Supporting Information

Partial Decarboxylation of Hafnium Oxide Clusters for High Resolution Lithographic Applications

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KEYWORDS: Hexameric Hf oxide clusters, partially decarboxylation, photoresist, EUV lithography, line/space/edge character.

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Content:

1. Representative Synthetic procedures ---------- 1
2. ESI-Mass and thermogravimetric analysis datas ---------- 5
3. SEM images E-beam lithography patterns ---------- 7
4. SEM images EUV lithography patterns ---------- 9
5. X-ray crystallographic structures and data ----------13
6. Spectral data of key compounds ----------15
7. ^{1}H and ^{13}C NMR of key compounds ---------- 17

1. Representative synthetic procedures

Unless otherwise noted, all reactions were carried out under nitrogen atmosphere inoven-dried glassware using standard syringe, cannula and septa apparatus. Dichloromethane and toluene were dried over CaH_2 and distilled. Reagents were purchased from commercial sources and used without purification, unless otherwise stated. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker 400 MHz and Bruker 500 MHz spectrometers using chloroform-d ($CDCl_3$) as the internal standard. The ESI-Mass were perdormed using JEOL JMS-700. The EA analysis was performed by elementar vario EL cube. The TGA were performed using Mettler-Toledo 2-HT. FTIR Spectroscopy of power samples was in a Bruker Vertex 80v spectrometer. The AFM measurements were using SEIKO SPA-300HV. Electron-beam lithography was done by utilizing Elionix ELS-7800 with an accelerating voltage of 80 kV and a beam current of 200 pA. The EUV-IL system at the Swiss Light Sources (SLS), Paul Scherrer Institute, utilizes 13.5 nm EUV light. HRXPS measurements were performed in a ULVAC-PHI Quantera II, with a monochromatic Al Ka source (energy of 1486.7 eV).

2. ESI-Mass, TGA data and AFM of species 1-OH

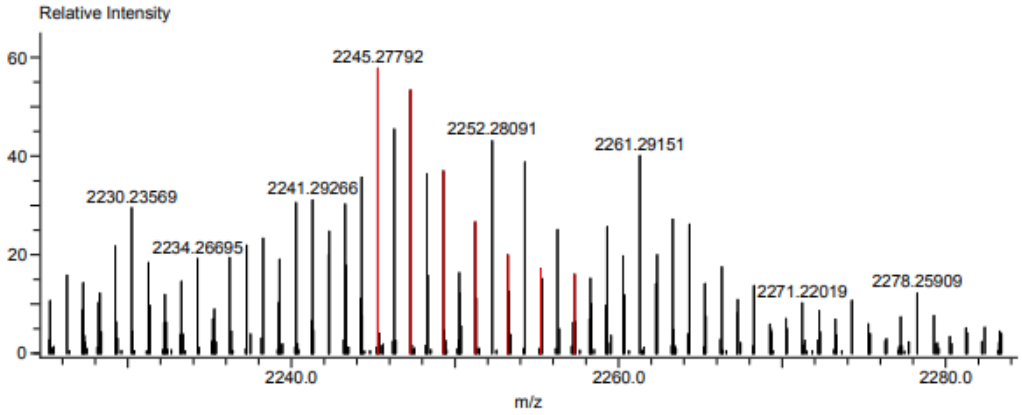
We attempted to conform the structure of partially decarboxylated sample **1-OH** with ESI-mass to confirm the formula $Hf_6O_4(OH)_6(i\text{-}C_4H_9CO_2)_{10.}$ We observed clusters of peaks due to six hafnium isotopes together with $[M+H]^+$ and $[M+2H]^{+2}$. We selected two major Hf isotopes ^{178}Hf (27%) and ^{180}Hf (35%), we were able to find seven fragments corresponding to $[M+H]^+$ which the exact mass between calculated and experimental data are well matched; see Figure S1. These are additional peaks that might be due to additional fragments of other Hf isotopes or different $[M+nH]^{+n}$ as 6-Hf clusters sometimes bear two or more protons because of the large sizes and more basic sites such as Hf-OH.

Apart from the fragments of $[M+H]^+$, and we are also able to find seven fragments corresponding to $[M+Na]^+$; the exact mass are calculated by two main Hf isotopes ^{178}Hf (27%) and ^{180}Hf (35%). As shown in Figure S-2, the calculated and the experimental values are well compatible. Additional peaks in Figure S2 is probably due to fragments of other Hf isotopes, or to different $[M+Na+H]^{+2}$ as 6-Hf clusters sometimes bear two or more protons because of the large sizes and more basic sites such as Hf-OH.

Data:2PC028 LiOH MeOH
Comment:
Description:
Ionization Mode:ESI+
History:Average(MS[1] 0.18..0.50)

Acquired:5/18/2022 12:01:52 PM
Operator:AccuTOF
m/z Calibration File:20220518 TFANa_...
Created:6/8/2022 3:51:56 PM
Created by:AccuTOF

Charge number:1 Tolerance:300.00[ppm], 250.00 .. 250.... Unsaturation Number:-100.0 .. 200.0 (...
Element:^{12}C:50 .. 50, ^{1}H:97 .. 97, ^{178}Hf:0 .. 6, ^{180}Hf:1 .. 6, ^{23}Na:0 .. 1, ^{16}O:30 .. 30



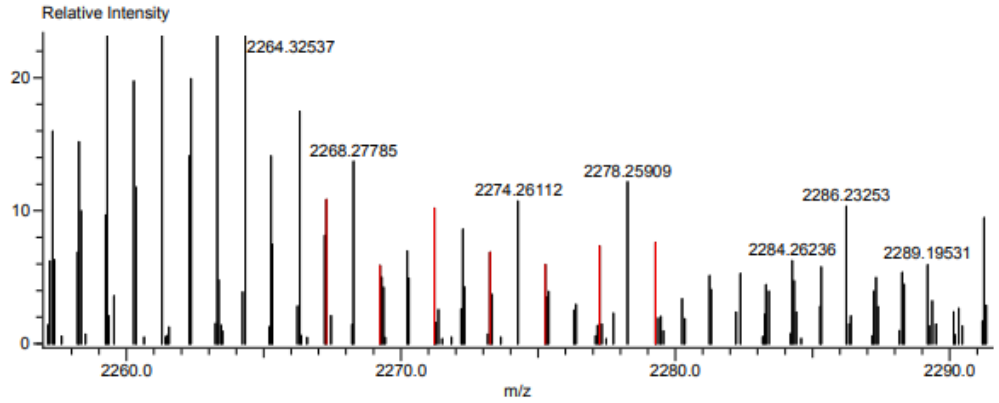
Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula
2245.27792	2184.53				
2247.28242	2018.18	2247.27150	10.92	4.86	$^{12}C_{50}{}^{1}H_{97}{}^{178}Hf_5{}^{180}Hf_1{}^{16}O_{30}$
2249.29040	1396.37	2249.27435	16.05	7.13	$^{12}C_{50}{}^{1}H_{97}{}^{178}Hf_4{}^{180}Hf_2{}^{16}O_{30}$
2251.24141	1005.19	2251.27720	-35.80	-15.90	$^{12}C_{50}{}^{1}H_{97}{}^{178}Hf_3{}^{180}Hf_3{}^{16}O_{30}$
2253.22847	751.38	2253.28005	-51.59	-22.89	$^{12}C_{50}{}^{1}H_{97}{}^{178}Hf_2{}^{180}Hf_4{}^{16}O_{30}$
2255.24941	646.32	2255.28291	-33.49	-14.85	$^{12}C_{50}{}^{1}H_{97}{}^{178}Hf_1{}^{180}Hf_5{}^{16}O_{30}$
2257.31199	604.00	2257.28576	26.24	11.62	$^{12}C_{50}{}^{1}H_{97}{}^{180}Hf_6{}^{16}O_{30}$

Figure S1. ESI-Mass of species **1-OH** $[M+H]^+$.

Data:2PC028 LiOH MeOH
Comment:
Description:
Ionization Mode:ESI+
History:Average(MS[1] 0.18..0.50)

Acquired:5/18/2022 12:01:52 PM
Operator:AccuTOF
m/z Calibration File:20220518 TFANa_...
Created:6/8/2022 3:49:46 PM
Created by:AccuTOF

Charge number:1 Tolerance:300.00[ppm], 250.00 .. 250.... Unsaturation Number:-100.0 .. 200.0 (...
Element:^{12}C:50 .. 50, ^{1}H:96 .. 96, ^{178}Hf:0 .. 6, ^{180}Hf:1 .. 6, ^{23}Na:1 .. 1, ^{16}O:30 .. 30



Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula
2267.28408	409.52				
2269.24046	221.47	2269.25345	-12.99	-5.72	$^{12}C_{50}{}^{1}H_{96}{}^{178}Hf_{5}{}^{180}Hf_{1}{}^{23}Na_{1}{}^{16}O_{30}$
2271.22019	384.97	2271.25630	-36.11	-15.90	$^{12}C_{50}{}^{1}H_{96}{}^{178}Hf_{4}{}^{180}Hf_{2}{}^{23}Na_{1}{}^{16}O_{30}$
2273.25093	259.39	2273.25915	-8.22	-3.62	$^{12}C_{50}{}^{1}H_{96}{}^{178}Hf_{3}{}^{180}Hf_{3}{}^{23}Na_{1}{}^{16}O_{30}$
2275.25915	224.25	2275.26200	-2.85	-1.25	$^{12}C_{50}{}^{1}H_{96}{}^{178}Hf_{2}{}^{180}Hf_{4}{}^{23}Na_{1}{}^{16}O_{30}$
2277.24485	277.36	2277.26485	-20.00	-8.78	$^{12}C_{50}{}^{1}H_{96}{}^{178}Hf_{1}{}^{180}Hf_{5}{}^{23}Na_{1}{}^{16}O_{30}$
2279.27785	287.47	2279.26770	10.15	4.45	$^{12}C_{50}{}^{1}H_{96}{}^{180}Hf_{6}{}^{23}Na_{1}{}^{16}O_{30}$

Figure S2. ESI-Mass of species 1-OH $[M+Na]^{+}$.

We employed TGA to see their calibration with formula. In the case of acid-containing 1, we obtained residual weight ca. 50%; the theoretical value of HfO_2 formation is 46% based on the formula from the x-ray diffraction; the discrepancy is 4%. For partially decarboxylated **1-OH**, the residual weight is 58% whereas the theoretical value is found to be 56% based on our proposed formula $Hf_6O_4(OH)_6(i\text{-}C_4H_9CO_2)_{10}$.

