Supporting information for

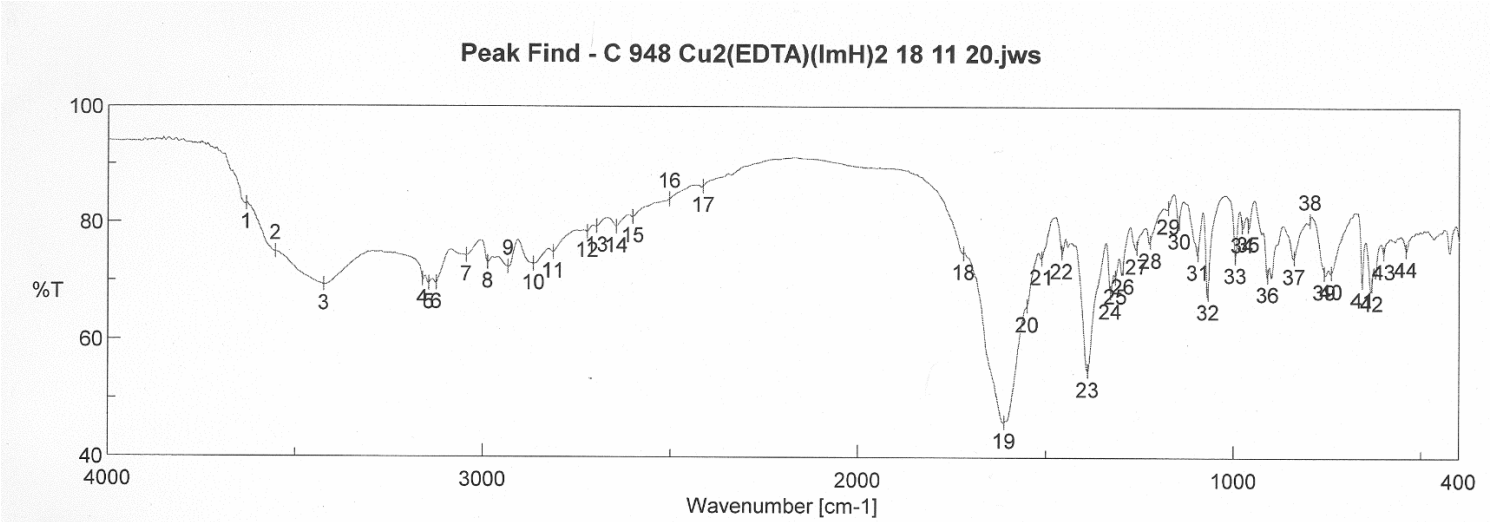
H-bonds, π-Stacking and (water)O-H/π Interactions in (μ4-EDTA)bis(Imidazole)Dicopper(II) Dihydrate

Jeannette Carolina Belmont-Sánchez,[1] María Eugenia García-Rubiño,[1] Antonio Frontera,[2] Josefa María González-Pérez,[1] Alfonso Castiñeiras,[3] Juan Niclós-Gutiérrez*[1]

[1] University of Granada, Department of Inorganic Chemistry, Faculty of Pharmacy, 18071 Granada, Spain.
[2] Departamento Fisicoquímica, Facultad de Farmacia, Universidad de Granada, 18071 Granada, Spain; rubino@ugr.es
[3] Departament de Química, Universitat de les Illes Balears, Crta. de Valldemossa km 7.5, 07122 Palma de Mallorca (Baleares), SPAIN; toni.frontera@uib.es
[4] University of Santiago de Compostela, Department of Inorganic Chemistry, Faculty of Pharmacy, 15782 Santiago de Compostela, Spain.
* Correspondence: jniclos@ugr.es; (J.N.-G.)

* Samples for these purposes have been studied in crystalline solid phase.

SI.1. Infrared spectrum of **1**.



[Comments]
Sample name
Comment
User
Division
Company Universidad de Granada

[Detailed Information]
Creation date 18/11/2020 13:02

[Measurement Information]
Model Name FT/IR-6300typeA
Serial Number A014961024

Measurement Date 18/11/2020 12:56

Light Source Standard
Detector TGS
Accumulation 250
Resolution 4 cm-1

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3632.27	83.0674	2	3553.2	74.7989	3	3423.99	69.2203
4	3160.76	70.1746	5	3144.37	69.498	6	3124.12	69.546
7	3045.05	74.2554	8	2988.16	73.0779	9	2934.16	72.3493
10	2865.7	72.8115	11	2813.63	74.8136	12	2723	78.3235
13	2697.93	79.2396	14	2645.86	79.1624	15	2602.47	80.8561
16	2505.08	83.9024	17	2414.44	86.1417	18	1720.19	74.6849
19	1611.23	46.0034	20	1550.49	65.7933	21	1511.92	73.8609
22	1458.89	74.9123	23	1389.46	54.7883	24	1329.68	68.0765
25	1316.18	70.6167	26	1295.93	72.3295	27	1259.29	75.7344
28	1223.61	76.7152	29	1175.4	82.5774	30	1146.47	80.0333
31	1096.33	74.7104	32	1069.33	67.9539	33	997.017	74.1867
34	978.697	79.4197	35	962.305	79.5912	36	910.236	70.9855
37	839.847	74.0766	38	797.421	80.496	39	758.852	71.4501
40	740.531	71.5321	41	656.643	70.1222	42	631.573	69.54
43	599.753	74.9537	44	540.935	75.3416			

SI.2. Electronic (Reflectance) spectrum of **1**.

