GERMAN FEDERAL INSTITUTE
FOR RISK ASSESSMENT

Bundesinstitut für Risikobewertung

IRMS – Part 2 –
^{13}C and ^{18}O analysis

Dr. Melanie Gimpel

Isotopic Analysis of Wine I

CO_2: ^{13}C

Wine Water:

^{18}O (Equilibration)

Ethanol:

^{13}C,

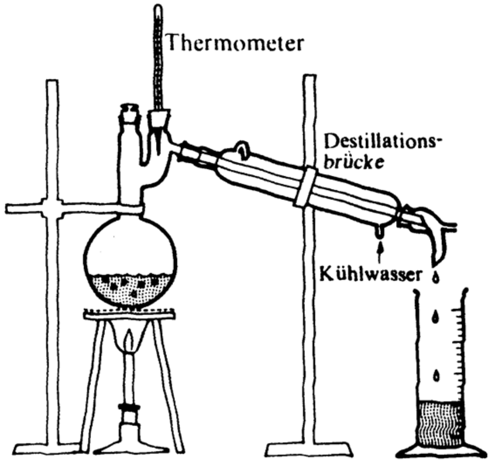
SNIF-NMR,

^{2}H-Pyr-IRMS,

^{18}O-Pyr-IRMS

Glycerol: ^{13}C

Isotopic Analysis of Wine II



Distillate

^{18}O of Wine Water
(OIV method)

SNIF-NMR
(OIV method)

^{13}C of Ethanol
(OIV method)

COMPENDIUM OF INTERNATIONAL METHODS OF ANALYSIS - OIV
Isotopic ratio of water

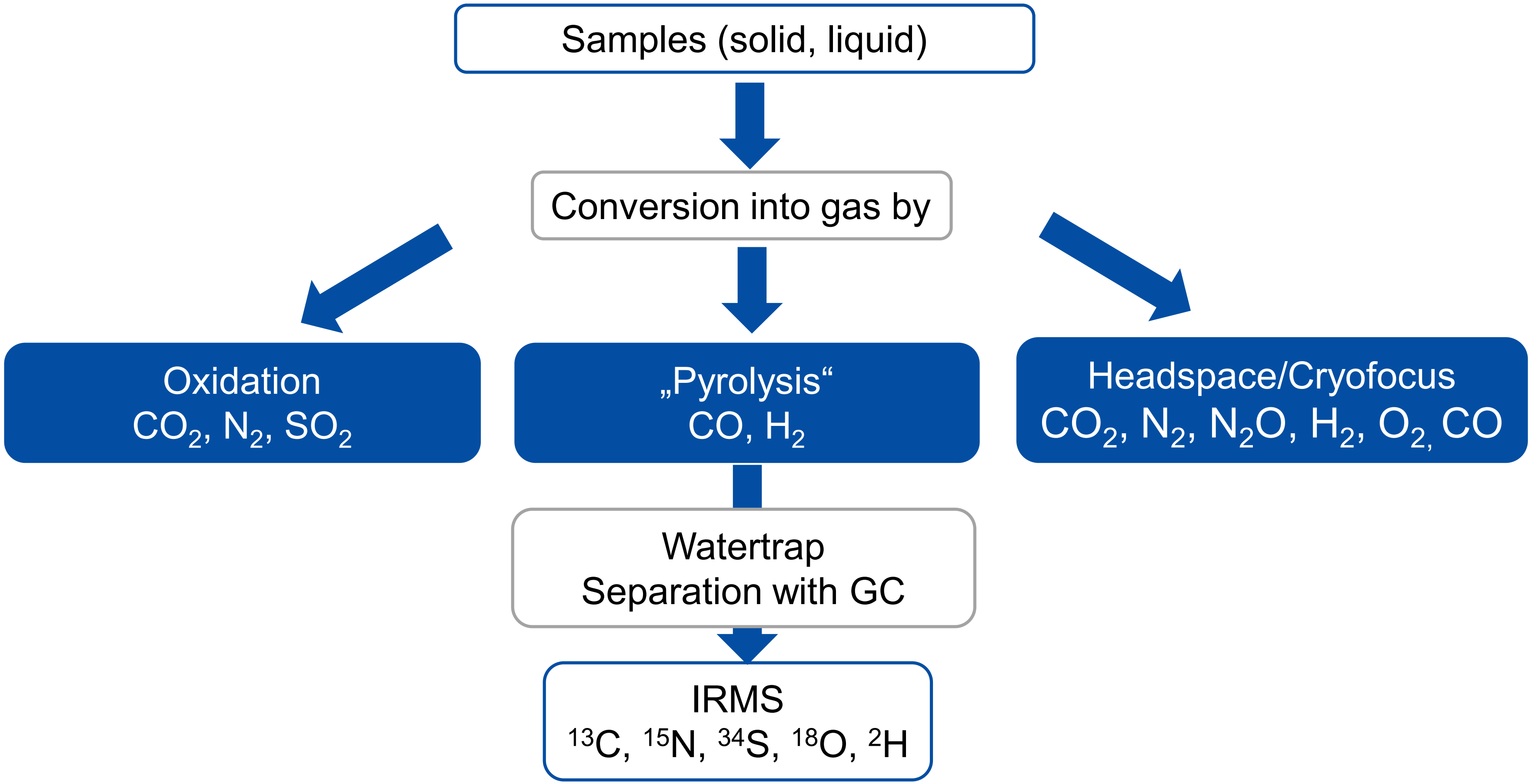
Method OIV-MA-AS2-12 Type II method

COMPENDIUM OF INTERNATIOAL METHODS OF ANALYSIS - OIV
Ethanol

Method OIV-MA-AS312-06 Type II method

IRMS Basics – Bulk analysis

- The IRMS instruments measure stable precisely small differences in the abundance of isotopes ($^2H/^1H$, $^{13}C/^{12}C$, $^{15}N/^{14}N$, $^{18}O/^{16}O$)
- Prior to analysis by IRMS, samples are converted into simple gas



IRMS basics – CO_2

- Example $^{13}C/^{12}C$: **CO_2** can contain **^{12}C, ^{13}C, ^{16}O, ^{17}O, ^{18}O**