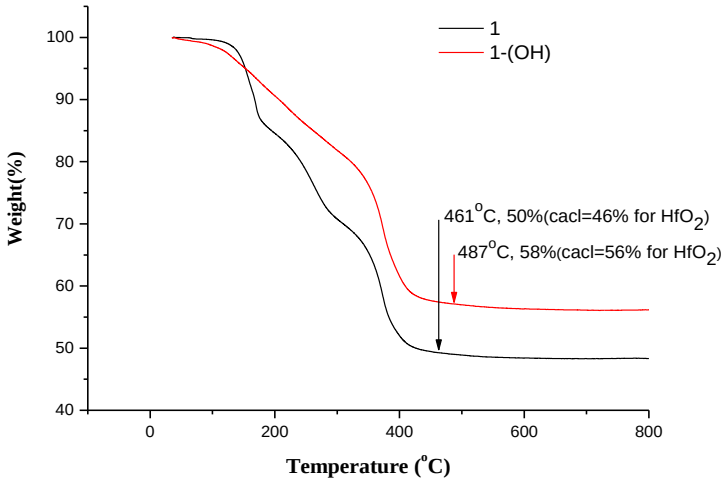


Fig. S3. TGA of species 1 and 1-OH

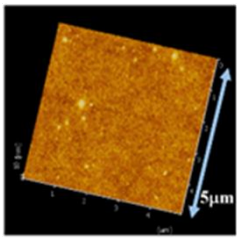
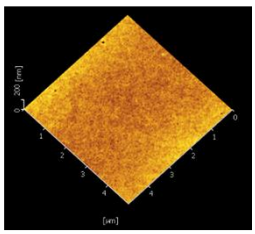
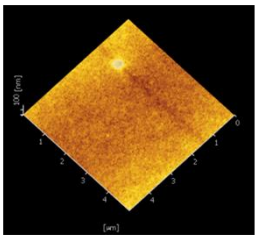
Days	1	3	7
AFM			
	RMS roughness = 0.85 nm	RMS roughness = 0.74 nm	RMS roughness = 1.06 nm

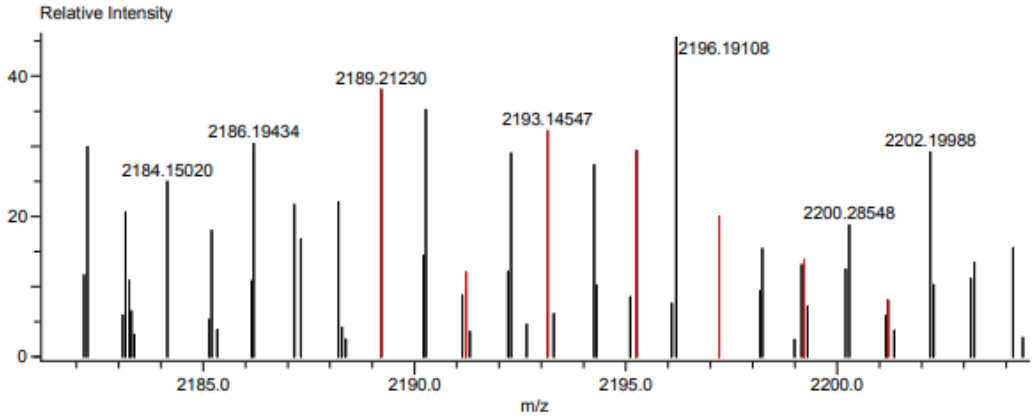
Fig. S4. AFM of species **1-OH** at different days after soft backing

2. ESI-Mass and TGA data of species 2-OH

Data:2PC023 LiOH ACN
Comment:
Description:
Ionization Mode:ESI+
History:Average(MS[1] 0.20..0.29)

Acquired:5/18/2022 12:30:41 PM
Operator:AccuTOF
m/z Calibration File:20220518 TFANa_...
Created:6/7/2022 4:50:48 PM
Created by:

Charge number:1 Tolerance:300.00[ppm], 250.00 .. 250.... Unsaturation Number:-100.0 .. 200.0 (...
Element:^{12}C:46 .. 46, ^{1}H:89 .. 89, ^{178}Hf:0 .. 6, ^{180}Hf:1 .. 6, ^{23}Na:0 .. 1, ^{16}O:30 .. 30



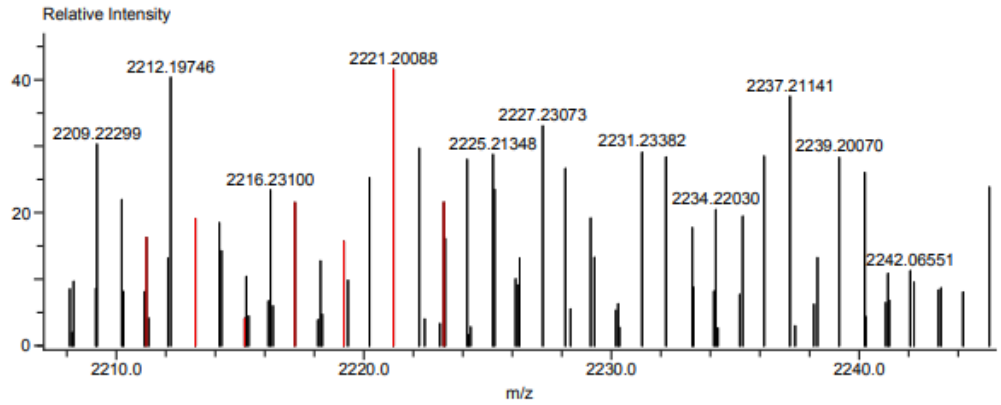
Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula
2189.21230	1020.22				
2191.21754	322.37	2191.20890	8.64	3.94	$^{12}C_{46}{}^{1}H_{89}{}^{178}Hf_{5}{}^{180}Hf_{1}{}^{16}O_{30}$
2193.14547	862.15	2193.21175	-66.29	-30.22	$^{12}C_{46}{}^{1}H_{89}{}^{178}Hf_{4}{}^{180}Hf_{2}{}^{16}O_{30}$
2195.24768	787.31	2195.21460	33.08	15.07	$^{12}C_{46}{}^{1}H_{89}{}^{178}Hf_{3}{}^{180}Hf_{3}{}^{16}O_{30}$
2197.21042	533.32	2197.21745	-7.03	-3.20	$^{12}C_{46}{}^{1}H_{89}{}^{178}Hf_{2}{}^{180}Hf_{4}{}^{16}O_{30}$
2199.22067	369.45	2199.22031	0.37	0.17	$^{12}C_{46}{}^{1}H_{89}{}^{178}Hf_{1}{}^{180}Hf_{5}{}^{16}O_{30}$
2201.20209	215.29	2201.22316	-21.07	-9.57	$^{12}C_{46}{}^{1}H_{89}{}^{180}Hf_{6}{}^{16}O_{30}$

Figure S5. ESI-Mass of species 2-OH $[M+H]^{+}$.

Data:2PC023 LiOH ACN
Comment:
Description:
Ionization Mode:ESI+
History:Average(MS[1] 0.20..0.29)

Acquired:5/18/2022 12:30:41 PM
Operator:AccuTOF
m/z Calibration File:20220518 TFANa_...
Created:6/7/2022 4:53:31 PM
Created by:

Charge number:1 Tolerance:300.00[ppm], 250.00 .. 250.... Unsaturation Number:-100.0 .. 200.0 (...
Element:^{12}C:46 .. 46, ^{1}H:88 .. 88, ^{178}Hf:0 .. 6, ^{180}Hf:1 .. 6, ^{23}Na:1 .. 1, ^{16}O:30 .. 30



Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula
2211.22533	435.21				
2213.19557	510.75	2213.19085	4.72	2.13	$^{12}C_{46}{}^{1}H_{88}{}^{178}Hf_{5}{}^{180}Hf_{1}{}^{23}Na_{1}{}^{16}O_{30}$
2215.18849	108.95	2215.19370	-5.21	-2.35	$^{12}C_{46}{}^{1}H_{88}{}^{178}Hf_{4}{}^{180}Hf_{2}{}^{23}Na_{1}{}^{16}O_{30}$
2217.21910	575.67	2217.19655	22.56	10.17	$^{12}C_{46}{}^{1}H_{88}{}^{178}Hf_{3}{}^{180}Hf_{3}{}^{23}Na_{1}{}^{16}O_{30}$
2219.19506	419.93	2219.19940	-4.33	-1.95	$^{12}C_{46}{}^{1}H_{88}{}^{178}Hf_{2}{}^{180}Hf_{4}{}^{23}Na_{1}{}^{16}O_{30}$
2221.20088	1113.12	2221.20225	-1.37	-0.62	$^{12}C_{46}{}^{1}H_{88}{}^{178}Hf_{1}{}^{180}Hf_{5}{}^{23}Na_{1}{}^{16}O_{30}$
2223.23436	577.78	2223.20510	29.26	13.16	$^{12}C_{46}{}^{1}H_{88}{}^{180}Hf_{6}{}^{23}Na_{1}{}^{16}O_{30}$

Figure S6. ESI-Mass of species 2-OH $[M+Na]^{+}$.

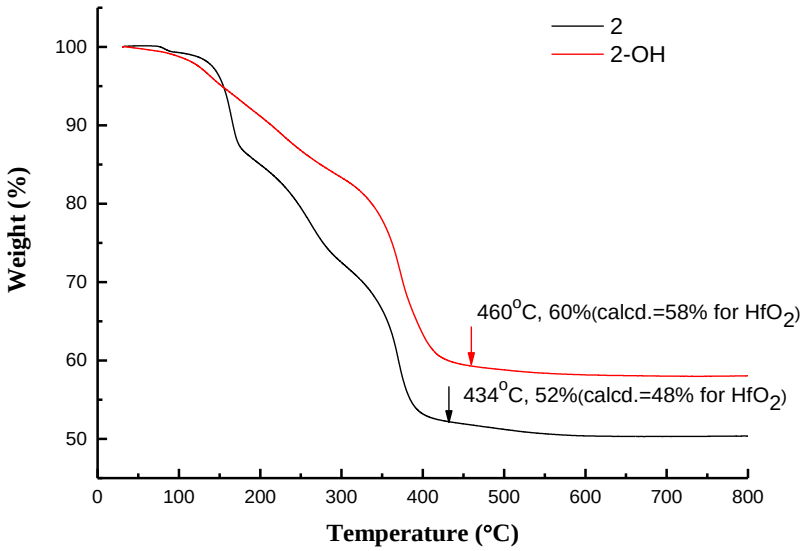


Figure S7. TGA of species 2 and 2-OH.

