Supplementary Information

Influence of intramolecular ring-ring π,π-interaction on crystal building in ternary compound of nickel(II) chelates of 2,2'-{[2-(4-methylphenyl)ethyl]azanediyl} diacetic acid and 1,10-phenanthroline – Synthesis, spectral, optical and quantum chemical study

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Fig. S1-Ortep diagram generated through mercury showing intramolecular weak π,π-interaction between phenethyl ring of H_2MEphedia and imine ring of 1,10-phen: centroid-centroid distance $d(C_I–C_J)$ = 5.169 Å.

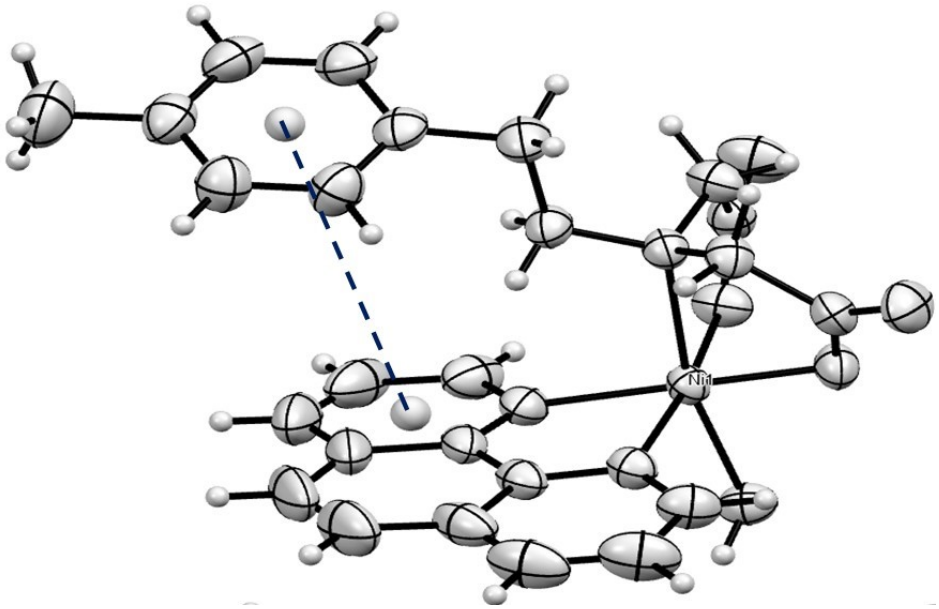


Fig. S1 FT-IR spectrum of Ni(II) complex**.**

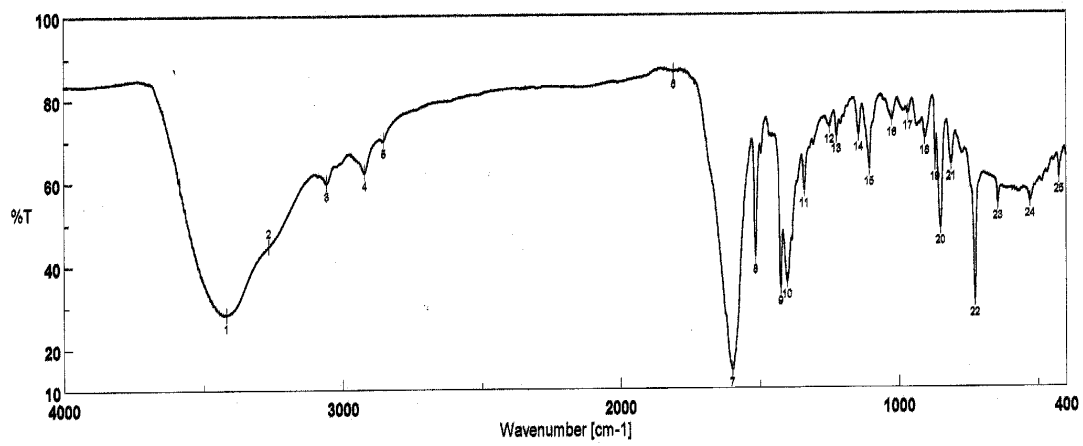


Fig. S2 FTIR spectrum of Ni(II) complex obtained by DFT.

