Second Virial Coefficients of the Lennard-Jones (6,*m*) Gases

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THE three-parameter Lennard-Jones (6, m) potential is used to calculate the second virial coefficient of gases. The reduced second virial coefficient for the Lennard-Jones (6, m) potential is given as follows (*11, 17*):

$$B^*(T) = -\left(\frac{3}{m}\right)\sum_{j=0}^{\infty}\frac{1}{(j!)}\cdot\left(\frac{T^*}{4}\right)^{\frac{(6-m)j-3}{m}}\cdot\Gamma\left(\frac{6j-3}{m}\right)$$

where $B^* = B/(2/3\ \pi\ N\sigma^3)$, $T^* = KT/\epsilon$, and N is Avogadro's

Table I. The Second Virial Coefficient for the Lennard-Jones (6-m) Potentials

	m							
T*	8	9	10	11	12	13	14	15
0.30	−6.83576	−10.93724	−15.69024	−21.28756	−27.88056	−35.59537	−44.53981	−51.80645
0.35	−5.33515	−8.26889	−11.42748	−14.90386	−18.75487	−23.01717	−27.71469	−32.86254
0.40	−4.32369	−6.57009	−8.86150	−11.26025	−13.79881	−16.49409	−19.35410	−22.38142
0.45	−3.59715	−5.39891	−7.16276	−8.93961	−10.75496	−12.62139	−14.54459	−16.52623
0.50	−3.05076	−4.54475	−5.96098	−7.34506	−8.72019	−10.09837	−11.48566	−12.88476
0.55	−2.62534	−3.89528	−5.06845	−6.18730	−7.27408	−8.34090	−9.39453	−10.43875
0.60	−2.28502	−3.38535	−4.38065	−5.31099	−6.19796	−7.05386	−7.88596	−8.69876
0.65	−2.00681	−2.97470	−3.83505	−4.62588	−5.36819	−6.07424	−6.75164	−7.40531
0.70	−1.77528	−2.63715	−3.39209	−4.07627	−4.71003	−5.30551	−5.87043	−6.40992
0.75	−1.57973	−2.35493	−3.02554	−3.62600	−4.17592	−4.68723	−5.16762	−5.62230
0.80	−1.41248	−2.11559	−2.71738	−3.25063	−3.73422	−4.17978	−4.59488	−4.98473
0.85	−1.26787	−1.91015	−2.45482	−2.93308	−3.36311	−3.75618	−4.11969	−4.45876
0.90	−1.14168	−1.73195	−2.22851	−2.66108	−3.04711	−3.39748	−3.71941	−4.01790
0.95	−1.03065	−1.57598	−2.03152	−2.42558	−2.77490	−3.09000	−3.37785	−3.64331
1.00	−0.93325	−1.43836	−1.85854	−2.21976	−2.53808	−2.82361	−3.08311	−3.32130
1.50	−0.34453	−.62696	−0.85347	−1.04121	−1.20088	−1.33937	−1.46135	−1.57006
2.00	−0.07713	−.26174	−0.40808	−0.52757	−0.62762	−0.71310	−0.78731	−0.85758
2.50	−0.07198	−.05772	−0.16030	−.24350	−0.31261	−0.37118	−0.42162	−0.50453
3.00	0.16507	0.07055	−0.00442	−0.06507	−0.11523	−0.15754	−0.19380	−0.22531
3.50	0.22750	0.15746	0.10153	0.05629	0.01895	−0.01243	−0.03925	−0.06248
4.00	0.27146	0.21946	0.17748	0.14346	0.11541	0.09188	0.07181	0.05448
4.50	0.30355	0.26539	0.23408	0.20861	0.18761	0.17002	0.15505	0.14215
5.00	0.32759	0.30038	0.27751	0.25878	0.24334	0.23041	0.21944	0.21000
5.50	0.34596	0.32764	0.31161	0.29835	0.28739	0.27824	0.27048	0.26383
6.00	0.36022	0.34924	0.33888	0.33014	0.32290	0.31686	0.31176	0.30741
7.00	0.38027	0.38073	0.37920	0.37752	0.37608	0.37491	0.37396	0.37320
8.00	0.39294	0.40189	0.40693	0.41053	0.41343	0.41590	0.41806	0.41999
9.00	0.40101	0.41649	0.42662	0.43432	0.44059	0.44590	0.45049	0.45453
10.0	0.40608	0.42672	0.44091	0.45189	0.46087	0.46846	0.47501	0.48075
20.0	0.40307	0.44589	0.47806	0.50388	0.52537	0.54366	0.55948	0.57334
30.0	0.38318	0.43238	0.47023	0.50104	0.52692	0.54911	0.56841	0.58540
40.0	0.36488	0.41672	0.45717	0.49043	0.51857	0.54283	0.56404	0.58277
50.0	0.34927	0.40232	0.44418	0.47885	0.50836	0.53392	0.55634	0.57622
60.0	0.33596	0.38957	0.43223	0.46780	0.49821	0.52466	0.54794	0.56863
70.0	0.32447	0.37829	0.42144	0.45760	0.48865	0.51574	0.53966	0.56097
80.0	0.31443	0.36828	0.41171	0.44827	0.47978	0.50737	0.53178	0.55357
90.0	0.30556	0.35931	0.40290	0.43975	0.47161	0.49957	0.52437	0.54656
100.0	0.29764	0.35121	0.39488	0.43193	0.46406	0.49233	0.51745	0.53996

