

Title: Interpreting gas-saturation vapor pressure measurements using virial coefficients derived from molecular models

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Pure and mixture virial coefficients using Mayer sampling Monte Carlo method unless noted otherwise

B2 of He (single sphere Lennard-Jones model, direct quadrature method)

T(K)	B2(cm ³ /mol)
200.00	12.2694210494
220.00	12.1856438145
240.00	12.0975331179
260.00	12.0076978367
280.00	11.9177582369

300.00 11.828725924
320.00 11.7412283502
323.15 11.7276148732
340.00 11.6556457938
360.00 11.5721972047
380.00 11.4909952293
400.00 11.4120821484
420.00 11.3354537181
440.00 11.2610751871

B3 of He (single sphere Lennard-Jones model, Fast Fourier transforms)

T(K) B3(cm³/mol)²
200.00 113.678622755
220.00 110.1310124121
240.00 106.9138461237
260.00 103.9785925709
280.00 101.2860303743
300.00 98.8041218585
320.00 96.5064320105
323.15 96.1598420693
340.00 94.3709428299
360.00 92.3791552187
380.00 90.5154014881
400.00 88.7663135636
420.00 87.1204074488
440.00 85.5677553901

B2 of CO2 (TraPPE)

T(K)	B2(cm ³ /mol)	Uncertainty(cm ³ /mol)
200.00	-275.9446664865	0.0296837366
220.00	-222.2739515368	0.0233171289
240.00	-183.0512793324	0.0193943060
260.00	-153.1459245660	0.0165078937
280.00	-129.6941489535	0.0141713029
300.00	-110.8408788864	0.0127645307
320.00	-95.3153915875	0.0115059031
323.15	-93.1365037327	0.0114583282
340.00	-82.3717871620	0.0105899355
360.00	-71.4038654362	0.0097076918
380.00	-61.9847655453	0.0091548592
400.00	-53.8306206754	0.0086273196
420.00	-46.7052247024	0.0082135985
440.00	-40.4195576092	0.0076360752
460.00	-34.8315316587	0.0074536043
480.00	-29.8406786532	0.0070212145
500.00	-25.3600375674	0.0068670477

B3 of CO2 (TraPPE)

T(K)	B3(cm ³ /mol) ²	Uncertainty(cm ³ /mol) ²
200.00	-8175.1500457878	12.2188032917
220.00	-744.2437159699	6.3364279684
240.00	1949.1940801923	3.7629794300
260.00	2875.3765547702	2.4340775867
280.00	3094.5176225532	1.7213382389

300.00	3038.2142992801	1.2709484784
320.00	2883.3916013582	0.9702292665
323.15	2855.9146160815	0.9507180586
340.00	2702.1881431083	0.7790339354
360.00	2524.0011142879	0.6521748177
380.00	2362.9202341806	0.5504481668
400.00	2223.1147997929	0.4752683638
420.00	2103.2358282647	0.4170611357
440.00	2001.0214909888	0.3738318424
460.00	1916.2978844676	0.3433428600
480.00	1844.1426545478	0.3109970490
500.00	1782.9562641617	0.2862780168

B2 of N2 (TraPPE)

T(K)	B2(cm ³ /mol)	Uncertainty(cm ³ /mol)
200.00	-33.4420974510	0.0066990300
220.00	-24.7398478487	0.0062347229
240.00	-17.7358819417	0.0060390033
260.00	-11.9562615170	0.0055991461
280.00	-7.1338676127	0.0054820154
300.00	-3.0415880497	0.0052847301
320.00	0.4758288095	0.0051392954
323.15	0.9832870185	0.0050487224
340.00	3.5023939610	0.0049810335
350.00	4.8764932114	0.0048902798
360.00	6.1583414543	0.0048362010
380.00	8.4890818292	0.0047935642

