Supporting Information: Coexistence Calculation Using the Isothermal-Isochoric Integration Method

S. Mostafa Razavi,[1, a)] Richard A. Messerly,[2, b)] and J. Richard Elliott[1, c)]

[1)] *Department of Chemical and Biomolecular Engineering, The University of Akron, Akron, Ohio 44325, USA*

[2)] *Thermodynamics Research Center, National Institute of Standards and Technology, Boulder, Colorado, 80305, USA*

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[a)]Electronic mail: sr87@uakron.edu

[b)]Electronic mail: richard.messerly@nist.gov

[c)]Electronic mail: elliot1@uakron.edu

I. TABLES OF EXAMPLE SIMULATIONS RESULTS

TABLE I. Cassandra simulation results of TraPPE-UA ethane.

[K]	[g/cm^3]			[$\frac{\text{kcal}}{\text{mol}}$]		[$\frac{\text{kcal}}{\text{mol}}$]		[$\frac{\text{kcal}}{\text{mol}}$]		[$\frac{\text{kcal}}{\text{mol}}$]		
T	ρ	Z	$\pm$	E^{tot}	$\pm$	E^{bonded}	$\pm$	E^{vdw}	$\pm$	E^{intra}	$\pm$	N
260.24	0.4286	0.0793	0.017	-1305.80	1.17	0.00	0.00	-1271.80	1.17	0.00	0.00	600
302.10	0.4286	0.6553	0.009	-1275.90	0.32	0.00	0.00	-1241.90	0.32	0.00	0.00	600
236.27	0.4714	0.0533	0.038	-1454.50	1.51	0.00	0.00	-1417.10	1.51	0.00	0.00	600
285.30	0.4714	0.9343	0.016	-1415.70	0.56	0.00	0.00	-1378.20	0.56	0.00	0.00	600
207.20	0.5143	0.0620	0.013	-1614.30	0.44	0.00	0.00	-1573.40	0.44	0.00	0.00	600
263.02	0.5143	1.3713	0.013	-1560.30	0.46	0.00	0.00	-1519.50	0.46	0.00	0.00	600
173.80	0.5571	0.0223	0.012	-1785.80	0.28	0.00	0.00	-1741.50	0.28	0.00	0.00	600
234.42	0.5571	2.0220	0.018	-1710.80	0.45	0.00	0.00	-1666.50	0.45	0.00	0.00	600
136.97	0.6000	-0.0907	0.030	-1969.80	0.66	0.00	0.00	-1922.20	0.66	0.00	0.00	600
198.44	0.6000	2.9710	0.016	-1869.80	0.52	0.00	0.00	-1822.10	0.52	0.00	0.00	600
360.00	0.0214	0.9267	0.001	-282.73	0.83	0.00	0.00	-275.92	0.83	0.00	0.00	2400
360.00	0.0286	0.9020	0.001	-377.38	0.49	0.00	0.00	-368.29	0.49	0.00	0.00	2400
360.00	0.0429	0.8577	0.001	-562.56	0.78	0.00	0.00	-548.92	0.78	0.00	0.00	2400
360.00	0.0857	0.7407	0.005	-1102.00	1.95	0.00	0.00	-1074.80	1.95	0.00	0.00	2400
360.00	0.1714	0.5760	0.009	-524.55	1.35	0.00	0.00	-510.93	1.35	0.00	0.00	600
360.00	0.2571	0.5267	0.008	-757.44	1.69	0.00	0.00	-737.00	1.69	0.00	0.00	600
360.00	0.3429	0.6587	0.005	-994.97	1.55	0.00	0.00	-967.72	1.55	0.00	0.00	600
360.00	0.4286	1.2170	0.008	-1240.40	0.64	0.00	0.00	-1206.30	0.64	0.00	0.00	600
360.00	0.4714	1.7697	0.013	-1360.30	0.58	0.00	0.00	-1322.80	0.58	0.00	0.00	600
360.00	0.5143	2.5573	0.008	-1473.90	0.74	0.00	0.00	-1433.00	0.74	0.00	0.00	600
360.00	0.5571	3.6940	0.020	-1572.70	1.40	0.00	0.00	-1528.40	1.40	0.00	0.00	600
360.00	0.6000	5.2740	0.012	-1649.30	0.88	0.00	0.00	-1601.60	0.88	0.00	0.00	600

TABLE II. Cassandra simulation results of TraPPE-UA n-dodecane.

[K]	[g/cm^3]			[$\frac{\text{kcal}}{\text{mol}}$]		[$\frac{\text{kcal}}{\text{mol}}$]		[$\frac{\text{kcal}}{\text{mol}}$]		[$\frac{\text{kcal}}{\text{mol}}$]		
T	ρ	Z	$\pm$	E^{tot}	$\pm$	E^{bonded}	$\pm$	E^{vdw}	$\pm$	E^{intra}	$\pm$	N
547.99	0.5336	-0.0778	0.072	539.58	2.30	1413.40	2.35	-842.53	0.90	-100.82	0.77	100
611.24	0.5336	0.6870	0.034	692.62	2.35	1546.40	1.97	-822.58	0.45	-97.28	1.68	100
496.88	0.5870	-0.1298	0.054	325.26	3.28	1302.00	2.59	-942.33	1.00	-101.08	0.59	100
578.08	0.5870	1.3135	0.030	527.83	3.43	1477.80	2.76	-915.60	0.78	-98.97	0.98	100
436.18	0.6404	-0.3040	0.044	62.32	1.55	1154.40	0.91	-1054.60	0.77	-102.66	0.24	100
534.79	0.6404	2.0660	0.062	329.60	2.49	1385.00	1.89	-1017.90	0.62	-100.14	0.61	100
368.10	0.6937	-0.3983	0.052	-229.46	2.23	986.52	1.86	-1175.40	0.54	-102.65	0.40	100
480.33	0.6937	3.4458	0.106	95.99	0.98	1263.10	0.31	-1126.50	0.77	-101.91	0.81	100
296.20	0.7471	-0.6928	0.064	-558.84	2.80	793.21	2.48	-1308.30	0.34	-99.60	0.21	100
414.66	0.7471	5.5373	0.106	-181.39	1.05	1105.90	1.11	-1243.50	1.17	-103.16	0.30	100
691.00	0.0267	0.8800	0.005	6254.10	2.84	6823.90	3.10	-563.52	2.05	-376.65	2.15	400
691.00	0.0356	0.8453	0.010	6193.00	2.09	6825.10	2.53	-623.75	1.48	-376.81	1.87	400
691.00	0.0534	0.7843	0.005	6062.30	4.10	6817.00	4.69	-742.13	2.27	-378.90	1.64	400
691.00	0.1067	0.5953	0.019	5727.10	5.15	6816.20	5.39	-1064.20	1.44	-376.56	1.54	400
691.00	0.2135	0.3968	0.032	1290.70	1.72	1701.00	1.90	-397.78	0.22	-94.47	0.85	100
691.00	0.3202	0.3218	0.052	1164.30	2.94	1701.60	2.71	-518.57	0.40	-94.09	0.84	100
691.00	0.4269	0.4833	0.030	1027.00	2.10	1701.40	1.16	-649.39	1.05	-94.02	1.33	100
691.00	0.5336	1.5103	0.045	870.35	3.33	1701.70	3.72	-800.11	0.48	-94.49	1.20	100
691.00	0.5870	2.6510	0.091	784.24	2.65	1701.00	2.19	-882.39	1.34	-92.90	2.05	100
691.00	0.6404	4.3288	0.027	703.23	2.43	1704.30	2.50	-963.56	0.73	-93.39	0.93	100
691.00	0.6937	6.9253	0.045	624.32	5.24	1705.40	3.88	-1040.50	1.96	-93.70	0.94	100
691.00	0.7471	10.5860	0.079	554.85	3.62	1706.60	3.24	-1108.00	1.04	-92.12	1.18	100

