Measured saturation vapour pressures of phenolic and nitro-aromatic compounds

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Supplementary Information

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Table S1: Estimates of the sub-cooled liquid vapour pressure at 298 K (Pa). The estimates are N_Tb/N_Vp (Nannoolal boiling point, Nannoolal Vapour pressure) N_Tb/M_Vp (Nannoolal boiling point, Moller vapour pressure) N_Tb/MY_Vp (Nannoolal boiling point, Myrdal and Yalkowsky vapour pressure) N_Tb/LK_Vp (Nannoolal boiling point, Lee-Kesler vapour pressure) S_Vp (SIMPOL vapour pressure) SB_Tb/N_Vp (Stein and Brown boiling point, Nannoolal vapour pressure) SB_Tb/M_Vp (Stein and Brown boiling point, Moller vapour pressure) SB_Tb/MY_Vp (Stein and Brown boiling point, Mydral and Yalkowsky vapour pressure) SB_Tb/LK_Vp (Stein and Brown boiling point, Lee-Kesler vapour pressure).

	N_Tb & N_Vp (Pa)	N_Tb & M_Vp (Pa)	N_Tb & MY_Vp (Pa)	N_Tb & LK_Vp (Pa)	S_Vp (Pa)	SB_Tb & N_Vp (Pa)	SB_Tb & M_Vp (Pa)	SB_Tb & MY_Vp (Pa)	SB_Tb & LK_Vp (Pa)	Experimental (Pa)
1-napthol	4.34×10^{-1}	7.34×10^{-1}	3.06×10^{-1}	4.69×10^{-2}	6.68×10^{-1}	1.37	2.50	9.99×10^{-1}	1.72×10^{-1}	8×10^{-2}
2-napthol	4.34×10^{-1}	7.34×10^{-1}	3.06×10^{-1}	4.69×10^{-2}	6.68×10^{-1}	1.37	2.50	9.99×10^{-1}	1.72×10^{-1}	1.26×10^{-1}
1,3-dihydroxynapthalene	4.48×10^{-3}	1.88×10^{-2}	8.98×10^{-3}	7.38×10^{-5}	5.13×10^{-3}	3.12×10^{-2}	1.46×10^{-1}	5.53×10^{-2}	7.40×10^{-4}	5.7×10^{-7}
2,3-dihydroxynapthalene	6.39×10^{-3}	2.39×10^{-2}	1.10×10^{-2}	1.28×10^{-4}	5.13×10^{-3}	3.53×10^{-2}	1.46×10^{-1}	5.53×10^{-2}	9.56×10^{-4}	5.46×10^{-5}
1,7-dihydroxynapthalene	4.29×10^{-3}	1.82×10^{-2}	8.72×10^{-3}	7.10×10^{-5}	5.13×10^{-3}	3.09×10^{-2}	1.46×10^{-1}	5.53×10^{-2}	7.40×10^{-4}	1.6×10^{-7}
2,7-dihydroxynapthalene	4.29×10^{-3}	1.82×10^{-2}	8.72×10^{-3}	7.10×10^{-5}	5.13×10^{-3}	3.09×10^{-2}	1.46×10^{-1}	5.53×10^{-2}	7.40×10^{-4}	1.04×10^{-7}
1,5-dihydroxynapthalene	4.29×10^{-3}	1.82×10^{-2}	8.72×10^{-3}	7.10×10^{-5}	5.13×10^{-3}	3.09×10^{-2}	1.46×10^{-1}	5.53×10^{-2}	7.40×10^{-4}	2×10^{-5}
1-nitronapthalene	8.85×10^{1}	7.71×10^{1}	7.18×10^{1}	1.35×10^{1}	8.70×10^{1}	4.62×10^{1}	3.78×10^{1}	3.58×10^{1}	5.93	3.98×10^{-2}