3. SEM image of E-beam lithography patterns

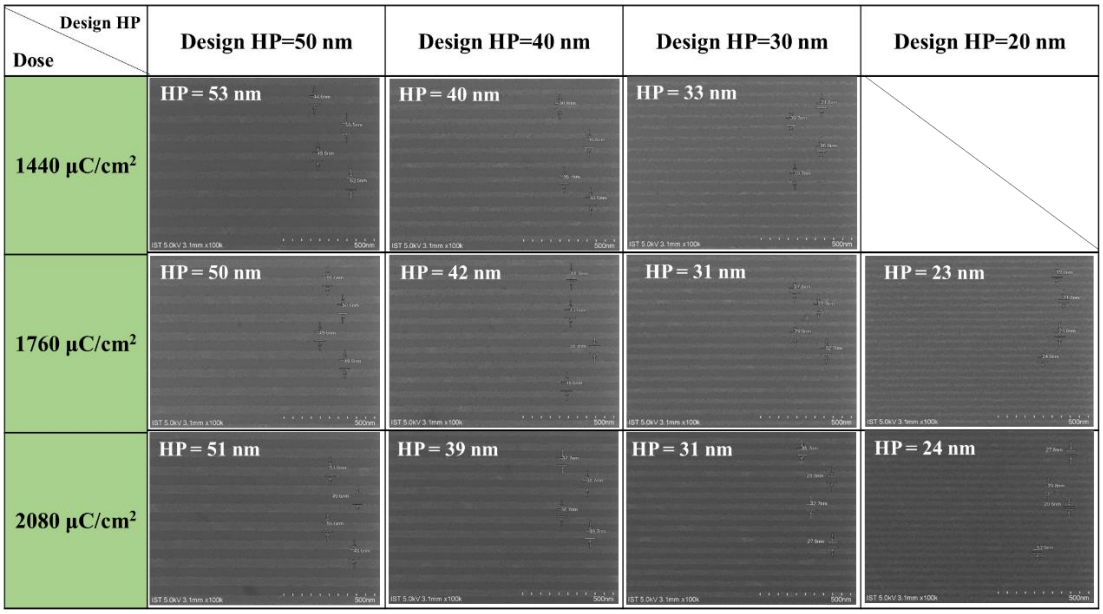


Figure S8. SEM images of E-beam lithography patterns on 1. Process parameter: 1.5 wt%, THK= 24 nm, Developer: 2-Heptanone : Hexane = 1 : 1 60 s, PEB= 80℃ 60 s

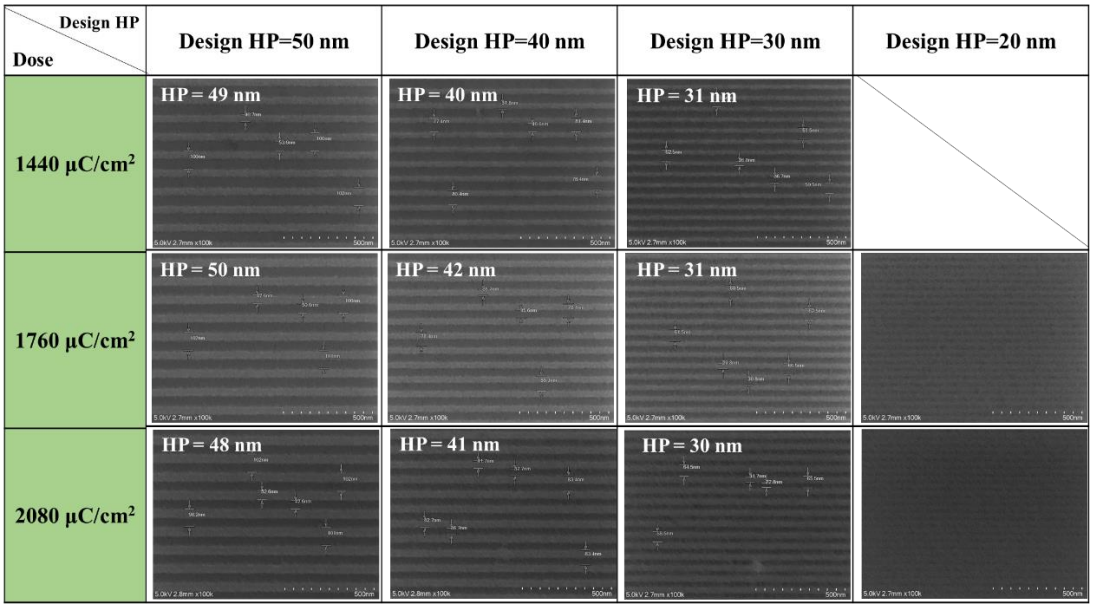


Figure S9. SEM images of E-beam lithography patterns on 1-(OH). Process parameter: 2.0 wt%, THK= 23 nm, Developer: 2-Heptanone : Hexane = 1 : 1 80 s, PEB= 80℃, 60s

.

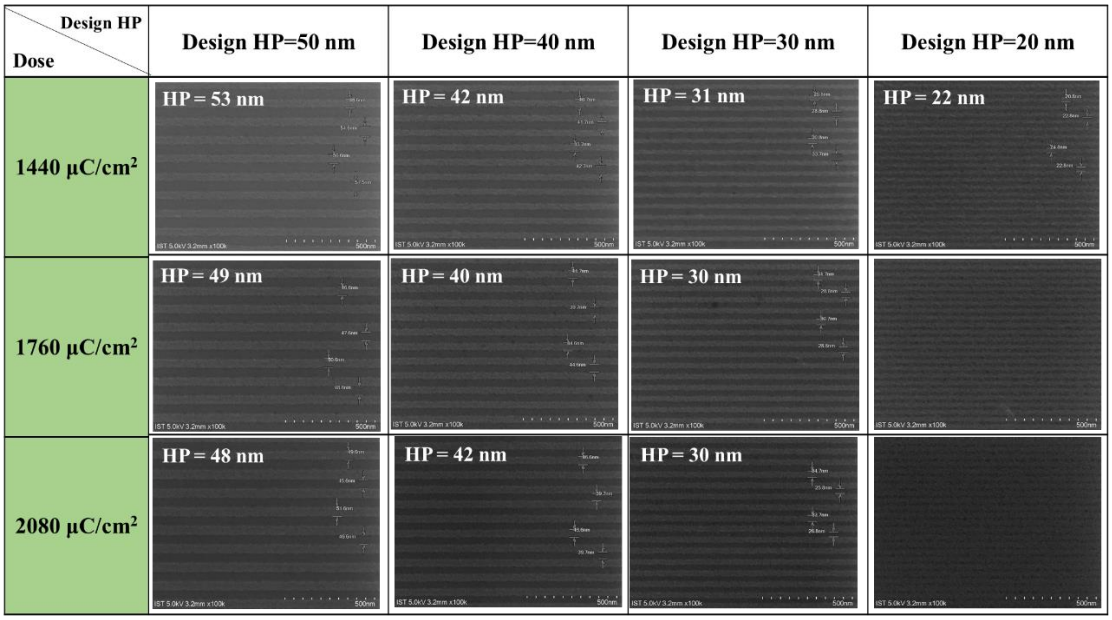


Figure S10. SEM images of E-beam lithography patterns on 2-(OH). Process parameter: 2.0 wt%, THK= 24 nm, Developer: 2-Heptanone : Hexane = 1 : 1 60 s, PEB= 80℃ 60 s

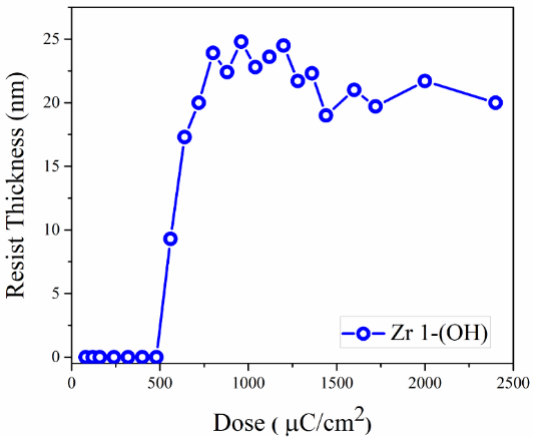


Figure S11. E-beam contrast curve of compound **Zr 1-(OH)** Intial thickness 30 nm..

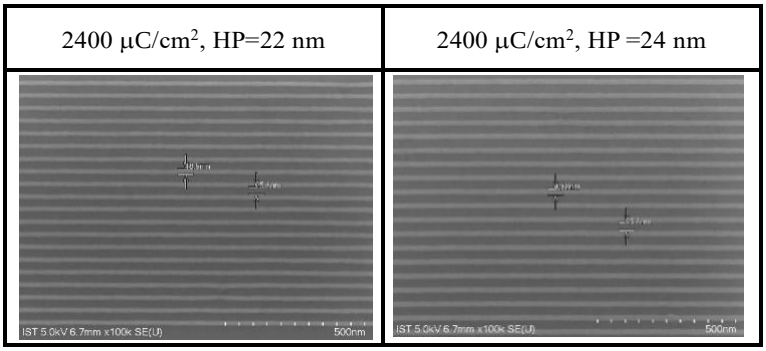


Figure S12. SEM images of E-beam lithography patterns on **Zr 1-(OH)**. Process parameter: 2.0 wt%, THK= 17 nm, Developer: 2-Heptanone : Hexane = 1 : 1 60 s, PEB= 80℃ 60 s

4. SEM image of EUV lithography patterns

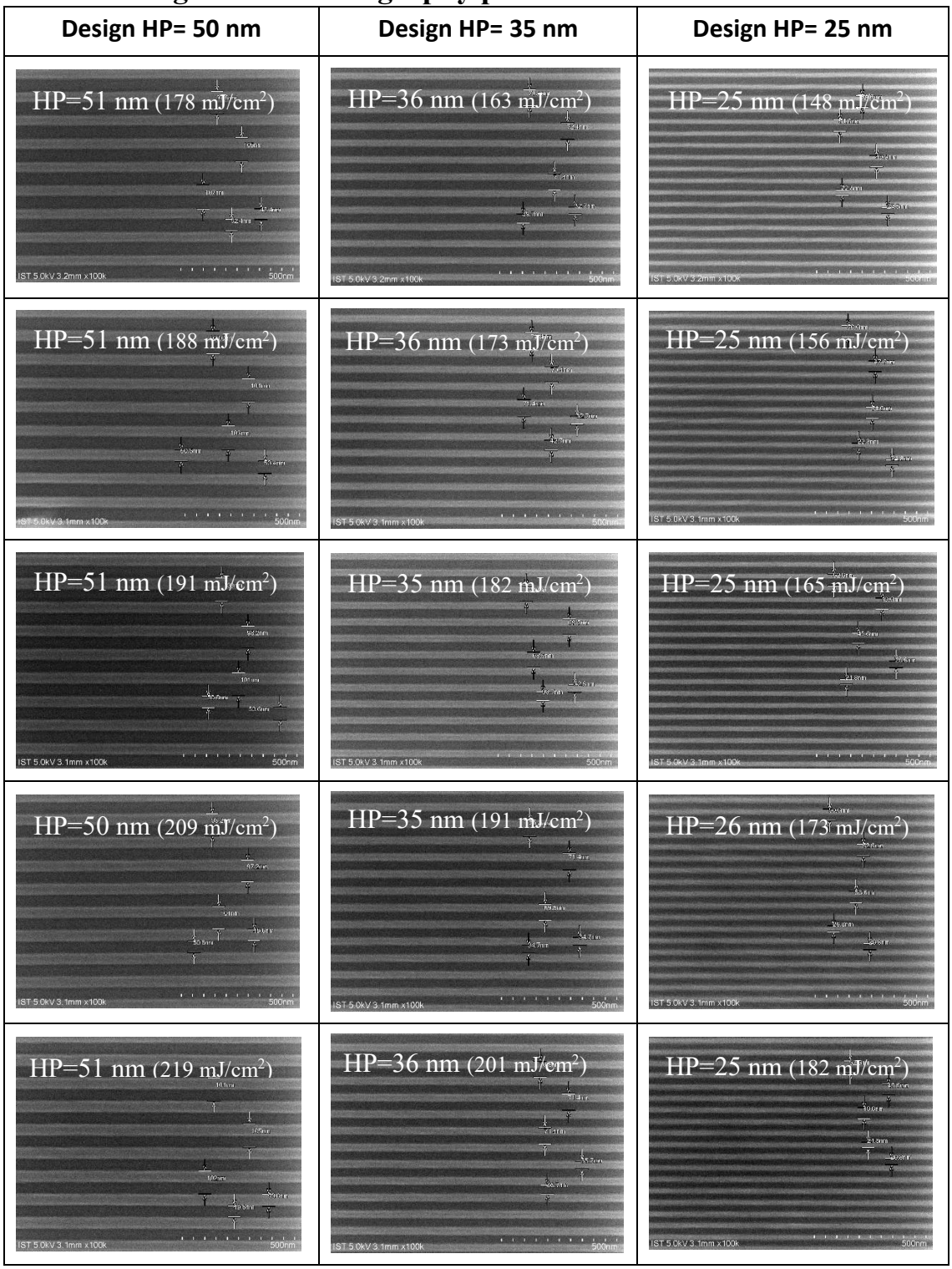


Figure S13. SEM images of EUV lithography patterns on 1-(OH) HP= 50, 35, 25 nm at different dose. Process parameter: 2.0 wt%, THK= 23 nm, Developer: 2-Heptanone : Hexane = 1 : 1 80 s, PEB= 80℃ 60 s

