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*Supplement of*

# Measurement of Henry's law and liquid-phase loss rate constants of peroxypropionic nitric anhydride (PPN) in deionized water and in $n$-octanol

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**Table S1.** Schedule of experiments: PAN in DI water.

| Internal reference | GC-ECD | $T$ (°C) | $V_l$ (mL) | $\Phi$ (mL min$^{-1}$) | $\frac{\Phi}{V_l}$ (min$^{-1}$) | $\frac{\mathrm{d}}{\mathrm{d}t}\ln\left(\frac{c_{g,0}}{c_{g,t}}\right)$ (min$^{-1}$) |
|---|---|---|---|---|---|---|
| KN 211026 | HP | 20.0±0.1 | 140±2 | 317±3 | 2.26±0.04 | 0.0532±0.0006 |
| KN 211028 | HP | 20.0±0.1 | 140±2 | 532±6 | 3.80±0.07 | 0.0592±0.0010 |
| AM 211108 | Varian | 20.00±0.01 | 140±2 | 124±1 | 0.89±0.02 | 0.0302±0.0001 |
| HO 211108 | HP | 5.0±0.1 | 100±2 | 240±3 | 2.40±0.05 | 0.0190±0.0003 |
| AM 211116 | Varian | 5.00±0.01 | 50.0±0.4 | 481±5 | 9.6±0.1 | 0.0466±0.0001 |
| KN 211118-1 | HP | 5.0±0.1 | 75.0±0.4 | 541±6 | 7.21±0.09 | 0.0394±0.0003 |
| KN 211104 | HP | 5.0±0.1 | 30.0±0.4 | 433±5 | 14.4±0.2 | 0.0639±0.0004 |
| KN 211116 | HP | 5.0±0.1 | 100±2 | 481±5 | 4.81±0.11 | 0.0299±0.0002 |
| KN 211118-2 | HP | 20.0±0.1 | 140±2 | 177±2 | 1.27±0.02 | 0.0299±0.0002 |
| KN 211123 | HP | 20.0±0.1 | 140±2 | 570±6 | 4.07±0.07 | 0.0654±0.0011 |
| AM 211123 | Varian | 5.00±0.01 | 75.0±0.4 | 451±5 | 6.01±0.07 | 0.0309±0.0001 |
| KN 211125 | HP | 20.0±0.1 | 100±2 | 697±8 | 6.97±0.16 | 0.0899±0.0023 |

**Table S2.** Schedule of experiments: PPN in DI water. Experiments were conducted with the Varian GC-ECD.

| Internal reference | $T$ (°C) | $V_l$ (mL) | $\Phi$ (mL min$^{-1}$) | $\frac{\Phi}{V_l}$ (min$^{-1}$) | $\frac{\mathrm{d}}{\mathrm{d}t}\ln\left(\frac{c_{g,0}}{c_{g,t}}\right)$ (min$^{-1}$) |
|---|---|---|---|---|---|
| MV 220301 | 20.00±0.01 | 100±2 | 125±15 | 1.25±0.15 | 0.043±0.005 |
| MV 220308 | 20.00±0.01 | 100±2 | 433±52 | 4.33±0.53 | 0.085±0.002 |
| MV 220315-1 | 20.00±0.01 | 150±2 | 496±5 | 3.33±0.06 | 0.0706±0.0010 |
| MV 220315-2 | 20.00±0.01 | 100±2 | 620±7 | 6.23±0.14 | 0.1235±0.0018 |
| MV 220317-1 | 5.00±0.01 | 150±2 | 118±1 | 0.79±0.01 | 0.01098±0.00004 |
| MV 220317-2 | 5.00±0.01 | 150±2 | 294±3 | 1.97±0.03 | 0.01818±0.00005 |
| MV 220322-1 | 5.00±0.01 | 150±2 | 235±3 | 1.58±0.02 | 0.01533±0.00005 |
| MV 220322-2 | 5.00±0.01 | 150±2 | 353±4 | 2.37±0.04 | 0.01932±0.00005 |
| MV 220324-1 | 5.00±0.01 | 150±2 | 176±2 | 1.18±0.02 | 0.01357±0.00002 |