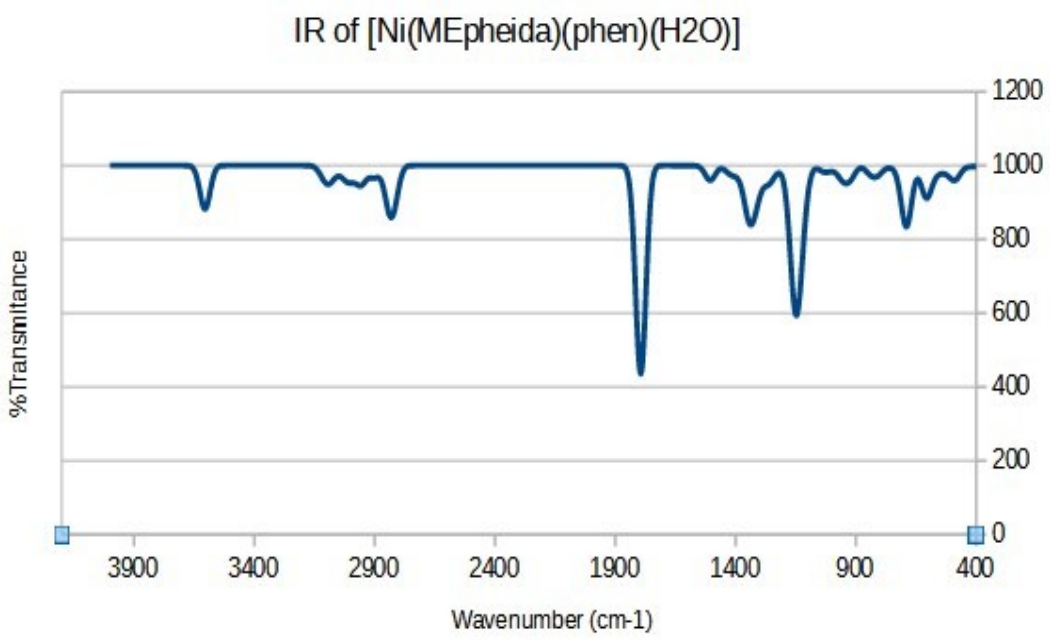


Fig. S3 Electronic spectrum of nickel(II) compound (experimental and computational).

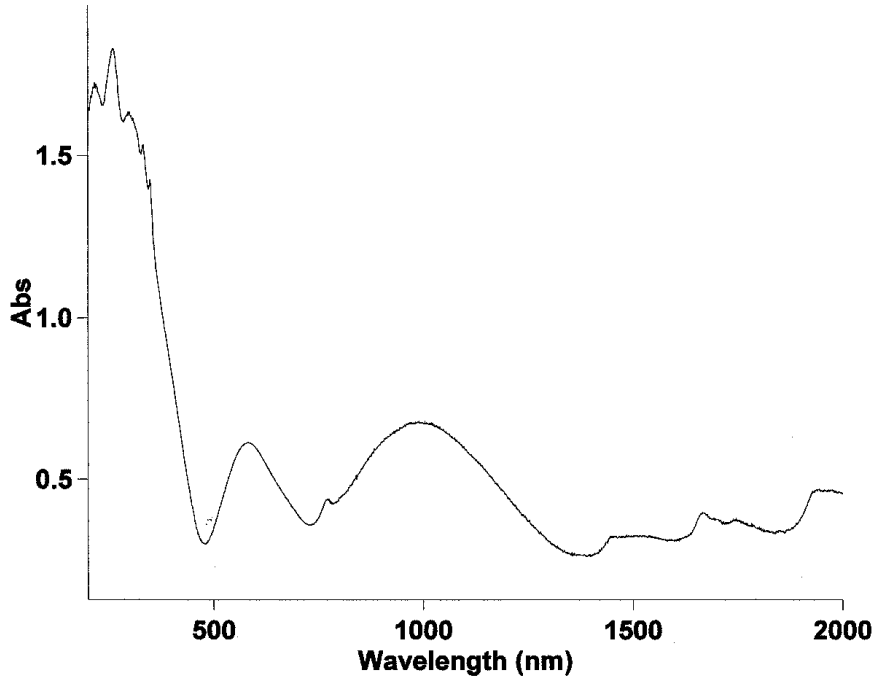


Fig. S4-Absorption spectrum of compound obtained through tddft measurements of complex [Ni(MEpheida)(phen)(H_2O)]·3H_2O

