

Supporting Information

‘Comparison of Approaches for Measuring the Mass Accommodation Coefficient for the Condensation of Water and Sensitivities to Uncertainties in Thermophysical Properties’, Rachael E. H. Miles, Jonathan P. Reid and Ilona Riipinen.

A literature survey was undertaken to determine the most accurate parameterisations to use for the diffusion coefficient and thermal conductivity of the gas mixtures water/air and water/nitrogen, required as input parameters in the semi-analytical model of Kulmala *et al.*¹ The thermodynamic properties investigated were the diffusion coefficient of water in air; the diffusion coefficient of water in water vapour; the viscosity of air; the viscosity of nitrogen; the viscosity of water; the thermal conductivity of air; the thermal conductivity of nitrogen; the thermal conductivity of water and formulae for determining the thermal conductivity of a mixture. The results of the literature survey are summarised below.

S1. The diffusion coefficient of water in air

The results of the literature survey are summarised in Figure S1. Winkler *et al.* based their parameterisation on a fit to collated data reported in Landolt-Börnstein over the temperature range 273 – 373 K.^{2,3} Marrero and Mason⁴, and Matsunaga and Nagashima⁵ performed similar fits to diffusion coefficient values they themselves had collated from the literature. An empirical method was used by Slattery and Bird who applied the principle of corresponding states to collated data on self diffusion and binary diffusion coefficients⁶. Fuller *et al.* performed a non-linear least squares fit to 340 experimental diffusion constants reported in the literature for 153 different binary gas systems using a function based on the Stefan-Maxwell hard sphere model and the principle of additive atomic volume.⁷ A later study by

the same group used an identical fitting procedure but applied it to a larger data set containing 512 data points.⁸

Massman used a local regression model (LOESS) to individually fit literature data collated for 30 different gas pairs in the temperature range – 50 °C to 100 °C near 1 atm pressure or less.⁹ Huang *et al.* used a generalized semi-empirical equation based on the Arnold modified Maxwell equation to predict the diffusion coefficient as a function of pressure and temperature through fitting experimental results from gas chromatography.¹⁰ Gilliland recast the Maxwell and Sutherland modified Maxwell equations in terms of the liquid molal volumes of the diffusing species at the normal boiling point and compared the results with 500 experimental points from 183 different systems.¹¹ An approximation to Chapman-Enskog theory was suggested by Chen and Othmer who replaced the collision diameter, σ , and collision integral, Ω , with critical constants (molal volume and temperature) of the 66 different binary gas systems they used to determine the proportionality constants in the new equation.¹² Predictions from full Chapman-Enskog theory using molecular interaction parameters σ and Ω from Poling *et al.* are also shown on the figure.^{13,14}

S2. The diffusion coefficient of water in water vapour

The results of the literature survey are summarised in Figure S2. Only two parameterisations were found which derived directly from experimental measurements of the diffusion process of water in water vapour. The first by Swinton measured the diffusion of H₂O in HTO in a two bulb diffusion apparatus¹⁵, while the second by Yoshida *et al.* looked at gas phase diffusion of water using NMR.¹⁶ Even between these two direct measurements there exists a

discrepancy of 18.9 % in their predictions at 1 atm total pressure and a temperature of 298.15 K, once reduced mass considerations are taken in to account. The remaining studies identified in the literature survey were either purely theoretical in origin, were based on a combination of theory and a fit to other experimental data for water vapour, such as viscosity, or were derived from a fit to self diffusion data for a range of other species with the results assumed to be applicable in the case of water vapour. Where tabulated data was given in references, values were corrected to 1 atm assuming an inverse pressure dependence and a fit of the form

$$D = aT^b \quad (S2.1)$$

was applied in order to derive diffusion coefficient (D) values over the temperature (T) range 270 K to 300 K. a and b were floated as constants in the fit.

Fokin and Kalashnikov used 182 experimental data points for the viscosity and self diffusion coefficient of steam as a function of temperature to calculate new values for ϵ/k and σ to be used in Chapman-Enskog theory.¹⁷ A correction was also made to the calculation of the collision integral to take in to account dipole-dipole interactions between water molecules. Gershenzon *et al.* state a single value for the self diffusion coefficient of water at 293 K and 1 atm which is referenced to Swinton, with the authors then assuming a temperature dependence of $T^{1.5}$.¹⁸ Predictions using kinetic gas theory¹⁹ and full Chapman-Enskog theory¹³ are also shown on Figure S2, using interaction parameters taken from Poling *et al.*¹⁴ and the temperature dependence of the collision integral taken from Table E2 in Bird *et al.*²⁰ A critical review of self diffusion measurements in the literature covering the entire fluid state for 27 fluids (not including water) was performed by Lee and Thodos.²¹ This data was used to determine a generalized method based on kinetic theory, the state properties of the fluids under consideration and dimensional analysis, which could be used to predict the self diffusion of any compound at a specific density.

