Supplement of

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

Einar Karu et al.

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

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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 ±5% for all components. MR certificate analysis date: June 9, 2015.

| RT 30°C (min) | Compound                          | CAS #     | Concentration (ppb) |
|--------------|-----------------------------------|-----------|---------------------|
| 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 (CS₂)            | 75-15-0   | 47.0                |
| Number | Compound                                      | CAS Number | RI  | DBE  |
|--------|-----------------------------------------------|------------|-----|------|
| 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|
|        | Hydroxyacetone                                | 116-09-6   | 53.1|
| 18.31  | 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|
| RT (s) | Compound                        | NPL Code   | Uncertainty (%) |
|-------|---------------------------------|------------|-----------------|
| 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            |
| 22.14 | 3-Hexanone                      | 598-38-8   | 50.9            |
| 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            |
| 24.71 | m-Xylene                        | 108-38-3   | 50.8            |
| 25.66 | p-Xylene                        | 106-42-3   | 51.5            |
| 25.70 | o-Xylene                        | 95-47-6    | 50.6            |
| 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 2σ, providing a coverage probability of ~95%. Calibration date 7 May – 21 June 2017.

IAGOS-CARIBIC-2018

NPL-2017 (Bottle: D51 7546)
| RT 30°C (min) | Compound            | MR (pmol mol⁻¹) | Uncertainty (pmol mol⁻¹) |
|--------------|---------------------|-----------------|--------------------------|
| 3.15         | Ethene              | 3930            | 80                       |
|              | Ethyne              | 4140            | 210                      |
| 3.46         | Ethane              | 4010            | 80                       |
|              | Propene             | 3930            | 80                       |
| 3.93         | Propene             | 3950            | 80                       |
| 4.31         | Isobutane           | 4030            | 110                      |
| 4.36         | 1-Butene            | 3980            | 80                       |
| 4.50         | n-Butane            | 3990            | 80                       |
| 4.60         | 1,3-Butadiene       | 4040            | 80                       |
| 4.88         | trans-2-Butene      | 4000            | 80                       |
| 5.90         | cis-2-Butene        | 3990            | 80                       |
| 6.58         | Isopentane          | 3940            | 80                       |
| 6.76         | 1-Pentene           | 4040            | 80                       |
| 7.28         | n-Pentane           | 3960            | 80                       |
| 7.61         | trans-2-Pentene     | 3980            | 80                       |
| 10.11        | Isoprene            | 4140            | 90                       |
| 11.81        | 2-Methylpentane     | 4150            | 80                       |
| 16.17        | n-Hexane            | 4150            | 80                       |
| 16.33        | Benzene             | 4140            | 80                       |
| 16.84        | 2,2,4-Trimethylpentane | 3900 | 80 |
| 20.84        | n-Heptane           | 4160            | 80                       |
| 21.08        | Toluene             | 4020            | 110                      |
| 24.41        | n-Octane            | 3910            | 80                       |
| 24.70        | Ethylbenzene        | 4350            | 110                      |
|              | m-Xylene            | 8460            | 220                      |
| 25.64        | p-Xylene            | 4160            | 110                      |
| 27.95        | o-Xylene            | 4160            | 110                      |
| 28.86        | 1,3,5-Trimethylbenzene | 3940 | 100 |
| 29.90        | 1,4,4-Trimethylbenzene | 4060 | 110 |
|              | 1,2,3-Trimethylbenzene | 3890 | 100 |