Mie potentials for phase equilibria: Application to alkenes

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Table S1: Vapor-liquid coexistence data predicted by optimized Mie potentials. Maximum uncertainties are: ρ_{liq} = 0.5 kg/m^3, ρ_{vap}=0.1 kg/m^3, P^{sat}=0.1 bar, ΔH_v=0.1 kJ/mol.

T (K)	ρ_{liq} (kg/m^3)	ρ_{vap}(kg/m^3)	P (bar)	ΔH_v (kJ/mol)	Z
Ethene					
280.00	320.08	121.15	49.32	4.32	0.41
260.00	397.15	61.57	30.92	7.68	0.54
240.00	448.24	33.09	18.22	9.78	0.64
220.00	486.13	17.62	9.82	11.17	0.71
200.00	519.83	8.61	4.66	12.32	0.76
180.00	549.15	3.64	1.86	13.17	0.80
160.00	576.45	1.24	0.58	13.92	0.82
Propene					
360.00	344.57	124.52	43.52	6.01	0.41
340.00	416.46	70.66	29.92	9.86	0.52
320.00	465.13	42.49	19.81	12.42	0.61
300.00	502.24	25.88	12.47	14.24	0.68
280.00	533.43	15.23	7.34	15.68	0.72
260.00	562.09	8.44	3.97	16.90	0.76
240.00	587.50	4.27	1.92	17.91	0.79
220.00	613.27	1.89	0.80	18.87	0.81
1-Butene					
420.00	338.75	143.92	42.48	6.11	0.39
400.00	402.36	91.49	30.65	9.97	0.47
380.00	456.57	55.57	21.45	13.44	0.57
360.00	495.32	35.44	14.52	15.78	0.64
340.00	527.75	22.41	9.41	17.62	0.69
320.00	556.21	13.74	5.77	19.15	0.74
300.00	581.61	7.99	3.30	20.45	0.77
280.00	605.62	4.31	1.74	21.63	0.81
260.00	627.72	2.11	0.83	22.70	0.85
240.00	651.17	0.91	0.36	23.85	0.92
1-pentene					
460.00	380.49	117.65	32.54	9.36	0.42
440.00	434.82	73.96	23.73	13.41	0.51
420.00	478.30	47.59	16.92	16.61	0.59
400.00	512.64	31.46	11.70	18.95	0.65
380.00	541.65	20.58	7.78	20.83	0.70
360.00	567.99	13.09	4.94	22.45	0.73
340.00	592.13	7.97	2.95	23.88	0.76
320.00	614.05	4.58	1.64	25.11	0.79
300.00	636.26	2.43	0.83	26.30	0.80

T (K)	ρ_{liq} (kg/m^3)	ρ_{vap}(kg/m^3)	P (bar)	ΔH_v (kJ/mol)	Z
1-Hexene					
500.00	376.45	117.45	29.27	10.38	0.43
480.00	435.03	74.25	21.73	15.06	0.52
460.00	477.29	48.93	15.82	18.49	0.61
440.00	510.76	33.13	11.22	21.04	0.66
420.00	539.17	22.25	7.70	23.14	0.71
400.00	564.20	14.62	5.09	24.93	0.75
380.00	587.14	9.31	3.21	26.49	0.78
360.00	609.09	5.68	1.91	27.91	0.80
340.00	630.58	3.26	1.05	29.26	0.82
320.00	649.63	1.72	0.53	30.42	0.83
300.00	668.30	0.82	0.24	31.54	0.84
1-heptene					
540.00	297.56	103.22	28.50	10.39	0.50
520.00	352.83	72.48	21.72	14.95	0.57
500.00	394.91	48.40	16.12	18.99	0.65
480.00	426.35	32.99	11.69	22.11	0.73
460.00	452.28	22.52	8.24	24.61	0.78
440.00	474.65	15.16	5.62	26.71	0.83
420.00	494.35	9.96	3.58	28.50	0.86
400.00	512.28	6.33	2.30	30.07	0.89
380.00	530.32	3.83	1.36	31.59	0.92
360.00	547.04	2.18	0.75	32.96	0.93
340.00	563.57	1.15	0.38	34.20	0.95
320.00	592.29	0.55	0.17	35.46	0.95
1-octene					
560.00	384.72	109.55	22.95	13.04	0.42
540.00	436.11	70.38	17.26	18.24	0.51
520.00	477.12	47.00	12.77	22.30	0.59
500.00	509.69	32.42	9.23	25.30	0.64
480.00	536.62	22.27	6.48	27.73	0.68
460.00	560.37	15.04	4.41	29.81	0.71
440.00	582.46	9.89	2.88	31.68	0.74
420.00	603.84	6.26	1.79	33.42	0.77
400.00	623.36	3.79	1.06	34.97	0.78
380.00	642.06	2.16	0.58	36.43	0.79
360.00	660.48	1.15	0.29	37.83	0.79

T (K)	ρ_{liq} (kg/m^3)	ρ_{vap}(kg/m^3)	P (bar)	ΔH_v (kJ/mol)	Z
cis-2-butene					
440.00	332.81	155.25	47.68	5.72	0.39
420.00	390.84	106.18	35.15	9.18	0.44
400.00	448.86	64.80	25.14	12.95	0.54
380.00	489.94	41.82	17.48	15.53	0.62
360.00	523.57	27.16	11.69	17.49	0.67
340.00	551.94	17.25	7.46	19.07	0.71
320.00	577.65	10.55	4.48	20.41	0.75
300.00	602.56	6.09	2.49	21.62	0.77
280.00	625.64	3.25	1.25	22.66	0.77
260.00	645.95	1.56	0.54	23.49	0.75
trans-2-butene					
420.00	378.61	109.70	35.16	8.80	0.43
400.00	437.06	65.93	25.02	12.73	0.53
380.00	479.66	41.83	17.33	15.50	0.61
360.00	513.01	26.93	11.57	17.52	0.67
340.00	542.38	16.97	7.37	19.20	0.72
320.00	568.40	10.30	4.42	20.60	0.75
300.00	592.08	5.92	2.47	21.80	0.78
280.00	614.28	3.15	1.25	22.87	0.80
260.00	636.01	1.50	0.56	23.86	0.81
240.00	654.50	0.62	0.21	24.68	0.81
cis-2-pentene					
460.00	406.94	97.27	28.82	11.40	0.45
440.00	457.57	60.93	20.86	15.26	0.55
420.00	494.97	39.89	14.77	18.02	0.62
400.00	526.69	26.48	10.13	20.17	0.67
380.00	554.46	17.30	6.67	21.96	0.71
360.00	579.11	10.93	4.18	23.48	0.75
340.00	602.49	6.59	2.47	24.86	0.77
320.00	624.25	3.73	1.35	26.07	0.79
300.00	646.75	1.95	0.67	27.28	0.81
280.00	668.01	0.91	0.30	28.40	0.82
trans-2-pentene					
460.00	389.95	105.62	29.86	10.43	0.43
440.00	443.68	65.04	21.59	14.63	0.53
420.00	484.84	41.93	15.25	17.71	0.61
400.00	517.70	27.61	10.44	19.99	0.66
380.00	546.06	17.92	6.86	21.87	0.71
360.00	571.72	11.26	4.29	23.48	0.74
340.00	594.25	6.76	2.53	24.85	0.77
320.00	615.23	3.83	1.38	26.06	0.79
300.00	635.56	2.00	0.69	27.19	0.80
280.00	656.19	0.94	0.30	28.27	0.81

T (K)	ρ_{liq} (kg/m^3)	ρ_{vap}(kg/m^3)	P (bar)	ΔH_v (kJ/mol)	Z
1,3-butadiene					
420.00	319.69	156.97	49.08	5.07	0.42
400.00	382.85	111.39	36.01	8.32	0.45
380.00	449.55	67.03	25.32	12.14	0.56
360.00	494.35	41.94	17.24	14.79	0.64
340.00	530.18	26.44	11.26	16.77	0.70
320.00	561.57	16.25	6.97	18.40	0.75
300.00	588.78	9.56	4.04	19.74	0.79
280.00	614.62	5.26	2.14	20.92	0.82
260.00	638.68	2.63	1.02	21.97	0.83
240.00	660.65	1.15	0.42	22.90	0.85
1,5-hexadiene					
480.00	416.13	93.39	25.59	12.74	0.47
460.00	469.07	59.81	18.69	16.78	0.56
440.00	507.32	40.03	13.31	19.63	0.62
420.00	538.70	26.84	9.18	21.87	0.67
400.00	566.24	17.66	6.08	23.77	0.71
380.00	591.73	11.25	3.84	25.45	0.74
360.00	615.25	6.85	2.29	26.94	0.76
340.00	636.41	3.93	1.27	28.24	0.78
320.00	657.10	2.09	0.65	29.48	0.80
300.00	676.57	1.01	0.30	30.60	0.81

Table S2: Selected coexistence points for ethane(1)-propene(2) at 344.26 K.

P (bar)	x_{ethene}	y_{ethene}
32.14	0.0019	0.0033
32.98	0.0202	0.0329
34.98	0.0655	0.1005
37.34	0.1167	0.1711
39.19	0.1560	0.2196
41.66	0.2090	0.2798
43.20	0.2418	0.3154
45.00	0.2795	0.3547

Table S3: Selected coexistence mole fractions for ethane(1)-propene(2) at 310.93 K.

P (bar)	x_{ethene}	y_{ethene}
16.17	0.0155	0.0348
16.91	0.0404	0.0888
18.02	0.0765	0.1606
20.18	0.1469	0.2767
21.93	0.2019	0.3546
23.06	0.2371	0.3992
25.97	0.3296	0.5018
27.88	0.3873	0.5588
30.21	0.4536	0.6172
33.06	0.5321	0.6742
36.43	0.6246	0.7370
38.32	0.6770	0.7735
40.46	0.7314	0.8109
42.98	0.7854	0.8470
46.04	0.8430	0.8835
49.33	0.9096	0.9225

Table S4: Selected coexistence mole fractions for ethane(1)-propene(2) at 277.59 K.

P (bar)	x_{ethene}	y_{ethene}
6.90	0.0063	0.0191
8.13	0.0779	0.2067
9.58	0.1581	0.3660
11.69	0.2670	0.5255
13.94	0.3895	0.6466
16.32	0.5097	0.7430
18.36	0.6115	0.8086
20.92	0.7272	0.8744
22.42	0.7962	0.9079
24.11	0.8690	0.9422
26.02	0.9460	0.9767
27.27	0.9946	0.9975

Table S5: Selected coexistence data for butene(1)-hexene(2) at 373.6 K.

Optimized Mie Potentials			TraPPE		
P (Bar)	x_{butene}	y_{butene}	P (Bar)	x_{butene}	y_{butene}
2.74	0.00	0.00	3.74	0.0015	0.0067
3.33	0.0472	0.2083	4.62	0.0597	0.2225
4.04	0.1003	0.3691	5.64	0.1243	0.3889
5.69	0.2217	0.5904	6.62	0.1868	0.5003
7.18	0.3199	0.7046	8.36	0.2961	0.6384
8.54	0.4092	0.7737	10.57	0.4432	0.7517
9.78	0.4859	0.8200	11.84	0.5045	0.7997
12.71	0.6661	0.8988	14.09	0.6253	0.8637
15.27	0.8083	0.9467	16.63	0.7551	0.9167
16.81	0.8928	0.9701	17.86	0.8154	0.9381
17.98	0.9543	0.9870	20.76	0.9530	0.9845
18.91	0.9981	0.9995	21.84	0.9985	0.9995

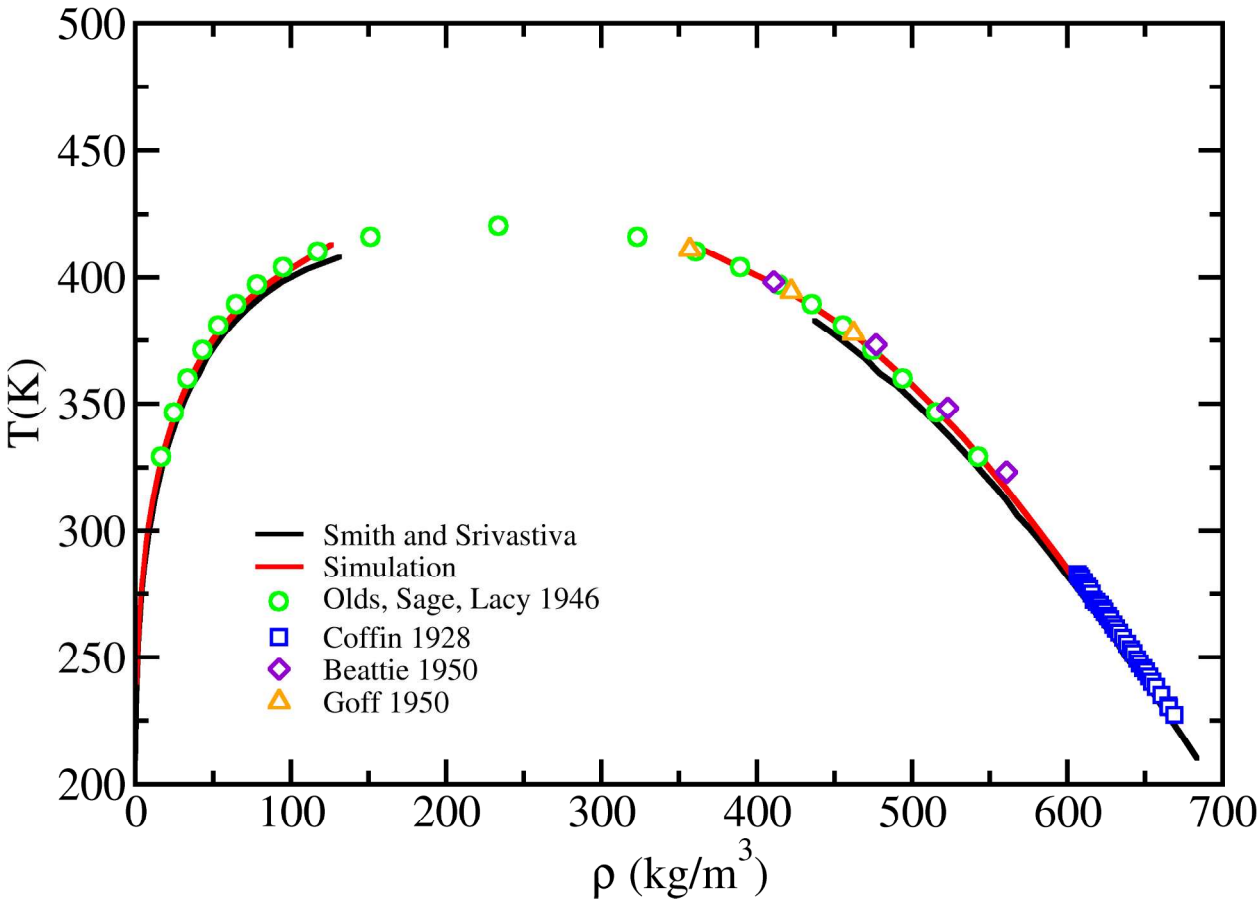

Figure S1: Comparison of experimental vapor-liquid coexistence data for 1-butene[1-5].

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