

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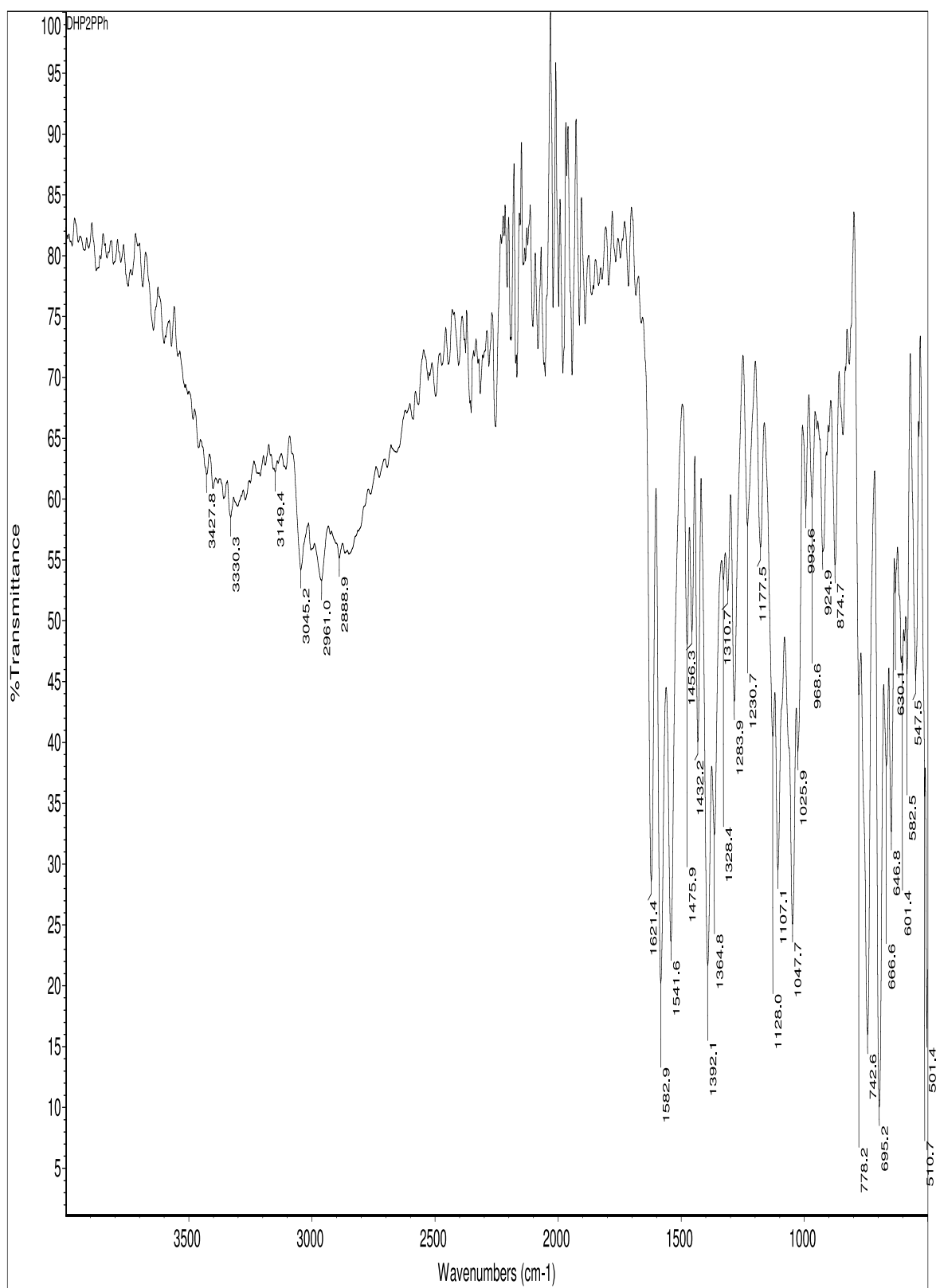
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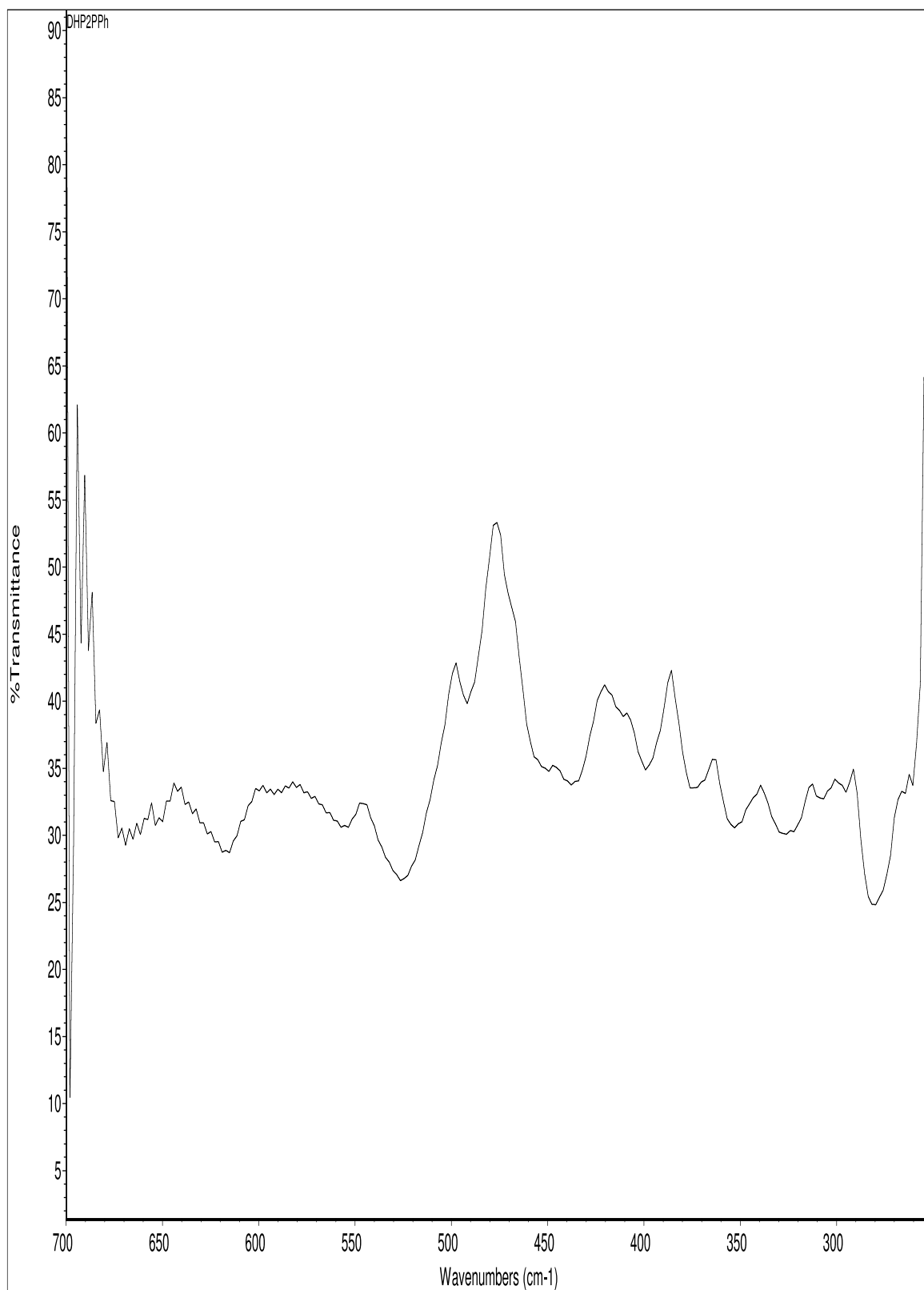
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Table S1 Crystallographic data and refinement details for the binuclear nickel(II) complex (**2**)

