Supplementary Information for: Simple liquid models with corrected dielectric constants

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SI 1 Structure comparison of chloromethane models

Fig. 1 shows a radial distribution function comparison between the flexible Fox & Kollman CCl_4 solvent model and the CCl_4-DC model with a single embedded dipole. In order to embed the dipole and match the experimental density, the diameters of the atom LJ parameters are larger than those of the flexible model. This results in a broader and shorter first-shell peak as discussed in the main text. If a narrower and more intense first-shell peak is desired, one could use an alternate to the LJ potential with a steeper repulsive term and correspondingly narrower attractive well. Such a change would also reduce the temperature dependence of volumetric expansion.

Figs. 2 and 3 show Cl-Cl radial distribution function comparisons between the united-atom $CHCl_3$-DC and CH_2Cl_2-DC models and their all-atom Fox & Kollman counterparts. Structural comparisons between united-atom and all-atom models are qualitative given the geometric distortions involved in making a united atom site as discussed in the main text, and the Cl-Cl packing is possibly the least perturbed. These plots illustrate the consequence of enhanced polarization of the dipole moment of a given model – the first solvation shell peaks are slightly more intense, indicating a more structured liquid. This intensity naturally dampens out at further separation distances as the fluid reaches bulk density behavior.

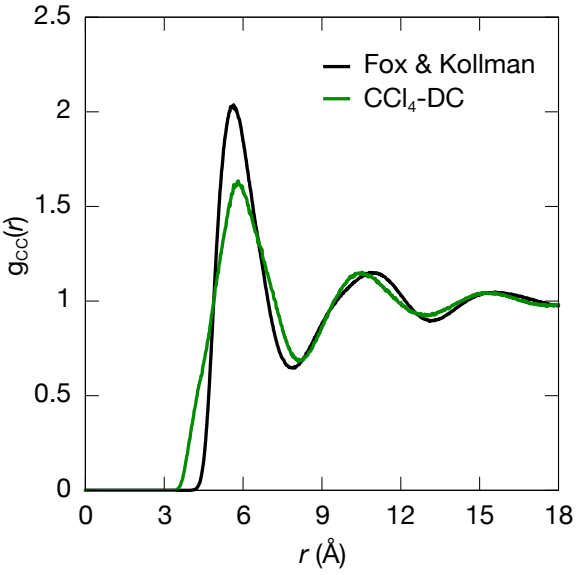

Figure 1: The C-C radial distribution function for the flexible Fox & Kollman CCl_4 and the localized dipole CCl_4-DC model.

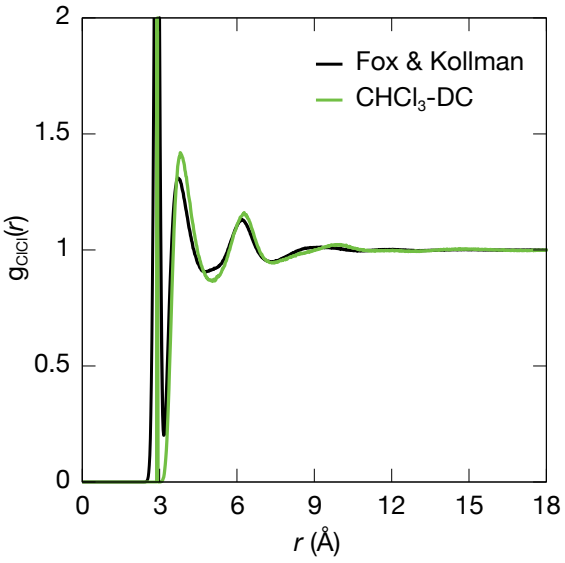

Figure 2: The Cl-Cl radial distribution function for the flexible Fox & Kollman $CHCl_3$ and $CHCl_3$-DC model.

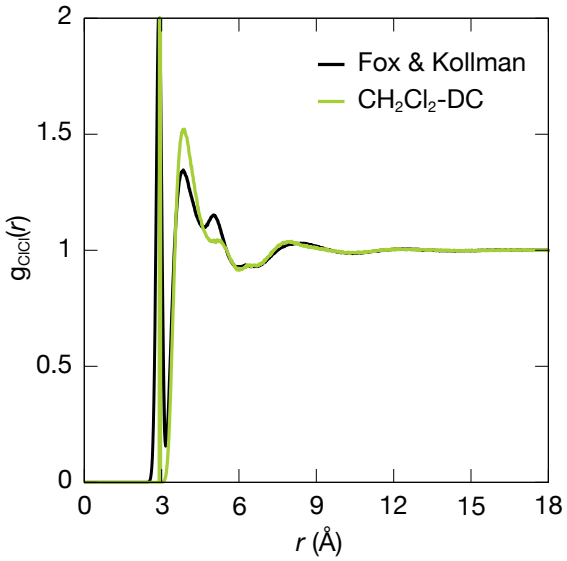

Figure 3: The Cl-Cl radial distribution function for the flexible Fox & Kollman CH_2Cl_2 and CH_2Cl_2-DC model.

