Supplementary material of the Article in *Crystals*

A tetranuclear Ni(II)-cubane cluster molecule build by four μ3-O-methanolate (MeO) ligands, externally cohesive by four unprecedented bridging μ2-N7,O6-acyclovirate (acv-H) anions.

by

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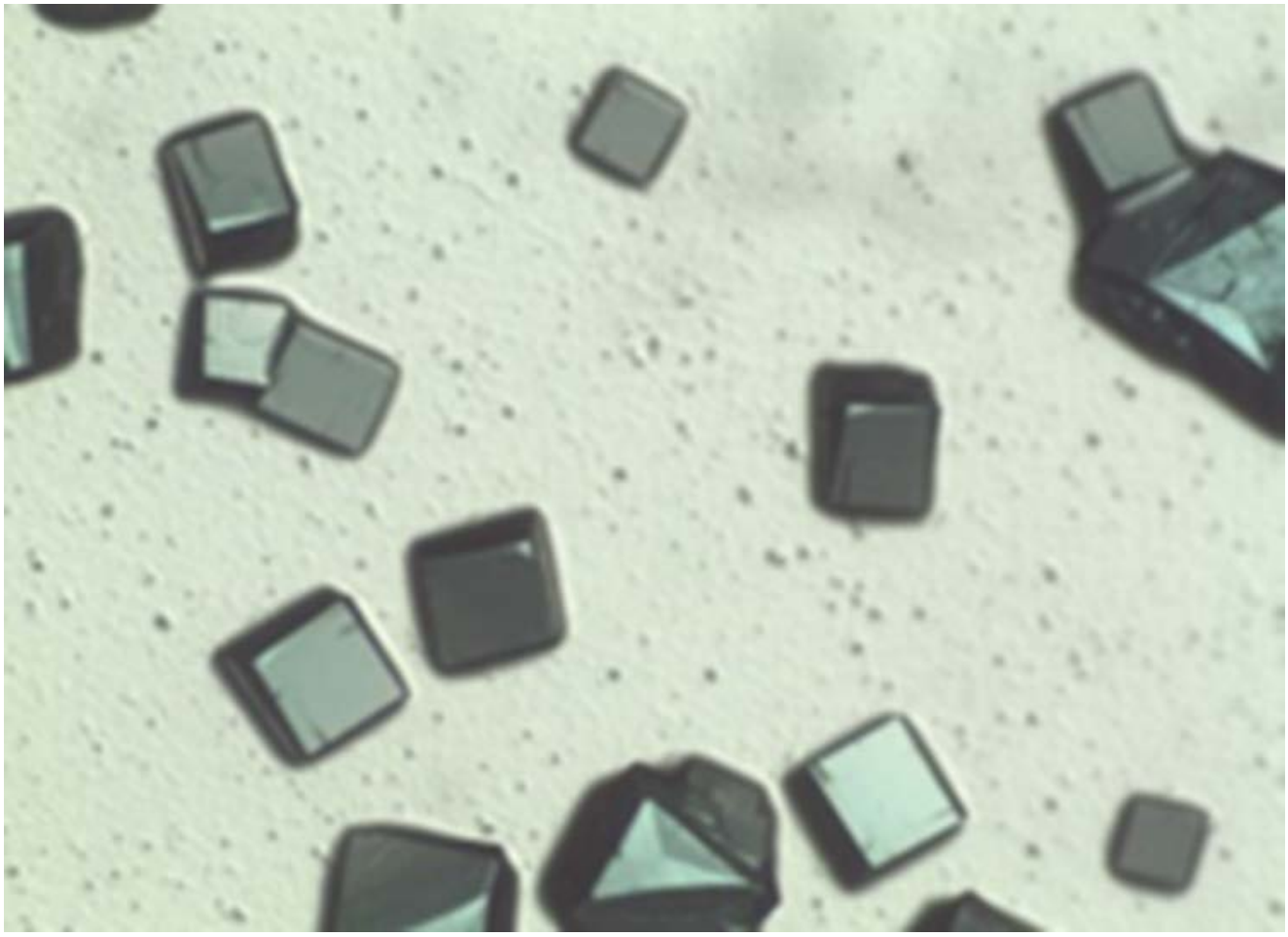
Contents

Figure S1. Crystals of compound [Ni(μ_2-N7,O6-acv-H)(μ_3-MeO)(H_2O)]$_4$·8H_2O (1).



S2. Supplementary structural information of compound 1.

Table A. Selected bond lengths [A] and angles [deg] for [Ni(acv)(MeO)(H2O)]4.8H2O.

Ni(1)-O(1)	2.038(2)
Ni(1)-O(1)#1	2.041(3)
Ni(1)-O(1)#2	2.049(2)
Ni(1)-O(16)	2.054(2)
Ni(1)-N(17)	2.069(3)
Ni(1)-O(2)	2.131(3)
Ni(1)-Ni(1)#3	3.0527(10)
Ni(1)-Ni(1)#1	3.0527(10)
Ni(1)-Ni(1)#2	3.0657(11)
O(1)-O(1)#2	2.694(5)
O(1)-O(1)#3	2.701(4)
O(1)-O(1)#1	2.701(4)
O(1)-Ni(1)-O(1)#1	82.94(10)
O(1)-Ni(1)-O(1)#2	82.44(10)
O(1)#1-Ni(1)-O(1)#2	82.66(11)
O(1)-Ni(1)-O(16)	175.74(10)
O(1)#1-Ni(1)-O(16)	96.29(10)
O(1)#2-Ni(1)-O(16)	93.30(10)
O(1)-Ni(1)-N(17)	94.82(10)
O(1)#1-Ni(1)-N(17)	95.31(11)
O(1)#2-Ni(1)-N(17)	176.76(12)
O(16)-Ni(1)-N(17)	89.43(11)
O(1)-Ni(1)-O(2)	91.31(10)
O(1)#1-Ni(1)-O(2)	171.96(11)
O(1)#2-Ni(1)-O(2)	91.04(10)
O(16)-Ni(1)-O(2)	89.03(10)
N(17)-Ni(1)-O(2)	90.75(12)
Ni(1)-O(1)-Ni(1)#3	96.90(11)
Ni(1)-O(1)-Ni(1)#2	97.18(10)
Ni(1)#3-O(1)-Ni(1)#2	96.54(10)