400.00	10.5440211031	0.0046611374
420.00	12.3776215076	0.0046245227
440.00	14.0343805979	0.0045913407
460.00	15.5077346756	0.0045593632
480.00	16.8457006212	0.0044315733
500.00	18.0544425380	0.0044548188

B3 of N2 (TraPPE)

T(K)	B3(cm ³ /mol) ²	Uncertainty(cm ³ /mol) ²
200.00	1576.9073680787	0.2604709991
220.00	1477.8408353965	0.2296882606
240.00	1405.5718678488	0.2117328721
260.00	1353.1370286959	0.2009944545
280.00	1313.9628857060	0.1917356973
300.00	1284.6516602400	0.1830717055
320.00	1262.6073312426	0.1794668466
323.15	1260.1534652763	0.1801667840
340.00	1246.2585945266	0.1790280258
360.00	1232.9705609517	0.1739144936
380.00	1222.8028962833	0.1737259094
400.00	1214.1967651965	0.1720213987
420.00	1207.7486689883	0.1710603448
440.00	1202.2078038779	0.1733451145
460.00	1197.9017861267	0.1718872138
480.00	1193.5192420826	0.1679922255
500.00	1190.1865534967	0.1686667765

B2 of SF6 (single sphere Lennard-Jones model, direct quadrature method)

T(K) B2(cm³/mol)

200.00 -606.7848597

220.00 -510.8413645

240.00 -434.3966547

260.00 -372.1113023

280.00 -320.4267508

283.15 -313.0801423

293.15 -291.0000851

300.00 -276.8813047

303.15 -270.642256

313.15 -251.8160029

320.00 -239.7184443

323.15 -234.3577059

340.00 -207.6515831

360.00 -179.7169988

380.00 -155.1786847

400.00 -133.4649444

420.00 -114.1250337

440.00 -96.79883252

460.00 -81.19519732

480.00 -67.07623094

500.00 -54.24566515

B3 of SF6 (single sphere Lennard-Jones model, Fast Fourier transforms)

T(K) B3(cm³/mol)²

200.00 48132.31083

220.00	50268.90433
240.00	49186.11832
260.00	47006.02107
280.00	44591.63627
283.15	44216.51302
293.15	43053.50701
300.00	42286.90765
303.15	41943.65882
313.15	40895.29529
320.00	40214.63713
323.15	39911.99574
340.00	38402.80281
360.00	36840.01572
380.00	35500.29813
400.00	34354.10913
420.00	33373.06503
440.00	32531.74474
460.00	31808.16141
480.00	31183.64895
500.00	30642.51842

B2 of SF6 (7-site model)

T(K)	B2(cm ³ /mol)	Uncertainty(cm ³ /mol)
200.00	-612.2429187961	0.0495941402
220.00	-493.1008414089	0.0388693087
240.00	-405.9130851267	0.0321594389
260.00	-339.6168615972	0.0283739209

280.00	-287.5013756262	0.0250864340
300.00	-245.5251148613	0.0223559951
320.00	-211.1209048382	0.0206703978
323.15	-206.2348399381	0.0204993690
340.00	-182.3297711616	0.0192600123
360.00	-157.9318453324	0.0179188814
380.00	-136.9969551566	0.0169643720
400.00	-118.8611920189	0.0161020014
420.00	-102.9856267009	0.0153757311
440.00	-88.9967365707	0.0145284159
460.00	-76.5030975063	0.0139502903
480.00	-65.4150485385	0.0138936822
500.00	-55.4129463913	0.0131270636

B3 of SF6 (7-site model)

T(K)	B3(cm ³ /mol) ²	Uncertainty(cm ³ /mol) ²
200.00	-63049.9356058261	55.0919627223
210.00	-36396.8015326056	40.3062388056
220.00	-19427.1729098447	29.8351030036
240.00	-1373.8693128679	17.6337074810
260.00	6288.9648073044	11.6265764789
280.00	9439.9916491643	8.2690530053
300.00	10526.7636804934	6.2515650938
323.15	10690.4277462585	4.7505076670
325.00	10684.5363414707	4.7000976689
350.00	10280.4234595359	3.6628847574
375.00	9726.8129405678	3.2811831527

