Supporting Information

Measurement and Correlation of the Physicochemical Properties of Novel Aqueous Bis(3-aminopropyl)amine and Its Blend with N-Methyldiethanolamine for CO_2 Capture

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Number of Tables: 4

Number of Figures: 6

Number of Pages: 10

Density (ρ) and viscosity (η) of pure APA and Henry's Constant (H_{N_2O}) in pure APA are calculated at various temperatures (T)= (298 to 323) K. Experimental data of these properties correlated by following equations

$$\rho / \mathrm{kg \cdot m^{-3}} = a + b(T / \mathrm{K}) + c(T / \mathrm{K})^2 \quad (1)$$

$$\eta / \mathrm{mPa \cdot s} = a + b(T / \mathrm{K}) + c(T / \mathrm{K})^2 \quad (2)$$

$$H_{N_2O} / \mathrm{kPa \cdot m^3 \cdot kmol^{-1}} = a \exp(b / (T / \mathrm{K})) \quad (3)$$

Table S1. Density ρ, Viscosity η, Molality M_{N_2O}, and Henry's Constant, H_{N_2O}, of Pure APA at Different Temperature T[a]

T/(K)	ρ/kg·m^{-3}	η/mPa·s	M_{N_2O}/ mol·kg^{-1}	$H_{N_2O}\cdot10^{-3}$/kPa·kg·kmol^{-1}
298	927.36	8.51	0.0493	2054
303	923.34	7.04	0.0466	2174
308	919.32	5.92	0.0442	2294
313	915.28	5.05	0.0419	2421
318	911.18	4.62	0.0396	2556
323	906.97	3.99	0.0376	2695

[a]Standard uncertainties u for density, viscosity and Henry's Constant $u(T)$ = 0.25 K and $u(p)$ = 0.2 kPa. The combined expanded uncertainty for density measurement $U_c(\rho)$ = 4.07 kg·m^{-3} for viscosity measurement $U_c(\eta)$ =0.113 mPa·s, and for solubility measurement uncertainty in terms of molality $U_c(M_{N_2O})$ = 4.07·10^{-4} mol·kg^{-1} and Henry constant $U_c(H_{N_2O})$ =22.27·10^3 kPa·kg·kmol^{-1} (95% level of confidence, k=2).

Table S2. Parameters of Density, Viscosity and Henry's Constant for pure APA[a]

parameters	density	viscosity	Henry's Constant
a	1032.1	539.31	9.743·10^4
b	79.61·10^{-2}	-3.262	-1.1281·10^3
c	14.47·10^{-4}	4.971·10^{-3}	
[a]AAD%	1.56·10^{-2}	1.38	0.15

Figure S1 shows the variation of Henry's law constant of CO_2 in pure water at various temperatures.

Figure S2 shows the variation of Henry's law constant of N_2O in pure water at various temperatures.

Figure S3 shows the variation of Diffusivity of CO_2 in pure water at various temperatures.

Figure S4 shows the variation of Diffusivity of N_2O in pure water at various temperatures.

