**SUPLEMENTRY INFORMATION OF THE MANUSCRIPT**

**Title**

Nitro–ring inter–laminar π,π–interactions affecting the crystal building of *N*–(*p*–nitro–benzyl)–iminodiacetato–nickel(II) complex. Synthesis, characterization, Hirshfeld surface analysis, time–dependent–DFT and optical bandgap energy plots of $H_2$NBIDA and their Ni(II) binary and ternary complexes.

**Journal Name-** Transition Metal Chemistry

**Name of authors-** D.K. Patel[a,*], P. Makwane[b], B. Jain[a], A. Singh[a], N.M. Gupta[a], A. Castiñeiras[c] and J. Niclós–Gutiérrez[d]

**Corresponding author**: Dheerendra Kumar Patel

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**CheckCIF report**

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

# Datablock: c492

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Bond precision: C-C = 0.0037 A Wavelength=0.71073

Cell: a=19.0730(13) b=7.6524(5) c=22.6758(15)
alpha=90 beta=110.494(1) gamma=90

Temperature: 293 K

| | Calculated | Reported |
|---|---|---|
| Volume | 3100.2(4) | 3100.2(4) |
| Space group | P 21/c | P21/c |
| Hall group | -P 2ybc | ? |
| Moiety formula | 2(C11 H16 N2 Ni O9), H2 O | 2(C11 H16 N2 Ni O9), H2 O |
| Sum formula | C22 H34 N4 Ni2 O19 | C22 H34 N4 Ni2 O19 |
| Mr | 775.91 | 775.95 |
| Dx,g cm-3 | 1.662 | 1.662 |
| Z | 4 | 4 |
| Mu (mm-1) | 1.304 | 1.304 |
| F000 | 1608.0 | 1608.0 |
| F000' | 1611.63 | |
| h,k,lmax | 22,9,27 | 22,9,27 |
| Nref | 5580 | 5578 |
| Tmin,Tmax | 0.683,0.878 | 0.508,0.881 |
| Tmin' | 0.453 | |

Correction method= # Reported T Limits: Tmin=0.508 Tmax=0.881
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.200

R(reflections)= 0.0300( 4985) wR2(reflections)= 0.1106( 5578)

S = 0.914 Npar= 424

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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.

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**Alert level A**

DIFF003_ALERT_1_A _diffrn_measurement_device_type is missing
Diffractometer make and type. Replaces _diffrn_measurement_type.

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**Alert level C**

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

PLAT220_ALERT_2_C NonSolvent Resd 1 N Ueq(max)/Ueq(min) Range 3.5 Ratio

**And 2 other PLAT220 Alerts**

More ...
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N45 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.3 Note

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**Alert level G**
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 14 Report
H20A H20B H21A H21B H22A H22B H50A H50B H51A H51B H52A
H52B H1A H1B
PLAT794_ALERT_5_G Tentative Bond Valency for Ni1 (II) . 2.04 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ni2 (II) . 2.07 Info
PLAT899_ALERT_4_G SHELXL-97 is Outdated and Succeeded by SHELXL 2019/3 Note

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

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

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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**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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**PLATON version of 04/06/2025; check.def file version of 30/05/2025**

# **Datablock c492** - ellipsoid plot

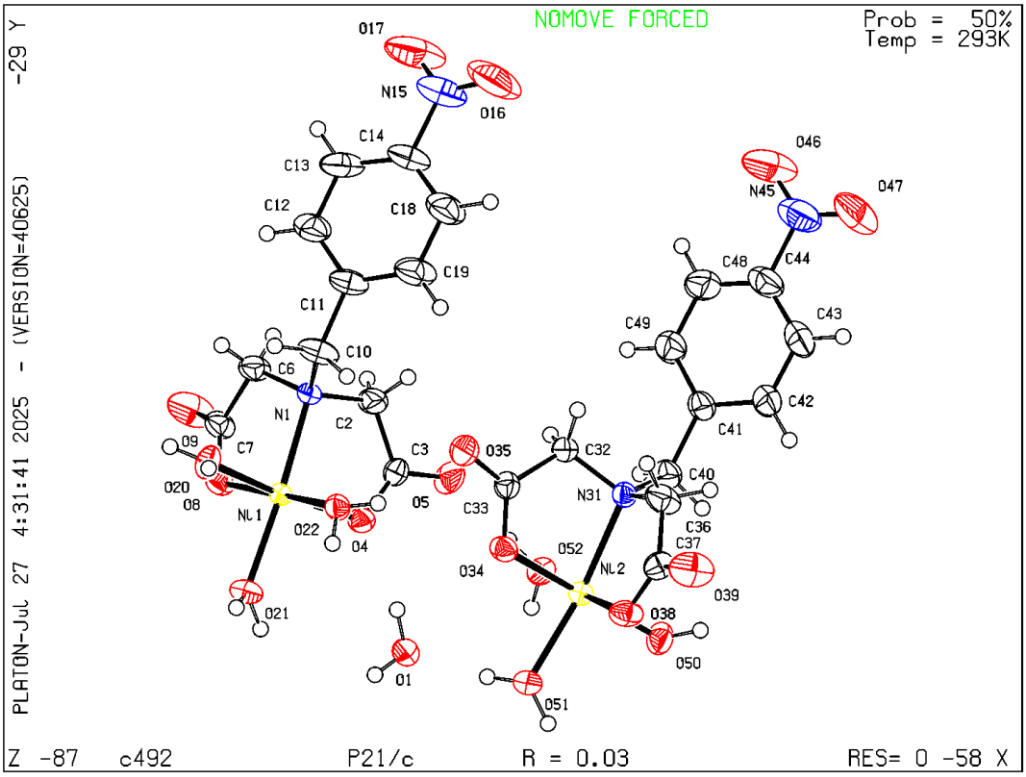
NOMOVE FORCED
Prob = 50%
Temp = 293K
PLATON-Jul 27 4:31:41 2025 - (VERSION=40625) -29 Y
Z -87 c492 P21/c R = 0.03 RES= 0 -58 X
O17
N15
O16
C14
C13
C12
C18
C19
C11
C10
C6
N1
C2
C3
O35
C32
O9
C7
O20
O8
NL1
O22
O4
O5
C33
N31
C40
C36
C37
O39
O52
O34
NL2
O38
O50
O21
O1
O51
O46
N45
O47
C48
C44
C49
C43
C42
C41