Liu and Macedo reported two equations with differing functional form for calculating the self diffusion coefficient of water; equation (4) in the original paper expresses the self diffusion coefficient in terms of an expansion in molar density, with the proportional coefficients in each term being temperature dependent, while equation (13) is a modified free volume model in which the effective molecular diameter is temperature dependent and the overlap factor is density dependent.²² Constants in both equations were determined from fits to 118 literature data points collated by the authors. Matsunaga and Nagashima calculated the viscosity of water using a fit to experimental data and then converted these values in to self diffusion coefficients.⁵ Molecular dynamics simulations of the self diffusion coefficient of water were performed by Yoshida *et al.*¹⁶ and Hellmann *et al.*²³ In the work of Swinton introduced previously, there is some ambiguity over the gas phase pressure to which the reported diffusion coefficients correspond. In this work we have assumed a pressure of 1 atm, in line with previous publications.^{18,23}

The nine studies in Figure S2 giving diffusion coefficients at 298.15 K grouped within the range $1.90 \times 10^{-5} \text{ m}^2 \cdot \text{s}^{-1}$ to $1.46 \times 10^{-5} \text{ m}^2 \cdot \text{s}^{-1}$ were deemed to be the most reliable. Given the significant degree of variation in the methods used to determine each of these parameterisations and the spread in their resulting values, it was deemed impractical to try and discriminate which was the most appropriate one to use. Equal weighting was therefore given to all nine studies and the average diffusion coefficient predicted by the different parameterisations was calculated in 5 K increments over the temperature range 270 K to 300 K at 1 atm pressure. These values were then fitted with an equation of the form shown in (S2.1) to determine a new parameterisation for the diffusion coefficient of water in water vapour, $D(\text{H}_2\text{O}-\text{H}_2\text{O})$. Assuming an inverse pressure dependence

$$D(H_2O - H_2O) = 7.5695 \times 10^{-10} \cdot T^{1.7575} \cdot p^{-1} \quad (S2.2)$$

where $D(H_2O-H_2O)$ is given in $m^2 \cdot s^{-1}$, T is the temperature in K and p is the pressure in atmospheres. This parameterisation is shown by the solid line on Figure S2b), with the shaded area denoting the standard deviation in the mean values of 9.2 %.

S3. The viscosity of air

The results of the literature survey are summarised in Figure S3. The parameterisation from Touloukian *et al.* arises from a fit to available literature data.²⁴ Tsilingiris reports an equation based on a fit to viscosity data between -23 °C and 327 °C taken from the Handbook of Heat Transfer.²⁵ The work of Lemmon and Jacobsen is the current National Institute of Standards and Technology (NIST) recommendation for the viscosity of air and is based on a fit to data from 37 theoretical and experimental studies covering the temperature range 70 K – 2500 K and pressures up to 325 MPa.²⁶ The parameterisation consists of dilute gas and residual contribution terms.

Due to its associations with the NIST, the study by Lemmon and Jacobsen was judged to be the most reliable to use for the viscosity of air. From equation (1) in the original paper:

$$\eta = \eta^0(T) + \eta^r(\tau, \delta) \quad (S3.1)$$

where η is the viscosity in $\mu Pa \cdot s$, $\eta^0(T)$ is the dilute gas viscosity and $\eta^r(\tau, \delta)$ is the residual fluid viscosity. Only the dilute term needs to be considered for pressures less than 1 atm.

The dilute gas term is given by:

$$\eta^0(T) = \frac{0.0266958\sqrt{MT}}{\sigma^2\Omega(T^*)} \quad (S3.2)$$

with

$$\Omega(T^*) = \exp\left(\sum_{i=0}^4 b_i [\ln(T^*)]^i\right) \quad (S3.3)$$

where $M = 28.9586 \text{ g.mol}^{-1}$, $\sigma = 0.360 \text{ nm}$, $T^* = T/(\varepsilon/k)$ and $\varepsilon/k = 103.3 \text{ K}$. The coefficients b_i for the collision integral equation are given in Table S1.