**Table S2 (continued).** Schedule of experiments: PPN in DI water. Experiments were conducted with the Varian GC-ECD.

| **Internal reference** | $T$ **(°C)** | $V_l$ **(mL)** | $\Phi$ **(mL min$^{-1}$)** | $\frac{\Phi}{V_l}$ **(min$^{-1}$)** | $\frac{\mathrm{d}}{\mathrm{d}t}\ln\left(\frac{c_{g,0}}{c_{g,t}}\right)$ **(min$^{-1}$)** |
|---|---|---|---|---|---|
| MV 220324-2 | 12.50±0.01 | 150±2 | 121±1 | 0.81±0.01 | 0.0204±0.00018 |
| MV 220329-1 | 12.50±0.01 | 150±2 | 243±3 | 1.62±0.03 | 0.0288±0.0001 |
| MV 220329-2 | 12.50±0.01 | 150±2 | 365±4 | 2.43±0.04 | 0.0373±0.0001 |
| MV 220331-1 | 12.50±0.01 | 150±2 | 182±2 | 1.22±0.02 | 0.0251±0.0001 |
| MV 220331-2 | 12.50±0.01 | 150±2 | 304±3 | 2.03±0.04 | 0.0332±0.0002 |
| MV 220405-1 | 20.00±0.01 | 150±2 | 375±4 | 2.50±0.04 | 0.0665±0.0001 |
| MV 220405-2 | 8.50±0.01 | 150±2 | 240±3 | 1.60±0.03 | 0.0212±0.0001 |
| MV 220405-3 | 8.50±0.01 | 150±2 | 481±5 | 3.20±0.06 | 0.0345±0.0001 |
| MV 220407-1 | 8.50±0.01 | 150±2 | 353±4 | 2.35±0.04 | 0.0285±0.0001 |
| MV 220407-2 | 8.50±0.01 | 150±2 | 530±6 | 3.54±0.06 | 0.0388±0.0002 |
| MV 220407-3 | 5.00±0.01 | 150±2 | 408±4 | 2.72±0.05 | 0.0231±0.0001 |
| HO 220411-1 | 16.00±0.01 | 150±2 | 430±5 | 2.87±0.05 | 0.0567±0.0003 |
| HO 220411-2 | 16.00±0.01 | 150±2 | 246±3 | 1.64±0.03 | 0.03744±0.00004 |
| HO 220412-1 | 16.00±0.01 | 150±2 | 213±2 | 1.42±0.02 | 0.03453±0.00005 |
| HO 220412-3 | 20.00±0.01 | 150±2 | 246±3 | 1.64±0.03 | 0.0487±0.0001 |
| HO 220414-1 | 16.00±0.01 | 150±2 | 336±4 | 2.24±0.04 | 0.0451±0.0001 |
| HO 220414-2 | 16.00±0.01 | 150±2 | 580±6 | 3.87±0.07 | 0.0665±0.0001 |
| KE 220531-1 | 25.00±0.01 | 100.0±0.4 | 312±3 | 3.12±0.04 | 0.1122±0.0006 |
| KE 220531-2 | 25.00±0.01 | 100.0±0.4 | 125±1 | 1.25±0.01 | 0.0628±0.0001 |
| KE 220531-3 | 25.00±0.01 | 100.0±0.4 | 281±3 | 2.81±0.03 | 0.1048±0.0006 |
| KE 220531-4 | 25.00±0.01 | 100.0±0.4 | 344±4 | 3.44±0.04 | 0.125±0.002 |
| KE 220603-1 | 25.00±0.01 | 100.0±0.4 | 189±2 | 1.89±0.02 | 0.0810±0.0003 |

**Table S3.** Schedule of experiments: PPN in n-octanol. Experiments were conducted with the Varian GC-ECD.

| Internal reference | $T$ (°C) | $V_l$ (mL) | $\Phi$ (mL min$^{-1}$) | $\frac{\Phi}{V_l}$ (min$^{-1}$) | $\frac{d}{dt}\ln\left(\frac{c_{g,0}}{c_{g,t}}\right)$ (min$^{-1}$) |
|---|---|---|---|---|---|
| KE 220607-1c | 20.00±0.01 | 50.0±0.4 | 277±3 | 5.54±0.08 | 0.00255±0.00004 |
| KE 220607-1d | 20.00±0.01 | 50.0±0.4 | 339±4 | 6.78±0.09 | 0.00381±0.00003 |
| KE 220609-1b | 20.00±0.01 | 50.0±0.4 | 186±2 | 3.73±0.05 | 0.00242±0.00005 |
| KE 220609-1c | 20.00±0.01 | 50.0±0.4 | 373±4 | 7.46±0.10 | 0.00413±0.00002 |
| KE 220609-1d | 20.00±0.01 | 50.0±0.4 | 311±3 | 6.22±0.08 | 0.00374±0.00005 |
| KE 220609-1e | 20.00±0.01 | 50.0±0.4 | 125±1 | 2.49±0.03 | 0.00221±0.00002 |
| KE 220609-1f | 20.00±0.01 | 50.0±0.4 | 100±1 | 2.00±0.03 | 0.0018152±0.0000009 |
| KE 220610-1 | 20.00±0.01 | 50.0±0.4 | 281±3 | 5.62±0.08 | 0.00363±0.00002 |
| KE 220621-2a | 20.00±0.01 | 50.0±0.4 | 259±3 | 5.17±0.07 | 0.00317±0.00002 |
| KE 220621-2b | 20.00±0.01 | 50.0±0.4 | 401±4 | 8.02±0.11 | 0.004642±0.000009 |
| KE 220621-2c | 20.00±0.01 | 50.0±0.4 | 130±1 | 2.60±0.04 | 0.002091±0.000001 |
| KE 220622-1 | 20.00±0.01 | 50.0±0.4 | 223±2 | 4.47±0.06 | 0.00346±0.00005 |
| KE 220622-2b | 5.00±0.01 | 50.0±0.4 | 384±4 | 7.68±0.10 | 0.00152±0.00001 |
| KE 220622-2c | 5.00±0.01 | 50.0±0.4 | 118±1 | 2.37±0.03 | 0.000562±0.000001 |
| KE 220623-1 | 5.00±0.05 | 50.0±0.4 | 177±2 | 3.54±0.05 | 0.0008265±0.0000009 |
| KE 220624-1a | 5.00±0.05 | 50.0±0.4 | 234±3 | 4.68±0.06 | 0.00144±0.00003 |
| KE 220624-1b | 5.00±0.05 | 50.0±0.4 | 321±4 | 6.42±0.09 | 0.00176±0.00004 |
| KE 220624-1c | 5.00±0.05 | 50.0±0.4 | 350±4 | 7.00±0.10 | 0.00202±0.00005 |
| KE 220627-1a | 25.00±0.01 | 50.0±0.4 | 312±3 | 6.25±0.09 | 0.00533±0.00009 |
| KE 220627-1b | 25.00±0.01 | 50.0±0.4 | 125±1 | 2.50±0.03 | 0.00379±0.00003 |
| KE 220627-1c | 25.00±0.01 | 50.0±0.4 | 282±3 | 5.64±0.08 | 0.00543±0.00002 |
| KE 220627-1d | 25.00±0.01 | 50.0±0.4 | 188±2 | 3.76±0.05 | 0.00439±0.00001 |
| KE 220627-1e | 25.00±0.01 | 50.0±0.4 | 345±4 | 6.89±0.09 | 0.005763±0.000005 |
| KE 220628-1a | 16.00±0.01 | 50.0±0.4 | 304±3 | 6.09±0.08 | 0.0027±0.0001 |
| KE 220628-1c | 16.00±0.01 | 50.0±0.4 | 275±3 | 5.49±0.07 | 0.00263±0.00003 |
| KE 220628-1d | 16.00±0.01 | 50.0±0.4 | 183±2 | 3.67±0.05 | 0.00192±0.00003 |
| KE 220628-1e | 16.00±0.01 | 50.0±0.4 | 337±4 | 6.74±0.09 | 0.002889±0.000001 |
| KE 220629-2c | 5.00±0.01 | 50.0±0.4 | 200±2 | 4.01±0.05 | 0.00095±0.00001 |

