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*Supplement of*

## **A versatile, refrigerant- and cryogen-free cryofocusing–thermodesorption unit for preconcentration of traces gases in air**

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## 1 Supplementary Information

2 **Table S-1** shows a list of substances detected up to the time of completion of this paper. Identifications based on ambient air samples as well as synthetic mixtures. Substances are separated into six classes (e.g. CFCs and HCFCs, PFCs and HFCs etc.), which are listed in arbitrary order. Within each class, substances are sorted according to their boiling point (bp) in [°C]. Chemical sum formula as well as retention time  $t_R$  in [min] on the GS GasPro PLOT column listed in columns two and three. Columns 5 & 6 show analyte residues in [%], expressed as chromatographic signal area determined in a blank gas measurement relative to a signal area determined in a preceding 1 L ambient air sample. Blank gas: purified helium 6.0 (Praxair, Germany). “Residue HayeSep D” denotes residues found with HayeSep D as adsorptive material, “Residue Unibeads 1S” shows the same for Unibeads 1S as adsorptive material. Residues that a constant background (contamination), are marked with a “c”, ones that represent a memory effect from a preceding sample are marked with an “m”. Substances that are not detected regularly in ambient air samples or show poor measurement precision  $\geq 10\%$  were excluded from the analysis (“not analysed”; n.a.). If no residue was detected or the detected residue was  $\leq 0.01\%$ , a “not detected” (n.d.) is assigned to the respective substance.

17 **Table S-1.** List of detectable substances and blank residues. Descriptions are given in the text.

Class/Name	Formula	$t_R$ [min]	bp [°C]	Residue HayeSep D	Residue Unibeads 1S
<b><u>CFCs &amp; HCFCs</u></b>					
HCFC-22	CHClF <sub>2</sub>	5.20	-41	n.d.	n.d.
CFC-115	CClF <sub>2</sub> CF <sub>3</sub>	4.48	-39	n.d.	n.d.
CFC-12	CF <sub>2</sub> Cl <sub>2</sub>	5.02	-30	n.d.	n.d.
HCFC-124	CHF <sub>2</sub> CF <sub>2</sub> Cl	6.85	-12	n.d.	n.d.
HCFC-142b	CH <sub>3</sub> CClF <sub>2</sub>	6.87	-10	n.d.	n.d.
HCFC-31	CH <sub>2</sub> ClF	6.40	-9	n.a.	n.a.
CFC-114	CClF <sub>2</sub> CClF <sub>2</sub>	6.67	4	n.d.	n.d.
HCFC-133a	C <sub>2</sub> H <sub>2</sub> ClF <sub>3</sub>	7.55	6	n.d.	n.d.
HCFC-21	CHCl <sub>2</sub>	7.32	9	n.d.	n.d.
CFC-11	CFCl <sub>3</sub>	7.28	24	n.d.	n.d.
HCFC-141b	CH <sub>3</sub> CCl <sub>2</sub> F	8.42	32	n.d.	n.d.
HCFC-1121	CHClCFCl	8.05	35	n.a.	n.a.

