Corrigendum

Corrigendum to 'Molecular simulation of the surface tension of 33 multi-site models for real fluids' [J. Mol. Liq. 235 (2017) 126–134]

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The authors regret that at typesetting stage, additional '1' digits were mistakenly introduced into the tables, leading to an incorrect reproduction of numerical data. Corrected versions of the tables are included here; the affected values, which in the published article [1] erroneously contained an additional leading digit, are highlighted in bold typeface. The text of the article, and the conclusions formulated therein, were based on the correct data and do not require any modification. The authors would like to apologize for any inconvenience caused.

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Table 1

Molecular models discussed in the present work. The deviations $\delta\rho'$ and δp^s are taken from the referenced publications, and $\delta\gamma$ is the root mean square relative deviation between predictions by the present MD simulations and DIPPR correlations to experimental data [2], determined in the present work. For all considered fluids, the models overestimate γ on average. Citations in the “Source” column refer to the literature list of the corrigendum.

Name	Formula	CAS RN	# model interaction sites	$\delta\rho'$	δp^s	$\delta\gamma$	Source
Acetonitrile	C ₂ H ₃ N	75-05-8	3 LJ + dipole	0.1	4.7	51.7	reference [3]
Cyclohexane	C ₆ H ₁₂	110-82-7	6 LJ	0.3	1.7	10.8	reference [4]
Cyclohexanone	C ₆ H ₁₀ O	108-94-1	7 LJ + dipole	0.9	2.7	26.0	reference [4]
Cyclohexanol	C ₆ H ₁₀ OH	108-93-0	7 LJ + 3 charges	0.2	3.0	28.3	reference [5]
Ethylene oxide	C ₂ H ₄ O	75-21-8	3 LJ + dipole	0.4	1.5	16.6	reference [6]
Isobutane	C ₄ H ₁₀	75-28-5	4 LJ + dipole + quadrupole	0.6	4.2	12.5	reference [7]
Formaldehyde	CH ₂ O	50-00-0	2 LJ + dipole	0.9	4.3	—	reference [7]
Dimethyl ether	C ₂ H ₆ O	115-10-6	3 LJ + dipole	0.4	2.6	18.9	reference [7]
Sulfur dioxide	SO ₂	7446-09-5	3 LJ + dipole + quadrupole	0.9	4.0	3.4	reference [7]
Dimethyl sulfide	C ₂ H ₆ S	75-18-3	3 LJ + dipole + 2 quadrupoles	0.7	4.0	18.1	reference [7]
Thiophene	C ₄ H ₄ S	110-02-1	5 LJ + dipole + quadrupole	1.2	3.8	22.4	reference [7]
Hydrogen cyanide	HCN	74-90-8	2 LJ + dipole + quadrupole	1.0	7.2	51.9	reference [7]
Nitromethane	CH ₃ NO ₂	75-52-5	4 LJ + dipole + quadrupole	0.2	18.7	31.5	reference [7]
Phosgene	COCl ₂	75-44-5	4 LJ + dipole + quadrupole	0.5	2.1	17.2	reference [8]
Benzene	C ₆ H ₆	71-43-2	6 LJ + 6 quadrupoles	0.4	3.4	11.9	reference [8]
Chlorobenzene	C ₆ H ₅ Cl	108-90-7	7 LJ + dipole + 5 quadrupoles	0.9	5.0	17.8	reference [8]
Ortho-dichlorobenzene	C ₆ H ₄ Cl ₂	95-50-1	8 LJ + dipole + 4 quadrupoles	0.5	6.4	34.3	reference [8]
Cyanogen chloride	NCCl	506-77-4	3 LJ + dipole + quadrupole	0.3	2.1	15.3	reference [9]
Cyanogen	C ₂ N ₂	460-19-5	4 LJ + quadrupole	0.6	13.0	2.5	reference [9]
Heptafluoropropane (R227ea)	C ₃ HF ₇	431-89-0	10 LJ + dipole + quadrupole	1.0	1.0	7.2	reference [10]
Ammonia	NH ₃	7664-41-7	LJ + 4 charges	0.7	1.6	36.7	reference [11]
Formic acid	CH ₂ O ₂	64-18-6	3 LJ + 4 charges	0.8	5.1	9.5	reference [12]
Methanol	CH ₃ OH	67-56-1	2 LJ + 3 charges	0.6	1.1	35.3	reference [13]
Dimethylamine	C ₂ H ₇ N	124-40-3	3 LJ + 3 charges	0.4	6.2	28.7	reference [14]
Ethylene glycol	C ₂ H ₆ O ₂	107-21-1	4 LJ + 6 charges	0.8	4.8	32.6	reference [15]
Water	H ₂ O	7732-18-5	LJ + 3 charges	1.1	7.2	30.7	reference [15]
Hydrazine	N ₂ H ₄	302-01-2	2 LJ + 6 charges	0.5	7.6	29.2	reference [16]
Methylhydrazine	CH ₆ N ₂	60-34-4	3 LJ + 3 charges	0.2	7.0	—	reference [16]
1,1-Dimethylhydrazine	C ₂ H ₈ N ₂	57-14-7	4 LJ + 3 charges	1.3	3.7	—	reference [16]
Ethyl acetate	C ₄ H ₈ O ₂	141-78-6	6 LJ + 5 charges	0.1	4.6	10.3	reference [17]
Decafluorobutane	C ₄ F ₁₀	355-25-9	14 LJ + 14 charges	0.5	3.5	10.3	reference [18]
Hexamethyldisiloxane	C ₆ H ₁₈ OSi ₂	107-46-0	9 LJ + 3 charges	0.5	5.0	12.9	reference [19]
Octamethylcyclotetrasiloxane	C ₈ H ₂₄ O ₂ Si ₄	556-67-2	16 LJ + 8 charges	0.5	6.0	10.5	reference [20]