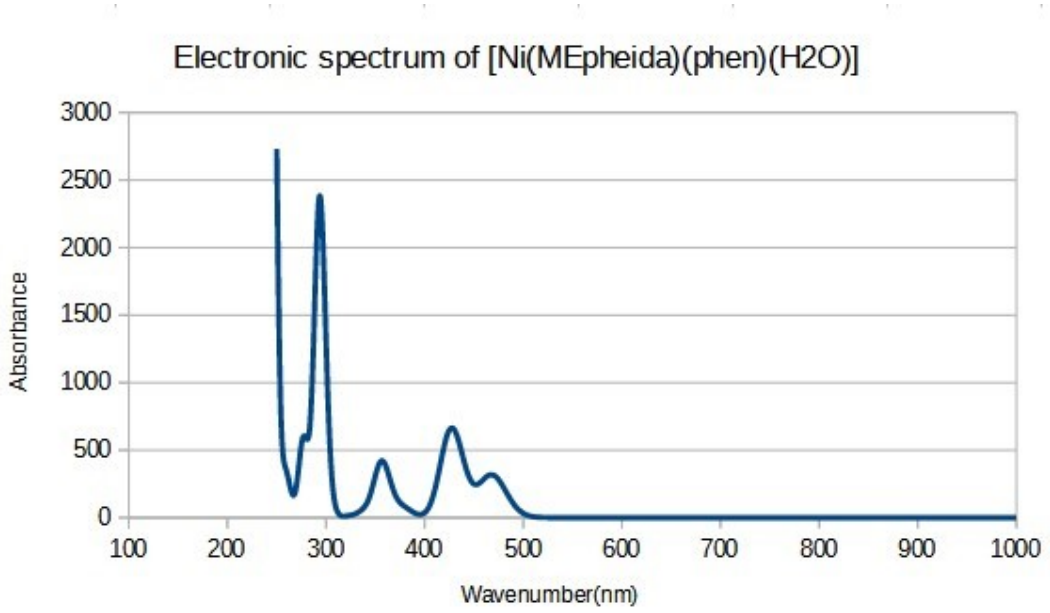
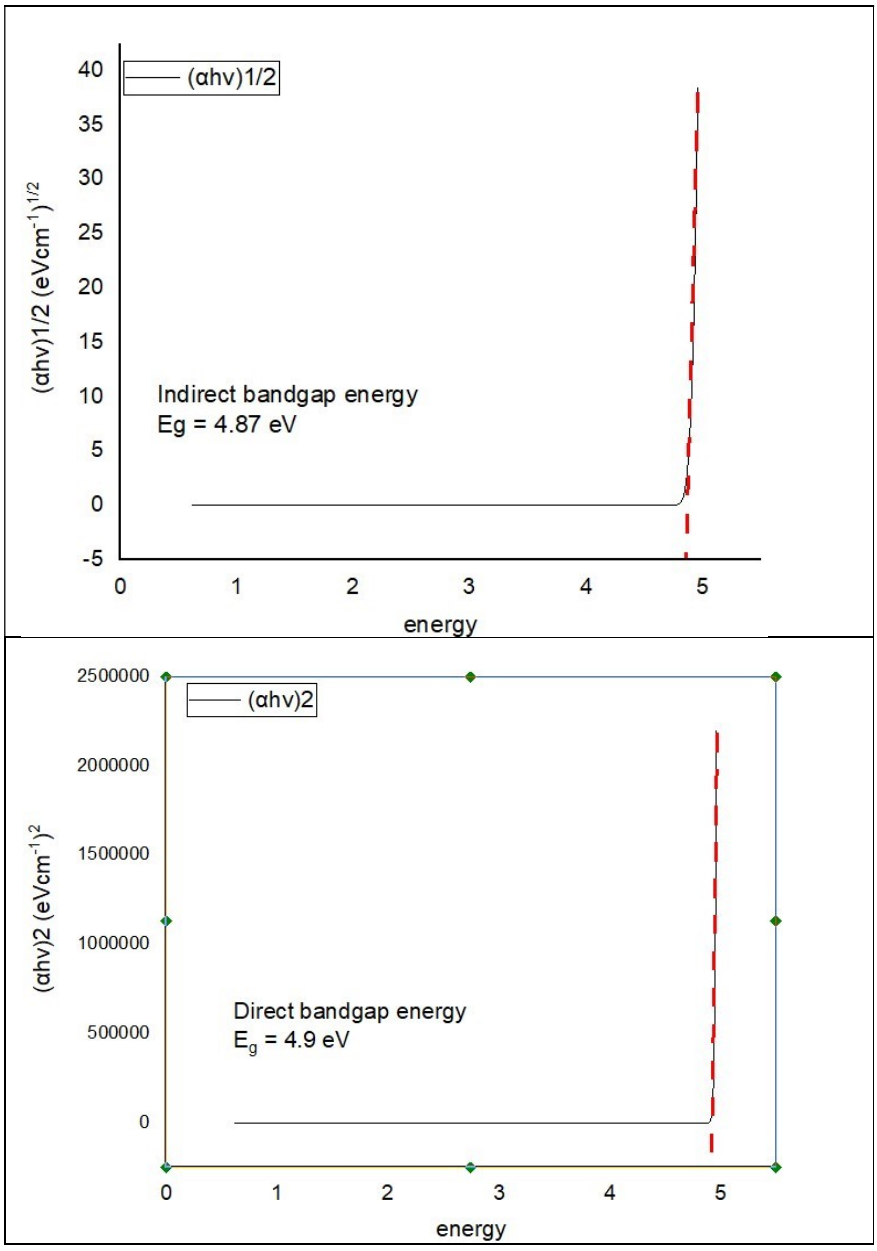


Fig. S5. HOMO-LUMO data measured from B3LYP method for Ni(II) complex.