Using equations (S3.2) and (S3.3), a quadratic fit to values calculated over the T range 270 to 300 K gives:

$$\mu = (8.4908E - 7) + (6.96344E - 8).T - (3.57384E - 11).T^2 \quad (S3.4)$$

where μ is in Pa.s and T is in K. The uncertainty in the viscosity over this temperature range is $\pm 1 \%$.

S4. The viscosity of nitrogen

The parameterisation deemed most reliable for the viscosity of nitrogen is also taken from the work of Lemmon and Jacobsen and uses equations (S3.2) and (S3.3).²⁶ For nitrogen the relevant constants are $M = 28.01348 \text{ g.mol}^{-1}$, $\sigma = 0.3656 \text{ nm}$ and $\varepsilon/k = 98.94 \text{ K}$, with the coefficients used in the collision integral equation the same as given in Table S1.

Using the dilute term only, a quadratic fit to values calculated over the T range 270 to 300 K gives:

$$\mu = (9.22223E - 7) + (6.69226E - 8).T - (3.46889E - 11).T^2 \quad (S4.1)$$

where μ is in Pa.s and T is in K. The uncertainty in the viscosity calculated over this temperature range is ± 0.5 %.

S5. The viscosity of water

The results of the literature survey are summarised in Figure S4. The studies of Huber *et al.* and Sengers and Watson originate from the NIST and are based on a fit to collated literature data, with the work of Huber *et al.* being the most recent.^{27,28} Both parameterisations consist of dilute gas, residual contribution and critical enhancement terms. Matsunaga and Nagashima report an equation determined from a fit to selected experimental data to calculate the viscosity as a function of temperature, with the authors stating the formalism reliability as 5% over the temperature range 273 to 373 K.⁵ Fokin and Kalashnikov used a fit to experimental data to determine new values of the interaction parameters σ and ϵ/k for use in a modified m-6-3 Stockmayer potential.¹⁷ This was then used to calculate viscosities over a range of temperatures. Experimental measurements of the viscosity of water vapour at low densities were made by Teske *et al.* using an all-quartz oscillating-disk viscometer, with a stated uncertainty of 0.2 %.²⁹ Touloukian *et al.* also report an equation to calculate the viscosity of gaseous water as a function of temperature based on a fit to literature data, with a quoted tolerance of ± 1 %.²⁴

The study of Huber *et al.* was judged to be the most reliable, as it is the most recent study from the NIST and is endorsed by the International Association for the Properties of Water and Steam. A database was created which included all experimental water viscosity

measurements to be found in the literature in the range 279.88 – 1346.24 K, 0.0008 – 15.779 MPa and 0.006 – 50 kg.m⁻³. These were fitted with a framework cast in terms of the dimensionless variables

$$\bar{T} = \frac{T}{T^*} \quad (S5.1)$$

$$\bar{\rho} = \frac{\rho}{\rho^*} \quad (S5.2)$$

$$\bar{\mu} = \frac{\mu}{\mu^*} \quad (S5.3)$$

where T = temperature, ρ = density, μ = viscosity and the reference constants are $T^* = 647.096$ K, $\rho^* = 322.0$ kg.m⁻³ and $\mu^* = 1 \times 10^{-6}$ Pa.s.

The viscosity is given by

$$\bar{\mu} = \bar{\mu}_0(\bar{T}) \times \bar{\mu}_1(\bar{T}, \bar{\rho}) \times \bar{\mu}_2(\bar{T}, \bar{\rho}) \quad (S5.4)$$

where $\bar{\mu}_0(\bar{T})$ is the viscosity in the zero density limit, $\bar{\mu}_1(\bar{T}, \bar{\rho})$ is the residual contribution term and $\bar{\mu}_2(\bar{T}, \bar{\rho})$ gives the enhancement near the critical point. For the conditions considered in this manuscript, only the zero density term need be considered.

The term $\bar{\mu}_0(\bar{T})$ has the form shown in (S5.5) and is based on a general expression for the viscosity given by the kinetic theory of gases. The constants H_i were estimated by applying orthogonal distance regression to the literature data, with each point given a weighting representative of its experimental uncertainty. The values of the H_i coefficients are given in Table S2.

$$\bar{\mu}_0(\bar{T}) = \frac{100\sqrt{\bar{T}}}{\sum_{i=0}^3 \frac{H_i}{\bar{T}^i}} \quad (S5.5)$$

Using the zero density term only, a quadratic fit to data calculated over the temperature range 270 to 300 K gives

$$\mu = (5.68432E - 6) - (5.00546E - 9).T + (6.20639E - 11).T^2 \quad (S5.6)$$

where μ is in Pa.s and T is in K. The uncertainty in the viscosity over this temperature range is $\pm 2\%$.