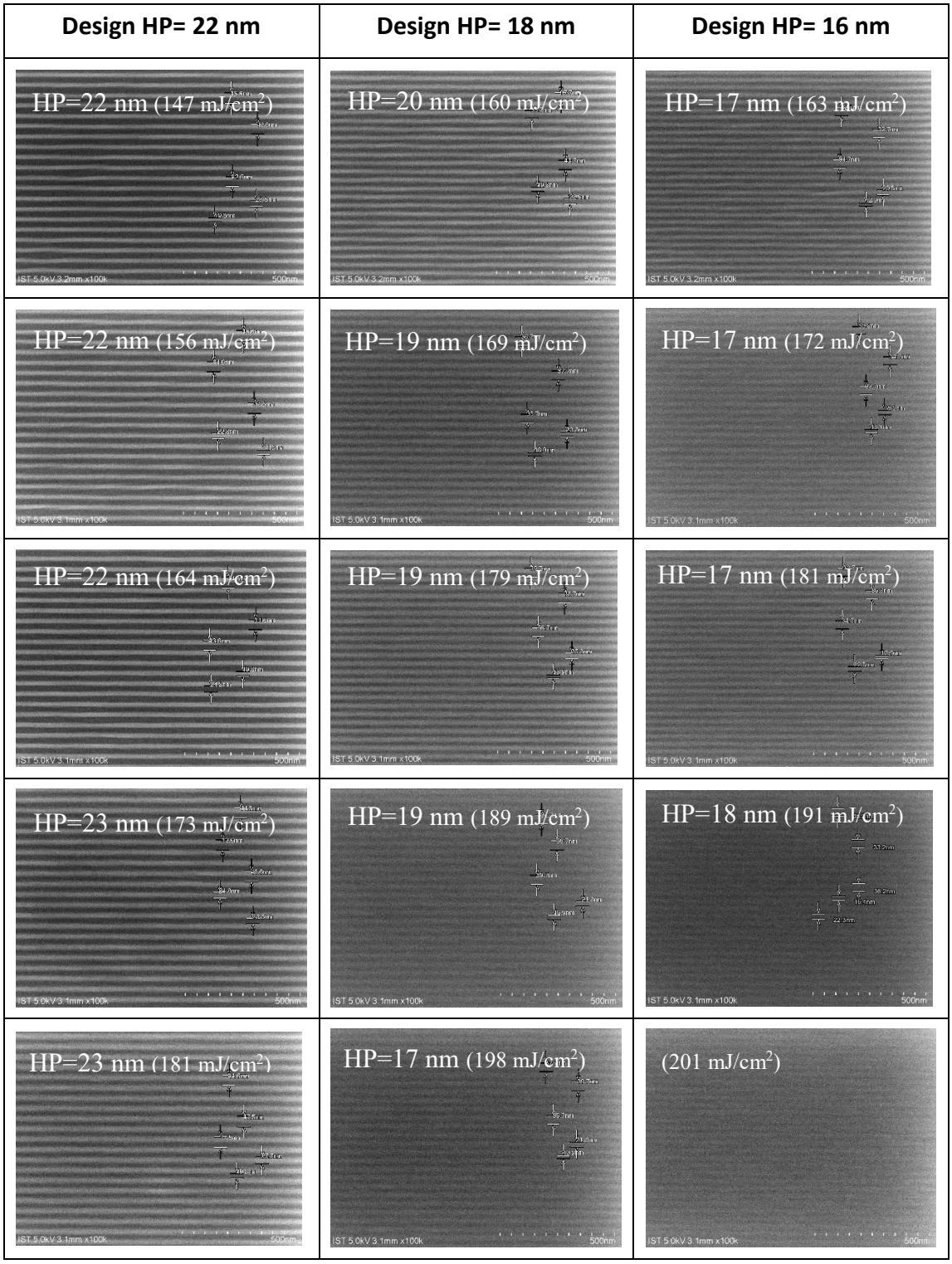


Figure S14. SEM images of EUV lithography patterns on 1-(OH) HP= 22, 18,16 nm at different dose. Process parameter: 2.0 wt%, THK= 23 nm, Developer: 2-Heptanone : Hexane = 1 : 1 80 s, PEB= 80℃ 60 s

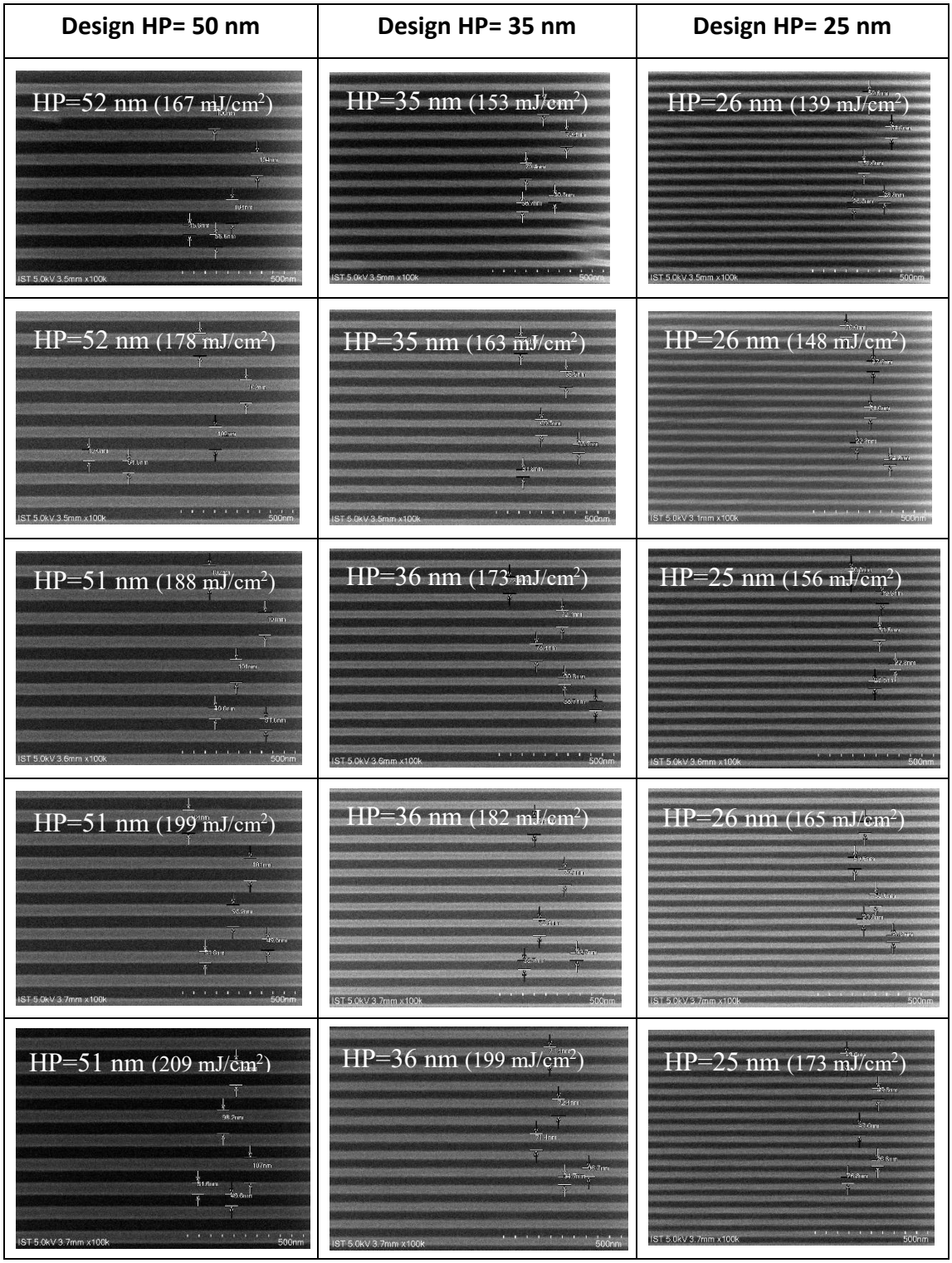


Figure S15. SEM images of EUV lithography patterns on **2-(OH)** HP= 50, 35, 25 nm at different dose. Process parameter: 2.0 wt%, THK= 24 nm, Developer: 2-Heptanone : Hexane = 1 : 1 60 s, PEB= 80℃ 60 s.

.

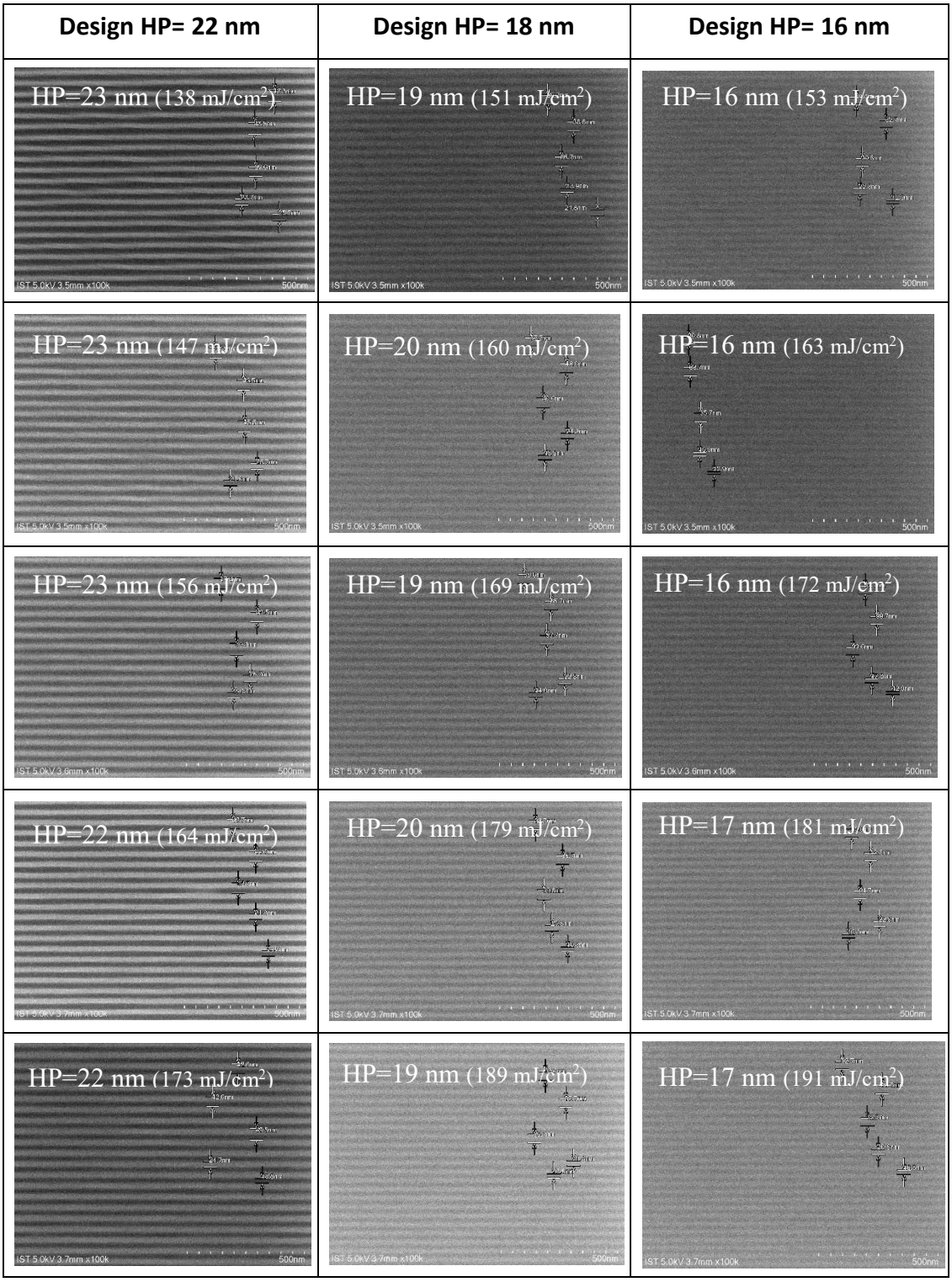
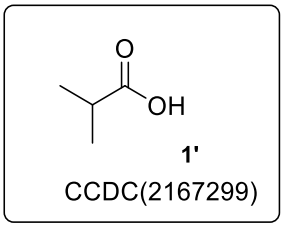


