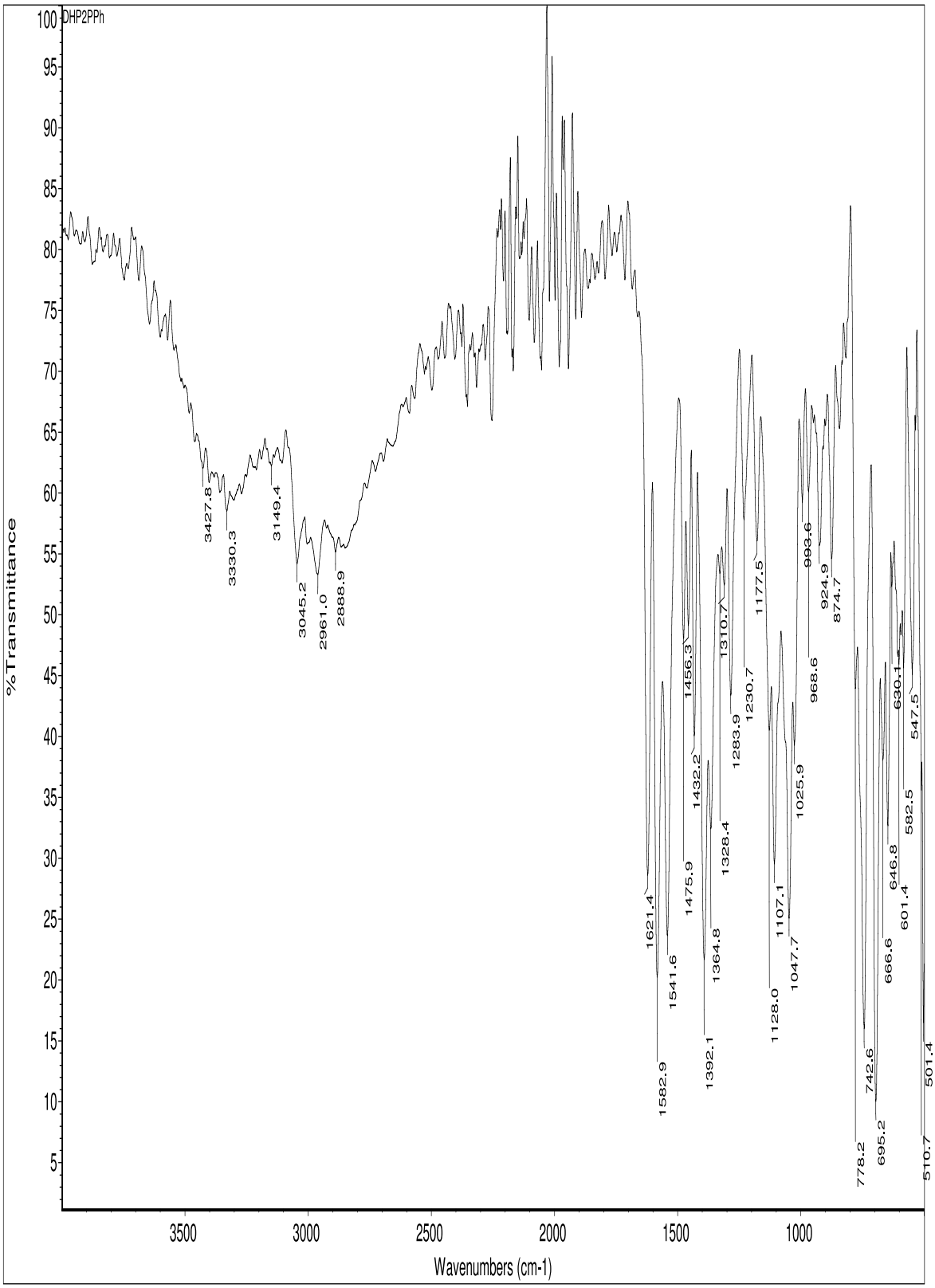
Table S1 Crystallographic data and refinement details for the binuclear nickel(II) complex (**2**)

Crystal data	
Chemical formula	$C_{47}H_{42}Cl_3N_6Ni_2O_2P_2 \cdot 2(CH_4O) \cdot Cl$
M_r	1108.11
Crystal system, space group	Triclinic, *P*–1
Temperature (K)	294
a, *b*, *c* (Å)	12.3956(5), 14.8378(6), 15.0593(6)
α, *β*, *γ* (°)	87.926(3), 72.807(4), 71.367(4)
V (Å^3)	2502.11(19)
Z	2
Radiation type	Mo *Kα*
μ (mm^{-1})	1.08
Crystal size (mm)	0.67 × 0.43 × 0.27
Data collection	
Diffractometer	Gemini S (Oxford Diffraction)
Absorption correction	Analytical