<i>Crystal data</i>	
Chemical formula	C ₄₇ H ₄₂ Cl ₃ N ₆ Ni ₂ O ₂ P ₂ ·2(CH ₄ O)·Cl
<i>M_r</i>	1108.11
Crystal system, space group	Triclinic, <i>P</i> -1
Temperature (K)	294
<i>a</i> , <i>b</i> , <i>c</i> (Å)	12.3956(5), 14.8378(6), 15.0593(6)
<i>α</i> , <i>β</i> , <i>γ</i> (°)	87.926(3), 72.807(4), 71.367(4)
<i>V</i> (Å ³)	2502.11(19)
<i>Z</i>	2
Radiation type	Mo <i>Kα</i>
<i>μ</i> (mm ⁻¹)	1.08
Crystal size (mm)	0.67 × 0.43 × 0.27
<i>Data collection</i>	
Diffractometer	Gemini S (Oxford Diffraction)
Absorption correction	Analytical
<i>T_{min}</i> , <i>T_{max}</i>	0.668, 0.816
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	22863, 11437, 9238
<i>R_{int}</i>	0.025
(sin <i>θ</i> /λ) _{max} (Å ⁻¹)	0.683
<i>Refinement</i>	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.038, 0.135, 1.12
No. of reflections	11437
No. of parameters	628
No. of restraints	8
Δ <i>ρ</i> _{max} , Δ <i>ρ</i> _{min} (e Å ⁻³)	0.54, -0.53

