Supplementary Information: Mie Potentials for High Accuracy Phase Equilibria Calculations

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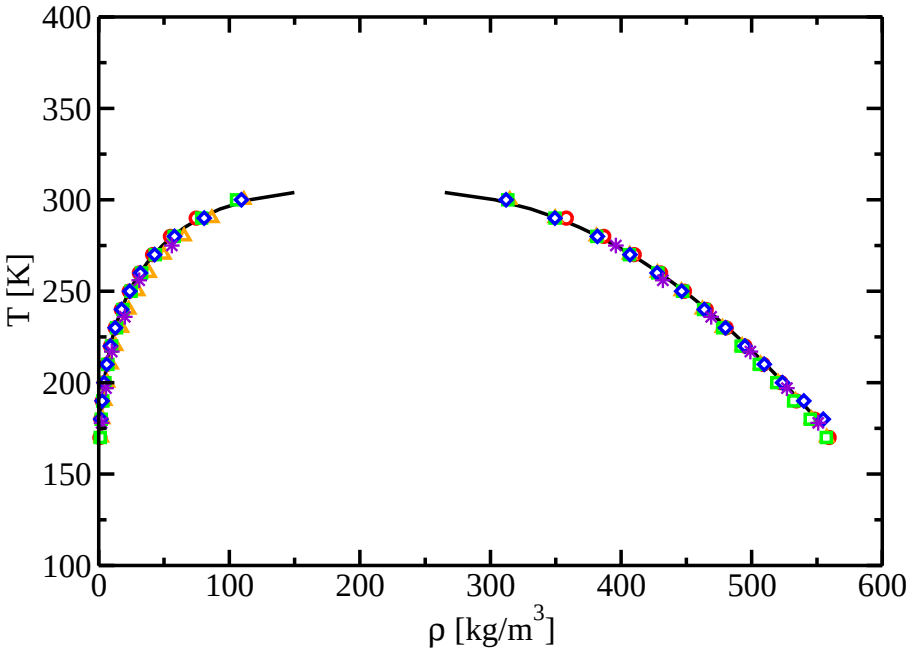

Figure 1: Vapor-liquid coexistence curves predicted by Mie potentials with various repulsion exponents. Line (experiment) [1, 2], triangle ($n = 9$), square ($n = 14$), circle($n = 16$), diamonds($n = 18$), stars($n = 12$, TraPPE-UA) [3]. The predictions of the TraPPE-UA force field should considered the best fit possible using $n = 12$.

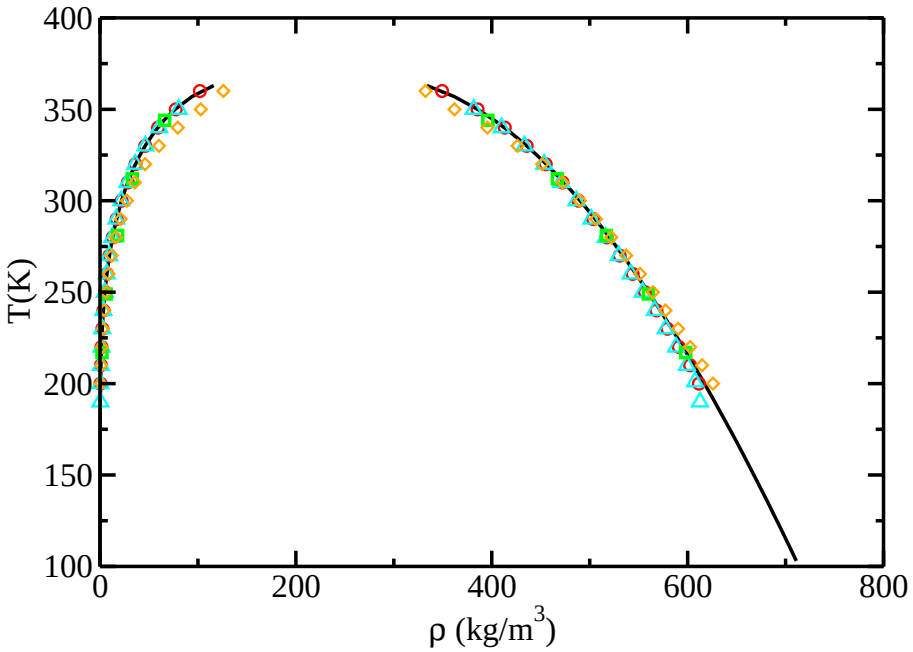

Figure 2: Vapor-liquid coexistence curves predicted by this work for n-propane (circle), TraPPE-UA (square) [3], Gordon (diamond) [4], and exponential-6 (triangle) [5]. Line represents experimental data [1, 2].