SI 2 Temperature Dependent Property Data for Chloromethane Models

Tables 1, 2, 3, and 4 list the investigated properties as a function of temperature for the CCl_4 (localized and distributed dipole), $CHCl_3$, and CH_2Cl_2 models respectively.

SI 3 Temperature Dependent Property Data for Water Models

Tables 5, 6, 7, and 8 list the investigated properties as a function of temperature for the SPC, SPC/E, SPC/DC , and H_2O-DC water models respectively.

Table 1: Temperature dependent property data for the localized dipole CCl_4-DC model with standard error of the last digit in parentheses

Temperature (K)	ρ (kg/m^3)	ΔH_{vap} (kJ/mol)	$\varepsilon(0)$	C_p (J/mol·K)	κ_T (10^5 atm^{-1})	α_p (10^6 K^{-1})	D (10^{-9} m^2/s)
253.15	1,718.86 (5)	38.287 (3)	2.30 (1)	140 (3)	82 (2)	170 (5)	0.53 (1)
258.15	1,705.8 (1)	37.669 (4)	2.29 (1)	141 (1)	86 (1)	173 (2)	0.62 (1)
263.15	1,692.2 (1)	37.041 (3)	2.285 (8)	144 (1)	91 (1)	178 (2)	0.66 (1)
268.15	1,678.3 (1)	36.400 (4)	2.27 (1)	147 (2)	98 (2)	188 (4)	0.71 (1)
273.15	1,664.2 (1)	35.750 (5)	2.27 (1)	146 (3)	100 (3)	185 (5)	0.80 (1)
278.15	1,649.63 (4)	35.095 (1)	2.232 (8)	152 (3)	111 (2)	200 (4)	0.85 (2)
283.15	1,634.7 (1)	34.427 (4)	2.224 (6)	154 (2)	118 (2)	207 (4)	0.99 (1)
288.15	1,619.7 (1)	33.754 (3)	2.21 (1)	156 (1)	127 (1)	214 (3)	1.06 (2)
293.15	1,604.62 (8)	33.084 (3)	2.197 (4)	155 (2)	130 (2)	215 (3)	1.17 (1)
298.15	1,588.7 (1)	32.392 (4)	2.202 (6)	154 (2)	134 (2)	213 (4)	1.24 (1)
303.15	1,573.2 (1)	31.711 (7)	2.170 (6)	155 (2)	147 (2)	223 (4)	1.34 (1)
308.15	1,557.4 (1)	31.026 (5)	2.16 (1)	153 (3)	151 (4)	222 (5)	1.42 (3)
313.15	1,541.8 (1)	30.348 (5)	2.139 (7)	157 (2)	161 (2)	230 (4)	1.56 (3)
318.15	1,526.02 (9)	29.670 (4)	2.128 (8)	154 (3)	168 (4)	230 (5)	1.75 (2)
323.15	1,510.2 (1)	28.994 (4)	2.11 (1)	156 (1)	179 (1)	236 (2)	1.84 (2)
328.15	1,494.4 (1)	28.321 (5)	2.10 (1)	157 (2)	192 (5)	244 (6)	1.95 (7)
333.15	1,478.9 (2)	27.661 (6)	2.075 (4)	151 (2)	194 (2)	235 (3)	2.16 (3)
338.15	1,463.3 (2)	27.006 (6)	2.072 (7)	155 (3)	214 (6)	250 (6)	2.25 (5)
343.15	1,447.80 (9)	26.351 (3)	2.07 (2)	151 (2)	218 (5)	245 (5)	2.41 (4)
348.15	1,432.5 (1)	25.708 (5)	2.034 (9)	150 (1)	230 (4)	249 (4)	2.63 (3)
353.15	1,417.6 (1)	25.081 (4)	2.03 (1)	145 (2)	233 (4)	240 (5)	2.76 (8)
358.15	1,402.8 (2)	24.460 (5)	2.018 (7)	147 (2)	252 (4)	250 (4)	3.01 (6)
363.15	1,388.30 (8)	23.858 (4)	1.995 (5)	147 (4)	265 (8)	254 (9)	3.13 (4)
368.15	1,373.85 (8)	23.254 (2)	1.991 (8)	142 (4)	269 (0)	248 (9)	3.31 (3)
373.15	1,359.6 (1)	22.666 (4)	1.969 (4)	140 (2)	280 (4)	247 (4)	3.56 (5)

Table 2: Temperature dependent property data for the localized dipole CCl_4-DC model with standard error of the last digit in parentheses