400.00	9187.2711380461	2.5801577828
425.00	8703.0509172142	2.2817958729
450.00	8289.7470256896	2.0203892063
475.00	7955.3339911412	1.8272355012
500.00	7676.3781747741	1.6966772326

B2 of SF6 (6-site model)

T(K)	B2(cm3/mol)	Uncertainty(cm3/mol)
200.00	-588.6700999558	0.0454466915
220.00	-479.1430159032	0.0371379431
240.00	-397.8962855967	0.0318143702
260.00	-335.3306053999	0.0276139267
280.00	-285.7198976159	0.0250346436
300.00	-245.4675446341	0.0231316469
323.15	-207.5010309649	0.0207890339
325.00	-204.7536099812	0.0209112834
350.00	-171.8491235067	0.0189980491
375.00	-144.7690394483	0.0177002777
400.00	-122.0540878235	0.0167162598
425.00	-102.7657984439	0.0158701489
450.00	-86.1708403053	0.0149716455
475.00	-71.7524180079	0.0142845191
500.00	-59.1443321170	0.0140749486

B3 of SF6 (6-site model)

T(K)	B3(cm3/mol)^2	Uncertainty(cm3/mol)^2
200.00	-86315.5402832777	74.9658324950

220.00	-28689.7974633865	39.1203345326
240.00	-5241.1111427930	22.4571101814
260.00	4604.5882054788	14.0183314269
280.00	8623.2276350258	6.8796954305
300.00	10077.5014757582	5.0203280888
320.00	10389.3713574461	5.4348505915
323.15	10375.6646025596	5.2310346278
340.00	10186.3472132911	4.4070668883
360.00	9782.6018016016	3.6206709172
380.00	9317.7098308144	3.1184567774
400.00	8866.9499840876	2.6738696067
420.00	8452.4638557755	2.3937133220
440.00	8087.5859956484	2.1890995022
460.00	7777.0612137204	1.9601510718
480.00	7514.7669748414	1.8173710986
500.00	7295.5402024827	1.6797046577

B2 of C14 (TraPPE-UA model)

T(K)	B2(cm ³ /mol)	Uncertainty(cm ³ /mol)
200.00	-671784.4908030243	785.8894383450
220.00	-231790.2559738071	202.1753273879
240.00	-101745.4497972382	66.3097977442
260.00	-53368.6884014208	27.1490173636
280.00	-31929.2559804559	12.6049439341
283.15	-29768.9325603978	11.2355090048
293.15	-24093.5896719405	7.9781327810
300.00	-21086.0272068195	6.6237532049

303.15	-19903.3096836668	5.9852857853
313.15	-16726.7269592891	4.5872456848
320.00	-14980.6619220168	3.9018657846
340.00	-11237.7766749235	2.4952742435
360.00	-8785.4420165277	1.7014355787
380.00	-7092.2125320236	1.2415848698
400.00	-5869.3738242010	0.9475237106
420.00	-4953.1335731672	0.7374112010
440.00	-4247.5543792091	0.5931688728
460.00	-3687.8536052339	0.4999160149
480.00	-3237.2494828414	0.4122517041
500.00	-2866.9529366489	0.3606720640

B2 of C14 (TraPPE-EH model)

T(K)	B2(cm ³ /mol)	Uncertainty(cm ³ /mol)
283.15	-46684.0687081318	27.1839457831
293.15	-36326.3241559753	18.8372579551
303.15	-28966.0434431153	13.4895964896
313.15	-23577.3308027003	9.7329847529

B2 of C20 (TraPPE-UA model)

T(K)	B2(cm ³ /mol)	Uncertainty(cm ³ /mol)
200.00	-61498591.8095555902	348278.4972245700
220.00	-9678154.5459260698	36080.4551107770
240.00	-2287953.5223172004	6086.5782018030
260.00	-727914.0144099643	1404.0020203506