**Fig. SI 1** Electronic spectrum of nickel(II) complex (**1)**

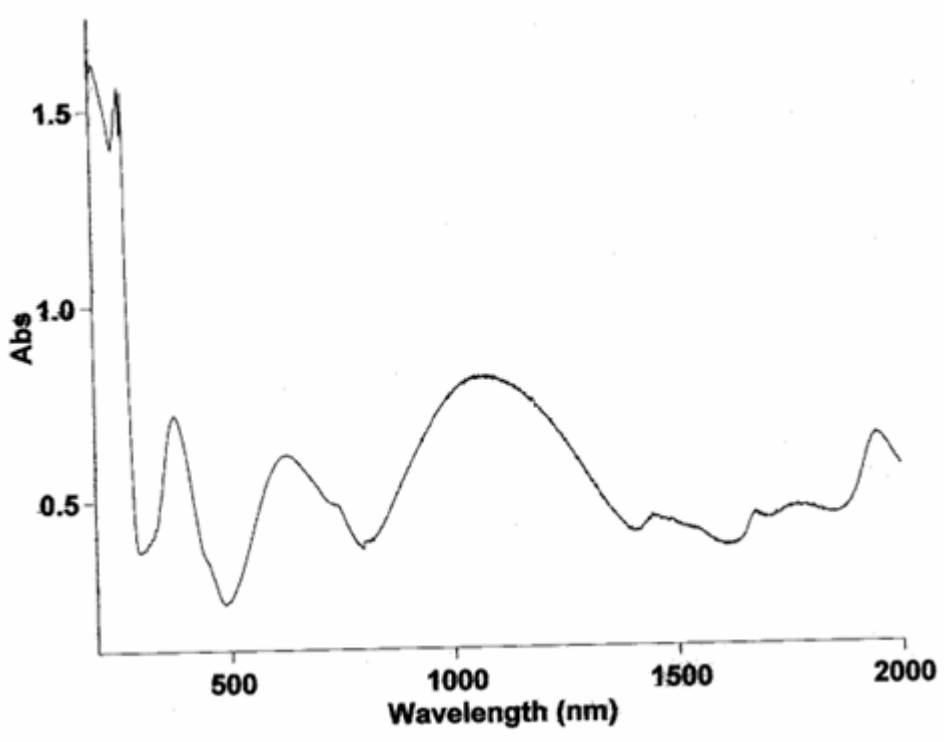


**Fig. SI 2** Electronic spectrum of nickel(II) compound **2.**: Typical spectra for Ni(II) octahedral complexes

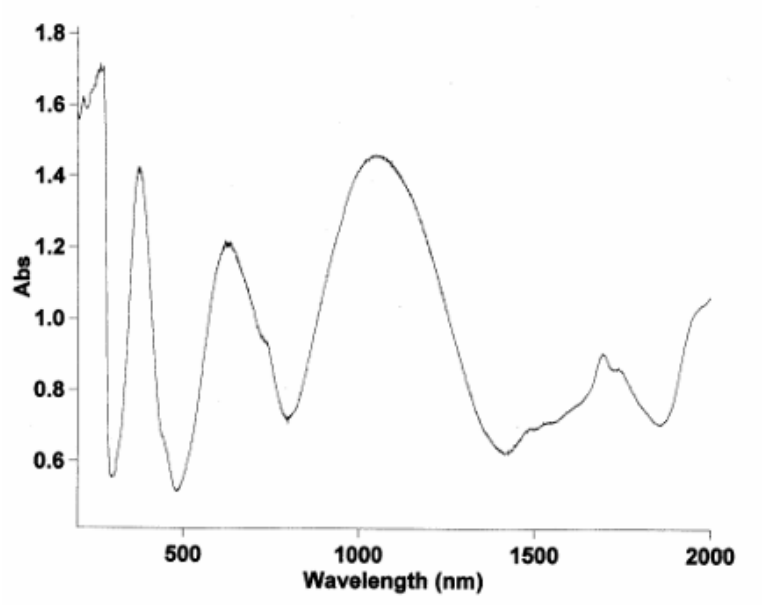

**Fig. SI 3** FMOs for Ni(II) complex 2 calculated at TD–SCF, B3LYP and LANL2DZ basis set for Ni(II) center and conductor–like polarizable continuum model (CPCM)

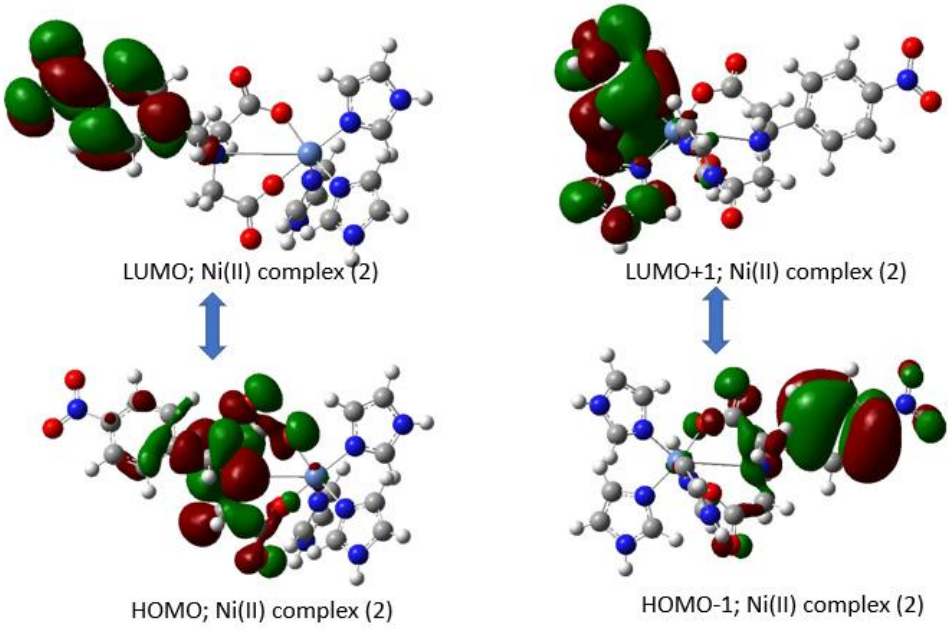


**Table SI 1** TD-DFT data for nickel(II) complex 1.

**Excitation energies and oscillator strengths:**

Excited State 1: 3.003-A 0.4120 eV 3009.55 nm f=0.0001 <S**2>=2.005

| | | | | | |
|---|---|---|---|---|---|
| 70B -> 94B | 0.10110 | 72B -> 94B | 0.16168 | 74B -> 94B | 0.10324 |
| 77B -> 94B | 0.16553 | 79B -> 94B | -0.57723 | 80B -> 94B | -0.13560 |
| 82B -> 94B | -0.16055 | 84B -> 94B | -0.36889 | 85B -> 94B | -0.56104 |
| 86B -> 94B | 0.10294 | 89B -> 94B | -0.19692 | 90B -> 94B | 0.22530 |
| 91B -> 94B | 0.20202 | 92B -> 94B | 0.37994 | 79B <- 94B | -0.27775 |
| 84B <- 94B | -0.17550 | 85B <- 94B | -0.26300 | 92B <- 94B | 0.15370 |

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -1384.48043999

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 3.003-A 0.5707 eV 2172.47 nm f=0.0001 <S**2>=2.004

| | | | | | |
|---|---|---|---|---|---|
| 72B -> 94B | 0.17439 | 73B -> 94B | 0.11347 | 76B -> 94B | 0.16403 |

| | | | | | |
|---|---|---|---|---|---|
| 77B -> 94B | -0.22471 | 78B -> 94B | -0.41785 | 79B -> 94B | 0.23761 |
| 82B -> 94B | -0.28029 | 84B -> 94B | -0.52621 | 85B -> 94B | 0.13794 |
| 86B -> 94B | -0.35193 | 87B -> 94B | 0.13776 | 89B -> 94B | -0.18912 |
| 90B -> 94B | -0.23446 | 91B -> 94B | 0.33371 | 78B <- 94B | -0.17032 |
| 82B <- 94B | -0.10756 | 84B <- 94B | -0.20169 | 86B <- 94B | -0.12490 |
| 90B <- 94B | -0.10485 | | | | |

Excited State 3: 3.005-A 0.9463 eV 1310.21 nm f=0.0002 <S**2>=2.007

| | | | | | |
|---|---|---|---|---|---|
| 76B -> 94B | -0.23728 | 77B -> 94B | -0.25636 | 78B -> 94B | -0.15695 |
| 85B -> 94B | -0.27076 | 88B -> 94B | -0.11575 | 90B -> 94B | -0.62615 |
| 91B -> 94B | -0.50016 | 92B -> 94B | 0.23570 | | |

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 3 LETran= 62.