S6. The thermal conductivity of air

The results of the literature survey are summarised in Figure S5. Tsilingiris reports an equation based on a fit to thermal conductivity data between $-23\text{ }^\circ\text{C}$ and $777\text{ }^\circ\text{C}$ taken from the Handbook of Heat Transfer.²⁵ The work of Lemmon and Jacobsen is based on a fit to literature data using a three part equation with dilute gas, residual contribution and critical contribution terms.²⁶ Touloukian *et al.* give recommended values for the thermal conductivity of air also based on a fit to literature data.³⁰ The authors comment that the composition of the ‘air’ (ie. presence of water vapour) being studied in each measurement is not clear, however, they found that when they included data sets where the air had not been dried, agreement with the overall correlation was seen to within individual experimental errors. Pruppacher and Klett also report an equation resulting from a fit to experimental data.³¹ The Engineering ToolBox is an online database for the thermophysical properties of air.³² Winkler *et al.* provide no reference for the origin of their equation.²

As described in the manuscript, the work of Lemmon and Jacobsen was deemed the most reliable. In this parameterisation, the thermal conductivity, λ , in $\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ is given by:

$$\lambda = \lambda^0(T) + \lambda^r(\tau, \delta) + \lambda^c(\tau, \delta) \quad (\text{S6.1})$$

where $\lambda^0(T)$ is the dilute gas thermal conductivity, $\lambda^r(\tau, \delta)$ is the residual fluid thermal conductivity, and $\lambda^c(\tau, \delta)$ is the thermal conductivity critical enhancement. For the conditions considered in this work, only the dilute gas term is required. This is based on Chapman-Enskog theory with a collision integral determined by fitting to experimental data and is given by:

$$\lambda^0 = N_1 \left[\frac{\eta^0(T)}{1 \mu\text{Pa}\cdot\text{s}} \right] + N_2 \tau^{t_2} + N_3 \tau^{t_3} \quad (\text{S6.2})$$

where $\eta^0(T)$ is the dilute gas viscosity as calculated in (S3.2). The values of the constants N_i and t_i are given in Table S3.

S7. Thermal conductivity of nitrogen

The formalism for the thermal conductivity of nitrogen was also taken from the work of Lemmon and Jacobsen²⁶. The parameterisation is again based on equations (S6.1) and (S6.2), with the viscosity of nitrogen calculated as in section S4 and values of N_i and t_i as given in Table S4.

S8. The thermal conductivity of water

The results of the literature survey are summarised in Figure S6. Touloukian *et al.* give recommended values for the thermal conductivity in increments of 10 K based on a fit to available literature data.³⁰ Tsilingiris reports an equation apparently based on a fit to the

Touloukian *et al.* data, however it can be seen from the figure that there are significant differences between the two parameterisations.²⁵ An empirical equation based on a fit to experimental data taken at temperatures up to 1190 K is presented by Matsunaga and Nagashima.⁵ Sengers and Watson report an equation containing dilute gas, residual contribution and critical enhancement terms which has been fitted to collated literature data.²⁸ Pruppacher and Klett also present the results of a fit to literature data.³¹ No reference is provided for the origin of the equation given by Winkler *et al.*.²

As described in the manuscript, the work of Sengers and Watson was deemed to be the most reliable parameterisation for the thermal conductivity of water as it originates from the NIST and is endorsed by the International Association for the Properties of Water and Steam. The parameterisation is cast in terms of dimensionless variables for T and ρ as given in section S5 with the dimensionless thermal conductivity given by:

$$\bar{\lambda} = \frac{\lambda}{\lambda^*} \quad (S8.1)$$

The reference values are $\lambda^* = 0.4945 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$, $T^* = 647.27 \text{ K}$ and $\rho^* = 317.763 \text{ kg}\cdot\text{m}^{-3}$.

The recommended interpolating equation for scientific use has the form:

$$\bar{\lambda} = \bar{\lambda}_0(\bar{T}) \times \bar{\lambda}_1(\bar{T}, \bar{\rho}) + \bar{\lambda}_2(\bar{T}, \bar{\rho}) \quad (S8.2)$$

where $\bar{\lambda}_0(\bar{T})$ represents the ideal gas limit, $\bar{\lambda}_1(\bar{T}, \bar{\rho})$ is the term for the residual contribution and $\bar{\lambda}_2(\bar{T}, \bar{\rho})$ gives the enhancement in the critical limit. Only the ideal gas limit term needs to be taken in to account for the conditions considered in this work. The term $\bar{\lambda}_0(\bar{T})$ is given by:

$$\bar{\lambda}_0(\bar{T}) = \bar{T}^{0.5} / \sum_{i=0}^3 \frac{L_i}{\bar{T}^i} \quad (S8.3)$$

with the value of the constants L_i as given in Table S5.