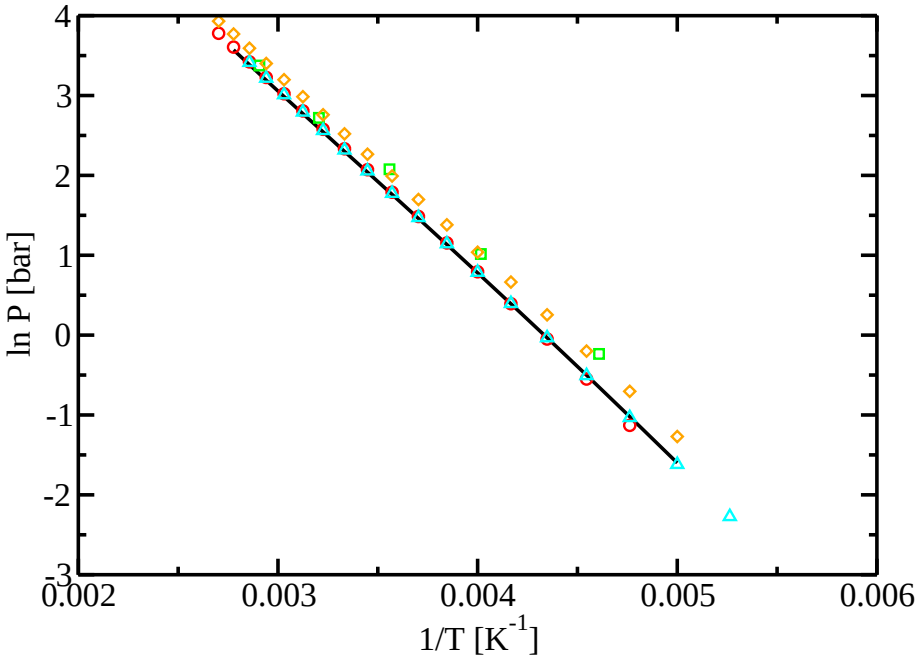

Figure 3: Vapor pressures predicted by this work for n-propane (circle), TraPPE-UA (square) [3], Gordon (diamond) [4], and exponential-6 (triangle) [5]. Line represents experimental data [1, 2].

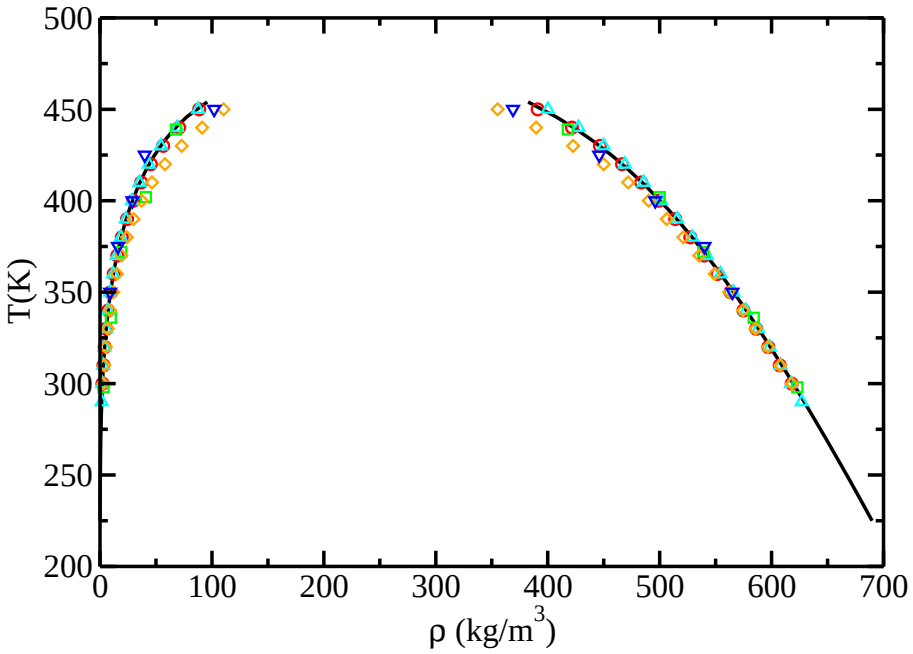

Figure 4: Vapor-liquid coexistence curves predicted by this work for *n*-pentane (circle), TraPPE-UA (square) [3], Gordon (diamond) [4], exponential-6 (triangle up) [5], and OPPE (triangle down) [6]. Line represents experimental data [1, 2].

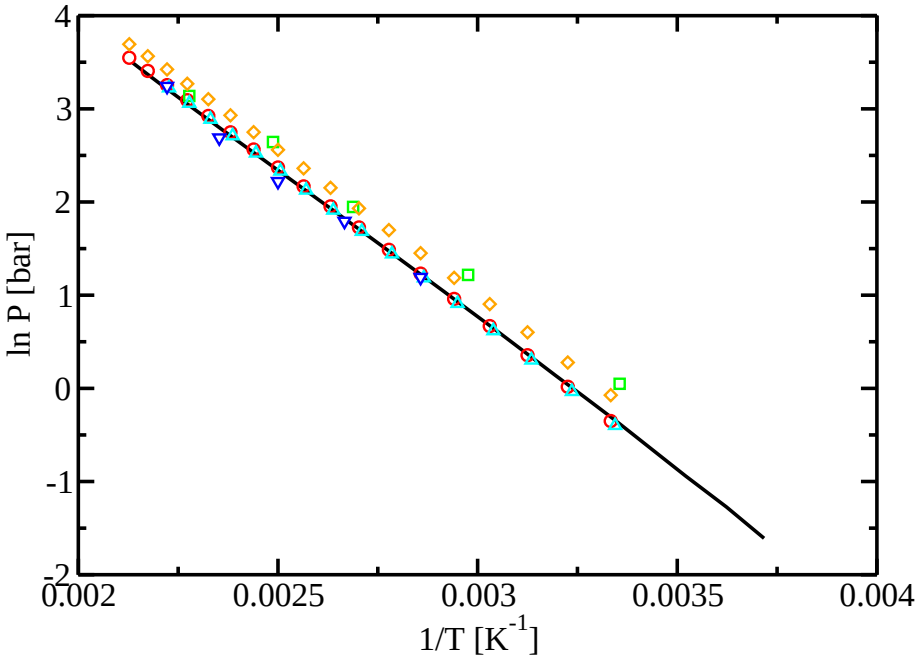

Figure 5: Vapor pressures predicted by this work for *n*-pentane (circle), TraPPE-UA (square) [3], Gordon (diamond) [4], exponential-6 (triangle up) [5], and OPPE (triangle down) [6]. Line represents experimental data [1, 2].