T_{min}, T_{max}	0.668, 0.816
No. of measured, independent and observed [$I>2\sigma(I)$] reflections	22863, 11437, 9238
R_{int}	0.025
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.683
Refinement	
$R[F^2>2\sigma(F^2)]$, $wR(F^2)$, *S*	0.038, 0.135, 1.12
No. of reflections	11437
No. of parameters	628
No. of restraints	8
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.54, −0.53

1,4-Bis-{2-[2-(diphenylphosphino)benzylidene}]phthalazinylhydrazone (**1**)


DHP2PPh
%Transmittance
Wavenumbers (cm-1)
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3045.2
2961.0
2888.9
1621.4
1582.9
1541.6
1475.9
1456.3
1432.2
1392.1
1364.8
1328.4
1310.7
1283.9
1230.7
1177.5
1128.0
1107.1
1047.7
1025.9
998.6
968.6
924.9
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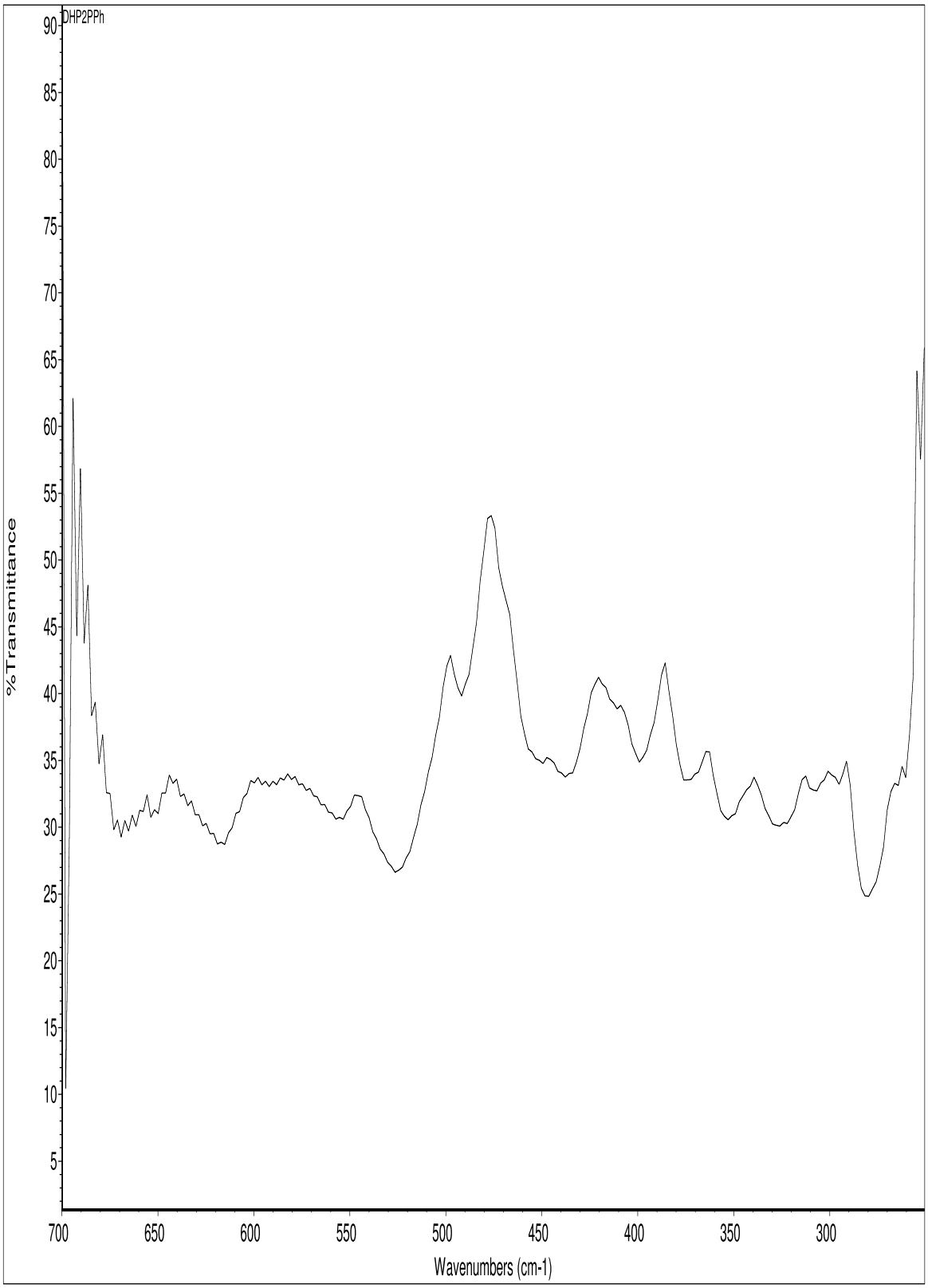
547.5
510.7
501.4


DHP2PPh
%Transmittance
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85
80
75
70
65
60
55
50
45
40
35
30
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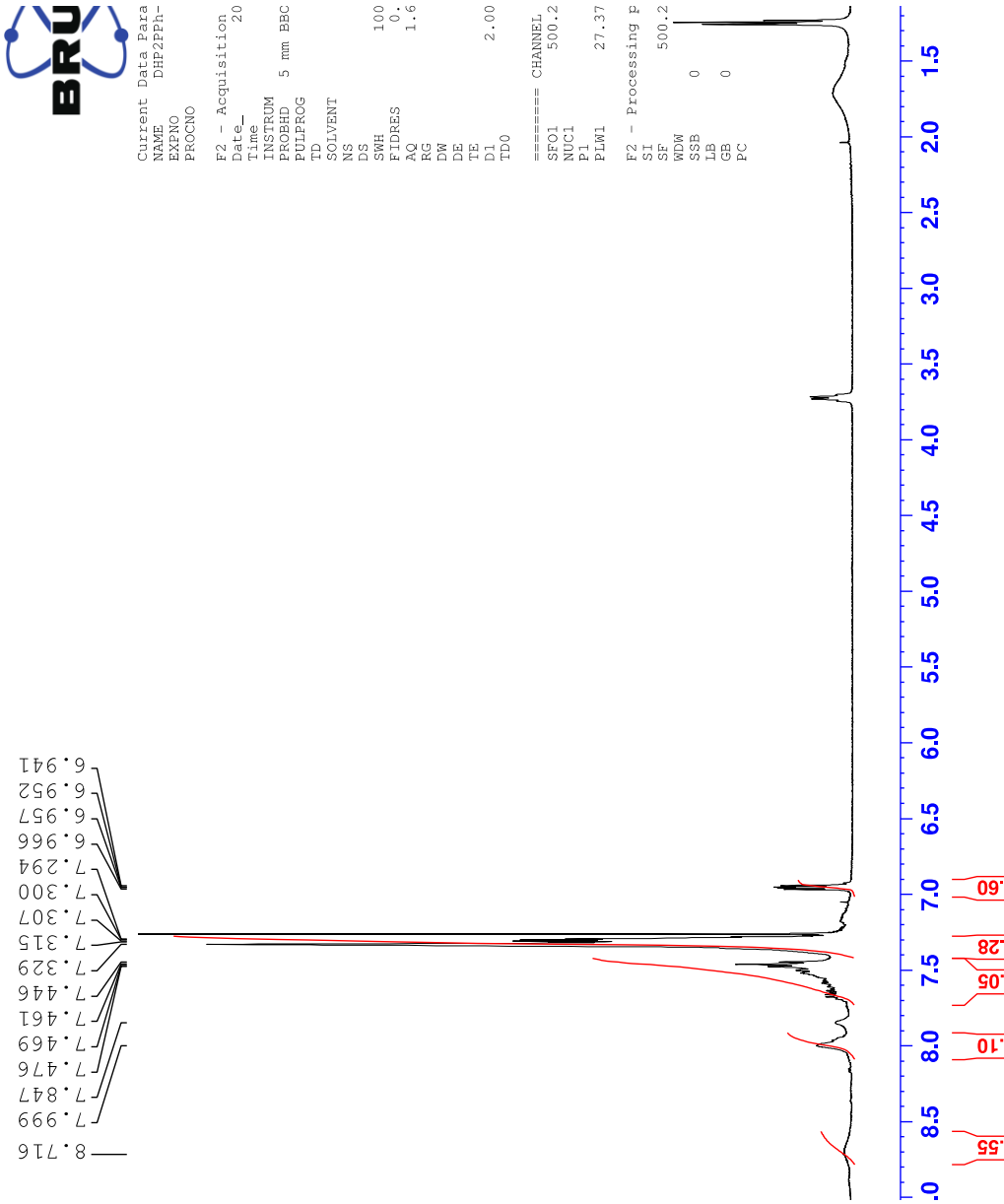
20
15
10
5
700
650
600
550
500
450
400
350
300
Wavenumbers (cm-1)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PROCNO
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FIDRES 0.