**Table S3 (continued).** Schedule of experiments: PPN in n-octanol. Experiments were conducted with the Varian GC-ECD.

| **Internal reference** | $\boldsymbol{T}$ **(°C)** | $\boldsymbol{V_l}$ **(mL)** | $\boldsymbol{\Phi}$ **(mL min$^{-1}$)** | $\boldsymbol{\frac{\Phi}{V_l}}$ **(min$^{-1}$)** | $\boldsymbol{\frac{d}{dt}\ln\left(\frac{c_{g,0}}{c_{g,t}}\right)}$ **(min$^{-1}$)** |
|---|---|---|---|---|---|
| KE 220711-1b | 8.50±0.01 | 50.0±0.4 | 118±1 | 2.37±0.03 | 0.000843±0.000009 |
| KE 220711-1c | 8.50±0.01 | 50.0±0.4 | 267±3 | 5.34±0.07 | 0.00155±0.00001 |
| KE 220711-1d | 8.50±0.01 | 50.0±0.4 | 178±2 | 3.56±0.05 | 0.0010546±0.0000009 |
| KE 220712-1a | 8.50±0.01 | 50.0±0.4 | 327±4 | 6.55±0.09 | 0.00197±0.00002 |
| KE 220712-1b | 8.50±0.01 | 50.0±0.4 | 238±3 | 4.77±0.06 | 0.00162±0.00002 |
| KE 220712-1c | 8.50±0.01 | 50.0±0.4 | 358±4 | 7.16±0.10 | 0.00223±0.00004 |
| KE 220712-2b | 12.50±0.01 | 50.0±0.4 | 121±1 | 2.43±0.03 | 0.001046±0.000002 |
| KE 220713-1a | 12.50±0.01 | 50.0±0.4 | 273±3 | 5.46±0.07 | 0.00214±0.00002 |
| KE 220713-1b | 12.50±0.01 | 50.0±0.4 | 182±2 | 3.64±0.05 | 0.00168±0.00002 |
| KE 220713-1c | 12.50±0.01 | 50.0±0.4 | 334±4 | 6.68±0.09 | 0.0025±0.0001 |
| KE 220713-1d | 12.50±0.01 | 50.0±0.4 | 152±2 | 3.03±0.04 | 0.00161±0.00008 |
| KE 220713-1e | 12.50±0.01 | 50.0±0.4 | 243±3 | 4.86±0.07 | 0.00206±0.00007 |
| KE 220713-2 | 5.00±0.01 | 50.0±0.4 | 147±2 | 2.94±0.04 | 0.000682±0.000001 |
| KE 220714-1a | 5.00±0.01 | 50.0±0.4 | 252±3 | 5.05±0.07 | 0.00127±0.00002 |
| KE 220714-1b | 5.00±0.01 | 50.0±0.4 | 211±2 | 4.23±0.06 | 0.00105±0.00004 |
| KE 220714-1c | 5.00±0.01 | 50.0±0.4 | 382±4 | 7.64±0.10 | 0.00181±0.00003 |
| KE 220714-1d | 5.00±0.01 | 50.0±0.4 | 265±3 | 5.29±0.07 | 0.00129±0.00003 |
| KE 220714-1e | 5.00±0.01 | 50.0±0.4 | 306±3 | 6.12±0.08 | 0.00167±0.00006 |
| KE 220718-1b | 5.00±0.01 | 50.0±0.4 | 354±4 | 7.09±0.10 | 0.00122±0.00003 |
| KE 220718-1c | 5.00±0.01 | 50.0±0.4 | 331±4 | 6.62±0.09 | 0.00142±0.00001 |
| KE 220718-1d | 5.00±0.01 | 50.0±0.4 | 401±4 | 8.02±0.11 | 0.001641±0.000001 |
| KE 220719-1a | 5.00±0.01 | 50.0±0.4 | 318±3 | 6.36±0.09 | 0.00167±0.00002 |
| KE 220719-1b | 5.00±0.01 | 50.0±0.4 | 365±4 | 7.30±0.10 | 0.00195±0.00004 |
| KE 220719-1c | 5.00±0.01 | 50.0±0.4 | 413±5 | 8.26±0.11 | 0.00206±0.00006 |
| KE 220719-2 | 5.00±0.01 | 100.0±0.6 | 94±1 | 0.94±0.01 | 0.000285±0.000001 |
| KE 220720-1a | 5.00±0.01 | 100.0±0.6 | 176±2 | 1.76±0.02 | 0.00062±0.00001 |
| KE 220720-1b | 5.00±0.01 | 100.0±0.6 | 129±1 | 1.29±0.02 | 0.000466±0.000007 |
| KE 220720-1c | 5.00±0.01 | 100.0±0.6 | 188±2 | 1.88±0.02 | 0.000667±0.000008 |