TABLE III. Cassandra simulation results of Mie-UA n-dodecane.

[K]	[g/cm^3]			[$\frac{\text{kcal}}{\text{mol}}$]		[$\frac{\text{kcal}}{\text{mol}}$]		[$\frac{\text{kcal}}{\text{mol}}$]		[$\frac{\text{kcal}}{\text{mol}}$]		
T	ρ	Z	$\pm$	E^{tot}	$\pm$	E^{bonded}	$\pm$	E^{vdw}	$\pm$	E^{intra}	$\pm$	N
547.99	0.5336	-0.0153	0.063	407.88	2.47	1400.40	2.15	-906.78	0.57	-122.15	0.85	100
611.24	0.5336	0.9015	0.066	559.66	2.20	1530.90	1.72	-885.46	0.74	-120.10	1.24	100
496.88	0.5870	-0.0500	0.075	175.14	3.30	1288.30	2.55	-1018.80	1.13	-121.86	1.03	100
578.08	0.5870	1.6285	0.066	378.49	1.85	1463.50	2.14	-990.66	0.61	-120.36	0.93	100
436.18	0.6404	0.0350	0.045	-102.43	1.17	1144.10	0.67	-1143.60	0.58	-122.64	0.17	100
534.79	0.6404	2.8502	0.113	160.90	1.77	1369.40	1.43	-1105.60	0.67	-122.40	0.97	100
368.10	0.6937	-0.0140	0.141	-416.93	1.60	976.69	1.15	-1282.20	1.05	-121.18	0.65	100
480.33	0.6937	4.8027	0.112	-92.08	2.81	1250.50	2.92	-1231.10	0.84	-122.57	0.21	100
296.20	0.7471	0.1143	0.244	-770.81	3.57	784.67	2.34	-1435.40	1.52	-116.21	0.23	100
414.66	0.7471	8.0452	0.056	-392.58	2.13	1094.90	2.14	-1367.40	0.54	-122.52	0.15	100
691.00	0.0267	0.8818	0.011	6084.00	7.82	6765.80	6.27	-664.64	1.69	-468.95	1.11	400
691.00	0.0356	0.8510	0.009	6016.80	4.40	6766.20	3.88	-726.49	0.98	-470.03	2.83	400
691.00	0.0534	0.7770	0.007	5886.30	5.75	6765.80	3.52	-845.19	2.42	-469.07	1.29	400
691.00	0.1067	0.6038	0.013	5514.60	6.73	6759.60	6.36	-1176.40	2.67	-468.99	0.76	400
691.00	0.2135	0.3505	0.055	1224.20	2.24	1685.80	0.88	-427.30	1.52	-116.83	1.79	100
691.00	0.3202	0.3143	0.036	1079.90	2.27	1686.60	1.34	-555.26	1.32	-117.34	0.35	100
691.00	0.4269	0.5490	0.035	922.36	2.86	1685.80	2.65	-694.81	0.45	-117.14	0.88	100
691.00	0.5336	1.8942	0.099	736.46	1.26	1684.20	0.20	-862.01	1.22	-117.53	0.72	100
691.00	0.5870	3.2350	0.087	632.54	0.88	1683.60	1.33	-956.78	0.62	-116.73	1.12	100
691.00	0.6404	5.6220	0.018	533.01	0.60	1687.20	0.69	-1051.30	0.24	-116.66	1.16	100
691.00	0.6937	9.2245	0.057	432.38	1.48	1686.90	2.44	-1143.00	0.99	-117.03	0.88	100
691.00	0.7471	14.4230	0.142	340.46	0.91	1686.40	0.81	-1225.80	1.02	-115.80	1.42	100
592.20	0.0267	0.8158	0.016	5254.60	6.38	6013.70	4.63	-741.96	2.23	-485.86	0.65	400
592.20	0.0356	0.7500	0.013	5159.60	3.87	6005.10	4.03	-822.56	0.96	-486.04	1.53	400
592.20	0.0534	0.6528	0.012	4978.20	6.83	5999.90	6.23	-987.40	6.16	-487.60	2.00	400
592.20	0.1067	0.3945	0.017	4525.10	25.56	5998.70	4.72	-1405.00	22.32	-484.97	2.34	400

TABLE IV. Cassandra simulation results of TIP4P/2005 water.

[K]	[g/cm^3]		[$\frac{\text{kcal}}{\text{mol}}$]	[$\frac{\text{kcal}}{\text{mol}}$]	[$\frac{\text{kcal}}{\text{mol}}$]	
T	ρ	Z	E^{tot}	E^{vdw}	E^{coul}	N
572.78	0.7129	0.0740	-2242.94	270.51	-2502.424	300
659.08	0.7129	0.4840	-2067.62	243.28	-2299.876	300
532.85	0.7841	0.0600	-2438.16	309.05	-2735.093	300
631.84	0.7841	0.6320	-2228.53	279.70	-2496.111	300
480.94	0.8554	0.0760	-2657.13	360.23	-3004.142	300
593.84	0.8554	0.7820	-2400.21	316.31	-2703.301	300
412.51	0.9267	0.0670	-2940.19	436.05	-3361.919	300
538.67	0.9267	1.0540	-2610.77	376.95	-2973.396	300
293.92	0.9980	-0.0590	-3434.88	610.33	-4029.781	300
426.35	0.9980	0.9710	-2965.60	462.30	-3412.474	300
776.00	0.0356	0.8560	-912.83	99.02	-1009.651	1200
776.00	0.0475	0.8140	-1186.59	127.57	-1311.222	1200
776.00	0.0713	0.7420	-1681.62	178.48	-1855.691	1200
776.00	0.1426	0.5970	-2845.35	296.92	-3133.459	1200
776.00	0.2851	0.4690	-1113.92	116.16	-1225.669	300
776.00	0.4277	0.4590	-1403.35	145.32	-1542.058	300
776.00	0.5703	0.5840	-1650.40	179.19	-1820.766	300
776.00	0.7129	0.9190	-1883.52	229.07	-2101.566	300
776.00	0.7841	1.1790	-1999.09	262.93	-2249.894	300
776.00	0.8554	1.5650	-2098.20	305.50	-2390.48	300
776.00	0.9267	2.1170	-2189.13	365.39	-2540.201	300
776.00	0.9980	2.7130	-2269.56	425.70	-2679.834	300