Temperature (K)	ρ (kg/m^3)	ΔH_{vap} (kJ/mol)	$\varepsilon(0)$	C_p (J/mol·K)	κ_T (10^5 atm^{-1})	α_p (10^6 K^{-1})	D (10^{-9} m^2/s)
253.15	1,718.55 (1)	38.325 (2)	2.33 (1)	140 (3)	82 (1)	170 (4)	0.56 (1)
258.15	1,705.45 (7)	37.703 (4)	2.313 (6)	143 (1)	86 (1)	175 (2)	0.60 (1)
263.15	1,691.88 (7)	37.067 (3)	2.30 (1)	146 (2)	92 (2)	182 (3)	0.66 (1)
268.15	1,678.16 (4)	36.431 (2)	2.26 (1)	147 (3)	96 (2)	185 (4)	0.73 (1)
273.15	1,663.9 (1)	35.776 (6)	2.252 (7)	147 (1)	102 (2)	191 (3)	0.81 (2)
278.15	1,649.4 (1)	35.115 (3)	2.210 (8)	153 (2)	110 (2)	201 (4)	0.88 (3)
283.15	1,634.7 (1)	34.451 (5)	2.177 (6)	152 (3)	115 (1)	202 (4)	0.97 (2)
288.15	1,619.4 (2)	33.765 (5)	2.168 (7)	156 (1)	124.7 (9)	212 (2)	1.06 (2)
293.15	1,604.34 (4)	33.093 (3)	2.148 (9)	154 (1)	130 (2)	213 (2)	1.13 (1)
298.15	1,588.77 (7)	32.406 (1)	2.112 (8)	156 (2)	137 (2)	219 (4)	1.26 (2)
303.15	1,573.0 (1)	31.719 (6)	2.096 (4)	159 (2)	154 (3)	233 (4)	1.36 (3)
308.15	1,557.34 (6)	31.033 (2)	2.06 (1)	156 (2)	151 (3)	224 (5)	1.47 (2)
313.15	1,541.29 (3)	30.340 (2)	2.062 (8)	156 (3)	161 (4)	229 (6)	1.65 (3)
318.15	1,525.59 (4)	29.662 (2)	2.038 (1)	156 (3)	172 (4)	235 (5)	1.68 (3)
323.15	1,509.7 (1)	28.981 (5)	2.016 (4)	158 (2)	182 (2)	240 (3)	1.84 (3)
328.15	1,494.0 (2)	28.306 (6)	1.985 (9)	158 (2)	192 (3)	245 (4)	2.05 (2)
333.15	1,478.15 (6)	27.630 (4)	1.973 (7)	155 (2)	201 (4)	244 (4)	2.08 (5)
338.15	1,462.8 (2)	26.979 (4)	1.956 (6)	154 (3)	208 (5)	244 (6)	2.27 (7)
343.15	1,447.3 (1)	26.324 (4)	1.926 (7)	152 (4)	220 (7)	247 (8)	2.42 (5)
348.15	1,432.0 (1)	25.684 (6)	1.916 (8)	148 (3)	225 (5)	243 (6)	2.59 (5)
353.15	1,416.9 (1)	25.047 (4)	1.896 (7)	152 (3)	247 (9)	256 (9)	2.89 (4)
358.15	1,402.0 (1)	24.418 (5)	1.870 (5)	146 (5)	244 (1)	243 (1)	2.86 (5)
363.15	1,387.0 (1)	23.798 (3)	1.849 (8)	150 (3)	270 (6)	260 (6)	3.17 (4)
368.15	1,372.50 (8)	23.195 (3)	1.834 (6)	145 (2)	275 (4)	254 (4)	3.37 (7)
373.15	1,358.5 (1)	22.608 (5)	1.818 (7)	140 (4)	277 (2)	245 (0)	3.37 (4)

Table 3: Temperature dependent property data for the united-atom $CHCl_3$-DC model with standard error of the last digit in parentheses