**Table S3 (continued).** Schedule of experiments: PPN in n-octanol. Experiments were conducted with the Varian GC-ECD.

| Internal reference | $T$ (°C) | $V_l$ (mL) | $\Phi$ (mL min$^{-1}$) | $\frac{\Phi}{V_l}$ (min$^{-1}$) | $\frac{\mathrm{d}}{\mathrm{d}t}\ln\left(\frac{c_{g,0}}{c_{g,t}}\right)$ (min$^{-1}$) |
|---|---|---|---|---|---|
| KE 220720-1d | 5.00±0.05 | 100.0±0.6 | 153±2 | 1.53±0.02 | 0.000444±0.000001 |
| KE 220721-1b | 16.00±0.01 | 50.0±0.4 | 257±3 | 5.14±0.07 | 0.00235±0.00004 |
| KE 220721-1c | 16.00±0.01 | 50.0±0.4 | 153±2 | 3.06±0.04 | 0.001639±0.000007 |
| KE 220721-1d | 16.00±0.01 | 50.0±0.4 | 221±2 | 4.42±0.06 | 0.00219±0.00002 |
| KE 220725-1a | 20.00±0.01 | 100.0±0.4 | 148±2 | 1.48±0.02 | 0.00140±0.00006 |
| KE 220725-1b | 20.00±0.01 | 100.0±0.4 | 432±5 | 4.32±0.05 | 0.00372±0.00009 |
| KE 220725-1c | 20.00±0.01 | 100.0±0.4 | 99±1 | 0.99±0.01 | 0.00149±0.00003 |
| KE 220725-1d | 20.00±0.01 | 100.0±0.4 | 185±2 | 1.85±0.02 | 0.00206±0.00001 |
| KE 220725-1e | 20.00±0.01 | 100.0±0.4 | 463±5 | 4.63±0.05 | 0.00325±0.00003 |
| KE 220725-1f | 20.00±0.01 | 100.0±0.4 | 111±1 | 1.11±0.01 | 0.001492±0.000001 |
| KE 220726-1a | 25.00±0.01 | 100.0±0.4 | 150±2 | 1.50±0.02 | 0.00350±0.00009 |
| KE 220726-1b | 25.00±0.01 | 100.0±0.4 | 100±1 | 1.00±0.01 | 0.00307±0.00007 |
| KE 220726-1c | 25.00±0.01 | 100.0±0.4 | 451±5 | 4.51±0.05 | 0.0050±0.0001 |
| KE 220726-1d | 25.00±0.01 | 100.0±0.4 | 201±2 | 2.01±0.02 | 0.0033±0.0001 |
| KE 220726-1e | 25.00±0.01 | 100.0±0.4 | 502±6 | 5.02±0.06 | 0.00513±0.00006 |
| KE 220726-2 | 12.50±0.01 | 100.0±0.4 | 102±1 | 1.02±0.01 | 0.000622±0.000002 |
| KE 220727-1a | 12.50±0.01 | 100.0±0.4 | 204±2 | 2.04±0.02 | 0.00115±0.00001 |
| KE 220727-1b | 12.50±0.01 | 100.0±0.4 | 450±5 | 4.50±0.05 | 0.00190±0.00002 |
| KE 220727-1c | 12.50±0.01 | 100.0±0.4 | 144±2 | 1.44±0.02 | 0.00088±0.00003 |
| KE 220727-1d | 12.50±0.01 | 100.0±0.4 | 390±4 | 3.90±0.05 | 0.00174±0.00007 |
| KE 220727-1e | 12.50±0.01 | 100.0±0.4 | 240±3 | 2.40±0.03 | 0.00131±0.00003 |
| KE 220727-2 | 8.50±0.01 | 100.0±0.4 | 101±1 | 1.01±0.01 | 0.000438±0.000001 |
| KE 220728-1a | 8.50±0.01 | 100.0±0.4 | 296±3 | 2.96±0.03 | 0.00118±0.00004 |

**Table S4.** Schedule of experiments: PPN in n-octanol containing ~(0.6±0.2) mM of α-tocopherol. Experiments were conducted with the Varian GC-ECD.

| **Internal reference** | $T$ (°C) | $V_l$ (mL) | $\Phi$ (mL min$^{-1}$) | $\frac{\Phi}{V_l}$ (min$^{-1}$) | $\frac{d}{dt}\ln\left(\frac{c_{g,0}}{c_{g,t}}\right)$ (min$^{-1}$) |
|---|---|---|---|---|---|
| KE 220809-1b | 20.00±0.01 | 100.0±0.4 | 123±1 | 1.23±0.01 | 0.0027±0.0002 |
| KE 220809-1c | 20.00±0.01 | 100.0±0.4 | 278±3 | 2.78±0.03 | 0.00345±0.00002 |
| KE 220809-1d | 20.00±0.01 | 100.0±0.4 | 185±2 | 1.85±0.02 | 0.003015±0.000004 |
| KE 220810-1a | 20.00±0.01 | 100.0±0.4 | 339±4 | 3.39±0.04 | 0.0033±0.0001 |
| KE 220810-1b | 20.00±0.01 | 100.0±0.4 | 197±2 | 1.97±0.02 | 0.00310±0.00009 |
| KE 220810-1c | 20.00±0.01 | 100.0±0.4 | 247±3 | 2.47±0.03 | 0.00341±0.00005 |
| KE 220810-1d | 20.00±0.01 | 100.0±0.4 | 370±4 | 3.70±0.04 | 0.00404±0.00003 |
| KE 220810-1e | 20.00±0.01 | 100.0±0.4 | 123±1 | 1.23±0.01 | 0.003100±0.000007 |