II. FIGURES OF EXAMPLE SIMULATIONS

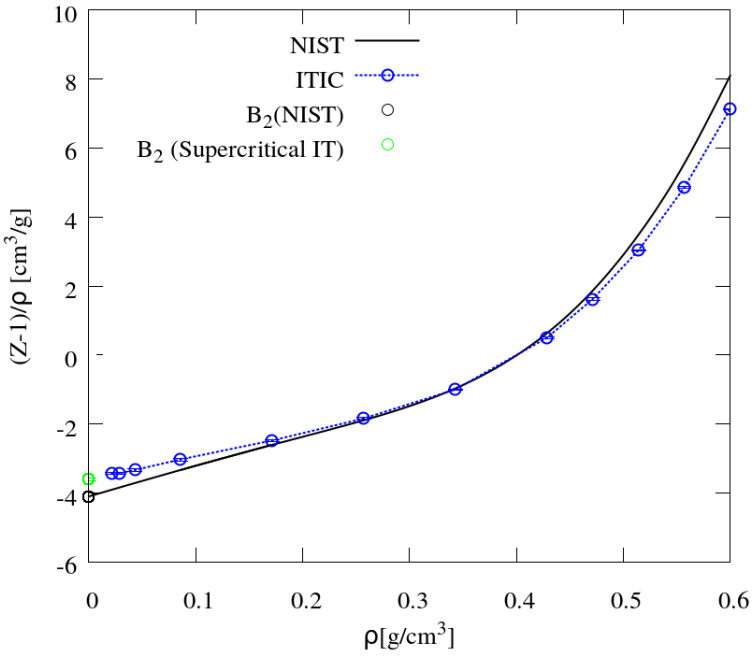

FIG. 1. Compressibility factor plot of TraPPE-UA ethane with repect to density.

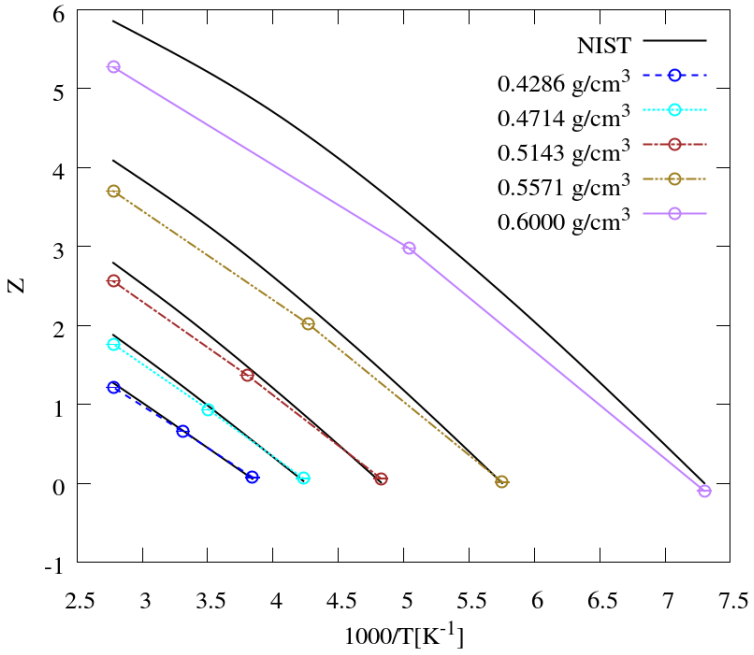

FIG. 2. Plot of TraPPE-UA ethane isochores at different densities compared to NIST values.

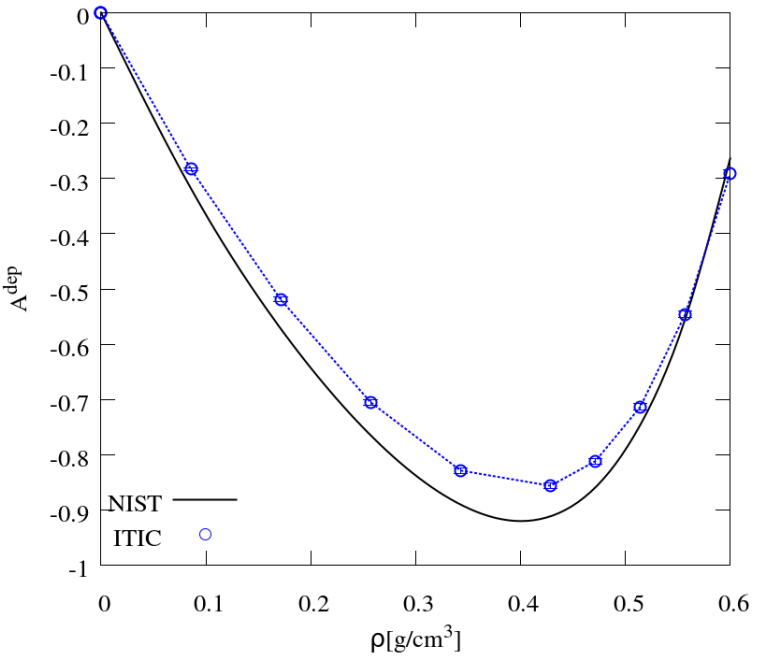

FIG. 3. Helmholtz energy departure function of TraPPE-UA ethane as a function of density compared to NIST data.

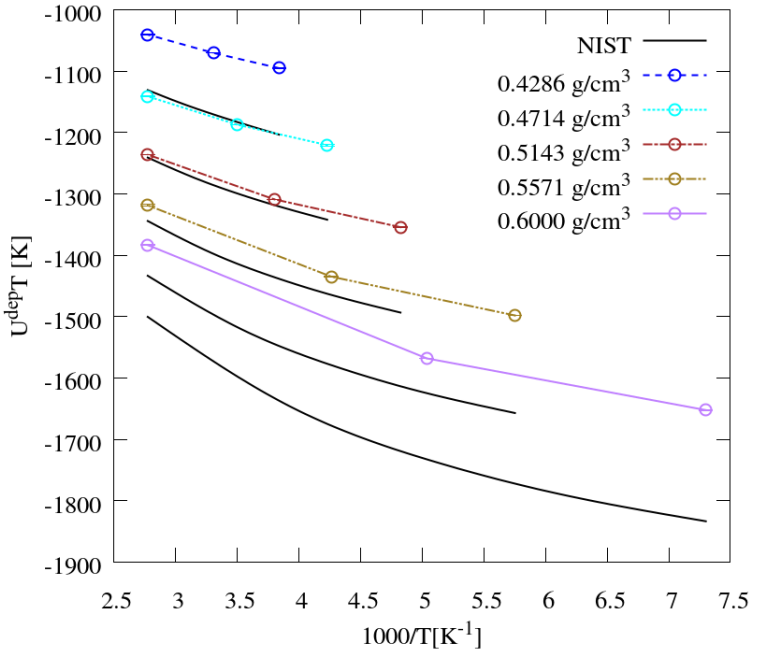

FIG. 4. Internal energy departure function of TraPPE-UA ethane.