**Pic** HOMO-LUMO data of Ni(II) complex 1.

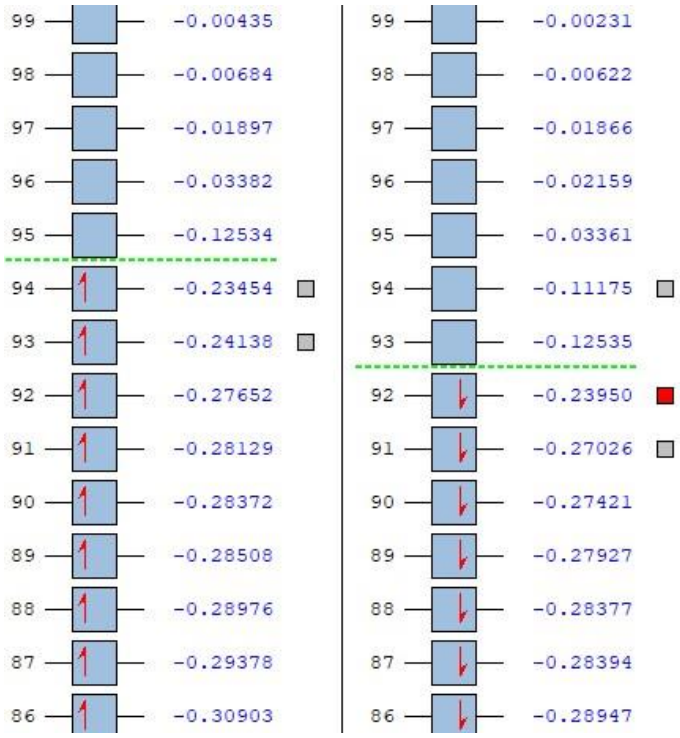

**Table SI 2** TD-DFT data for $H_2$NBIDA.

Excitation energies and oscillator strengths:

Excited State 1:
Singlet-A 1.4951 eV 829.27 nm f=0.0000 <S**2>=0.000
70 -> 71 0.70182
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -981.584289516
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2:
Singlet-A 2.7761 eV 446.61 nm f=0.0056 <S**2>=0.000
69 -> 71 0.70340

Excited State 3:
Singlet-A 3.1673 eV 391.45 nm f=0.0001 <S**2>=0.000
65 -> 71 0.69035
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 3 LETran= 62.