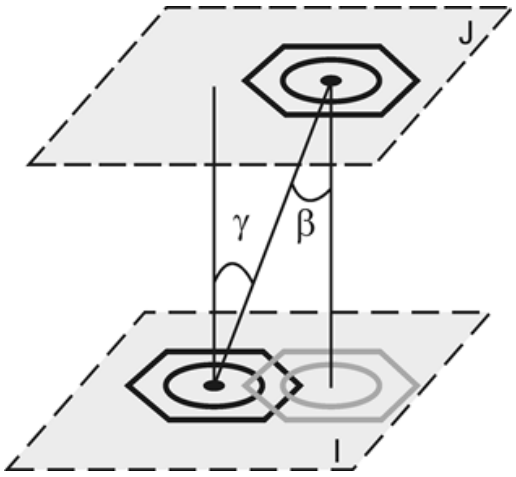
Symmetry transformations used to generate equivalent atoms:
#1 -z+1/4,-y+3/4,x #2 -x+1/4,y,-z+1/4
#3 z,-y+3/4,-x+1/4

Table B. Hydrogen bonds for [Ni(acv)(MeO)(H2O)]4.8H2O [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2A)...O(4)#4	0.98	1.77	2.714(6)	159.8
N(12)-H(12A)...O(4)#5	0.84	2.15	2.935(6)	156.4

Symmetry transformations used to generate equivalent atoms:
#1 -z+1/4,-y+3/4,x #2 -x+1/4,y,-z+1/4 #3 z,-y+3/4,-x+1/4
#4 y,z,x #5 -x,-y+1/2,-z+1/2

Table C. Selected data for π-sacking interactions between the six-membered ring of guanine moieties of acv-H.

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================================================================================================================
Analysis of Short Ring-Interactions with Cg-Cg Distances <   6.0 Angstrom and Beta < 60.0Deg.
================================================================================================================
- Cg(I)    = Plane number I (= ring number in () above)
- Alpha    = Dihedral Angle between Planes I and J (Deg)
- Beta     = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma    = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg    = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)
- Slippage = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).
- P,Q,R,S  = J-Plane Parameters for Carth. Coord. (Xo, Yo, Zo)
================================================================================================================
  6-Membered Ring (21)   N(11)  -->   C(12)  -->   N(13)  -->   C(14)  -->   C(15)  -->   C(16)a -->
================================================================================================================
  6-Membered Ring (22)   C(16)  -->   N(11)c -->   C(12)c -->   N(13)c -->   C(14)c -->   C(15)c -->
================================================================================================================


Cg(I) Res(I)   Cg(J)  [   ARU(J)]       Cg-Cg Transformed J-Plane P, Q, R, S     Alpha  Beta Gamma    CgI_Perp    CgJ_Perp  Slippage

Cg(21) [ 1] -> Cg(21) [ 10554.10]      3.7561 -0.2580 0.6911-0.6752  10.2640         1 25.32 25.32     -3.3954     -3.3954
Cg(22) [ 1] -> Cg(22) [  6455.10]      3.7561 -0.6752 0.6911 0.2580   6.8318         1 25.32 25.32      3.3954      3.3954
                                ----------                                    ------------------------------------------
                           Min or Max  3.745                                      0.67  1.98 89.44      -3.421      -5.352


[  1555] = X,Y,Z
[103555] = 1/4-X,Y,1/4-Z
[  6455] = -1/4+Y,1/4+X,-Z
================================================================================================================
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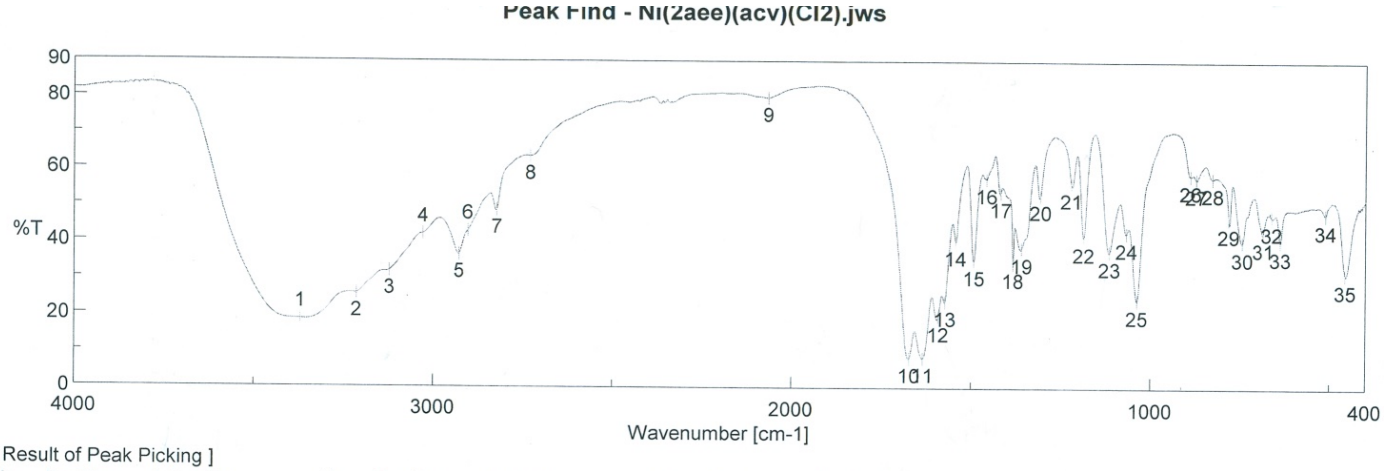
S3. FT-IR spectrum (KBr disk) of compound 1.



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3369.51	18.54	2	3212.34	25.6522	3	3122.19	31.8255
4	3028.66	41.9277	5	2927.89	36.3618	6	2903.79	42.8008
7	2823.76	48.4978	8	2730.71	63.3809	9	2065.87	79.8039
10	1671.98	8.20386	11	1634.38	8.29311	12	1591.95	19.491
13	1573.63	23.7284	14	1544.22	40.2333	15	1493.6	34.8934
16	1458.89	57.4153	17	1418.87	53.5897	18	1384.64	34.2486
19	1360.53	38.286	20	1307.5	52.9018	21	1222.17	56.0861
22	1187.45	41.2979	23	1115.62	37.3534	24	1067.89	42.4665
25	1038.48	24.0948	26	889.505	58.3826	27	873.596	57.4321
28	828.277	57.6666	29	782.958	46.4963	30	745.835	40.0812
31	687.498	42.7729	32	663.393	47.1947	33	639.287	40.338
34	511.526	47.619	35	456.082	31.374			

S4. TGA study of compound 1 with FT-IR spectra to identification of evolved gases.