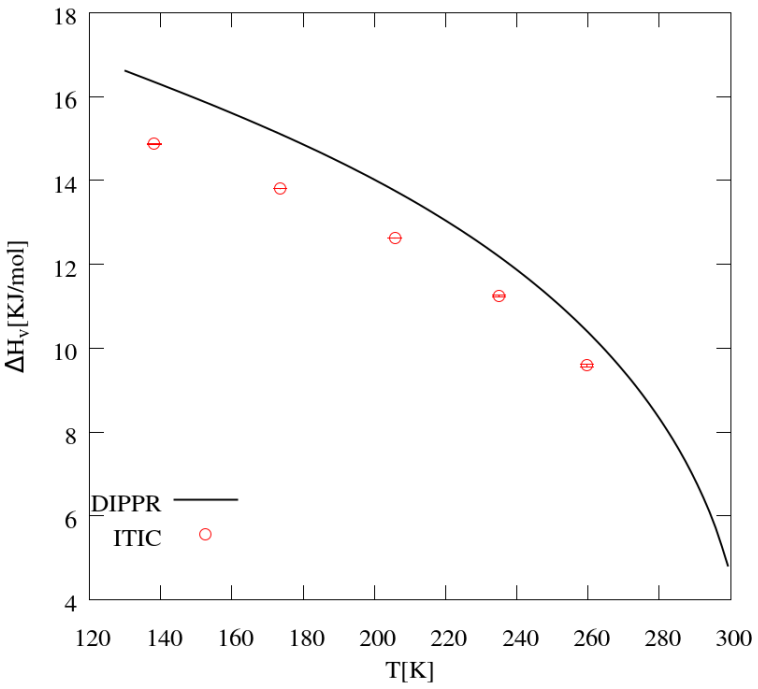

FIG. 5. Heat of vaporization of TraPPE-UA ethane.

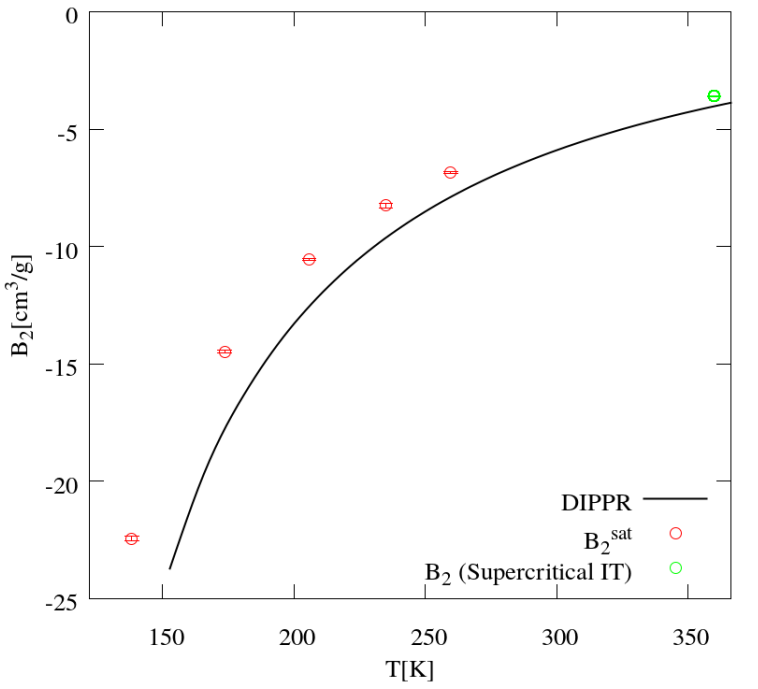

FIG. 6. Second virial coefficient plot of TraPPE-UA ethane.

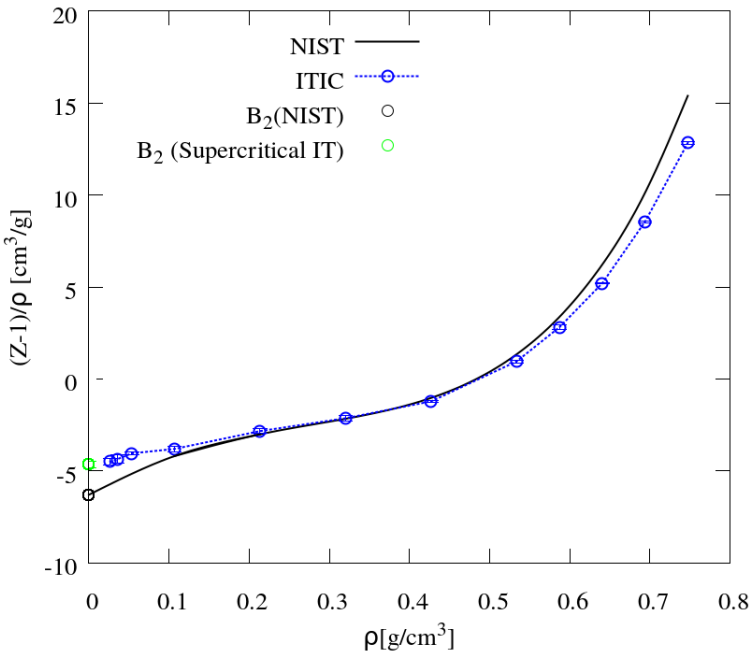

FIG. 7. Compressibility factor plot of TraPPE-UA *n*-dodecane with repect to density.

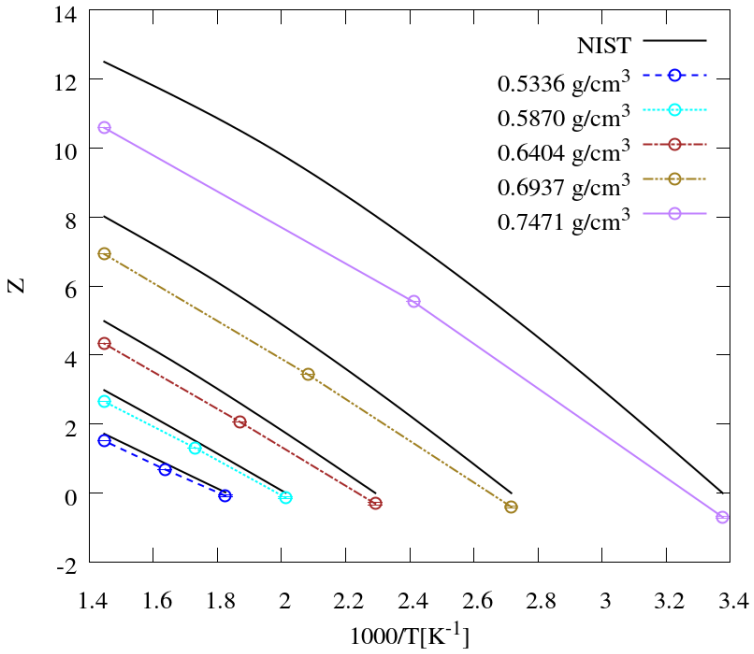

FIG. 8. Plot of TraPPE-UA *n*-dodecane isochores at different densities compared to NIST values.