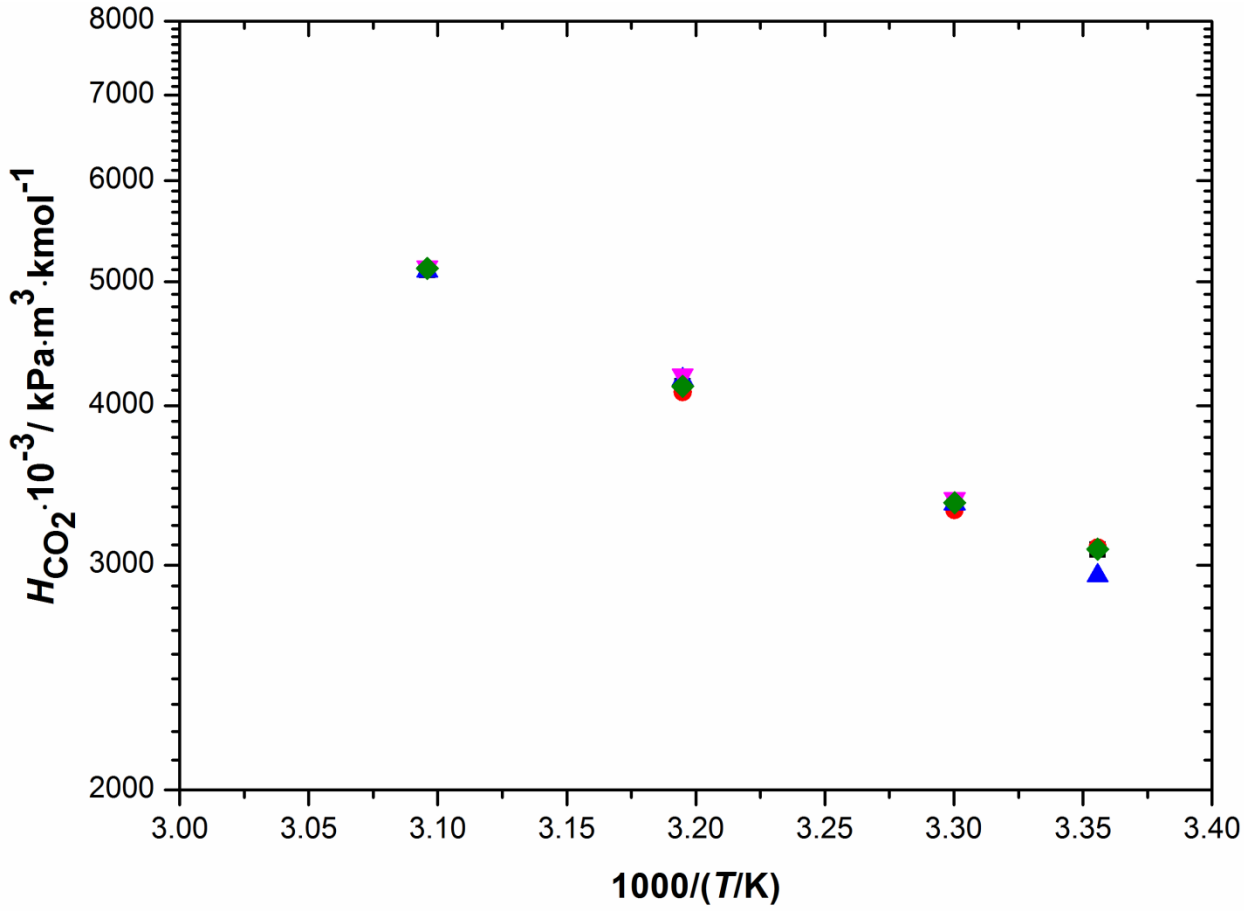

Figure S1. Henry's law constant of CO_2 (H_{CO_2}) in water as a function of temperature (T): ■, Paul et al.[26]; ●, Mandal et al.[27]; ▲, Al-Ghawas et al.[22]; ▼, Li and Lai[28]; ♦, this study.