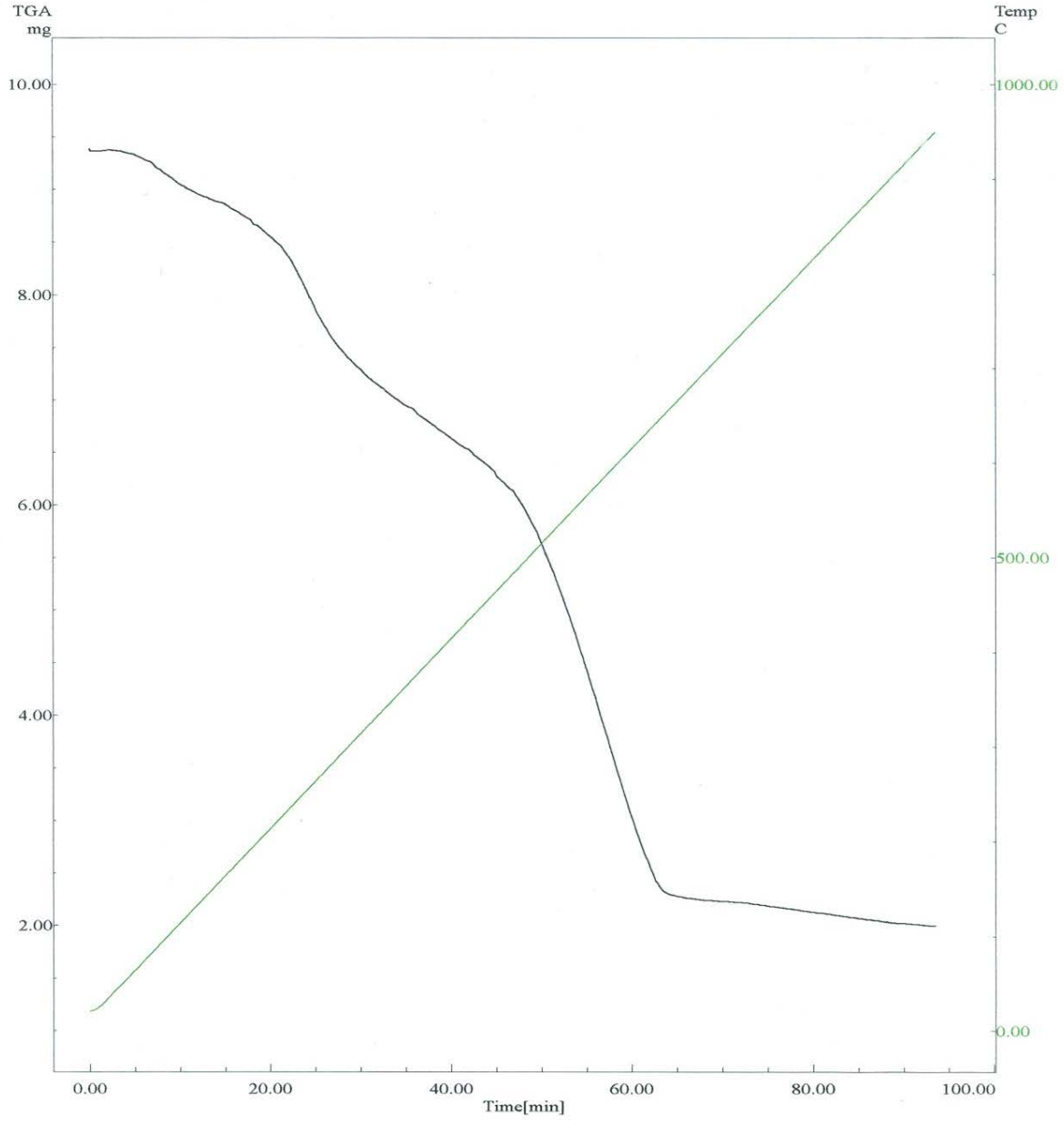
S4.1. TGA curve versus time (abscissas) and temperature (right ordinates).

File Name:	18C-0055.D20
Detector Type:	Shimadzu TGA-50H
Acquisition Date:	11/11/30
Acquisition Time:	08:45:37
Sample Name:	C-884
Weight:	9.382[mg]
Cell:	Alumina
Atmosphere:	Air
Rate Flow:	100.0[ml/min]
Operator:	MASP

C-884

Temp Program

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



S4.2. First derivative of TGA curve, to decide the beginning and end of steps.

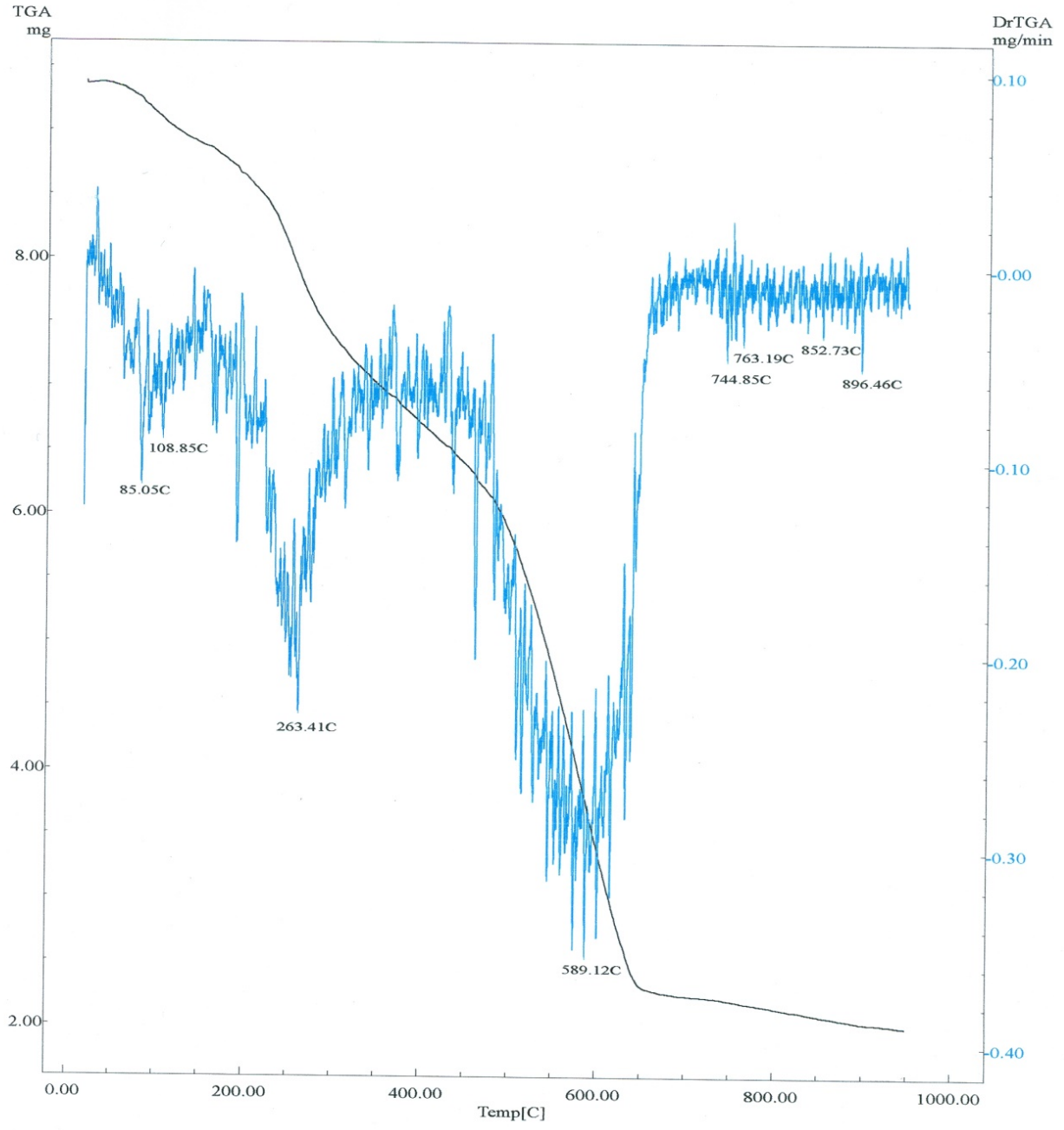
Unidades de TA y UVNIR
Centro de Instrumentación Científica
Universidad de Granada

