

Supplemental Information to “Modeling the surface tension of complex, reactive organic-inorganic mixtures”

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Table S1. Fit parameters for all species in Millipore H₂O and in 3.1 M (NH₄)₂SO₄ at 25°C.

Solution	σ_o^+	a (dyn cm ⁻¹ K ⁻¹)	b (kg H ₂ O (mol C) ⁻¹)
Acetaldehyde	72.5	0.00339 ± 0.00213	1281.1 ± 4450
Acetaldehyde in 3.1 M (NH ₄) ₂ SO ₄	78.5	0.02601 ± 0.00484	8.9282 ± 3.61
Formaldehyde	72.5	--	--
Formaldehyde in 3.1 M (NH ₄) ₂ SO ₄	78.5	0.0119 ± 0.0043	50.23 ± 44.8
Glyoxal	72.5	--	--
Glyoxal in 3.1 M (NH ₄) ₂ SO ₄	78.5	--	--
Methylglyoxal	72.5	0.02453 ± 0.00363	2.9998 ± 1.25
Methylglyoxal in 3.1 M (NH ₄) ₂ SO ₄	78.5	0.0185 ± 0.0008	140 ± 34
Alanine	72.5	0.0135 ± 0.0268	5.9931 ± 17.4
Alanine in 3.1 M (NH ₄) ₂ SO ₄	78.5	--	--
Serine	72.5	0.00330 ± 0.00519	392.1 ± 2.27×10 ³
Serine in 3.1 M (NH ₄) ₂ SO ₄	78.5	0.00160 ± 0.00171	1392.9 ± 8.01×10 ³
Glycine	72.5	0.04030 ± 0.0951	3.3357 ± 9.62
Glycine in 3.1 M (NH ₄) ₂ SO ₄	78.5	--	--
Leucine	72.5	0.01289 ± 0.00913	13.731 ± 18.6
Leucine in 3.1 M (NH ₄) ₂ SO ₄	78.5	0.03338 ± 0.00851	32.709 ± 14.7
‡Oxalic Acid	72.5	0.00291 ± 0.00050	6.943 ± 2.83
Oxalic Acid in 3.1 M (NH ₄) ₂ SO ₄	78.5	0.01297 ± 0.0238	1.0583 ± 2.92
‡Succinic Acid	72.5	0.00986 ± 7.4×10 ⁻⁴	2.5101 ± 0.385
Succinic Acid in 3.1 M (NH ₄) ₂ SO ₄	78.5	0.0349 ± 0.0222	0.74884 ± 0.751

‡ Calculated from surface tension data from (Hyvärinen et al., 2006)

⁺ The surface tension of (NH₄)₂SO₄ was taken from the International Critical Tables (Washburn, 2003).

Table S2. k values calculated for all organics in 3.1 M $(\text{NH}_4)_2\text{SO}_4$ using Eqn. (5).

Organic	k
Acetaldehyde	-0.36197 ± 0.0176
Methylglyoxal	-2.339 ± 0.0487
Alanine	1.0389 ± 0.179
Serine	0.05173 ± 0.0553
Glycine	3.5809 ± 0.241
Leucine	-4.629 ± 0.129
Oxalic Acid	-0.28876 ± 0.0904
Succinic Acid	-0.92445 ± 0.102

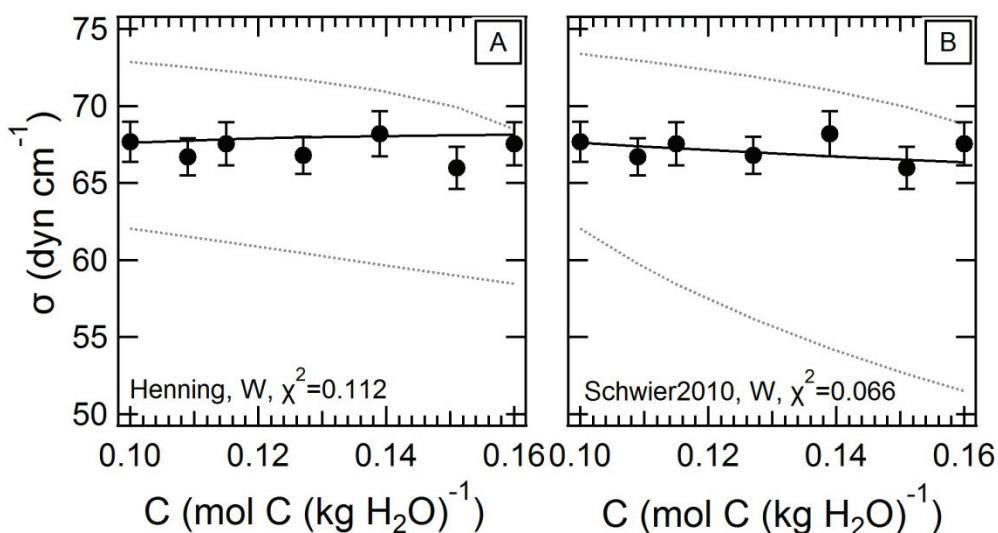


Figure S1. 0.05 M acetaldehyde with varying amounts of alanine in Millipore H_2O .