Figure S16. SEM images of EUV lithography patterns on 2-(OH) HP= 22, 18, 16 nm at different dose. Process parameter: 2.0 wt%, THK= 24 nm, Developer: 2-Heptanone : Hexane = 1 : 1 60 s, PEB= 80℃ 60 s.

5. X-ray crystallographic structures and data.

5.1 X-ray structure of isobutyrate derivative 1':



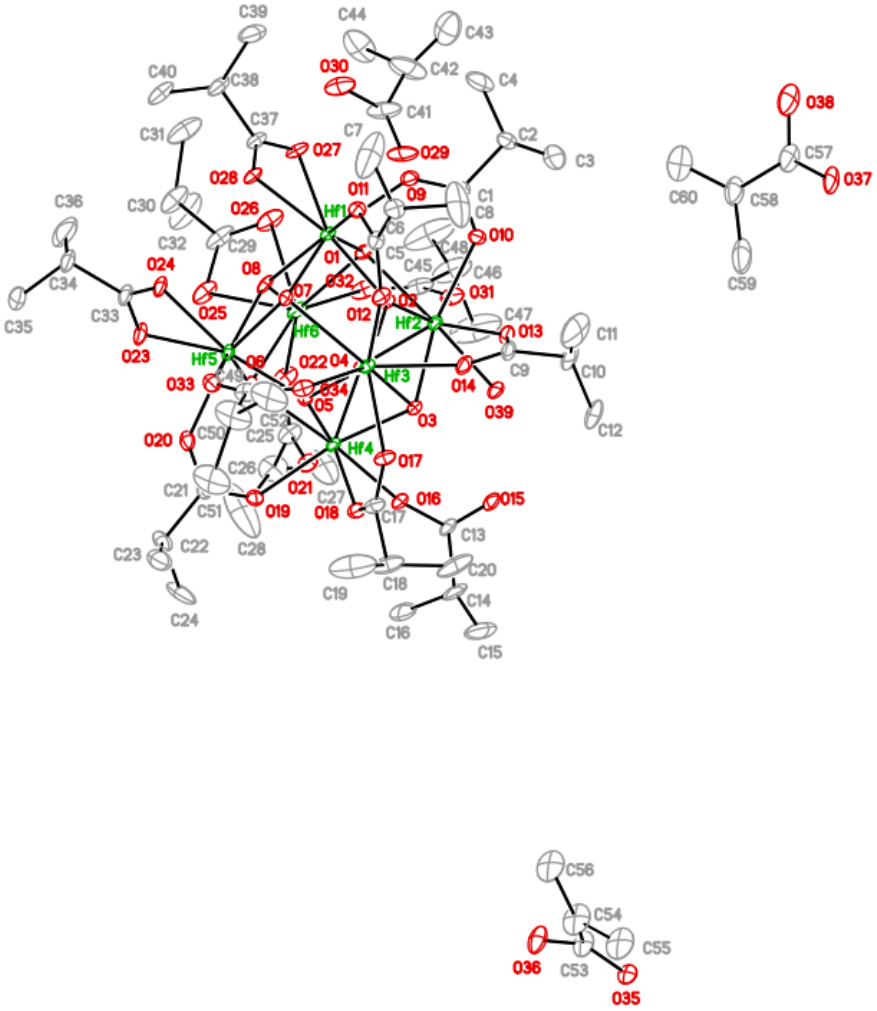


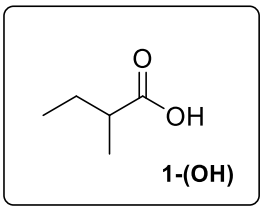
Table S1. Crystal data and structure refinement for mo_200723lt_0m_a.

Identification code	mo_200723LT_0m_a
Empirical formula	C60 H108 Hf6 O39
Formula weight	2524.40
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic

Space group	P-1	
Unit cell dimensions	a = 13.6866(9) Å	= 90.858(2)°.
	b = 14.8851(9) Å	= 97.847(2)°.
	c = 22.7136(14) Å	= 104.937(2)°.
Volume	4423.0(5) Å ^{3}	
Z	2	
Density (calculated)	1.895 Mg/m^3	
Absorption coefficient	7.091 mm^{-1}	
F(000)	2424	
Crystal size	0.15 x 0.15 x 0.14 mm^3	
Theta range for data collection	0.906 to 26.526°.	
Index ranges	-16<=h<=17, -18<=k<=18, -28<=l<=28	
Reflections collected	153604	
Independent reflections	18291 [R(int) = 0.0520]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.6769	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	18291 / 137 / 1036	
Goodness-of-fit on F^2	1.090	
Final R indices [I>2sigma(I)]	R1 = 0.0563, wR2 = 0.1338	
R indices (all data)	R1 = 0.0978, wR2 = 0.1739	
Extinction coefficient	n/a	
Largest diff. peak and hole	4.917 and -3.842 e.Å $^{-3}$	

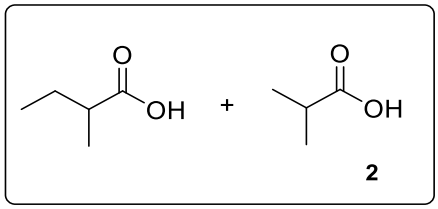
6. Spectral data of key compounds.

6.1 Spectral data for partially decarboxylated 6-Hafnium Cluster with 2-methylbutanoic acid ligand 1-(OH).



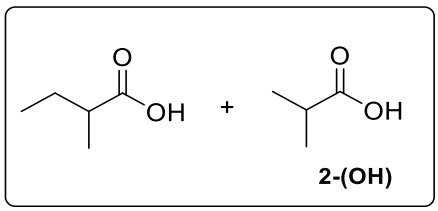
White solid (34%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.13 (s, 10H), 1.66 ~ 1.33 (m, 20H), 1.03 (s, 30H), 0.85 (s, 30H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 182.4, 42.8, 42.2, 26.6, 16.1, 11.9; EA Anal. Calcd. for $C_{50}H_{96}O_{30}Hf_6$: C: 26.71%; H: 4.30%, found: C: 26.50% ; H: 4.36%.

6.2 Spectral data for 6-Hafnium Cluster with 2-methylbutanoic acid and isobutyric acid ligand 2.



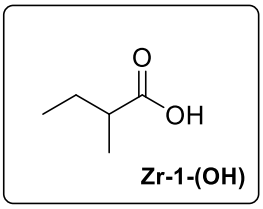
White solid (90%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.22 (s, 2H), 2.40 (s, 6H), 2.22-2.12 (m, 9H), 1.65-1.40 (m, 18H), 1.05 (s, 63H), 0.87 (s, 27H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 182.4, 42.8, 35.9, 26.6, 18.9, 16.1, 11.8; HRMS (ESI+, m/z) Calcd. for $C_{54}H_{103}O_{33}{}^{180}Hf_6$ $[M+H]^+$: 2359.32, found: 2359.27 ; EA Anal. Calcd. for $C_{69}H_{132}O_{39}Hf_6$: C: 31.19%, H: 5.01%, found: C: 30.86%, H: 4.86%.

6.3 Spectral data for partially decarboxylated 6-Hafnium Cluster with 2-methylbutanoic acid and isobutyric acid ligand 2-(OH).



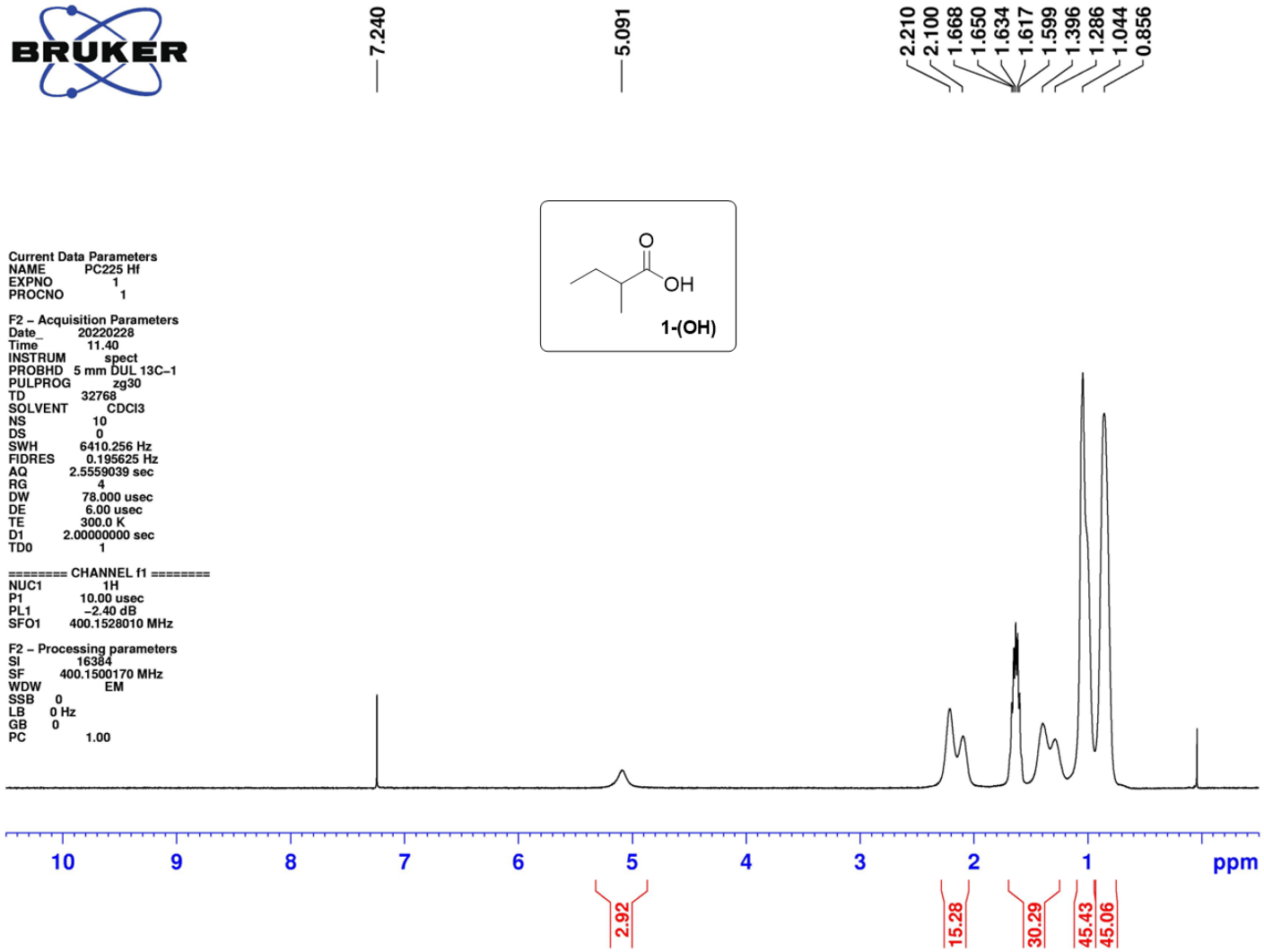
White solid (30%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.15 (s, 4H), 2.07 (s, 6H), 1.64-1.24 (m, 12H), 1.05 (s, 42H), 0.85 (s, 18H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 182.4, 42.8, 36.0, 35.5, 26.6, 19.0, 16.2, 11.9. EA Anal. Calcd. for $C_{46}H_{88}O_{30}Hf_6$: C: 25.20%, H: 4.05%, found: C: 25.17%, H: 4.36%.

