

# Atomic emission detector with gas chromatographic separation and cryogenic pre-concentration (CryoTrap-GC-AED) for atmospheric trace gas measurements

Einar Karu<sup>1</sup>, Mengze Li<sup>1</sup>, Lisa Ernle<sup>1</sup>, Carl A.M. Brenninkmeijer<sup>1</sup>, Jos Lelieveld<sup>1</sup>, Jonathan Williams<sup>1</sup>

5 <sup>1</sup>Atmospheric Chemistry Department, Max Planck Institute for Chemistry, 55128 Mainz, Germany

*Correspondence to:* Jonathan Williams (jonathan.williams@mpic.de)

## Supplementary

Apel-Riemer-2015, 84 multi-component gas calibration standard

10 **Table S1: Retention times of Apel-Riemer-2015, Apel-Riemer Environmental, Inc. 84 multi-component gas phase calibration mix in UHP nitrogen balance. Stated uncertainty better than  $\pm 5\%$  for all components. MR certificate analysis date: June 9, 2015.**

---

<b>IAGOS- CARIBIC-2018</b>			
<b>RT 30°C (min)</b>	<b>Compound</b>	<b>CAS #</b>	<b>Concentration (ppb)</b>
3.46	Propene	115-07-1	51.8
3.50	Carbonyl Sulfide (OCS)	463-58-1	51.2
3.55	Dichlorodifluoromethane (R-12)	75-71-8	49.6
3.61	Chlorodifluoromethane (HCFC-22)	75-45-6	50.8
3.91	1,2-Dichlorotetrafluoroethane (R-114)	76-14-2	55.5
4.06	Chloromethane	74-87-3	52.5
4.31	Isobutene	115-11-7	51.3
4.39	Vinyl Chloride	75-01-4	52.3
4.50	1,3-Butadiene	106-99-0	51.7
4.77	Acetaldehyde	75-07-0	58.2
5.20	Methanol	67-56-1	51.7
5.38	Bromomethane	74-83-9	55.0
5.72	Chloroethane	75-00-3	54.8
6.50	Trichlorofluoromethane (F-11)	75-69-4	51.8
6.77	Pentane	109-66-0	61.8
	Ethanol	64-17-5	45.3

7.61	Isoprene	78-79-5	52.4
8.24	Acrolein	107-02-8	46.1
	Propanal	123-38-6	43.2
8.38	1,1-Dichloroethene	75-35-4	75.4
	1,1,2-Trichloro-1,2,2-Trifluoroethane (CFC-113)	76-13-1	70.6
	Acetone	67-64-1	43.2
8.85	Methyl Iodide	74-88-4	69.4
9.00	Carbon Disulfide (CS <sub>2</sub> )	75-15-0	47.0
9.44	2-Propanol	67-63-0	50.7
9.95	Acetonitrile	75-05-8	50.0
	Dichloromethane	75-09-2	52.2
10.22	Cyclopentane	287-92-3	52.8
11.14	Acrylonitrile	107-13-1	64.3
	trans-1,2-Dichloroethene	156-60-5	62.3
11.03	Methyl Tertiary Butyl Ether (MTBE)	1634-04-4	61.0
11.82	Hexane	110-54-3	52.1
12.25	Methacrolein	78-85-3	48.9
12.36	1,1-Dichloroethane	75-34-3	57.8
12.58	Vinyl Acetate	108-05-4	56.4
12.93	1-Propanol	71-23-8	51.4
13.57	Butanal	123-72-8	59.6
13.66	Methyl Vinyl Ketone	78-94-4	74.4
14.05	cis-1,2-Dichloroethene	156-59-2	52.3
14.10	Methyl Ethyl Ketone	78-93-3	51.1
14.90	Chloroform	67-66-3	51.9
	1,1,1-Trichloroethane	71-55-6	52.4
15.32	Cyclohexane	110-82-7	53.4
15.65	Tetrachloromethane	56-23-5	51.4
16.18	Benzene	71-43-2	48.1
16.36	1,2-Dichloroethane	107-06-2	58.5
	Trichloroethylene	79-01-6	54.8
17.83	1-Butanol	71-36-3	40.5
18.04	Isopropyl nitrate	1712-64-7	44.7