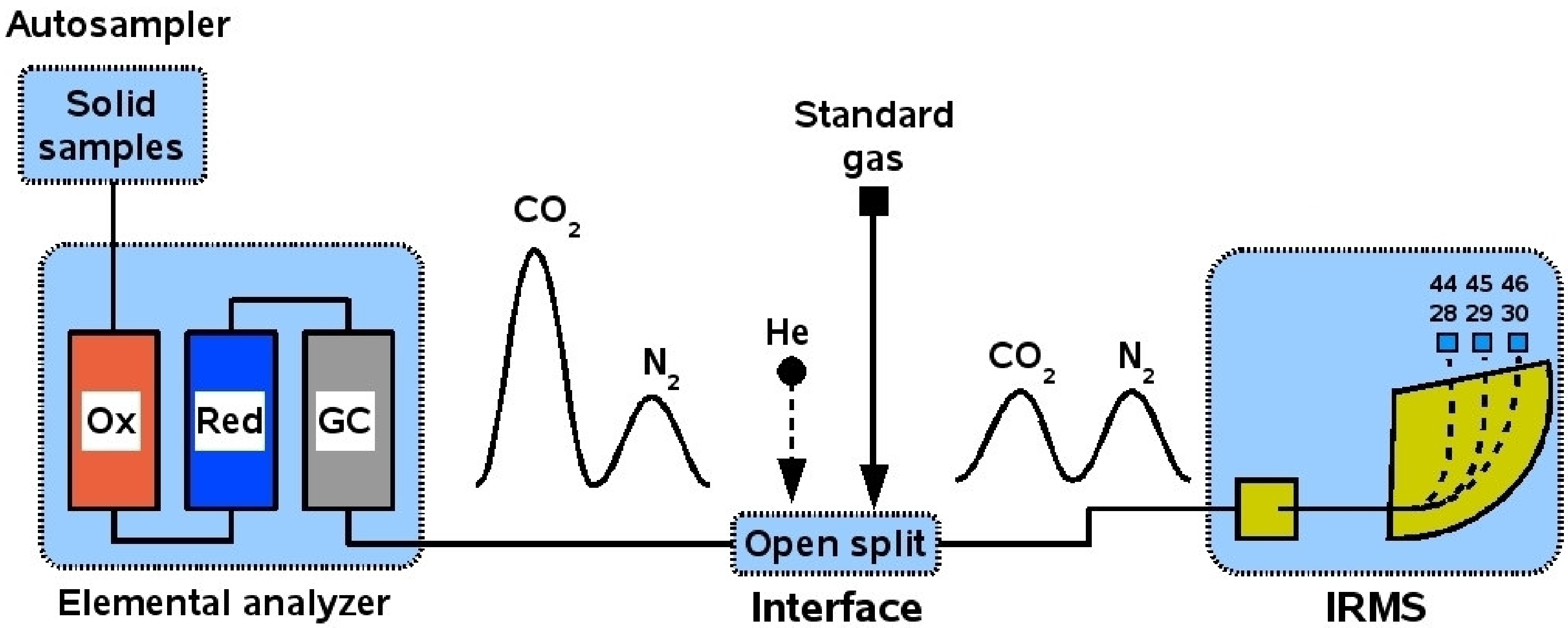
$$O{=}C{=}O$$

- Mass to charge ratios (*m/z*):
  - **44** ($^{12}C^{16}O^{16}O$)
  - **45** ($^{13}C^{16}O^{16}O$, $^{12}C^{16}O^{17}O$)
  - **46** ($^{12}C^{16}O^{18}O$, $^{12}C^{17}O^{17}O$, $^{13}C^{17}O^{16}O$)

→ Separation in the Mass Spectrometer

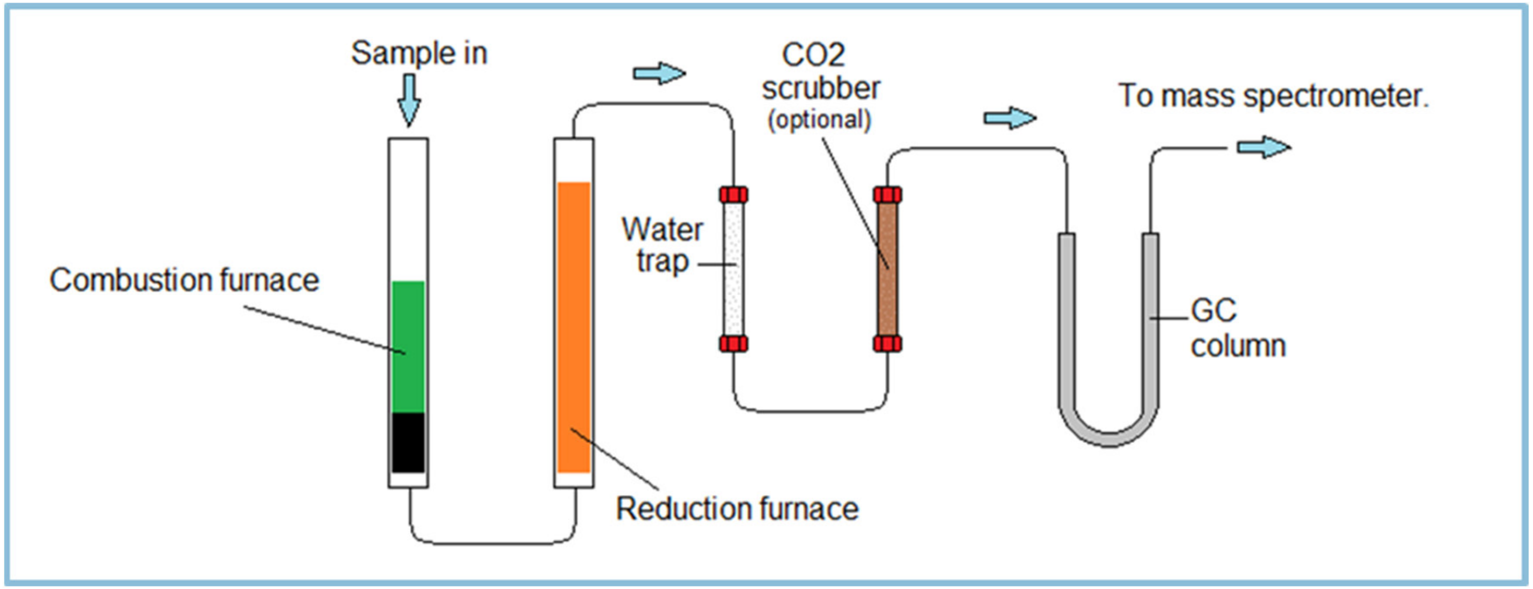
Principles of EA-IRMS measurements I

- **Combustion**: for $^{13}C/^{12}C$ and $^{15}N/^{14}N$ analysis
- Carrier gas in the EA-IRMS-system is helium