S9. The thermal conductivity of a mixture

Seven methods for calculating the thermal conductivity of a binary mixture were identified in the literature. Tsilingiris provides two formulae relating explicitly to humid air, with equation (29) in the original paper based on the Wassiljewa equation, and equation (55) based on mole fractions and relative molecular masses of the pure components.²⁵ Lindsay and Bromley report an equation for calculating the values of the A parameters incorporating pure component viscosities, molecular masses and normal boiling points.³³ In the work of Mason and Saxena, the values of the A parameters are determined from pure component viscosities and molecular masses.³⁴ Winkler *et al.* state the values of A used in their equation and reference the work of Lindsay and Bromley.² Tondon and Saxena report the same equation as Mason and Saxena but change a constant from 1.065 to 0.85 as they state that this better fits sample experimental data.³⁵ Poling *et al.* give an equation for calculating the A parameters using the molecular masses, critical temperatures and critical pressures of the pure components and the reduced temperature.¹⁴ A comparison of all the different parameterisations with experimental data from Touloukian *et al.* for humid air is shown in Figure S7.³⁰

References

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Tables

i	b_i
0	0.431
1	-0.4623
2	0.08406
3	0.005341
4	-0.00331

Table S1. Coefficients required for calculating the viscosity of air and the viscosity of nitrogen using equation (S3.3).

i	H_i
0	1.67752
1	2.20462
2	0.6366564
3	-0.241605

Table S2. Coefficients for calculating the viscosity of water using equation (S5.5).

i	N_i	t_i
1	1.308	
2	1.405	-1.1
3	-1.036	-0.3
4	8.743	0.1
5	14.76	0.0
6	-16.62	0.5
7	3.793	2.7
8	-6.142	0.3
9	-0.3778	1.3

Table S3. Coefficients for calculating the thermal conductivity of air using equation (S6.2)

i	N_i	t_i
1	1.511	
2	2.117	-1.0
3	-3.332	-0.7
4	8.862	0.0
5	31.11	0.03
6	-73.13	0.2
7	20.03	0.8
8	-0.7096	0.6
9	0.2672	1.9

Table S4. Coefficients for calculating the thermal conductivity of nitrogen using equation (S6.2).

i	L_i
0	1.000000
1	6.978267
2	2.599096
3	-0.998254

Table S5. Coefficients for calculating the thermal conductivity of water using (S8.3)

Figure captions

Figure S1. Summary of the temperature dependence for the diffusion coefficient of water in air for the 11 different literature parameterisations found. All values are calculated for a pressure of 1 atm. Filled squares: Winkler *et al.*²; filled circles: Marrero and Mason⁴; filled triangles: Slattery and Bird⁶; empty squares: Fuller *et al.*⁷; empty circles: Massman⁹; empty triangles: Matsunaga and Nagashima⁵; solid line: Huang *et al.*¹⁰; dotted line: Fuller *et al.*⁸; dashed line: Gilliland¹¹; dot-dashed line: Chen and Othmer¹²; dot-dot-dashed line: Chapman-Enskog theory.¹⁴

Figure S2. a) Literature parameterisations for the diffusion coefficient of water in water vapour at 1 atm pressure. Filled squares: Fokin and Kalashnikov¹⁷; filled circles: Hellmann *et al.*²³; filled triangles: Matsunaga and Nagashima⁵; empty squares: Swinton¹⁵, assuming tabulated data at 1 atm; empty circles: Hirschfelder *et al.* (Chapman-Enskog theory)¹³; empty triangles: Yoshida *et al.*¹⁶ Molecular Dynamics; crossed squares: Yoshida *et al.*¹⁶ NMR; dotted line: Liu and Macedo²² Eq 4; dashed line: Gershenzon *et al.*¹⁸; dot-dashed line: Lee and Thodos²¹; dot-dot-dashed line: Liu and Macedo²² Eq 13; dot-dot-dashed-dashed line: Plawsky *et al.* (Kinetic gas theory)¹⁹. **b)** Expanded version of panel a). Solid line shows the average of the different parameterisations with the shaded area indicating the standard deviation.