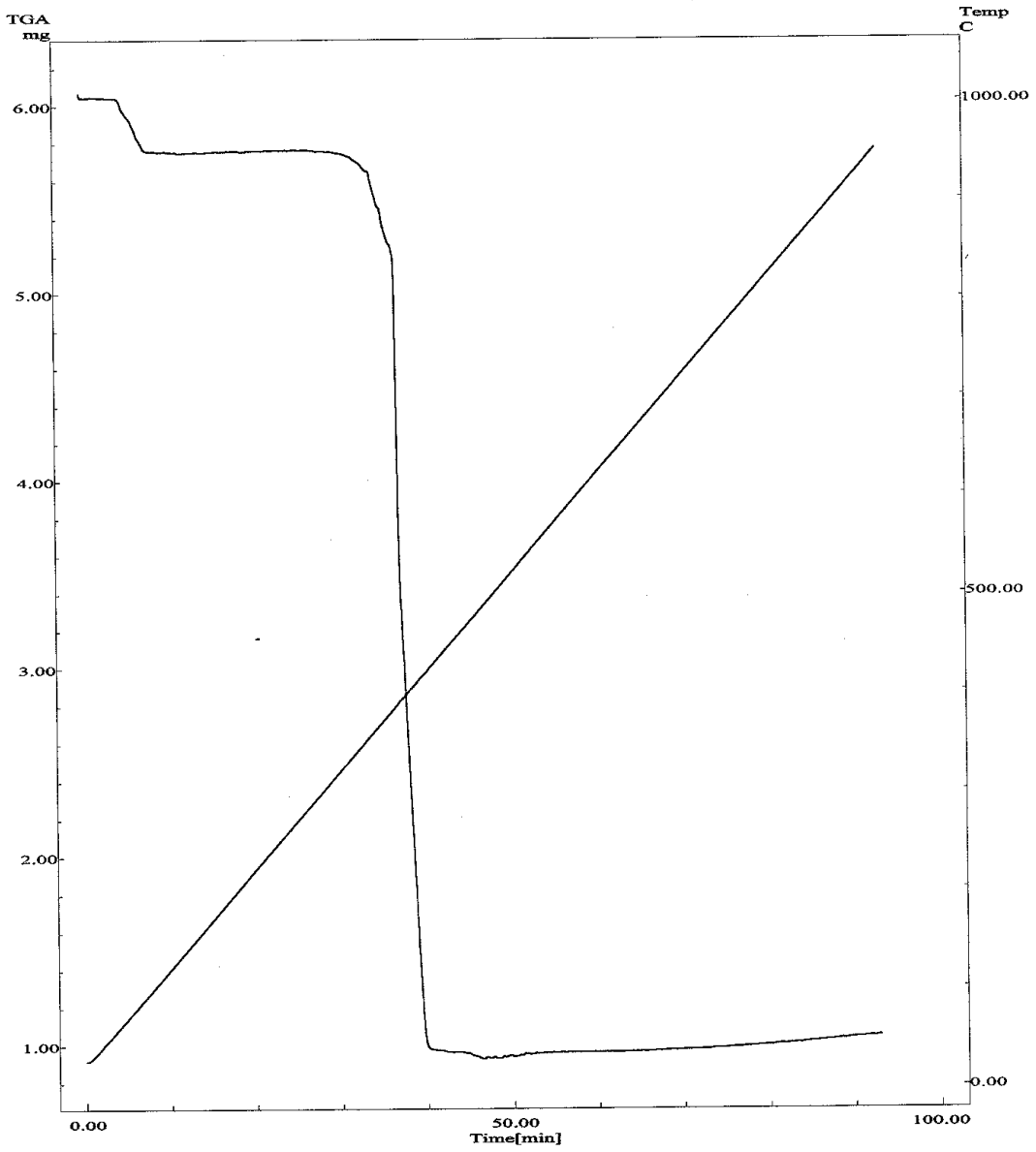
99	HOMO-5	-10.807			
100	HOMO-4	-10.689			1
101	HOMO-3	-10.420			1
102	HOMO-2	-9.954			1
103	HOMO-1	-9.696			1
104	HOMO	-9.353			1
105	LUMO	0.583			1
106	LUMO+1	0.926			1
107	LUMO+2	2.238			1
108	LUMO+3	3.282			1
109	LUMO+4	3.871			1
110	LUMO+5	4.161			

Fig. S6. Top; indirect and bottom direc bandgap of H_2MEpheida.