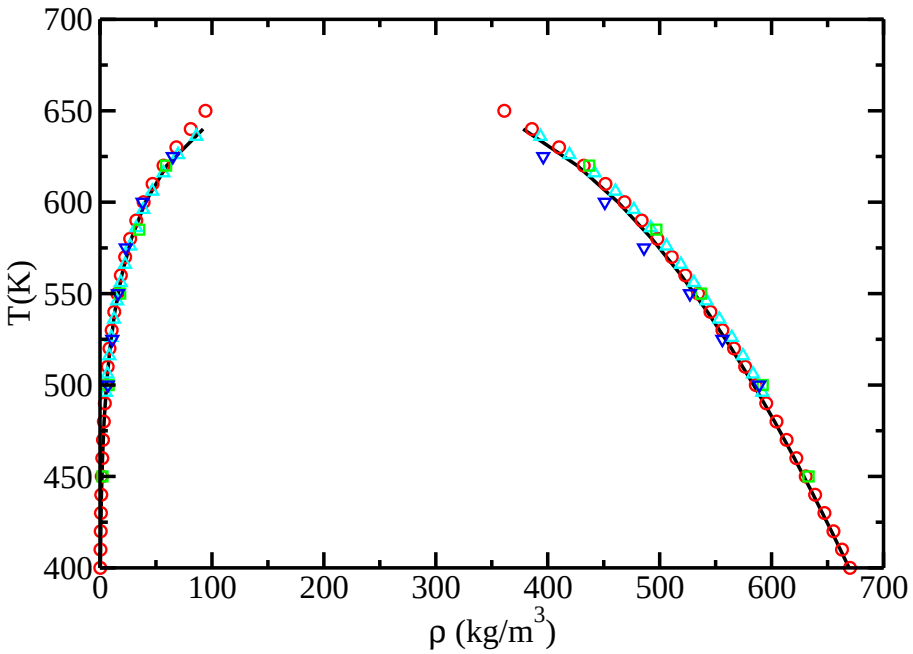

Figure 6: Vapor-liquid coexistence predicted by this work for *n*-dodecane (circle), TraPPE-UA (square) [3], exponential-6 (triangle up) [5], and OPPE (triangle down) [6]. Line represents experimental data [1, 2].

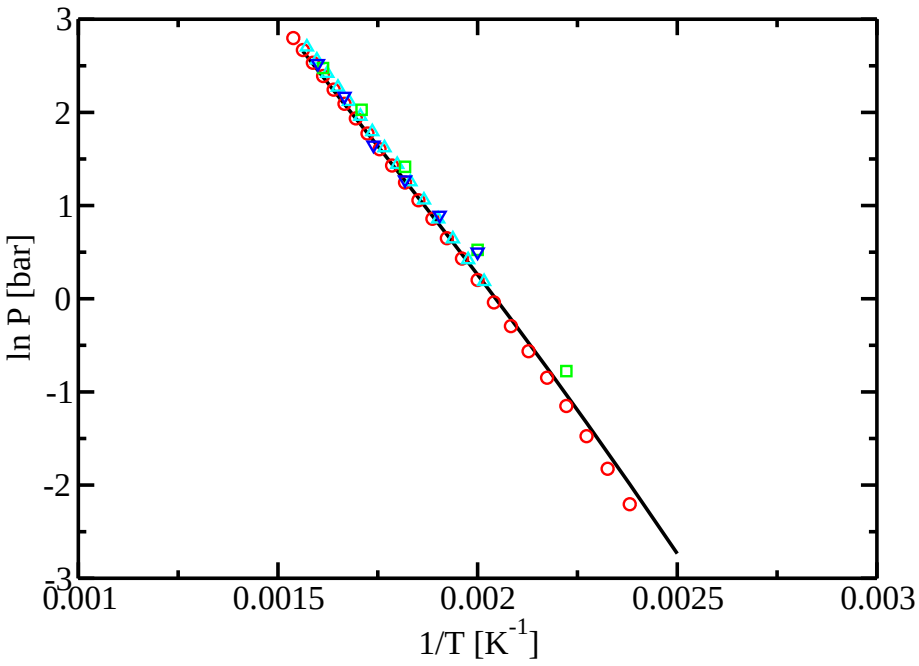

Figure 7: Vapor pressures predicted by this work for *n*-dodecane (circle), TraPPE-UA (square) [3], exponential-6 (triangle up) [5], and OPPE (triangle down) [6]. Line represents experimental data [1, 2].