	m							
T*	16	17	18	19	20	22	24	26
0.30	−66.47425	−79.60976	−94.26790	−110.49259	−128.31806	−168.86108	−215.99577	−269.70712
0.35	−38.46922	−44.53815	−51.06864	−58.05673	−65.49581	−81.68986	−99.56145	−119.00339
0.40	−25.57506	−28.93174	−32.44653	−36.11341	−39.92568	−47.95720	−56.48108	−65.43674
0.45	−18.56564	−20.66071	−22.80848	−25.00547	−27.24796	−31.85398	−36.59610	−41.44545
0.50	−14.29650	−15.72056	−17.15594	−18.60130	−20.05509	−22.98139	−25.92190	−28.86459
0.55	−11.47557	−12.50599	−13.53037	−14.54871	−15.56078	−17.56468	−19.53878	−21.47979
0.60	−9.49509	−10.27680	−11.04506	−11.80070	−12.54424	−13.99646	−15.40371	−16.76721
0.65	−8.03858	−8.65376	−9.25257	−9.83625	−10.40580	−11.50544	−12.55632	−13.56199
0.70	−6.92759	−7.42603	−7.90722	−8.37266	−8.82358	−9.68568	−10.49983	−11.27076
0.75	−6.05499	−6.46844	−6.86475	−7.24555	−7.61220	−8.30728	−8.95698	−9.56661

(*Continued on page 78*)

Table I. The Second Virial Coefficient for the Lennard-Jones (6-m) Potentials (Continued)

	m							
T*	16	17	18	19	20	22	24	26
0.80	−5.35306	−5.70268	−6.03573	−6.35391	−6.65862	−7.23202	−7.76323	−8.25771
0.85	−4.77711	−5.07752	−5.36214	−5.63268	−5.89054	−6.37265	−6.81579	−7.22542
0.90	−4.29658	−4.55820	−4.80489	−5.03832	−5.25988	−5.67177	−6.04774	−6.39313
0.95	−3.88994	−4.12041	−4.33679	−4.54073	−4.73358	−5.09027	−5.41384	−5.70947
1.00	−3.54160	−3.74662	−3.93838	−4.11847	−4.28819	−4.60069	−4.88260	−5.13890
1.50	−1.66797	−1.75679	−1.83793	−1.91247	−1.98130	−2.10452	−2.21194	−2.30668
2.00	−0.91059	−0.96262	−1.00963	−1.05237	−1.09146	−1.16052	−1.21977	−1.27128
2.50	−0.50453	−0.53915	−0.57024	−0.59835	−0.62392	−0.66875	−0.70687	−0.73974
3.00	−0.25300	−0.27756	−0.29953	−0.31932	−0.33725	−0.36856	−0.39502	−0.41773
3.50	−0.08283	−0.10083	−0.11689	−0.13131	−0.14435	−0.16705	−0.18616	−0.20249
4.00	0.03934	0.02597	0.01407	0.00340	−0.00622	−0.02293	−0.03696	−0.04892
4.50	0.13090	0.12099	0.11219	0.10431	0.09721	0.08491	−0.07461	0.06585
5.00	0.20179	0.19457	0.18817	0.18245	0.17730	0.16841	0.16098	0.15468
5.50	0.25806	0.25300	0.24853	0.24454	0.24096	0.23479	0.22965	0.22530
6.00	0.30366	0.30038	0.29749	0.29493	0.29263	0.28869	0.28543	0.28268
7.00	0.37259	0.37208	0.37167	0.37132	0.37102	0.37056	0.37020	0.36993
8.00	0.42173	0.42330	0.42473	0.42604	0.42725	0.42938	0.43120	0.43278
9.00	0.45810	0.46131	0.46419	0.46680	0.46918	0.47335	0.47689	0.47992
10.0	0.48581	0.49033	0.49439	0.49806	0.50139	0.50722	0.51215	0.51637
20.0	0.58559	0.59652	0.60634	0.61520	0.62325	0.63732	0.64923	0.65943
30.0	0.60048	0.61397	0.62613	0.63713	0.64715	0.66473	0.67964	0.69246
40.0	0.59946	0.61444	0.62796	0.64024	0.65144	0.67113	0.68789	0.70234
50.0	0.59398	0.60995	0.62441	0.63756	0.64957	0.67074	0.68881	0.70442
60.0	0.58716	0.60387	0.61902	0.63281	0.64544	0.66773	0.68679	0.70329
70.0	0.58009	0.59736	0.61304	0.62735	0.64046	0.66364	0.68350	0.70072
80.0	0.57316	0.59089	0.60700	0.62172	0.63522	0.65914	0.67966	0.69748
90.0	0.56654	0.58463	0.60111	0.61617	0.63001	0.65453	0.67562	0.69395
100.0	0.56026	0.57867	0.59545	0.61081	0.62492	0.64998	0.67155	0.69032