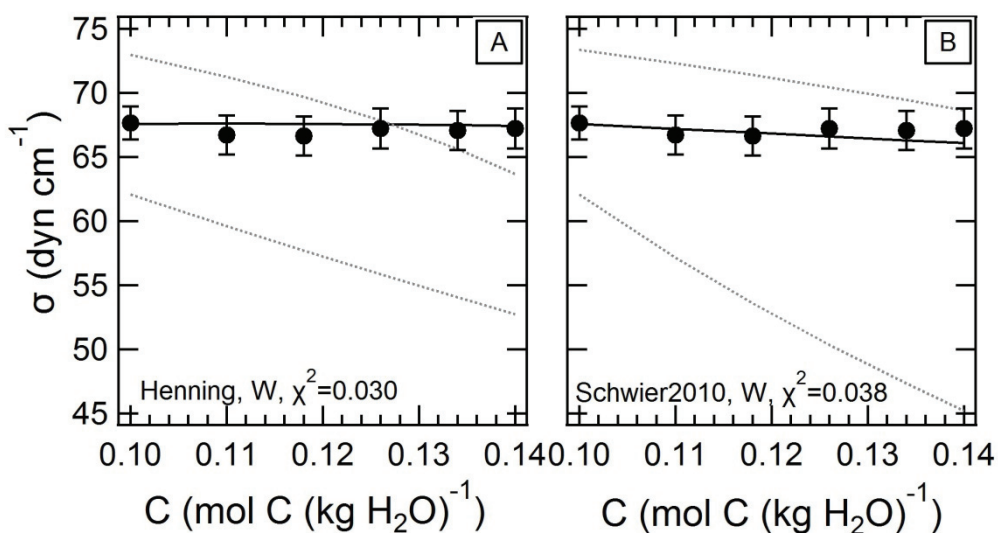


Figure S2. 0.05 M acetaldehyde with varying amounts of glycine in Millipore H_2O .

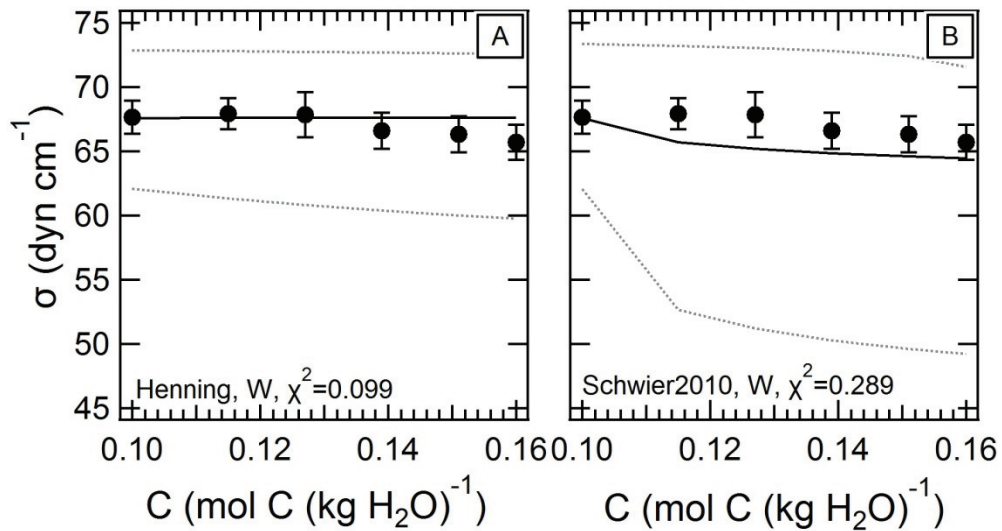


Figure S3. 0.05 M acetaldehyde and varying amounts of serine in Millipore H₂O.