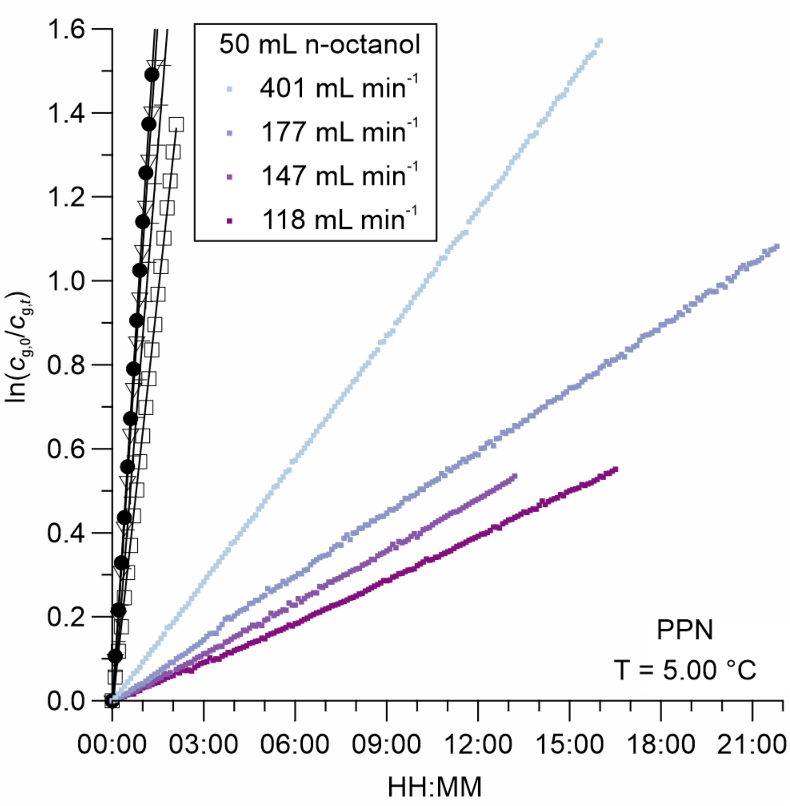


**Figure S1.** Plots of $\ln(c_{g,0}/c_{g,t})$ versus $t$ for PPN, observed in overnight experiments downstream from 50 mL of n-octanol at 5.00 °C for four different volumetric flow rates. Each data point shown is derived from the peak area of an individual chromatogram, of which there were between 119 and 219 at each flow rate. The data from Figure 3 are superimposed in black colour.

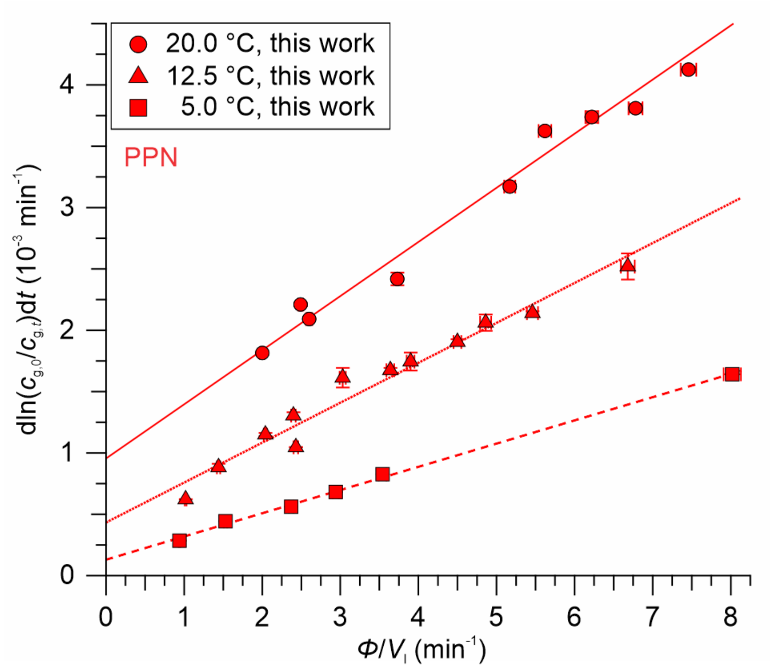


**Figure S2.** Plots of dln($c_{g,0}$/$c_{g,t}$)/d$t$ versus $\Phi/V_l$ for PPN in n-octanol at 20.00 °C (●), 12.50 °C (▲), and 5.00 °C (■).