File Name:	18C-0055.D20
Detector Type:	Shimadzu TGA-50H
Acquisition Date:	11/11/30
Acquisition Time:	08:45:37
Sample Name:	C-884
Weight:	9.382[mg]
Cell:	Alumina
Atmosphere:	Air
Rate Flow:	100.0[ml/min]
Operator:	MASP

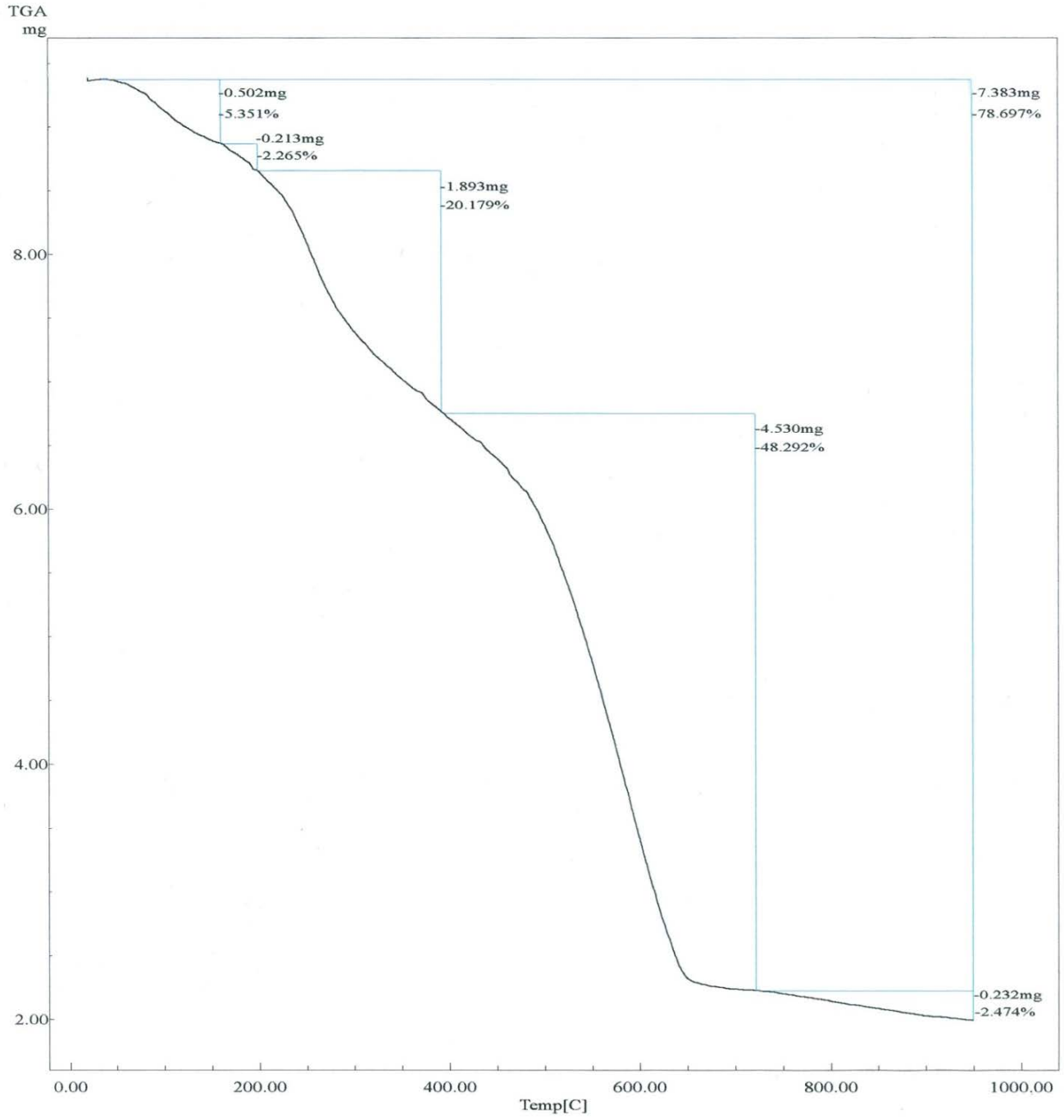
C-884

Temp Program

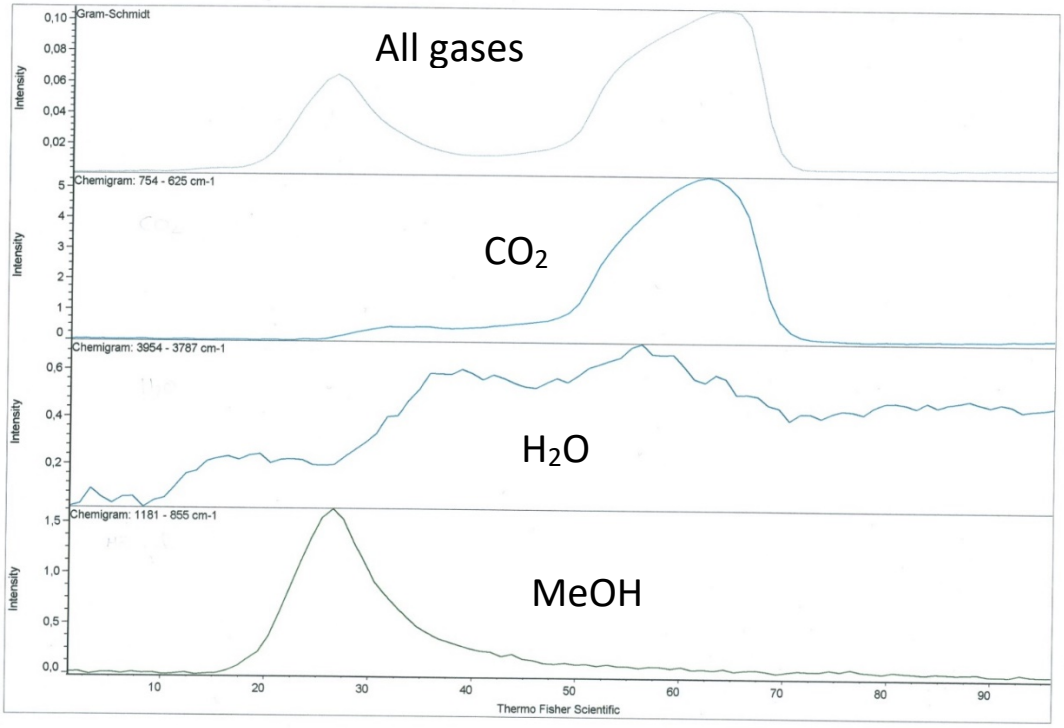
Rate [C/min]	Hold Temp [C]	Hold Time [min]
10.0	950.0	0.0