<b>Class/Name</b>	<b>Formula</b>	<b>t<sub>R</sub> [min]</b>	<b>bp [°C]</b>	<b>Residue HayeSep D</b>	<b>Residue Unibeads 1S</b>
HCFC-132b	CH <sub>2</sub> ClCClF <sub>2</sub>	9.08	46	n.d.	n.d.
CFC-113	CCl <sub>2</sub> FCClF <sub>2</sub>	8.45	48	0.2% (m)	n.d.
HCFC-225ca	CF <sub>3</sub> CF <sub>2</sub> CHCl <sub>2</sub>	9.37	51	n.a.	n.a.
HCFC-225cb	CClF <sub>2</sub> CF <sub>2</sub> CHClF	9.57	56	n.a.	n.a.
CFC-112	CFCl <sub>2</sub> CFCl <sub>2</sub>	10.33	92	n.d.	n.d.
HCFC-131	CCl <sub>3</sub> CH <sub>2</sub> F	12.38	103	n.a.	n.a.
<b><u>PFCs &amp; HFCs</u></b>					
HFC-23	CHF <sub>3</sub>	3.01	-82	2.6% (c)	n.a.
HFC-41	CH <sub>3</sub> F	4.38	-78	n.a.	n.a.
HFC-32	CH <sub>2</sub> F <sub>2</sub>	4.20	-52	n.d.	n.d.
HFC-125	CHF <sub>2</sub> CF <sub>3</sub>	4.87	-49	0.4% (c)	1.3% (c)
HFC-143a	CH <sub>3</sub> CF <sub>3</sub>	5.00	-48	n.d.	n.d.
HFC-161	C <sub>2</sub> H <sub>5</sub> F	6.85	-38	n.a.	n.a.
PFC-218	C <sub>3</sub> F <sub>8</sub>	4.02	-37	n.d.	n.d.
PFC-216	C <sub>3</sub> F <sub>6</sub>	4.58	-30	n.a.	n.a.
HFO-1234yf	CHFCHCF <sub>3</sub>	5.72	-28	6.9% (c)	14.9% (c)
HFC-134a	CH <sub>2</sub> FCF <sub>3</sub>	5.92	-26	n.d.	n.d.
HFC-152a	CH <sub>3</sub> CHF <sub>2</sub>	6.53	-25	n.d.	n.d.
HFC-134	CHF <sub>2</sub> CHF <sub>2</sub>	6.32	-23	1.1% (c)	3.0% (c)
HFC-227ea	CF <sub>3</sub> CHFCF <sub>3</sub>	6.52	-16	n.d.	n.d.
HFO-1234ze	CHFCHCF <sub>3</sub>	6.27	-16	n.d.	n.d.
PFC-318	c-C <sub>4</sub> F <sub>8</sub>	5.68	-6	n.d.	n.d.
HFC-236fa	CF <sub>3</sub> CH <sub>2</sub> CF <sub>3</sub>	7.22	-1	n.d.	n.d.
HFC-329ccb	C <sub>4</sub> HF <sub>9</sub>	7.67	15	n.a.	n.a.
HFC-245fa	CF <sub>3</sub> CH <sub>2</sub> CHF <sub>2</sub>	7.92	15	n.d.	n.d.
HFO-1233zd	CHClCHCF <sub>3</sub>	7.82	19	n.a.	n.a.
HFC-356mff	C <sub>4</sub> H <sub>4</sub> F <sub>6</sub>	8.35	25	n.a.	n.a.
HFC-365mfc	CF <sub>3</sub> CH <sub>2</sub> CF <sub>2</sub> CH <sub>3</sub>	9.27	40	n.a.	n.a.
<b><u>Halons</u></b>					
Halon-1301	CBrF <sub>3</sub>	3.87	-58	n.d.	n.d.
Halon-1211	CBrClF <sub>2</sub>	6.32	-4	n.d.	n.d.
Halon-1202	CF <sub>2</sub> Br <sub>2</sub>	7.45	23	n.a.	n.a.
Halon-2402	CBrF <sub>2</sub> CBrF <sub>2</sub>	8.53	47	n.d.	n.d.
Halon-2311	CF <sub>3</sub> CHBrCl	9.30	50	n.a.	n.a.

<b>Class/Name</b>	<b>Formula</b>	<b>t<sub>R</sub> [min]</b>	<b>bp [°C]</b>	<b>Residue HayeSep D</b>	<b>Residue Unibeads 1S</b>
<b><u>Chloro-, Bromo- &amp; Iodocarbons</u></b>					
Chloromethane	CH <sub>3</sub> Cl	6.02	-24	0.5% (c)	0.6% (c)
Bromomethane	CH <sub>3</sub> Br	7.00	4	3.4% (c)	1.8% (c)
Chloroethane	C <sub>2</sub> H <sub>5</sub> Cl	7.92	12	25.5% (c)	8.6% (c)
Dichloromethane	CH <sub>2</sub> Cl <sub>2</sub>	8.17	40	0.4% (c, m)	0.2% (c)
Iodomethane	CH <sub>3</sub> I	8.00	42	43.9% (c, m)	46.2% (c, m)
Trichloromethane	CHCl <sub>3</sub>	8.92	61	1.4% (c, m)	0.7% (c, m)
Bromochloromethane	CH <sub>2</sub> BrCl	9.03	68	n.d.	n.d.
Methyl chloroform	CH <sub>3</sub> CCl <sub>3</sub>	9.93	74	n.d.	n.d.
Tetrachloromethane	CCl <sub>4</sub>	9.08	77	1.1% (m)	n.d.
Trichloroethene	C <sub>2</sub> HCl <sub>3</sub>	9.55	87	n.d.	n.d.
Bromodichloromethane	CHBrCl <sub>2</sub>	10.10	90	n.d.	n.d.
Dibromomethane	CH <sub>2</sub> Br <sub>2</sub>	10.03	96	n.d.	n.d.
Dibromochloromethane	CHBr <sub>2</sub> Cl	11.53	119	n.d.	n.d.
Tetrachloroethene	C <sub>2</sub> Cl <sub>4</sub>	10.62	121	23.9% (c, m)	5.2% (c, m)
Tribromomethane	CHBr <sub>3</sub>	13.50	147	11.2% (m)	n.d.
Diiodomethane	CH <sub>2</sub> I <sub>2</sub>	15.00	181	n.a.	n.a.
<b><u>Sulfur-containing and other halogenated compounds</u></b>					
Sulfuryldifluoride	SO <sub>2</sub> F <sub>2</sub>	4.20	-55	n.d.	n.d.
Carbonyl sulfide	COS	3.77	-50	0.4% (c)	0.1% (c)
Chlorotrifluoroethylene	C <sub>2</sub> F <sub>3</sub> Cl	4.92	-28	n.a.	n.a.
Perfluorotetrahydrofuran	C <sub>4</sub> F <sub>8</sub> O	5.87	2	n.a.	n.a.
3-chloropentafluoropropene	CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> Cl	8.07	8	n.d.	7.6% (c)
Desflurane	CF <sub>3</sub> CHFOCHF <sub>2</sub>	8.42	24	n.a.	n.a.
Carbon disulfide	CS <sub>2</sub>	6.54	46	4.0% (c)	0.8% (c)
Isoflurane	CHF <sub>2</sub> OCHClCF <sub>3</sub>	9.83	49	n.a.	n.a.
Sevoflurane	CF <sub>3</sub> CF <sub>3</sub> CHOCH <sub>2</sub> F	10.35	59	n.a.	n.a.