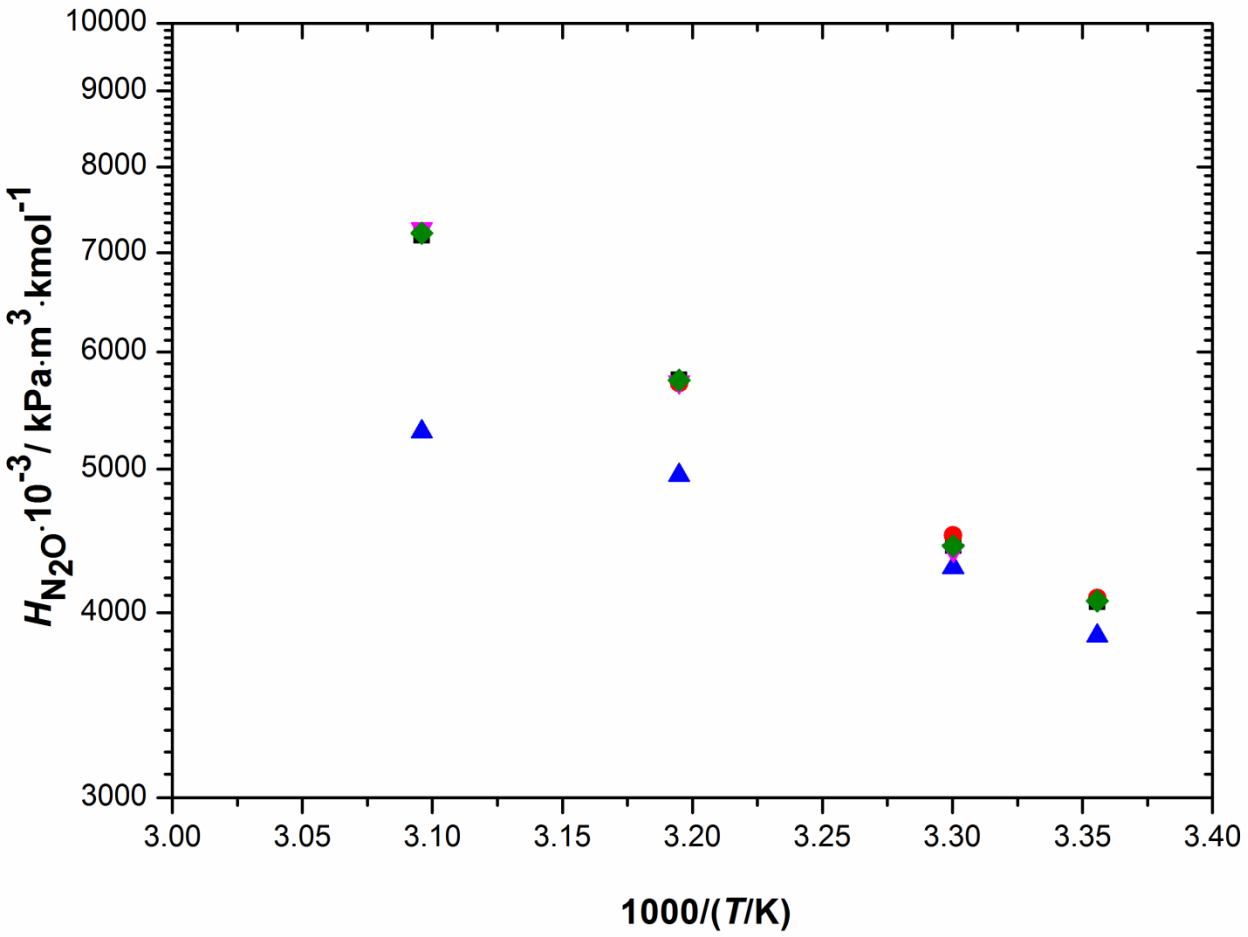

Figure S2. Henry's law constant of N_2O (H_{N_2O}) in water as a function of temperature (T): ■, Paul et al.[26]; ●, Mandal et al.[27]; ▲, Al-Ghawas et al.[22]; ▼, Li and Lai[28]; ♦, this study.