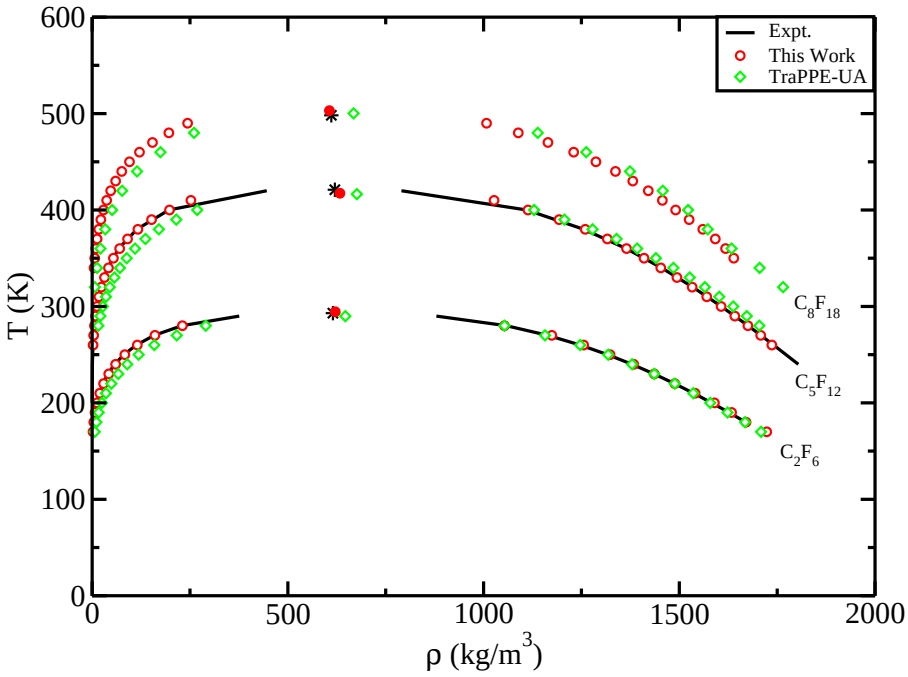

Figure 8: Vapor-liquid coexistence predicted by this work for selected perfluorocarbons (circle), TraPPE-UA (diamond) [7]. Line represents experimental data [2, 14, 17, 18, 25, 26].

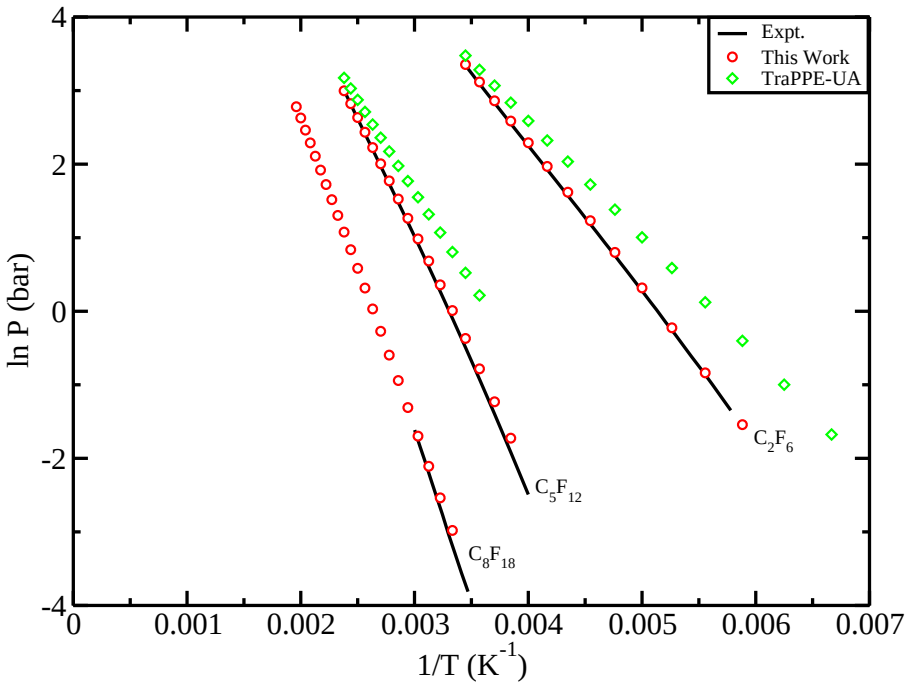

Figure 9: Vapor pressures predicted by this work for selected perfluorocarbons (circle), TraPPE-UA (diamond) [7]. Line represents experimental data [2, 14, 17, 18, 25, 26].

Table 1: Densities and heats of vaporization for selected perfluorocarbons predicted from NPT simulations at 1 atm

		density (g/cm^3)		ΔH_v (kJ/mol)	
Compound	T (K)	calcd	expt [8–24]	calcd	expt [8–24]
CF_4	145.13	1.598	1.608	12.01(4)	12.55
C_2F_6	195.05	1.610	1.590	15.83(5)	16.15
C_3F_8	236.5	1.609	1.600	19.16(2)	19.63
C_4F_{10}	273.15	1.601	1.600	22.32(2)	22.84
C_5F_{12}	298.15	1.607	1.600	25.74(4)	26.99
C_6F_{14}	298.15	1.687	1.675	30.64(9)	31.42

Table 2: Selected phase coexistence data predicted for methane by grand canonical histogram-reweighting Monte Carlo simulations.

$T(K)$	ρ_l (kg/m^3)	ρ_v (kg/m^3)	P (bar)	ΔH_v [kJ/mol]
190.000	236.947	96.319	45.239	2.570
180.000	279.516	58.706	32.955	4.194
170.000	312.322	37.427	23.402	5.373
165.000	325.153	30.436	19.464	5.798
160.000	336.721	24.727	16.018	6.165
155.000	347.379	19.984	13.027	6.492
150.000	357.599	16.030	10.457	6.792
145.000	367.471	12.730	8.269	7.068
140.000	376.584	9.986	6.430	7.314
135.000	385.355	7.721	4.909	7.541
130.000	393.468	5.873	3.669	7.744
125.000	401.204	4.383	2.679	7.929
120.000	409.737	3.197	1.902	8.120
115.000	418.053	2.267	1.307	8.297
110.000	425.428	1.555	0.865	8.451
105.000	429.969	1.026	0.549	8.544
100.000	431.713	0.650	0.333	8.571

Table 3: Selected phase coexistence data predicted for ethane by grand canonical histogram-reweighting Monte Carlo simulations.