Table 2

Molecular simulation results for the vapour-liquid equilibrium of the pure components from the present work. The numbers in parentheses indicate the statistical uncertainties in terms of the last given decimal digits.

T K	p^s MPa	ρ' mol l ⁻¹	ρ'' mol l ⁻¹	γ mN m ⁻¹
<i>Acetonitrile</i>				
300	0.005(4)	18.885(1)	0.002(1)	41.9(15)
370	0.137(38)	17.013(20)	0.053(12)	27.1(6)
440	0.839(90)	14.810(21)	0.307(58)	15.7(30)
510	2.72(14)	11.84(9)	1.09(15)	5.9(3)
<i>Cyclohexane</i>				
280	0.008(6)	9.355(3)	0.003(1)	29.2(12)
335	0.049(8)	8.750(4)	0.017(3)	22.3(13)
390	0.270(33)	8.093(3)	0.090(9)	15.5(10)
445	0.855(34)	7.325(13)	0.273(11)	9.5(7)
510	2.387(93)	6.117(26)	0.834(41)	3.5(4)
<i>Cyclohexanone</i>				
250	0.000(0)	9.902(8)	0.000(0)	50.6(38)
315	0.002(2)	9.327(4)	0.001(1)	40.5(12)
380	0.020(6)	8.741(5)	0.006(1)	30.8(21)
445	0.148(22)	8.118(11)	0.042(5)	22.3(13)
510	0.558(37)	7.423(14)	0.146(9)	14.8(6)
<i>Cyclohexanol</i>				
300	0.000(0)	9.700(22)	0.000(0)	40.3(62)
375	0.009(7)	9.028(4)	0.003(1)	32.0(13)
450	0.122(20)	8.277(3)	0.034(8)	22.9(4)
525	0.633(24)	7.422(13)	0.165(12)	14.0(7)
600	2.093(91)	6.325(20)	0.575(31)	5.7(11)
<i>Ethylene oxide</i>				
180	0.000(0)	23.230(4)	0.000(0)	48.1(33)
245	0.006(4)	21.325(6)	0.004(3)	38.6(23)
310	0.331(68)	19.323(27)	0.145(30)	25.0(13)
375	1.304(57)	16.851(13)	0.495(27)	14.3(19)
440	4.77(40)	13.39(13)	2.16(34)	3.7(11)
<i>Isobutane</i>				
120	0.000(0)	12.654(6)	0.000(0)	37.9(13)
185	0.001(1)	11.539(3)	0.001(1)	26.7(8)
250	0.067(17)	10.383(23)	0.032(7)	17.4(5)
315	0.584(10)	8.983(28)	0.263(16)	9.1(7)
380	2.32(12)	7.112(41)	1.13(12)	2.3(4)
<i>Formaldehyde</i>				
180	0.001(1)	31.984(54)	0.001(1)	51.6(14)
235	0.030(9)	29.228(5)	0.017(5)	36.3(15)
290	0.331(54)	26.222(77)	0.155(20)	24.2(14)
345	1.66(13)	22.594(39)	0.782(66)	12.7(9)
<i>Dimethyl ether</i>				
205	0.016(8)	17.016(5)	0.016(4)	30.0(12)
260	0.205(39)	15.415(53)	0.100(35)	19.8(13)
315	0.95(13)	13.563(13)	0.442(38)	10.9(10)
370	3.34(35)	10.94(12)	1.70(31)	3.6(6)