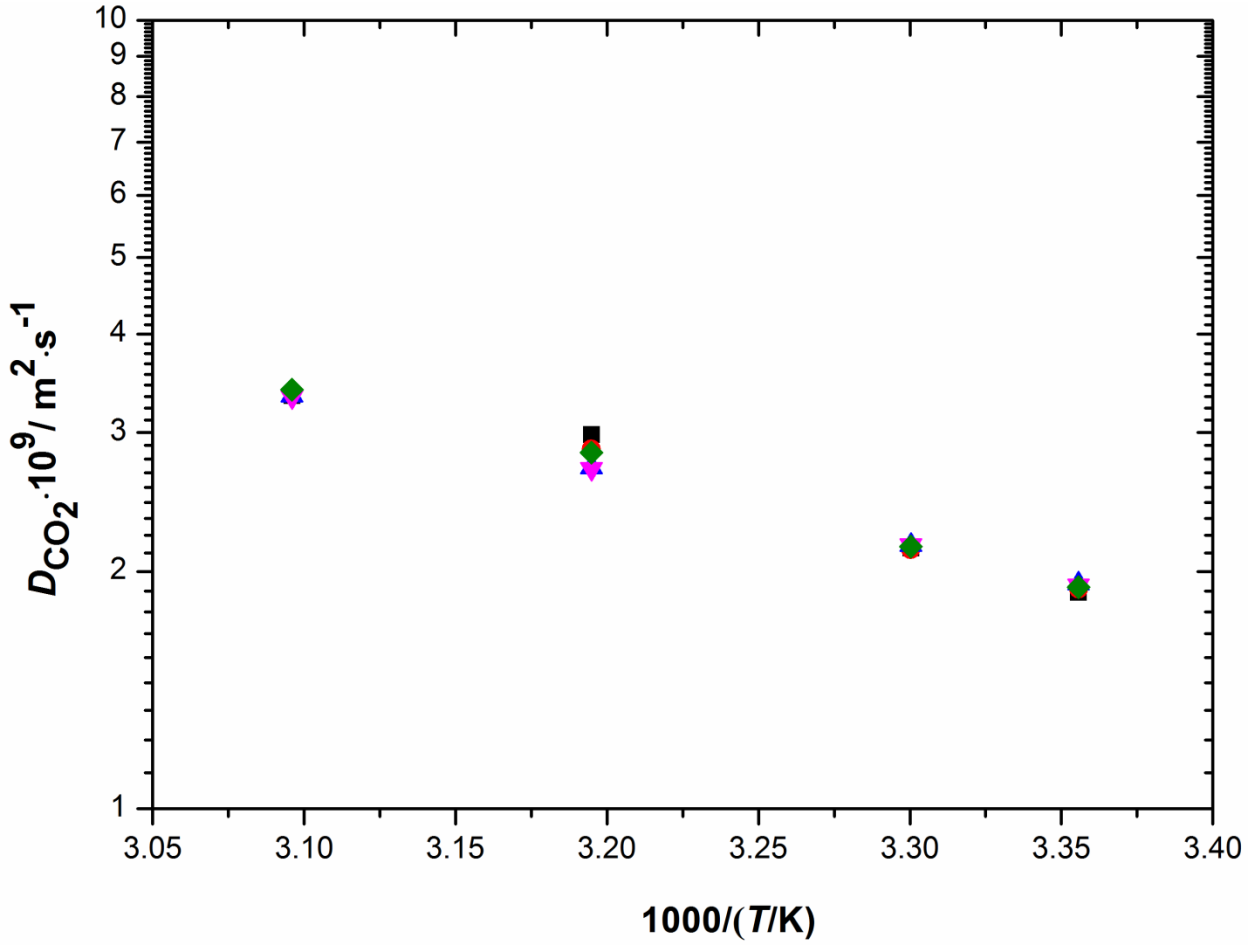

Figure S3. Diffusivity of CO_2 (D_{CO_2}) in water as a function of temperature: ■, Paul et al.[26]; ●, Mandal et al.[27]; ▲, Al-Ghawas et al.[22]; ▼, Li and Lai[28]; ♦, this study.