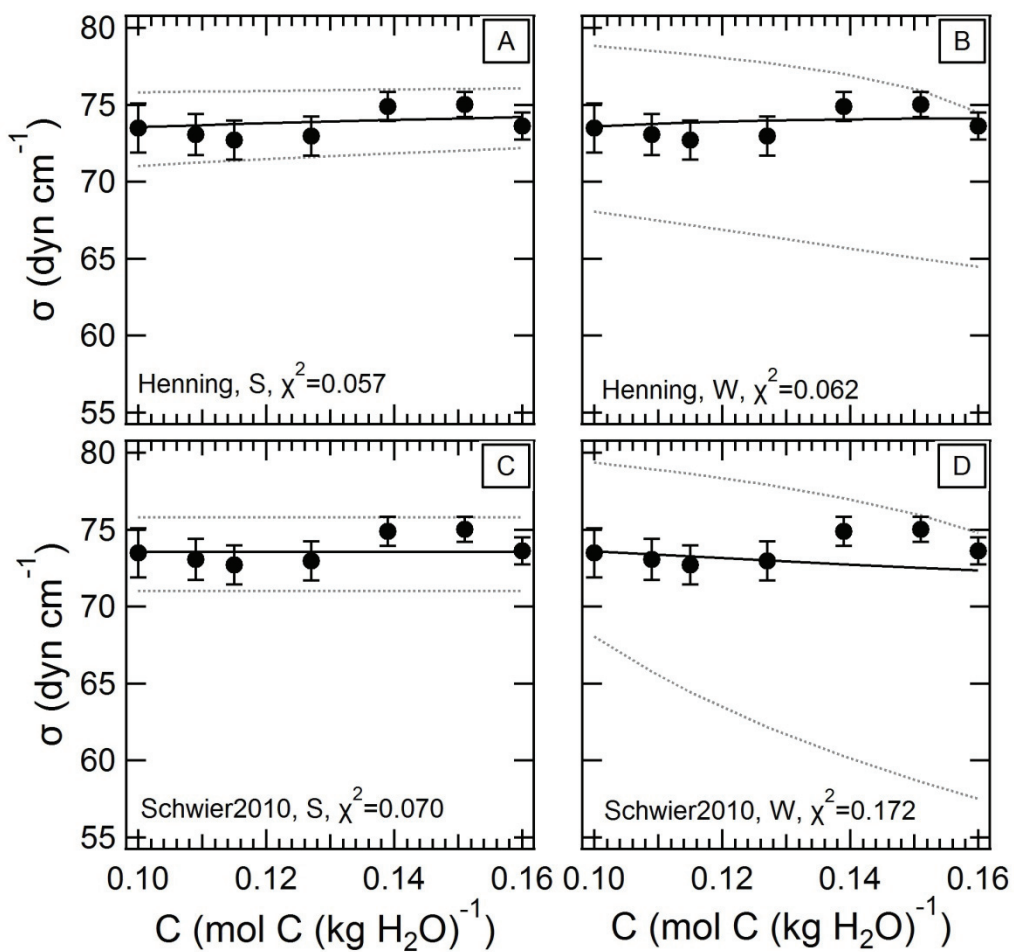


Figure S4. 0.05 M acetaldehyde with varying amounts of alanine in 3.1 M (NH₄)₂SO₄.