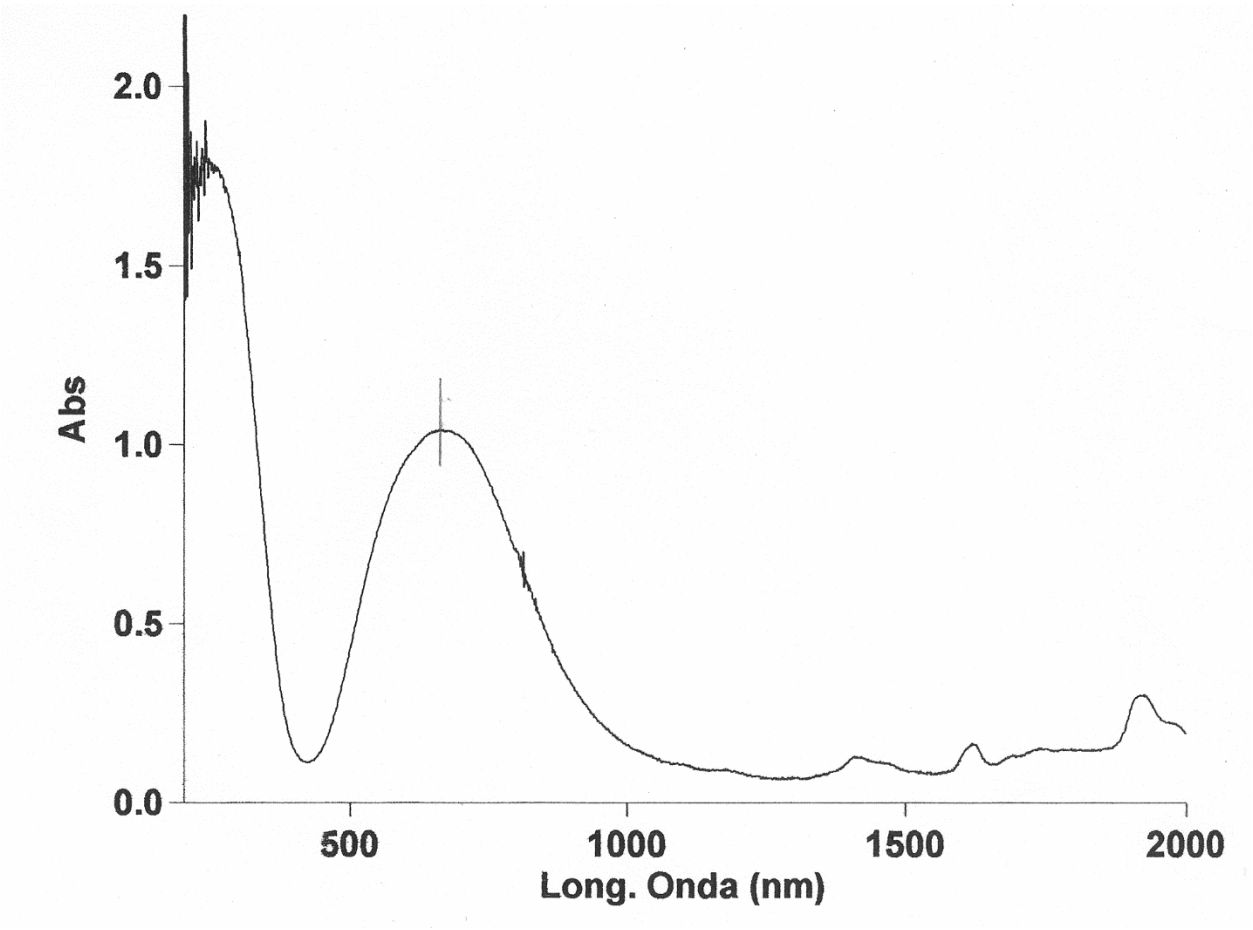


Tabla Picos

Peak Style	Picos
Umbral Picos	0.01000
Rango	2000.000nm a200.000nm

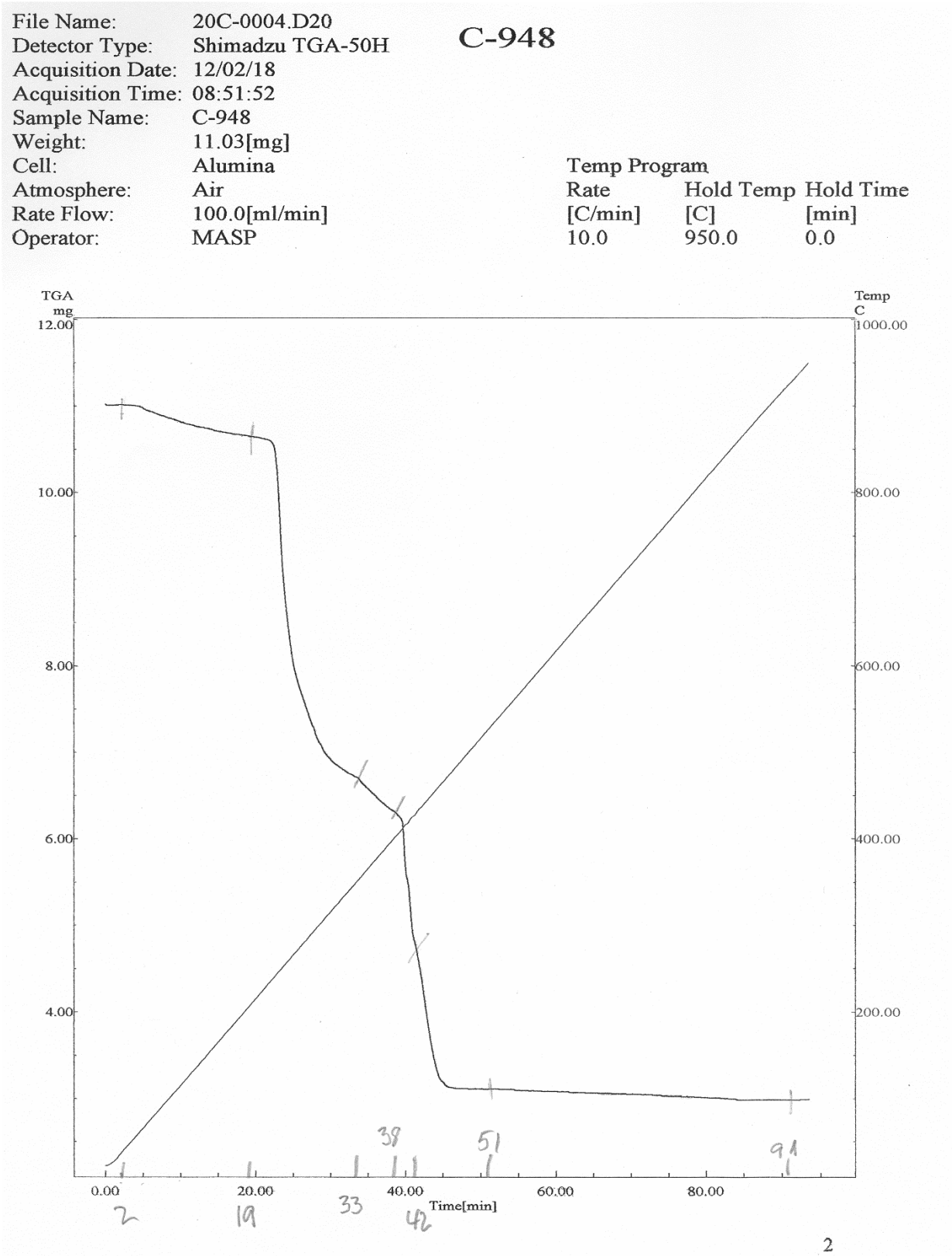
Long. Onda (nm)	Abs
1924.000	0.303
1742.000	0.154
1620.000	0.166
1422.000	0.131
851.000	0.498
845.000	0.521
838.000	0.549
835.000	0.571
824.000	0.609
816.000	0.642
813.000	0.702
809.000	0.689
665.000	1.042
300.000	1.542
276.000	1.722
262.000	1.776
260.000	1.777
256.000	1.784
251.000	1.789

λ_{max} 665 nm

15.040 cm^{-1}

SI.3. Termogravimetric analysis (TGA) of 1 with FT-IR spectra for identification of evolved gases.

A) Plot to estimate the initial and final temperatures (°C) as well as the weight lost in each step or the final residue (%).