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

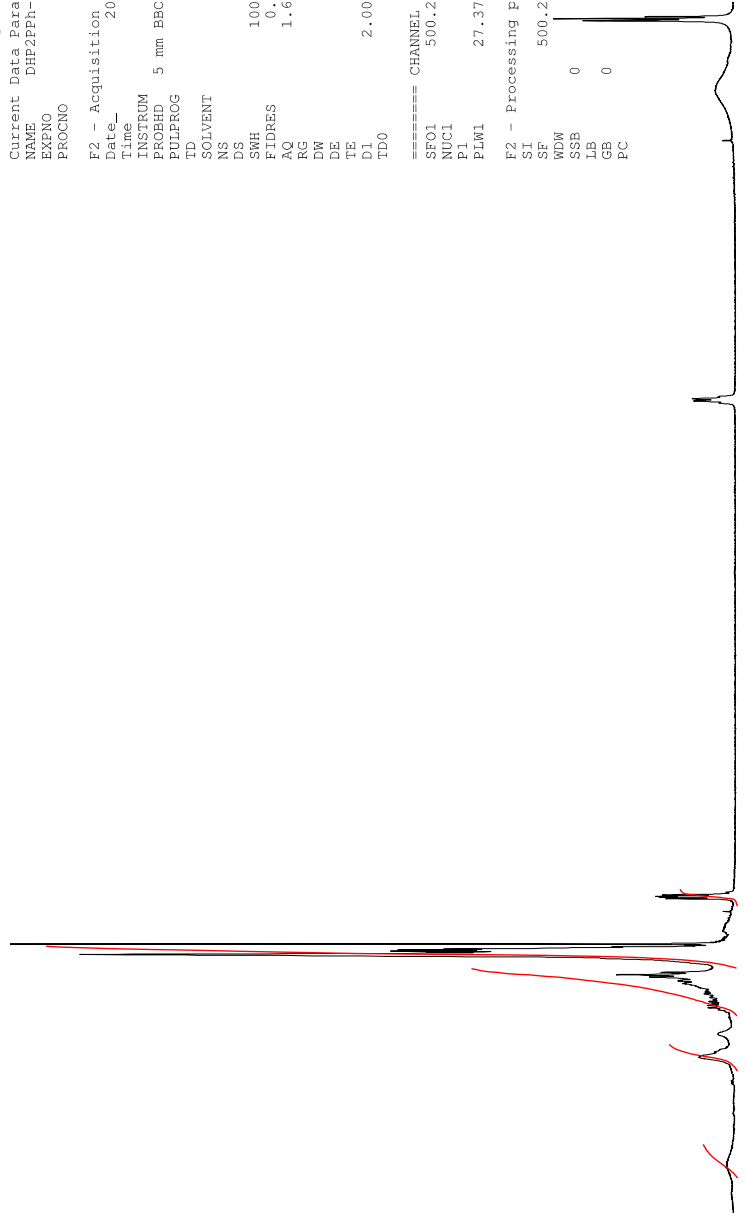






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SF 0.
FIDRES 1.6
AQ
RG
DW
DE
TE
D1 2.00
TDO
==== CHANNEL
SFO1 500.2
NUC1
PL 27.37
PLW1
F2 - Processing P
SI
SF 500.2
WDW
SSB 0
LB
GB 0
PC

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7.476
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6.952
6.941

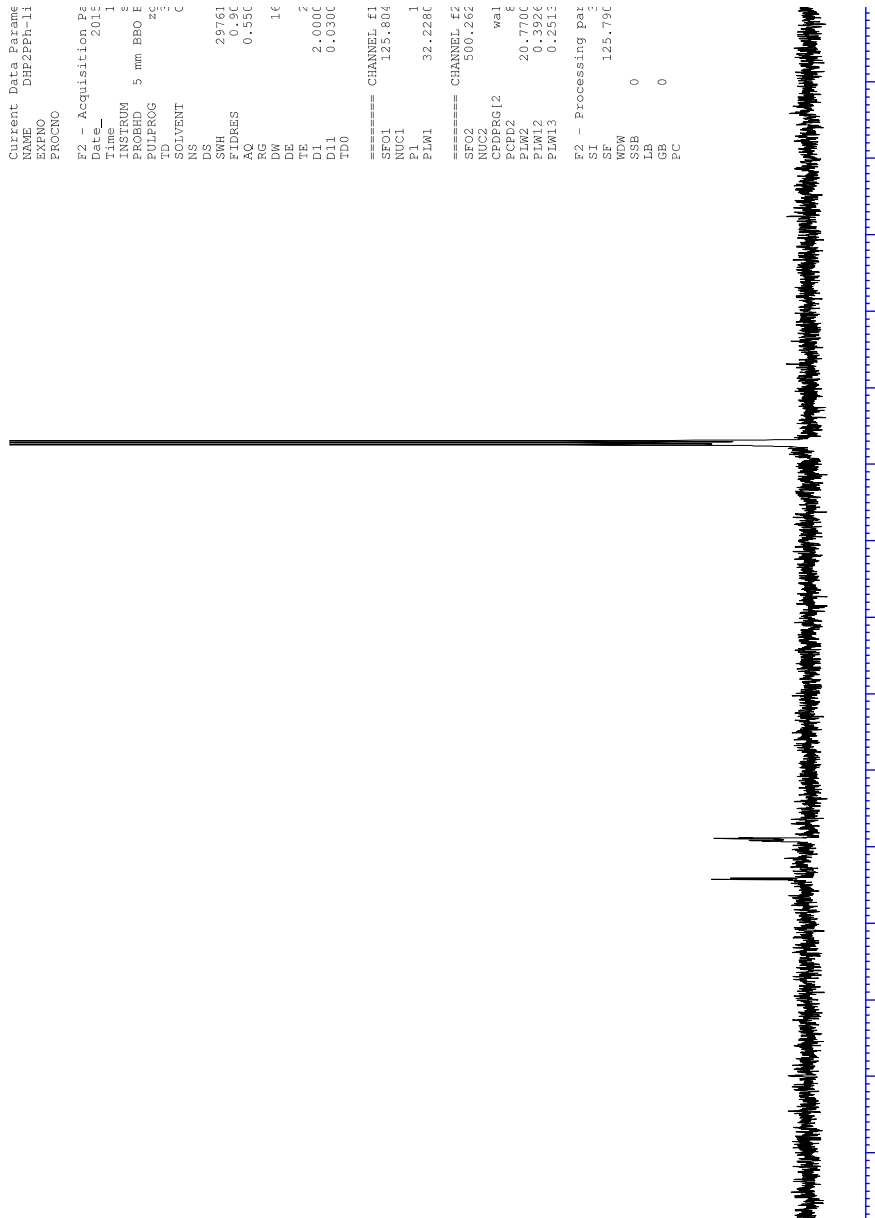


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D11       0.030C
TD0
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NUC1
P1        1
PLW1     32.228C
===== CHANNEL f2
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NUC2
CPDPRG12  wal
PCPD2
PLW2     20.770C
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FC
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129.00
129.11
133.92
134.08





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 PROCNO :

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 Time_ :
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 PROBHD : 5 mm
 PULPROG :

TD :
 NS :
 DS :
 SWH :
 FIDRES :
 AQ :
 RG :
 DW :
 DE :
 TE :
 D1 :
 TDO :

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 SFOL : CHAN
 NUCL : 2
 P1 :
 PL1 : 3

F2 - Processi
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 SF : 2
 WDW :
 SSB : 0
 LB :
 GB : 0
 PC :

— 11.46

— 40.19

*Aqua- μ -chloro-dichloro-{1,4-bis-{2-[2-(diphenylphosphino-
 1 κ P,2 κ P)benzylidene]]phthalazinylylhydrazone-1 κ^2 N,N',
 2 κ^2 N,N'}dinickelate(II) (2)*