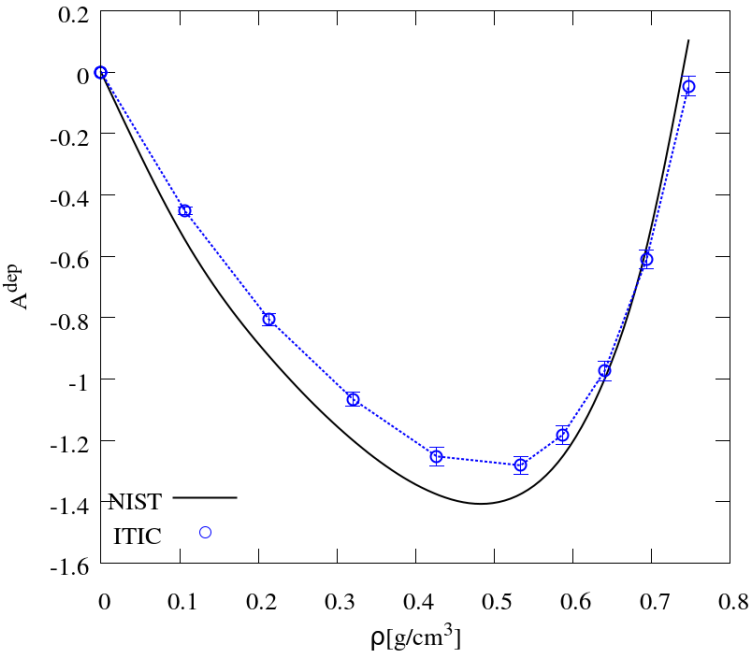

FIG. 9. Helmholtz energy departure function of TraPPE-UA *n*-dodecane as a function of density compared to NIST data.

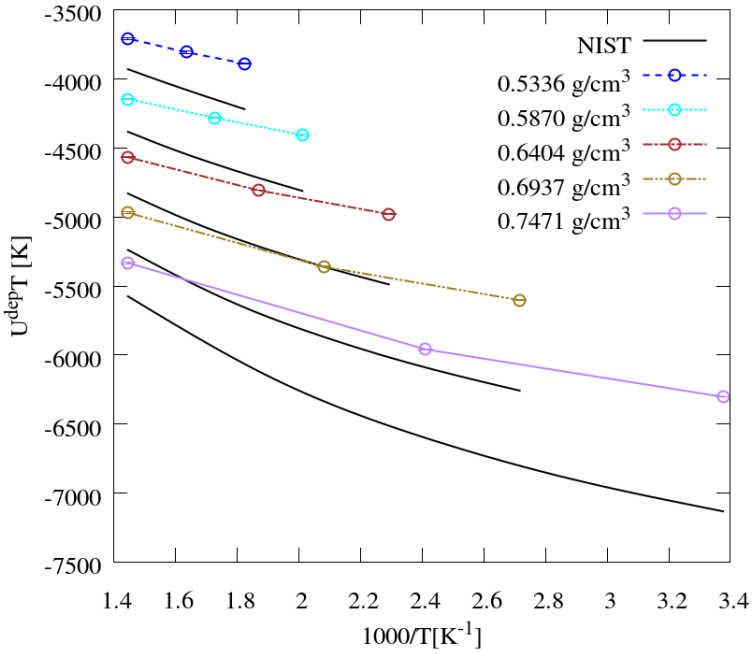

FIG. 10. Internal energy departure function of TraPPE-UA *n*-dodecane.

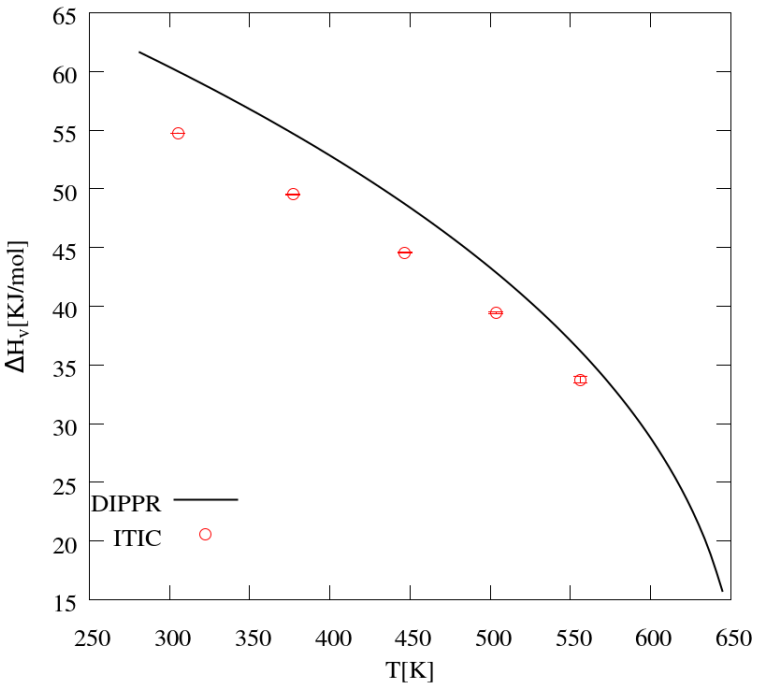

FIG. 11. Heat of vaporization of TraPPE-UA *n*-dodecane.