Table 2 (continued)

<i>T</i> K	<i>p</i> ^s MPa	ρ' mol l ⁻¹	ρ'' mol l ⁻¹	γ mN m ⁻¹
<i>Sulfur dioxide</i>				
220	0.013(8)	24.771(11)	0.007(4)	39.8(29)
265	0.106(39)	22.923(25)	0.049(14)	29.6(27)
310	0.65(17)	20.932(52)	0.278(74)	20.0(14)
355	1.95(46)	18.48(12)	0.83(19)	11.1(9)
400	4.65(26)	14.87(28)	2.30(25)	3.6(10)
<i>Dimethyl sulfide</i>				
190	0.001(1)	19.996(5)	0.000(0)	48.6(16)
260	0.036(14)	18.300(17)	0.022(14)	36.1(10)
330	0.342(26)	16.471(18)	0.134(16)	23.6(7)
400	1.70(15)	14.315(56)	0.635(65)	11.8(13)
470	5.32(33)	10.85(26)	2.60(57)	2.1(8)
<i>Thiophene</i>				
250	0.002(1)	13.107(7)	0.001(1)	43.6(22)
320	0.035(16)	12.168(6)	0.013(4)	33.3(7)
390	0.263(37)	11.166(7)	0.084(9)	22.4(13)
460	1.12(11)	10.001(16)	0.342(35)	13.6(10)
530	3.13(29)	8.458(65)	1.01(16)	5.0(8)
<i>Hydrogen cyanide</i>				
280	0.038(21)	25.756(38)	0.021(11)	34.0(11)
315	0.122(12)	24.015(12)	0.063(10)	25.5(21)
340	0.343(32)	22.589(23)	0.153(23)	19.2(12)
375	0.949(50)	20.50(12)	0.431(41)	13.2(17)
410	2.03(10)	17.766(69)	1.00(12)	7.6(7)
<i>Nitromethane</i>				
260	0.001(1)	19.569(16)	0.001(1)	55.3(37)
330	0.030(7)	18.014(6)	0.014(6)	41.6(34)
400	0.109(22)	16.259(52)	0.044(15)	28.3(14)
470	0.826(69)	14.337(25)	0.266(32)	16.5(15)
540	2.84(26)	11.70(20)	1.06(15)	6.0(9)
<i>Phosgene</i>				
160	0.000(0)	17.047(11)	0.000(0)	49.2(32)
225	0.007(0)	15.578(10)	0.004(3)	34.8(17)
290	0.133(34)	14.047(7)	0.058(8)	23.1(21)
355	0.937(36)	12.311(20)	0.367(8)	12.5(12)
420	3.35(33)	9.873(48)	1.46(22)	3.7(7)
<i>Benzene</i>				
290	0.007(7)	11.208(13)	0.003(3)	33.2(13)
350	0.092(23)	10.403(7)	0.033(3)	24.3(7)
410	0.423(47)	9.523(3)	0.137(16)	15.7(10)
470	1.441(67)	8.450(19)	0.468(22)	8.5(11)
530	3.337(92)	6.884(36)	1.21(13)	2.6(9)
<i>Chlorobenzene</i>				
250	0.004(3)	10.320(8)	0.002(2)	46.7(28)
335	0.011(6)	9.466(11)	0.005(3)	33.3(19)
420	0.122(13)	8.567(23)	0.037(2)	21.9(8)
505	0.79(14)	7.520(30)	0.222(44)	11.7(9)
590	2.91(8)	5.992(20)	0.94(7)	3.2(9)