Class/Name	Formula	t <sub>R</sub> [min]	bp [°C]	Residue HayeSep D	Residue Unibeads 1S
<b><u>Hydrocarbons and Aldehydes</u></b>					
Ethyne	C <sub>2</sub> H <sub>2</sub>	3.75	-81	0.3% (c)	1.4% (c)
Propene	C <sub>3</sub> H <sub>6</sub>	5.38	-48	35.2% (c)	28.5% (c)
Propane	C <sub>3</sub> H <sub>8</sub>	4.09	-42	0.4% (c)	0.1% (c)
Propyne	C <sub>3</sub> H <sub>4</sub>	7.17	-23	n.d.	n.d.
Formaldehyde	CH <sub>2</sub> O	7.62	-19	n.a.	n.a.
Isobutane	C <sub>4</sub> H <sub>10</sub>	5.79	-13	0.7% (c)	1.0% (c)
Isobutene	C <sub>4</sub> H <sub>8</sub>	7.32	-7	n.d.	75.3% (c)
1-butene	C <sub>4</sub> H <sub>8</sub>	7.38	-6	n.a.	n.a.
1,3-butadiene	C <sub>4</sub> H <sub>6</sub>	7.32	-4	n.a.	n.a.
n-butane	C <sub>4</sub> H <sub>10</sub>	6.05	-1	0.3% (c)	0.1% (c)
trans-2-butene	C <sub>4</sub> H <sub>8</sub>	7.02	1	25.3% (c)	19.8% (c)
cis-2-butene	C <sub>4</sub> H <sub>8</sub>	7.24	4	n.a.	n.a.
Acetaldehyde	C <sub>2</sub> H <sub>4</sub> O	11.26	20	99.2% (c, m)	82.0% (c, m)
2-methylbutane	C <sub>5</sub> H <sub>10</sub>	7.40	28	0.4% (m)	0.2% (m)
Isoprene	C <sub>5</sub> H <sub>8</sub>	8.67	34	n.a.	n.a.
n-pentane	C <sub>5</sub> H <sub>12</sub>	7.57	36	0.7% (m)	0.3% (m)
trans-2-pentene	C <sub>5</sub> H <sub>10</sub>	8.47	36	n.d.	22.2% (c, m)
cis-2-pentene	C <sub>5</sub> H <sub>10</sub>	8.56	37	n.a.	n.a.
2-methylpentane	C <sub>6</sub> H <sub>14</sub>	8.61	60	0.8% (m)	1.0% (m)
3-methylpentane	C <sub>6</sub> H <sub>14</sub>	8.71	63	1.8% (m)	n.d.
n-hexane	C <sub>6</sub> H <sub>14</sub>	8.71	68	1.5% (c)	n.d.
Benzene	C <sub>6</sub> H <sub>6</sub>	11.00	80	2.5% (c)	5.2% (c)
Cyclohexane	c-C <sub>6</sub> H <sub>12</sub>	8.82	81	n.d.	n.d.
n-heptane	C <sub>7</sub> H <sub>16</sub>	10.06	98	23.1% (c, m)	4.0% (m)
Toluene	C <sub>7</sub> H <sub>8</sub>	14.52	111	17.4% (c, m)	9.8% (c, m)