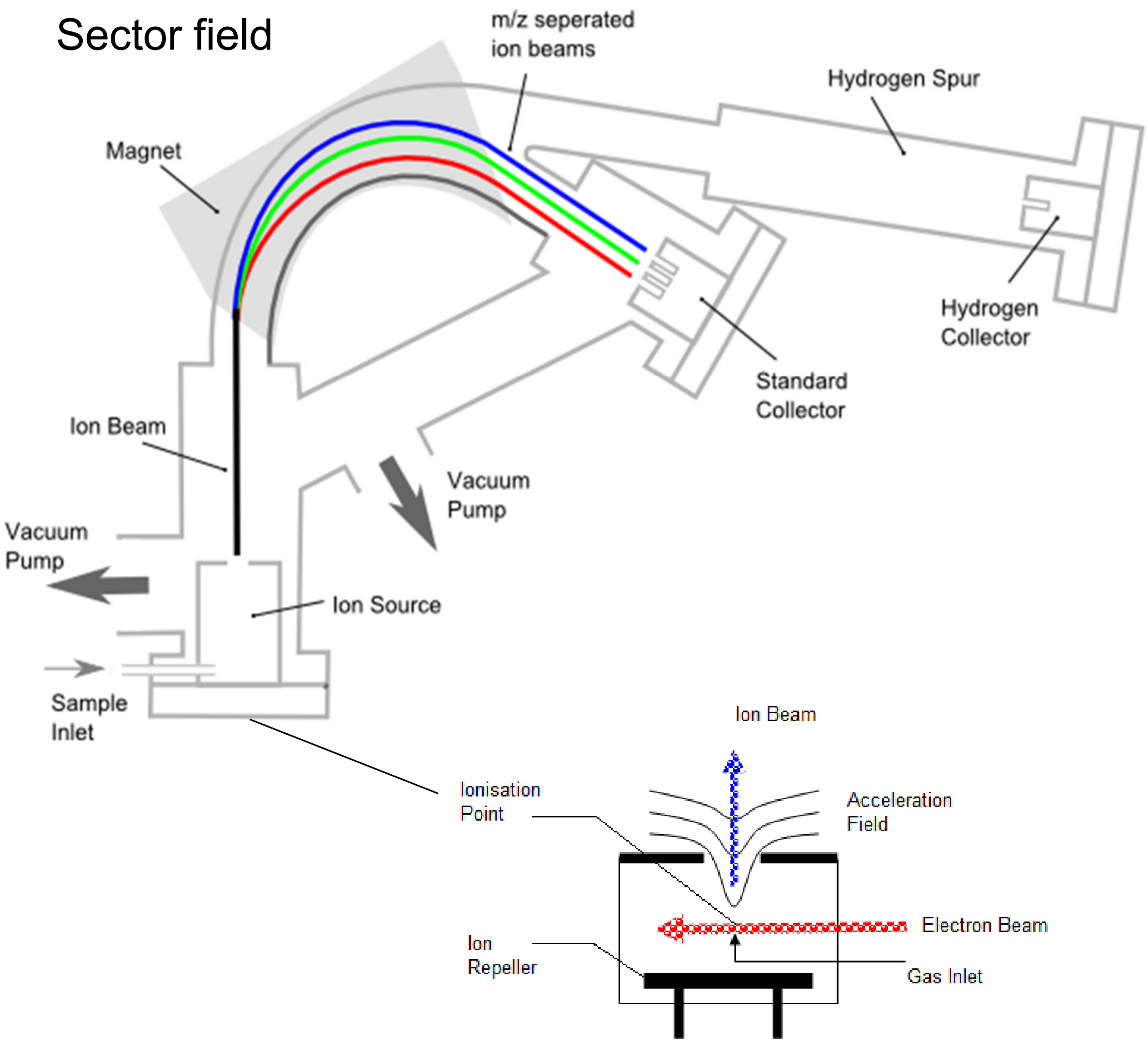
Principles of EA-IRMS measurements II

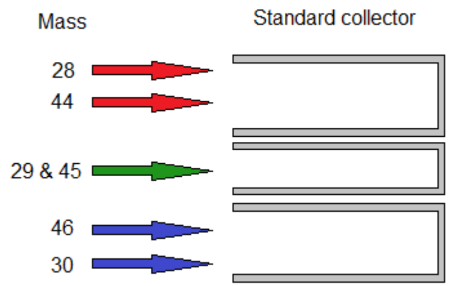
- **Combustion**: for $^{13}C/^{12}C$ and $^{15}N/^{14}N$ analysis
- Carrier gas in the EA-IRMS-system is helium



IRMS Basics – Mass Spectrometer

Sector field





Faraday Cups:
simple metal „buckets“ coated with specialized high carbon content paint

Source: Sercon 20-22 User‘s Manual V5.1

$\delta^{13}C$ of wine ethanol

COMPENDIUM OF INTERNATIATIOAL METHODS OF ANALYSIS - OIV
Ethanol

Method OIV-MA-AS312-06 Type II method

Determination by isotope ratio mass spectometry $^{13}C/^{12}C$ of wine ethanol or that obtained through the fermentation of musts, concentrated musts or grape sugar.
(Resolution Oeno 17/2001)

- The distillate that is produced according to the SNIF-NMR method OIV-MA-AS311-05 is used.
- Elemental Analyzer EA-IRMS

EA-IRMS – Combustion

Distillate

https://www.elementalmicroanalysis.com

Tin Capsules/ Liquid Injector

https://www.palsystem.com

EA-IRMS – Sequence

Make Sample List

Delete | Add | Insert | Copy | Paste | Clear | Revert | Quick File | Import | Special

Select Sample File: EA_LIQ_SEQ069 — References: MOW_JAN2015 (Edit)

Description: TEST SAMPLE — SetUp: CO2 PRESISION (Edit)

	Sample Name	Weight	Setup
1	MOW_JAN2015	100	13C_DESTILLAT
2	MOW_JAN2015	100	13C_DESTILLAT
3	MOW_JAN2015	100	13C_DESTILLAT
4	MOW_JAN2015	100	13C_DESTILLAT
5	MOW_JAN2015	100	13C_DESTILLAT
6	MOW_JAN2015	100	13C_DESTILLAT
7	MOW_JAN2015	100	13C_DESTILLAT
8	BCR656-337	100	13C_DESTILLAT
9	BCR656_337	100	13C_DESTILLAT
10	BCR656-337	100	13C_DESTILLAT
11	W-PTS05729_15A 0712151 PP_W286	100	13C_DESTILLAT
12	W-PTS05729_15A 0712151 PP_W286	100	13C_DESTILLAT
13	W-FAS06607_17P 0905181 PP_W310	100	13C_DESTILLAT
14	W-FAS06607_17P 0905181 PP_W310	100	13C_DESTILLAT
15	W-FAS06607_17P 0905181 PP_W310	100	13C_DESTILLAT
16	MOW 2017	100	13C_DESTILLAT
17	MOW 2017	100	13C_DESTILLAT
18	MOW 2017	100	13C_DESTILLAT
19	W-PTS05624_15A 2204152 PP_W278	100	13C_DESTILLAT
20	W-PTS05624_15A 2204152 PP_W278	100	13C_DESTILLAT
21	BCR656_337	100	13C_DESTILLAT
22	BCR656-337	100	13C_DESTILLAT
23	W-PTS05729_15A 0712151 PP_W286	100	13C_DESTILLAT
24	W-PTS05729_15A 0712151 PP_W286	100	13C_DESTILLAT
25	W-FAS06610_17P 0905182 PP_W310	100	13C_DESTILLAT
26	W-FAS06610_17P 0905182 PP_W310	100	13C_DESTILLAT
27	W-FAS06610_17P 0905182 PP_W310	100	13C_DESTILLAT
28	W-FAS06620_17P 0905183 PP_W310	100	13C_DESTILLAT
29	W-FAS06620_17P 0905183 PP_W310	100	13C_DESTILLAT
30	W-FAS06620_17P 0905183 PP_W310	100	13C_DESTILLAT
31	W-PTS05624_15A 2204152 PP_W278	100	13C_DESTILLAT
32	W-PTS05624_15A 2204152 PP_W278	100	13C_DESTILLAT
33	BCR656_337	100	13C_DESTILLAT
34	BCR656-337	100	13C_DESTILLAT
35	W-PTS05729_15A 0712151 PP_W286	100	13C_DESTILLAT
36	W-PTS05729_15A 0712151 PP_W286	100	13C_DESTILLAT
37	W-FAS06627_17P 0905184 PP_W310	100	13C_DESTILLAT
38	W-FAS06627_17P 0905184 PP_W310	100	13C_DESTILLAT
39	W-FAS06627_17P 0905184 PP_W310	100	13C_DESTILLAT
40	W-QSP06605_17P 0905185 PP_W310	100	13C_DESTILLAT
41	W-QSP06605_17P 0905185 PP_W310	100	13C_DESTILLAT
42	W-QSP06605_17P 0905185 PP_W310	100	13C_DESTILLAT
43	W-PTS05624_15A 2204152 PP_W278	100	13C_DESTILLAT
44	W-PTS05624_15A 2204152 PP_W278	100	13C_DESTILLAT
45	BCR656_337	100	13C_DESTILLAT
46	BCR656_337	100	13C_DESTILLAT
47	W-PTS05729_15A 0712151 PP_W286	100	13C_DESTILLAT
48	W-PTS05729_15A 0712151 PP_W286	100	13C_DESTILLAT
49	W-FAS06811_17P 0305184 PP_W310	100	13C_DESTILLAT