$T(K)$	ρ_l (kg/m^3)	ρ_v (kg/m^3)	P (bar)	ΔH_v [kJ/mol]
305.000	299.827	117.078	49.142	4.579
300.000	317.048	103.799	44.450	5.331
290.000	354.321	76.737	35.899	7.039
280.000	385.593	55.916	28.616	8.567
270.000	410.132	41.707	22.506	9.739
260.000	430.632	31.398	17.410	10.669
250.000	448.772	23.534	13.208	11.453
240.000	465.570	17.424	9.795	12.143
230.000	481.226	12.672	7.073	12.758
220.000	495.550	9.011	4.954	13.301
210.000	509.441	6.228	3.346	13.801
200.000	522.503	4.154	2.165	14.249
190.000	535.060	2.653	1.332	14.660
180.000	547.943	1.606	0.770	15.061
170.000	560.451	0.910	0.412	15.436
160.000	571.367	0.476	0.200	15.748

Table 4: Selected phase coexistence data predicted for propane by grand canonical histogram-reweighting Monte Carlo simulations.

$T(K)$	ρ_l (kg/m^3)	ρ_v (kg/m^3)	P (bar)	ΔH_v [kJ/mol]
370.000	312.771	128.054	43.775	5.447
360.000	349.247	101.991	36.812	7.289
350.000	385.491	77.365	30.590	9.243
340.000	413.318	59.272	25.189	10.834
330.000	435.632	46.244	20.539	12.090
320.000	455.087	36.267	16.552	13.143
310.000	472.216	28.398	13.164	14.046
300.000	488.368	22.105	10.311	14.860
290.000	503.491	17.034	7.935	15.595
280.000	517.293	12.953	5.986	16.246
270.000	530.652	9.689	4.415	16.850
260.000	543.856	7.105	3.172	17.422
250.000	556.405	5.088	2.209	17.945
240.000	568.163	3.545	1.482	18.415
230.000	579.331	2.391	0.952	18.833
220.000	591.007	1.551	0.577	19.236
210.000	602.573	0.960	0.323	19.590
200.000	611.544	0.561	0.160	19.790

Table 5: Selected phase coexistence data predicted for butane by grand canonical histogram-reweighting Monte Carlo simulations.

$T(K)$	ρ_l (kg/m^3)	ρ_v (kg/m^3)	P (bar)	ΔH_v [kJ/mol]
420.000	339.772	111.441	36.390	7.890
410.000	367.823	94.748	31.196	9.357
400.000	397.770	77.419	26.411	10.992
390.000	425.604	61.697	22.129	12.625
380.000	449.307	48.859	18.373	14.104
370.000	469.197	38.815	15.116	15.369
360.000	486.370	30.917	12.312	16.444
350.000	501.822	24.590	9.914	17.383
340.000	516.251	19.455	7.881	18.229
330.000	529.952	15.265	6.174	19.004
320.000	542.972	11.847	4.756	19.719
310.000	555.375	9.070	3.596	20.380
300.000	567.192	6.832	2.661	20.992
290.000	578.439	5.049	1.922	21.557
280.000	589.399	3.650	1.349	22.088
270.000	600.329	2.571	0.916	22.597
260.000	610.984	1.757	0.598	23.070

Table 6: Selected phase coexistence data predicted for pentane by grand canonical histogram-reweighting Monte Carlo simulations.

$T(K)$	ρ_l (kg/m^3)	ρ_v (kg/m^3)	P (bar)	ΔH_v [kJ/mol]
470.000	335.698	125.273	34.723	8.115
460.000	364.461	106.951	30.078	9.849
450.000	395.200	87.481	25.784	11.803
440.000	422.936	69.916	21.931	13.724
430.000	445.806	55.870	18.538	15.418
420.000	465.089	45.037	15.569	16.857
410.000	482.357	36.519	12.978	18.106
400.000	498.285	29.635	10.723	19.218
390.000	513.022	23.977	8.773	20.221
380.000	526.654	19.295	7.100	21.131
370.000	539.384	15.415	5.678	21.965
360.000	551.557	12.207	4.482	22.744
350.000	563.440	9.565	3.485	23.480
340.000	574.930	7.402	2.665	24.171
330.000	585.917	5.647	2.001	24.816
320.000	596.473	4.236	1.470	25.422
310.000	606.834	3.117	1.055	26.000
300.000	618.164	2.241	0.736	26.608

Table 7: Selected phase coexistence data predicted for hexane by grand canonical histogram-reweighting Monte Carlo simulations.

$T(K)$	ρ_l (kg/m^3)	ρ_v (kg/m^3)	P (bar)	ΔH_v [kJ/mol]
500.000	366.018	112.352	27.697	10.594
490.000	395.855	90.541	23.906	12.917
480.000	422.477	72.249	20.521	15.112
470.000	444.562	58.283	17.529	16.972
460.000	463.473	47.563	14.889	18.534
450.000	480.498	39.028	12.563	19.899
440.000	496.217	32.053	10.522	21.125
430.000	510.897	26.270	8.738	22.247
420.000	524.727	21.441	7.190	23.283
410.000	537.821	17.397	5.857	24.245
400.000	550.308	14.013	4.717	25.146
390.000	562.197	11.190	3.753	25.990
380.000	573.494	8.846	2.946	26.778
370.000	584.216	6.913	2.279	27.514
360.000	594.369	5.331	1.734	28.201
350.000	604.257	4.050	1.296	28.856
340.000	614.026	3.023	0.949	29.489
330.000	623.440	2.213	0.680	30.086
320.000	631.598	1.584	0.476	30.596

Table 8: Selected phase coexistence data predicted for octane by grand canonical histogram-reweighting Monte Carlo simulations.