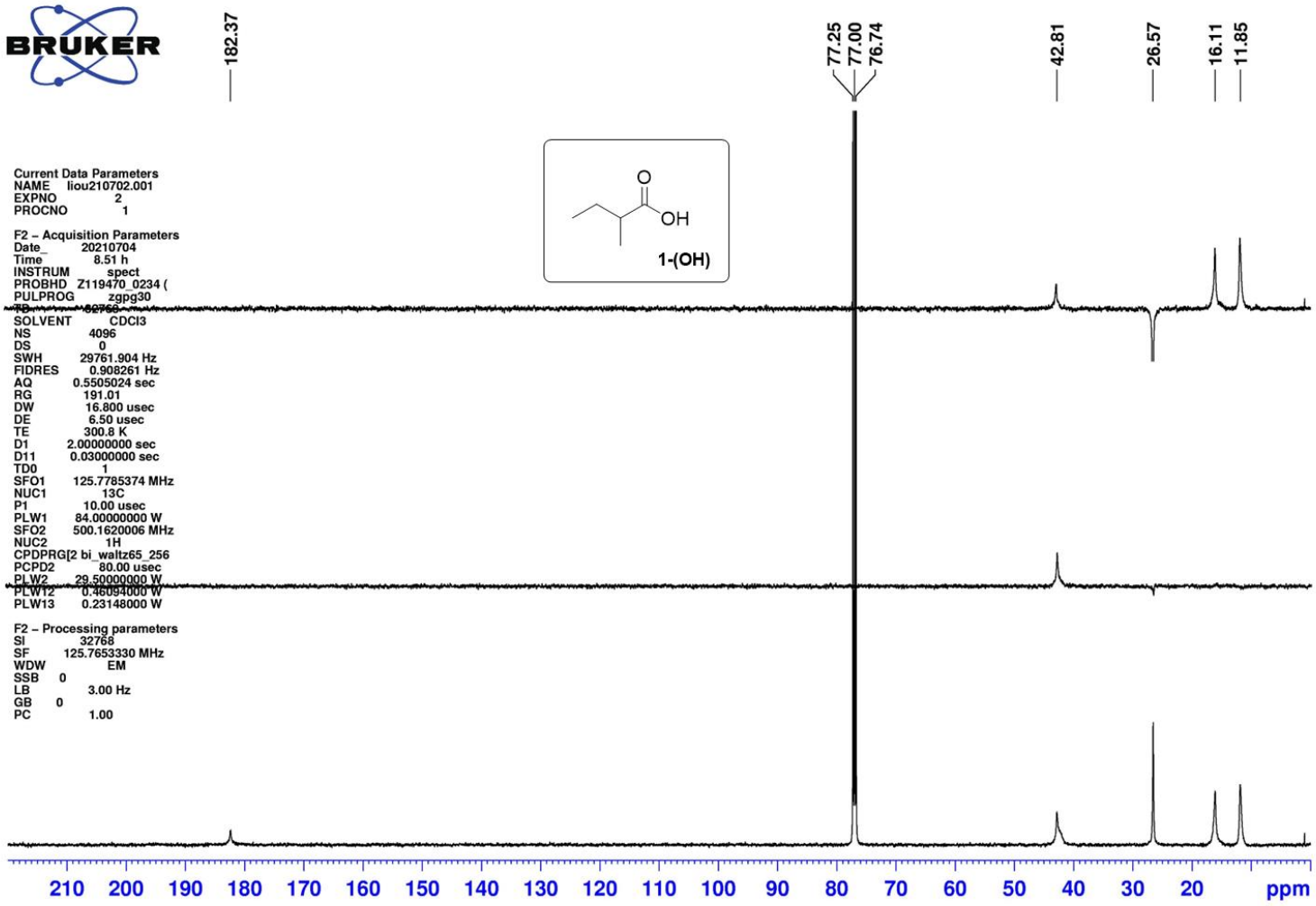
6.4 Spectral data for partially decarboxylated 12-Zirconium Cluster with 2-methylbutanoic acid ligand Zr-1-OH.



White solid; ^{1}H NMR (400 MHz, CDCl3): δ2.13(s, 18H), 1.63(s, 18H), 1.32(s, 18H), 1.02,(d, J = 5.6 Hz, 54H), 0.84(s, 54H); ^{13}C NMR (100 MHz, CDCl3): δ182.6, 42.6, 26.7, 16.2, 12.0,; HRMS(ESI, m/z) Calcd. for $C_{90}H_{177}O_{58}Zr_{12}$ [M+H]+ : 3264.95, found: 3264.92; EA Calc. for $C_{90}H_{177}O_{58}Zr_{12}$: C: 32.95%, H: 5.41%, found: C: 33.64%, H: 5.62%.