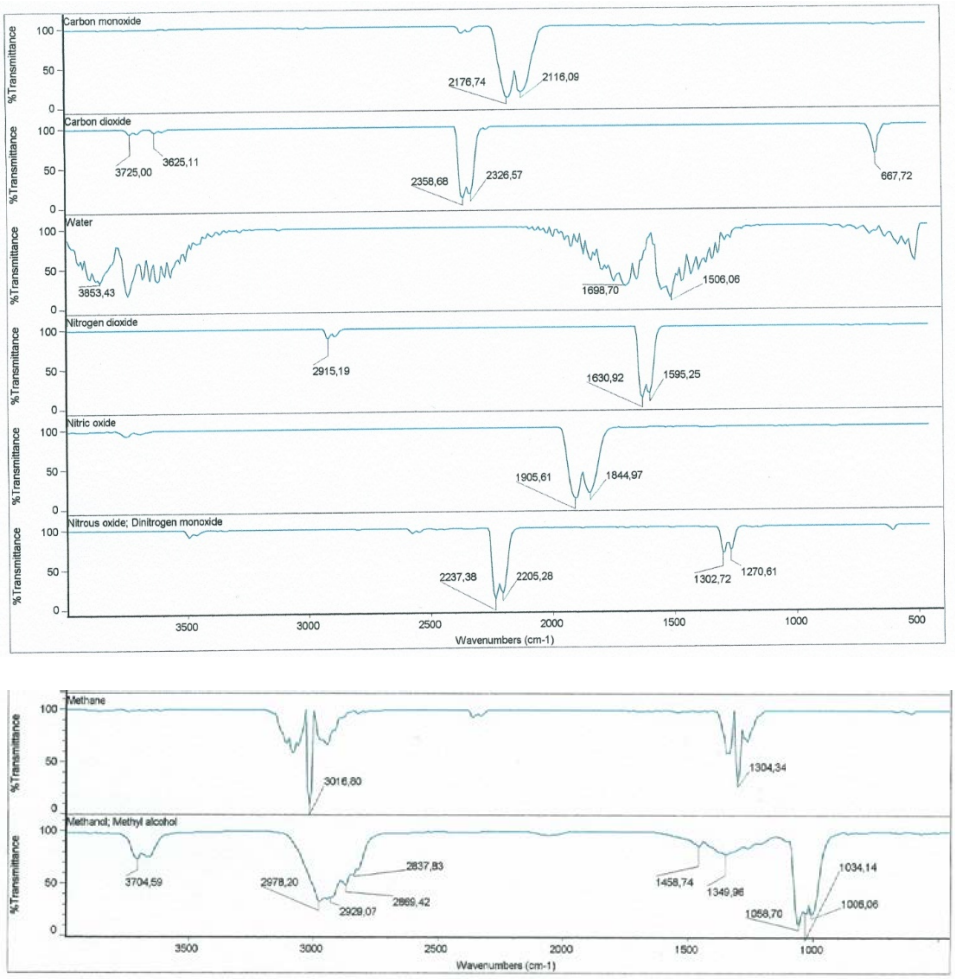
S4.3. TGA curve of weight versus temperature, with data of partial or total experimental weight loss (in mg or %).



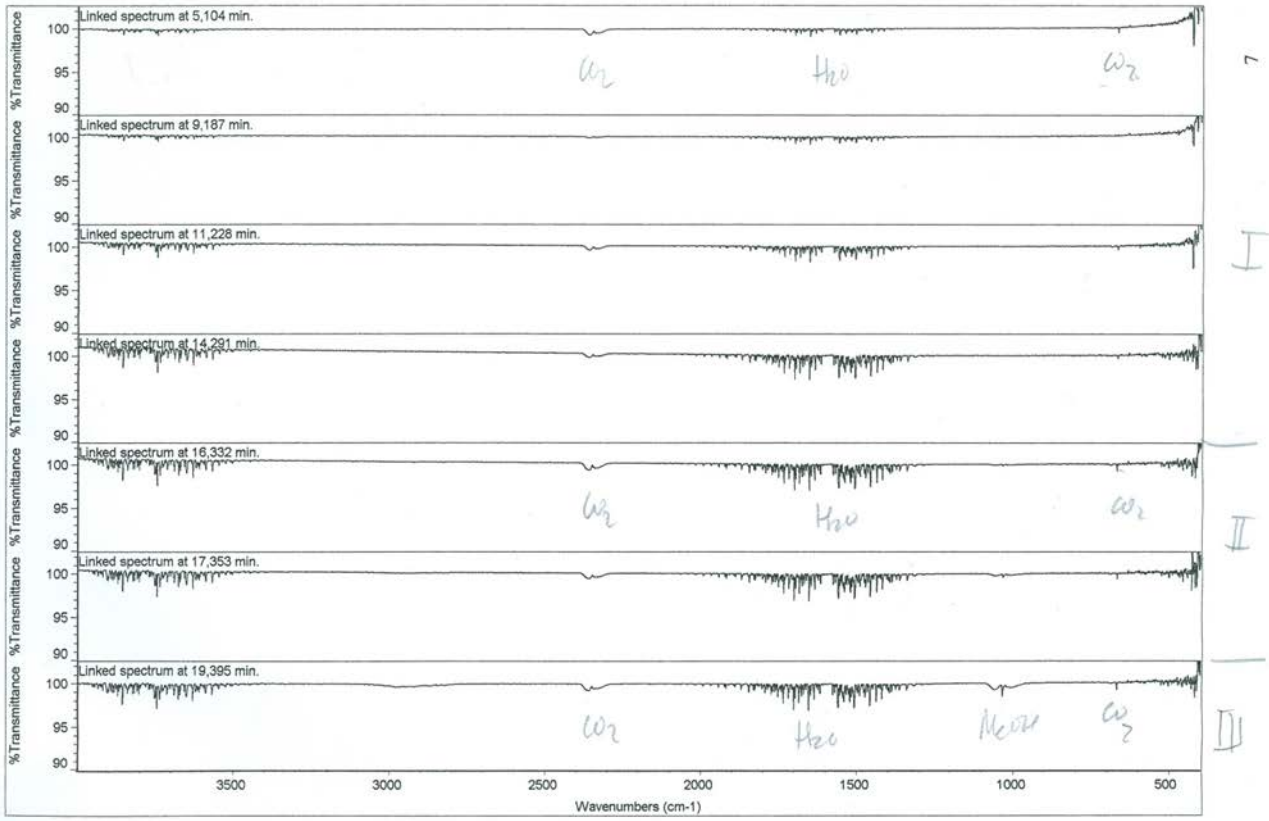
S4.4. Plot for all losses gases (up) and for CO_2, water and methanol versus time (min), as monitored by continuous IR spectra.