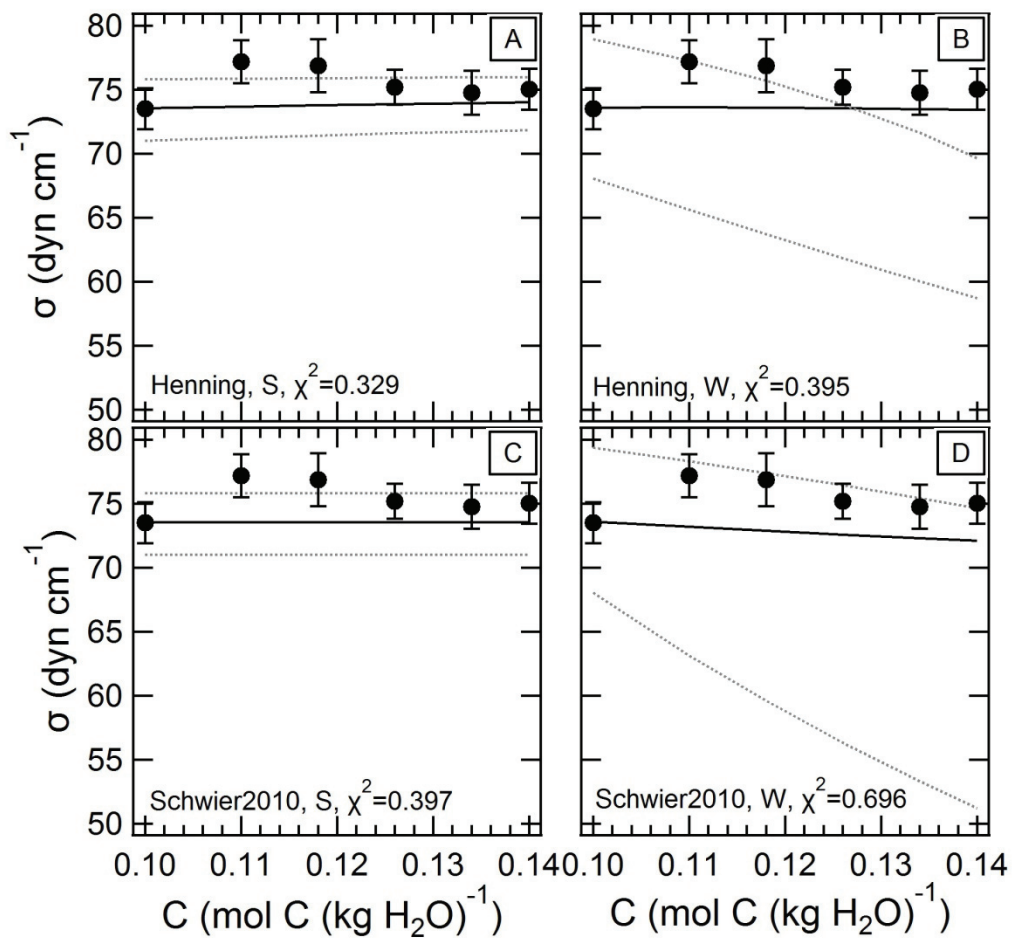


Figure S5. 0.05 M acetaldehyde with varying amounts of glycine in 3.1 M (NH₄)₂SO₄.

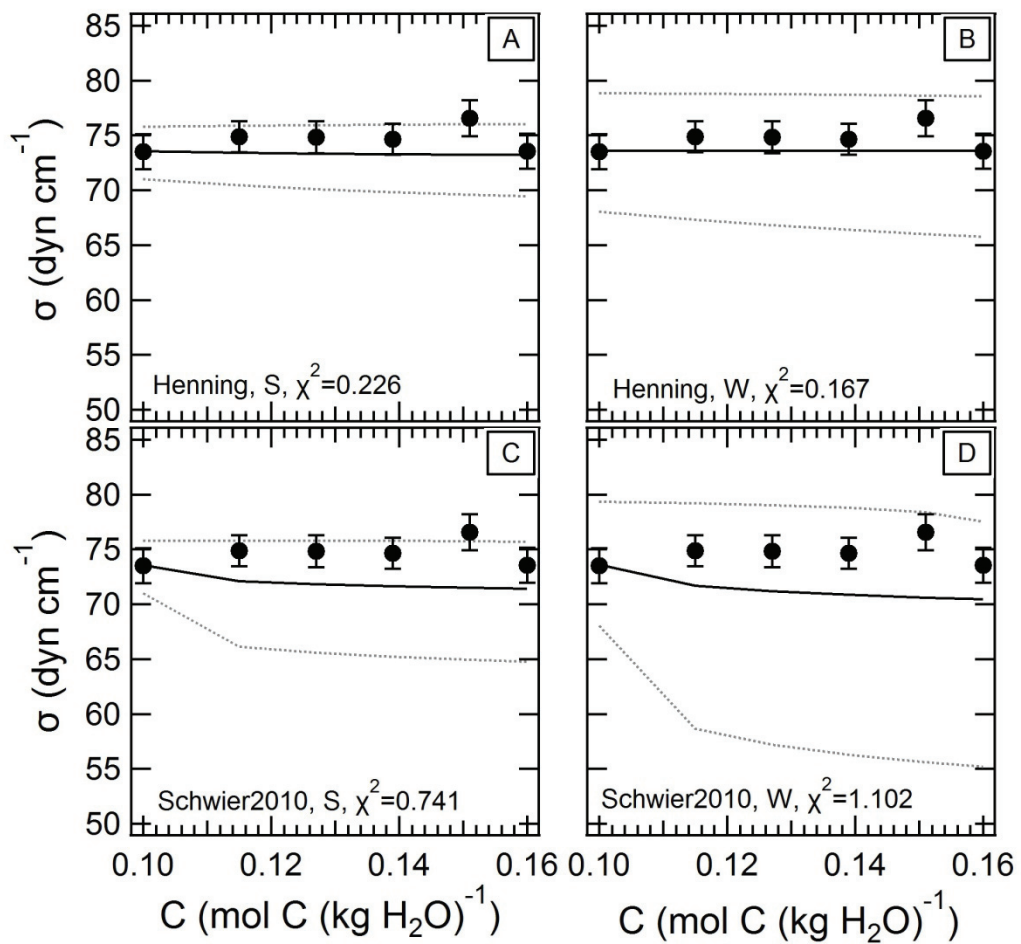


Figure S6. 0.05 M acetaldehyde and varying amounts of serine in 3.1 M (NH₄)₂SO₄.

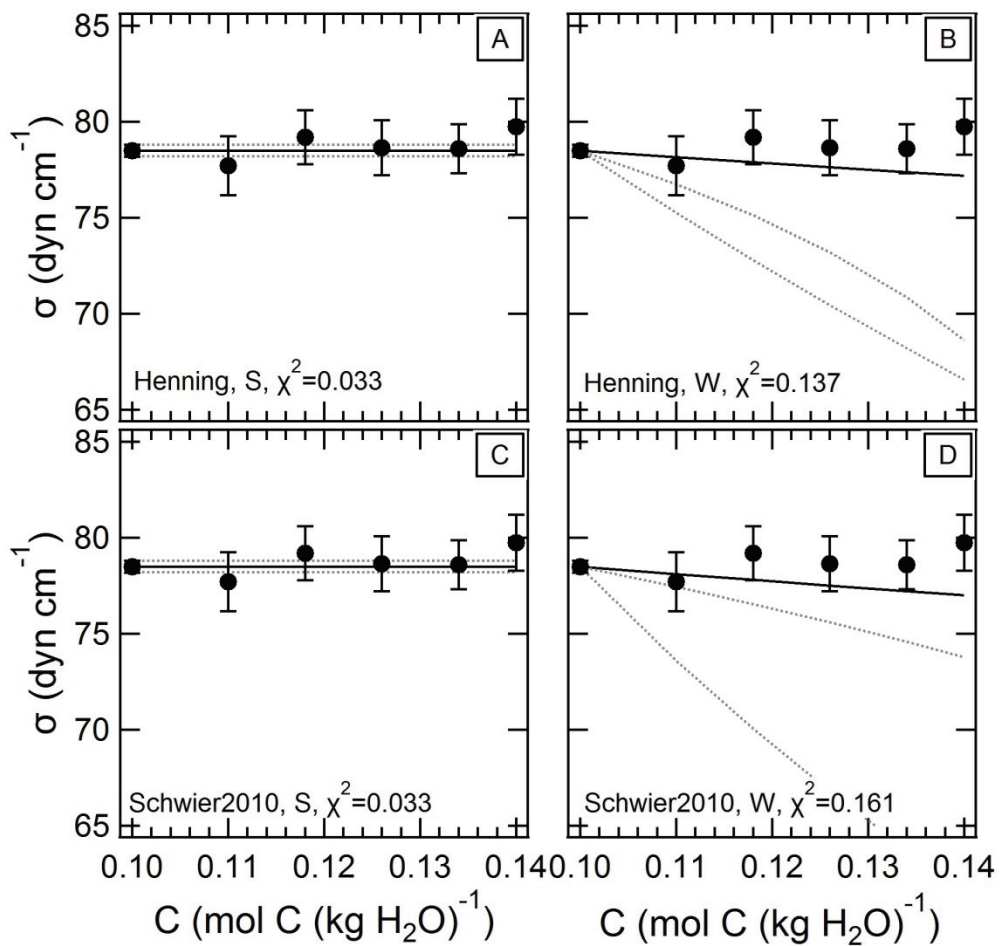


Figure S7. 0.05 M glyoxal and varying amounts of glycine in 3.1 M (NH₄)₂SO₄.

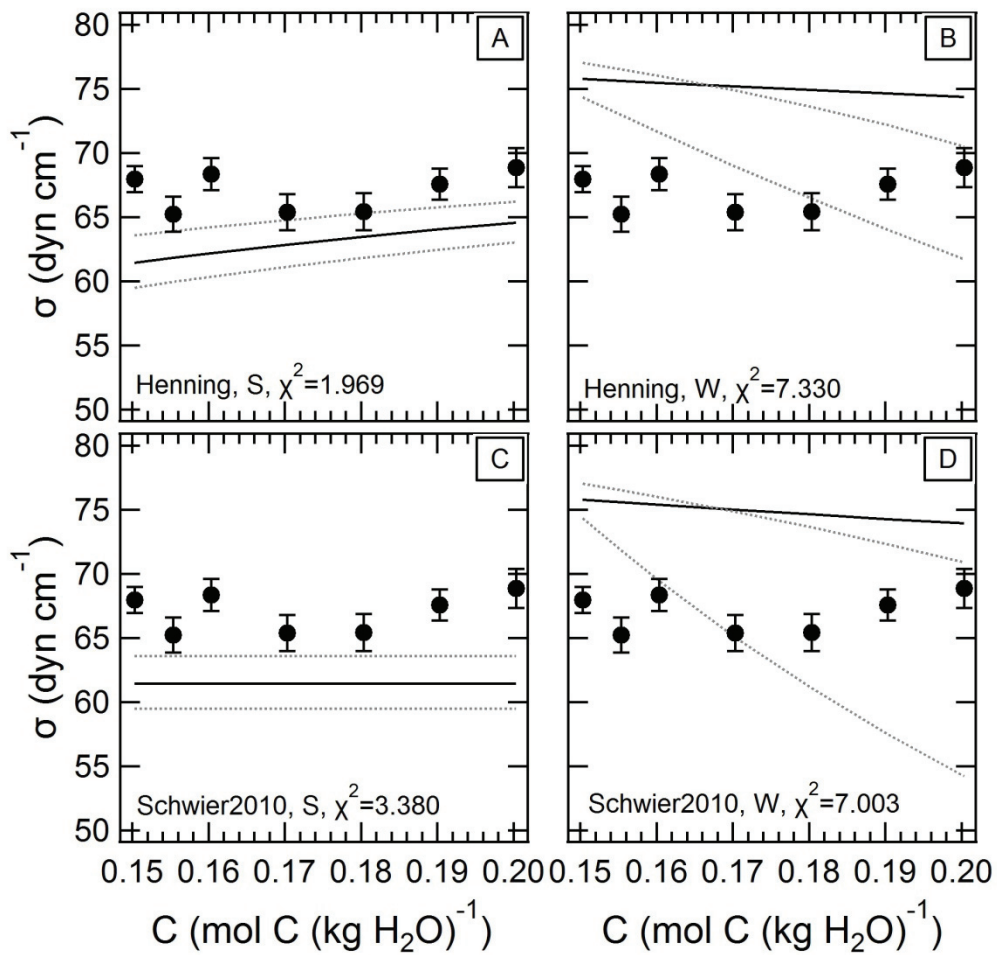


Figure S8. 0.05 M methylglyoxal and varying amounts of glycine in 3.1 M $(\text{NH}_4)_2\text{SO}_4$.

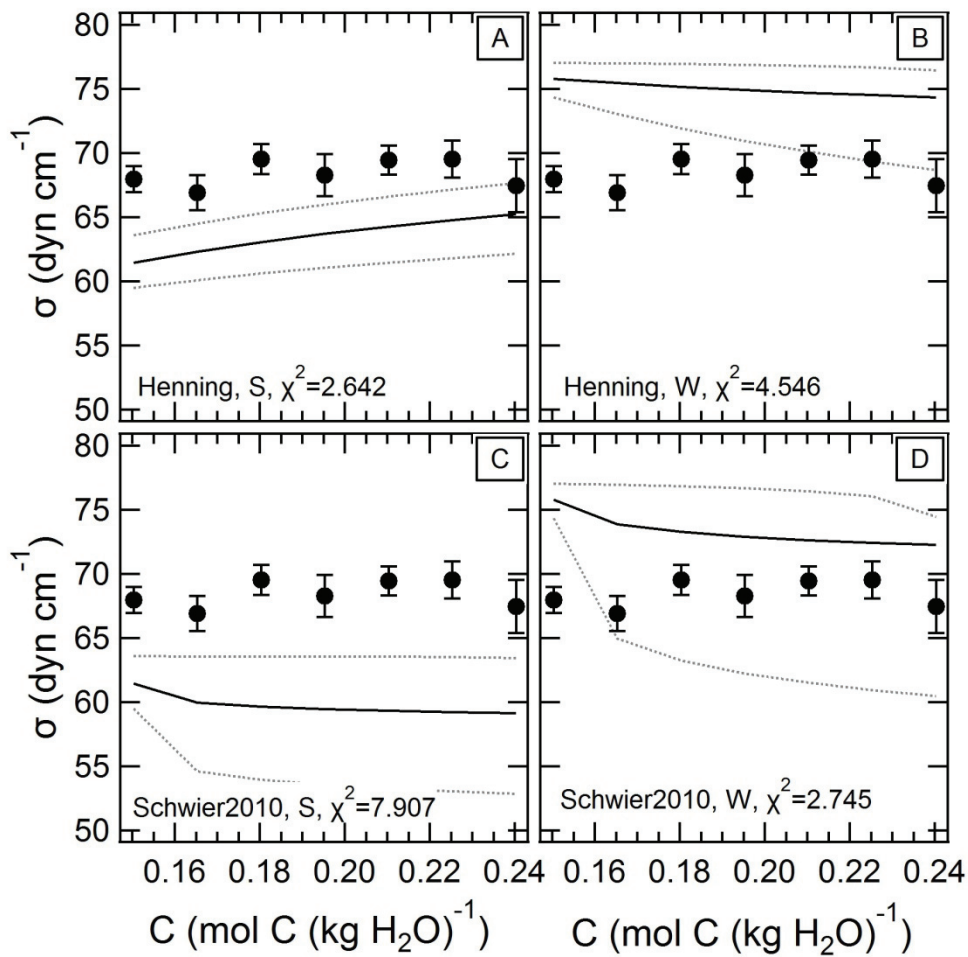


Figure S9. 0.05 M methylglyoxal and varying amounts of serine in 3.1 M (NH₄)₂SO₄.

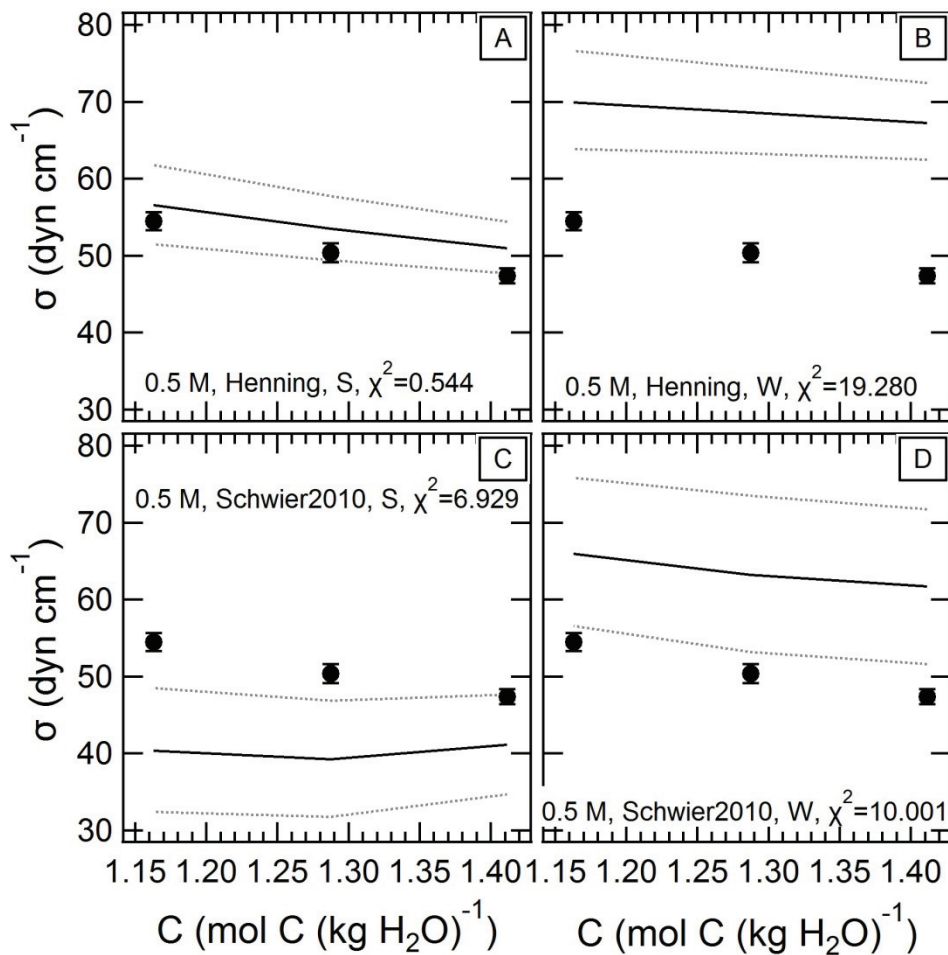


Figure S10. 0.5 M total organic, varying ratio of acetaldehyde and methylglyoxal in 3.1 M (NH₄)₂SO₄.

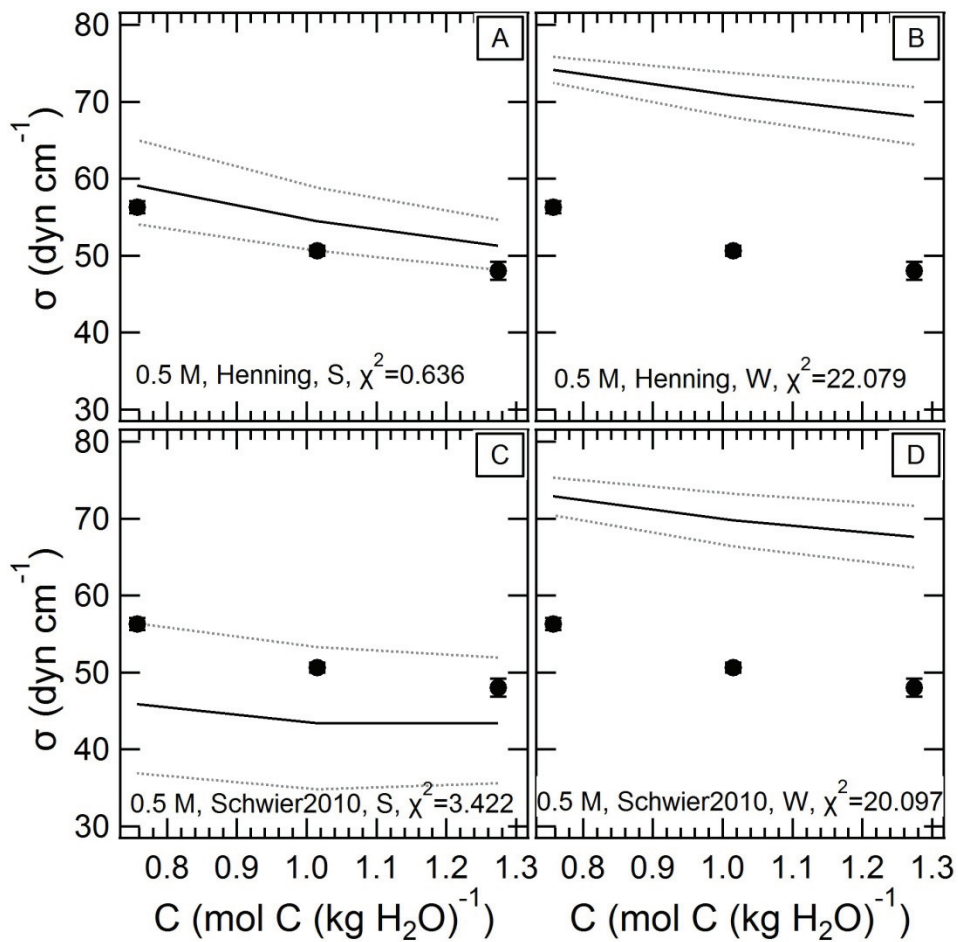


Figure S11. 0.5 M total organic, varying ratio of formaldehyde and methylglyoxal in 3.1 M $(\text{NH}_4)_2\text{SO}_4$.

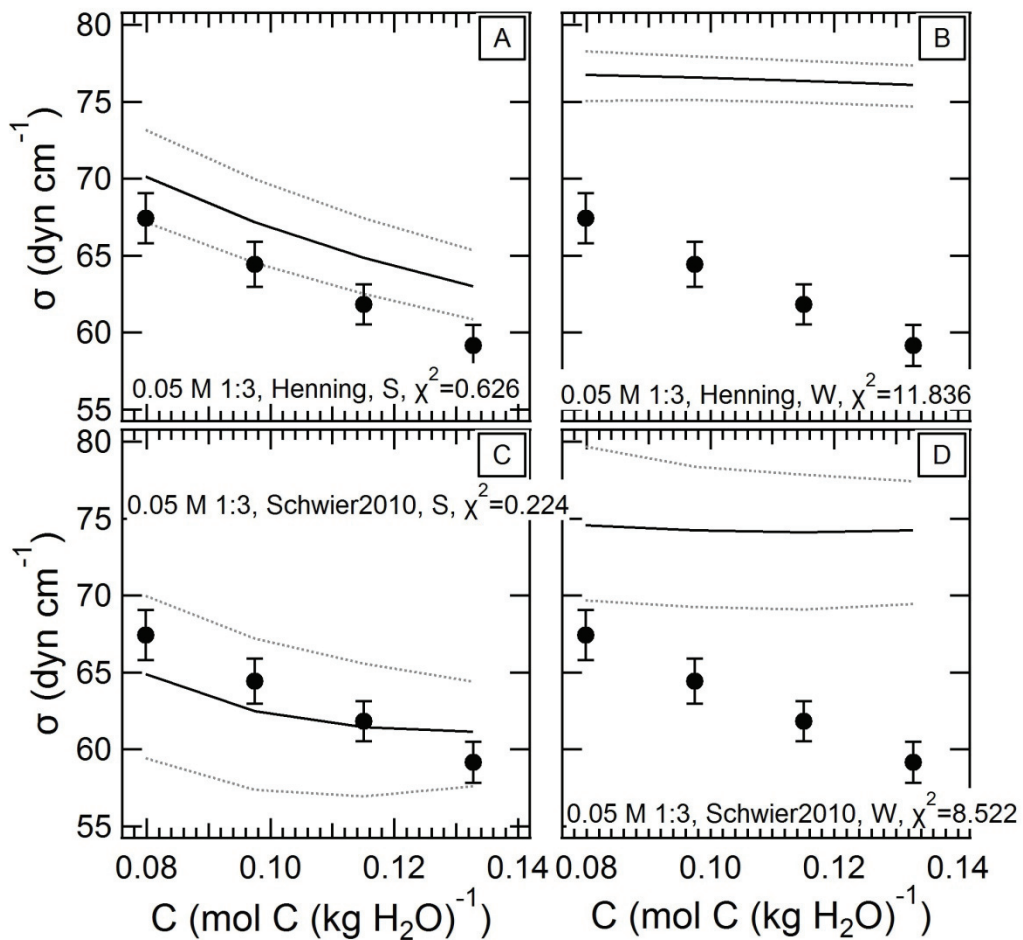


Figure S12. 0.05 M total organic with varying amounts of acetaldehyde:formaldehyde (3:1) and methylglyoxal in 3.1 M $(\text{NH}_4)_2\text{SO}_4$.

References:

- Hyvärinen, A. R., Lihavainen, H., Gaman, A., Vairila, L., Ojala, H., Kulmala, M., and Viisanen, Y.: Surface tensions and densities of oxalic, malonic, succinic, maleic, malic, and cis-pinonic acids, *Journal of Chemical and Engineering Data*, 51 (1), 255-260, 2006.
- Washburn, E. W., *International Critical Tables Of Numerical Data, Physics, Chemistry and Technology* (1st Electronic Edition), Knovel, 1926-1930;2003.