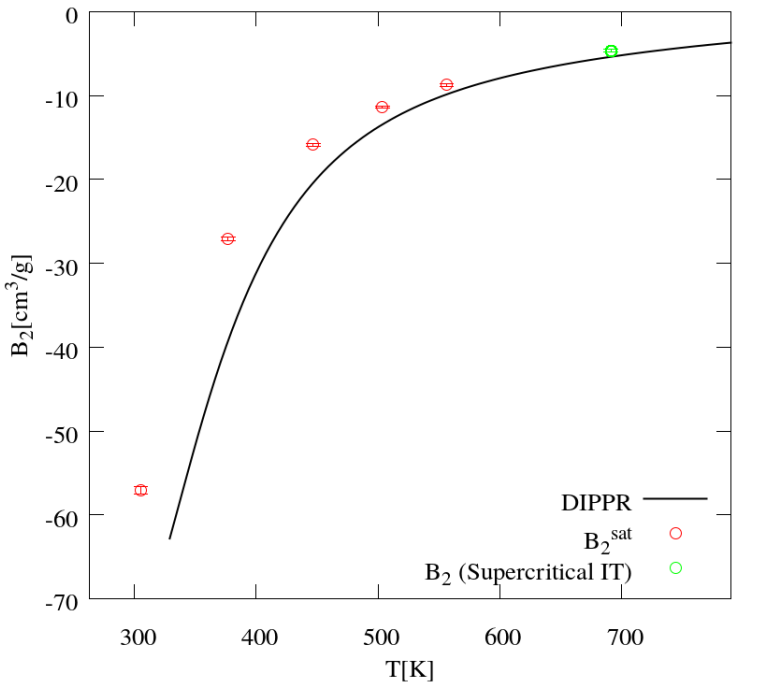

FIG. 12. Second virial coefficient plot of TraPPE-UA *n*-dodecane.

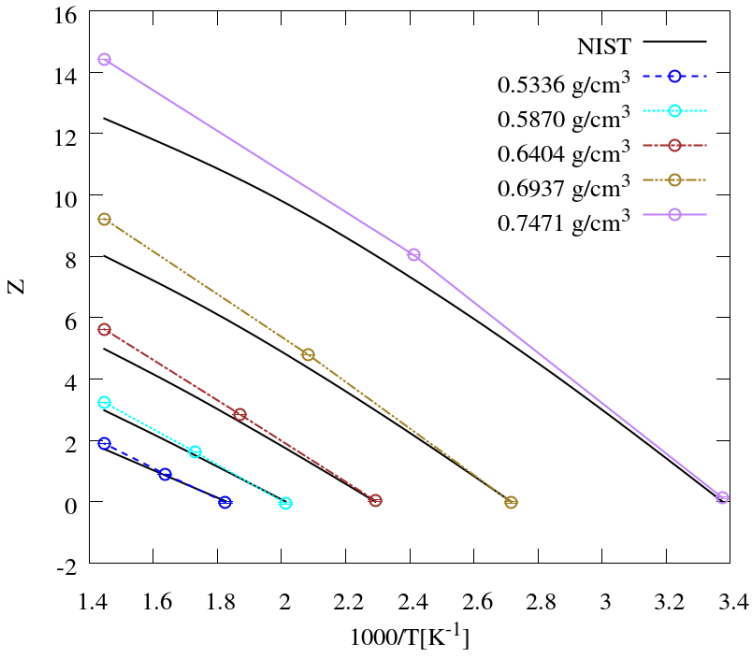

FIG. 13. Plot of Mie-UA n-dodecane isochores at different densities compared to NIST values.

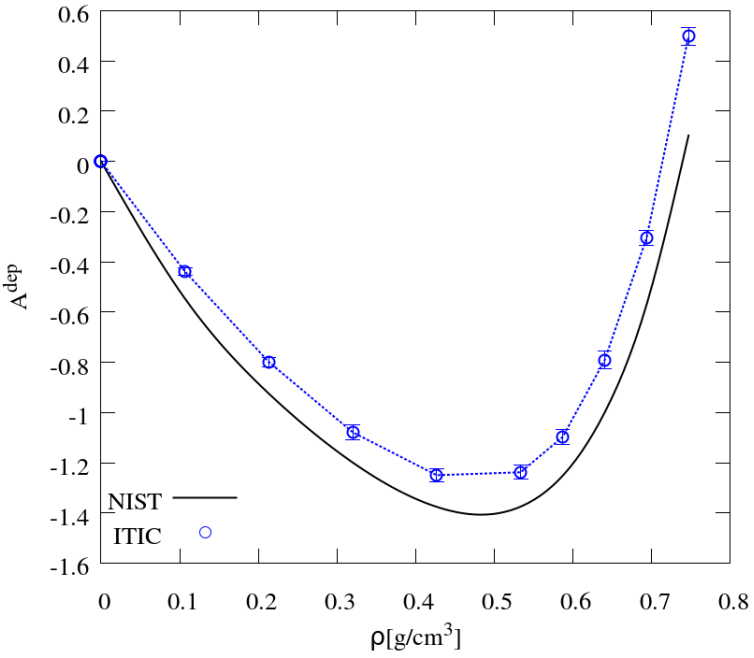

FIG. 14. Helmholtz energy departure function of Mie-UA n-dodecane as a function of density compared to NIST data.

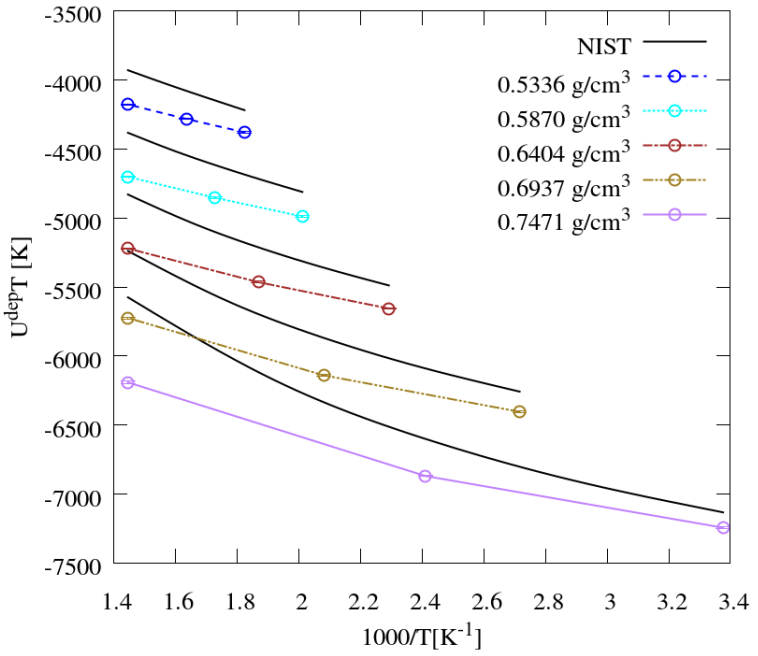

FIG. 15. Internal energy departure function of Mie-UA *n*-dodecane.