	m							
T*	28	30	35	40	60	80	100	150
0.30	−329.88847	−396.36114	−588.43736	−813.75123	−1947.5184	−3259.0126	−4587.2760	−7592.7558
0.35	−139.89842	−162.12466	−222.71645	−289.05247	−583.60598	−883.61158	−1163.6472	−1745.1426
0.40	−74.76563	−84.41254	−109.59509	−135.77281	−241.75839	−339.81038	−425.90159	−593.63918
0.45	−46.37570	−51.36336	−63.95394	−76.52519	−123.94014	−164.63261	−198.70244	−261.90830
0.50	−31.79891	−34.71579	−41.88520	−48.81678	−73.53588	−93.51101	−109.61276	−138.34755
0.55	−23.38485	−25.25168	−29.74161	−33.96993	−48.37995	−59.46465	−68.12801	−83.11002
0.60	−18.08794	−19.36687	−22.38798	−25.17153	−34.30918	−41.05572	−46.19503	−54.85520
0.65	−14.52537	−15.44893	−17.59780	−19.54151	−25.72499	−30.13497	−33.42259	−38.84345
0.70	−12.00228	−12.69760	−14.29462	−15.71660	−20.12124	−23.17092	−25.40299	−29.01612
0.75	−10.14036	−10.68168	−11.91126	−12.99127	−16.26084	−18.46748	−20.05708	−22.58986
0.80	−8.71978	−9.15293	−10.12733	−10.97311	−13.48317	−15.13985	−16.31697	−18.16695
0.85	−7.60581	−7.96038	−8.75124	−9.43060	−11.41197	−12.69436	−13.59458	−14.99252
0.90	−6.71209	−7.00791	−7.66281	−8.22022	−9.82113	−10.83948	−11.54676	−12.63357
0.95	−5.98112	−6.23195	−6.78354	−7.24919	−8.56846	−9.39481	−9.96333	−10.82877
1.00	−5.37338	−5.58902	−6.06039	−6.45541	−7.56103	−8.24404	−8.71002	−9.41344
1.50	−2.39101	−2.46668	−2.62613	−2.75384	−3.08570	−3.27407	−3.39605	−3.57116
2.00	−1.31655	−1.35670	−1.43986	−1.50507	−1.66882	−1.75814	−1.81467	−1.89389
2.50	−0.76842	−0.79370	−0.84555	−0.88573	−0.98471	−1.03753	−1.07051	−1.11618
3.00	−0.43746	−0.45477	−0.49007	−0.51722	−0.58333	−0.61814	−0.63969	−0.66931
3.50	−0.21664	−0.22902	−0.25417	−0.27342	−0.31992	−0.34419	−0.35914	−0.37959
4.00	−0.05926	−0.06829	−0.08657	−0.10051	−0.13402	−0.15140	−0.16207	−0.17662
4.50	0.05829	0.05170	0.03839	0.02827	0.00403	−0.00847	−0.01614	−0.02657
5.00	0.14925	0.14452	0.13499	0.12776	0.11051	0.10163	0.09619	0.08881
5.50	0.22156	0.21831	0.21178	0.20683	0.19505	0.18900	0.18531	0.18029
6.00	0.28032	0.27828	0.27418	0.27108	0.26375	0.25998	0.25769	0.25456
7.00	0.36971	0.36953	0.36920	0.36897	0.36845	0.36818	0.36802	0.36778
8.00	0.43416	0.43538	0.43786	0.43976	0.44431	0.44664	0.44805	0.44994
9.00	0.48256	0.48497	0.48955	0.49312	0.50161	0.50602	0.50866	0.51223
10.0	0.52002	0.52322	0.52971	0.53465	0.54642	0.55244	0.55610	0.56103
20.0	0.66827	0.67601	0.69172	0.70370	0.73239	0.74712	0.75610	0.76823
30.0	0.70361	0.71338	0.73328	0.74852	0.78518	0.80412	0.81569	0.83137
40.0	0.71493	0.72599	0.74856	0.76590	0.80780	0.82955	0.84288	0.86096
50.0	0.71804	0.73003	0.75455	0.77343	0.81923	0.84310	0.85774	0.87766
60.0	0.71771	0.73043	0.75647	0.77657	0.82546	0.85103	0.86674	0.88814
70.0	0.71579	0.72909	0.75637	0.77747	0.82893	0.85591	0.87252	0.89517
80.0	0.71309	0.72688	0.75521	0.77715	0.83081	0.85900	0.87638	0.90013
90.0	0.71002	0.72423	0.75347	0.77614	0.83170	0.86096	0.87901	0.90369
100.0	0.70679	0.72137	0.75140	0.77472	0.83197	0.86217	0.88082	0.90635