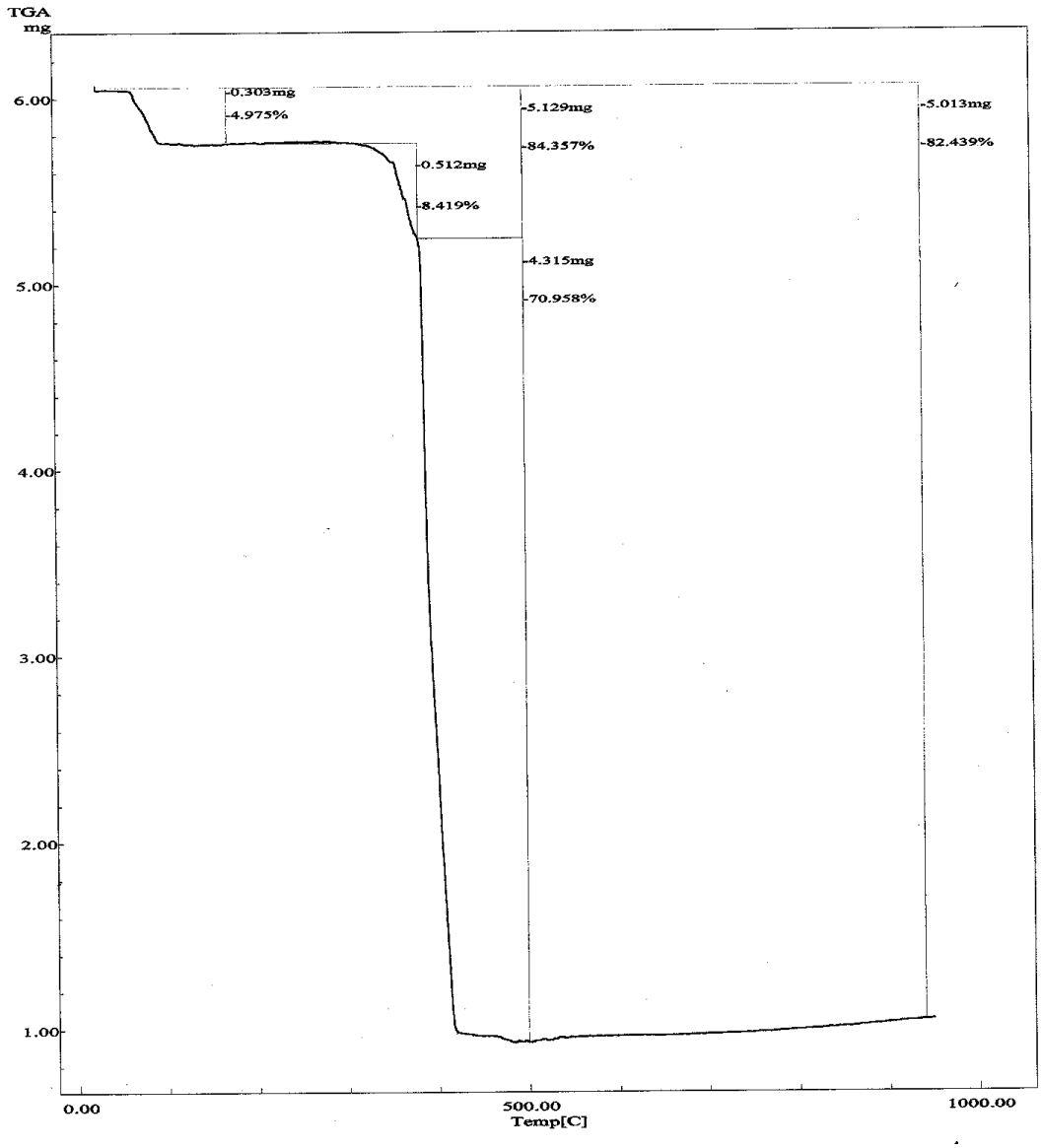


Thermo-gravimetric analysis of Ni(II) complex**,** with FT-IR spectra for identification of omitted gases.

Fig. (S7-A) TG-spectra of complex as a function of time versus temperature



(S7-B) TG-spectra of 1 as a function of the temperature.



(S7-C-1) Three sheets bellow showing a sequential series of spectra, recorded with the increase of time (minutes) which enable to identification of evolved gases.

Sheet 1: First step corresponds; only lose of water and trace amount of CO_2 followed by pyrolysis of organic ligand.