Figure S3. The variation in the viscosity of air with temperature calculated for different literature parameterisations. Filled squares: Lemmon and Jacobsen²⁶, dilute gas term; empty circles: Touloukian *et al.*²⁴; filled triangles: Tsilingiris.²⁵

Figure S4. The variation in the viscosity of water vapour with temperature calculated using different literature parameterisations. Filled squares: Touloukian *et al.*²⁴; filled circles: Matsunaga and Nagashima⁵; filled triangles: Fokin and Kalashnikov¹⁷; empty squares: Sengers and Watson²⁸; empty circles: Teske *et al.*²⁹; empty triangles: Huber *et al.*²⁷, dilute gas term.

Figure S5. The variation in the thermal conductivity of air with temperature calculated using parameterisations found in the literature. Filled squares: Lemmon and Jacobsen²⁶, dilute term only; filled circles: Touloukian *et al.*³⁰; filled triangles: Tsilingiris²⁵; empty squares: Winkler *et al.*²; empty circles: The Engineering ToolBox³²; empty triangles: Pruppacher and Klett.³¹

Figure S6. Variation in the thermal conductivity of water with temperature calculated using different literature parameterisations. Filled squares: Tsilingiris²⁵; filled circles: Winkler *et al.*²; filled triangles: Matsunaga and Nagashima⁵; empty squares: Sengers and Watson²⁸, dilute gas term; empty circles: Touloukian *et al.*³⁰; empty triangles: Pruppacher and Klett.³¹

Figure S7. Comparison of different theoretical predictions for the thermal conductivity of humid air with experimental data recorded as a function of mole fraction of air. Filled squares (Experimental data): Touloukian *et al.*³⁰; filled circles: Tondon and Saxena³⁵; filled triangles: Tsilingiris²⁵ eq 29; empty squares: Tsilingiris²⁵ eq 55; empty circles: Mason and Saxena³⁴; empty triangles: Lindsay and Bromley³³; crossed squares: Winkler *et al.*²; crossed circles: Poling *et al.*¹⁴

Figures

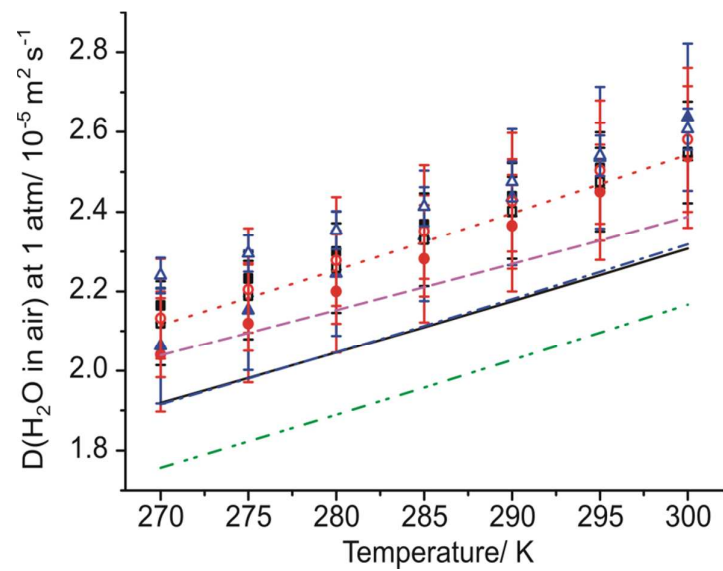


Figure S1.