Table 2 (continued)

<i>T</i> K	<i>p</i> ^s MPa	ρ' mol l ⁻¹	ρ'' mol l ⁻¹	γ mN m ⁻¹
<i>Ortho-dichlorobezene</i>				
375	0.003(2)	8.472(5)	0.001(1)	36.1(51)
470	0.097(17)	7.631(3)	0.026(6)	23.4(8)
565	0.701(89)	6.647(16)	0.173(28)	12.6(15)
660	2.79(14)	5.240(33)	0.807(80)	3.0(7)
<i>Cyanogen chloride</i>				
280	0.079(21)	19.777(13)	0.036(8)	28.3(21)
315	0.312(36)	18.490(46)	0.135(9)	21.6(16)
350	0.86(17)	17.08(39)	0.361(83)	14.9(21)
385	1.86(43)	15.27(7)	0.79(23)	9.4(17)
420	3.74(36)	12.92(9)	1.86(54)	4.2(7)
<i>Cyanogen</i>				
260	0.094(31)	18.030(33)	0.049(21)	21.9(24)
290	0.349(95)	16.866(58)	0.168(25)	16.6(12)
320	0.79(30)	15.546(99)	0.36(17)	11.5(16)
350	2.17(34)	13.820(16)	1.04(26)	5.7(6)
380	4.40(5)	11.15(28)	2.89(40)	1.2(6)
<i>Heptafluoropropane</i>				
200	0.002(1)	10.364(13)	0.001(1)	21.9(10)
250	0.063(10)	9.381(8)	0.031(2)	14.8(19)
300	0.466(39)	8.215(3)	0.213(21)	7.7(9)
350	1.776(68)	6.531(20)	0.938(46)	1.8(6)
<i>Ammonia</i>				
220	0.029(2)	41.985(19)	0.015(1)	55.1(19)
260	0.233(38)	38.927(14)	0.116(23)	40.1(36)
300	1.029(80)	35.470(30)	0.467(39)	26.2(13)
340	3.080(66)	31.410(26)	1.421(43)	15.2(25)
380	7.23(15)	25.572(21)	3.86(21)	4.8(1)
<i>Formic acid</i>				
300	0.014(10)	26.192(5)	0.007(2)	39.3(29)
360	0.072(9)	24.478(9)	0.038(14)	30.2(23)
420	0.333(28)	22.607(11)	0.169(20)	22.0(15)
480	1.14(17)	20.36(17)	0.543(61)	15.3(13)
540	3.20(25)	17.45(14)	1.57(18)	6.7(15)
<i>Methanol</i>				
245	0.001(1)	26.175(9)	0.001(1)	36.0(16)
320	0.045(17)	23.958(6)	0.020(7)	27.1(16)
395	0.58(13)	21.317(36)	0.359(49)	14.0(20)
470	3.61(14)	17.318(91)	1.61(26)	6.0(14)
<i>Dimethylamine</i>				
210	0.003(1)	16.653(10)	0.002(1)	35.2(13)
260	0.033(11)	15.523(4)	0.016(6)	27.3(4)
310	0.257(24)	14.279(7)	0.109(10)	19.0(2)
360	1.04(10)	12.888(6)	0.407(45)	11.8(9)
410	2.65(74)	10.814(77)	1.07(50)	5.3(18)