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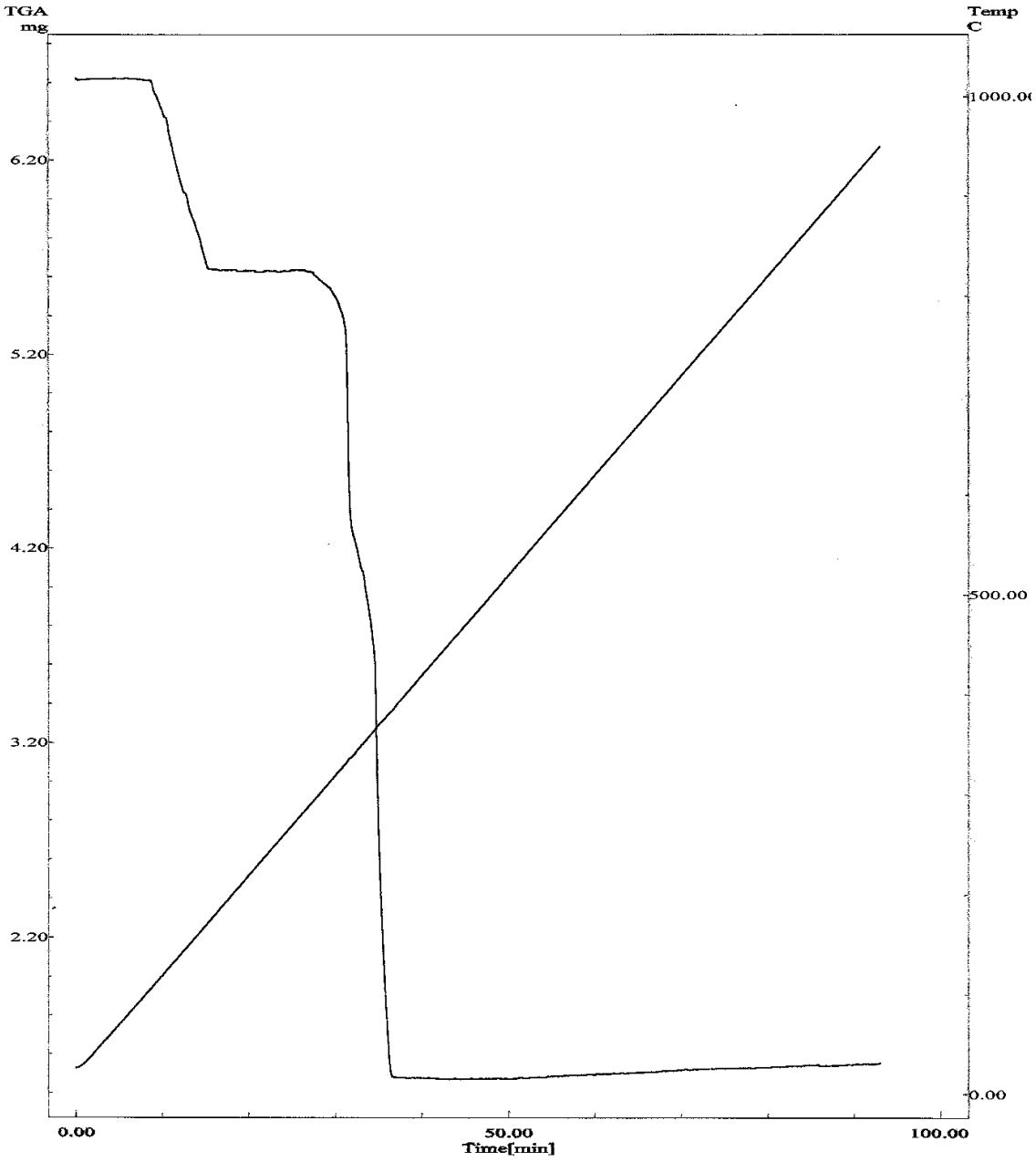
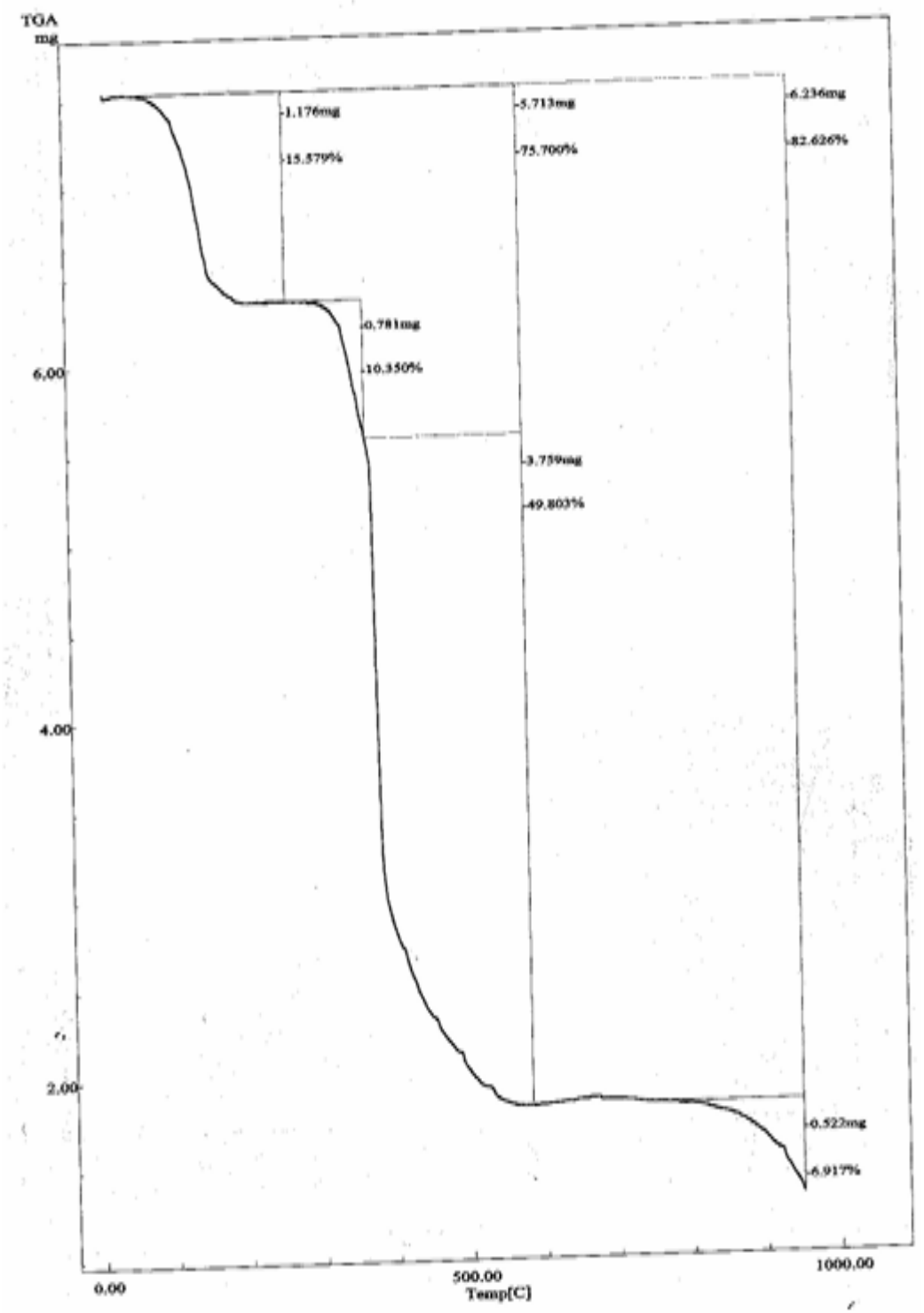
**Fig. SI 4** Thermo-gravimetric analysis of complex **1,** with FT-IR spectra for identification of omitted gases. As an example, for the thermal stability of a binary compound