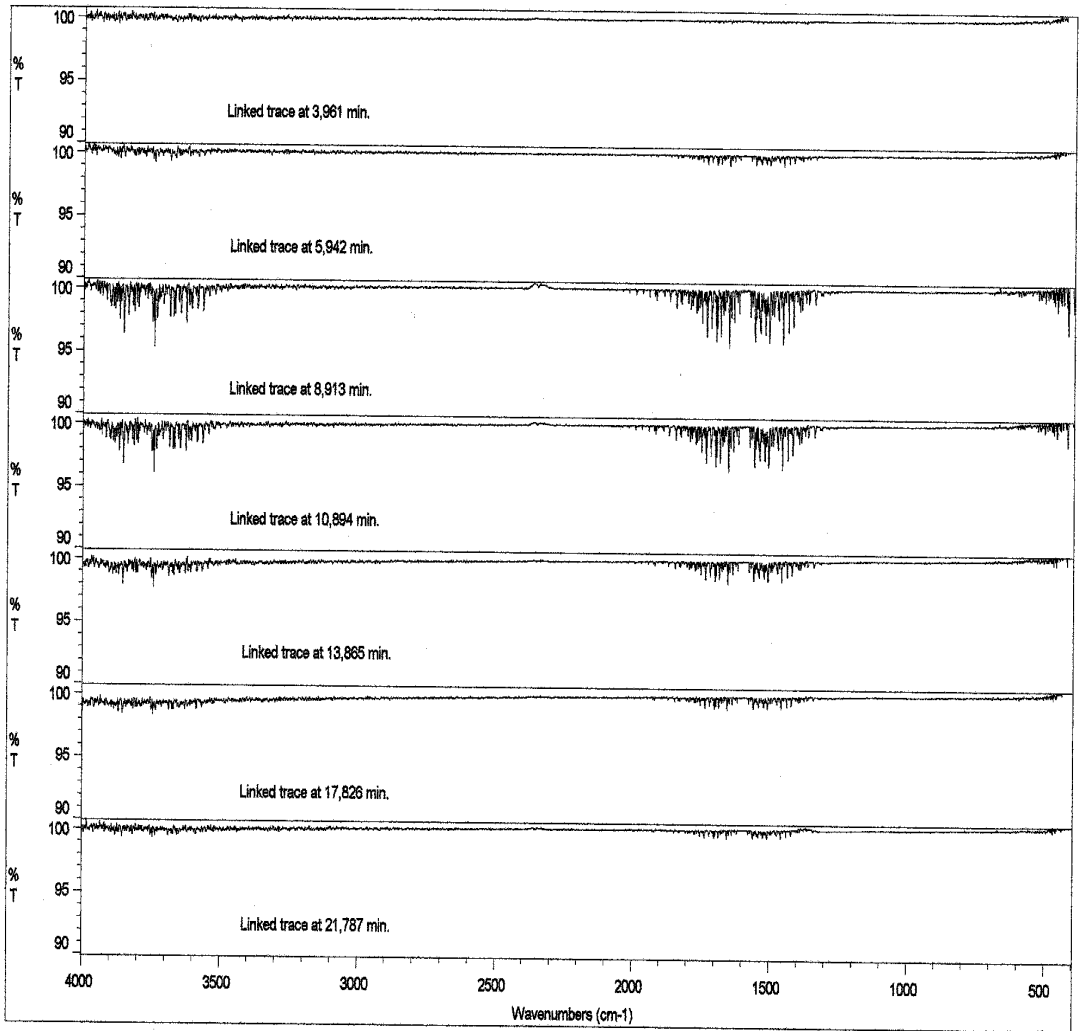


Fig. (S7-2) Sheet 2: Showings lose of H_2O, CO_2 and trace amount of CO, NO, NO_2, N_2O gases with traces of CH_4.