$T(K)$	ρ_l (kg/m^3)	ρ_v (kg/m^3)	P (bar)	ΔH_v [kJ/mol]
550.000	397.631	89.470	19.649	15.270
540.000	420.504	73.420	16.985	17.492
530.000	442.446	59.669	14.604	19.689
520.000	462.402	48.580	12.493	21.710
510.000	480.277	39.808	10.629	23.494
500.000	496.417	32.787	8.986	25.058
490.000	511.137	27.050	7.543	26.446
480.000	524.607	22.287	6.283	27.691
470.000	536.981	18.298	5.188	28.820
460.000	548.524	14.947	4.245	29.858
450.000	559.578	12.133	3.438	30.834
440.000	570.408	9.773	2.753	31.767
430.000	581.072	7.803	2.177	32.663
420.000	591.464	6.165	1.697	33.520
410.000	601.541	4.815	1.303	34.339
400.000	611.378	3.712	0.982	35.131
390.000	620.878	2.820	0.726	35.885
380.000	629.771	2.108	0.523	36.570
370.000	638.119	1.548	0.367	37.181
360.000	646.175	1.115	0.248	37.726
350.000	653.743	0.785	0.160	38.181

Table 9: Selected phase coexistence data predicted for decane by grand canonical histogram-reweighting Monte Carlo simulations.

$T(K)$	ρ_l (kg/m^3)	ρ_v (kg/m^3)	P (bar)	ΔH_v [kJ/mol]
600.000	394.289	85.557	16.919	18.074
590.000	418.032	70.894	14.716	20.570
580.000	439.381	58.384	12.736	22.934
570.000	458.107	48.211	10.970	25.062
560.000	474.774	40.009	9.401	26.949
550.000	489.982	33.308	8.010	28.636
540.000	504.037	27.740	6.782	30.166
530.000	517.062	23.056	5.702	31.568
520.000	529.196	19.090	4.758	32.861
510.000	540.632	15.727	3.940	34.066
500.000	551.623	12.880	3.234	35.207
490.000	562.379	10.478	2.631	36.306
480.000	572.897	8.461	2.119	37.368
470.000	583.039	6.775	1.688	38.383
460.000	592.838	5.377	1.329	39.348
450.000	602.416	4.223	1.033	40.268
440.000	611.662	3.279	0.791	41.147
430.000	620.510	2.514	0.596	41.988
420.000	629.347	1.900	0.442	42.818
410.000	638.350	1.414	0.321	43.646
400.000	646.965	1.033	0.228	44.441
390.000	655.058	0.740	0.158	45.175
380.000	663.164	0.519	0.106	45.860
370.000	671.403	0.355	0.069	46.471

Table 10: Selected phase coexistence data predicted for dodecane by grand canonical histogram-reweighting Monte Carlo simulations.

$T(K)$	ρ_l (kg/m^3)	ρ_v (kg/m^3)	P (bar)	ΔH_v [kJ/mol]
650.000	361.232	94.233	16.411	17.847
640.000	385.879	81.059	14.423	20.368
630.000	410.129	68.257	12.587	22.978
620.000	432.201	56.750	10.922	25.522
610.000	451.558	46.992	9.430	27.893
600.000	468.610	38.960	8.103	30.050
590.000	483.938	32.385	6.927	31.995
580.000	497.931	26.962	5.889	33.752
570.000	510.839	22.446	4.976	35.351
560.000	522.901	18.652	4.177	36.825
550.000	534.352	15.446	3.480	38.203
540.000	545.374	12.731	2.877	39.510
530.000	556.070	10.432	2.358	40.761
520.000	566.435	8.491	1.914	41.960
510.000	576.383	6.859	1.539	43.100
500.000	585.906	5.494	1.223	44.182
490.000	595.182	4.361	0.961	45.225
480.000	604.378	3.426	0.745	46.244
470.000	613.407	2.661	0.570	47.229
460.000	622.093	2.042	0.428	48.162
450.000	630.514	1.545	0.316	49.054
440.000	638.906	1.152	0.229	49.926

Table 11: Selected phase coexistence data predicted for tetradecane by grand canonical histogram-reweighting Monte Carlo simulations.

$T(K)$	ρ_l (kg/m^3)	ρ_v (kg/m^3)	P (bar)	ΔH_v [kJ/mol]
690.000	350.462	103.114	15.238	17.820
680.000	373.510	86.877	13.411	20.853
670.000	396.930	71.727	11.744	24.047
660.000	418.740	58.857	10.244	27.131
650.000	438.103	48.523	8.904	29.917
640.000	455.218	40.318	7.709	32.366
630.000	470.574	33.706	6.645	34.527
620.000	484.504	28.265	5.700	36.457
610.000	497.247	23.717	4.863	38.206
600.000	509.135	19.879	4.125	39.823
590.000	520.557	16.619	3.476	41.356
580.000	531.737	13.840	2.909	42.831
570.000	542.664	11.468	2.416	44.252
560.000	553.240	9.447	1.991	45.614
550.000	563.360	7.730	1.626	46.907
540.000	572.949	6.278	1.315	48.125
530.000	582.058	5.058	1.054	49.275
520.000	590.790	4.038	0.835	50.372
510.000	599.138	3.193	0.655	51.418
500.000	607.073	2.498	0.508	52.418
490.000	614.782	1.931	0.389	53.410
480.000	622.201	1.473	0.293	54.403
470.000	628.013	1.109	0.219	55.221
460.000	631.267	0.823	0.161	55.711
450.000	632.711	0.603	0.117	55.963
440.000	633.297	0.436	0.084	56.106
430.000	633.519	0.311	0.060	56.214
420.000	633.583	0.218	0.043	56.334
410.000	633.574	0.151	0.030	56.484
400.000	633.533	0.102	0.021	56.719