1,3-dinitronapthalene	2.63×10^{2}	2.22×10^{2}	2.33×10^{2}	2.43×10^{1}	8.70×10^{1}	4.21×10^{1}	2.95×10^{1}	3.28×10^{1}	1.80×10^{1}	3.55×10^{-8}
2-methyl-1-nitronapthalene	4.27×10^{1}	3.52×10^{1}	3.57×10^{1}	5.57	3.28×10^{1}	1.77×10^{1}	1.32×10^{1}	1.41×10^{1}	1.86	3.6×10^{-2}
ortho-amino-benzoic acid	7.37×10^{-3}	2.10×10^{-3}	3.61×10^{-2}	6.62×10^{-3}	1.32×10^{-2}	1.14×10^{-2}	3.62×10^{-3}	5.32×10^{-2}	1.02×10^{-2}	3.08×10^{-2}
meta-amino-benzoic acid	5.05×10^{-3}	1.54×10^{-3}	2.89×10^{-2}	5.51×10^{-3}	1.32×10^{-2}	1.01×10^{-2}	3.62×10^{-3}	5.32×10^{-2}	1.08×10^{-2}	1.28×10^{-4}
para-amino-benzoic acid	4.06×10^{-3}	1.18×10^{-3}	2.41×10^{-2}	4.50×10^{-3}	1.32×10^{-2}	1.00×10^{-2}	3.62×10^{-3}	5.32×10^{-2}	1.08×10^{-2}	5.14×10^{-3}
meta-nitrophenol	1.11×10^{3}	1.46×10^{3}	9.40×10^{2}	4.05×10^{2}	3.32×10^{1}	1.70×10^{2}	2.29×10^{2}	1.23×10^{2}	3.89×10^{1}	9.44×10^{-3}
para-nitrophenol	9.60×10^{2}	1.27×10^{3}	8.07×10^{2}	3.40×10^{2}	3.32×10^{1}	1.69×10^{2}	2.29×10^{2}	1.23×10^{2}	3.89×10^{1}	4.01×10^{-3}
ortho-nitroanaline	8.43×10^{2}	8.09×10^{2}	8.30×10^{2}	3.12×10^{2}	1.13×10^{2}	1.07×10^{2}	8.94×10^{1}	9.35×10^{1}	2.47×10^{1}	1.05×10^{-2}
meta-nitroanaline	6.80×10^{2}	6.78×10^{2}	6.96×10^{2}	2.59×10^{2}	1.13×10^{2}	9.99×10^{1}	8.94×10^{1}	9.35×10^{1}	2.54×10^{1}	5.14×10^{-3}
para-nitroanaline	5.89×10^{2}	5.86×10^{2}	6.01×10^{2}	2.19×10^{2}	1.13×10^{2}	9.94×10^{1}	8.94×10^{1}	9.35×10^{1}	2.54×10^{1}	9.44×10^{-3}
Glutarimide	4.39×10^{-6}	3.75×10^{-10}	4.52×10^{-4}	8.39×10^{-5}	1.38×10^{-11}	1.24×10^{-4}	1.16×10^{-7}	5.86×10^{-3}	1.22×10^{-3}	6.33×10^{-2}

Figure S1a: Fraction of a component in the condensed phase as a function of its volatility, represented by the C* value (replicated from (1)), for 5 existing condensed mass loadings [red lines, each value given in $\mu g.m^{-3}$] against the measured volatility [solid black line] and range of estimates from predictive techniques [dashed blue lines].

