Supporting Information: Prediction of cloud condensation nuclei activity for organic compounds using functional group contribution methods

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Keywords

Cloud condensation nuclei, organic aerosol, thermodynamic modeling, UNIFAC, functional group composition

Model Parameters and Validation

Tables S1 and S2 summarize group interaction parameters a_{mn} and van der Waals volume and surface parameters for functional groups examined in this work, respectively. These parameters were compiled from Hansen et al. (1991), Raatikainen and Laaksonen (2005), and Compernolle et al. (2009). An instance of the model was executed for the mixtures ethanol/water and acetone/water using parameters from Hansen et al. (1991) only. For these mixtures UNIFAC predictions are available from the Dortmund Data Bank Software & Separation GmbH (DDBST) online tool for prediction of activity coefficients (http://ddbonline.ddbst.com/UNIFAC Calculation/UNIFACCalculationCGI.exe). Calculations were also compared against the software package xlUNIFAC (Randhol and Engelien, 2000, http://www.pvv.org/~randhol/xlunifac/). Figure 1 shows a benchmark comparison for the activity coefficients predicted for the two mixtures. Agreement between this work and DDBST prediction is taken as indication for correct implementation of the UNIFAC model.
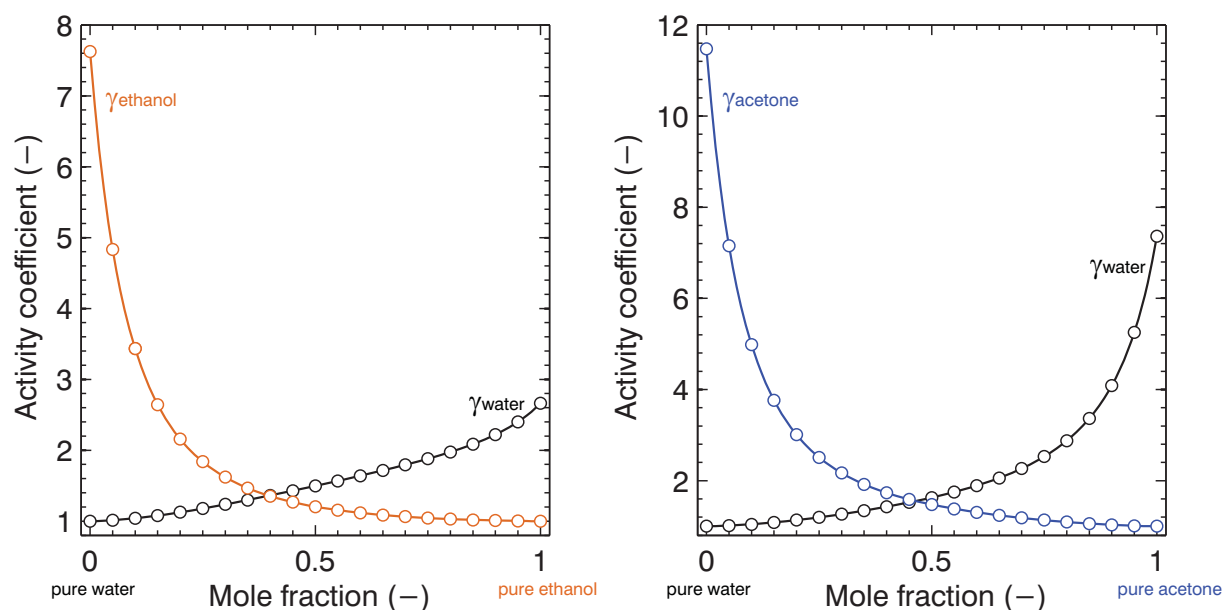
Figure S1. Activity coefficients γ_{water} and γ_{solute} (ethanol or acetone) vs. mole fraction of solute. Symbols are from the DDBST online calculator. Solid lines are computed from the code using a_{mn} interaction parameter values from Hansen (1991). The Q_k parameter for the $CH_3C(=O)$ was taken from xlUNFAC (Table 2).