(SI 4-A) TG-spectra of 1 as a function of time versus temperature

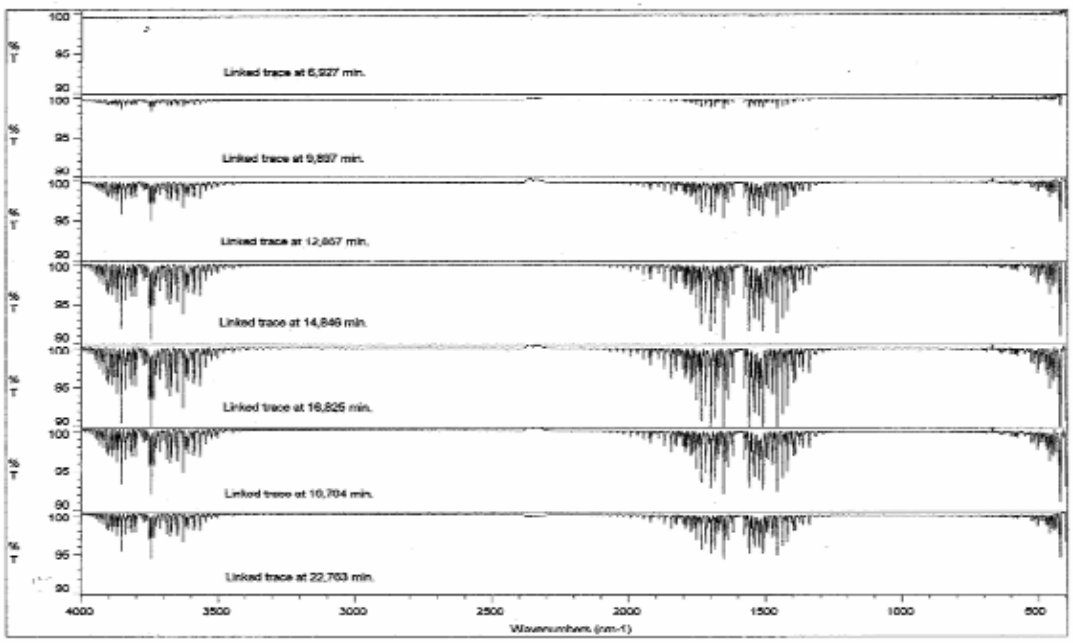


(SI 4-B) TG-spectra of 1 as a function of the temperature

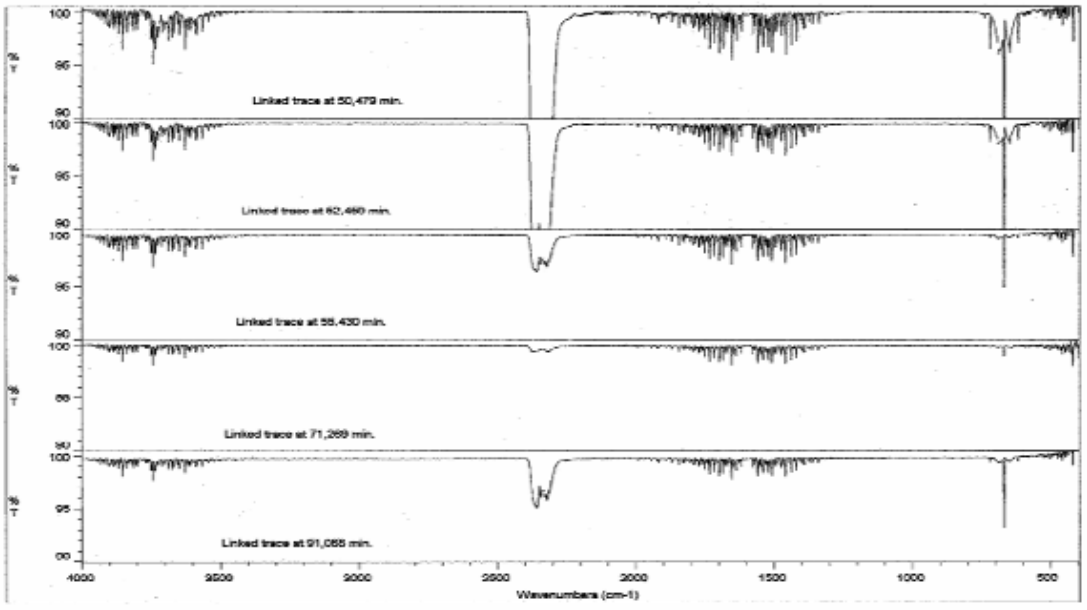


(SI 4-C-1) Three sheets bellow showing a sequential series of spectra, recorded with the increase of time (minutes) which enable to identification of evolved gases.

Sheet 1: First step corresponds; only loss of $H_2O$ and trace amount of $CO_2$ followed by pyrolysis of organic ligand.




Sheet 2: Showings loss of $H_2O$, $CO_2$ and CO.



Sheet 3: Lose of various nitrogenous gases as $N_2O$, NO and $NO_2$ along with $H_2O$, $CO_2$ and CO.