Table 2 (continued)

T K	p^s MPa	ρ' mol l ⁻¹	ρ'' mol l ⁻¹	γ mN m ⁻¹
<i>Ethylene glycol</i>				
380	0.005(3)	16.867(29)	0.002(1)	65.6(21)
480	0.107(60)	15.527(25)	0.028(11)	42.3(36)
580	1.144(52)	13.759(14)	0.268(9)	23.6(31)
680	5.45(58)	10.906(97)	1.44(19)	6.2(12)
<i>Water</i>				
300	0.006(5)	56.348(12)	0.002(1)	94.0(21)
375	0.069(16)	52.650(12)	0.024(8)	75.1(13)
450	0.63(10)	48.475(11)	0.31(13)	56.9(19)
525	3.31(16)	43.412(11)	0.94(6)	34.1(21)
600	10.43(20)	36.485(46)	3.28(3)	13.7(20)
<i>Hydrazine</i>				
280	0.000(0)	32.321(8)	0.000(0)	96.7(23)
360	0.028(10)	29.955(5)	0.010(5)	72.6(13)
440	0.358(24)	27.220(18)	0.153(19)	49.4(30)
520	2.24(64)	24.063(80)	1.16(33)	29.9(20)
<i>Methylhydrazine</i>				
270	0.009(5)	19.384(10)	0.004(3)	57.3(13)
345	0.031(13)	17.944(6)	0.012(3)	43.1(16)
420	0.420(64)	16.358(48)	0.137(40)	29.7(12)
495	1.93(21)	14.598(16)	0.573(51)	16.7(8)
570	5.21(22)	12.21(12)	1.73(13)	5.7(9)
<i>1,1-Dimethylhydrazine</i>				
260	0.003(2)	13.783(6)	0.001(1)	35.5(21)
315	0.045(13)	12.833(4)	0.018(6)	27.6(16)
370	0.290(14)	11.806(6)	0.101(9)	19.4(9)
425	1.03(13)	10.603(3)	0.344(40)	11.9(4)
480	2.97(19)	9.026(33)	1.10(12)	4.6(4)
<i>Ethylacetate</i>				
190	0.000(0)	11.726(4)	0.000(0)	42.4(19)
265	0.002(1)	10.709(18)	0.001(1)	29.9(6)
340	0.063(12)	9.636(10)	0.024(3)	19.7(9)
415	0.497(39)	8.379(6)	0.170(6)	10.9(12)
490	2.078(53)	6.584(19)	0.831(37)	3.0(7)
<i>Decafluorobutane</i>				
260	0.077(13)	6.848(12)	0.038(7)	11.8(17)
310	0.357(6)	6.021(28)	0.157(5)	6.5(6)
360	1.329(67)	4.852(77)	0.657(43)	1.7(3)
<i>Hexamethyldisiloxane</i>				
210	0.000(0)	5.211(31)	0.000(0)	26.3(17)
280	0.002(1)	4.788(5)	0.001(0)	18.4(9)
350	0.047(15)	4.327(8)	0.017(4)	12.1(11)
420	0.299(20)	3.771(10)	0.097(10)	6.7(4)
490	1.161(26)	3.020(25)	0.421(10)	1.8(2)

Table 2 (continued)

T K	p^s MPa	ρ' mol l ⁻¹	ρ'' mol l ⁻¹	γ mN m ⁻¹
<i>Octamethylcyclotetrasiloxane</i>				
310	0.000(0)	3.135(14)	0.000(0)	18.6(33)
355	0.004(2)	2.970(12)	0.001(0)	14.6(10)
420	0.044(14)	2.709(8)	0.013(4)	10.1(11)
485	0.217(15)	2.403(12)	0.061(4)	5.7(2)
550	0.699(12)	1.985(27)	0.211(7)	1.9(3)