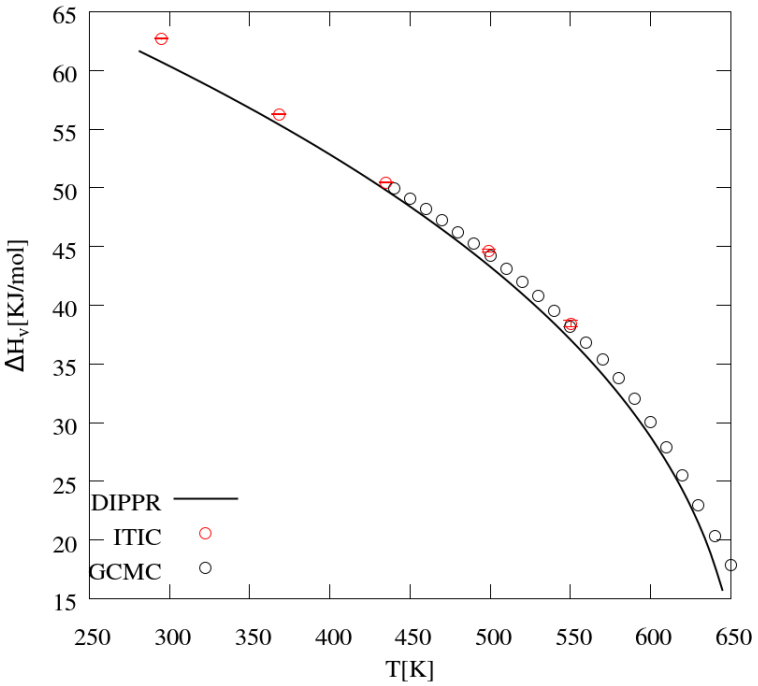

FIG. 16. Heat of vaporization of Mie-UA *n*-dodecane. GCMC data were obtained from Ref. 1.

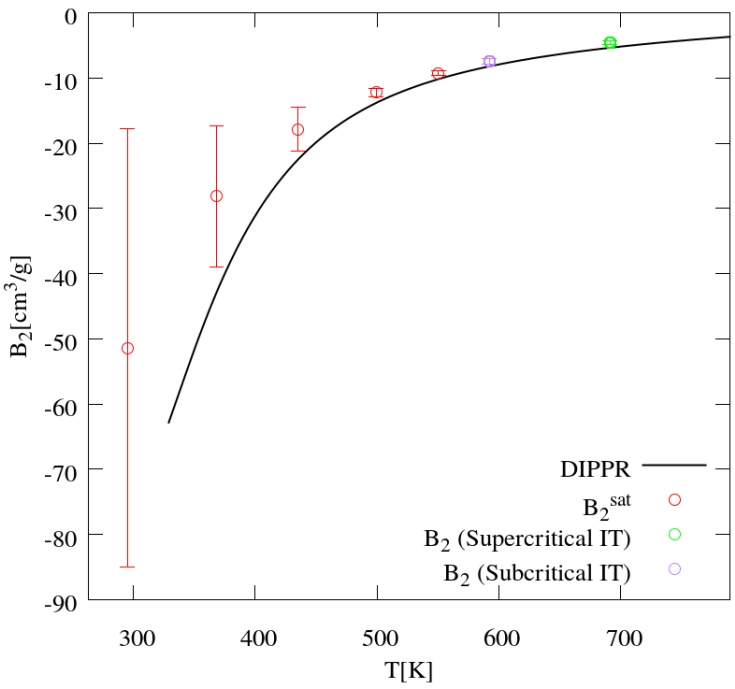

FIG. 17. Second virial coefficient plot of Mie-UA n-dodecane.

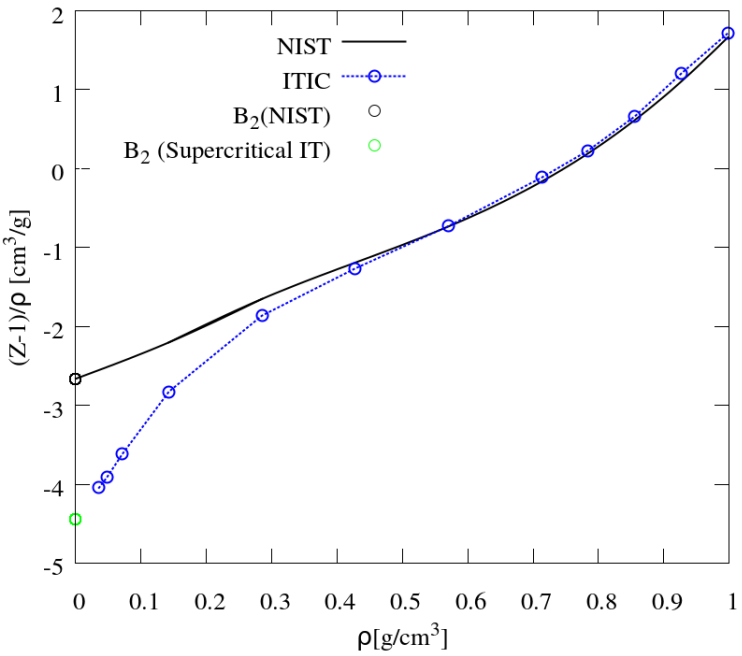

FIG. 18. Compressibility factor plot of TIP4P/2005 water with repect to density.

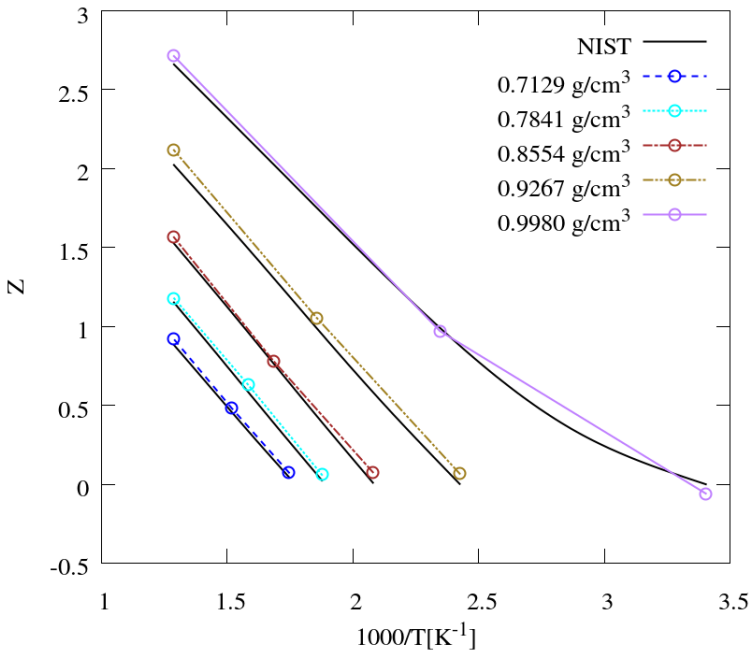

FIG. 19. Plot of TIP4P/2005 isochores at different densities compared to NIST values.