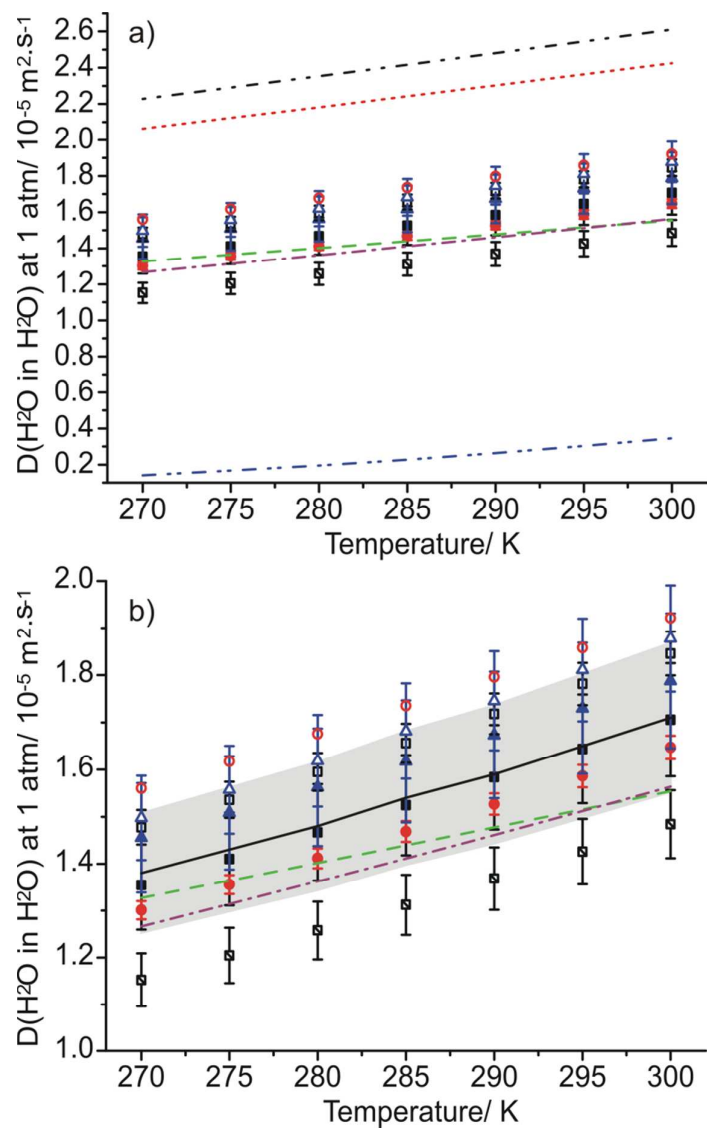


Figure S2.

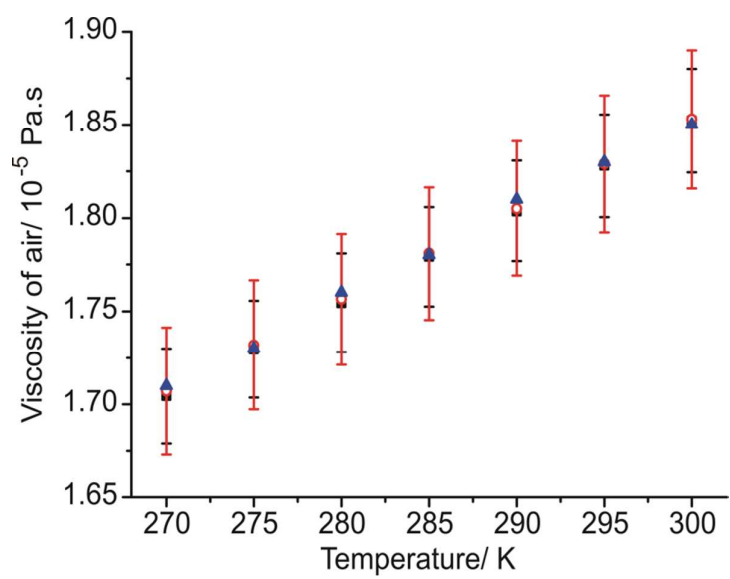


Figure S3.

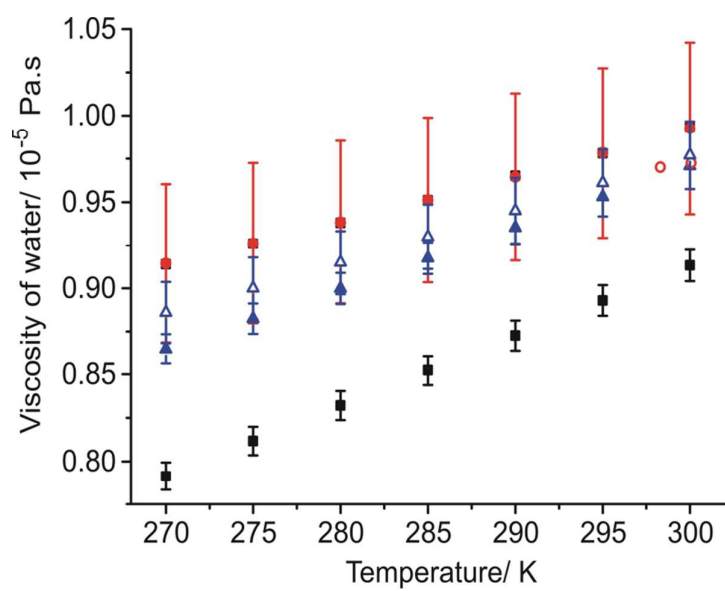


Figure S4.