Print | Save As | Save+Exit | Exit

EA-IRMS – Combustion

Distillate

https://www.elementalmicroanalysis.com

https://www.palsystem.com

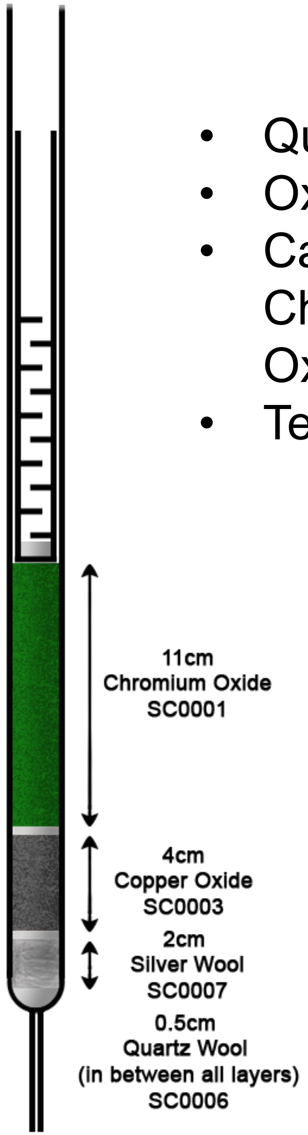
Tin Capsules/ Liquid Injector

Combustion at 900-1050°C
+ Catalyst (Cr_2O_3 and Co_3O_4+Ag)

Sample Gas $CO_2 + H_2O + (NO_x)$

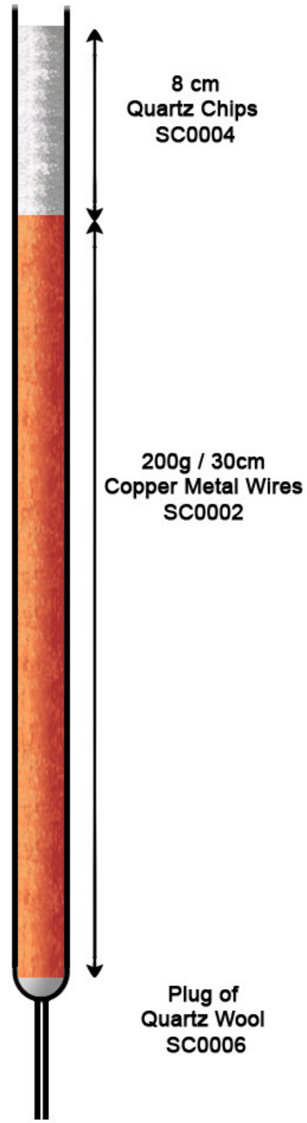
Reduction (in 2nd quartz tube), 650°C,
$NO_x \rightarrow N_2$

Combustion and Reduction tubes



Standard Combustion Tube

- Quartz or steel stube
- Oxygen atmosphere
- Catalyst: Cobalt Oxide, Chromium Oxide, Copper Oxide
- Temperature 900-1050 °C



Standard Reduction Tube

- Quartz or steel stube
- Copper
- Temperature 600-650 °C

EA-IRMS – Combustion II

Reduction (in 2nd quartz tube), 650°C, NO_x → N_2

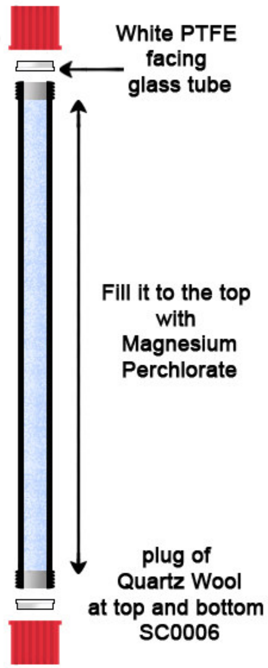
↓

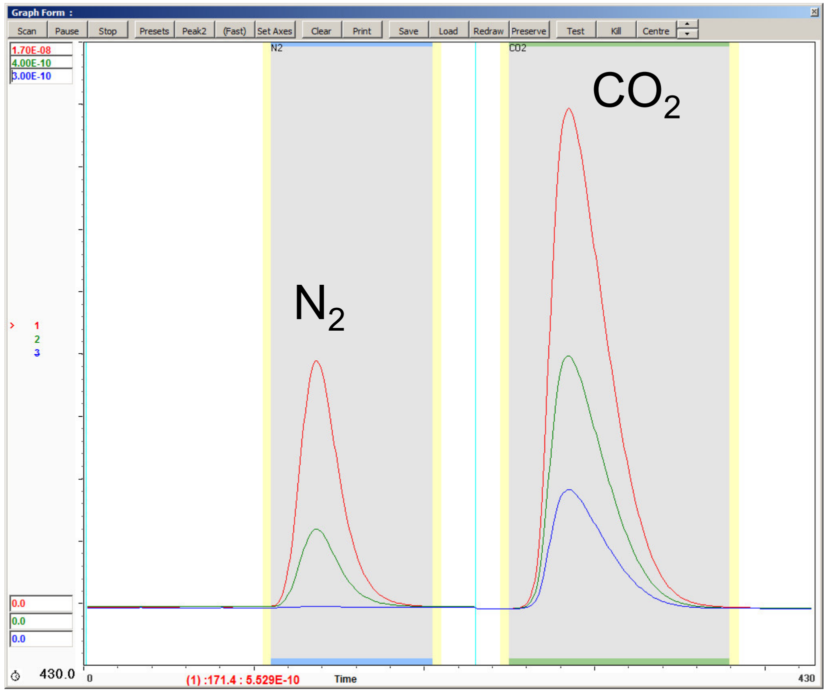
Water trap → Removal of H_2O, $Mg(ClO_4)_2$

↓

GC (packed column, isothermal 65-100°C) → separation of CO_2 + N_2

Watertrap and GC





Water trap: $Mg(ClO_4)_2$

Separation of N_2 and CO_2:

- packed GC column
- isothermal, approx. 70 °C

- alternativ purge-and-trap system

EA-IRMS – Combustion II

Reduction (in 2nd quartz tube), 650°C, NO_x → N_2

↓

Water trap → Removal of H_2O, $Mg(ClO_4)_2$

↓

GC (packed column, isothermal 65-100°C) → separation of CO_2 + N_2

↓

Interface

Dilution with Helium, Transfer into MS

↓

IRMS

EA-IRMS – Results and Data handling

Automatically:
- Peak integration
- Correction of raw data (e.g. ^{17}O correction)
- Calculation of isotope delta ratios ($\delta^{13}C$)

Reference Gas Calibration

Reference gas is previously calibrated against reference material

Reference gas is measured in each run of each sample

Chromatogramm

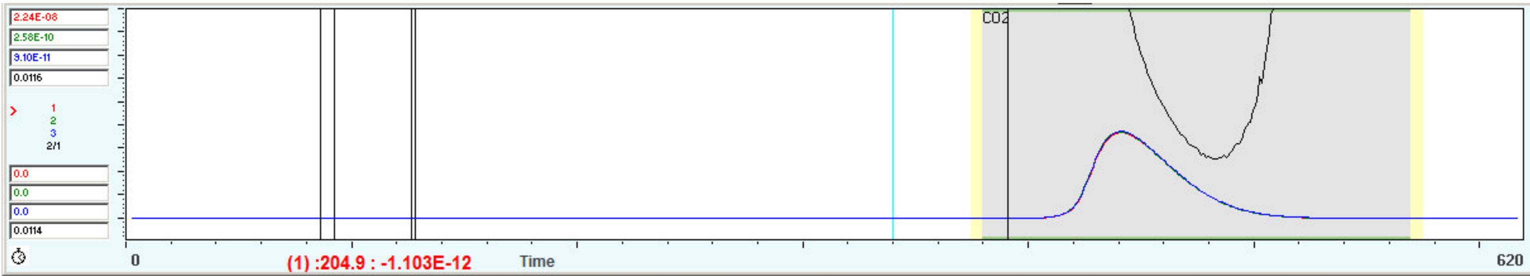
Calibration Intra-Sequence

Raw ratios

Recalibration against the reference samples in the sequence

Results ($\delta^{13}C_{VPDB}$)

Results and Data handling – intra-sequence calibration



Data Reprocess [EA_LIQ_SEQ068.rec]

Replay | abc SampleList | Setup | Show Info | Tall

Labe | Label4 | Original Timing | Original Names | Original Blank | Blank On | < >

	SampleName		CO2 >>	C (Sam)	13C (Sam)	180 (Sam)	2/1	3/1
			Beam Area	ug	DeltaPDB	DeltaSMO\		
	Drift Corrected Results							
1	MOW_JAN2015	100.	4.01E-07	28882.12	**-29.76**	**0.09**	0.010903	0.004011
2	MOW_JAN2015	100.	4.01E-07	28907.12	**-29.23**	**0.05**	0.010909	0.004011
3	MOW_JAN2015	100.	3.98E-07	28698.26	**-29.01**	**0.06**	0.010911	0.004011
4	MOW_JAN2015	100.	3.98E-07	28695.66	**-28.89**	**0.55**	0.010913	0.004013
5	MOW_JAN2015	100.	3.97E-07	28632.4	**-28.75**	**0.54**	0.010914	0.004013
6	MOW_JAN2015	100.	4.01E-07	28871.86	**-28.52**	**0.81**	0.010917	0.004014
7	MOW_JAN2015	100.	3.98E-07	28648.25	**-28.39**	**0.85**	0.010918	0.004014
8	BCR656-337	100.	4.07E-07	29307.95	**-27.02**	**1.19**	0.010934	0.004015
9	BCR656_337	100.	4.06E-07	29270.	**-26.91**	**1.00**	0.010935	0.004014
10	BCR656-337	100.	4.08E-07	29411.37	**-26.94**	**1.07**	0.010934	0.004015
11	W-PTS05729_15A 0712151 PF	100.	4.02E-07	28973.31	**-28.06**	**1.23**	0.010922	0.004015
12	W-PTS05729_15A 0712151 PF	100.	4.02E-07	28963.57	**-28.09**	**1.29**	0.010922	0.004016
13	W-FAS06623_17P 2404185 PF	100.	4.03E-07	29062.48	**-28.11**	**1.15**	0.010921	0.004015
14	W-FAS06623_17P 2404185 PF	100.	4.06E-07	29235.18	**-28.11**	**1.11**	0.010921	0.004015
15	W-FAS06623_17P 2404185 PF	100.	4.04E-07	29094.62	**-28.13**	**1.12**	0.010921	0.004015
16	W-FAS06624_17P 2504181 PF	100.	4.02E-07	28991.83	**-27.84**	**1.10**	0.010924	0.004015
17	W-FAS06624_17P 2504181 PF	100.	4.05E-07	29178.78	**-27.89**	**1.03**	0.010924	0.004015
18	W-FAS06624_17P 2504181 PF	100.	4.02E-07	28960.3	**-27.85**	**1.12**	0.010924	0.004015
19	W-PTS05624_15A 2204152 PF	100.	3.97E-07	28635.98	**-26.94**	**1.35**	0.010934	0.004016
20	W-PTS05624_15A 2204152 PF	100.	3.97E-07	28576.63	**-26.90**	**1.22**	0.010935	0.004015
21	BCR656_337	100.	4.06E-07	29270.	**-26.91**	**1.00**	0.010935	0.004014
22	BCR656-337	100.	4.06E-07	29255.83	**-26.95**	**0.96**	0.010934	0.004014
23	W-PTS05729_15A 0712151 PF	100.	4.03E-07	29032.71	**-28.17**	**0.57**	0.010921	0.004013
24	W-PTS05729_15A 0712151 PF	100.	4.03E-07	28986.43	**-28.10**	**0.20**	0.010921	0.004011
25	W-FAS06625_17P 2504182 PF	100.	4.03E-07	28979.31	**-26.65**	**0.13**	0.010938	0.004011
26	W-FAS06625_17P 2504182 PF	100.	4.05E-07	29147.04	**-26.75**	**0.22**	0.010937	0.004011
27	W-FAS06625_17P 2504182 PF	100.	4.03E-07	28956.39	**-26.73**	**0.54**	0.010937	0.004013
28	W-FAS06626_17P 2504183 PF	100.	4.06E-07	29212.87	**-23.31**	**0.70**	0.010975	0.004013
29	W-FAS06626_17P 2504183 PF	100.	4.04E-07	28990.98	**-23.20**	**0.76**	0.010976	0.004013
30	W-FAS06626_17P 2504183 PF	100.	4.07E-07	29213.81	**-23.30**	**0.82**	0.010975	0.004014
31	W-PTS05624_15A 2204152 PF	100.	3.99E-07	28610.18	**-26.87**	**1.14**	0.010935	0.004015
32	W-PTS05624_15A 2204152 PF	100.	3.98E-07	28595.85	**-26.87**	**1.20**	0.010935	0.004015
33	BCR656_337	100.	4.08E-07	29270.	**-26.91**	**1.00**	0.010935	0.004014
34	BCR656-337	100.	4.08E-07	29230.81	**-26.93**	**1.15**	0.010935	0.004015
35	W-PTS05729_15A 0712151 PF	100.	4.04E-07	28942.89	**-28.10**	**1.29**	0.010921	0.004016
36	W-PTS05729_15A 0712151 PF	100.	4.04E-07	28933.45	**-28.11**	**1.17**	0.010921	0.004015

$\delta^{18}O$ of Wine water

COMPENDIUM OF INTERNATIONAL METHODS OF ANALYSIS - OIV
Isotopic ratio of water

Method OIV-MA-AS2-12 Type II method

Method for $^{18}O/^{16}O$ isotope ratio determination of water in wines and must

(Resolution OIV-Oeno 353/2009)

Example Gasbench

- The technique is based on the equilibration of water in samples of wine with a Carbon dioxide standard gas.

$$C^{16}O_2 + H_2{}^{18}O \leftrightarrow C^{16}O^{18}O + H_2{}^{16}O$$

- Headspace-Method

Principles of equilibration-IRMS measurements I

Headspace Method

He + CO_2 | Sample | Closed system (vials)

CO_2 (gas phase) | Water (liquid phase) | CO_2 (gas phase) | Water vapor (gas phase)

$^{12}C^{16}O^{16}O$ + $^{1}H^{1}H^{\mathbf{18}}\mathbf{O}$ ⟷ $^{12}C^{16}O^{\mathbf{18}}\mathbf{O}$ + $^{1}H^{1}H^{16}O$

m/z 44 | *m/z 20* | *m/z 46* | *m/z 18*

Injection of the gas phase into IRMS

He + CO_2 (*m/z 44* + *46*) + H_2O (*m/z 18* + *20*)

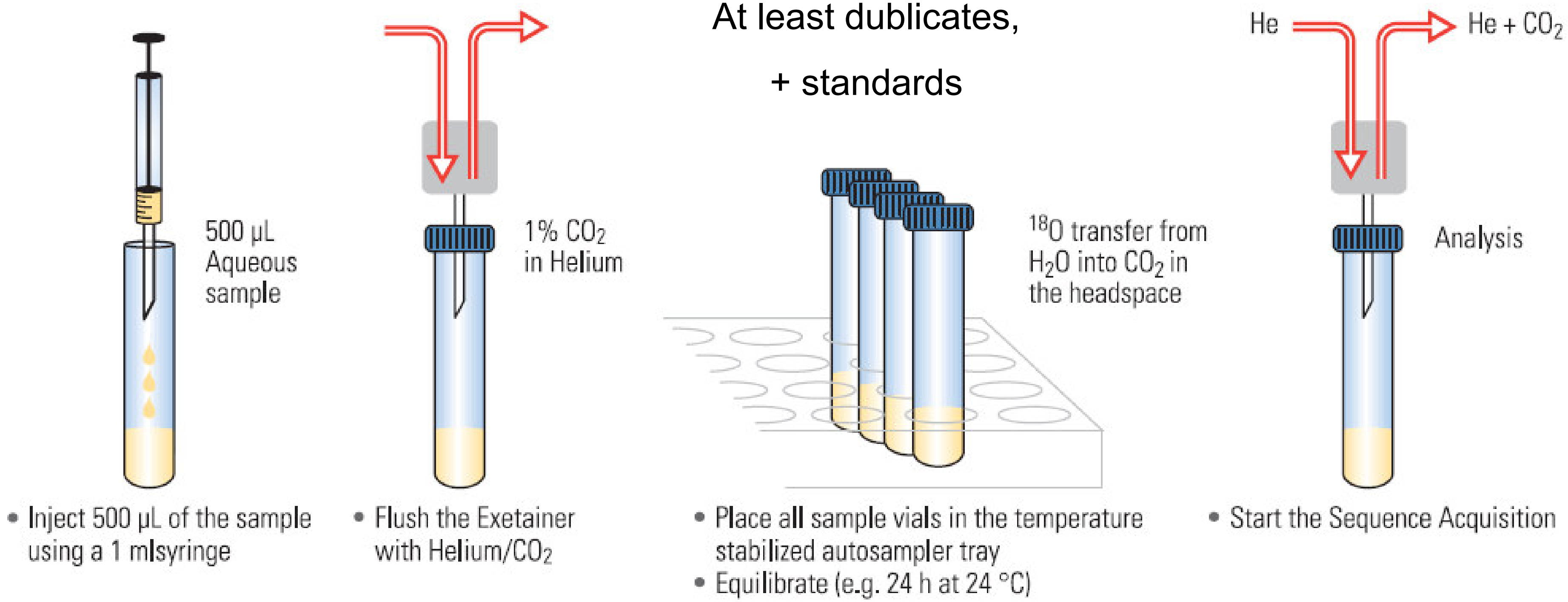
Principles of equilibration-IRMS measurements II