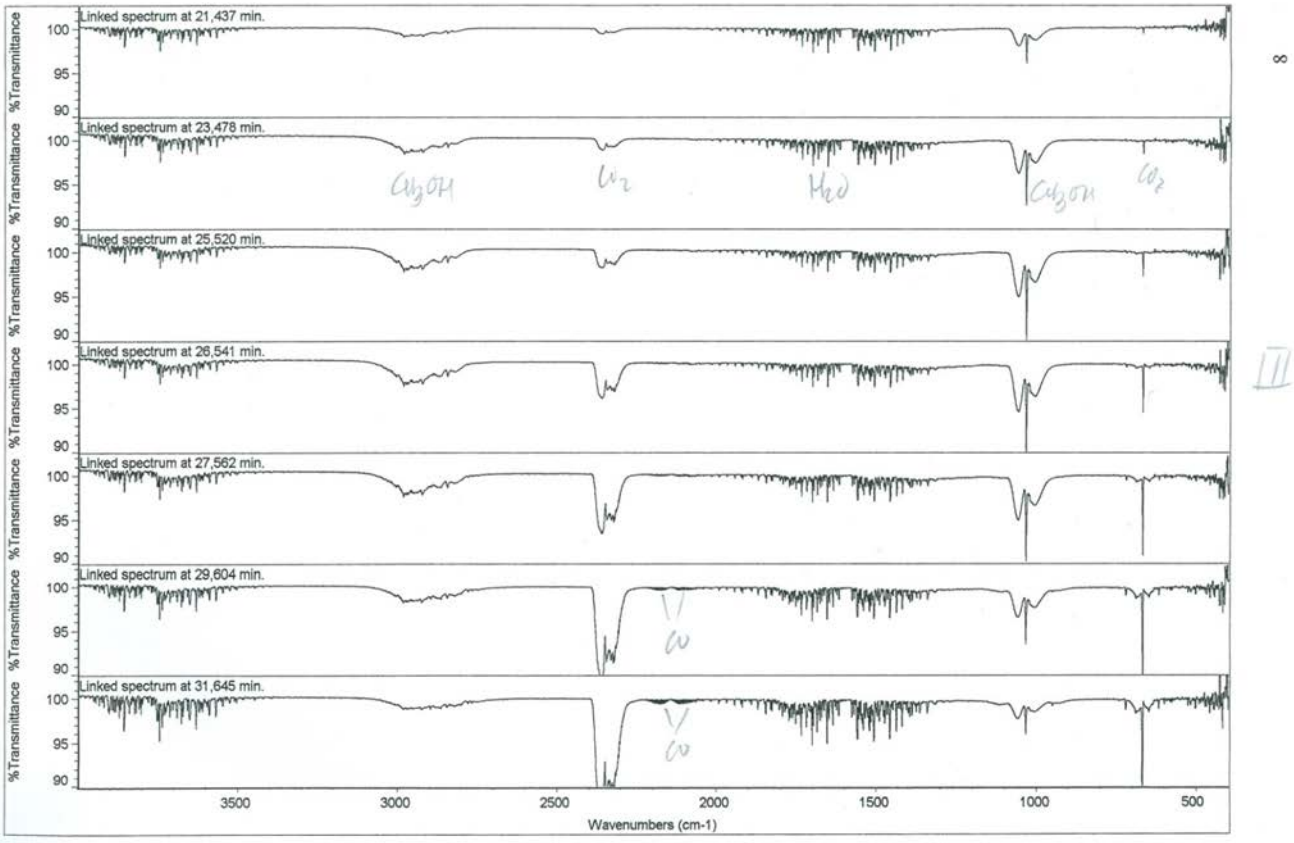


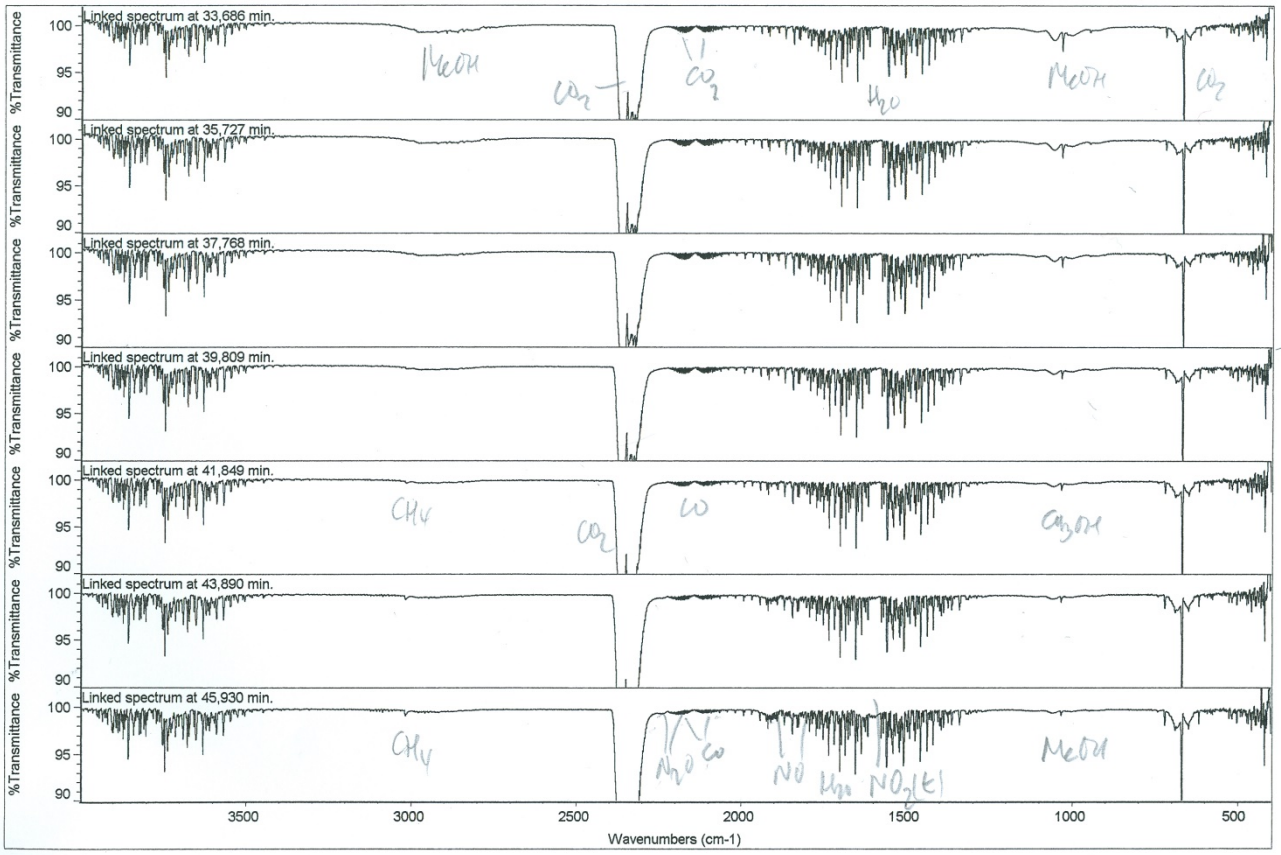
S4.5. FT-IR spectra of pure samples of the observed evolved gases.