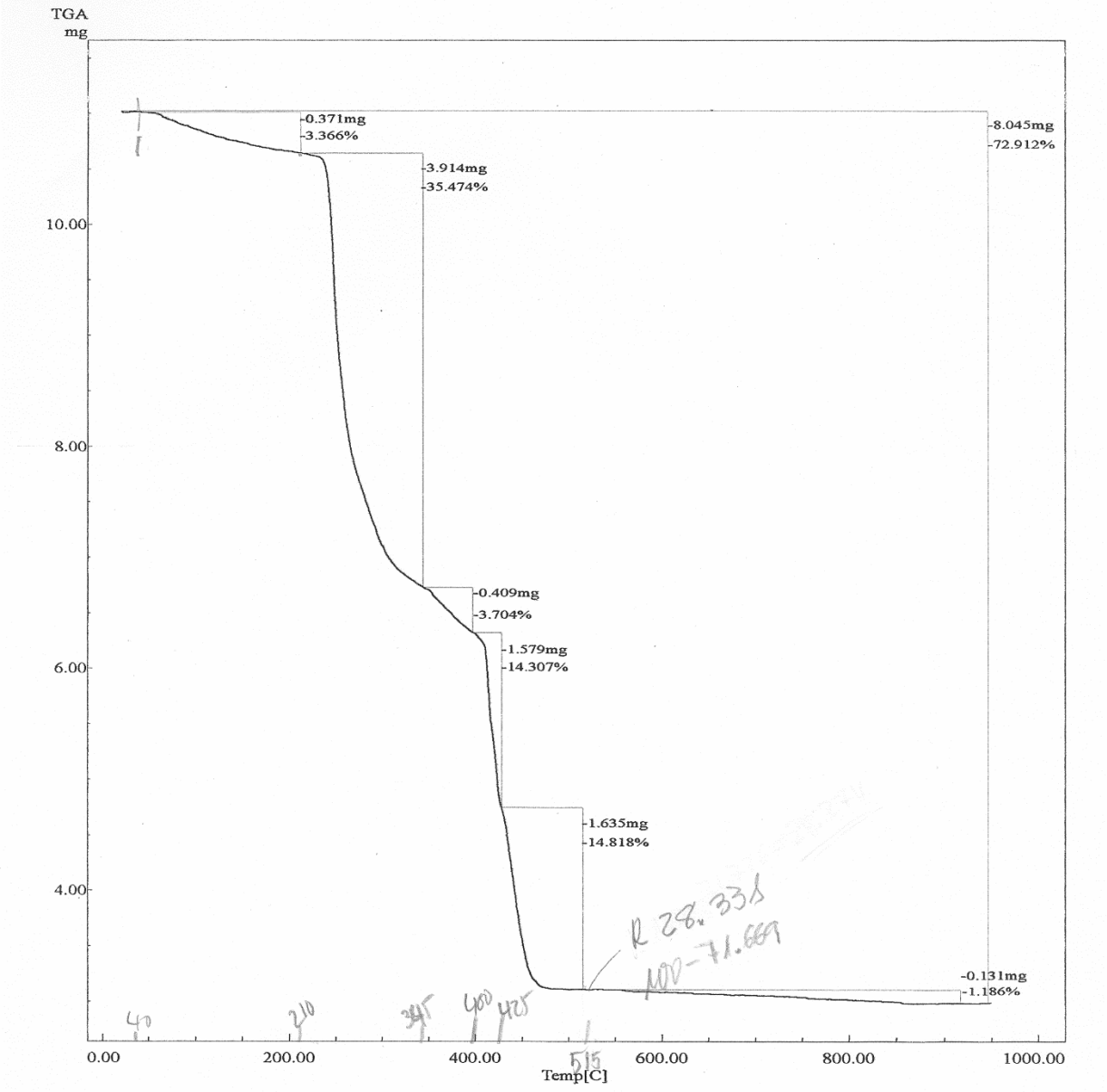
B) Plot to estimate the initial and final time (min.) of each step as well as the time in which the final residue (CuO) has formed.

File Name:	20C-0004.D20
Detector Type:	Shimadzu TGA-50H
Acquisition Date:	12/02/18
Acquisition Time:	08:51:52
Sample Name:	C-948
Weight:	11.03[mg]
Cell:	Alumina
Atmosphere:	Air
Rate Flow:	100.0[ml/min]
Operator:	MASP