280.00 -295972.7213973137 427.8249615242
300.00 -143799.3001212970 152.8118352338
320.00 -80561.0482757793 64.9969709430
323.15 -74348.2163682252 57.6427319996
340.00 -50344.2798753612 31.3994446861
360.00 -34149.3673047485 16.6765136603
380.00 -24648.7479060325 9.6884209074
400.00 -18691.2624487844 6.0600807801
420.00 -14730.1267943865 3.9541981924
440.00 -11937.9542500372 2.7926475804
460.00 -9907.0047045784 2.0365677415
480.00 -8379.3306172236 1.5913508359
500.00 -7192.0421046616 1.2380920278

B2 of C20 (TraPPE-EH model)

T(K) B2(cm³/mol) Uncertainty(cm³/mol)
323.15 -135190.2392312719 177.5748802182

B11 of He (single sphere Lennard-Jones model)-C20 (TraPPE-UA)

T(K) B11(cm³/mol) Uncertainty(cm³/mol)
323.15 130.4188303079 0.0276705348

B11 of He (single sphere Lennard-Jones model)-C20 (TraPPE-EH)

T(K) B11(cm³/mol) Uncertainty(cm³/mol)
323.15 145.2353392126 0.0314506329

B11 of CO₂ (TraPPE)-C20 (TraPPE-UA)

T(K)	B11(cm ³ /mol)	Uncertainty(cm ³ /mol)
200.00	-3219.4736942751	0.5270879164
220.00	-2471.9006906152	0.3495250805
240.00	-1968.4696819098	0.2545137573
260.00	-1609.6632953776	0.2077488192
280.00	-1342.3120052419	0.1495990229
300.00	-1137.4480845538	0.1377203492
320.00	-974.9352409069	0.1030328154
323.15	-952.4301474230	0.1024697451
340.00	-843.7127948545	0.0935750425
360.00	-735.5103810081	0.0845568858
380.00	-645.0678423626	0.0762734305
400.00	-568.1504951097	0.0654275541
420.00	-502.1626283628	0.0662947424
440.00	-444.9657086352	0.0590711839
460.00	-395.0400415827	0.0553766002
480.00	-350.7378747804	0.0564846742
500.00	-311.4237015536	0.0500168945

B11 of CO₂ (TraPPE)-C₂₀ (TraPPE-EH)

T(K)	B11(cm ³ /mol)	Uncertainty(cm ³ /mol)
323.15	-947.4990089672	0.1143152970

B11 of N₂ (TraPPE)-C₂₀ (TraPPE-UA)

T(K)	B11(cm ³ /mol)	Uncertainty(cm ³ /mol)
200.00	-1099.9669206917	0.1098227796
220.00	-889.0540459616	0.0896245177

240.00	-730.7494153113	0.0764902276
260.00	-607.9687165978	0.0662013992
280.00	-510.0731140679	0.0595108003
300.00	-430.5059535387	0.0537626664
320.00	-364.5622270941	0.0493002596
323.15	-355.0969353860	0.0479693665
340.00	-309.1184597574	0.0456960081
360.00	-261.8630794538	0.0431877862
380.00	-221.0470051046	0.0398665754
400.00	-185.6453432523	0.0387223685
420.00	-154.5534970242	0.0370903682
440.00	-127.1164692204	0.0353921243
460.00	-102.7912463386	0.0342629728
480.00	-80.9470023037	0.0333897624
500.00	-61.2952672446	0.0319354153

B11 of N2 (TraPPE)-C20 (TraPPE-EH)

T(K)	B11(cm ³ /mol)	Uncertainty(cm ³ /mol)
323.15	-361.5318738813	0.0430402438

B11 of SF6 (single sphere Lennard-Jones model)-C20 (TraPPE-UA)