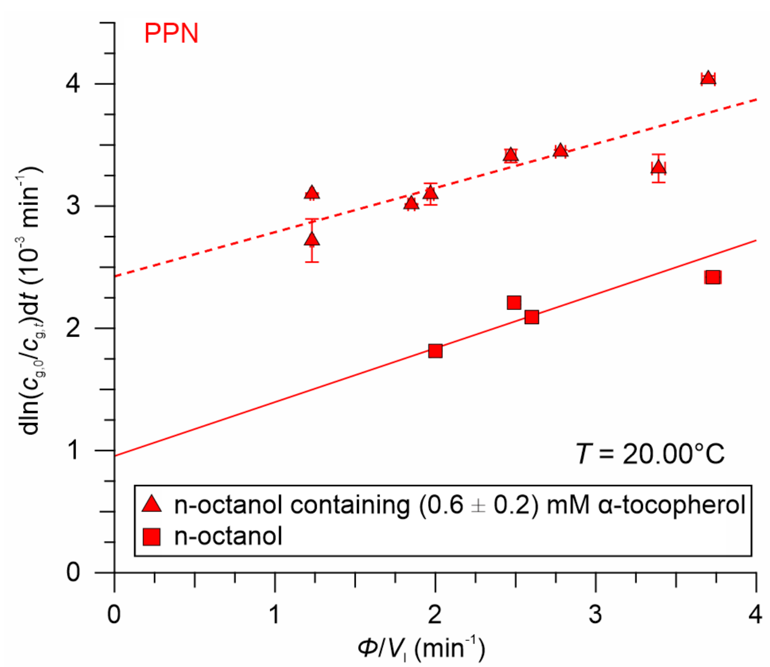


**Figure S3**. Effect of adding Vitamin E on plots of dln($c_{g,0}$/$c_{g,t}$)/d$t$ versus $\Phi/V_l$ for PPN in n-octanol at 20.00 ºC. Results with unadulterated n-octanol are shown as (■), whereas results with n-octanol containing ~(0.6±0.2) mM of α-tocopherol are shown as (▲).

**Table S5.** Dimensionless Henry's law constants of PAN in deionized water, $H_{\mathrm{S,aq}}^{cc}(\mathrm{PAN})$. N/A = not available. n/d = not determined.

| | $\boldsymbol{H_{\mathrm{S,aq}}^{cc}(\mathrm{PAN})}$ **(unitless)** | |
|---|---|---|
| **Reference** | **293.15 K** | **278.15 K** |
| (Lee, 1984) | 98.3±4.8 (295 K) | n/d |
| (Kames et al., 1991) | 97.4±3.6 | N/A |
| (Kames and Schurath, 1995) | 97.9±2.0 | N/A |
| This work | 101±10 | 269±13 |

**Table S6.** Dimensionless Henry's law constants of PPN in deionized water, $H_{\mathrm{S,aq}}^{cc}(\mathrm{PPN})$. N/A = not available.

| | $\boldsymbol{H_{\mathrm{S,aq}}^{cc}(\mathrm{PPN})}$ **(unitless)** | | | | | |
|---|---|---|---|---|---|---|
| **Reference** | **298.15** | **293.15 K** | **289.15 K** | **285.65 K** | **281.65 K** | **278.15 K** |
| (Kames and Schurath, 1995) | N/A | 70.8±1.5 | N/A | N/A | N/A | N/A |
| This work | 36.5±1.1 | 64.2±4.4 | 74.5±4.5 | 96.4±1.7 | 114.7±7.1 | 160.1±5.6 |

**Table S7.** Dimensionless Henry's law constants of PPN in n-octanol, $H_{\mathrm{S,oct}}^{cc}(\mathrm{PPN})$.

| | $\boldsymbol{H_{\mathrm{S,oct}}^{cc}(\mathrm{PPN})}$ **(unitless)** | | | | | |
|---|---|---|---|---|---|---|
| **Reference** | **298.15 K** | **293.15 K** | **289.15 K** | **285.65 K** | **281.65 K** | **278.15 K** |
| This work | (2.15±0.11) $\times 10^3$ | (2.35±0.21) $\times 10^3$ | (2.98±0.19) $\times 10^3$ | (3.07±0.18) $\times 10^3$ | (3.62±0.26) $\times 10^3$ | (4.65±0.36) $\times 10^3$ |

**Table S8.** Loss rate constants of PPN at 293.15 K.

| **Compound and solvent / medium** | ***k*** **($10^{-4}$ $s^{-1}$)** |
|---|---|
| PPN in DI water | 3.8±0.6 |
| PPN in n-octanol | 0.18±0.03 |
| PPN in n-octanol containing ~(0.6±0.2) mM α-tocopherol | 0.40±0.04 |
| PPN in air (Kabir et al., 2014) | 1.7 |

**Table S9a.** Estimated lifetimes of PAN with respect to wet deposition in the atmosphere at 293 K.

| **Type** | ***L*** **(g $m^{-3}$)** | $H_S^{cc}(\mathbf{PAN}) \times \boldsymbol{L}$ | $\boldsymbol{k_{l,aq}}$**(PAN) ($10^{-4}$ $s^{-1}$)** | $\boldsymbol{\tau_{wet}}$ **(PAN)=** $\left(\boldsymbol{k_{l,aq}} \times H_S^{cc} \times \boldsymbol{L}\right)^{-1}$ |
|---|---|---|---|---|
| Aerosol (low load) | $2.4\times10^{-6}$ (Nenes et al., 2021) | $2.4\times10^{-10}$ | 3.8 (this work) | 350 ky |
| Aerosol (high load) | $1.0\times10^{-4}$ (Nenes et al., 2021) | $1.0\times10^{-8}$ | 3.8 (this work) | 8.3 ky |
| Stratus clouds (continental) | 0.28 (Hess et al., 1998) | $2.8\times10^{-5}$ | 3.8 (this work) | 3.0 y |
| Stratus clouds (maritime) | 0.30 (Hess et al., 1998) | $3.0\times10^{-5}$ | 44 (Kames and Schurath, 1995) | 87 d |
| Cumulus clouds (continental, clean) | 0.26 (Hess et al., 1998) | $2.6\times10^{-5}$ | 3.8 (this work) | 3.2 y |
| Cumulus clouds (continental, polluted) | 0.30 (Hess et al., 1998) | $3.0\times10^{-5}$ | 3.8 (this work) | 2.8 y |
| Cumulus clouds (maritime) | 0.44 (Hess et al., 1998) | $4.4\times10^{-5}$ | 44 (Kames and Schurath, 1995) | 59 d |
| Cumulonimbus clouds (Java) | 3.0 (Rosenfeld and Lensky, 1998) | $3.0\times10^{-4}$ | 3.8 (this work) | 101 d |
| Fog | 0.058 (Hess et al., 1998) | $5.8\times10^{-6}$ | 3.8 (this work) | 14 y |
| Fog (Po Valley) | 0.3 (Wobrock et al., 1992) | $3.0\times10^{-5}$ | 3.8 (this work) | 2.8 y |
| Fog (maritime) | 0.058 (Hess et al., 1998) | $5.8\times10^{-6}$ | 44 (Kames and Schurath, 1995) | 1.2 y |
| Fog (maritime) | 0.8 (Dimitrova et al., 2021) | $8.1\times10^{-5}$ | 44 (Kames and Schurath, 1995) | 33 d |
| Fog (maritime) | 1.8 (Osthoff et al., 2006) | $1.8\times10^{-4}$ | 44 (Kames and Schurath, 1995) | 14 d |