Headspace Method

Removal of residual air

At least dublicates,

+ standards



Borosilicate sample bottles

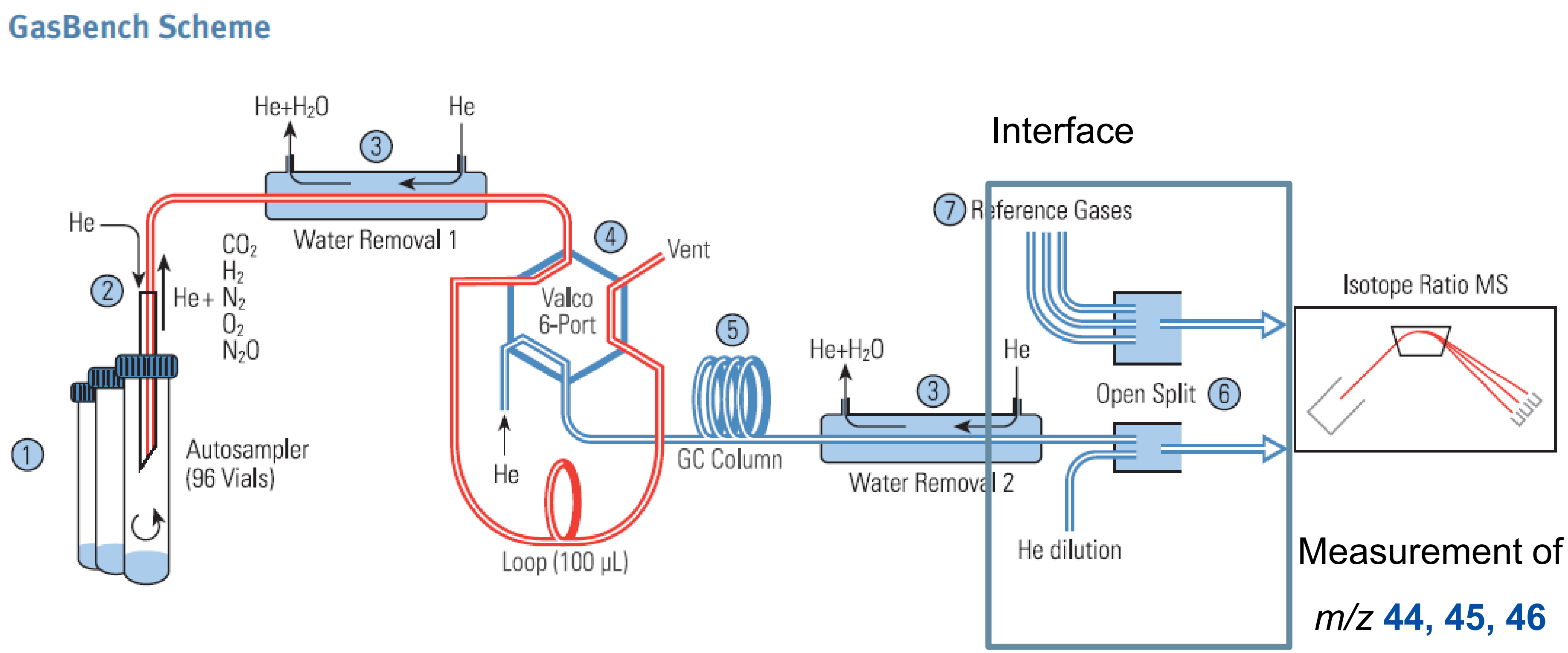
- Sealed with new septa

Required temperature stability ± 0.1 °C

(temperature dependance ≈ 0.25 ‰ per °C)

Thermo Fisher Scientific, Application Note 30048

Principles of Equilibration-IRMS measurements II



Measurement of

m/z **44, 45, 46**

Equilibration-IRMS measurements - Sequence

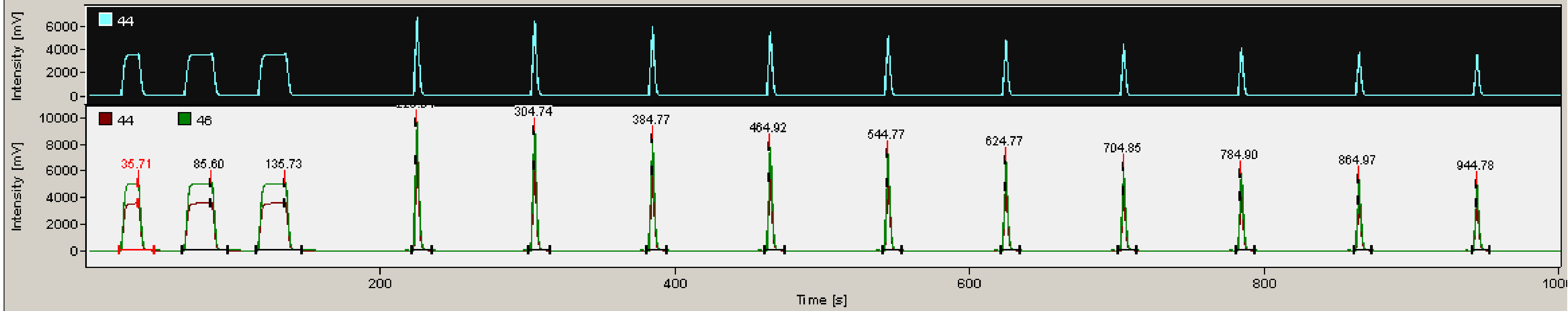
GB_SEQ_IRMS2_094.ods

GB_SEQ_IRMS2_094		26.07.2018			C=CO2 in He	H=He					
Nr	Identifier1	Identifier2	AS	Nr	Identifier1	Identifier2	AS	Nr	Identifier1	Identifier2	AS
1	Laborwasser		C	29	W-DBW07080/18A	RHG-28/17 W330	C	57	W-PTS07029/18A	18/1/A W327	C
2	Laborwasser		C	30	W-PTS07029/18A	18/1/A W327	C	58	W-DBW07081/18A	RHG-29/17 W330	C
3	Laborwasser		C	31	W-DBW07081/18A	RHG-29/17 W330	C	59	W-DBW07082/18A	RHG-30/17 W330	C
4	**STD 16**	**20160016**	C	32	W-DBW07082/18A	RHG-30/17 W330	C	60	**W-MOW04612_12P_24_30**	**PP:W224**	C
5	**STD 17**	**20160017**	C	33	**STD 16**	**20160016**	C	61	**STD 16**	**20160016**	C
6	**STD 18**	**20160018**	C	34	**STD 17**	**20160017**	C	62	**STD 17**	**20160017**	C
7	**Laborwasser**		C	35	**STD 18**	**20160018**	C	63	**STD 18**	**20160018**	C
8	**W-MOW04612_12P_24_30**	**PP:W224**	C	36	W-PTS07084/18P	JUE/0718/1 W332	C	64			C
9	W-PTS07084/18P	JUE/0718/1 W332	C	37	W-DBW07077/18A	RHG-25/17 W330	C	65			C
10	W-DBW07077/18A	RHG-25/17 W330	C	38	W-DBW07078/18A	RHG-26/17 W330	C	66			C
11	W-DBW07078/18A	RHG-26/17 W330	C	39	W-DBW07079/18A	RHG-27/17 W330	C	67			C
12	W-DBW07079/18A	RHG-27/17 W330	C	40	W-DBW07080/18A	RHG-28/17 W330	C	68			C
13	W-DBW07080/18A	RHG-28/17 W330	C	41	**W-MOW04612_12P_24_30**	**PP:W224**	C	69			C
14	W-PTS07029/18A	18/1/A W327	C	42	**STD 16**	**20160016**	C	70			C
15	**STD 16**	**20160016**	C	43	**STD 17**	**20160017**	C	71			C
16	**STD 17**	**20160017**	C	44	**STD 18**	**20160018**	C	72			C
17	**STD 18**	**20160018**	C	45	**Laborwasser**		C	73			C
18	**W-MOW04612_12P_24_30**	**PP:W224**	C	46	W-PTS07029/18A	18/1/A W327	C	74			C
19	W-DBW07081/18A	RHG-29/17 W330	C	47	W-DBW07081/18A	RHG-29/17 W330	C	75			C
20	W-DBW07082/18A	RHG-30/17 W330	C	48	W-DBW07082/18A	RHG-30/17 W330	C	76			C
21	W-PTS07084/18P	JUE/0718/1 W332	C	49	W-DBW07077/18A	RHG-25/17 W330	C	77			C
22	W-DBW07077/18A	RHG-25/17 W330	C	50	W-DBW07078/18A	RHG-26/17 W330	C	78			C
23	W-DBW07078/18A	RHG-26/17 W330	C	51	**STD 16**	**20160016**	C	79			C
24	**STD 16**	**20160016**	C	52	**STD 17**	**20160017**	C	80			C
25	**STD 17**	**20160017**	C	53	**STD 18**	**20160018**	C	81			C
26	**STD 18**	**20160018**	C	54	**Laborwasser**		C	82			C
27	**W-MOW04612_12P_24_30**	**PP:W224**	C	55	W-DBW07079/18A	RHG-27/17 W330	C	83			C
28	W-DBW07079/18A	RHG-27/17 W330	C	56	W-DBW07080/18A	RHG-28/17 W330	C	84			C