Temperature (K)	ρ (kg/m^3)	ΔH_{vap} (kJ/mol)	$\varepsilon(0)$	C_p (J/mol·K)	κ_T (10^5 atm^{-1})	α_p (10^6 K^{-1})	D (10^{-9} m^2/s)
253.15	1,535.12 (4)	34.419 (1)	5.19 (5)	85 (1)	58 (1)	106 (2)	0.76 (1)
258.15	1,527.99 (7)	34.054 (2)	5.17 (7)	87 (1)	60 (1)	109 (2)	0.82 (2)
263.15	1,520.94 (3)	33.699 (2)	5.18 (3)	87 (2)	63.7 (3)	112 (3)	0.90 (2)
268.15	1,513.88 (5)	33.340 (2)	5.07 (5)	84 (2)	64.4 (6)	110 (3)	0.99 (4)
273.15	1,506.68 (5)	32.980 (2)	5.05 (6)	86 (1)	67 (2)	113 (4)	1.04 (2)
278.15	1,499.7 (1)	32.632 (2)	4.99 (2)	85 (1)	68.3 (4)	112 (2)	1.12 (2)
283.15	1,492.43 (4)	32.272 (2)	4.83 (2)	84.3 (7)	70.6 (0)	112 (2)	1.21 (1)
288.15	1,485.43 (5)	31.924 (1)	4.86 (4)	86 (1)	74 (1)	117 (3)	1.30 (2)
293.15	1,478.31 (5)	31.573 (1)	4.81 (3)	89 (2)	80 (3)	123 (5)	1.44 (2)
298.15	1,471.16 (7)	31.222 (4)	4.77 (3)	85 (1)	78 (1)	116 (2)	1.48 (1)
303.15	1,464.02 (8)	30.875 (2)	4.75 (3)	84.5 (9)	81 (1)	117 (2)	1.54 (2)
308.15	1,456.81 (5)	30.522 (2)	4.67 (2)	86 (1)	85 (2)	121 (3)	1.64 (2)
313.15	1,449.61 (5)	30.177 (2)	4.56 (2)	84 (2)	85 (2)	117 (3)	1.85 (2)
318.15	1,442.31 (6)	29.831 (3)	4.56 (3)	86 (2)	91 (2)	123 (3)	1.81 (5)
323.15	1,435.0 (0)	29.487 (1)	4.51 (3)	86 (1)	94 (1)	124 (2)	2.07 (3)
328.15	1,427.85 (4)	29.141 (2)	4.51 (3)	85 (1)	95.4 (5)	122 (2)	2.14 (5)
333.15	1,420.54 (7)	28.800 (4)	4.45 (3)	84 (1)	99 (3)	125 (4)	2.20 (3)
338.15	1,413.15 (6)	28.452 (3)	4.44 (3)	85 (1)	106 (2)	129 (2)	2.33 (3)
343.15	1,405.86 (9)	28.114 (3)	4.34 (3)	86 (1)	108 (3)	130 (4)	2.54 (5)
348.15	1,398.46 (6)	27.771 (2)	4.35 (4)	85.7 (5)	113 (2)	131 (2)	2.65 (5)
353.15	1,390.93 (4)	27.425 (2)	4.26 (2)	86 (1)	119 (2)	135 (3)	2.82 (7)
358.15	1,383.50 (9)	27.085 (2)	4.23 (3)	86.9 (6)	122 (1)	136 (2)	2.87 (5)
363.15	1,376.11 (0)	26.749 (3)	4.15 (1)	84.9 (8)	123 (2)	134 (2)	3.09 (3)
368.15	1,368.57 (4)	26.402 (2)	4.21 (2)	82 (1)	119 (3)	126 (3)	3.2 (1)
373.15	1,360.83 (4)	26.061 (2)	4.14 (2)	86 (2)	134 (3)	139 (3)	3.40 (5)

Table 4: Temperature dependent property data for the united-atom CH_2Cl_2-DC model with standard error of the last digit in parentheses

Temperature (K)	ρ (kg/m^3)	ΔH_{vap} (kJ/mol)	$\varepsilon(0)$	C_p (J/mol·K)	κ_T (10^5 atm^{-1})	α_p (10^6 K^{-1})	D (10^{-9} m^2/s)
253.15	1,374.57 (4)	31.733 (2)	9.93 (8)	91.0 (9)	72 (1)	144 (2)	1.15 (2)
258.15	1,368.16 (5)	31.395 (2)	9.89 (0)	94 (1)	78 (2)	152 (4)	1.25 (2)
263.15	1,361.76 (6)	31.060 (4)	9.67 (7)	91.5 (6)	76 (2)	146 (3)	1.32 (2)
268.15	1,355.30 (3)	30.725 (2)	9.58 (6)	91 (1)	80 (2)	148 (3)	1.47 (3)
273.15	1,348.76 (3)	30.389 (2)	9.4 (1)	92 (2)	84 (2)	153 (4)	1.54 (3)
278.15	1,342.40 (2)	30.063 (1)	9.30 (7)	92 (1)	84 (3)	149 (5)	1.67 (5)
283.15	1,335.88 (6)	29.729 (3)	9.25 (5)	92 (1)	91 (3)	156 (5)	1.80 (3)
288.15	1,329.28 (3)	29.395 (2)	9.26 (4)	95 (1)	95 (1)	161 (3)	1.91 (2)
293.15	1,322.89 (4)	29.067 (2)	9.05 (3)	92.7 (6)	96 (2)	158 (2)	2.02 (6)
298.15	1,316.34 (1)	28.740 (1)	8.8 (1)	92.3 (8)	98 (1)	159 (2)	2.13 (2)
303.15	1,309.72 (4)	28.409 (3)	8.87 (6)	97 (2)	110 (5)	174 (7)	2.27 (4)
308.15	1,303.22 (3)	28.082 (1)	8.65 (7)	93 (2)	107 (2)	164 (4)	2.34 (5)
313.15	1,296.65 (7)	27.755 (2)	8.64 (6)	94 (1)	110 (1)	166 (2)	2.60 (3)
318.15	1,290.01 (6)	27.431 (3)	8.65 (6)	96.1 (9)	119 (2)	174 (2)	2.66 (4)
323.15	1,283.42 (9)	27.106 (4)	8.41 (6)	94 (2)	119 (3)	169 (4)	2.74 (2)
328.15	1,276.72 (4)	26.779 (1)	8.37 (4)	95.6 (7)	127 (3)	178 (3)	3.10 (5)
333.15	1,270.06 (8)	26.457 (3)	8.23 (6)	95 (1)	129 (3)	176 (4)	3.19 (6)
338.15	1,263.18 (4)	26.130 (2)	8.24 (7)	96 (1)	137 (3)	184 (4)	3.30 (5)
343.15	1,256.56 (5)	25.807 (2)	8.22 (3)	95.5 (1)	138 (1)	181 (1)	3.4 (1)
348.15	1,249.67 (9)	25.482 (5)	7.94 (5)	99.0 (7)	151 (4)	192 (4)	3.6 (1)
353.15	1,242.84 (4)	25.158 (2)	7.89 (8)	96 (1)	148 (4)	185 (4)	3.7 (1)
358.15	1,236.09 (4)	24.835 (2)	7.83 (7)	95 (1)	149 (3)	182 (4)	4.1 (1)
363.15	1,229.12 (4)	24.511 (2)	7.73 (3)	95 (2)	154 (7)	184 (7)	4.29 (8)
368.15	1,222.12 (7)	24.186 (2)	7.69 (5)	97 (2)	166 (5)	192 (6)	4.3 (1)
373.15	1,215.13 (5)	23.865 (3)	7.53 (3)	98 (2)	174 (4)	198 (4)	4.39 (3)

Table 5: Temperature dependent property data for the SPC water model with standard error of the last digit in parentheses

Temperature (K)	ρ (kg/m^3)	ΔH_{vap} (kJ/mol)	$\varepsilon(0)$	C_p (J/mol·K)	κ_T (10^5 atm^{-1})	α_p (10^6 K^{-1})	D (10^{-9} m^2/s)
233.15	1,009.1 (1)	41.873 (2)	70 (1)	89.7 (4)	50 (1)	16 (1)	0.76 (1)
238.15	1,008.05 (2)	41.470 (2)	71 (2)	88.3 (8)	50.5 (4)	20 (2)	0.93 (2)
243.15	1,007.04 (8)	41.065 (1)	68.5 (9)	89.2 (6)	49.0 (4)	26 (3)	1.09 (1)
248.15	1,005.34 (9)	40.665 (1)	68.8 (6)	87 (1)	49.3 (6)	30 (3)	1.25 (2)
253.15	1,003.58 (6)	40.270 (1)	67 (1)	87 (1)	49.1 (7)	36.6 (9)	1.48 (3)
258.15	1,001.59 (6)	39.875 (1)	67 (2)	86.4 (5)	49.1 (4)	40 (1)	1.73 (2)
263.15	999.41 (7)	39.484 (1)	66.7 (9)	85.6 (4)	49.5 (8)	49 (2)	1.96 (3)
268.15	996.83 (5)	39.1010 (6)	67.7 (7)	84.3 (6)	50.0 (4)	51.4 (6)	2.19 (3)
273.15	994.16 (3)	38.714 (2)	66.9 (7)	84.9 (7)	50.9 (6)	59 (2)	2.43 (4)
278.15	991.34 (4)	38.3319 (9)	66.5 (6)	84.9 (4)	51.5 (7)	60.5 (7)	2.71 (5)
283.15	988.40 (3)	37.949 (1)	67.4 (6)	84.1 (1)	50.4 (4)	63 (3)	3.09 (4)
288.15	985.24 (5)	37.5714 (5)	66.9 (8)	83.3 (7)	52.7 (6)	68 (2)	3.20 (3)
293.15	981.84 (2)	37.1933 (7)	65.8 (3)	82.5 (3)	54.2 (9)	73 (2)	3.63 (7)
298.15	978.41 (3)	36.820 (1)	65.6 (2)	82.9 (3)	53.7 (5)	71.5 (7)	3.99 (1)
303.15	974.77 (5)	36.445 (2)	64.9 (7)	83.0 (6)	54.4 (2)	75 (2)	4.34 (4)
308.15	970.97 (3)	36.074 (3)	64.5 (9)	82.0 (3)	56.1 (6)	78 (3)	4.49 (7)
313.15	966.95 (3)	35.701 (1)	63.2 (5)	82.3 (5)	56 (1)	82 (2)	4.89 (9)
318.15	963.10 (4)	35.3336 (8)	63.1 (5)	81.5 (7)	58.4 (7)	86 (2)	5.45 (8)
323.15	958.81 (4)	34.968 (1)	63.1 (5)	81.7 (3)	58 (1)	86 (2)	5.79 (4)
328.15	954.56 (2)	34.598 (1)	61.9 (4)	81.8 (4)	61.5 (7)	91.9 (7)	6.33 (9)
333.15	950.17 (2)	34.233 (2)	61.6 (3)	81.1 (4)	61.6 (8)	95 (1)	6.6 (2)
338.15	945.69 (4)	33.866 (1)	60.8 (4)	81.9 (7)	63 (1)	99 (3)	7.09 (8)
343.15	941.00 (3)	33.499 (2)	60.9 (4)	82.3 (6)	67.9 (8)	106 (2)	7.57 (9)
348.15	936.21 (3)	33.135 (1)	60.9 (3)	80.8 (4)	65 (2)	101 (3)	7.99 (5)
353.15	931.38 (6)	32.771 (1)	59.9 (3)	80.2 (6)	70 (1)	108 (3)	8.6 (1)
358.15	926.32 (6)	32.403 (2)	59.8 (4)	81.8 (4)	70.8 (5)	109 (1)	8.9 (3)
363.15	921.22 (5)	32.039 (1)	57.9 (3)	81.8 (9)	74 (1)	117 (2)	9.6 (1)
368.15	915.96 (6)	31.673 (2)	58.0 (1)	81.3 (3)	76 (2)	116 (3)	9.9 (1)
373.15	910.65 (3)	31.311 (2)	57.4 (4)	82.1 (7)	79 (2)	124 (3)	10.8 (2)

Table 6: Temperature dependent property data for the SPC/E water model with standard error of the last digit in parentheses

Temperature (K)	ρ (kg/m^3)	ΔH_{vap} (kJ/mol)	$\varepsilon(0)$	C_p (J/mol·K)	κ_T (10^5 atm^{-1})	α_p (10^6 K^{-1})	D (10^{-9} m^2/s)	
233.15	1,011.4 (2)	47.295 (5)	71 (1)	23.2 (3)	97 (1)	45.5 (5)	-22 (4)	0.238 (5)
238.15	1,012.7 (1)	46.839 (5)	70 (1)	95.9 (8)	45.5 (9)	-12 (2)	0.345 (2)	
243.15	1,013.0 (2)	46.416 (3)	74 (1)	94.7 (7)	44.1 (4)	-7 (1)	0.419 (6)	
248.15	1,013.2 (1)	45.985 (2)	75 (3)	92.6 (7)	46.2 (5)	2 (2)	0.54 (1)	
253.15	1,012.98 (6)	45.562 (2)	71 (1)	93.2 (5)	46.2 (8)	7 (1)	0.68 (1)	
258.15	1,012.68 (2)	45.137 (1)	74 (1)	91.6 (4)	44.8 (7)	14 (2)	0.82 (1)	
263.15	1,011.60 (3)	44.722 (2)	71.5 (9)	90.5 (9)	44.0 (4)	18 (2)	0.97 (2)	
268.15	1,010.81 (7)	44.309 (2)	71 (1)	90.6 (5)	44.6 (4)	24 (3)	1.14 (1)	
273.15	1,009.4 (1)	43.907 (1)	73 (1)	89.9 (7)	45.2 (5)	28 (3)	1.31 (1)	
278.15	1,007.78 (4)	43.491 (2)	73.0 (8)	88.9 (5)	44.4 (4)	34 (1)	1.51 (3)	
283.15	1,006.09 (9)	43.093 (2)	72.9 (6)	88.7 (7)	45.9 (2)	40 (1)	1.73 (3)	
288.15	1,004.07 (6)	42.697 (2)	70.8 (5)	87.8 (5)	46.1 (7)	40 (2)	2.00 (2)	
293.15	1,001.89 (3)	42.299 (2)	71.5 (5)	87.0 (7)	45.4 (3)	44 (2)	2.21 (5)	
298.15	999.53 (2)	41.905 (1)	71.1 (1)	86.3 (2)	46.1 (2)	49.1 (4)	2.456 (3)	
303.15	996.95 (7)	41.512 (2)	70.3 (3)	86.2 (4)	47.2 (5)	54 (2)	2.72 (4)	
308.15	994.16 (5)	41.125 (2)	69.4 (4)	85.2 (7)	47.6 (6)	56 (2)	2.97 (9)	
313.15	991.32 (4)	40.736 (2)	70.8 (9)	85.5 (5)	47.4 (7)	58 (1)	3.37 (6)	
318.15	988.28 (4)	40.353 (2)	69.4 (5)	84.8 (3)	48.9 (5)	62.3 (5)	3.66 (5)	
323.15	985.16 (3)	39.967 (2)	69.9 (6)	83.5 (5)	50.0 (7)	65 (2)	3.92 (5)	
328.15	981.83 (7)	39.592 (1)	68.3 (5)	84.6 (4)	50.6 (8)	67 (2)	4.20 (5)	
333.15	978.39 (7)	39.210 (1)	69.0 (5)	83.3 (3)	50.4 (5)	70 (1)	4.60 (6)	
338.15	974.84 (4)	38.831 (1)	67.7 (6)	83.4 (4)	53.1 (6)	78 (1)	5.00 (7)	
343.15	971.14 (5)	38.455 (2)	68.3 (5)	83.1 (7)	54.0 (7)	79 (1)	5.36 (8)	
348.15	967.36 (4)	38.0788 (9)	67.0 (6)	84.7 (8)	54.6 (5)	82 (2)	5.59 (5)	
353.15	963.37 (3)	37.707 (2)	66.5 (8)	82.7 (7)	55 (1)	83 (4)	6.0 (1)	
358.15	959.35 (3)	37.332 (1)	65.7 (6)	83.4 (5)	57 (1)	87 (2)	6.27 (8)	
363.15	955.19 (5)	36.963 (2)	65.6 (7)	83.0 (8)	59 (1)	89 (2)	6.83 (7)	
368.15	950.91 (4)	36.587 (1)	64.6 (3)	82.2 (3)	58 (1)	90 (1)	7.4 (1)	
373.15	946.56 (4)	36.2192 (9)	64.4 (7)	82.1 (6)	62.7 (5)	96 (1)	7.4 (1)	

Table 7: Temperature dependent property data for the SPC/DC water model with standard error of the last digit in parentheses

Temperature (K)	ρ (kg/m^3)	ΔH_{vap} (kJ/mol)	$\varepsilon(0)$	C_p (J/mol·K)	κ_T (10^5 atm^{-1})	α_p (10^6 K^{-1})	D (10^{-9} m^2/s)	
233.15	1,016.3 (1)	49.044 (2)	82 (2)	21.4 (2)	89.5 (8)	49.6 (7)	-3 (2)	0.344 (5)
238.15	1,016.69 (8)	48.638 (3)	80 (4)	88.3 (8)	49.8 (5)	-3 (3)	0.438 (9)	
243.15	1,016.2 (2)	48.236 (3)	81 (2)	87.6 (8)	47.9 (6)	8 (2)	0.54 (1)	
248.15	1,015.6 (1)	47.841 (3)	83 (3)	86.3 (4)	46.6 (7)	9 (1)	0.645 (9)	
253.15	1,014.70 (4)	47.452 (2)	79.2 (8)	87.3 (5)	46.0 (2)	14 (2)	0.769 (9)	
258.15	1,013.74 (8)	47.054 (1)	79.5 (9)	86.9 (3)	46.7 (3)	25 (2)	0.92 (1)	
263.15	1,012.51 (5)	46.663 (2)	79 (1)	85.9 (7)	44.2 (4)	24 (1)	1.08 (2)	
268.15	1,010.94 (4)	46.279 (2)	82 (1)	85.1 (7)	43.9 (5)	30.2 (7)	1.25 (2)	
273.15	1,009.33 (8)	45.8941 (5)	80 (2)	84.7 (4)	43.4 (2)	34.7 (4)	1.44 (2)	
278.15	1,007.53 (4)	45.505 (1)	78 (2)	85.2 (7)	42.8 (4)	37 (2)	1.62 (3)	
283.15	1,005.46 (3)	45.127 (2)	79 (2)	83.5 (5)	43.2 (3)	39 (1)	1.84 (2)	
288.15	1,003.32 (8)	44.7459 (9)	78.0 (4)	84.6 (6)	43.6 (5)	46 (1)	2.08 (3)	
293.15	1,001.15 (4)	44.370 (3)	77.2 (7)	81.9 (6)	42.8 (5)	43 (1)	2.26 (3)	
298.15	998.69 (2)	43.993 (0)	78.3 (6)	83.2 (3)	43.7 (3)	48.8 (9)	2.48 (1)	
303.15	996.15 (4)	43.623 (1)	77.7 (6)	83.4 (6)	44.4 (3)	55 (2)	2.67 (4)	
308.15	993.44 (4)	43.251 (1)	76 (1)	82.5 (7)	44.6 (6)	57 (2)	3.02 (8)	
313.15	990.70 (4)	42.879 (2)	76.9 (6)	82.1 (2)	45.1 (6)	57.3 (7)	3.26 (9)	
318.15	987.80 (2)	42.508 (2)	76.0 (5)	82.0 (6)	43.8 (6)	58 (2)	3.62 (3)	
323.15	984.80 (3)	42.141 (1)	76.0 (9)	81.4 (6)	45.9 (6)	62.2 (7)	3.82 (3)	
328.15	981.63 (4)	41.7773 (8)	75.3 (8)	81.4 (5)	45.8 (7)	63 (1)	4.06 (7)	
333.15	978.45 (6)	41.413 (2)	76.0 (8)	80.6 (5)	47 (1)	66 (2)	4.48 (9)	
338.15	975.19 (2)	41.047 (2)	74.1 (3)	80.3 (8)	47.8 (9)	69 (2)	4.77 (8)	
343.15	971.71 (4)	40.6832 (8)	74.8 (5)	81 (1)	48.9 (3)	72 (1)	5.1 (1)	
348.15	968.24 (3)	40.322 (1)	73.8 (2)	80.4 (6)	51 (1)	75 (3)	5.5 (1)	
353.15	964.79 (6)	39.9640 (9)	73.5 (5)	80.6 (4)	51.5 (8)	77 (1)	5.8 (1)	
358.15	961.12 (5)	39.601 (1)	73.3 (4)	80.0 (6)	52.3 (9)	82 (2)	6.32 (8)	
363.15	957.33 (5)	39.240 (2)	72.0 (7)	80.0 (3)	51.3 (5)	78 (2)	6.6 (1)	
368.15	953.50 (2)	38.882 (2)	72.3 (2)	80.6 (6)	51.9 (6)	81 (1)	6.9 (1)	
373.15	949.62 (4)	38.525 (2)	70.6 (5)	80.0 (4)	54 (1)	82.3 (9)	7.27 (4)	