AQ 1.6
RG
DW
DE
TE
D1 2.00
TD0
======== CHANNEL
SFO1 500.2
NUC1
P1
PLW1 27.37
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SF 500.2
WDW
SSB 0
LB
GB 0
PC
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7.476
7.469
7.461
7.446
7.329
7.315
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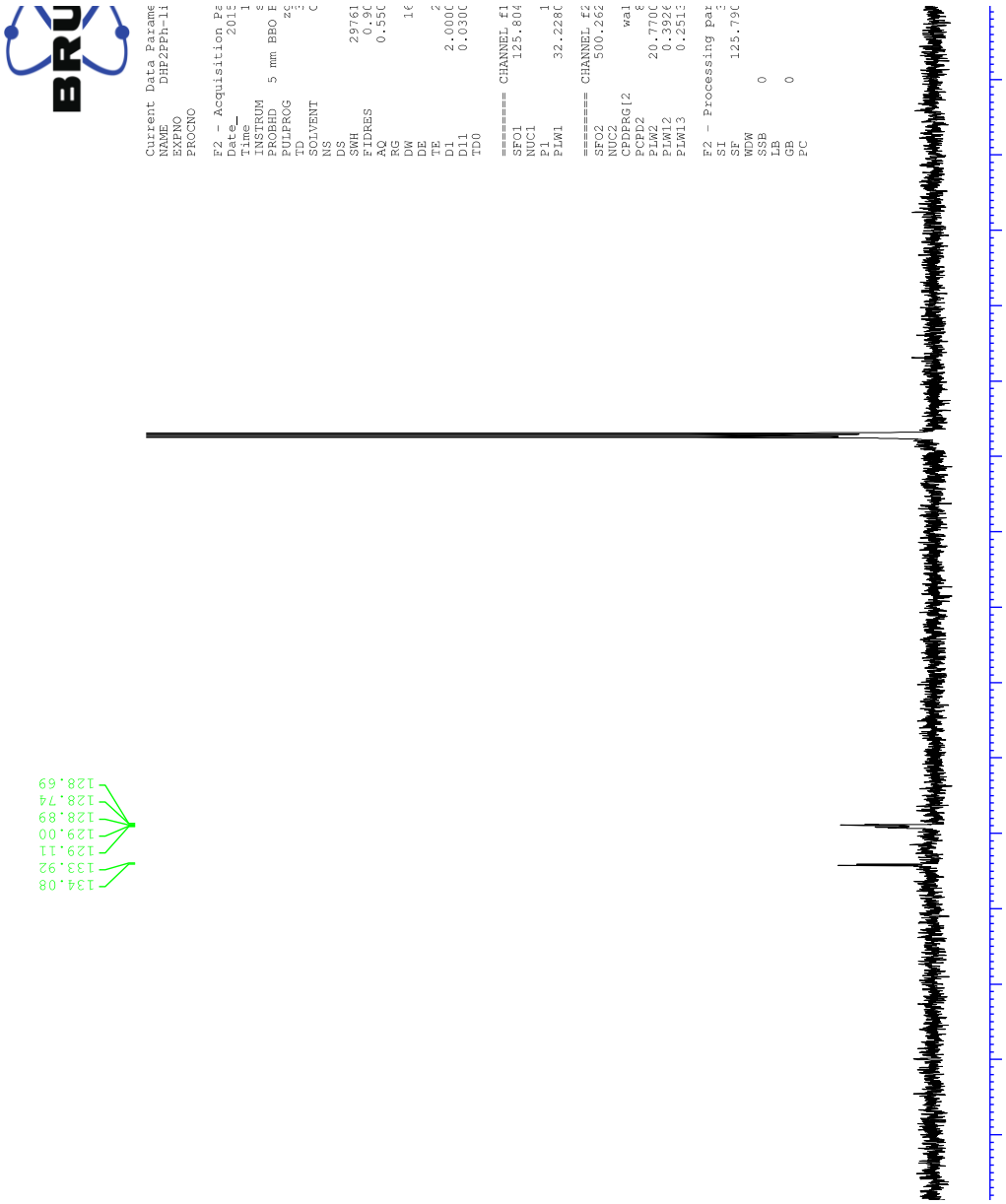
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TD
SOLVENT
NS