Table 12: Selected phase coexistence data predicted for perfluoromethane by grand canonical histogram-reweighting Monte Carlo simulations.

$T(K)$	ρ_l (kg/m^3)	ρ_v (kg/m^3)	P (bar)	ΔH_v [kJ/mol]
230.000	852.297	369.699	39.747	3.236
220.000	1000.626	260.039	29.945	4.974
210.000	1146.782	165.892	21.863	6.819
200.000	1250.684	109.779	15.537	8.128
190.000	1334.748	73.208	10.665	9.124
180.000	1400.446	47.991	7.021	9.884
170.000	1464.499	30.378	4.393	10.573
160.000	1524.403	18.274	2.577	11.186
150.000	1579.068	10.292	1.397	11.725
140.000	1640.053	5.297	0.684	12.287

Table 13: Selected phase coexistence data predicted for perfluoroethane by grand canonical histogram-reweighting Monte Carlo simulations.

$T(K)$	ρ_l (kg/m^3)	ρ_v (kg/m^3)	P (bar)	ΔH_v [kJ/mol]
290.000	923.207	332.865	28.845	5.131
280.000	1063.165	232.893	22.645	7.368
270.000	1174.898	161.084	17.488	9.288
260.000	1254.471	115.644	13.287	10.648
250.000	1322.134	83.622	9.887	11.747
240.000	1381.927	59.975	7.341	12.623
230.000	1437.696	42.325	5.057	13.250
220.000	1491.766	29.139	3.437	14.032
210.000	1539.931	19.396	2.238	14.709
200.000	1585.796	12.375	1.387	15.338
190.000	1626.622	7.505	0.810	15.899
180.000	1666.804	4.289	0.440	16.439
170.000	1709.499	2.272	0.217	16.893
160.000	1724.669	1.104	0.095	17.169
150.000	1730.031	0.487	0.034	17.162

Table 14: Selected phase coexistence data predicted for perfluoropropane by grand canonical histogram-reweighting Monte Carlo simulations.

$T(K)$	ρ_l (kg/m^3)	ρ_v (kg/m^3)	P (bar)	ΔH_v [kJ/mol]
330.000	1051.399	251.536	20.293	8.410
320.000	1149.215	179.981	16.189	10.550
310.000	1228.631	131.924	12.774	12.260
300.000	1294.416	98.588	9.941	13.603
290.000	1352.456	73.813	7.606	14.738
280.000	1405.047	54.828	5.703	15.733
270.000	1454.148	40.146	4.179	16.634
260.000	1501.250	28.828	2.982	17.471
250.000	1545.102	20.212	2.064	18.233
240.000	1586.061	13.773	1.379	18.930
230.000	1624.717	9.069	0.885	19.572
220.000	1665.266	5.726	0.541	20.228
210.000	1705.120	3.428	0.312	20.877

Table 15: Selected phase coexistence data predicted for perfluorobutane by grand canonical histogram-reweighting Monte Carlo simulations.

$T(K)$	ρ_l (kg/m^3)	ρ_v (kg/m^3)	P (bar)	ΔH_v [kJ/mol]
400.000	809.110	379.599	28.913	5.537
390.000	876.190	338.880	24.798	6.821
380.000	970.652	285.325	20.836	8.596
370.000	1076.958	225.220	17.179	10.675
360.000	1169.581	171.143	13.967	12.697
350.000	1242.416	129.747	11.232	14.434
340.000	1303.366	99.202	8.929	15.888
330.000	1357.947	76.019	7.001	17.145
320.000	1408.026	57.949	5.401	18.265
310.000	1453.826	43.720	4.092	19.270
300.000	1495.584	32.532	3.037	20.172
290.000	1535.039	23.798	2.203	21.004
280.000	1573.350	17.051	1.556	21.793
270.000	1611.806	11.910	1.066	22.567
260.000	1648.264	8.068	0.705	23.290
250.000	1680.776	5.276	0.449	23.934
240.000	1714.185	3.310	0.273	24.592

Table 16: Selected phase coexistence data predicted for perfluoropentane by grand canonical histogram-reweighting Monte Carlo simulations.