Table 8: Temperature dependent property data for the H_2O-DC water model with standard error of the last digit in parentheses

Temperature (K)	ρ (kg/m^3)	ΔH_{vap} (kJ/mol)	$\varepsilon(0)$	C_p (J/mol·K)	κ_T (10^5 atm^{-1})	α_p (10^6 K^{-1})	D (10^{-9} m^2/s)
233.15	1005.5 (1)	48.903 (7)	82.9 (8)	96 (1)	43.0 (2)	-29 (3)	0.154 (5)
238.15	1006.7 (2)	48.447 (4)	79 (6)	97 (2)	45 (1)	-22 (4)	0.214 (5)
243.15	1007.7 (1)	48.001 (4)	80 (2)	97 (2)	44.5 (7)	-12 (3)	0.297 (5)
248.15	1008.0 (2)	47.556 (4)	76 (1)	97.4 (9)	43.6 (6)	-14 (4)	0.385 (7)
253.15	1008.4 (1)	47.115 (2)	79 (2)	94 (1)	43.6 (4)	-4 (3)	0.499 (8)
258.15	1008.4 (1)	46.684 (2)	79 (1)	93.2 (5)	43.3 (8)	8 (2)	0.64 (1)
263.15	1008.03 (7)	46.246 (1)	77 (2)	94.9 (8)	43.5 (7)	9 (2)	0.77 (1)
268.15	1007.20 (4)	45.826 (3)	79.3 (6)	94.9 (5)	43 (1)	14 (1)	0.95 (1)
273.15	1006.21 (5)	45.406 (2)	79 (2)	91.5 (6)	44.1 (4)	22 (1)	1.14 (2)
278.15	1004.83 (4)	44.990 (2)	78 (2)	90.9 (4)	43.8 (3)	25 (2)	1.31 (3)
283.15	1003.45 (4)	44.580 (3)	78 (1)	90.6 (6)	44.4 (8)	35 (2)	1.49 (2)
288.15	1001.66 (3)	44.171 (1)	77 (1)	89.9 (4)	44.4 (8)	36 (1)	1.73 (3)
293.15	999.69 (5)	43.766 (1)	79.8 (7)	88.2 (8)	43.8 (3)	41 (2)	1.96 (4)
298.15	997.55 (2)	43.366 (1)	78.7 (6)	87.8 (2)	45.0 (2)	44.8 (4)	2.17 (1)
303.15	995.20 (5)	42.966 (2)	78 (2)	88.0 (8)	45.9 (6)	48.2 (6)	2.45 (2)
308.15	992.70 (3)	42.570 (2)	78.2 (8)	86.7 (8)	45.9 (7)	52 (2)	2.69 (3)
313.15	990.08 (4)	42.181 (2)	77.0 (7)	85.4 (9)	47.6 (4)	56 (2)	2.96 (4)
318.15	987.20 (4)	41.788 (2)	77 (1)	85.6 (6)	48.3 (7)	60 (2)	3.24 (5)
323.15	984.26 (3)	41.401 (1)	77.3 (9)	86.4 (4)	48.3 (8)	63 (2)	3.61 (7)
328.15	981.14 (3)	41.014 (2)	76.2 (6)	85 (1)	48.5 (6)	63 (2)	3.76 (6)
333.15	977.93 (4)	40.630 (2)	76.9 (8)	85.1 (7)	49.9 (7)	67 (2)	4.29 (5)
338.15	974.63 (1)	40.248 (1)	75.4 (9)	84.7 (6)	51.0 (8)	70 (2)	4.47 (4)
343.15	971.03 (5)	39.869 (1)	74.4 (8)	84.7 (5)	52.4 (6)	75 (2)	4.98 (3)
348.15	967.41 (3)	39.490 (2)	73.8 (7)	82.8 (9)	51.5 (7)	71 (2)	5.20 (8)
353.15	963.61 (2)	39.110 (2)	73.2 (8)	83.2 (1)	53.9 (6)	77 (1)	5.59 (5)
358.15	959.71 (6)	38.737 (1)	73.1 (4)	83.4 (7)	56 (1)	83 (3)	6.03 (8)
363.15	955.73 (4)	38.360 (1)	73.3 (8)	82.4 (3)	58.9 (6)	85 (1)	6.33 (2)
368.15	951.64 (5)	37.984 (2)	72.2 (3)	82.7 (7)	57 (2)	87 (3)	6.74 (8)
373.15	947.44 (4)	37.614 (1)	71.9 (7)	82.8 (3)	59.0 (8)	88 (2)	7.23 (3)