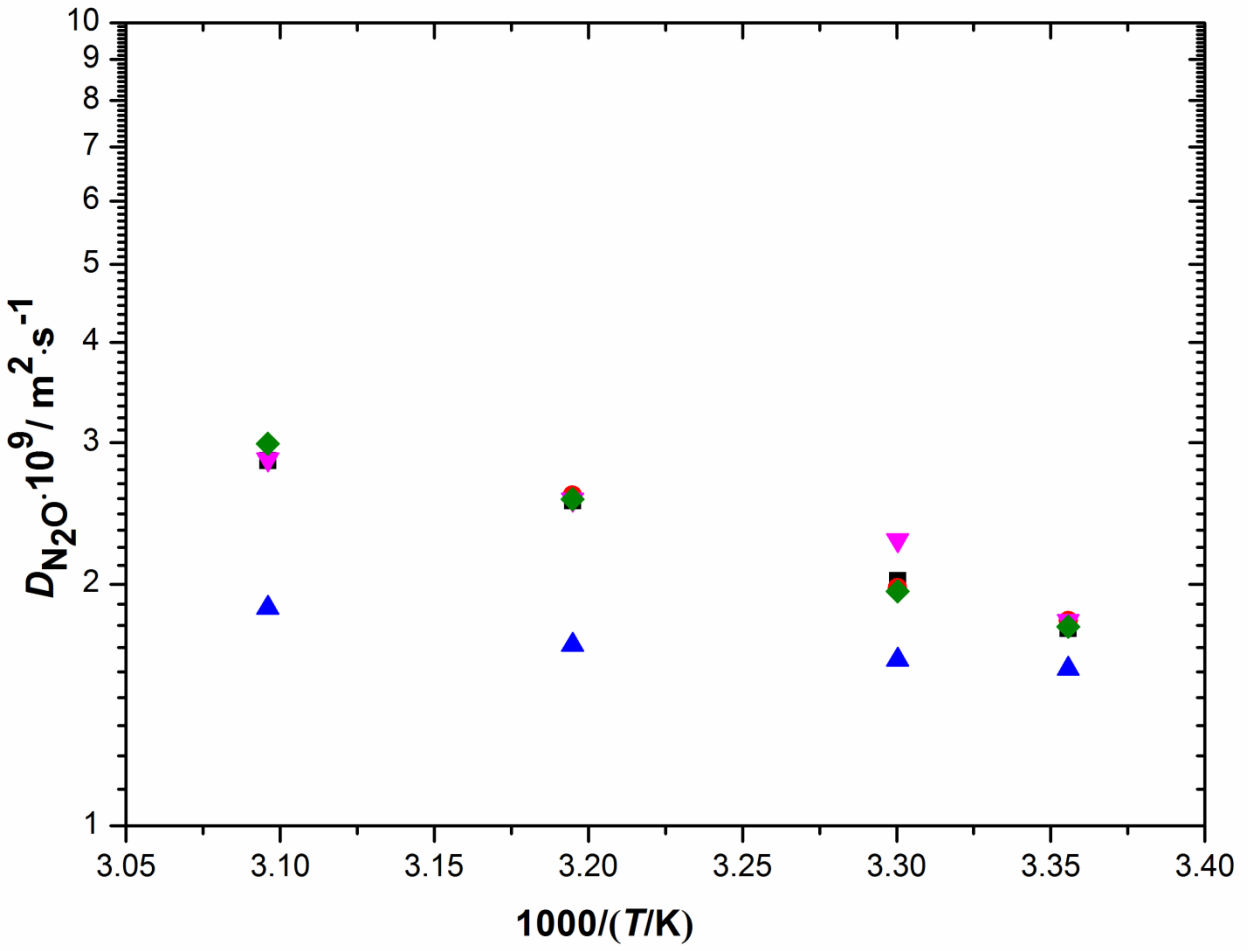

Figure S4. Diffusivity of N_2O (D_{N_2O}) in water as a function of temperature: ■, Paul et al.[26]; ●, Mandal et al.[27]; ▲, Al-Ghawas et al.[22]; ▼, Versteeg and van Swaaij.[31]; ♦, this study.

Multiple experimental data of density (ρ) and viscosity (η) of pure MDEA, and 10, 20 and 30 weight % of MDEA water solution are compared with various literature data [22, 32-36] as shown in figures S5 and S6 with the AAD of 0.07% and 0.92%, respectively.

Figure S5 shows the variation of experimental data of density of pure MDEA and aqueous MDEA solutions at various temperatures.

Figure S6 shows the variations of experimental data of viscosity of pure MDEA and aqueous MDEA solutions at various temperatures.