$T(K)$	ρ_l (kg/m^3)	ρ_v (kg/m^3)	P (bar)	ΔH_v [kJ/mol]
420.000	946.091	307.439	20.030	8.908
410.000	1026.727	252.206	16.810	10.825
400.000	1113.426	197.691	13.921	12.973
390.000	1192.799	151.815	11.404	15.056
380.000	1259.710	116.824	9.251	16.869
370.000	1316.176	90.519	7.424	18.390
360.000	1365.208	70.258	5.885	19.687
350.000	1409.863	54.312	4.601	20.838
340.000	1452.733	41.631	3.540	21.908
330.000	1494.024	31.523	2.675	22.911
320.000	1532.812	23.504	1.980	23.839
310.000	1570.172	17.205	1.432	24.718
300.000	1606.748	12.320	1.009	25.559
290.000	1641.776	8.598	0.691	26.338
280.000	1675.166	5.826	0.457	27.020
270.000	1707.821	3.815	0.292	27.585
260.000	1736.248	2.402	0.178	28.027
250.000	1756.071	1.448	0.104	28.297

Table 17: Selected phase coexistence data predicted for perfluorohexane by grand canonical histogram-reweighting Monte Carlo simulations.

$T(K)$	ρ_l (kg/m^3)	ρ_v (kg/m^3)	P (bar)	ΔH_v [kJ/mol]
450.000	950.001	311.801	17.609	9.728
440.000	1034.400	247.338	14.792	12.144
430.000	1119.002	189.672	12.314	14.663
420.000	1192.749	145.726	10.173	16.908
410.000	1253.706	113.626	8.336	18.766
400.000	1305.504	89.365	6.767	20.339
390.000	1351.745	70.341	5.435	21.737
380.000	1394.871	55.125	4.312	23.001
370.000	1436.068	42.859	3.374	24.152
360.000	1475.757	32.973	2.600	25.234
350.000	1514.493	25.042	1.969	26.280
340.000	1549.772	18.736	1.463	27.228
330.000	1580.976	13.783	1.065	28.063
320.000	1612.762	9.941	0.758	28.878
310.000	1645.581	7.000	0.526	29.695
300.000	1676.635	4.794	0.355	30.502
290.000	1703.623	3.181	0.232	31.227

Table 18: Selected phase coexistence data predicted for perfluorooctane by grand canonical histogram-reweighting Monte Carlo simulations.

$T(K)$	ρ_l (kg/m^3)	ρ_v (kg/m^3)	P (bar)	ΔH_v [kJ/mol]
510.000	891.415	317.399	16.217	10.739
500.000	958.692	270.729	13.925	12.820
490.000	1034.602	221.283	11.819	15.247
480.000	1109.866	175.601	9.937	17.790
470.000	1176.921	138.123	8.289	20.179
460.000	1233.958	109.128	6.864	22.260
450.000	1283.028	86.715	5.638	24.042
440.000	1326.761	69.024	4.589	25.602
430.000	1367.100	54.817	3.698	27.014
420.000	1405.400	43.307	2.946	28.327
410.000	1442.219	33.952	2.318	29.566
400.000	1477.235	26.357	1.798	30.726
390.000	1510.164	20.222	1.373	31.807
380.000	1541.339	15.305	1.031	32.819
370.000	1571.665	11.403	0.760	33.792
360.000	1602.164	8.343	0.548	34.756
350.000	1633.019	5.977	0.387	35.724

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Table 19: Selected phase coexistence data predicted for perfluoroethane(1)-ethane(2) at 242.93 K by grand canonical histogram-reweighting Monte Carlo simulations.

P (bar)	x_1	y_1
7.791	0.9988	0.9976
7.897	0.9885	0.9767
8.001	0.9789	0.9570
8.118	0.9678	0.9356
8.197	0.9599	0.9214
8.293	0.9499	0.9041
8.409	0.9374	0.8833
8.551	0.9220	0.8584
8.724	0.9030	0.8289
8.934	0.8792	0.7939
9.188	0.8486	0.7529
9.489	0.8081	0.7047
9.659	0.7839	0.6775
9.843	0.7580	0.6480
10.044	0.7287	0.6159
10.261	0.6924	0.5811
10.488	0.6487	0.5429
10.725	0.6019	0.5012
10.972	0.5473	0.4557
11.203	0.4698	0.4048
11.389	0.3866	0.3469
11.508	0.2964	0.2804
11.510	0.1880	0.2014
11.484	0.1659	0.1831
11.446	0.1432	0.1637
11.395	0.1195	0.1429
11.327	0.0961	0.1204
11.244	0.0740	0.0963
11.147	0.0518	0.0705
11.031	0.0295	0.0424
10.894	0.0076	0.0118

Table 20: Selected phase coexistence data predicted for perfluoroethane(1)-ethane(2) at 242.93 K by grand canonical histogram-reweighting Monte Carlo simulations with $k_{ij} = 0.045$.

P (bar)	x_1	y_1
7.719	0.9992	0.9977
7.822	0.9937	0.9818
7.925	0.9881	0.9665
8.038	0.9818	0.9498
8.115	0.9774	0.9386
8.210	0.9719	0.9251
8.327	0.9651	0.9088
8.471	0.9567	0.8893
8.648	0.9462	0.8660
8.866	0.9329	0.8384
9.133	0.9156	0.8060
9.458	0.8928	0.7680
9.852	0.8629	0.7237
10.079	0.8446	0.6990
10.327	0.8235	0.6723
10.598	0.7985	0.6436
10.893	0.7687	0.6126
11.209	0.7325	0.5792
11.543	0.6885	0.5430
11.889	0.6346	0.5038
12.227	0.5655	0.4611
12.519	0.4803	0.4135
12.684	0.3629	0.3559
12.489	0.2137	0.2716
12.376	0.1811	0.2494
12.225	0.1495	0.2245
12.031	0.1195	0.1965
11.790	0.0911	0.1648
11.499	0.0651	0.1290
11.162	0.0411	0.0885
10.776	0.0171	0.0418
10.687	0.0123	0.0313
10.495	0.0030	0.0084

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