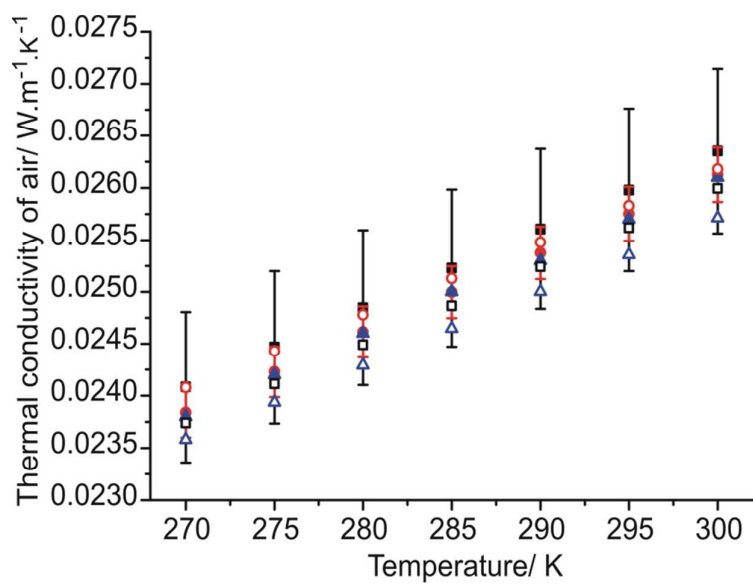


Figure S5.

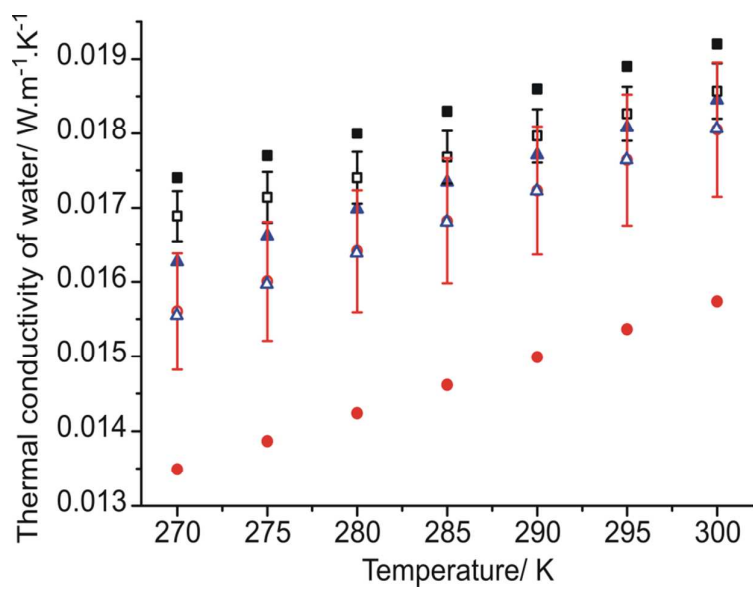


Figure S6.

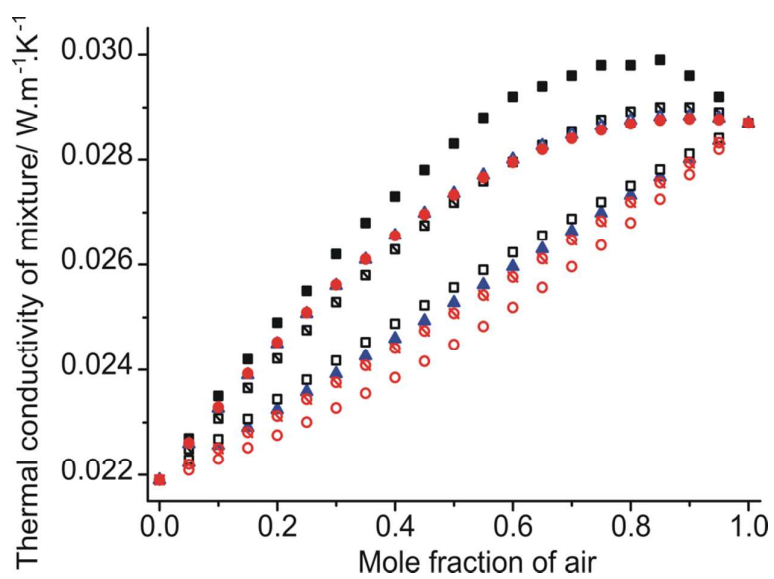


Figure S7.