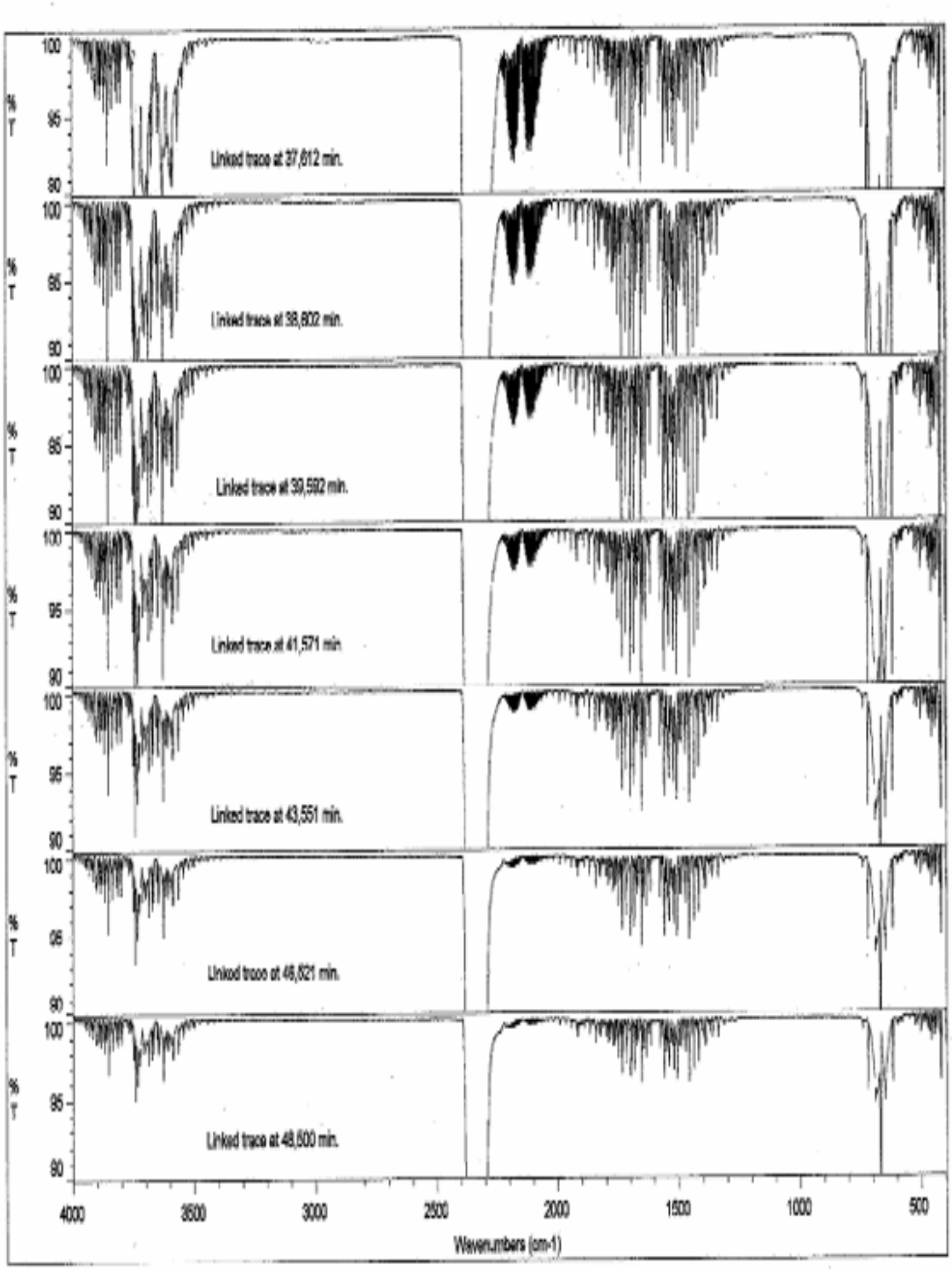
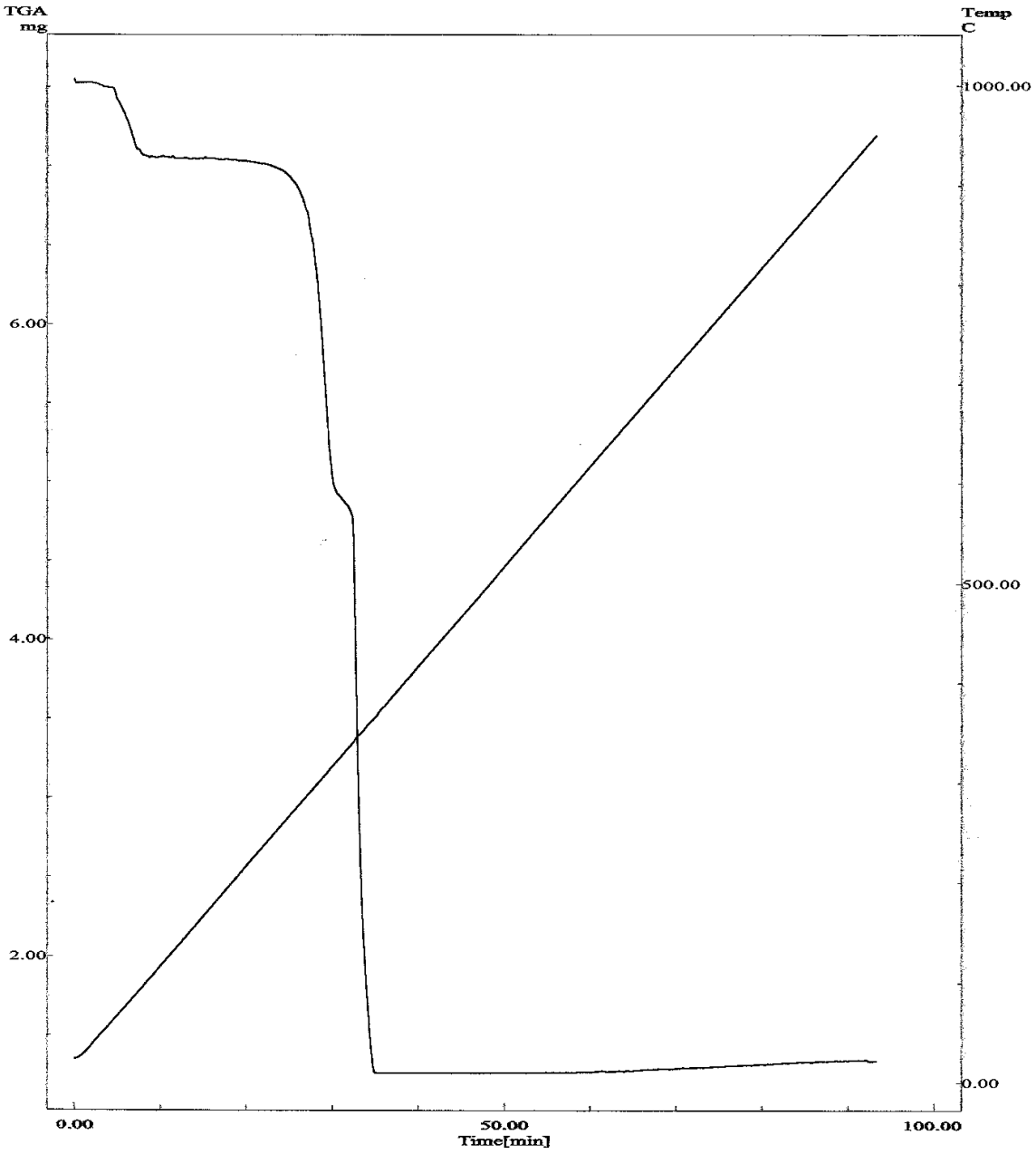
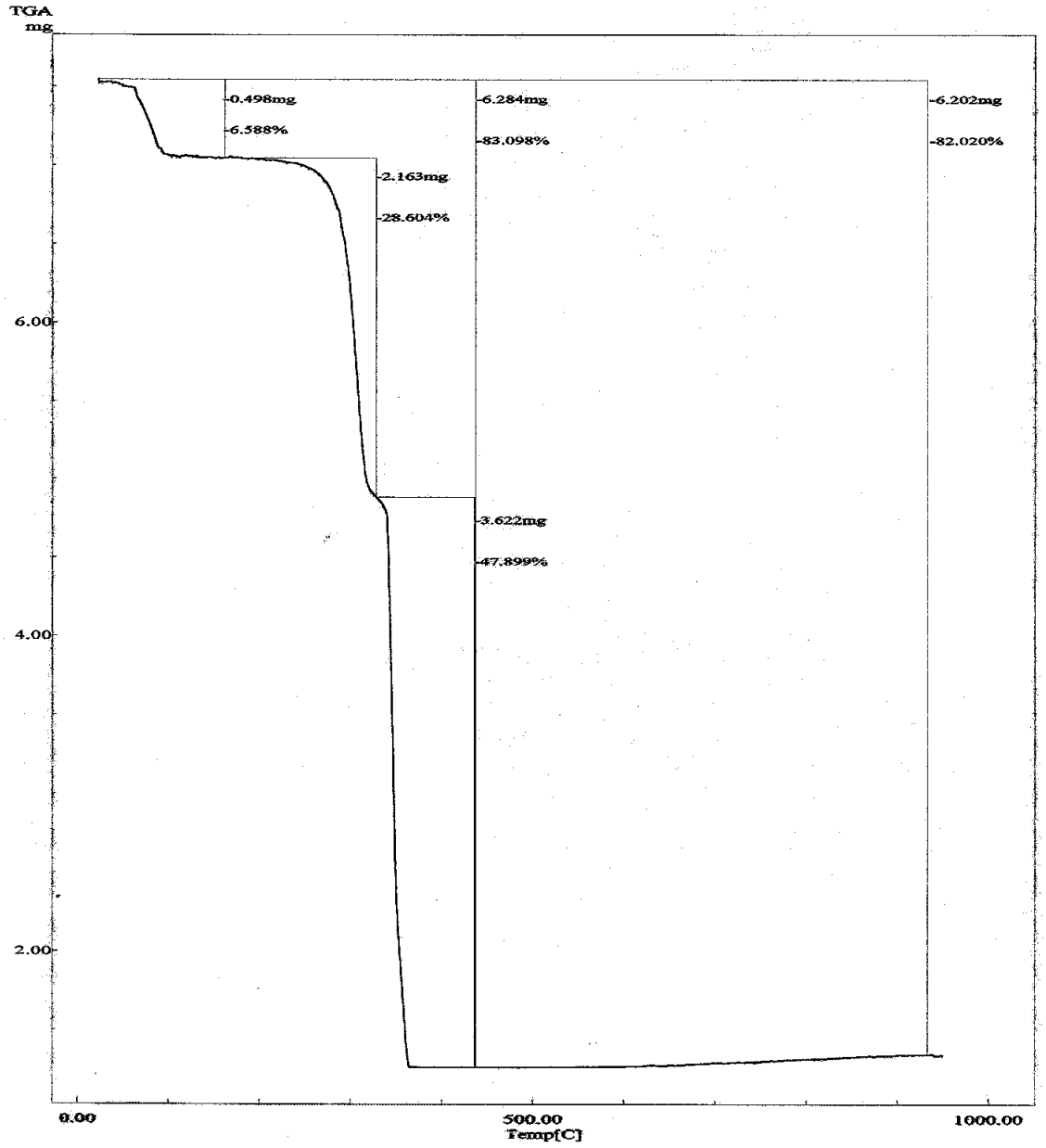


**Fig. SI 5** Thermogravimetric analysis of nickel(II) complex **2**, with FT-IR spectra for the step-wise identification of omitted gases

(SI 5-A) TG-spectra of complex **2** as a function of the time (bottom axis) and temperature (right axis). Weight sample in the left axis:

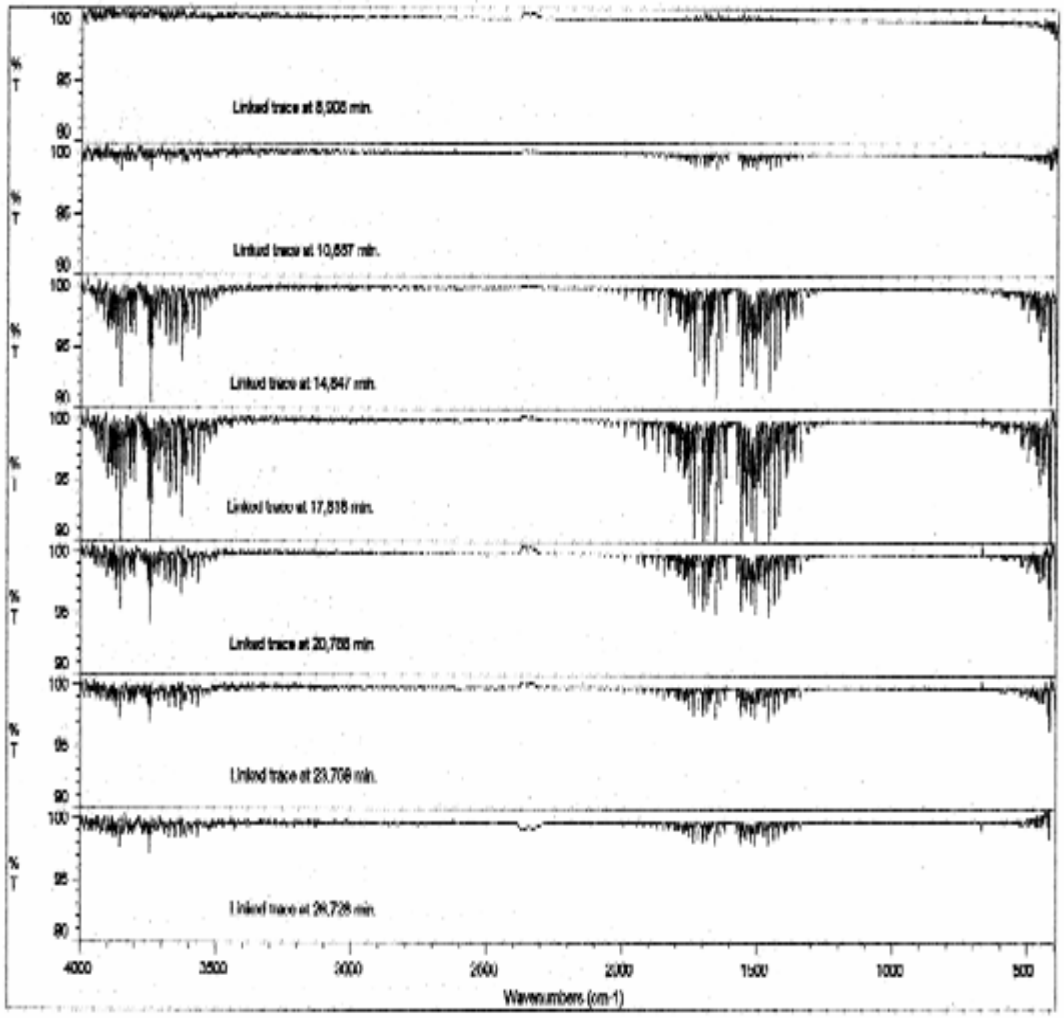


(SI 5-B) TG-spectra of compound **2** as a function of the temperature (bottom axis):

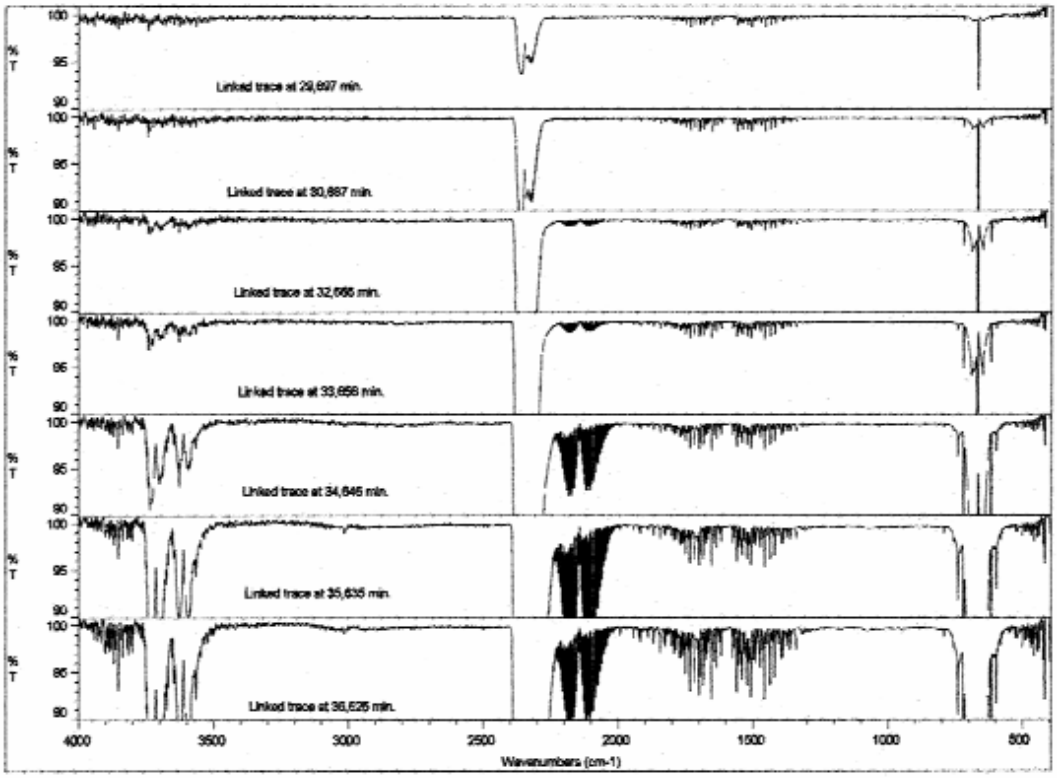


(SI 5-C) Three sheets bellow showing a sequential series of FT-IR spectra, recorded at increasing of time (minutes) which enable the identification of evolved gases in different steps.

Sheet 1: Showing loses of $H_2O$ and very trace amount of $CO_2$.



Sheet 2: The 1st 4 steps are shows loss of $H_2O$ and $CO_2$ while last two CO as well. The trace of methane also can be observed.




Sheet 3: In these spectra the evaluation of $CH_4$ and HCNO (t) along with various nitrogenous gasses has been observed.