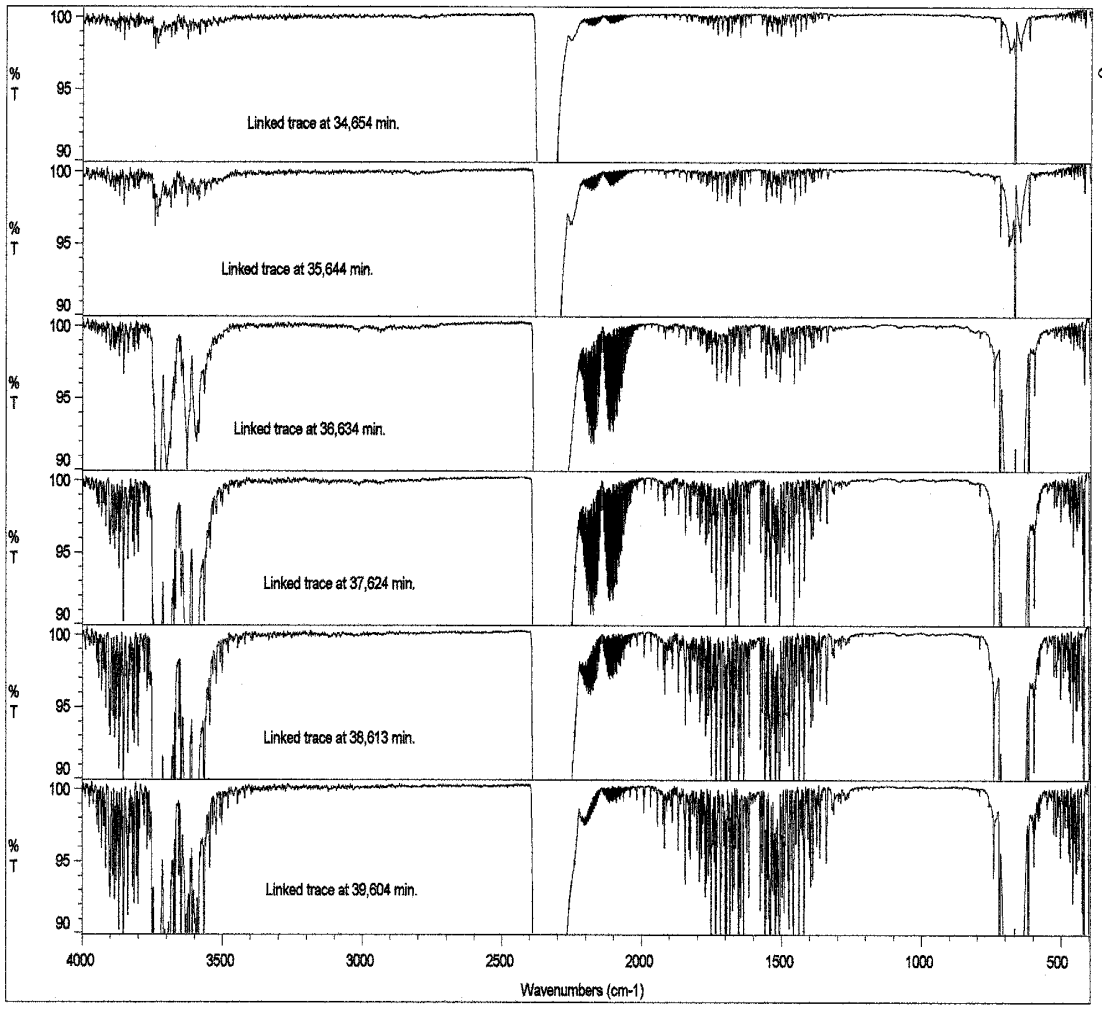
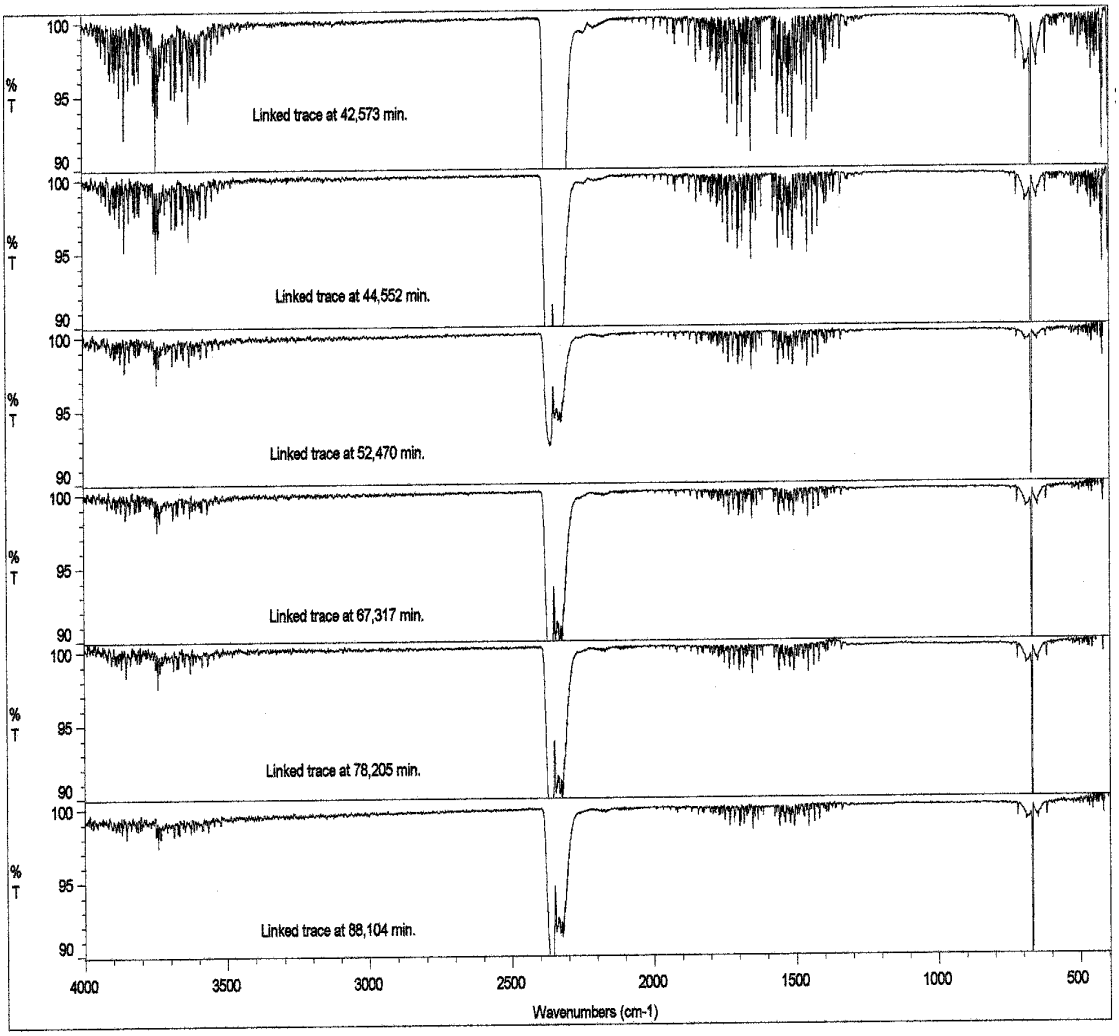


Fig. (S7-3) Sheet 3: Lose of H_2O, CO_2 and CO.



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: q

```
     Bond precision:   C-C = 0.0039 A           Wavelength=1.54178
Cell:           a=9.8693(5)         b=11.4745(6)      c=12.6233(6)
                alpha=112.758(1)    beta=93.195(2)    gamma=94.503(1)
Temperature:    293 K

                 Calculated                  Reported
Volume           1308.39(11)                 1308.39(11)
Space group      P -1                        P-1
Hall group       -P 1                        ?
Moiety formula   C25 H25 N3 Ni O5, 3(H2 O)   C25 H25 N3 Ni O5,3(H2 O)
Sum formula      C25 H31 N3 Ni O8            C25 H31 N3 Ni O8
Mr               560.22                      560.24
Dx,g cm-3        1.422                       1.422
Z                2                           2
Mu (mm-1)        1.525                       1.525
F000             588.0                       588.0
F000'            583.77
h,k,lmax                                     11,13,14
Nref                                         4080
Tmin,Tmax        0.665,0.796                 0.543,0.753
Tmin'            0.603

    Correction method= # Reported T Limits: Tmin=0.543
    Tmax=0.753 AbsCorr = MULTI-SCAN

    Data completeness=Theta(max)= 66.490
    R(reflections)= 0.0381( 4044)wR2(reflections)=
                          0.1083( 4080)
    S = 1.090                  Npar= 335
```

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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low .0.884 Why?

Alert level B

PLAT417_ALERT_2_B Short Inter D-H..H-DH1BH3A1.95 Ang.
1-x,1-y,1-z =2_666 Check PLAT417_ALERT_2_B Short Inter D-H..H-DH3B ..H33A2.05 Ang.
x,y,1+z =1_556 Check

Alert level C

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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 MULTI-SCAN
PLAT199_ALERT_1_C Reported _cell_measurement_temperature ..... (K)         293 Check
PLAT200_ALERT_1_C Reported    _diffrn_ambient_temperature ..... (K)         293 Check
PLAT230_ALERT_2_C Hirshfeld Test Diff for     C24      --C25      .         7.0 s.u.
PLAT355_ALERT_3_C Long    O-H (X0.82,N0.98A)  O1       - H1A      .        1.01 Ang.
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Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIFPlease Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .....8 Report
H33A H33B H1A H1B H2A H2B H3A H3B
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ni1 --O4 . 5.0 s.u. PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ni1 --N30 . 5.4 s.u. PLAT794_ALERT_5_G Tentative Bond Valency for Ni1 (II) . 2.01 Info PLAT899_ALERT_4_G SHELXL-97 is Deprecated and Succeeded by SHELXL 2019/3 Note

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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* or *IUCrData*, 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

Fig. S8 Ortep diagram of Ni(II) ternary complex $[Ni(MEpheida)(phen)(H_2O)]\cdot 3H_2O$ generated through x-ray diffractometer.