7. ^{1}H and ^{13}C NMR of key compounds

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77.25
77.00
76.74
42.81
26.57
16.11
11.85
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PROCNO 1
F2 – Acquisition Parameters
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Time 8.51 h
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PULPROG zgpg30
TD 32768
SOLVENT CDCl3
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DS 0
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505024 sec
RG 191.01
DW 16.800 usec
DE 6.50 usec
TE 300.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7785374 MHz
NUC1 13C
P1 10.00 usec
PLW1 84.00000000 W
SFO2 500.1620006 MHz
NUC2 1H
CPDPRG[2 bi_waltz65_256
PCPD2 80.00 usec
PLW2 29.50000000 W
PLW12 0.46094000 W
PLW13 0.23148000 W
F2 – Processing parameters
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SF 125.7653330 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
OH
1-(OH)
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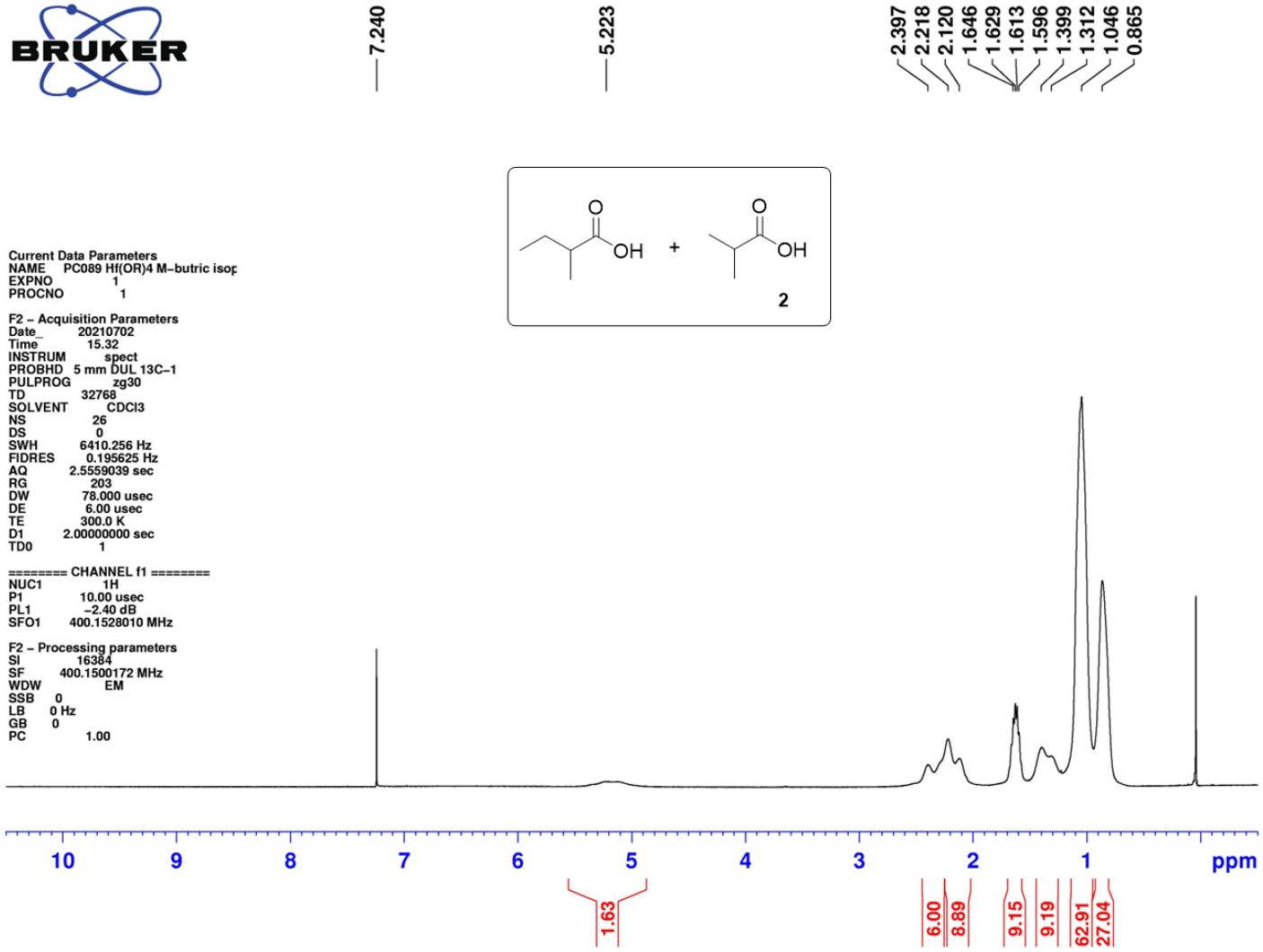
7.240
5.223
2.397
2.218
2.120
1.646
1.629
1.613
1.596
1.399
1.312
1.046
0.865
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PROCNO 1
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TD 32768
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SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559039 sec
RG 203
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
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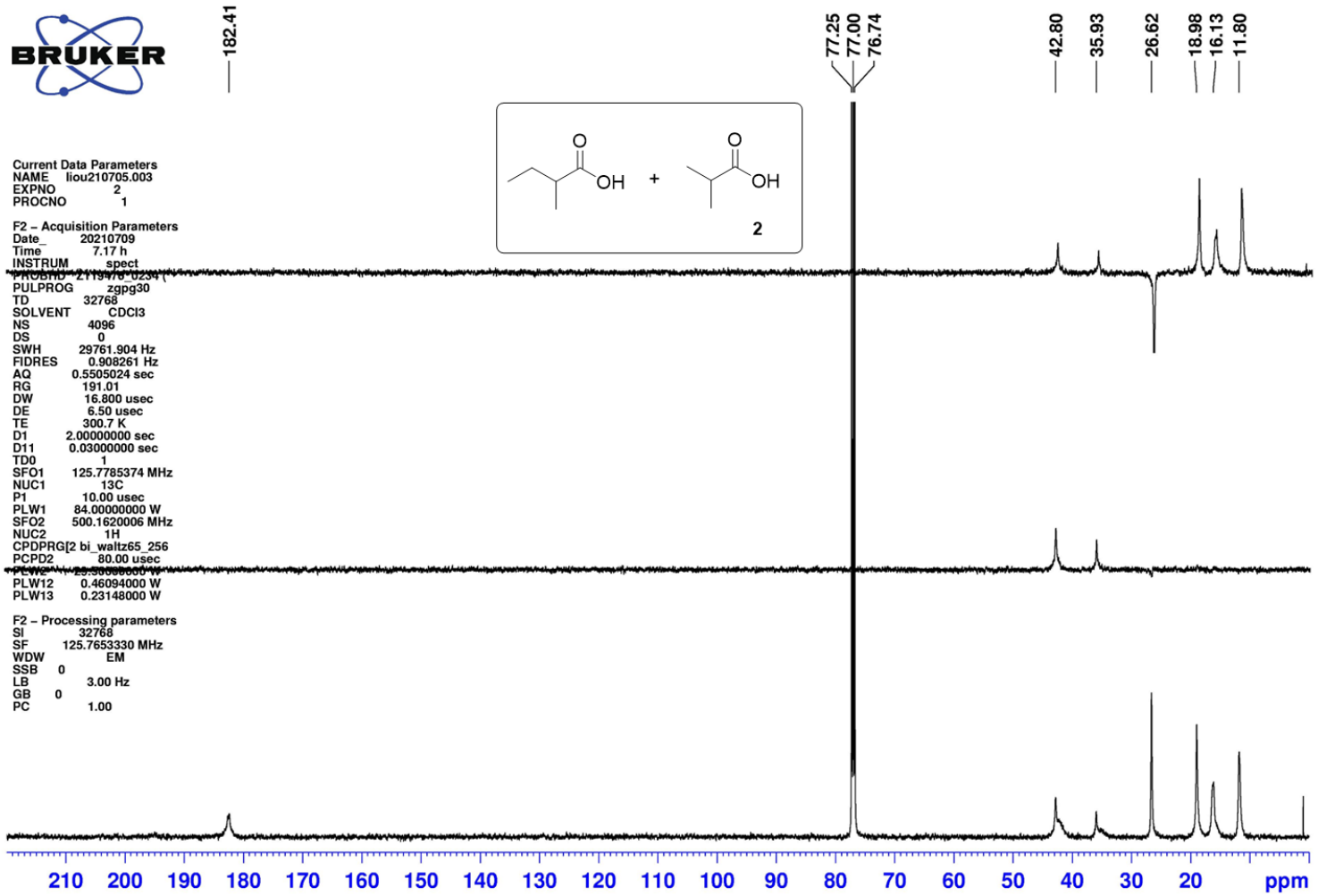
P1 10.00 usec
PL1 –2.40 dB
SFO1 400.1528010 MHz
F2 – Processing parameters
SI 16384
SF 400.1500172 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
O
OH
+
O
OH
2
10
9
8
7
6
5
4
3
2
1
ppm
1.63
6.00
8.89
9.15
9.19
62.91
27.04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76.74
42.80
35.93
26.62
18.98
16.13
11.80
OH
OH
2
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EXPNO 2
PROCNO 1
F2 – Acquisition Parameters
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Time 7.17 h
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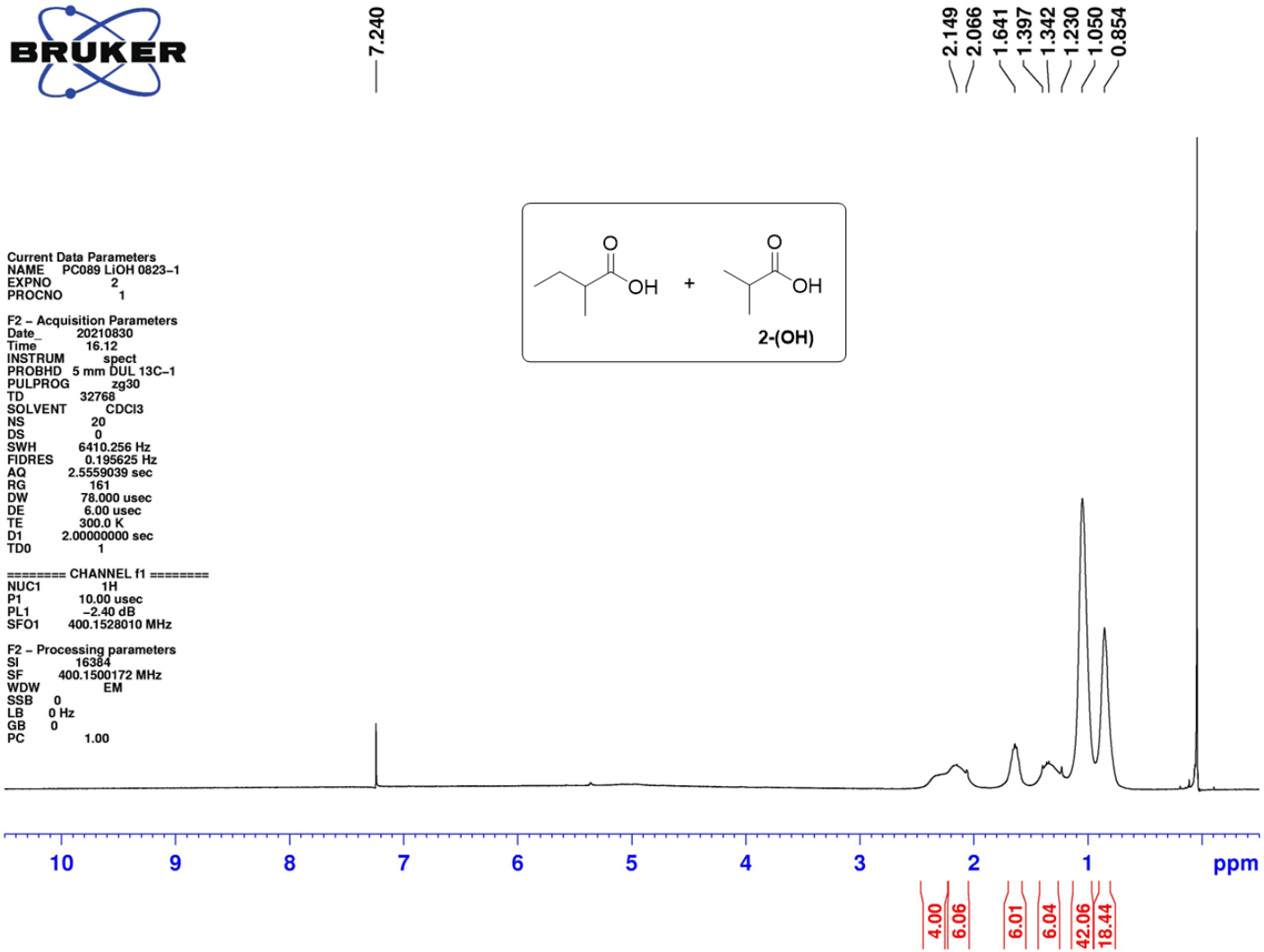
TD 32768
SOLVENT CDCl3
NS 4096
DS 0
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505024 sec
RG 191.01
DW 16.800 usec
DE 6.50 usec
TE 300.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7785374 MHz
NUC1 13C
P1 10.00 usec
PLW1 84.00000000 W
SFO2 500.1620006 MHz
NUC2 1H
CPDPRG[2 bi_waltz65_256
PCPD2 80.00 usec
PLW12 0.46094000 W
PLW13 0.23148000 W
F2 – Processing parameters
SI 32768
SF 125.7653330 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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2.066
1.641
1.397
1.342
1.230
1.050
0.854
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EXPNO 2
PROCNO 1
F2 – Acquisition Parameters
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PULPROG zg30
TD 32768
SOLVENT CDCl3
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SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559039 sec
RG 161
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
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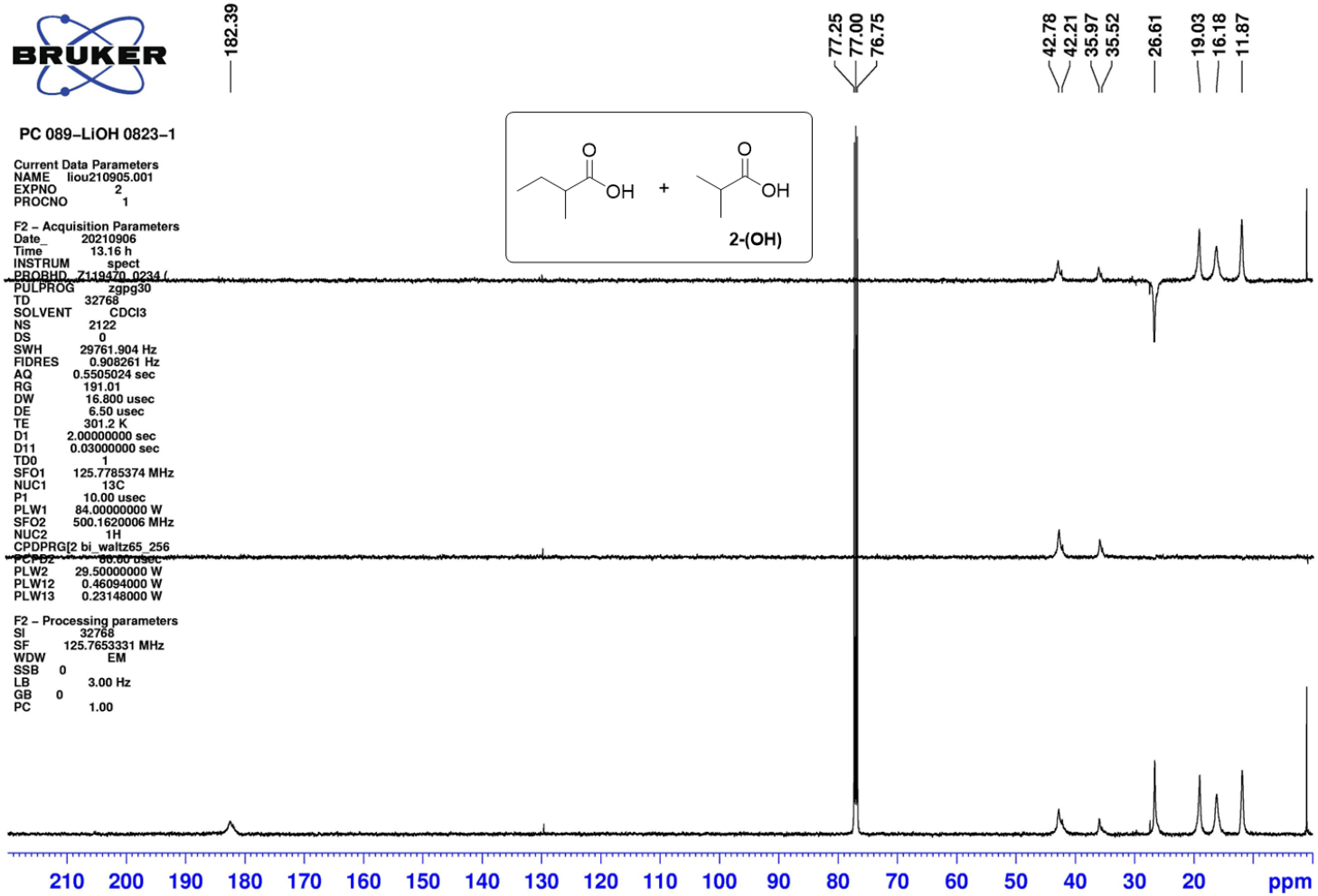
P1 10.00 usec
PL1 –2.40 dB
SFO1 400.1528010 MHz
F2 – Processing parameters
SI 16384
SF 400.1500172 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
OH
+
OH
2-(OH)
10
9
8
7
6
5
4
3
2
1
ppm
4.00
6.06
6.01
6.04
42.06
18.44