Table II. Potential Parameters Determined from Second Virial Coefficients for the Lennard-Jones (6-m) Potential Functions

b_0 = [cc./mole]

Gas	Force Constants for the Lennard-Jones (6-m) Potentials				Force Constants for the Lennard-Jones (6–12) Potential			Temp. Ranges
	m	$\frac{\epsilon}{K}$ °K.	σ, A	$b_0 = \frac{2}{3}\pi N\sigma^3$	$\frac{\epsilon}{K}$ °K.	σ A	$b_0 = \frac{2}{3}\pi N\sigma^3$	T, °K.
A	16	103.5	3.41	50.1	119.7	3.43	51.3	133.2–673.2
CO_2	12	190.5	4.44	110.9	...	...	...	273.2–510.9
CH_4	12	146.2	3.87	73.3	...	...	...	108.6–477.6
C_2H_6	30	164.1	4.52	115.3	215.5	4.88	147.2	191.9–510.9
C_3H_8	40	190.5	5.02	158.5	240.4	5.71	233.3	244–570.5
n-C_4H_{10}	40	421.7	3.38	48.42	770.9	3.39	48.98	244–573.2

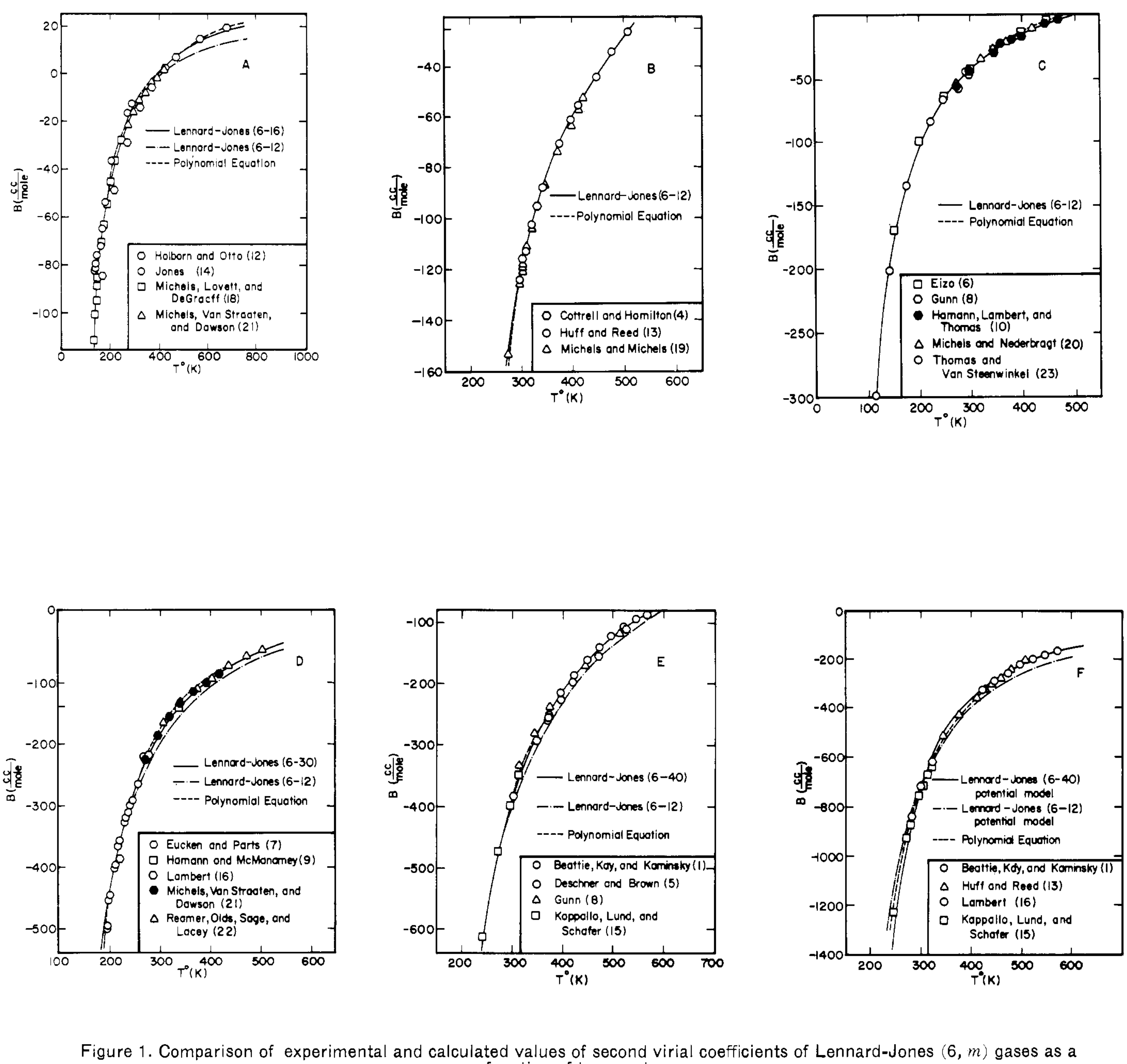

Figure 1. Comparison of experimental and calculated values of second virial coefficients of Lennard-Jones (6, m) gases as a function of temperature

A. Argon
B. Carbon dioxide
C. Methane
D. Ethane
E. Propane
F. n-Butane

Table III. Constants of Empirical Equations for Second Virial Coefficients

$B(T) = a_0 + a_1T^1 + \ldots\ldots a_nT_n \quad B(T) = [cc/mole];\ T = [°K.]$

Gas	$a_1 10^{-3}$	$a_2 10^{-1}$	$a_2 10$	$a_3 10^3$	$a_4 10^6$	$a_5 10^9$	$a_6 10^{11}$	$a_7 10^{14}$	$a_8 10^{17}$	Data Source	Mean Dev. 0/0	Max. Dev. 0/0
A	−3.97608	10.0484	−0.112481	7.08665	−27.2092	64.9270	−9.38577	7.50948	−2.54611	(12) (14) (18)	0.98	2.40
CO_2	−3.09046	2.69846	−0.923568	1427.36	−0.0829279	...	...	...	...	(4) (13) (19)	1.13	2.44
CH_4	+0.786618	−4.42534	6.32889	−4.36795	16.8230	−37.0016	4.35439	−2.12653	...	(6) (8) (10) (20) (23) (24)	1.10	2.94
C_2H_6	−15.5491	28.636	−23.7155	11.0419	−30.7553	50.9059	−4.62263	1.77474	...	(7) (9) (16) (21) (24)	0.82	2.67
C_3H_8	−8.79907	8.76505	−3.69862	0.793069	−0.849993	0.361841	...	...	...	(1) (5) (8) (15)	1.51	3.50
$n\text{-}C_4H_{10}$	−12.600	10.6422	−3.77283	0.67577	−0.59709	0.205589	...	...	...	(3) (13) (15) (16)	1.02	3.96

number, σ, ϵ, and m are the characteristics of the potential. The above equation was used for the calculation of the second virial coefficients of gases with the values of $m = 8(1)\ 20(2)30(5)\ 40(20)100(50)150$ and $T^* = 0.30\ (0.05)1.0(0.5)5.0(1.0)10(10)\ 100$. (The numbers in the parentheses between two numbers are the interval for the tabulation.) The tabulated data are reported to five decimal places in Table I.

The three potential parameters; m, ϵ/K, and σ for six gases; argon, carbon dioxide, methane, ethane, propane, and n-butane have been determined by Buckingham's translational method (*2*). The potential parameters, thus determined, are listed in Table II. Comparisons of the second virial coefficients for the six gases calculated by the Lennard-Jones (6, m) and (6, 12) potentials, with the most probable values calculated by a polynomial obtained by a least-square curve fitting of experimental data as in Table III, and the experimental data points are given in Figure 1.

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