Supplement to: **Predicting vapor-liquid phase equilibria with augmented *ab initio* interatomic potentials**

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In this supplement, the numerical values are provided for the coexistence densities and saturated vapor pressures illustrated in Figs. 1 and 2.

Table S1. Vapor-liquid coexistence properties of argon calculated from molecular simulation using the *ab initio* two-body JHBV potential (Eq. (1)).

T, K	p, MPa	ρ vapor, kg/m^3	ρ liquid, kg/m^3
85.02	0.051 ± 0.017	2.87 ± 1.08	1507.51 ± 2.23
95.03	0.139 ± 0.019	7.01 ± 0.98	1442.86 ± 1.78
110.06	0.463 ± 0.039	20.26 ± 1.70	1355.23 ± 7.98
119.94	0.836 ± 0.068	33.57 ± 2.75	1289.27 ± 4.91
129.96	1.455 ± 0.064	50.19 ± 2.37	1206.21 ± 2.95
141.98	2.709 ± 0.141	133.36 ± 6.47	1098.24 ± 13.58
147.99	3.559 ± 0.174	186.11 ± 11.72	1016.90 ± 17.44
149.99	3.949 ± 0.153	224.68 ± 24.22	986.51 ± 18.14

Table S2. Vapor-liquid coexistence properties of argon calculated from molecular simulation using the *ab initio* two-body JHBV potential (Eq. (1)) combined with the effective MWS three-body potential (Eq. (9)).

T, K	p, MPa	ρ vapor, kg/m^3	ρ liquid, kg/m^3
85.02	0.054 ± 0.005	3.03 ± 0.27	1463.09 ± 2.96
95.03	0.144 ± 0.014	7.29 ± 0.72	1398.94 ± 4.25
110.06	0.485 ± 0.029	21.19 ± 1.29	1289.49 ± 6.41
119.94	0.887 ± 0.045	35.62 ± 1.82	1204.67 ± 6.71
129.96	1.105 ± 0.048	52.63 ± 1.84	1155.01 ± 9.45
141.98	1.851 ± 0.025	92.75 ± 0.88	1024.99 ± 6.58
147.99	2.904 ± 0.084	145.02 ± 8.22	896.95 ± 33.46
149.99	3.534 ± 0.102	193.38 ± 6.04	788.01 ± 51.28

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Table S3. Vapor-liquid coexistence properties of argon calculated from molecular simulation using the *ab initio* two-body JHBV potential (Eq. (1)) combined with the three-body dispersion term (Eq. (7)).

T, K	p, MPa	ρ vapor, kg/m^3	ρ liquid, kg/m^3
98.75	0.233 ± 0.033	14.79 ± 1.84	1335.91 ± 10.05
107.34	0.423 ± 0.036	17.22 ± 0.96	1285.93 ± 21.58
120.22	1.021 ± 0.083	36.71 ± 3.29	1171.51 ± 23.54
127.38	1.414 ± 0.062	66.42 ± 6.76	1114.13 ± 23.19
134.54	2.053 ± 0.107	96.03 ± 5.89	1012.91 ± 34.65
141.69	2.858 ± 0.139	155.27 ± 13.26	872.37 ± 35.08

Table S4. Vapor-liquid coexistence properties of argon calculated from molecular simulation using the *ab initio* two-body PS potential (Eq. (2)).

T, K	p, MPa	ρ vapor, kg/m^3	ρ liquid, kg/m^3
88.91	0.076 ± 0.015	4.08 ± 1.60	1478.63 ± 2.41
99.92	0.211 ± 0.034	10.46 ± 2.41	1414.45 ± 3.60
114.90	0.628 ± 0.036	26.33 ± 1.97	1318.06 ± 9.50
129.79	1.378 ± 0.049	59.33 ± 3.60	1203.03 ± 17.60
139.80	2.353 ± 0.076	99.68 ± 15.60	1110.59 ± 19.60
143.80	2.968 ± 0.082	145.88 ± 21.00	1061.93 ± 21.60
147.80	3.423 ± 0.125	191.21 ± 24.00	1023.40 ± 26.23

Table S5. Vapor-liquid coexistence properties of argon calculated from molecular simulation using the *ab initio* two-body PS potential (Eq. (2)) combined with the effective MWS three-body potential (Eq. (9)).

T, K	p, MPa	ρ vapor, kg/m^3	ρ liquid, kg/m^3
88.91	0.077 ± 0.008	4.15 ± 1.06	1425.00 ± 3.59
99.92	0.232 ± 0.016	11.18 ± 2.05	1363.63 ± 9.95
114.90	0.673 ± 0.051	28.24 ± 4.51	1251.15 ± 16.64
129.79	1.387 ± 0.055	65.54 ± 7.81	1104.58 ± 18.00
139.80	2.384 ± 0.142	109.63 ± 14.00	926.41 ± 23.15
144.80	3.102 ± 0.214	182.80 ± 19.00	832.78 ± 26.00

Table S6. Vapor-liquid coexistence properties of argon calculated from molecular simulation using the *ab initio* two-body PS potential (Eq. (2)) combined with the three-body dispersion term (Eq. (7)).

T, K	p, MPa	ρ vapor, kg/m^3	ρ liquid, kg/m^3
98.63	0.193 ± 0.011	7.60 ± 1.06	1310.56 ± 12.36
107.21	0.384 ± 0.024	18.91 ± 2.35	1278.25 ± 18.99
120.07	0.969 ± 0.061	46.52 ± 5.61	1217.60 ± 22.41
127.22	1.306 ± 0.092	65.52 ± 4.36	1091.97 ± 24.66
134.37	1.898 ± 0.170	89.15 ± 8.36	1029.13 ± 29.50
141.51	2.436 ± 0.228	127.07 ± 12.56	942.44 ± 42.57

Table S7. Vapor-liquid coexistence properties of argon calculated from molecular simulation using the empirical two-body BFW potential (Eq. (4)). Results taken from Ref. 48.

T, K	p, MPa	ρ vapor, kg/m^3	ρ liquid, kg/m^3
99.47	0.207 ± 0.052	10.49 ± 1.75	1408.89 ± 6.99
106.57	0.310 ± 0.052	13.98 ± 1.75	1365.19 ± 5.24
117.23	0.775 ± 0.103	36.71 ± 3.50	1295.27 ± 6.99
120.78	0.879 ± 0.155	40.20 ± 3.50	1270.80 ± 8.74
124.33	1.137 ± 0.155	52.44 ± 3.50	1242.83 ± 8.74
127.89	1.292 ± 0.155	57.68 ± 5.24	1216.61 ± 8.74
131.44	1.603 ± 0.155	71.67 ± 3.50	1185.15 ± 5.24
134.99	1.913 ± 0.362	85.65 ± 8.74	1155.43 ± 17.48
138.54	2.171 ± 0.310	99.64 ± 8.74	1125.72 ± 10.49
142.10	2.636 ± 0.620	127.60 ± 12.24	1087.26 ± 12.24
145.65	2.998 ± 0.569	143.34 ± 10.49	1043.56 ± 13.98
149.20	3.567 ± 0.672	181.79 ± 12.24	1003.35 ± 15.73
152.75	3.877 ± 0.982	195.78 ± 17.48	943.92 ± 20.98

Table S8. Vapor-liquid coexistence properties of argon calculated from molecular simulation using the empirical two-body BFW potential (Eq. (4)) combined with the effective MWS three-body potential (Eq. (9)).

T, K	p, MPa	ρ vapor, kg/m^3	ρ liquid, kg/m^3
83.81	0.037 ± 0.006	2.13 ± 3.76	1461.15 ± 2.53
94.95	0.107 ± 0.012	5.40 ± 7.38	1388.88 ± 4.55
105.99	0.298 ± 0.024	13.50 ± 3.74	1324.91 ± 9.81
117.02	0.613 ± 0.067	25.14 ± 9.98	1236.60 ± 17.85
128.06	1.210 ± 0.096	41.00 ± 12.44	1140.00 ± 22.68
139.09	1.997 ± 0.103	62.22 ± 15.24	992.57 ± 25.35

Table S9. Vapor-liquid coexistence properties of argon calculated from molecular simulation using the empirical two-body BFW potential (Eq. (4)) combined with the three-body dispersion term (Eq. (7)). Results taken from Ref. 48.

T, K	p, MPa	ρ vapor, kg/m^3	ρ liquid, kg/m^3
106.57	0.346 ± 0.083	16.61 ± 2.97	1297.02 ± 8.74
117.23	0.662 ± 0.088	30.42 ± 2.62	1197.38 ± 13.98
120.78	0.837 ± 0.109	38.11 ± 3.15	1172.91 ± 17.48
124.33	1.117 ± 0.238	51.57 ± 6.47	1150.19 ± 17.48
127.89	1.339 ± 0.331	61.18 ± 8.39	1116.97 ± 19.23
131.44	1.556 ± 0.264	70.09 ± 6.64	1071.53 ± 19.23
134.99	2.006 ± 0.429	93.69 ± 9.79	1048.80 ± 17.48
138.54	2.275 ± 0.429	105.75 ± 9.09	985.87 ± 19.23
142.10	2.533 ± 0.289	114.49 ± 5.59	896.73 ± 52.44

Table S10. Vapor-liquid coexistence properties of krypton calculated from molecular simulation using the *ab initio* two-body JHBV2 potential (Eq. (5)).

T, K	p, MPa	ρ vapor, kg/m^3	ρ liquid, kg/m^3
115.91	0.053 ± 0.009	4.61 ± 1.71	2616.07 ± 8.38
123.58	0.085 ± 0.012	8.73 ± 1.92	2574.17 ± 4.70
131.00	0.140 ± 0.023	10.79 ± 2.22	2515.66 ± 6.41
137.64	0.224 ± 0.029	16.43 ± 1.59	2475.37 ± 3.97
146.00	0.346 ± 0.034	23.95 ± 2.83	2405.97 ± 4.48
153.07	0.505 ± 0.025	33.28 ± 2.23	2353.19 ± 2.29
160.10	0.685 ± 0.047	43.17 ± 1.90	2292.54 ± 4.39
166.53	0.851 ± 0.040	51.64 ± 2.44	2210.54 ± 6.10
176.00	1.278 ± 0.036	73.37 ± 3.13	2141.22 ± 7.52
182.62	1.587 ± 0.047	87.87 ± 3.45	2074.77 ± 7.06
189.02	2.163 ± 0.061	98.23 ± 8.64	1994.79 ± 6.67
192.64	2.500 ± 0.062	147.30 ± 13.45	1950.50 ± 12.27
197.66	2.935 ± 0.068	191.50 ± 18.64	1883.73 ± 10.85
201.08	3.536 ± 0.079	245.49 ± 28.61	1870.03 ± 17.80
204.09	3.839 ± 0.087	301.39 ± 33.19	1833.04 ± 18.97
206.90	4.376 ± 0.115	352.70 ± 34.37	1790.28 ± 33.19
209.91	4.537 ± 0.137	390.85 ± 47.72	1726.79 ± 47.72
212.93	4.963 ± 0.148	466.26 ± 28.06	1684.60 ± 28.06

Table S11. Vapor-liquid coexistence properties of krypton calculated from molecular simulation using the *ab initio* two-body JHBV2 potential (Eq. (5)) combined with the effective MWS three-body potential (Eq. (9)).

T, K	p, MPa	ρ vapor, kg/m^3	ρ liquid, kg/m^3
115.91	0.044 ± 0.007	3.87 ± 2.20	2572.89 ± 11.47
123.58	0.077 ± 0.015	6.26 ± 2.59	2499.05 ± 12.24
137.64	0.199 ± 0.017	14.57 ± 3.57	2385.24 ± 16.42
145.54	0.323 ± 0.009	29.81 ± 4.02	2333.34 ± 17.94
153.07	0.507 ± 0.044	33.42 ± 4.90	2281.95 ± 18.19
160.10	0.629 ± 0.037	39.63 ± 5.93	2208.20 ± 21.30
166.53	0.860 ± 0.037	52.13 ± 6.02	2145.02 ± 25.83
182.60	1.535 ± 0.039	84.86 ± 6.73	1963.75 ± 25.43
189.02	2.072 ± 0.078	130.16 ± 7.36	1863.64 ± 25.70
192.64	2.565 ± 0.050	155.13 ± 8.65	1807.05 ± 27.67
198.06	2.858 ± 0.028	199.49 ± 8.38	1734.45 ± 28.25
201.08	3.479 ± 0.085	242.10 ± 10.15	1689.05 ± 32.29
204.09	3.762 ± 0.064	286.57 ± 15.28	1633.14 ± 38.21
206.90	4.040 ± 0.076	310.76 ± 20.34	1538.72 ± 46.16
208.91	4.251 ± 0.093	331.71 ± 24.13	1397.22 ± 99.33

Table S12. Vapor-liquid coexistence properties of krypton calculated from molecular simulation using the *ab initio* two-body JHBV2 potential (Eq. (5)) combined with the three-body dispersion term (Eq. (7)).

T, K	p, MPa	ρ vapor, kg/m^3	ρ liquid, kg/m^3
115.91	0.059 ± 0.004	5.90 ± 2.93	2452.20 ± 18.19
137.60	0.240 ± 0.028	18.73 ± 2.33	2288.59 ± 25.83
153.07	0.555 ± 0.055	41.41 ± 2.26	2195.97 ± 25.43
160.10	0.637 ± 0.069	44.02 ± 2.14	2091.76 ± 17.94
166.53	0.637 ± 0.068	74.79 ± 4.16	2061.39 ± 12.24
175.97	1.015 ± 0.068	106.74 ± 5.73	1919.01 ± 16.42
182.60	1.431 ± 0.038	151.65 ± 9.33	1861.63 ± 19.89
192.64	2.020 ± 0.047	230.16 ± 10.12	1640.49 ± 28.16
197.66	2.344 ± 0.061	296.06 ± 15.24	1577.39 ± 25.62
206.90	3.438 ± 0.216	485.31 ± 20.28	1216.43 ± 32.19

Table S13. Vapor-liquid coexistence properties of krypton calculated from molecular simulation using the empirical two-body Barker potential (Eq. (6)). Results taken from Ref. 48.

T, K	p, MPa	ρ vapor, kg/m^3	ρ liquid, kg/m^3
141.33	0.306 ± 0.061	21.35 ± 6.10	2440.53 ± 12.20
151.43	0.428 ± 0.061	30.51 ± 3.05	2361.21 ± 9.15
166.57	1.039 ± 0.122	73.22 ± 6.10	2242.24 ± 15.25
171.62	1.161 ± 0.122	79.32 ± 6.10	2190.37 ± 12.20
176.66	1.406 ± 0.244	94.57 ± 12.20	2135.46 ± 15.25
181.71	1.833 ± 0.244	125.08 ± 12.20	2095.80 ± 15.25
186.76	2.078 ± 0.611	244.05 ± 21.35	2031.74 ± 21.35
191.81	2.506 ± 0.306	179.99 ± 9.15	1973.78 ± 9.15
196.85	2.872 ± 0.428	204.39 ± 15.25	1903.61 ± 27.46
201.90	3.606 ± 0.428	265.41 ± 12.20	1857.85 ± 18.30
206.95	3.972 ± 1.222	298.96 ± 36.61	1748.03 ± 51.86
212.00	4.889 ± 2.017	399.64 ± 54.91	1671.76 ± 54.91
215.02	5.011 ± 2.017	430.14 ± 48.81	1616.85 ± 70.17

Table S14. Vapor-liquid coexistence properties of krypton calculated from molecular simulation using the empirical two-body Barker potential (Eq. (6)) combined with the effective MWS three-body potential (Eq. (9)).

T, K	p, MPa	ρ vapor, kg/m^3	ρ liquid, kg/m^3
115.77	0.042 ± 0.005	3.64 ± 0.63	2564.79 ± 4.33
132.31	0.128 ± 0.008	9.73 ± 0.58	2425.87 ± 4.86
148.84	0.351 ± 0.007	23.73 ± 1.81	2289.16 ± 8.52
165.38	0.763 ± 0.006	46.41 ± 3.45	2097.52 ± 9.58
181.92	1.506 ± 0.005	83.19 ± 2.60	1905.70 ± 11.44

Table S15. Vapor-liquid coexistence properties of krypton calculated from molecular simulation using the empirical two-body Barker potential (Eq. (6)) combined with the three-body dispersion term (Eq. (7)). Results taken from Ref. 48.

T, K	p, MPa	ρ vapor, kg/m^3	ρ liquid, kg/m^3
151.43	0.452 ± 0.073	32.03 ± 3.66	2172.07 ± 18.30
166.57	0.904 ± 0.110	61.93 ± 4.58	2046.99 ± 27.46
171.62	1.118 ± 0.153	75.05 ± 6.10	1958.52 ± 27.46
176.66	1.546 ± 0.306	106.16 ± 11.29	1924.97 ± 24.41
181.71	1.931 ± 0.153	130.87 ± 5.19	1879.21 ± 21.35
186.76	2.139 ± 0.275	145.52 ± 9.46	1784.64 ± 42.71
191.81	2.499 ± 0.281	176.33 ± 10.07	1610.75 ± 70.17
196.85	3.098 ± 0.636	224.83 ± 18.61	1552.79 ± 70.17