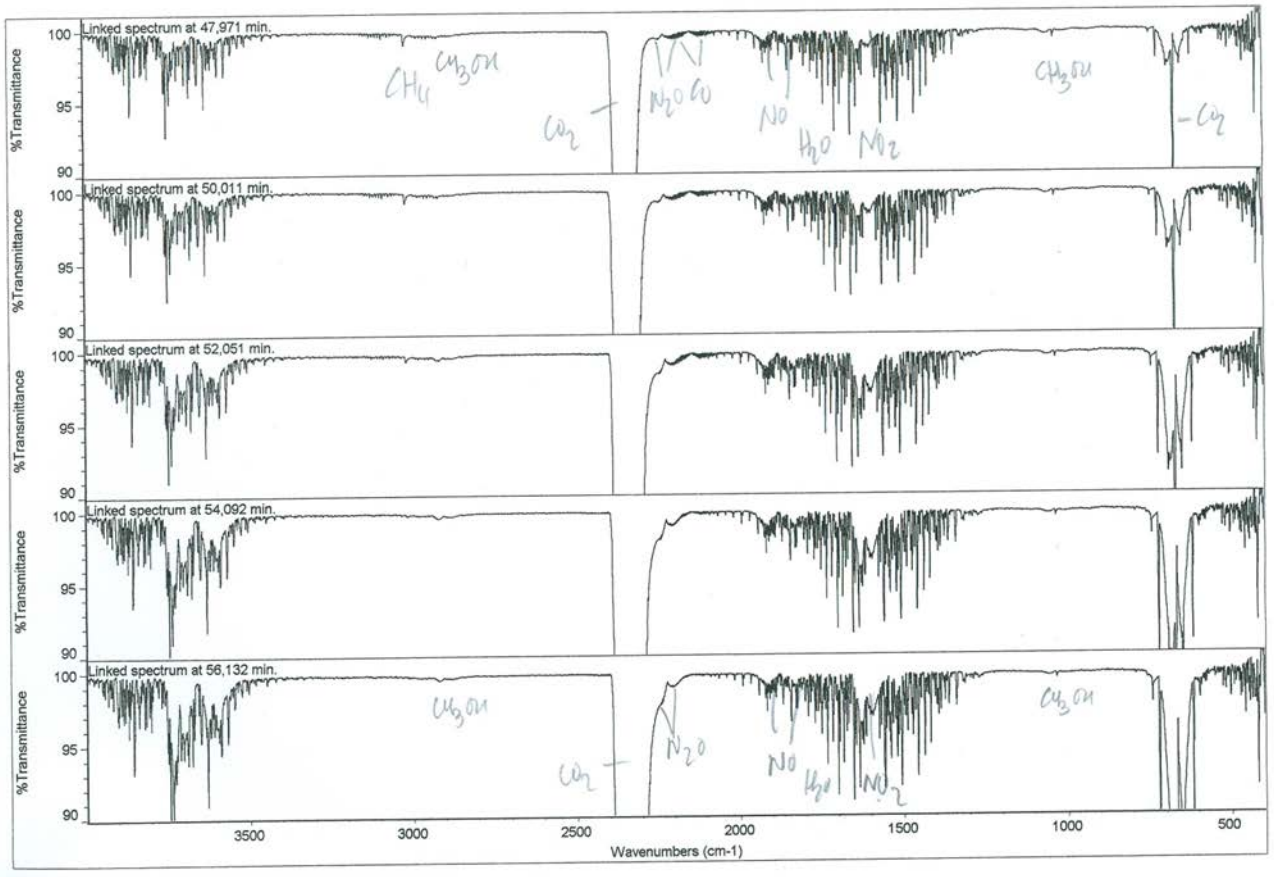


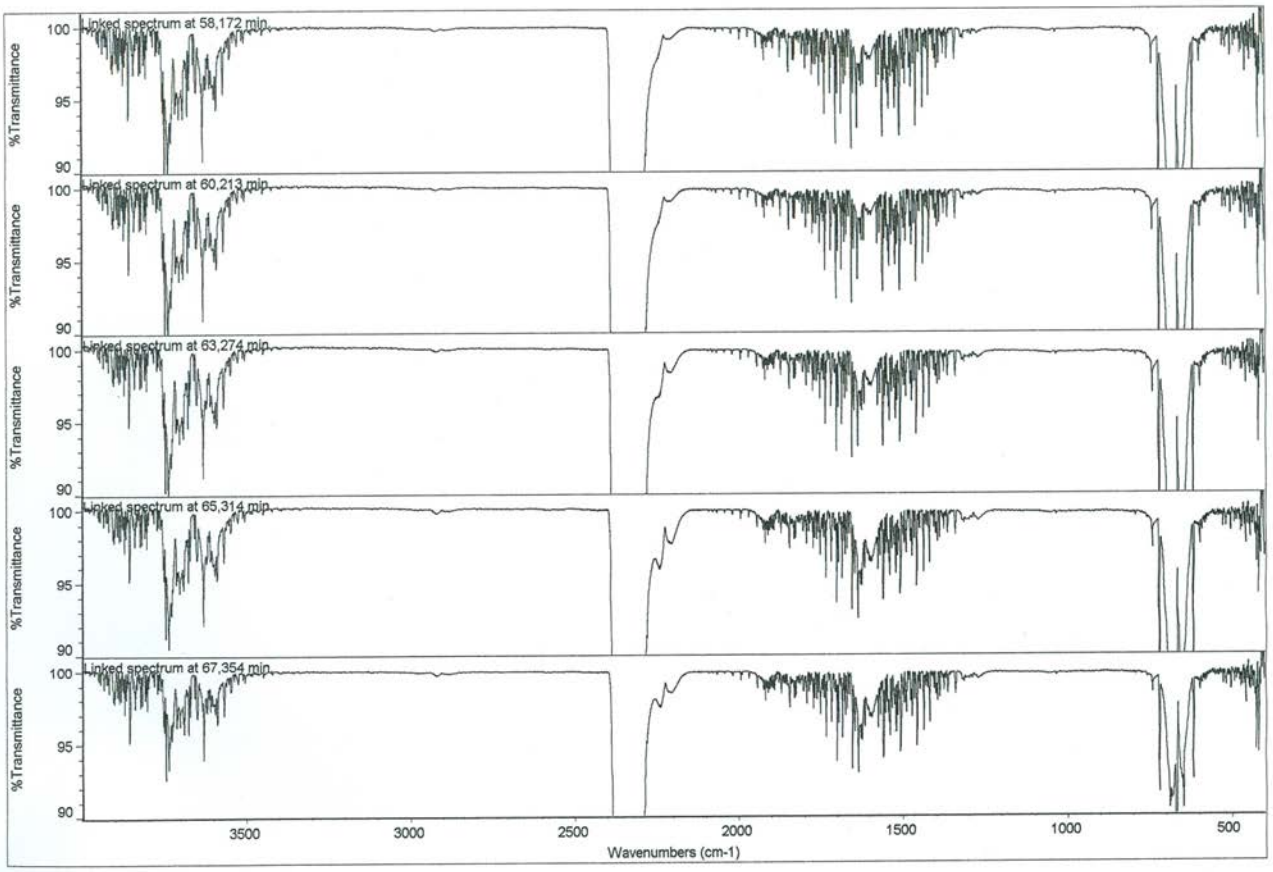
S4.6. Sheets with thirty-seven time-spaced IR spectra to identify evolved gases.



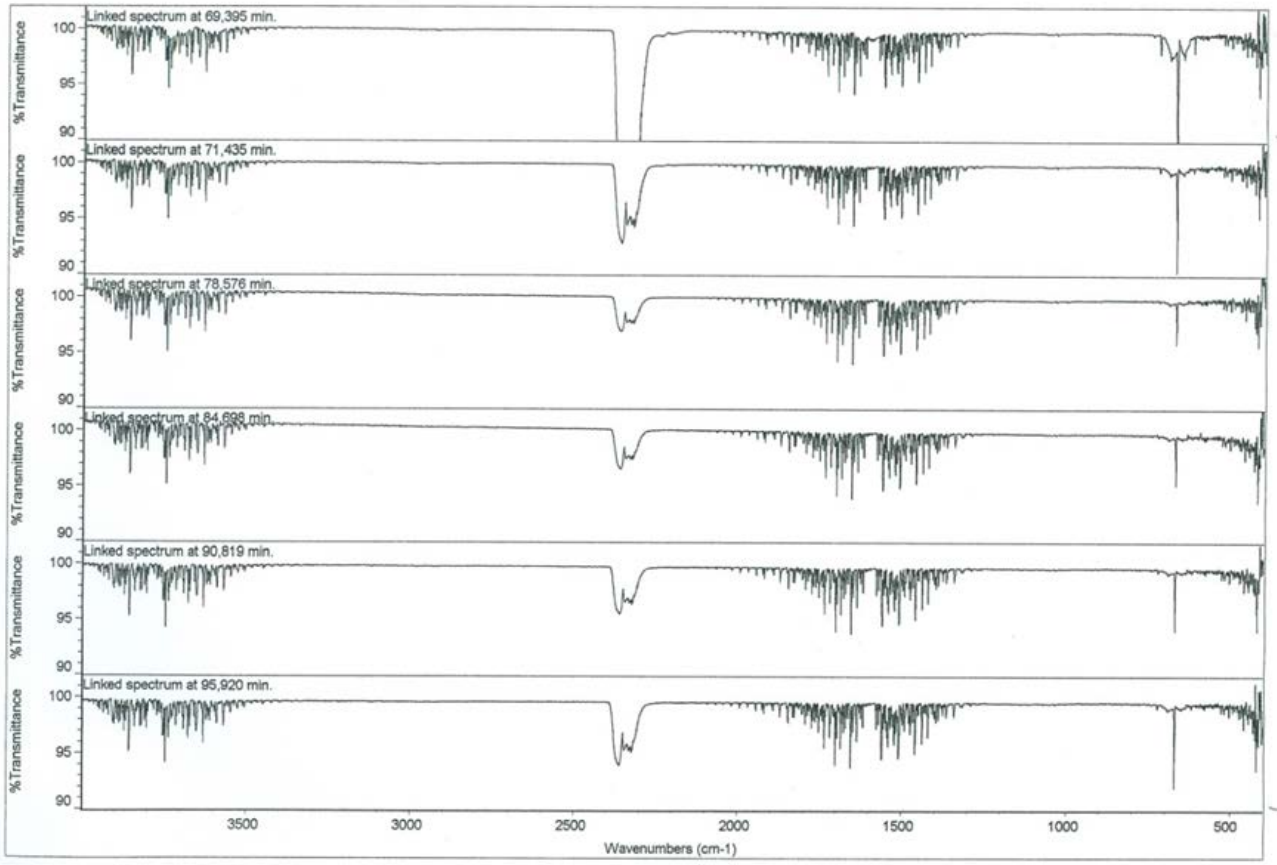



Linked spectrum at 33,686 min.
Linked spectrum at 35,727 min.
Linked spectrum at 37,768 min.
Linked spectrum at 39,809 min.
Linked spectrum at 41,849 min.
Linked spectrum at 43,890 min.
Linked spectrum at 45,930 min.
%Transmittance
Wavenumbers (cm-1)


Linked spectrum at 47,971 min.
Linked spectrum at 50,011 min.
Linked spectrum at 52,051 min.
Linked spectrum at 54,092 min.
Linked spectrum at 56,132 min.
%Transmittance
Wavenumbers (cm-1)


Linked spectrum at 58,172 min.
Linked spectrum at 60,213 min.
Linked spectrum at 63,274 min.
Linked spectrum at 65,314 min.
Linked spectrum at 67,354 min.
%Transmittance
100
95
90
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)

12


Linked spectrum at 69,395 min.
Linked spectrum at 71,435 min.
Linked spectrum at 78,576 min.
Linked spectrum at 84,698 min.
Linked spectrum at 90,819 min.
Linked spectrum at 95,920 min.
%Transmittance
100
95
90
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)

13

S4.7. Selected of four time-spaced IR spectra enhancing the production of methanol, during the step 3 (first two spectra) and the step 4 (the two below).

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