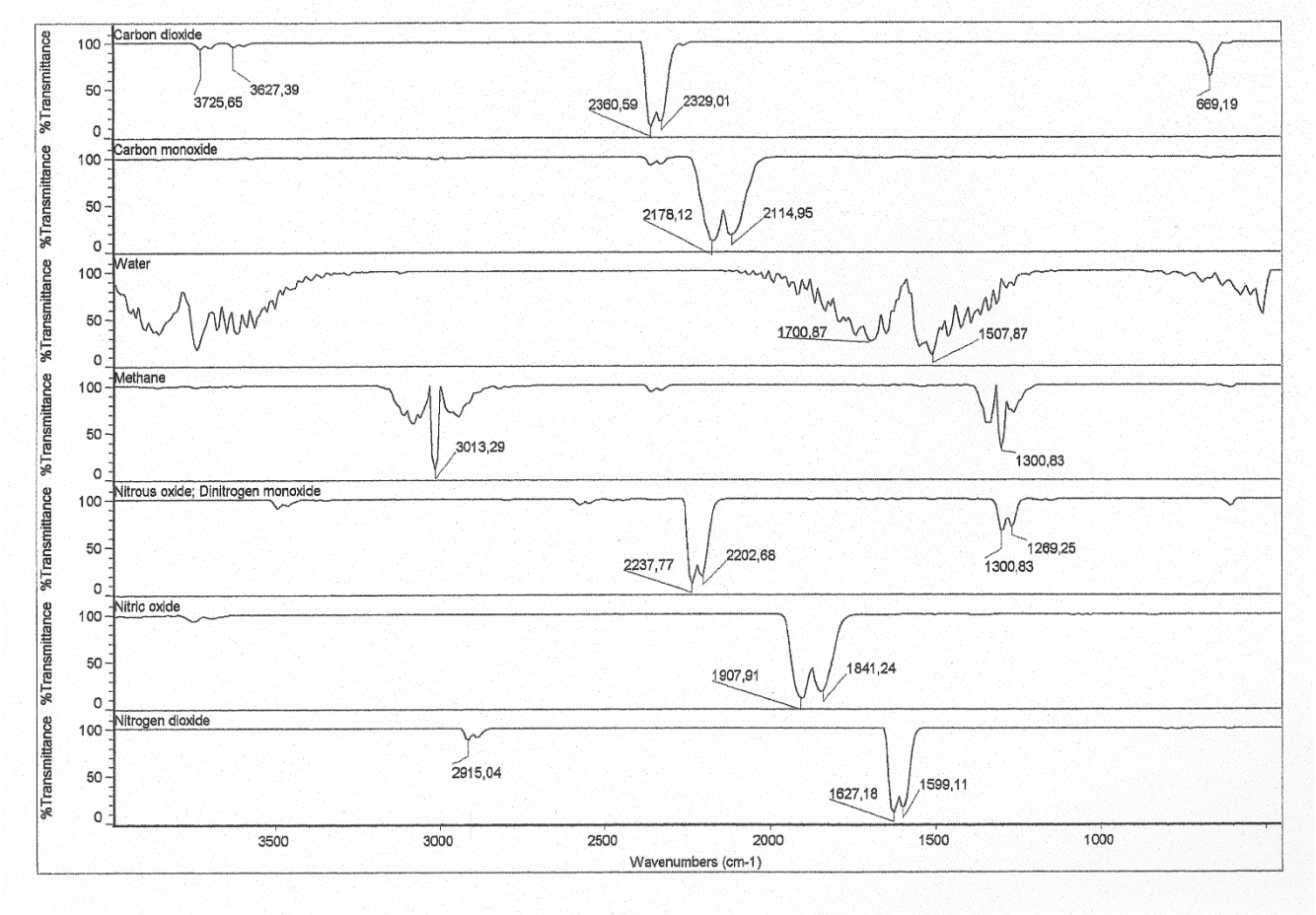
C-948

Temp Program

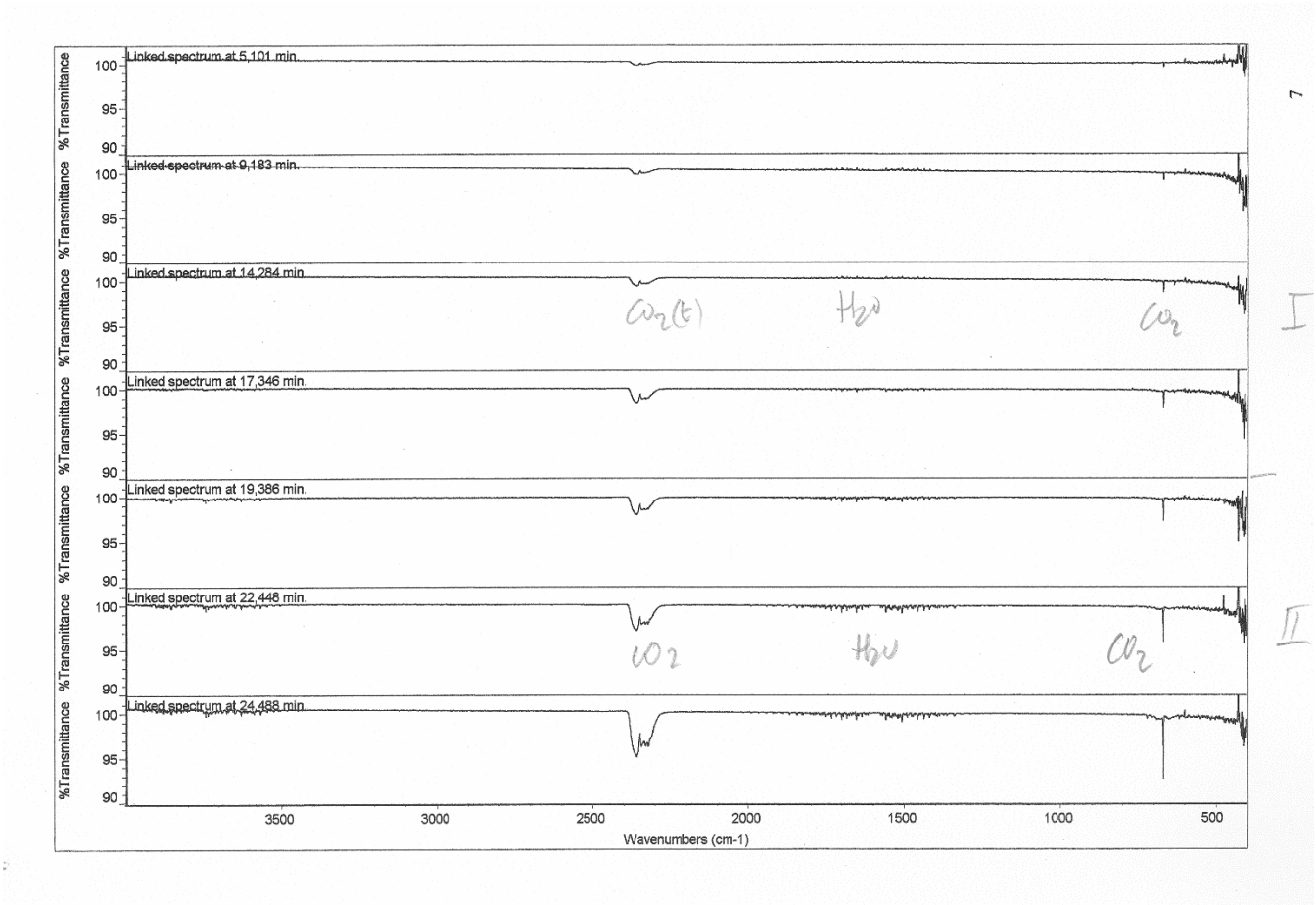
Rate [C/min]	Hold Temp [C]	Hold Time [min]
10.0	950.0	0.0