T(K)	B11(cm ³ /mol)	Uncertainty(cm ³ /mol)
200.00	-8283.3730577084	1.1343907548
220.00	-6295.1553669866	0.7638182905
240.00	-4985.8925314598	0.5459974401
260.00	-4072.0280420945	0.4213692261
280.00	-3403.3684004347	0.3353128270

300.00	-2897.0593765669	0.2822125962
320.00	-2501.5312683436	0.2402473046
323.15	-2446.8091825553	0.2388170461
340.00	-2184.6141537137	0.2308196424
360.00	-1924.9354052093	0.1893060115
380.00	-1709.5288274940	0.1708361041
400.00	-1527.7716139792	0.1536820347
420.00	-1372.6789655682	0.1457900185
440.00	-1238.5200087172	0.1343268725
460.00	-1121.6206361457	0.1248028561
480.00	-1018.9969544865	0.1155317696
500.00	-928.0752572648	0.1121744258

B11 of SF6 (single sphere Lennard-Jones model)-C20 (TraPPE-EH)

T(K)	B11(cm ³ /mol)	Uncertainty(cm ³ /mol)
323.15	-3484.6938050805	0.4072774154

B11 of SF6 (7-site model)-C20 (TraPPE-UA)

T(K)	B2(cm ³ /mol)	Uncertainty(cm ³ /mol)
200.00	-9268.5522748361	2.9317891549
220.00	-6498.7013701300	1.5751813865
240.00	-4850.8484414081	0.9560149298
260.00	-3784.0062083718	0.6792072054
280.00	-3051.4422543643	0.4944479106
300.00	-2521.4474514981	0.3662064118
320.00	-2123.5304377085	0.2896680071
323.15	-2070.3608785763	0.2640588513

340.00	-1815.5538395839	0.2430837332
360.00	-1570.7337294701	0.2079204502
380.00	-1371.8333364225	0.1818746891
400.00	-1207.5938733062	0.1546606326
420.00	-1069.7319886800	0.1388404674
440.00	-952.3265785693	0.1253960370
460.00	-851.5516468299	0.1176786629
480.00	-764.0468548448	0.1076096427
500.00	-686.8661638111	0.1008377448

B11 of SF6 (6-site model)-C20 (TraPPE-UA)

T(K)	B11(cm3/mol)	Uncertainty(cm3/mol)
200.00	-10227.3753891327	3.7039180004
220.00	-7032.7305887675	1.9347634429
240.00	-5177.7009275096	1.2538098166
260.00	-3997.4201339148	0.8003425774
280.00	-3196.8317666889	0.5409689521
300.00	-2624.9071103539	0.4018574883
320.00	-2199.8465233143	0.2962471965
323.15	-2142.3462345565	0.2510359707
340.00	-1872.2567952577	0.2390759981
360.00	-1614.0405081095	0.1975292454
380.00	-1405.3020121054	0.1707698606
400.00	-1233.4719564345	0.1520500344
420.00	-1089.7490553359	0.1314723776
440.00	-968.2239584272	0.1211594606
460.00	-863.7408558222	0.1093139087

480.00 -773.4441256318 0.1007684902

500.00 -694.3991615264 0.0887874401

B11 of SF6 (single sphere Lennard-Jones model)-C14 (TraPPE-UA)

T(K)	B11(cm3/mol)	Uncertainty(cm3/mol)
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283.15	-2178.9835521505	0.2040783240
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293.15	-2018.9613758714	0.1941387798
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303.15	-1877.4705809898	0.1800921353
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313.15	-1750.5612344819	0.1645158668
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B11 of SF6 (single sphere Lennard-Jones model)-C14 (TraPPE-EH)

T(K)	B11(cm3/mol)	Uncertainty(cm3/mol)
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283.15	-3083.9162197750	0.3661763011
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293.15	-2837.0587400557	0.3327835277
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303.15	-2621.5464473273	0.3038772495
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313.15	-2431.2963198224	0.2771690529
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