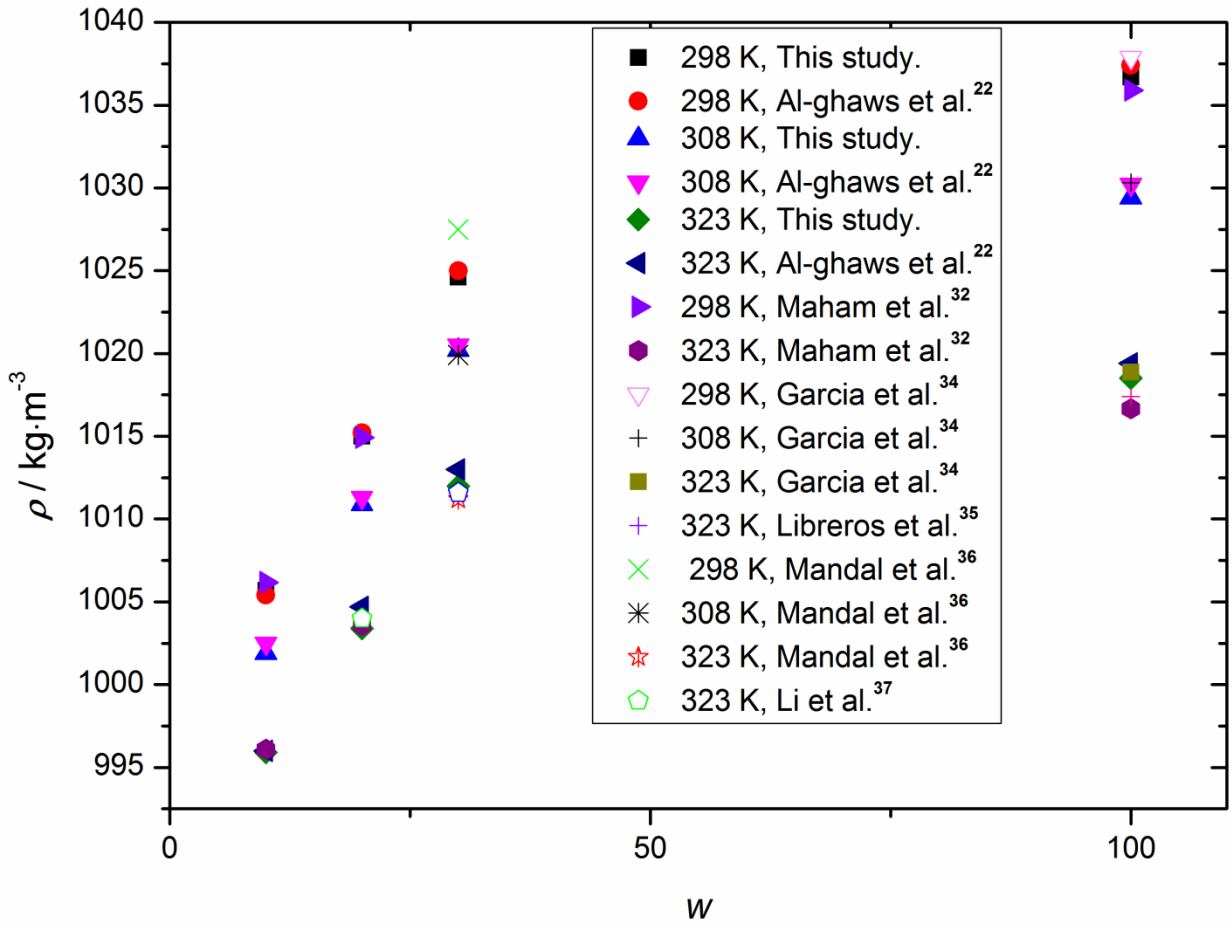

Figure S5. Experimental density data as a function of temperature and weight %.