**Table S9b.** Estimated lifetimes of PPN with respect to wet deposition in the atmosphere at 293 K.

| **Type** | $\boldsymbol{L}$ (g m$^{-3}$) | $H_S^{cc}$(PPN) × $L$ | $k_{l,aq}$(PPN) ($10^{-4}$ s$^{-1}$) | $\tau_{wet}$ (PPN) $= (k_{l,aq} \times H_S^{cc} \times L)^{-1}$ |
|---|---|---|---|---|
| Aerosol (low load) | 2.4×10$^{-6}$ (Nenes et al., 2021) | 1.5 ×10$^{-10}$ | 3.8 (this work) | 540 ky |
| Aerosol (high load) | 1.0×10$^{-4}$ (Nenes et al., 2021) | 6.4 ×10$^{-9}$ | 3.8 (this work) | 13 ky |
| Stratus clouds (continental) | 0.28 (Hess et al., 1998) | 1.8 ×10$^{-5}$ | 3.8 (this work) | 4.6 y |
| Stratus clouds (maritime) | 0.30 (Hess et al., 1998) | 1.9 ×10$^{-5}$ | 44 (Kames and Schurath, 1995) | 137 d |
| Cumulus clouds (continental, clean) | 0.26 (Hess et al., 1998) | 1.7 ×10$^{-5}$ | 3.8 (this work) | 5.0 y |
| Cumulus clouds (continental, polluted) | 0.30 (Hess et al., 1998) | 1.9 ×10$^{-5}$ | 3.8 (this work) | 4.3 y |
| Cumulus clouds (maritime) | 0.44 (Hess et al., 1998) | 2.8 ×10$^{-5}$ | 44 (Kames and Schurath, 1995) | 93 d |
| Cumulonimbus clouds (Java) | 3.0 (Rosenfeld and Lensky, 1998) | 1.9 ×10$^{-4}$ | 3.8 (this work) | 158 d |
| Fog | 0.058 (Hess et al., 1998) | 3.7 ×10$^{-6}$ | 3.8 (this work) | 22 y |
| Fog (Po Valley) | 0.3 (Wobrock et al., 1992) | 1.9 ×10$^{-5}$ | 3.8 (this work) | 4.3 y |
| Fog (maritime) | 0.058 (Hess et al., 1998) | 3.7 ×10$^{-6}$ | 44 (Kames and Schurath, 1995) | 1.9 y |
| Fog (maritime) | 0.8 (Dimitrova et al., 2021) | 5.1 ×10$^{-5}$ | 44 (Kames and Schurath, 1995) | 51 d |
| Fog (maritime) | 1.8 (Osthoff et al., 2006) | 1.2 ×10$^{-4}$ | 44 (Kames and Schurath, 1995) | 23 d |

**Table S10a.** Estimated lifetimes of PAN with respect to wet deposition in the atmosphere at 278 K.

| **Type** | $L$ (g m$^{-3}$) | $H_S^{cc}(\mathrm{PAN}) \times L$ | $k_{\mathrm{l,aq}}$(PAN) ($10^{-4}$ s$^{-1}$) | $\tau_{\mathrm{wet}}$(PAN) $= \left(k_{\mathrm{l,aq}} \times H_S^{cc} \times L\right)^{-1}$ |
|---|---|---|---|---|
| Aerosol (low load) | $2.4\times10^{-6}$ (Nenes et al., 2021) | $6.4 \times10^{-10}$ | 1.8 (this work) | 274 ky |
| Aerosol (high load) | $1.0\times10^{-4}$ (Nenes et al., 2021) | $2.7 \times10^{-8}$ | 1.8 (this work) | 6.5 ky |
| Stratus clouds (continental) | 0.28 (Hess et al., 1998) | $7.5 \times10^{-5}$ | 1.8 (this work) | 2.3 y |
| Stratus clouds (maritime) | 0.30 (Hess et al., 1998) | $8.1 \times10^{-5}$ | 44 (Kames and Schurath, 1995) | 33 d |
| Cumulus clouds (continental, clean) | 0.26 (Hess et al., 1998) | $7.0 \times10^{-5}$ | 1.8 (this work) | 2.5 y |
| Cumulus clouds (continental, polluted) | 0.30 (Hess et al., 1998) | $8.1 \times10^{-5}$ | 1.8 (this work) | 2.2 y |
| Cumulus clouds (maritime) | 0.44 (Hess et al., 1998) | $1.2 \times10^{-4}$ | 44 (Kames and Schurath, 1995) | 22 d |
| Cumulonimbus clouds (Java) | 3.0 (Rosenfeld and Lensky, 1998) | $8.1 \times10^{-4}$ | 1.8 (this work) | 80 d |
| Fog | 0.058 (Hess et al., 1998) | $1.6 \times10^{-5}$ | 1.8 (this work) | 11 y |
| Fog (Po Valley) | 0.3 (Wobrock et al., 1992) | $8.1 \times10^{-5}$ | 1.8 (this work) | 2.2 y |
| Fog (maritime) | 0.058 (Hess et al., 1998) | $1.6\times10^{-5}$ | 44 (Kames and Schurath, 1995) | 168 d |
| Fog (maritime) | 0.8 (Dimitrova et al., 2021) | $2.2\times10^{-4}$ | 44 (Kames and Schurath, 1995) | 12 d |
| Fog (maritime) | 1.8 (Osthoff et al., 2006) | $4.8\times10^{-4}$ | 44 (Kames and Schurath, 1995) | 5 d |

**Table S10b.** Estimated lifetimes of PPN with respect to wet deposition in the atmosphere at 278 K.

| **Type** | ***L*** **(g m$^{-3}$)** | $H_S^{cc}$(PPN) × $L$ | **$k_{l,aq}$(PPN) (10$^{-4}$ s$^{-1}$)** | **$\tau_{wet}$(PPN) $= \left(k_{l,aq} \times H_S^{cc} \times L\right)^{-1}$** |
|---|---|---|---|---|
| Aerosol (low load) | 2.4×10$^{-6}$ (Nenes et al., 2021) | 3.8×10$^{-10}$ | 1.0 (this work) | 840 ky |
| Aerosol (high load) | 1.0×10$^{-4}$ (Nenes et al., 2021) | 1.6×10$^{-8}$ | 1.0 (this work) | 20 ky |
| Stratus clouds (continental) | 0.28 (Hess et al., 1998) | 4.5×10$^{-5}$ | 1.0 (this work) | 7.2 y |
| Stratus clouds (maritime) | 0.30 (Hess et al., 1998) | 4.8×10$^{-5}$ | 44 (Kames and Schurath, 1995) | 55 d |
| Cumulus clouds (continental, clean) | 0.26 (Hess et al., 1998) | 4.2×10$^{-5}$ | 1.0 (this work) | 7.7 y |
| Cumulus clouds (continental, polluted) | 0.30 (Hess et al., 1998) | 4.8×10$^{-5}$ | 1.0 (this work) | 6.7 y |
| Cumulus clouds (maritime) | 0.44 (Hess et al., 1998) | 7.0×10$^{-5}$ | 44 (Kames and Schurath, 1995) | 37 d |
| Cumulonimbus clouds (Java) | 3.0 (Rosenfeld and Lensky, 1998) | 4.8×10$^{-4}$ | 1.0 (this work) | 244 d |
| Fog | 0.058 (Hess et al., 1998) | 9.3×10$^{-6}$ | 1.0 (this work) | 35 y |
| Fog (Po Valley) | 0.3 (Wobrock et al., 1992) | 4.8×10$^{-5}$ | 1.0 (this work) | 6.7 y |
| Fog (maritime) | 0.058 (Hess et al., 1998) | 9.3×10$^{-6}$ | 44 (Kames and Schurath, 1995) | 283 d |
| Fog (maritime) | 0.8 (Dimitrova et al., 2021) | 1.3×10$^{-4}$ | 44 (Kames and Schurath, 1995) | 21 d |
| Fog (maritime) | 1.8 (Osthoff et al., 2006) | 2.9×10$^{-4}$ | 44 (Kames and Schurath, 1995) | 9 d |

**Table S11.** Reactive uptake probabilities of PAN and PPN calculated using Eq. (8-9). The water viscosities were obtained from Korson et al. (1969) and those for n-octanol were calculated by linear extrapolation of the above-room temperature data by Venkatesan et al. (2020). Molar volume data were obtained using the PhysChem module of the ACD/Labs percepta platform via the Royal Society of Chemistry's Chemspider web site (2022).

| **Compound and solvent** | $T$ (K) | $\mu$ (mPa s) | $D_l$ ($10^{-9}$ m$^2$ s$^{-1}$) | $k_l$ ($10^{-5}$ s$^{-1}$) | $\omega$ (m s$^{-1}$) | $H_S^{cc}$ | $\gamma$ ($10^{-5}$) |
|---|---|---|---|---|---|---|---|
| PAN and DI water | 278.15 | 1.5192 | 0.88 | 18 | 221 | 269 | 0.2 |
| PAN and DI water | 293.15 | 1.0020 | 1.4 | 38 | 226 | 101 | 0.1 |
| PPN and DI water | 278.15 | 1.5192 | 0.86 | 10 | 209 | 160 | 0.09 |
| PPN and DI water | 293.15 | 1.0020 | 1.4 | 38 | 214 | 64 | 0.09 |
| PAN and n-octanol | 278.15 | 12.2 | 2.3 | 0.5 | 221 | 1920 | 0.4 |
| PAN and n-octanol | 293.15 | 9.3 | 3.2 | 0.3 | 226 | 1010 | 0.2 |
| PPN and n-octanol | 278.15 | 12.2 | 2.3 | 0.3 | 209 | 4652 | 0.7 |
| PPN and n-octanol | 293.15 | 9.3 | 3.2 | 1.8 | 214 | 2351 | 1.1 |

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