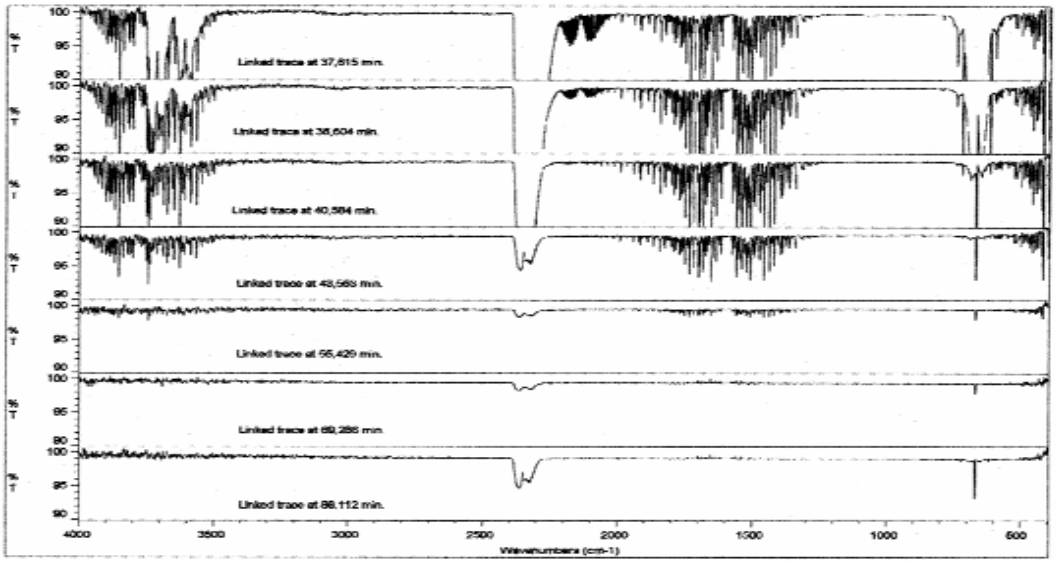


**Fig. SI 6** FT-IR spectrum of complex [Ni(NBIDA)($H_2O$)$_3$].0.5$H_2O$ (**1)**

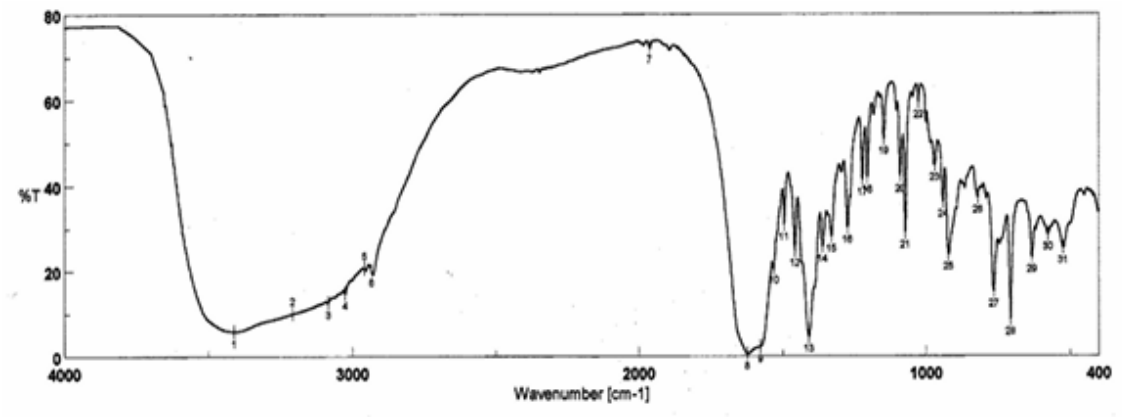



**Fig. SI 7** FTIR spectrum of complex **2**

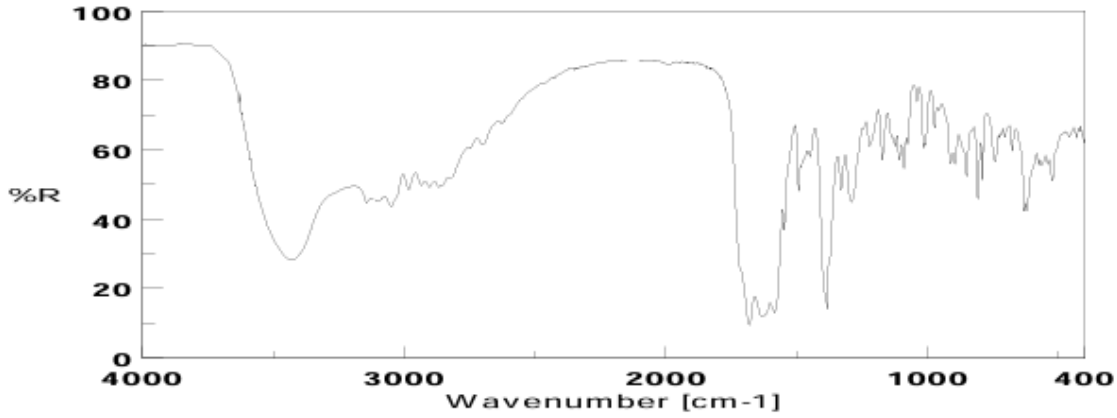


**Fig. SI 8** Showing direct bandgap energy plot for $H_2$NBIDA

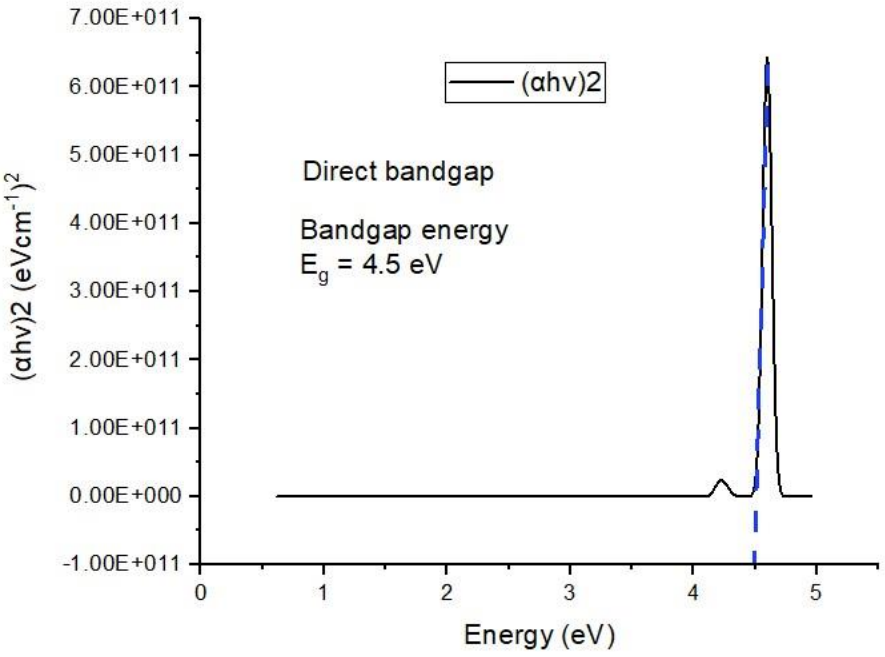



**Fig. SI 9** Showing indirect bandgap energy plot for $H_2$NBIDA