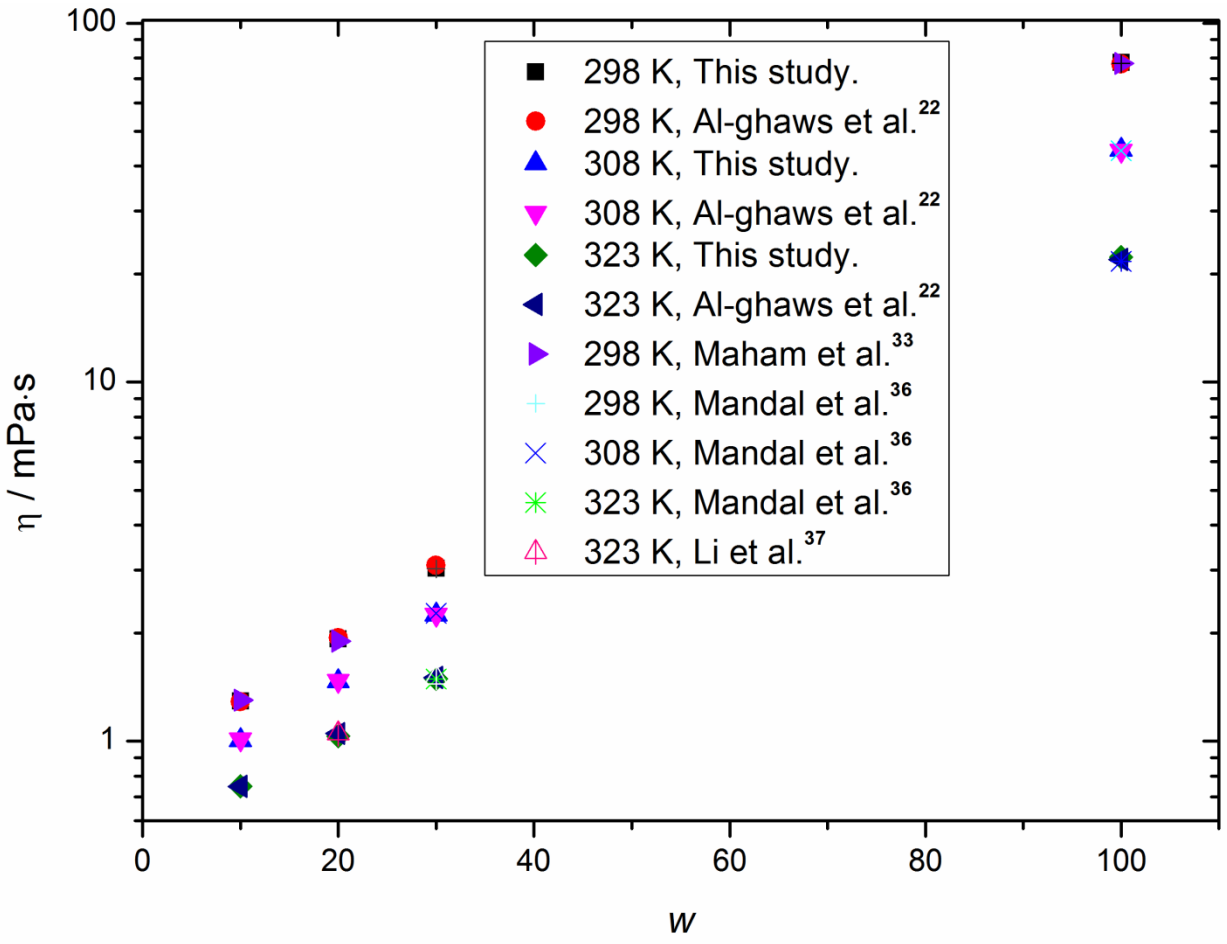

Figure S6. Experimental viscosity data at as a function of temperature and weight %.

The amount of N_2O absorbed at various concentrations and temperature as shown below in table S3 and S4.

Table S3. Measured Solubility of N_2O in APA (1) + H_2O (2) at various Temperatures as a Function of Molality *m* at a pressure 0.1 MPa[a]

	M_{N_2O} /mol·kg^{-1}					
m_1 /mol·kg^{-1}	298K	303K	308K	313K	318K	323K
0.102	0.0250	0.0226	0.0211	0.0192	0.0176	0.0162
0.313	0.0240	0.0218	0.0203	0.0186	0.0171	0.0158
0.537	0.0231	0.0212	0.0197	0.0181	0.0167	0.0154
0.773	0.0224	0.0207	0.0193	0.0177	0.0163	0.0150
1.024	0.0218	0.0202	0.0188	0.0173	0.0159	0.0148
1.291	0.0213	0.0197	0.0183	0.0168	0.0155	0.0144

[a]Standard uncertainties *u* are $u(T) = 0.25$ K, $u(m) = 0.001$ mol·kg^{-1}, $u(p) = 0.2$ kPa. The combined expanded uncertainty for solubility measurement on the molality basis with uncertainty $U_c(M_{N_2O}) = 2.29 \cdot 10^{-4}$ mol·kg^{-1} (95% level of confidence, k = 2). Solvent = Water.

Table S4. Measured Solubility of N_2O in APA (1) + MDEA (2) + H_2O (3) at various Temperatures as a Function of Molality *m* at a pressure 0.1 MPa[a]

m_1/m_2	M_{N_2O} / mol·kg^{-1}					
mol·kg^{-1}	298K	303K	308K	313K	318K	323K
0/4.416	0.0194	0.0184	0.0173	0.0161	0.0150	0.0139
0.148/4.294	0.0194	0.0183	0.0172	0.0160	0.0149	0.0138
0.447/4.025	0.0192	0.0182	0.0171	0.0160	0.0148	0.0138
0.751/3.753	0.0191	0.0182	0.0170	0.0159	0.0148	0.0138
1.058/3.478	0.0191	0.0181	0.0170	0.0159	0.0147	0.0138
1.371/3.199	0.0190	0.0181	0.0170	0.0158	0.0147	0.0138
1.688/2.915	0.0190	0.0180	0.0169	0.0158	0.0147	0.0138

[a]Standard uncertainties *u* are $u(T) = 0.25$ K, $u(m) = 0.001$ mol·kg^{-1}, $u(p) = 0.2$ kPa. The combined expanded uncertainty for solubility measurement on the molality basis with uncertainty $U_c(M_{N_2O}) = 1.74 \cdot 10^{-4}$ mol·kg^{-1} (95% level of confidence, k = 2). Solvent = water.

References

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