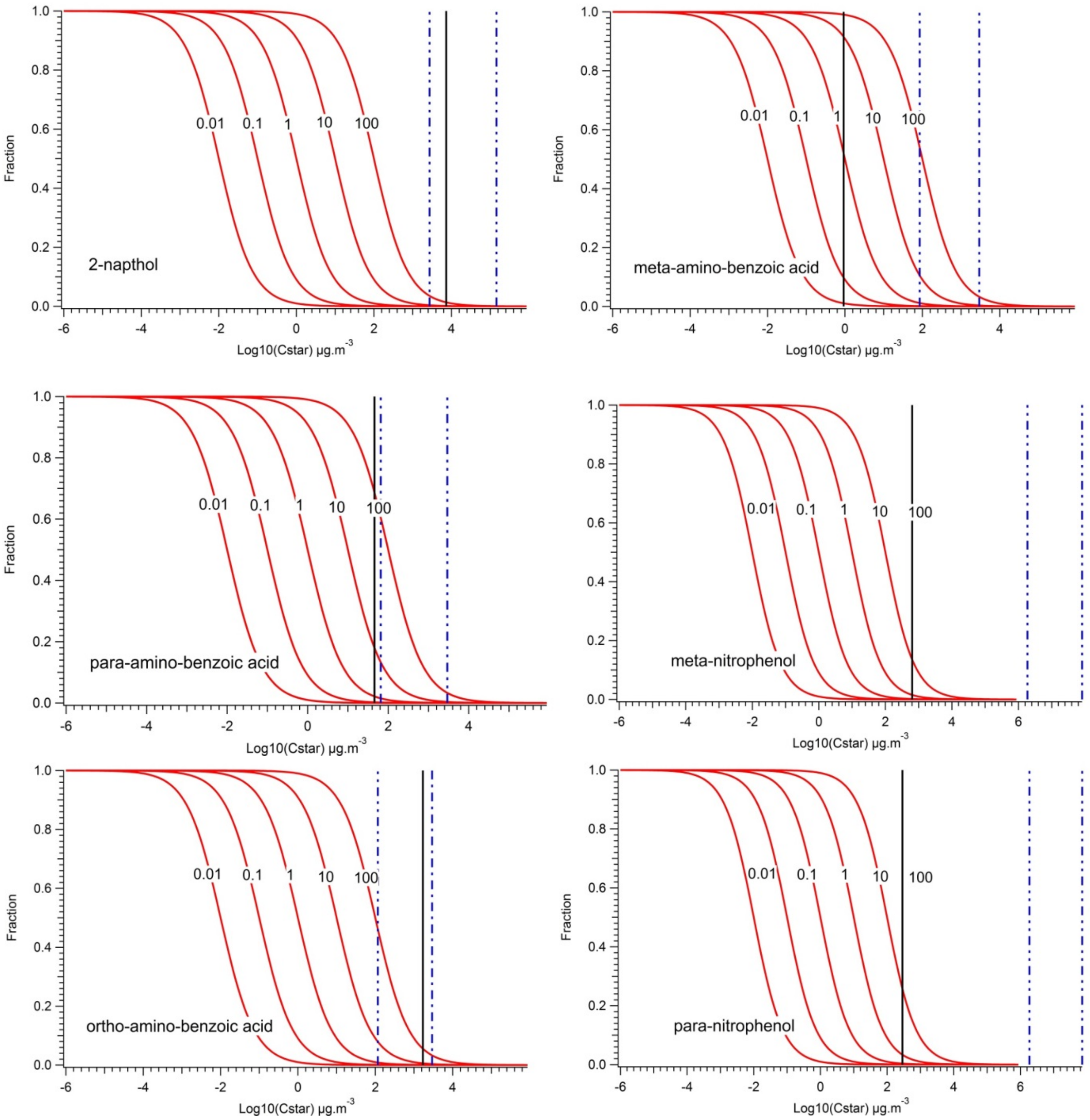
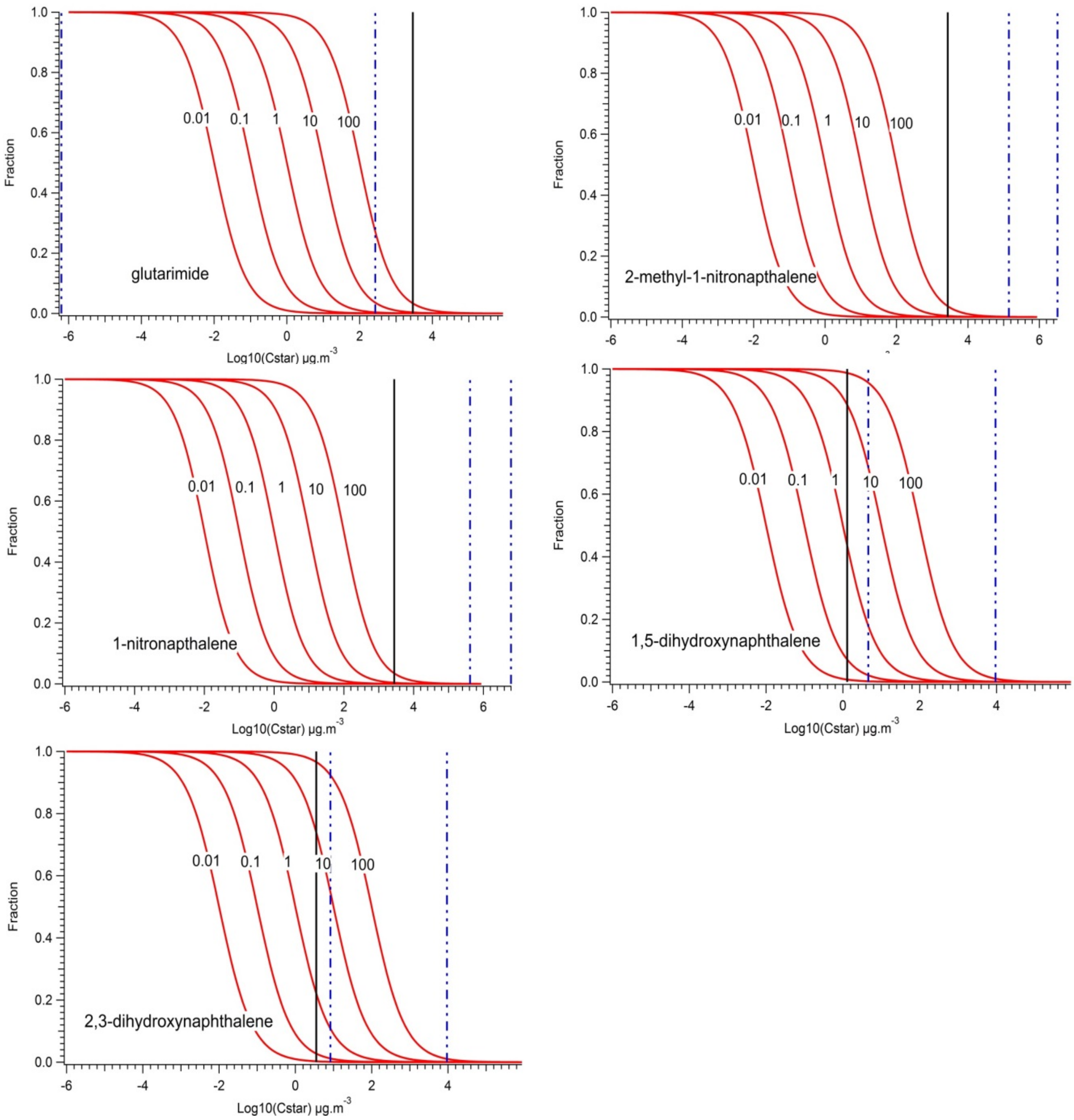


Figure S1b: Fraction of a component in the condensed phase as a function of its volatility, represented by the C* value (replicated from (1)), for 5 existing condensed mass loadings [red lines, each value given in $\mu g.m^{-3}$] against the measured volatility [solid black line] and range of estimates from predictive techniques [dashed blue lines].



References

1. Valorso, R., Aumont, B., Camredon, M., Raventos-Duran, T., Mouchel-Vallon, C., Ng, N. L., Seinfeld, J. H., Lee-Taylor, J., and Madronich, S.: Explicit modelling of SOA formation from α-pinene photooxidation: sensitivity to vapour pressure estimation, *Atmos. Chem. Phys.,* **2011,** 11, 6895-6910, doi:1.5194/acp-11-6895-2