Erstellt von Werner-Karl Blaas 31.08.2018 Seite 1

$\delta^{18}O$ in wine water - Chromatogram

File Name: D:\FINNIGAN\Gasbench_Results\GB_SEQ_IRMS2_094a\60_W_MOW04612_12P_24_30_.cf



CO2 | Error | Extended | Sequence Line

Peak Nr.	Start [s]	Rt [s]	Width [s]	Ampl. 46 [mV]	d 18O/16O [per mil] vs. VSMOW
1	23.2	35.7	23.8	5038	0.215
2	66.3	85.6	31.0	5041	0.033
3*	116.2	135.7	31.3	5041	0.000
4	221.8	225.0	14.0	9566	3.030
5	301.7	304.7	13.7	8987	3.078
6	381.7	384.8	13.5	8368	3.009
7	461.6	464.9	13.5	7731	2.898
8	541.7	544.8	13.2	7208	2.975
9	621.7	624.8	13.0	6692	3.019
10	701.8	704.8	12.7	6226	3.049
11	781.6	784.9	12.7	5769	2.882
12	861.7	865.0	12.5	5311	3.149
13	941.8	944.8	12.2	4933	3.176

$\delta^{18}O$ in wine water - data evaluation I

The final results are presented as relative $\delta^{18}O_{V\text{-}SMOW}$ values expressed in ‰. $\delta^{18}O_{V\text{-}SMOW}$ values are calculated using the following equation:

$$\delta^{18}O_{V-SMOW} = \left[\frac{\left(\frac{^{18}O}{^{16}O}\right)_{sample} - \left(\frac{^{18}O}{^{16}O}\right)_{V-SMOW}}{\left(\frac{^{18}O}{^{16}O}\right)_{V-SMOW}} \right] \times 1000 \quad [‰]$$

The $\delta^{18}O$ value normalized versus the V-SMOW/SLAP scale is calculated using the following equation:

$$\delta^{18}O_{V-SMOW/SLAP} = \left[\frac{\delta^{18}O_{sample} - \delta^{18}O_{V-SMOW}}{\delta^{18}O_{V-SMOW} - \delta^{18}O_{SLAP}} \right] \times 55.5 \quad [‰]$$

The $\delta^{18}O_{V\text{-}SMOW}$ value accepted for SLAP is -55.5‰ (see also 5.1).

Gasbench – data evaluation II

Auswertung
Sequenz **SEQ090** **PROBEN**

gemessen: 15.03. - 16.03.2018 Blaas

Streuung	Innerhalb	Probe
	0,200	0,150

		Delta 18/16 vs Ref CO2			Delta 18/16 vs Std 4		$\delta^{18}O$ (VSMOW, SLAP)				
Probe Nr.	Line No	Mittelwert	s n-1	n	Probe/STD 4	SKAL	ALL	Reduced	Mittelwert	s n-1	n
W-MOW04612/12P-22/30	8	3,537	0,192	5	-17,17	-17,17	-1,48	-1,48	**-1,32**	**0,137**	**3**
	34	3,783	0,052	5	-16,93	-16,93	-1,23	-1,23			
	47	3,766	0,179	5	-16,95	-16,95	-1,25	-1,25			
W-PTS06854/17A	9	8,267	0,156	5	-12,54	-12,54	3,23	3,23	**3,16**	**0,061**	**3**
Ref:17/3/F	22	8,152	0,105	5	-12,65	-12,65	3,11	3,11			
PP:W 321	35	8,174	0,073	5	-12,63	-12,63	3,14	3,14			
W-PTS07006/18A	10	-12,255	0,145	5	-32,64	-32,64	-17,19	-17,19	**-17,15**	**0,084**	**3**
JUE/0118/1	36	-12,271	0,170	5	-32,66	-32,66	-17,21	-17,21			
PP:W 325	49	-12,117	0,103	5	-32,50	-32,50	-17,05	-17,05			
W-DBW06909/18A	11	8,525	0,026	5	-12,29	-12,29	3,49	3,49	**3,53**	**0,062**	**3**
No22C_2016	24	8,552	0,136	5	-12,26	-12,26	3,51	3,51			
PP:W 323	37	8,644	0,129	5	-12,17	-12,17	3,60	3,60			
W-DBW06910/18A	12	8,515	0,125	5	-12,30	-12,30	3,48	3,48	**3,43**	**0,038**	**3**
No23C_2016	25	8,448	0,114	5	-12,36	-12,36	3,41	3,41			
PP:W 323	51	8,450	0,177	5	-12,36	-12,36	3,41	3,41			
W-DBW06911/18A	16	8,591	0,146	5	-12,22	-12,22	3,55	3,55	**3,63**	**0,076**	**3**
No24C_2016	29	8,741	0,143	5	-12,08	-12,08	3,70	3,70			
PP:W 323	55	8,693	0,139	5	-12,12	-12,12	3,65	3,65			
W-DBW06912/18A	30	10,483	0,060	5	-10,37	-10,37	5,43	5,43	**5,52**	**0,083**	**3**
No25C_2016	43	10,649	0,141	5	-10,21	-10,21	5,60	5,60			
PP:W 323	56	10,580	0,089	5	-10,28	-10,28	5,53	5,53			
W-DBW06913/18A	18	8,632	0,079	5	-12,18	-12,18	3,59	3,59	**3,60**	**0,036**	**3**
No26C_2016	31	8,673	0,042	5	-12,14	-12,14	3,63	3,63			
PP:W 323	57	8,601	0,109	5	-12,21	-12,21	3,56	3,56			
W-DBW06914/18A	32	8,392	0,046	5	-12,42	-12,42	3,35	3,35	**3,33**	**0,075**	**3**
No27C_2016	45	8,421	0,051	5	-12,39	-12,39	3,38	3,38			
PP:W 323	58	8,278	0,090	5	-12,53	-12,53	3,24	3,24			
Laborwasser	7	-1,809	0,093	5	-22,41	-22,41	-6,80	-6,80	**-6,76**	**0,031**	**3**
	33	-1,750	0,173	5	-22,35	-22,35	-6,74	-6,74			
	46	-1,763	0,138	5	-22,36	-22,36	-6,75	-6,75			

Data handling - Corrections

- Correction for interferences
  - e.g. mass 45: $^{13}C^{16}O^{16}O$, $^{12}C^{17}O^{16}O$ → ^{17}O-Correction,
- Drift correction
  - Traces of water, changes of working gas canlead to drift effects → determination of slope of linear drift curve
- Linearity correction
  - correlation between the signal intensity and the measured value → can be corrected or avoided by closely controlling the weight of each sample
- Memory correction
  - preceding samples with deviating isotope values → memory correction is possible, but quite complex
- Blank correction
  - Blank effects can arrise → can usually be corrected by IRMS software, unlikely with sufficiently large sample peaks

GERMAN FEDERAL INSTITUTE
FOR RISK ASSESSMENT

Bundesinstitut für Risikobewertung

Thank you for your attention

Melanie Gimpel

German Federal Institute for Risk Assessment
Max-Dohrn-Str. 8-10 ● 10589 Berlin, GERMANY
Phone +49 30 - 184 12 - 0 ● Fax +49 30 - 184 12 - 47 41
bfr@bfr.bund.de ● www.bfr.bund.de/en