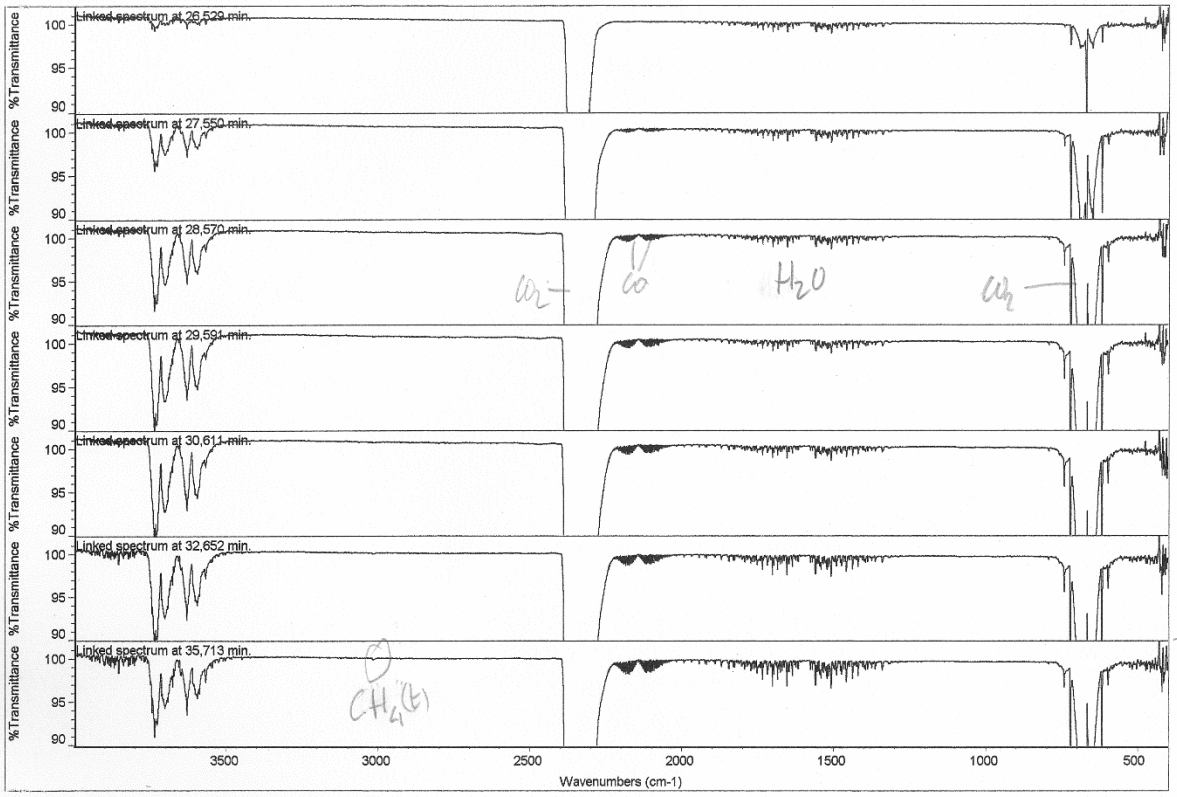


C) FT-IR spectra of identified gasses during the TGA analysis of **1**.

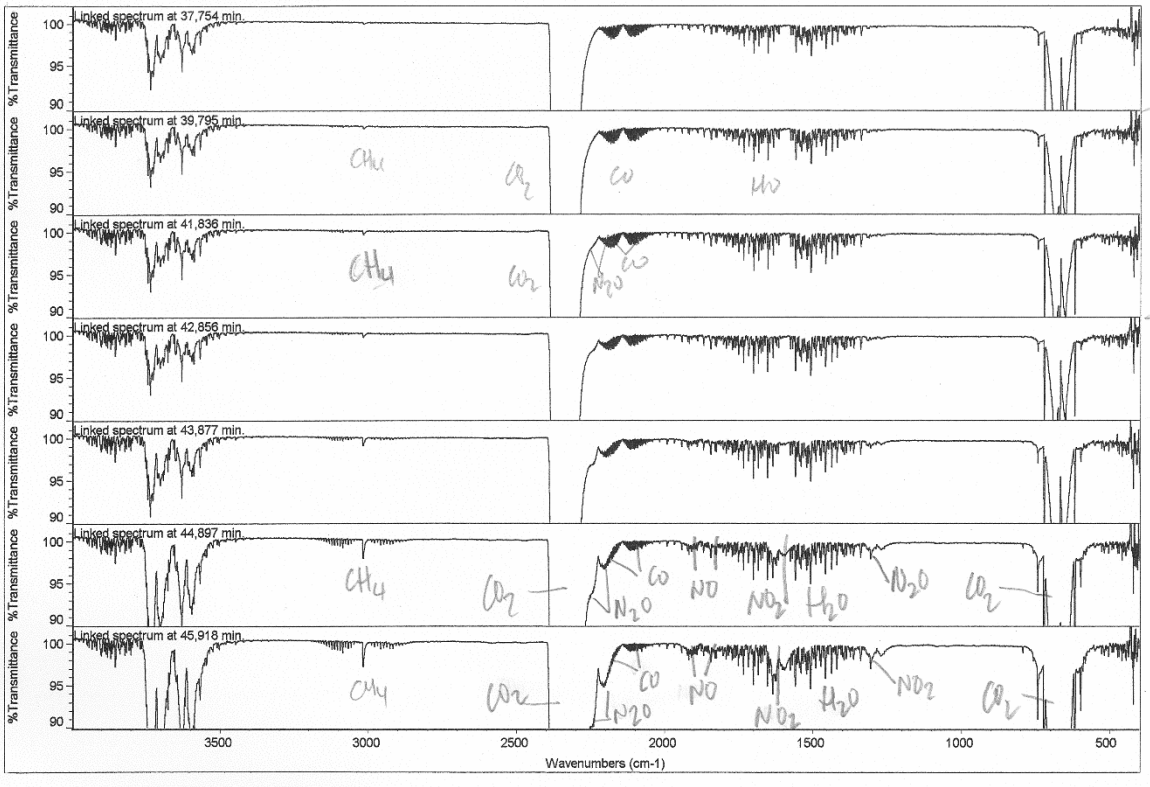


D) Five sheets showing 36 time-spaced FT-IR spectra to identify evolved gases during the TGA of **1**.

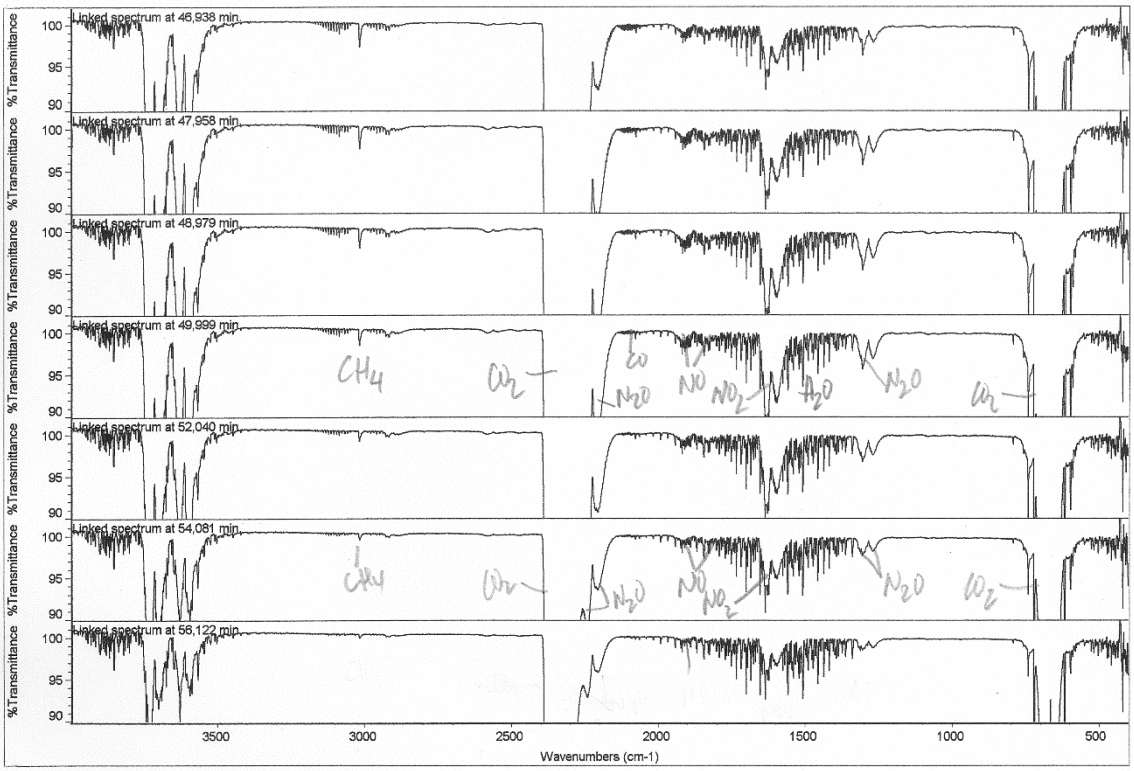



Linked spectrum at 26,529 min.
Linked spectrum at 27,550 min.
Linked spectrum at 28,570 min.
Linked spectrum at 29,591 min.
Linked spectrum at 30,611 min.
Linked spectrum at 32,652 min.
Linked spectrum at 35,713 min.
%Transmittance
100
95
90
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)
CO
H2O
CH4(g)
II cont.
II

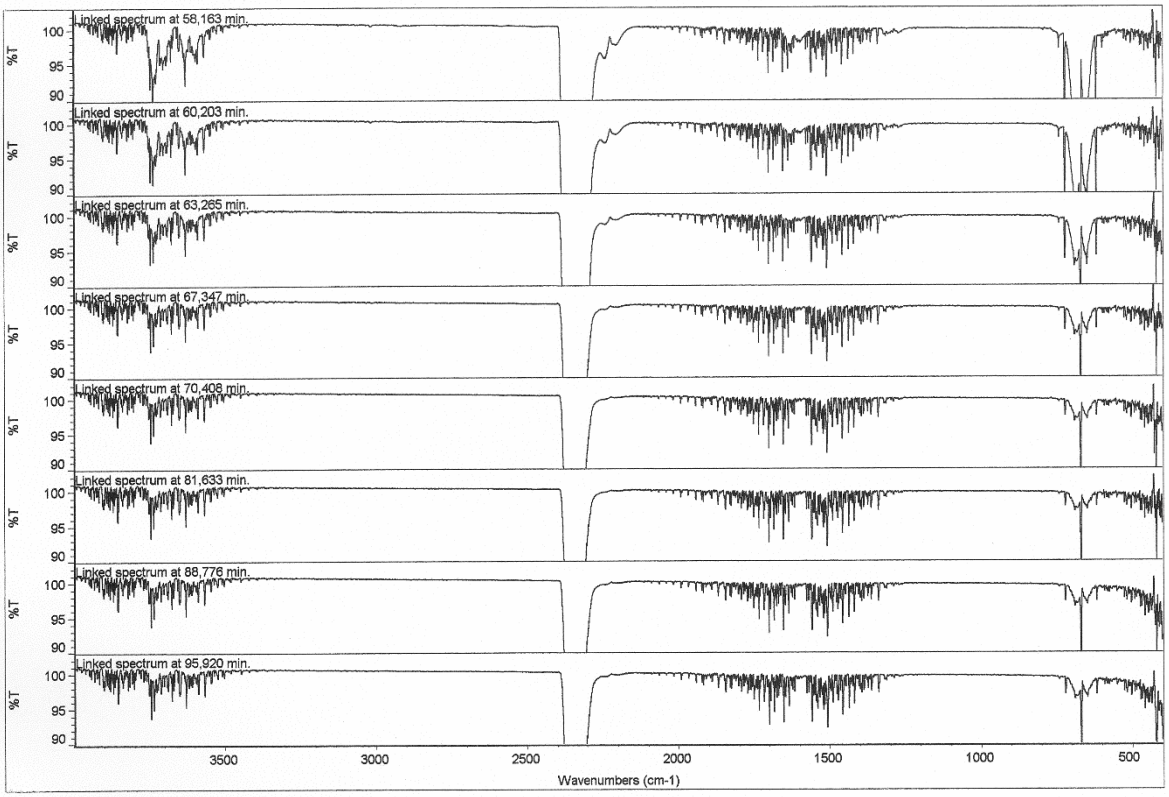
8


Linked spectrum at 37,754 min.
Linked spectrum at 39,795 min.
Linked spectrum at 41,836 min.
Linked spectrum at 42,856 min.
Linked spectrum at 43,877 min.
Linked spectrum at 44,897 min.
Linked spectrum at 45,918 min.
%Transmittance
100
95
90
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)
CH4
CO
H2O
N2O
NO
NO2
III cont.
IV
V

9


Linked spectrum at 46,938 min.
Linked spectrum at 47,958 min.
Linked spectrum at 48,979 min.
Linked spectrum at 49,999 min.
Linked spectrum at 52,040 min.
Linked spectrum at 54,081 min.
Linked spectrum at 56,122 min.
%Transmittance
100
95
90
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)

10


Linked spectrum at 58,163 min.
Linked spectrum at 60,203 min.
Linked spectrum at 63,265 min.
Linked spectrum at 67,347 min.
Linked spectrum at 70,408 min.
Linked spectrum at 81,633 min.
Linked spectrum at 88,776 min.
Linked spectrum at 95,920 min.
%T
100
95
90
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)

11

E) Three selected FT-IR spectra of step 5 (top and middle) or step 3 (down) from TGA of **1.**