DS
SWH 28761
FIDRES 0.9(
AQ 0.55(
RG 1(
DW
DE
TE 2
D1 2.000(
D11 0.030(
TD0
======== CHANNEL f1
SFO1 125.804
NUC1
P1 32.228(
PIW1
======== CHANNEL f2
SFO2 500.262
NUC2
CPDPRG[2 wal
PCPD2
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PIW12 0.392(
PIW13 0.251(
F2 - Processing par
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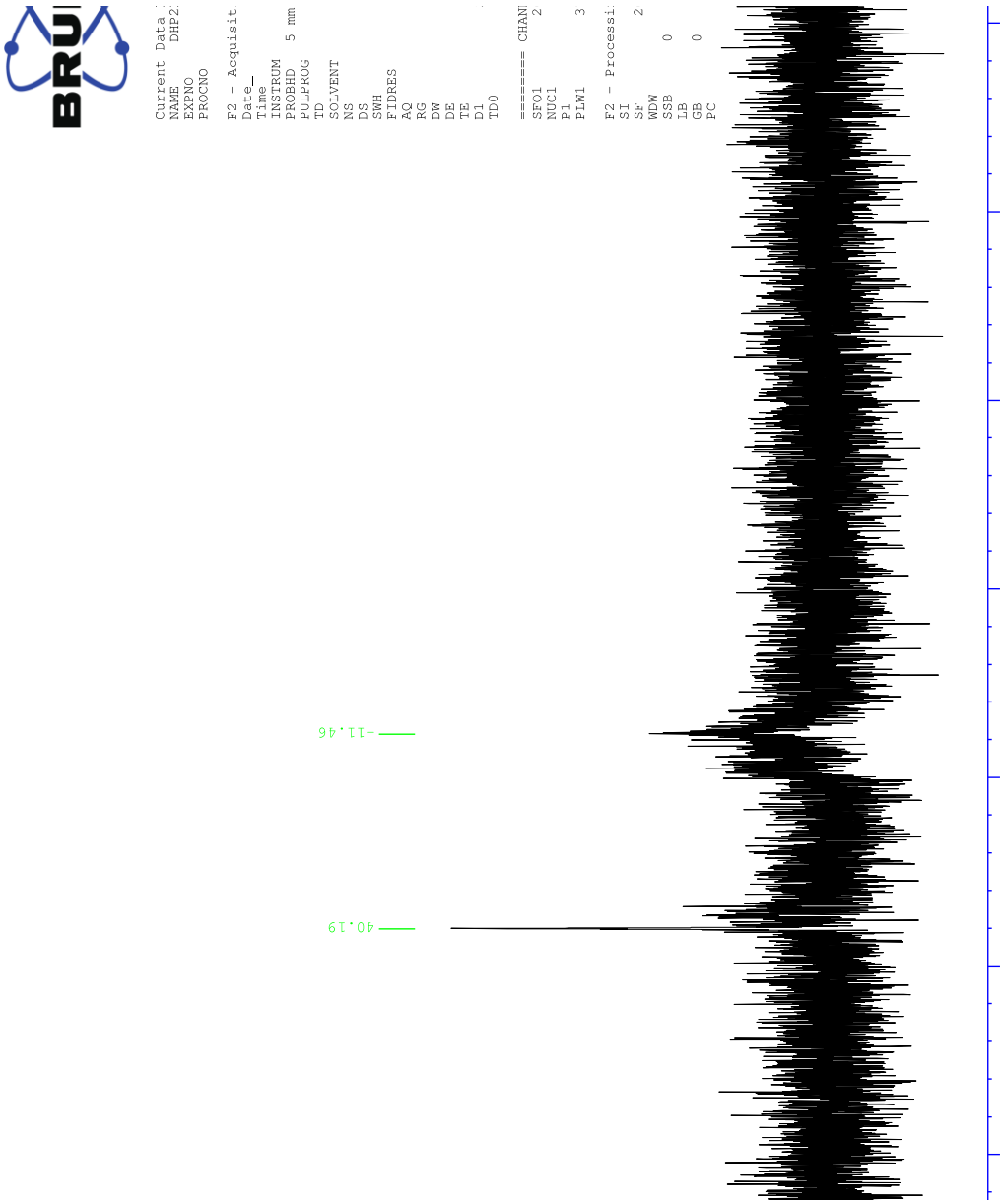
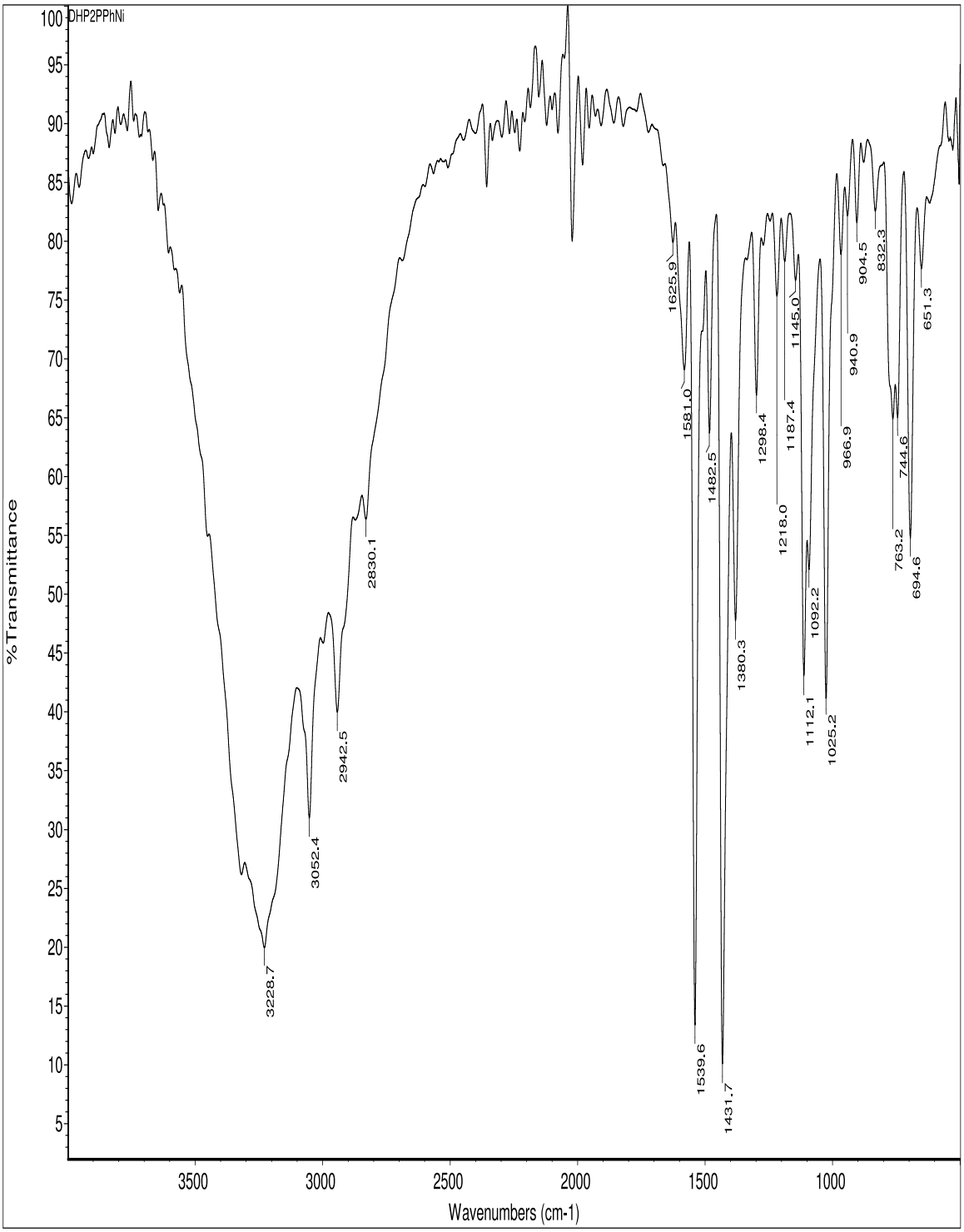


Aqua-μ-chloro-dichloro-{1,4-bis-{2-[2-(diphenylphosphino-1κP,2κP)benzylidene]}phthalazinylhydrazone-1κ²N,N', 2κ²N,N'}dinickelate(II) (**2**)


DHP2PPhNi
%Transmittance
Wavenumbers (cm-1)
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3052.4
2942.5
2830.1
1625.9
1581.0
1539.6
1482.5
1431.7
1380.3
1298.4
1218.0
1187.4
1145.0
1112.1
1092.2
1025.2
966.9
940.9
904.5
832.3
763.2
744.6
694.6
651.3