18.31	Hydroxyacetone	116-09-6	53.1
	2-Pentanone	107-87-9	50.2
18.40	1,2-Dichloropropane	78-87-5	50.5
18.56	Pentanal	110-62-3	59.9
18.64	3-Pentanone	96-22-0	52.5
18.69	1,4-Dioxane	123-91-1	50.7
19.07	Bromodichloromethane	75-27-4	49.2
19.81	Propyl nitrate	627-13-4	47.4
20.14	cis-1,3-Dichloropropene	10061-01-5	49.6
20.47	4-Methyl-2-Pentanone	108-10-1	51.7
20.85	Toluene	108-88-3	51.6
21.33	trans-1,3-Dichloropropene	10061-02-6	51.3
21.49	1,1,2-Trichloroethane	79-00-5	52.9
21.90	Isobutyl nitrate	543-29-3	45.0
	3-Hexanone	598-38-8	50.9
22.14	Tetrachloroethylene	127-18-4	55.5
22.44	2-Hexanone	591-78-6	52.0
22.68	Hexanal	66-25-1	55.8
23.06	1,2-Dibromoethane	106-93-4	50.2
24.21	Chlorobenzene	108-90-7	53.3
24.42	Ethyl Benzene	100-41-4	50.8
	m-Xylene	108-38-3	50.8
24.71	p-Xylene	106-42-3	51.5
25.66	o-Xylene	95-47-6	50.6
25.70	Styrene	100-42-5	52.5
26.16	Bromoform	75-25-2	52.4
27.34	1,1,2,2-Tetrachloroethane	79-34-5	50.7
27.96	1,3,5-Trimethylbenzene	108-67-8	51.2
28.88	1,2,4-Trimethylbenzene	95-63-6	50.7
29.61	(m-)1,3-Dichlorobenzene	541-73-1	52.9
29.84	(p-)1,4-Dichlorobenzene	106-46-7	55.6
29.91	1,2,3-Trimethylbenzene	526-73-8	46.2
30.15	Benzyl Chloride	100-44-7	61.7

30.75	(o-)1,2-Dichlorobenzene	95-50-1	61.8
	1,2,4-Trichlorobenzene	120-82-1	52.7

NPL-2017, National Physical Laboratory (NPL) 30 component NMHC primary calibration standard

**Table S2: Retention times of NPL-2017 30 ozone precursor NMHC gas phase primary calibration reference material in UHP nitrogen balance. Stated uncertainties are based on  $2\sigma$ , providing a coverage probability of ~95%. Calibration date 7 May – 21 June 2017.**

15

<b>IAGOS-CARIBIC-2018</b>		NPL-2017 (Bottle: D51 7546)	
<b>RT 30°C (min)</b>	<b>Compound</b>	<b>MR (pmol mol<sup>-1</sup>)</b>	<b>Uncertainty (pmol mol<sup>-1</sup>)</b>
	Ethene	3930	80
	Ethyne	4140	210
3.15	Ethane	4010	80
3.46	Propene	3930	80
	Propane	3950	80
3.93	Isobutane	4030	110
4.31	1-Butene	3980	80
4.36	n-Butane	3990	80
4.50	1,3-Butadiene	4040	80
4.60	trans-2-Butene	4000	80
4.88	cis-2-Butene	3990	80
5.90	Isopentane	3940	80
6.58	1-Pentene	4040	80
6.76	n-Pentane	3960	80
7.28	trans-2-Pentene	3980	80
7.61	Isoprene	4140	90
10.11	2-Methylpentane	4150	80
11.81	n-Hexane	4150	80
16.17	Benzene	4140	80
16.33	2,2,4-Trimethylpentane	3900	80
16.84	n-Heptane	4160	80
20.84	Toluene	4020	110
21.08	n-Octane	3910	80

24.41	Ethylbenzene	4350	110
24.70	m-Xylene	8460	220
	p-Xylene		
25.64	o-Xylene	4160	110
27.95	1,3,5-Trimethylbenzene	3940	100
28.86	1,4,4-Trimethylbenzene	4060	110
29.90	1,2,3-Trimethylbenzene	3890	100

---