Modelled phase boundaries were compared against published values computed with the UHAERO model (Table 3, Amundson et al., 2007). Three compounds, common to both studies, were compared adipic acid, palmitic acid and pinonic acid. For this comparison the model was executed using the parameters of Hansen et al. (1991), which is identical to the standard UNI-FAC calculations in (Amundson et al., 2007). For adipic acid, no phase separation is predicted by

either model. For pinonic acid, this model predicts $x_a = 0.9899$, $x_b = 0.5075$ while UHAERO predicts $x_a = 0.9990$, $x_b = 0.5078$. For palmitic acid, this model predicts $x_a = 0.9999$ (limit of model resolution), $x_b = 0.1562$ while UHAERO predicts $x_a = 1 - 1 \times 10^{-7}$, $x_b = 0.1567$ (see Amundson et al., Table 3). Here (x_a, x_b) are the mole fraction of water corresponding to the phase boundary as described in Eq. (10) in the main text.

Experimental Data for Model Evaluation

Tables S3- S7 summarize selected data from the literature to evaluate predictions by the proposed modelling approach. These include model compounds for primary organic aerosol (Table S3), functionalized hydroperoxy ethers (Table S4), hydroxynitrates (Table S5), carboxylic acids (Table S6), and carbohydrates (Table S7). These compounds represent of mix of the functional groups that evaluated in this work, i.e. alkane [CHn] acohol [OH], carbonyl [CHnC(=O)], aldehyde [HC(=O)], ether [CHn(O)], carboxyl [C(=O)OH], nitrate [CHnONO2], and hydroperoxide [CHn(OOH)]. Data in Table S3 are taken from Raymond and Pandis (2002) and Shilling et al., (2007). Data in Tables S4 and S5 are taken from the supplement of Suda et al. (2014). Data in Tables S6 and S7 are from various sources are summarized in the supplement of Petters et al. (2009). Values were updated with new compounds from Christensen and Petters (2012), and were re-screened for data quality based on summary provided by Kuwata et al. (2013).

The tables include the following information. Chemical name, elemental formula, molecular structure, decomposition into functional groups for UNIFAC, molecular weight, density, molar volume (1/density), solubility in water, observed CCN activity, and apparent κ-value. The abbreviations *obs* denotes observed value, *mod* denotes model predicted value, *insoluble* denotes that the compound is insoluble in water and precise solubility value is unknown, N/A denotes that information is not available. The UNIFAC representation lists the groups used to initialize the activity coefficient calculation. Note that the alpha-olefin group (HxC=CHx) was not implemented and the double bonded carbon for oleic acid and maleic acid was approximated as alkane group. For sufficiently soluble compounds the relationship between critical supersaturation and dry diameter follows a -3/2 slope when graphed in log-log coordinates and these compounds are well characterized using a single κ-value (Petters and Kreidenweis, 2008). For compounds that are sparingly soluble, this is not the case. Therefore, the supersaturation and dry diameter of the CCN data are included under the CCN column. For example, myristic acid (Table S3, column 1) did not show CCN activation at s_c = 1% and D < 200 nm. This data pair is used to compute an upper bound apparent κ-value for this substance, i.e. κ< 2×10^-5. Apparent kappa values were calculated numerically seeking the κ that reproduces the s_c, D_d data pair using Eq. (6) in Petters and Kreidenweis (2007). For sufficiently soluble compounds the supersaturation and dry diameter for which the CCN activity the compounds are marked as *dissolved*. Maleic acid (Table S6) falls into that category. For many compounds, two entries are

listed for observed κ-values. These denote the observed range and were derived from measurement uncertainty in a single study, the range between multiple studies, or the range of observation from differences between isomers. More details about the data can be found in the previous data compilations (Petters et al., 2009, Kuwata et al., 2013, Suda et al., 2014, and references therein).

Tables

Table S1. Group interaction parameters a_{mn}. Grey shaded entries are from Table 8 in Raatikainen and Laaksonen (2005). Purple entries are from Table 5, blue entries are from Table 6, and orange entries from Table 7 in Compernolle et al. (2009). The remaining entries are from Table 2, supporting information in Hansen et al. (1991).
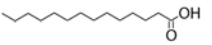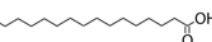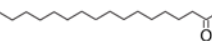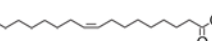
	CH_n	OH	H_2O	$CH_nC(=O)$	$HC(=O)$	$CH_n(O)$	$C(=O)OH$	CH_nONO_2	$CH_n(OOH)$
CH_n	0	143.480	2650.80	586.570	644.590	649.800	-150.91	500.950	977.56
OH	19.236	0	-407.50	84.000	-203.600	28.060	-492.09	37.631	-330.28
H_2O	170.220	-1.393	0	-195.400	-116.000	540.500	-437.73	142.650	-341.18
$CH_nC(=O)$	-180.670	164.500	472.50	0	-37.360	-103.600	669.40	-197.930	-350.58
$HC(=O)$	474.880	529.000	480.80	128.000	0	304.100	497.50	402.000	-387.63
$CH_n(O)$	-272.450	237.700	-314.70	191.100	-7.838	0	664.60	1133.100	-438.74
$C(=O)OH$	2693.300	238.130	271.04	-297.800	-165.500	-338.500	0	-100.170	-501.23
CH_nONO_2	-75.718	818.970	681.78	188.720	-179.380	-289.810	1173.30	0	545.66
$CH_n(OOH)$	-23.233	342.920	795.55	380.940	408.880	490.360	1479.00	-86.279	0

Table S2. Van der Waals volume and surface parameters for groups used in the work. Entries are from from Table 1, supporting information in Hansen (1991) except for CH_nONO_2 and $CH_n(OOH)$ which are taken from Table 1 in Compernolle et al., (2009).

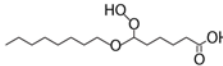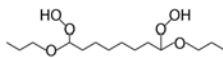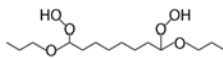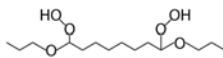| Main Group		Subgroup			
		CH_3	CH_2	CH	C
CH_n	R_k	0.9011	0.6744	0.4469	0.2195
	Q_k	0.8480	0.5400	0.2280	0
		OH			
OH	R_k	1.0			
	Q_k	1.2			
		H_2O			
H_2O	R_k	0.92			
	Q_k	1.40			
		$CH_3C(=0)$	$CH_2C(=0)$		
$CH_nC(=O)$	R_k	1.6724	1.4457		
	Q_k	1.4880[*]	1.1800		
		HC(=O)			
HC(=O)	R_k	0.998			
	Q_k	0.948			
		$CH_3(O)$	$CH_2(O)$	CH(O)	THF
$CH_n(O)$	R_k	1.145	0.9183	0.6908	0.9183
	Q_k	1.088	0.7800	0.46800	1.100
		C(=O)OH	HC(=O)OH		
C(=O)OH	R_k	1.3013	1.5280		
	Q_k	1.2240	1.5320		
		$CH2(ONO_2)$	$CH(ONO_2)$	$C(ONO_2)$	
CH_nONO_2	R_k	2.1246	1.8971	1.6697	
	Q_k	1.8682	1.5562	1.3282	
		CH2(OOH)	CH(OOH)	C(OOH)	
$CH_n(OOH)$	R_k	1.5869	1.3594	1.1320	
	Q_k	1.4370	1.1250	0.8970	
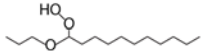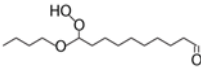
[*] Hansen et al. (1991) report $Q_k = 1.448$. The table used in xlUNIFAC gives 1.488. Using $Q_k = 1.488$ results in exact agreement between this code and output for acetone/water from the DDBST online calculator.

Table S3. Data for primary organic aerosol model compounds

#	Name	Formula	Structure	UNIFAC representation #	Subgroup	MW	ρ	Molar volume obs	mod	Solubility (v/v)	CCN s_c (%) / D_d (nm)	Apparent κ obs	model
	Myristic acid	$C_{14}H_{28}O_2$		1	CH₃	228.4	0.866	264	272.7	<2.3e-5	1% / > 200 nm	<2e-5	<1e-6
				12	CH₂								
				1	C(=O)OH								
	Cetyl alcohol	$C_{16}H_{34}O$		1	CH₃	242.5	0.830	292	309.1	1.2e-9	1% / > 200 nm	<2e-5	<1e-6
				15	CH₂								
				1	OH								
	Palmitic acid	$C_{16}H_{32}O_2$		1	CH₃	256.4	0.853	301	309.1	Insoluble	1% / > 200 nm	<2e-5	<1e-6
				14	CH₂								
				1	C(=O)OH								
	Stearic acid	$C_{18}H_{36}O_2$		1	CH₃	284.5	0.847	336	345.5	3.5e-6	1% / > 200 nm	<2e-5	<1e-6
				16	CH₂								
				1	C(=O)OH								
	Oleic acid	$C_{18}H_{34}O_2$		1	CH₃	282.5	0.890	317	336.4	insoluble	0.66% / >350 nm	<1e-5	<1e-6
				14	CH₂								
				2	CH								
				1	C(=O)OH								

(Row group label: POA model compounds)

Notes: Myristic acid κ-values are taken from Raymond and Pandis (2002), density and molecular weight are from Petters et al. (2009). The upper κ limits from Kuwata et al. (2013). Oleic acid κ-values are based on Shilling et al. (2007) and are imported from supplement of Kuwata et al. (2013). Density and molecular weight are from Petters et al. (2009).
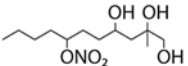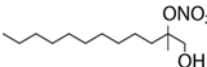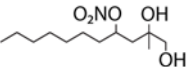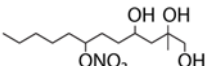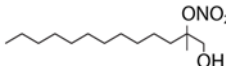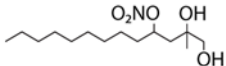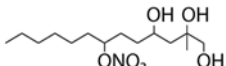
Table S4. Data for functionalized hydroperoxide ethers. Apparent κ-values are identical to those reported in Suda et al. (2014).
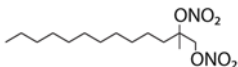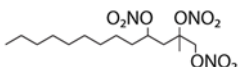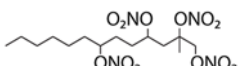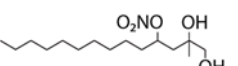
#	Name	Formula	Structure	UNIFAC representation #	Subgroup	MW	ρ	Molar volume obs	Molar volume mod	Solubility (v/v)	CCN s_c (%)	Apparent κ obs	Apparent κ model
Functionalized hydroperoxide ethers	Peroxide-ether	$C_{14}H_{30}O_3$		2	CH_3	246.4	N/A	N/A	320	N/A	0.59%	2.5e-3	<1e-6
				10	CH_2								
				1	$CH_2(O)$						205 nm	4.9e-3	
				1	$CH(OOH)$								
	Peroxide-ether with aldehyde	$C_{14}H_{28}O_4$		1	$CH3$	260.4	N/A	N/A	320	N/A	0.53%		8.3e-5
				10	CH_2							9.2e-4	
				1	$CH_2(O)$								
				1	$CH(OOH)$						264 nm		
				1	$C(=O)H$								
	Peroxide-ether with acid	$C_{14}H_{28}O_5$		1	$CH3$	276.4	N/A	N/A	300	N/A	0.83%	1.2e-2	8.5e-5
				10	CH_2								
				1	$CH_2(O)$								
				1	$CH(OOH)$						123 nm	2.8e-2	
				1	$C(=O)OH$								
	Diperoxide-diether	$C_{14}H_{30}O_6$		2	CH_3	294.4	N/A	N/A	350	N/A	0.31	1.0-e2	<1e-6
				8	CH_2								
				2	CH_2O						205 nm	1.1e-2	
				2	$CH(OOH)$								
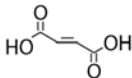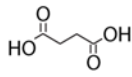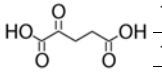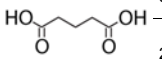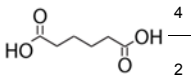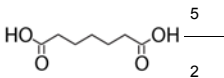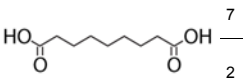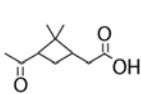
Table S5. Data for hydroxynitrates. Apparent κ-values are identical to those reported in Suda et al. (2014).
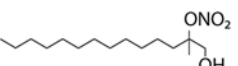
	Name	Formula	Structure	UNIFAC representation #	Subgroup	MW	ρ	Molar volume obs	Molar volume mod	Solubility obs	CCN s_c (%) / D_d (nm)	Apparent κ obs	Apparent κ model
Hydroxynitrates	Dihydroxynitrate	$C_{10}H_{21}O_5N$		2	CH₃	235.3	N/A	N/A	220.8	N/A	0.35% / 100 nm	9.8e-2	7.5e-2
				6	CH₂								
				1	C								
				1	CH(ONO₂)								
				2	OH								
	Trihydroxynitrate	$C_{10}H_{21}O_6N$		2	CH₃	251.3	N/A	N/A	211.5	N/A	0.36% / 88 nm	1.5e-1	8.6e-2
				5	CH₂								
				1	CH								
				1	C								
				1	CH(ONO₂)								
				3	OH								
	Dihydroxynitrate	$C_{11}H_{23}O_5N$		2	CH₃	249.3	N/A	N/A	237.5	N/A	0.85% / 100 nm	2.4e-2	2.8e-2
				7	CH₂								
				1	C								
				1	CH(ONO₂)								
				2	OH								
	Trihydroxynitrate	$C_{11}H_{23}O_6N$		2	CH₃	265.3	N/A	N/A	226.9	N/A	0.35% / 88 nm	1.7e-1	7.8e-1
				6	CH₂								
				1	CH								
				1	C								
				1	CH(ONO₂)								
				3	OH								
	Dihydroxynitrate	$C_{12}H_{25}O_5N$		2	CH₃	263.3	N/A	N/A	263.3	N/A	0.3% / 222 nm	1.8e-2	8.0e-3
				8	CH₂								
				1	C								
				1	CH(ONO₂)								
				2	OH								

Hydroxynitrates

Name	Formula	Fragments							Value
Trihydroxynitrate	$C_{12}H_{25}O_6N$	2 CH_3; 7 CH_2; 1 CH; 1 C; 1 $CH(ONO_2)$; 3 OH	279.3	N/A	N/A	242.3	N/A	0.3% / 100 nm	1.8e-1 7.2e-2
Hydroxynitrate	$C_{13}H_{27}O_4N$	2 CH_3; 10 CH_2; 1 OH; 1 $C(ONO_2)$	261.4	N/A	N/A	286.4	N/A	0.35% / 302 nm	2.7e-3 <1e-6
Dihydroxynitrate	$C_{13}H_{27}O_5N$	2 CH_3; 9 CH_2; 1 C; 1 $CH(ONO_2)$; 2 OH	277.4	N/A	N/A	270.8	N/A	0.21% / 222 nm	2.8e-2 1.9e-3
Trihydroxynitrate	$C_{13}H_{27}O_6N$	2 CH_3; 8 CH_2; 1 CH; 1 C; 1 $CH(ONO_2)$; 3 OH	293.4	N/A	N/A	257.7	N/A	0.3% / 111 nm	1.0e-1 6.6e-2
Hydroxynitrate	$C_{14}H_{29}O_4N$	2 CH_3; 11 CH_2; 1 $C(ONO_2)$; 1 OH	275.4	N/A	N/A	304.5	N/A	0.7% / 302 nm	4.8e-5 1.1e-4
Dihydroxynitrate	$C_{14}H_{29}O_5N$	2 CH_3; 10 CH_2; 1 C; 1 $CH(ONO_2)$; 2 OH	291.4	N/A	N/A	291.4	N/A	0.22% / 222 nm	2.6e-2 2.7e-4
Trihydroxynitrate	$C_{14}H_{29}O_6N$	2 CH_3; 9 CH_2; 1 CH; 1 C; 1 $CH(ONO_2)$; 3 OH	307.4	N/A	N/A	273.1	N/A	0.3% / 111 nm	1.0e-1 5.9e-2
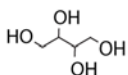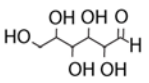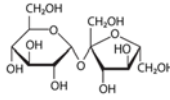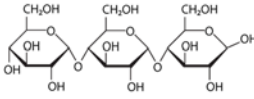
	Name	Formula	Structure	Count	Group								
Hydroxynitrates	Dinitrate	$C_{14}H_{28}O_6N_2$		2	CH_3	320.4	N/A	N/A	360	N/A	0.7% / 220 nm	3.6e-3	<1e-6
				10	CH_2								
				1	$CH_2(ONO_2)$								
				1	$C(ONO_2)$								
	Trinitrate	$C_{14}H_{27}O_9N_3$		2	CH_3	381.4	N/A	N/A	395	N/A	0.46% / 332 nm	2.9e-4	<1e-6
				9	CH_2								
				1	$CH_2(ONO_2)$								
				1	$CH(ONO_2)$								
				1	$C(ONO_2)$								
	Tetranitrate	$C_{14}H_{26}O_{12}N_4$		2	CH_3	442.4	N/A	N/A	430	N/A	0.37% / 332 nm	1.2e-3	<1e-6
				8	CH_2								
				1	$CH_2(ONO_2)$								
				2	$CH(ONO_2)$								
				1	$C(ONO_2)$								
	Hydroxynitrate	$C_{15}H_{31}O_4N$		2	CH_3	289.4	N/A	N/A	322.7	N/A	0.6% / 302 nm	8.4e-4	<1e-6
				12	CH_2								
				1	OH								
				1	$C(ONO_2)$								
	Dihydroxynitrate	$C_{15}H_{31}O_5N$		2	CH_3	305.4	N/A	N/A	304.2	N/A	0.23% / 223 nm	2.2e-2	5.3e-5
				11	CH_2								
				1	C								
				1	$CH(ONO_2)$								
				2	OH								
	Trihydroxynitrate	$C_{15}H_{31}O_6N$		2	CH_3	321.4	N/A	N/A	288.5	N/A	0.35% / 111 nm	8.1e-2	5.3e-2
				10	CH_2								
				1	CH								
				1	C								
				1	$CH(ONO_2)$								
				3	OH								

Table S6. Data for carboxylic acids.

	Name	Formula	Structure	UNIFAC representation #	Subgroup	MW (g mol^{-1})	ρ (g cm^{-3})	Molar volume obs	Molar volume mod	Solubility (v/v)	CCN s_c (%)	Apparent κ obs	Apparent κ model
Carboxylic acids	Maleic acid	$C_4H_4O_4$		2	CH	116.1	1.63	63.8	83.3	9.1e-1	dissolved	3.3e-1	2.2e-1
				2	C(=O)OH							3.8e-1	
	Succinic acid	$C_4H_6O_4$		2	CH$_2$	118.1	1.552	76.1	91.7	5.7e-2	dissolved	1.7e-1	2.0e-1
				2	C(=O)OH							3.0e-1	
	α-ketoglutaric acid	$C_5H_6O_5$		1	CH$_2$	146.1	1.499	102.2	108.3	Soluble	dissolved	2.7e-1	1.7e-1
				1	CH$_2$C(=O)							3.5e-1	
				2	C(=O)OH								
	Glutaric acid	$C_5H_8O_4$		3	CH$_2$	132.1	1.429	92.5	108.3	8.1e-1	dissolved	5.4e-2	1.7e-1
				2	C(=O)OH							1.6e-1	
	Adipic acid	$C_6H_{10}O_4$		4	CH$_2$	146.2	1.352	107	125.0	1.8e-2	~0.6%	1e-3	1.4e-1
				2	C(=O)OH						~200m	1e-2	
	Pimelic acid	$C_7H_{12}O_4$		5	CH$_2$	160.2	1.321	121	141.7	5.1e-2	dissolved	1.4e-1	1.3e-1
				2	C(=O)OH							1.6e-1	
	Azelaic acid	$C_9H_{16}O_4$		7	CH$_2$	188.2	1.251	150	175.0	4.0e-3	0.73%	2e-2	1.2e-2
				2	C(=O)OH						113 nm	4e-2	
	Cis-pinonic acid	$C_{10}H_{16}O_3$		2	CH$_3$	184.2	1.169	157	190.9	5.5e-3	1%	5e-3	5.3e-5
				2	CH$_2$								
				2	CH								
				1	C						115 nm		
				1	CH$_3$C(=O)								
				1	C(=O)OH								

Notes: The range for cis-pinonic acid is taken from the atomized alcohol solution data, which is thought to be the most pure (Huff Hartz et al., 2006). Overall results range from 0.1 (Raymond and Pandis, 2002), 0.005-0.04 (Huff-Hartz), and ~0.009 (Kuwata et al., 2013).

Table S7. Data for carbohydrates.

Name	Formula	Structure	UNIFAC representation #	UNIFAC representation Subgroup	MW (g mol⁻¹) $(g\ mol^{-1})$	ρ (g cm⁻³) $(g\ cm^{-3})$	Molar volume obs	Molar volume mod	Solubility (v/v)	CCN s_c (%)	Apparent κ obs	Apparent κ model
Carbohydrates Threitol	$C_4H_{10}O_4$		2	CH_2	122.1	1.451	84.2	100.0	4.4e-1	dissolved	1.2e-1 / 1.6e-1	2.1e-1
			2	CH								
			4	OH								
Glucose	$C_6H_{12}O_6$		1	CH_2	180.2	1.556	115.8	138.5	5.8e-1	dissolved	1.4e-1 / 2.0e-1	1.7e-1
			4	CH								
			5	OH								
			1	C(=O)H								
Sucrose	$C_{12}H_{22}O_{11}$		3	CH_2	342.3	1.589	215.4	261.5	1.3e-0	dissolved	7.0e-2 / 1.1e-1	1.1e-1
			6	CH								
			8	OH								
			2	CH(O)								
			1	C(O)								
Maltotriose	$C_{18}H_{32}O_{16}$		3	CH_2	504.4	N/A	N/A	384.6	soluble	dissolved	3e-2 / 7e-2	9.1e-1
			10	CH								
			11	OH								
			5	CH(O)								

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