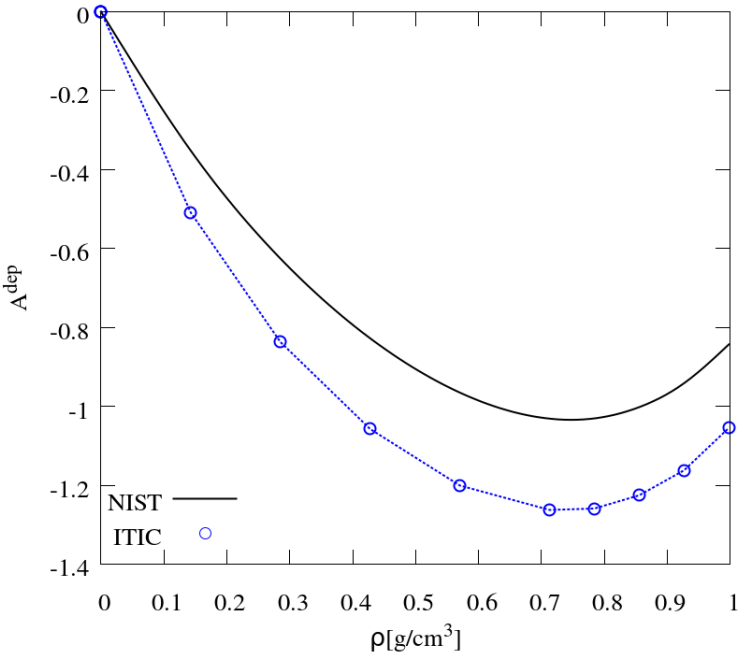

FIG. 20. Helmholtz energy departure function of TIP4P/2005 water as a function of density compared to NIST data.

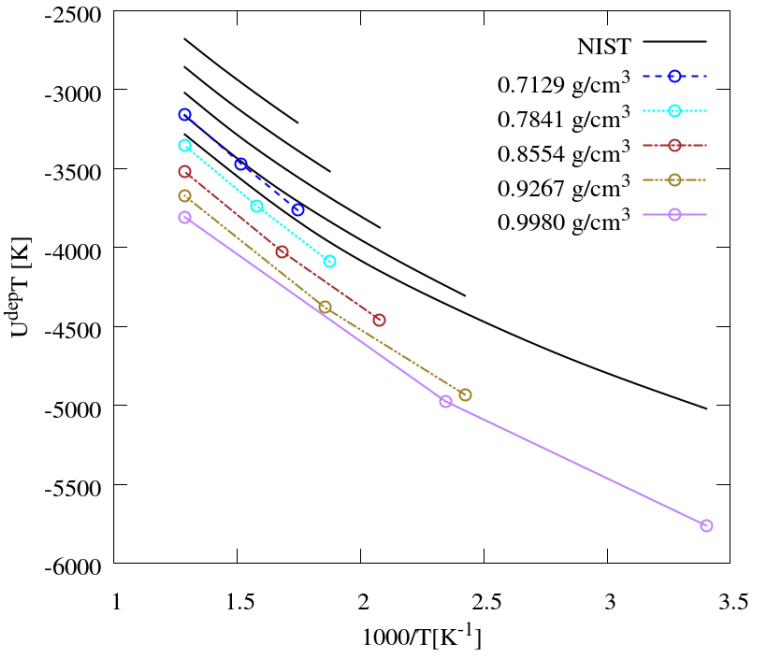

FIG. 21. Internal energy departure function of TIP4P/2005 water.

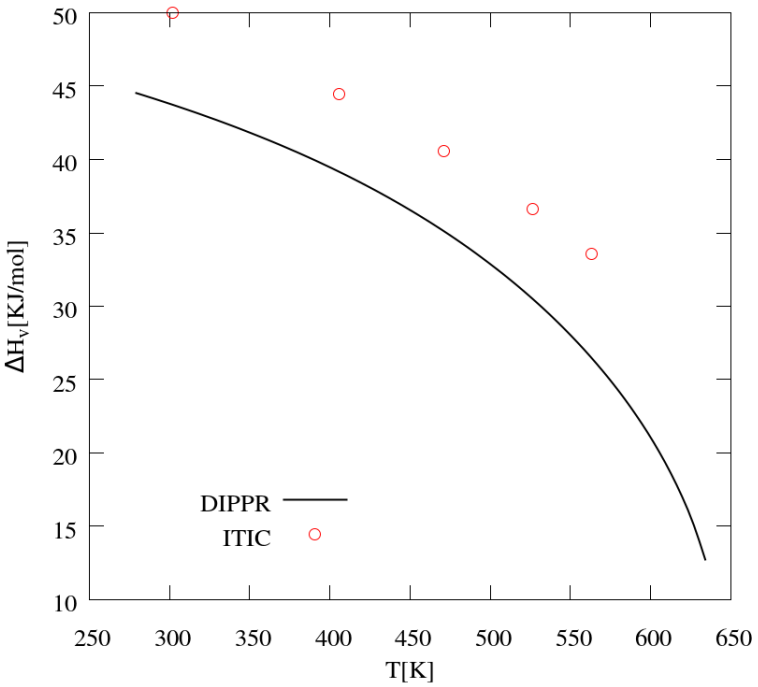

FIG. 22. Heat of vaporization of TIP4P/2005 water.

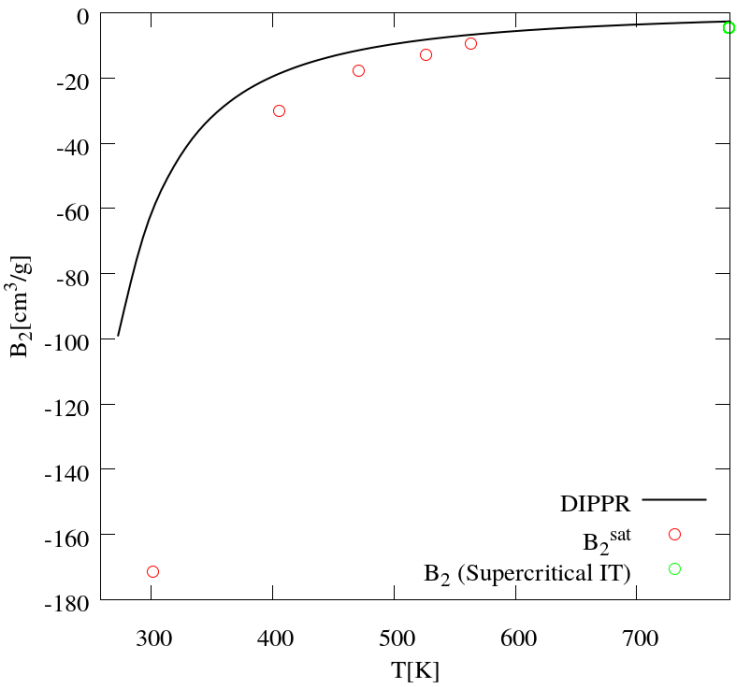

FIG. 23. Second virial coefficient plot of TIP4P/2005 water.

REFERENCES

[1]J. J. Potoff and D. A. Bernard-Brunel, The Journal of Physical Chemistry B **113**, 14725 (2009).