182.39
77.25
77.00
76.75
42.78
42.21
35.97
35.52
26.61
19.03
16.18
11.87
PC 089–LiOH 0823–1
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EXPNO 2
PROCNO 1
F2 – Acquisition Parameters
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Time 13.16 h
INSTRUM spect
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2122
DS 0
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505024 sec
RG 191.01
DW 16.800 usec
DE 6.50 usec
TE 301.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7785374 MHz
NUC1 13C
P1 10.00 usec
PLW1 84.00000000 W
SFO2 500.1620006 MHz
NUC2 1H
CPDPRG[2 bi_waltz65_256
PCPD2 80.00 usec
PLW2 29.50000000 W
PLW12 0.46094000 W
PLW13 0.23148000 W
F2 – Processing parameters
SI 32768
SF 125.7653331 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OH
OH
2-(OH)
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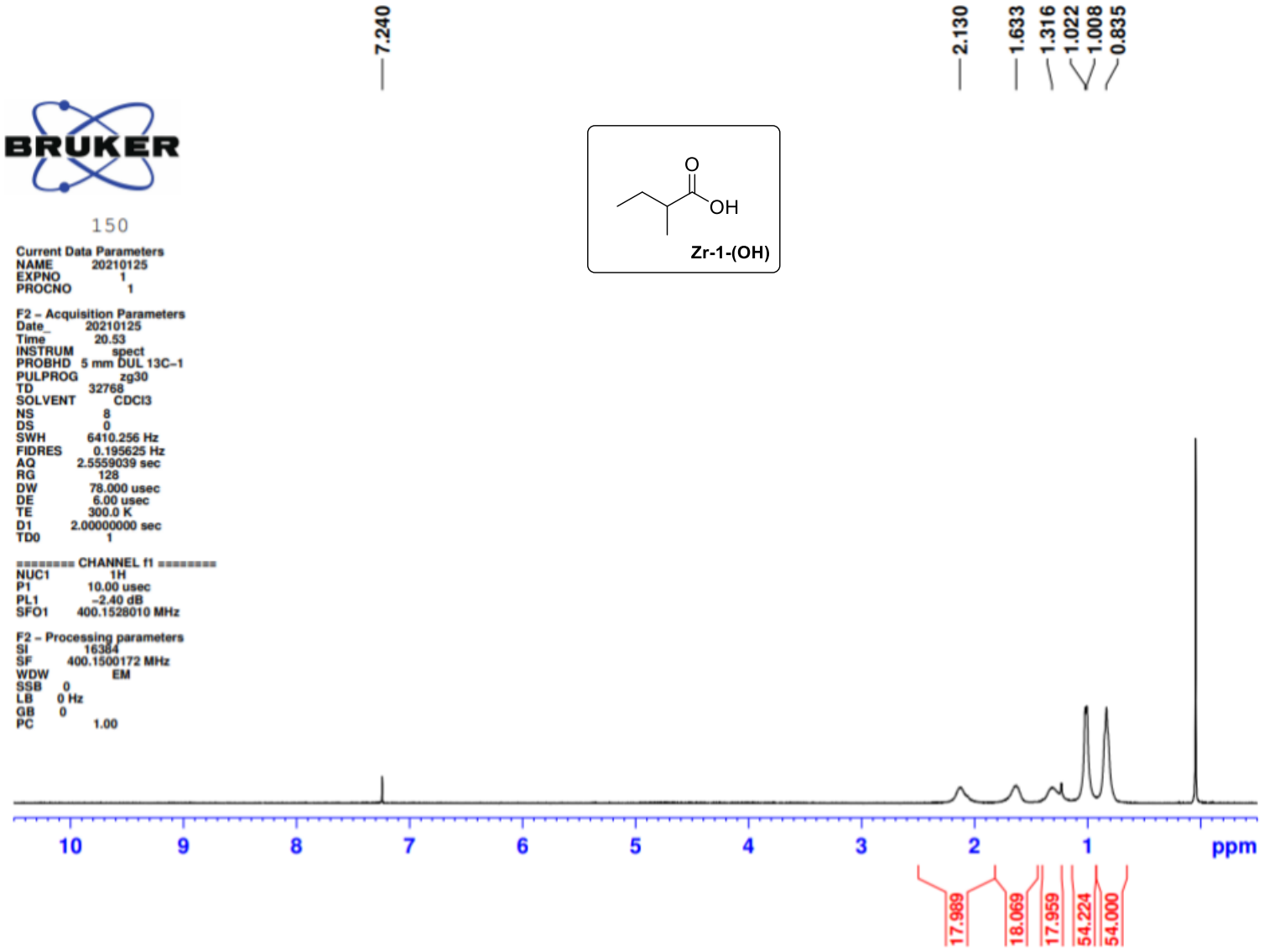
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2.130
1.633
1.316
1.022
1.008
0.835
O
OH
Zr-1-(OH)
150
Current Data Parameters
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EXPNO 1
PROCNO 1
F2 – Acquisition Parameters
Date_ 20210125
Time 20.53
INSTRUM spect
PROBHD 5 mm DUL 13C–1
PULPROG zg30
TD 32768
SOLVENT CDCl3
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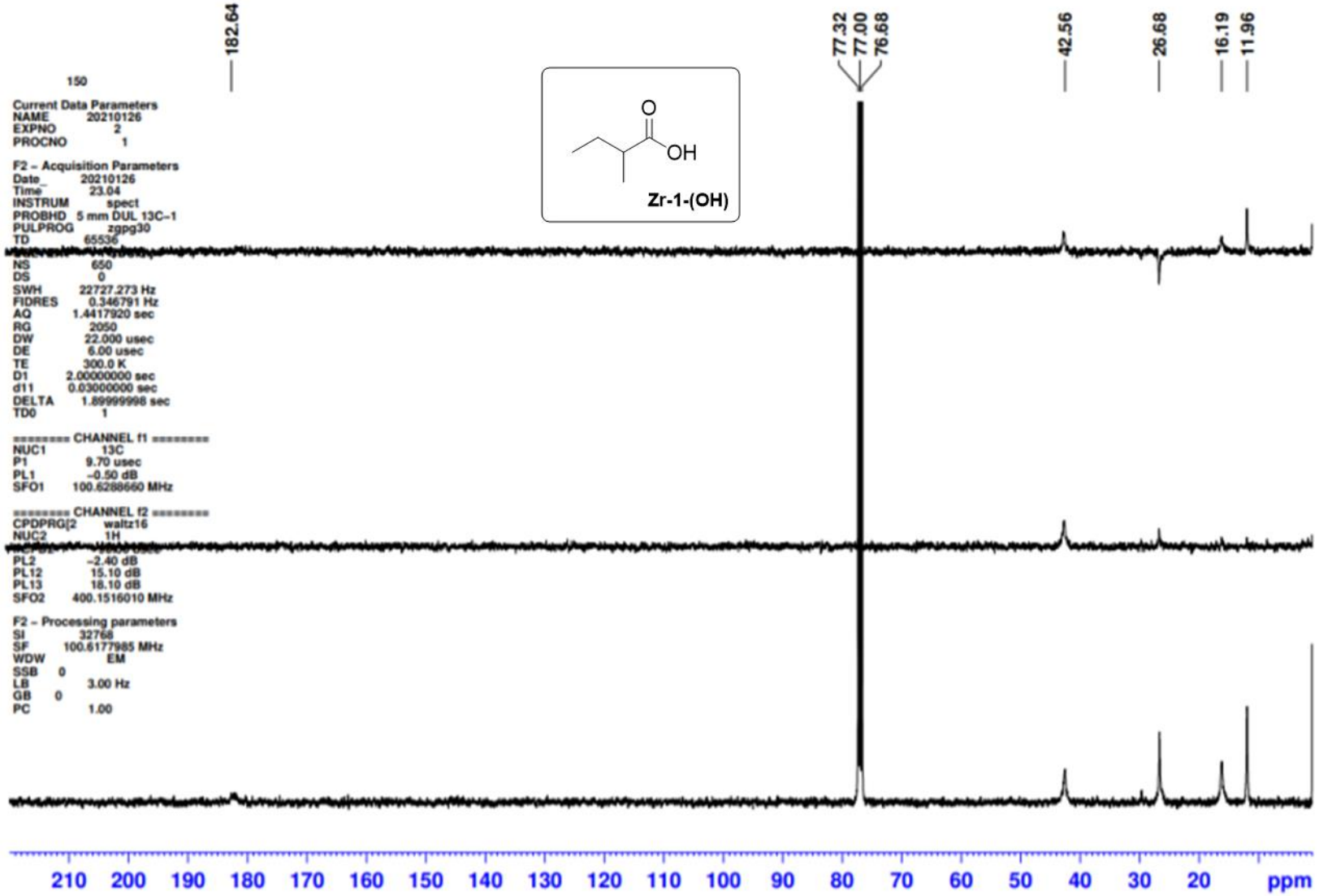
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559039 sec
RG 128
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 –2.40 dB
SFO1 400.1528010 MHz
F2 – Processing parameters
SI 16384
SF 400.1500172 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
17.989
18.069
17.959
54.224
54.000


182.64
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77.00
76.68
42.56
26.68
16.19
11.96
O
OH
Zr-1-(OH)
150
Current Data Parameters
NAME 20210126
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210126
Time 23.04
INSTRUM spect
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PULPROG zgpg30
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NS 650
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4417920 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6177985 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm