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@zips.uakron.edu

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

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

I. TABLES OF SIMULATION RESULTS

TABLE I: GOMC simulation results of Mie-UA n-dodecane.

[K]	[g/cm^3]			$\left[\frac{\text{kcal}}{\text{mol}}\right]$		$\left[\frac{\text{kcal}}{\text{mol}}\right]$		$\left[\frac{\text{kcal}}{\text{mol}}\right]$		$\left[\frac{\text{kcal}}{\text{mol}}\right]$		
T	ρ	Z	±	E^{tot}	±	E^{bonded}	±	E^{vdw}	±	E^{intra}	±	N
546.60	0.5336	-0.1261	0.056	406.10	1.32	1398.50	1.45	-992.43	0.77	-120.92	0.27	100
610.38	0.5336	0.8729	0.039	563.06	2.05	1534.00	1.60	-970.97	0.65	-119.24	0.08	100
495.91	0.5870	-0.0513	0.127	174.62	2.45	1287.80	0.97	-1113.20	1.49	-121.80	0.19	100
577.42	0.5870	1.6286	0.030	379.64	2.40	1465.00	1.75	-1085.40	0.78	-120.07	0.29	100
436.90	0.6404	-0.0915	0.065	-97.85	2.61	1149.30	1.97	-1247.20	0.75	-121.95	0.57	100
535.33	0.6404	2.9012	0.058	163.20	2.30	1371.70	2.41	-1208.50	0.43	-121.07	0.28	100
370.34	0.6937	0.0900	0.076	-409.79	5.38	982.86	4.40	-1392.70	1.09	-120.11	0.58	100
482.23	0.6937	4.8706	0.153	-90.93	2.37	1251.60	2.13	-1342.50	0.64	-121.45	0.59	100
296.98	0.7471	0.0618	0.395	-771.37	6.03	785.23	5.17	-1556.60	1.28	-115.43	1.12	100
415.42	0.7471	8.0692	0.193	-394.09	6.64	1093.20	4.29	-1487.30	2.83	-121.32	0.64	100
592.20	0.0267	0.8128	0.006	5278.70	2.49	6035.40	3.22	-756.67	1.79	-482.63	0.27	400
592.20	0.0356	0.7558	0.004	5189.60	4.39	6035.70	4.21	-846.12	1.47	-481.63	0.66	400
592.20	0.0534	0.6512	0.014	5019.00	10.65	6035.60	6.76	-1016.60	8.01	-481.85	0.30	400
592.20	0.1067	0.4037	0.011	4553.40	38.71	6020.00	7.59	-1466.60	31.26	-481.14	0.69	400
691.00	0.0267	0.8812	0.002	6129.00	4.16	6808.00	3.32	-679.03	1.01	-466.54	0.41	400
691.00	0.0356	0.8403	0.006	6058.10	2.94	6805.60	5.24	-747.48	2.31	-466.46	0.98	400
691.00	0.0534	0.7771	0.004	5921.20	6.45	6800.50	4.36	-879.30	2.54	-465.74	0.71	400
691.00	0.1067	0.6035	0.007	5540.70	16.26	6788.20	3.31	-1247.50	15.58	-466.46	0.63	400
691.00	0.2135	0.3401	0.034	1237.50	2.59	1697.10	1.42	-459.62	2.20	-116.36	0.29	100
691.00	0.3202	0.2706	0.032	1086.90	3.98	1692.00	3.01	-605.14	1.75	-116.25	0.17	100
691.00	0.4269	0.5763	0.032	931.11	3.33	1693.70	2.31	-762.60	1.24	-115.99	0.25	100
691.00	0.5336	1.8589	0.020	742.31	2.60	1690.60	2.38	-948.28	0.86	-115.89	0.28	100
691.00	0.5870	3.2749	0.072	641.63	4.85	1691.50	4.66	-1049.90	0.35	-115.77	0.39	100
691.00	0.6404	5.5809	0.060	533.58	2.72	1688.40	2.63	-1154.80	0.85	-115.80	0.38	100
691.00	0.6937	9.1539	0.101	434.13	2.06	1689.40	3.06	-1255.30	1.88	-115.69	0.46	100
691.00	0.7471	14.5340	0.037	346.35	5.20	1691.60	3.73	-1345.30	1.57	-115.34	0.28	100

TABLE II: Cassandra simulation results of TIP4P/2005 water.

[K]	[g/cm^3]			[$\frac{\text{kcal}}{\text{mol}}$]		[$\frac{\text{kcal}}{\text{mol}}$]		[$\frac{\text{kcal}}{\text{mol}}$]		[$\frac{\text{kcal}}{\text{mol}}$]		
T	ρ	Z	$\pm$	E^{tot}	$\pm$	E^{bonded}	$\pm$	E^{vdw}	$\pm$	E^{intra}	$\pm$	N
572.01	0.7129	0.0710	0.039	-2241.50	8.50	0.00	0.00	270.58	3.52	0.00	0.00	300
658.57	0.7129	0.4645	0.036	-2074.40	4.51	0.00	0.00	243.86	3.36	0.00	0.00	300
533.15	0.7841	0.0828	0.016	-2433.80	3.68	0.00	0.00	309.05	0.59	0.00	0.00	300
632.05	0.7841	0.6038	0.012	-2226.80	1.15	0.00	0.00	276.31	1.64	0.00	0.00	300
482.75	0.8554	0.0560	0.018	-2651.00	7.53	0.00	0.00	354.98	2.38	0.00	0.00	300
595.22	0.8554	0.7990	0.042	-2395.00	4.70	0.00	0.00	316.58	3.14	0.00	0.00	300
413.24	0.9267	0.0658	0.020	-2932.90	8.09	0.00	0.00	432.75	4.74	0.00	0.00	300
539.29	0.9267	1.0180	0.025	-2606.70	1.56	0.00	0.00	372.09	2.07	0.00	0.00	300
288.64	0.9980	0.0535	0.042	-3470.40	10.99	0.00	0.00	634.65	6.26	0.00	0.00	300
420.77	0.9980	0.9220	0.056	-2977.80	5.65	0.00	0.00	462.91	6.79	0.00	0.00	300
776.00	0.1426	0.5975	0.024	-711.47	6.46	0.00	0.00	74.78	2.98	0.00	0.00	300
776.00	0.2851	0.4625	0.012	-1106.80	8.08	0.00	0.00	113.53	2.81	0.00	0.00	300
776.00	0.4277	0.4790	0.007	-1392.90	4.24	0.00	0.00	146.57	1.09	0.00	0.00	300
776.00	0.5703	0.5763	0.010	-1655.40	4.35	0.00	0.00	180.24	1.05	0.00	0.00	300
776.00	0.7129	0.9113	0.017	-1889.60	3.57	0.00	0.00	230.02	3.21	0.00	0.00	300
776.00	0.7841	1.1960	0.014	-1993.90	3.54	0.00	0.00	263.57	1.08	0.00	0.00	300
776.00	0.8554	1.5645	0.016	-2100.40	3.29	0.00	0.00	305.41	1.18	0.00	0.00	300
776.00	0.9267	2.0420	0.043	-2191.80	4.06	0.00	0.00	355.62	5.31	0.00	0.00	300
776.00	0.9980	2.7380	0.021	-2270.00	3.31	0.00	0.00	428.68	2.89	0.00	0.00	300
776.00	0.0356	0.8560	0.000	-912.83	0.00	0.00	0.00	99.02	0.00	0.00	0.00	1200
776.00	0.0475	0.8140	0.000	-1186.60	0.00	0.00	0.00	127.57	0.00	0.00	0.00	1200
776.00	0.0713	0.7420	0.000	-1681.60	0.00	0.00	0.00	178.48	0.00	0.00	0.00	1200
776.00	0.1426	0.5970	0.000	-2845.40	0.00	0.00	0.00	296.92	0.00	0.00	0.00	1200

TABLE III: Cassandra simulation results of TraPPE-UA methane.

[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
167.20	0.3179	0.0690	0.025	-1507.30	3.00	0.00	0.00	-1439.50	3.00	0.00	0.00	1200
192.92	0.3179	0.5450	0.027	-1474.90	2.22	0.00	0.00	-1407.10	2.22	0.00	0.00	1200
153.67	0.3496	0.0668	0.006	-1671.80	0.53	0.00	0.00	-1597.20	0.53	0.00	0.00	1200
183.60	0.3496	0.7665	0.029	-1627.50	1.15	0.00	0.00	-1552.90	1.15	0.00	0.00	1200
137.14	0.3814	0.0740	0.023	-1844.50	0.83	0.00	0.00	-1763.20	0.83	0.00	0.00	1200
171.27	0.3814	1.1050	0.023	-1785.20	1.25	0.00	0.00	-1703.90	1.25	0.00	0.00	1200
117.81	0.4132	0.1023	0.014	-2029.80	1.13	0.00	0.00	-1941.70	1.13	0.00	0.00	1200
155.35	0.4132	1.5693	0.020	-1948.70	1.26	0.00	0.00	-1860.60	1.26	0.00	0.00	1200
135.01	0.4450	2.2950	0.026	-2116.40	1.68	0.00	0.00	-2021.50	1.68	0.00	0.00	1200
95.90	0.4450	0.0528	0.022	-2227.90	0.73	0.00	0.00	-2133.00	0.73	0.00	0.00	1200
171.51	0.0159	0.8765	0.001	-374.07	0.53	0.00	0.00	-360.51	0.53	0.00	0.00	4800
171.51	0.0212	0.8365	0.001	-499.01	1.97	0.00	0.00	-480.93	1.97	0.00	0.00	4800
171.51	0.0318	0.7548	0.003	-752.77	1.56	0.00	0.00	-725.65	1.56	0.00	0.00	4800
171.51	0.0636	0.5433	0.001	-1511.00	15.92	0.00	0.00	-1456.70	15.92	0.00	0.00	4800
228.00	0.0159	0.9293	0.001	-325.59	0.38	0.00	0.00	-312.02	0.38	0.00	0.00	4800
228.00	0.0212	0.9068	0.002	-434.57	0.88	0.00	0.00	-416.49	0.88	0.00	0.00	4800
228.00	0.0318	0.8630	0.001	-647.04	1.46	0.00	0.00	-619.91	1.46	0.00	0.00	4800
228.00	0.0636	0.7430	0.002	-1274.30	2.51	0.00	0.00	-1220.10	2.51	0.00	0.00	4800
228.00	0.1271	0.5813	0.012	-609.99	3.25	0.00	0.00	-582.89	3.25	0.00	0.00	1200
228.00	0.1907	0.5100	0.012	-886.99	4.15	0.00	0.00	-846.33	4.15	0.00	0.00	1200
228.00	0.2543	0.6045	0.003	-1157.10	1.27	0.00	0.00	-1102.90	1.27	0.00	0.00	1200
228.00	0.3179	1.0090	0.007	-1434.40	0.81	0.00	0.00	-1366.60	0.81	0.00	0.00	1200
228.00	0.3496	1.4165	0.013	-1568.40	0.22	0.00	0.00	-1493.80	0.22	0.00	0.00	1200
228.00	0.3814	2.0200	0.025	-1694.50	1.64	0.00	0.00	-1613.20	1.64	0.00	0.00	1200
228.00	0.4132	2.8875	0.026	-1803.30	2.42	0.00	0.00	-1715.20	2.42	0.00	0.00	1200
228.00	0.4450	4.0118	0.030	-1893.70	2.60	0.00	0.00	-1798.80	2.60	0.00	0.00	1200

TABLE IV: Cassandra simulation results of TraPPE-UA ethane.

[K]	[g/cm^3]			$\left[\frac{\text{kcal}}{\text{mol}}\right]$		$\left[\frac{\text{kcal}}{\text{mol}}\right]$		$\left[\frac{\text{kcal}}{\text{mol}}\right]$		$\left[\frac{\text{kcal}}{\text{mol}}\right]$		
T	ρ	Z	$\pm$	E^{tot}	$\pm$	E^{bonded}	$\pm$	E^{vdw}	$\pm$	E^{intra}	$\pm$	N
259.42	0.4286	0.0560	0.042	-1305.70	0.49	0.00	0.00	-1271.70	0.49	0.00	0.00	600
301.54	0.4286	0.6645	0.011	-1276.10	0.92	0.00	0.00	-1242.10	0.92	0.00	0.00	600
235.56	0.4714	0.0393	0.047	-1456.30	1.20	0.00	0.00	-1418.80	1.20	0.00	0.00	600
284.78	0.4714	0.9320	0.013	-1416.30	0.51	0.00	0.00	-1378.80	0.51	0.00	0.00	600
207.11	0.5143	0.0235	0.039	-1615.90	0.80	0.00	0.00	-1575.10	0.80	0.00	0.00	600
262.95	0.5143	1.3585	0.028	-1560.20	1.13	0.00	0.00	-1519.30	1.13	0.00	0.00	600
174.46	0.5571	0.0368	0.058	-1784.80	1.37	0.00	0.00	-1740.50	1.37	0.00	0.00	600
235.02	0.5571	2.0335	0.050	-1709.40	1.74	0.00	0.00	-1665.10	1.74	0.00	0.00	600
137.97	0.6000	0.0355	0.031	-1966.70	0.63	0.00	0.00	-1919.10	0.63	0.00	0.00	600
199.49	0.6000	3.0205	0.037	-1867.50	1.04	0.00	0.00	-1819.90	1.04	0.00	0.00	600
274.79	0.0214	0.8710	0.002	-329.87	0.96	0.00	0.00	-323.07	0.96	0.00	0.00	2400
274.79	0.0286	0.8315	0.004	-440.88	1.05	0.00	0.00	-431.79	1.05	0.00	0.00	2400
274.79	0.0429	0.7490	0.004	-664.05	0.64	0.00	0.00	-650.41	0.64	0.00	0.00	2400
274.79	0.0857	0.5315	0.006	-1333.40	16.47	0.00	0.00	-1306.20	16.47	0.00	0.00	2400
360.00	0.0214	0.9258	0.002	-283.85	0.94	0.00	0.00	-277.05	0.94	0.00	0.00	2400
360.00	0.0286	0.9015	0.002	-376.75	2.12	0.00	0.00	-367.66	2.12	0.00	0.00	2400
360.00	0.0429	0.8565	0.004	-563.25	1.06	0.00	0.00	-549.61	1.06	0.00	0.00	2400
360.00	0.0857	0.7373	0.006	-1103.80	4.31	0.00	0.00	-1076.60	4.31	0.00	0.00	2400
360.00	0.1714	0.5763	0.017	-524.24	1.96	0.00	0.00	-510.62	1.96	0.00	0.00	600
360.00	0.2571	0.5178	0.020	-757.74	3.23	0.00	0.00	-737.31	3.23	0.00	0.00	600
360.00	0.3429	0.6870	0.009	-994.67	1.22	0.00	0.00	-967.42	1.22	0.00	0.00	600
360.00	0.4286	1.2093	0.010	-1241.50	0.47	0.00	0.00	-1207.40	0.47	0.00	0.00	600
360.00	0.4714	1.7380	0.018	-1361.30	1.41	0.00	0.00	-1323.80	1.41	0.00	0.00	600
360.00	0.5143	2.5470	0.026	-1475.10	1.17	0.00	0.00	-1434.20	1.17	0.00	0.00	600
360.00	0.5571	3.7083	0.016	-1572.30	0.82	0.00	0.00	-1528.10	0.82	0.00	0.00	600
360.00	0.6000	5.2710	0.052	-1649.60	2.71	0.00	0.00	-1601.90	2.71	0.00	0.00	600

TABLE V: 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	±	E^{tot}	±	E^{bonded}	±	E^{vdw}	±	E^{intra}	±	N
546.60	0.5336	-0.0918	0.023	2146.90	7.84	5648.90	9.50	-3377.00	4.68	-397.50	2.00	400
610.38	0.5336	0.7345	0.045	2762.00	4.27	6178.50	5.64	-3291.50	1.47	-388.46	4.40	400
495.91	0.5870	-0.1640	0.015	1297.40	10.02	5209.20	9.31	-3774.20	2.34	-406.11	3.83	400
577.42	0.5870	1.2368	0.035	2102.00	7.98	5906.80	7.01	-3667.30	2.15	-393.19	1.49	400
436.90	0.6404	-0.2223	0.045	279.16	8.16	4644.30	7.28	-4215.10	2.03	-409.62	3.89	400
535.33	0.6404	2.0715	0.076	1322.80	10.84	5544.40	6.88	-4071.60	3.99	-401.14	3.05	400
370.34	0.6937	-0.4023	0.080	-892.69	8.02	3970.80	6.65	-4701.00	1.56	-411.37	1.86	400
482.23	0.6937	3.4830	0.055	413.70	4.70	5078.30	4.79	-4502.10	0.62	-407.61	1.99	400
296.98	0.7471	-0.8395	0.199	-2232.60	9.13	3174.30	5.85	-5231.90	3.51	-400.28	1.80	400
415.42	0.7471	5.4290	0.123	-708.79	4.19	4441.30	5.16	-4975.10	3.99	-411.21	1.63	400
592.20	0.0267	0.8085	0.012	5418.20	5.54	6056.20	7.61	-631.68	2.56	-397.26	1.33	400
592.20	0.0356	0.7620	0.012	5343.40	5.77	6058.80	2.96	-707.07	4.86	-399.08	0.82	400
592.20	0.0534	0.6578	0.023	5177.40	9.08	6052.50	4.87	-862.54	4.36	-398.22	1.16	400
592.20	0.1067	0.3863	0.024	4717.60	27.21	6047.70	7.71	-1305.00	22.52	-395.04	5.35	400
691.00	0.0267	0.8818	0.004	6252.00	7.32	6820.80	7.64	-562.53	1.89	-376.43	3.55	400
691.00	0.0356	0.8308	0.006	6189.10	13.47	6821.70	15.42	-624.30	3.21	-373.12	8.18	400
691.00	0.0534	0.7510	0.013	6056.60	5.95	6813.30	5.89	-744.18	1.48	-370.22	6.53	400
691.00	0.1067	0.6170	0.024	5723.10	12.36	6815.90	4.42	-1067.80	9.95	-375.87	1.72	400
691.00	0.2135	0.3883	0.032	5142.50	23.80	6808.10	7.97	-1615.60	16.05	-375.93	2.30	400
691.00	0.3202	0.2998	0.049	4648.20	1.93	6810.10	4.84	-2087.00	5.97	-375.98	4.16	400
691.00	0.4269	0.5150	0.021	4101.20	5.47	6807.80	5.09	-2606.60	2.18	-374.96	5.37	400
691.00	0.5336	1.4888	0.037	3479.00	3.37	6809.80	3.58	-3205.80	1.29	-368.90	5.79	400
691.00	0.5870	2.6080	0.035	3142.30	7.75	6809.10	10.24	-3529.20	3.50	-370.94	5.43	400
691.00	0.6404	4.3133	0.109	2805.60	16.79	6811.50	16.90	-3855.90	3.06	-373.88	3.96	400
691.00	0.6937	6.8885	0.036	2495.40	6.98	6819.80	7.26	-4161.80	1.50	-365.29	4.97	400
691.00	0.7471	10.4940	0.059	2220.40	10.34	6830.00	12.61	-4434.60	3.27	-364.64	6.13	400

TABLE VI: Cassandra simulation results of TraPPE-UA isobutane.

[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
348.59	0.4784	0.0640	0.026	-648.13	1.79	320.04	1.20	-935.53	0.60	0.00	0.00	300
407.15	0.4784	0.7205	0.021	-571.51	1.86	375.48	1.52	-914.35	0.79	0.00	0.00	300
316.83	0.5263	0.0003	0.031	-794.08	2.13	291.04	1.56	-1049.20	1.06	0.00	0.00	300
384.63	0.5263	1.0867	0.033	-700.22	3.67	355.19	2.12	-1019.50	1.61	0.00	0.00	300
278.44	0.5741	0.0153	0.056	-955.54	1.17	253.28	1.27	-1169.70	1.51	0.00	0.00	300
354.93	0.5741	1.6015	0.017	-845.51	0.84	324.37	1.13	-1130.70	0.63	0.00	0.00	300
233.85	0.6220	-0.0460	0.050	-1131.80	1.60	213.25	1.16	-1302.60	0.88	0.00	0.00	300
316.47	0.6220	2.4330	0.046	-999.43	1.31	290.60	0.53	-1247.60	0.91	0.00	0.00	300
183.51	0.6698	-0.3825	0.054	-1326.60	1.05	166.73	0.88	-1447.70	0.55	0.00	0.00	300
266.92	0.6698	3.5745	0.065	-1175.40	0.28	244.25	1.29	-1373.90	1.28	0.00	0.00	300
367.02	0.0240	0.8690	0.008	272.88	2.02	335.93	1.56	-61.41	0.53	0.00	0.00	300
367.02	0.0319	0.8198	0.013	251.89	0.77	335.50	0.69	-81.43	1.00	0.00	0.00	300
367.02	0.0478	0.7368	0.010	210.47	1.07	335.89	1.00	-122.16	1.00	0.00	0.00	300
367.02	0.0957	0.4943	0.014	82.98	2.48	337.26	1.39	-247.75	2.68	0.00	0.00	300
489.36	0.0240	0.9308	0.006	403.51	3.17	454.84	3.29	-49.69	0.21	0.00	0.00	300
489.36	0.0319	0.9030	0.006	385.51	2.48	454.77	2.06	-67.08	0.49	0.00	0.00	300
489.36	0.0478	0.8640	0.005	352.29	3.16	454.44	3.20	-98.88	0.61	0.00	0.00	300
489.36	0.0957	0.7608	0.005	254.98	3.30	455.63	3.38	-194.12	1.05	0.00	0.00	300
489.36	0.1914	0.6015	0.024	71.69	3.17	455.41	2.16	-370.66	1.51	0.00	0.00	300
489.36	0.2871	0.5430	0.024	-94.27	2.31	455.56	2.62	-530.23	1.16	0.00	0.00	300
489.36	0.3827	0.7328	0.013	-273.46	1.82	455.96	2.08	-703.31	1.61	0.00	0.00	300
489.36	0.4784	1.3948	0.022	-464.47	1.79	455.17	2.57	-887.00	1.25	0.00	0.00	300
489.36	0.5263	2.0635	0.062	-558.36	3.54	456.48	2.20	-978.94	2.33	0.00	0.00	300
489.36	0.5741	3.1127	0.029	-647.51	1.32	456.85	0.93	-1065.20	0.55	0.00	0.00	300
489.36	0.6220	4.5415	0.044	-732.74	4.05	454.80	3.21	-1145.10	1.37	0.00	0.00	300
489.36	0.6698	6.5442	0.041	-797.36	2.40	456.93	1.27	-1208.60	1.96	0.00	0.00	300

TABLE VII: Cassandra simulation results of TraPPE-UA isohexane.

[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
421.04	0.5093	-0.0243	0.031	-246.92	4.12	682.75	2.57	-897.34	1.57	-51.92	0.97	200
476.00	0.5093	0.6258	0.058	-133.79	1.82	776.31	0.88	-877.78	1.14	-47.94	2.55	200
382.27	0.5602	-0.0418	0.089	-420.59	3.18	618.74	2.94	-1003.80	1.39	-51.31	0.69	200
450.19	0.5602	0.9870	0.110	-276.88	2.98	736.47	2.12	-977.79	0.97	-48.50	2.24	200
336.12	0.6112	-0.1500	0.029	-619.26	1.38	539.81	1.43	-1120.30	0.81	-53.51	0.95	200
416.52	0.6112	1.5350	0.093	-444.33	3.01	679.94	1.11	-1085.50	2.26	-51.02	0.19	200
283.16	0.6621	-0.2815	0.058	-840.16	2.70	449.29	2.21	-1247.40	0.79	-54.55	0.79	200
373.26	0.6621	2.5400	0.091	-634.88	2.97	604.34	1.94	-1197.20	1.68	-51.90	0.47	200
223.97	0.7130	-0.4680	0.063	-1083.00	0.45	346.21	0.50	-1384.00	0.69	-55.19	0.71	200
317.89	0.7130	3.9067	0.080	-857.42	1.81	507.50	0.99	-1319.70	0.90	-53.86	0.82	200
447.93	0.0255	0.8523	0.009	2484.60	7.36	2927.10	6.84	-436.04	0.69	-199.34	1.92	800
447.93	0.0340	0.8020	0.010	2408.00	2.83	2928.70	3.58	-512.07	1.42	-199.11	0.37	800
447.93	0.0509	0.7063	0.009	2245.50	8.17	2928.60	5.51	-670.21	3.86	-200.15	1.92	800
447.93	0.1019	0.4858	0.016	1774.30	20.05	2923.50	8.40	-1123.30	18.23	-198.57	1.31	800
547.47	0.0255	0.9068	0.006	3189.50	0.42	3570.40	2.25	-374.42	2.02	-177.17	0.80	800
547.47	0.0340	0.8780	0.005	3117.60	2.56	3566.40	1.05	-440.13	1.77	-180.69	0.74	800
547.47	0.0509	0.8243	0.006	2996.60	5.22	3572.90	5.49	-563.37	0.31	-183.15	2.70	800
547.47	0.1019	0.6748	0.009	2623.60	5.88	3570.60	3.72	-921.09	3.57	-180.24	3.61	800
547.47	0.2037	0.4728	0.023	486.46	1.61	892.03	2.67	-392.64	2.78	-45.15	1.84	200
547.47	0.3056	0.4145	0.049	336.87	2.16	890.49	2.70	-534.22	2.37	-45.02	0.78	200
547.47	0.4074	0.5418	0.046	182.00	3.93	892.48	3.37	-684.62	1.39	-44.17	2.70	200
547.47	0.5093	1.2415	0.033	4.26	4.36	891.45	3.71	-854.86	1.49	-42.82	1.22	200
547.47	0.5602	1.9972	0.030	-86.21	2.99	891.50	3.91	-942.15	1.13	-44.38	1.86	200
547.47	0.6112	3.1675	0.096	-176.90	6.71	891.86	4.99	-1030.00	2.10	-44.27	1.08	200
547.47	0.6621	4.8715	0.037	-257.62	1.92	894.60	0.63	-1110.20	1.50	-44.57	0.88	200
547.47	0.7130	7.3948	0.112	-326.69	3.55	894.79	1.87	-1176.20	3.75	-43.86	2.56	200

TABLE VIII: GROMACS 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	E^{tot}	E^{bonded}	E^{vdw}	E^{intra}	N
259.38	0.4286	0.0646	-1306.40	0.00	-1272.34	0.00	600
301.48	0.4286	0.6455	-1276.91	0.00	-1242.85	0.00	600
235.32	0.4714	0.0435	-1455.46	0.00	-1417.99	0.00	600
284.78	0.4714	0.9208	-1416.45	0.00	-1378.99	0.00	600
207.11	0.5143	0.0324	-1615.47	0.00	-1574.60	0.00	600
262.94	0.5143	1.3748	-1560.07	0.00	-1519.20	0.00	600
174.46	0.5571	0.0494	-1784.86	0.00	-1740.59	0.00	600
235.11	0.5571	2.0381	-1709.51	0.00	-1665.24	0.00	600
138.01	0.6000	0.0024	-1967.50	0.00	-1919.82	0.00	600
199.47	0.6000	3.0080	-1867.76	0.00	-1820.08	0.00	600
274.75	0.0214	0.8648	-494.67	0.00	-484.46	0.00	3600
274.81	0.0286	0.8252	-662.24	0.00	-648.60	0.00	3600
274.79	0.0429	0.7465	-988.74	0.00	-968.28	0.00	3600
274.77	0.0857	0.5281	-1985.60	0.00	-1944.73	0.00	3600
359.97	0.0214	0.9237	-422.31	0.00	-412.11	0.00	3600
359.95	0.0286	0.8981	-563.63	0.00	-549.99	0.00	3600
359.98	0.0429	0.8554	-843.19	0.00	-822.73	0.00	3600
359.99	0.0857	0.7379	-1647.05	0.00	-1606.19	0.00	3600
360.11	0.1714	0.5735	-522.35	0.00	-508.72	0.00	600
359.93	0.2571	0.5198	-757.14	0.00	-736.71	0.00	600
359.98	0.3429	0.6569	-994.61	0.00	-967.35	0.00	600
359.84	0.4286	1.2086	-1240.44	0.00	-1206.37	0.00	600
359.99	0.4714	1.7497	-1360.83	0.00	-1323.36	0.00	600
360.01	0.5143	2.5589	-1473.55	0.00	-1432.68	0.00	600
359.88	0.5571	3.7067	-1571.94	0.00	-1527.67	0.00	600
360.05	0.6000	5.2765	-1648.66	0.00	-1600.97	0.00	600

TABLE IX: GROMACS simulation results of TraPPE-UA isobutane

[K]	[g/cm^3]			
T	ρ	Z	U^{dep}	N
184.00	0.6734	-0.2603	-13.67	300
267.00	0.6734	3.7086	-8.94	300
232.00	0.6253	-0.1424	-9.78	300
315.00	0.6253	2.4430	-6.90	300
276.00	0.5772	-0.0698	-7.39	300
353.00	0.5772	1.6294	-5.58	300
315.00	0.5291	-0.0271	-5.81	300
383.00	0.5291	1.0644	-4.64	300
347.00	0.4810	0.0107	-4.71	300
406.00	0.4810	0.7182	-3.93	300
489.00	0.0962	0.7376	-0.69	300
489.00	0.1924	0.5767	-1.31	300
489.00	0.2886	0.5474	-1.90	300
489.00	0.3848	0.7335	-2.51	300
489.00	0.4810	1.4208	-3.16	300
489.00	0.5291	2.0977	-3.49	300
489.00	0.5772	3.1310	-3.80	300
489.00	0.6253	4.6048	-4.09	300
489.00	0.6734	6.6846	-4.31	300

TABLE X: GROMACS simulation results of TraPPE-UA n-dodecane.

[K]	[g/cm^3]			
T	ρ	Z	U^{dep}	N
546.61	0.5336	-0.1193	-7.13	400
610.26	0.5336	0.7008	-6.24	400
495.80	0.5870	-0.1642	-8.90	400
577.29	0.5870	1.1938	-7.42	400
436.81	0.6404	-0.2707	-11.40	400
535.32	0.6404	2.0699	-8.97	400
370.40	0.6937	-0.4648	-15.11	400
482.25	0.6937	3.4362	-11.11	400
297.12	0.7471	-0.7890	-21.19	400
415.49	0.7471	5.4379	-14.33	400
592.19	0.0267	0.7787	-0.50	800
592.21	0.0356	0.7105	-0.66	800
592.19	0.0534	0.6150	-0.97	800
592.32	0.1067	0.3710	-1.85	800
691.06	0.0267	0.8393	-0.34	800
690.96	0.0356	0.8043	-0.46	800
691.14	0.0534	0.7456	-0.68	800
691.10	0.1067	0.5513	-1.26	800
691.18	0.2135	0.3253	-2.29	400
690.90	0.3202	0.2555	-3.22	400
690.90	0.4269	0.4966	-4.24	400
691.12	0.5336	1.4953	-5.37	400
691.00	0.5870	2.5720	-6.01	400
691.00	0.6404	4.3033	-6.60	400
690.74	0.6937	6.8075	-7.20	400
691.11	0.7471	10.4604	-7.71	400

TABLE XI: GOMC simulation results of TraPPE-UA 1-phenanthrenyl, 4-naphthalenyl butane

[K]	[g/cm^3]			[$\frac{kcal}{mol}$]		[$\frac{kcal}{mol}$]		[$\frac{kcal}{mol}$]		[$\frac{kcal}{mol}$]		
T	ρ	Z	±	E^{tot}	±	E^{bonded}	±	E^{vdw}	±	E^{intra}	±	N
1068.30	0.7143	1.6686	0.090	-1033.00	15.63	927.11	10.74	-1776.80	6.16	-412.58	3.94	100
897.19	0.7143	-0.0338	0.166	-1199.20	23.04	825.00	20.34	-1840.80	3.30	-413.57	7.67	100
1007.10	0.7857	2.4437	0.130	-1291.10	17.14	882.20	14.06	-1971.60	11.00	-407.71	4.04	100
814.09	0.7857	0.0765	0.139	-1472.40	13.92	772.32	3.87	-2043.00	11.45	-413.38	6.67	100
728.82	0.8571	0.2752	0.357	-1762.40	20.03	725.89	11.68	-2268.20	13.25	-415.69	5.36	100
939.12	0.8571	4.1479	0.302	-1541.40	22.75	853.86	15.65	-2175.20	7.52	-410.59	10.21	100
602.37	0.9286	-0.2570	0.506	-2155.00	8.22	615.28	5.25	-2531.80	6.60	-413.41	0.60	100
827.24	0.9286	6.0287	0.337	-1880.40	10.10	772.29	17.47	-2414.20	10.58	-411.00	5.24	100
486.63	1.0000	-0.4291	0.315	-2549.50	16.36	522.80	15.24	-2815.50	10.47	-407.97	3.45	100
711.10	1.0000	8.8936	0.586	-2228.70	23.30	691.25	26.45	-2663.20	5.68	-408.49	0.86	100
1320.00	0.0357	0.9304	0.016	2301.80	11.85	4232.20	10.61	-1893.80	1.26	-1611.00	1.50	400
1320.00	0.0476	0.9090	0.012	2186.60	13.16	4222.90	13.47	-1987.40	1.11	-1611.80	2.73	400
1320.00	0.0714	0.8665	0.004	1994.30	23.62	4229.20	16.01	-2161.60	9.15	-1614.30	7.77	400
1320.00	0.1429	0.7612	0.011	1424.60	19.93	4232.30	6.26	-2661.00	16.86	-1607.10	3.83	400
1320.00	0.2857	0.6646	0.052	80.91	13.20	1052.50	3.39	-898.21	9.99	-401.82	0.68	100
1320.00	0.4286	0.8130	0.062	-187.00	13.26	1053.30	4.05	-1130.20	9.56	-402.42	1.30	100
1320.00	0.5714	1.3929	0.074	-488.48	17.95	1057.70	12.96	-1399.50	8.27	-400.93	0.80	100
1320.00	0.7143	3.2638	0.189	-835.95	22.40	1055.80	22.28	-1708.30	0.84	-402.60	6.95	100
1320.00	0.7857	4.8092	0.034	-1019.50	6.47	1049.30	4.55	-1867.10	4.07	-397.29	6.28	100
1320.00	0.8571	7.3940	0.163	-1220.20	25.82	1043.30	25.99	-2043.50	3.75	-394.11	9.96	100
1320.00	0.9286	11.3790	0.150	-1393.70	9.47	1045.90	10.25	-2201.20	19.48	-401.07	3.02	100
1320.00	1.0000	17.0990	0.720	-1530.60	11.12	1056.50	15.30	-2330.30	4.29	-391.98	7.13	100
990.00	0.0357	0.8179	0.003	1382.70	13.94	3541.30	9.20	-2121.90	6.36	-1662.70	1.52	400
990.00	0.0476	0.7600	0.017	1234.30	12.08	3552.50	18.20	-2269.30	6.19	-1665.70	2.39	400
990.00	0.0714	0.6650	0.013	926.27	17.00	3543.50	7.95	-2543.90	10.91	-1661.10	3.12	400
990.00	0.1429	0.4478	0.029	108.20	174.04	3547.20	30.28	-3292.30	144.22	-1657.50	10.97	400

II. TABLES OF EXAMPLE SIMULATIONS RESULTS

TABLE XII: Mie-UA n-dodecane

	[K]		[MPa]		[g/cm^3]	[g/cm^3]		[kJ/mol]	
T_r^{sat}	T^{sat}	±	P^{sat}	±	ρ_{liq}	ρ_{vap}	±	ΔH_v	±
0.84	555.05	0.46	0.3789	0.0035	0.5336	0.01647	0.00017	39.12	0.03
0.76	498.11	0.74	0.1163	0.0021	0.5870	0.00512	0.00009	45.39	0.03
0.67	439.23	0.27	0.0222	0.0002	0.6404	0.00106	0.00001	51.37	0.02
0.56	368.94	0.22	0.0013	0.0000	0.6937	0.000070	0.0000008	57.37	0.04
0.45	296.11	0.61	0.0000097	0.0000005	0.7471	0.00000067	0.00000004	64.11	0.04

TABLE XIII: TIP4P/2005 water

	[K]		[MPa]		[g/cm^3]	[g/cm^3]		[kJ/mol]	
T_r^{sat}	T^{sat}	±	P^{sat}	±	ρ_{liq}	ρ_{vap}	±	ΔH_v	±
0.87	562.08	1.29	4.2904	0.0765	0.7129	0.02007	0.00032	33.76	0.04
0.81	524.66	0.73	2.3085	0.0308	0.7841	0.01113	0.00015	36.65	0.04
0.74	476.44	0.64	0.8604	0.0126	0.8554	0.00421	0.00006	40.32	0.03
0.63	408.18	0.60	0.1336	0.0025	0.9267	0.00072	0.00001	44.33	0.03
0.46	296.42	0.22	0.0007	0.0000	0.9980	0.000005	0.000000	50.40	0.01

TABLE XIV: TraPPE-UA methane

	[K]		[MPa]		[g/cm^3]	[g/cm^3]		[kJ/mol]	
T_r^{sat}	T^{sat}	±	P^{sat}	±	ρ_{liq}	ρ_{vap}	±	ΔH_v	±
0.88	167.56	0.18	2.1791	0.0154	0.3179	0.036	0.000	5.41	0.01
0.80	152.49	0.14	1.1963	0.0075	0.3496	0.0185	0.0001	6.44	0.00
0.71	135.76	0.08	0.5344	0.0024	0.3814	0.0084	0.0000	7.26	0.00
0.61	116.03	0.11	0.1532	0.0012	0.4132	0.00266	0.00002	7.95	0.00
0.50	95.35	0.06	0.0228	0.0002	0.4450	0.00047	0.00000	8.55	0.00

TABLE XV: TraPPE-UA ethane

	[K]		[MPa]		[g/cm^3]	[g/cm^3]		[kJ/mol]	
T_r^{sat}	T^{sat}	±	P^{sat}	±	ρ_{liq}	ρ_{vap}	±	ΔH_v	±
0.85	259.10	0.12	2.002000	0.006116	0.4286	0.03791500	0.00014413	9.594	0.007
0.77	234.56	0.09	1.016900	0.002912	0.4714	0.01853900	0.00005394	11.252	0.002
0.68	206.81	0.07	0.392300	0.001143	0.5143	0.00744330	0.00002068	12.625	0.001
0.57	173.63	0.07	0.083227	0.000328	0.5571	0.00177920	0.00000645	13.798	0.001
0.45	137.54	0.05	0.005918	0.000026	0.6000	0.00015609	0.00000064	14.852	0.001

TABLE XVI: TraPPE-UA *n*-dodecane

	[K]		[MPa]		[g/cm^3]	[g/cm^3]		[kJ/mol]	
T_r^{sat}	T^{sat}	±	P^{sat}	±	ρ_{liq}	ρ_{vap}	±	ΔH_v	±
0.84	555.32	0.25	0.4842	0.0048	0.5336	0.0222	0.0003	34.48	0.17
0.77	505.25	0.13	0.1875	0.0015	0.5870	0.0084	0.0001	40.29	0.16
0.68	445.13	0.28	0.0397	0.0005	0.6404	0.0019	0.0000	45.65	0.08
0.58	379.79	0.29	0.0044	0.0001	0.6937	0.00024	0.00000	50.70	0.03
0.47	309.17	0.31	0.000101	0.000002	0.7471	0.0000067	0.0000001	55.22	0.02

TABLE XVII: TraPPE-UA isobutane

	[K]		[MPa]		[g/cm^3]	[g/cm^3]		[kJ/mol]	
T_r^{sat}	T^{sat}	±	P^{sat}	±	ρ_{liq}	ρ_{vap}	±	ΔH_v	±
0.85	348.50	0.12	1.4228	0.0051	0.4784	0.0375	0.0002	14.326	0.019
0.78	317.29	0.13	0.7225	0.0027	0.5263	0.0186	0.0001	16.663	0.005
0.68	278.17	0.10	0.2476	0.0008	0.5741	0.0067	0.0000	18.731	0.002
0.58	234.94	0.11	0.0482	0.0002	0.6220	0.00146	0.00001	20.590	0.001
0.46	188.68	0.04	0.0031	0.0000	0.6698	0.000117	0.000000	22.348	0.001

TABLE XVIII: TraPPE-UA isohexane

	[K]		[MPa]		[g/cm^3]	[g/cm^3]		[kJ/mol]	
T_r^{sat}	T^{sat}	±	P^{sat}	±	ρ_{liq}	ρ_{vap}	±	ΔH_v	±
0.86	426.63	0.42	1.1097	0.0118	0.5093	0.03588	0.00057	19.16	0.07
0.78	386.02	0.77	0.4994	0.0081	0.5602	0.01540	0.00025	22.63	0.02
0.69	342.25	0.20	0.1704	0.0013	0.6112	0.00548	0.00005	25.57	0.02
0.58	289.73	0.22	0.0290	0.0003	0.6621	0.00105	0.00001	28.17	0.01
0.46	230.63	0.15	0.0012	0.0000	0.7130	0.000054	0.000001	30.70	0.01

TABLE XIX: TraPPE-UA ethane (Gromacs)

	[K]	[MPa]	[g/cm^3]	[g/cm^3]	[kJ/mol]
T_r^{sat}	T^{sat}	P^{sat}	ρ_{liq}	ρ_{vap}	ΔH_v
0.85	259.46	2.0250	0.4286	0.03935	9.47
0.77	234.86	1.0187	0.4714	0.01865	11.23
0.68	206.51	0.3850	0.5143	0.00730	12.64
0.57	173.49	0.0817	0.5571	0.00174	13.81
0.45	137.98	0.0061	0.6000	0.00016	14.86

TABLE XX: TraPPE-UA isobutane (Gromacs)

	[K]	[MPa]	[g/cm^3]	[g/cm^3]	[kJ/mol]
T_r^{sat}	T^{sat}	P^{sat}	ρ_{liq}	ρ_{vap}	ΔH_v
0.86	350.57	1.4574	0.4810	0.0381	14.40
0.78	317.87	0.7209	0.5291	0.0185	16.74
0.68	278.73	0.2486	0.5772	0.0067	18.82
0.58	235.22	0.0477	0.6253	0.0015	20.68
0.46	187.41	0.0028	0.6734	0.0001	22.43

TABLE XXI: TraPPE-UA n-dodecane (Gromacs)

	[K]	[MPa]	[g/cm^3]	[g/cm^3]	[kJ/mol]
T_r^{sat}	T^{sat}	P^{sat}	ρ_{liq}	ρ_{vap}	ΔH_v
0.85	557.28	0.4853	0.5336	0.0220	33.99
0.77	505.15	0.1844	0.5870	0.0083	39.48
0.68	446.23	0.0447	0.6404	0.0021	44.59
0.58	380.32	0.00476	0.6937	0.00026	49.48
0.47	307.34	0.000093	0.7471	0.000006	54.69

TABLE XXII: TraPPE-UA 1-phenanthrenyl, 4-naphthalenyl butane (GOMC)

[K]		[MPa]		[g/cm^3]	[g/cm^3]		[kJ/mol]	
T^{sat}	±	P^{sat}	±	ρ_{liq}	ρ_{vap}	±	ΔH_v	±
899.59	1.34	0.2853	0.0052	0.7143	0.0156	0.0003	71.574	0.069
809.90	0.95	0.0785	0.0012	0.7857	0.0044	0.0001	82.465	0.066
717.69	1.57	0.0144	0.0005	0.8571	0.0009	0.0000	92.112	0.099
608.31	1.37	0.0007	0.0000	0.9286	0.00005	0.00000	103.510	0.043
493.44	0.55	0.0000	0.0000	1.0000	0.000000	0.000000	114.680	0.062

III. FIGURES OF EXAMPLE SIMULATIONS

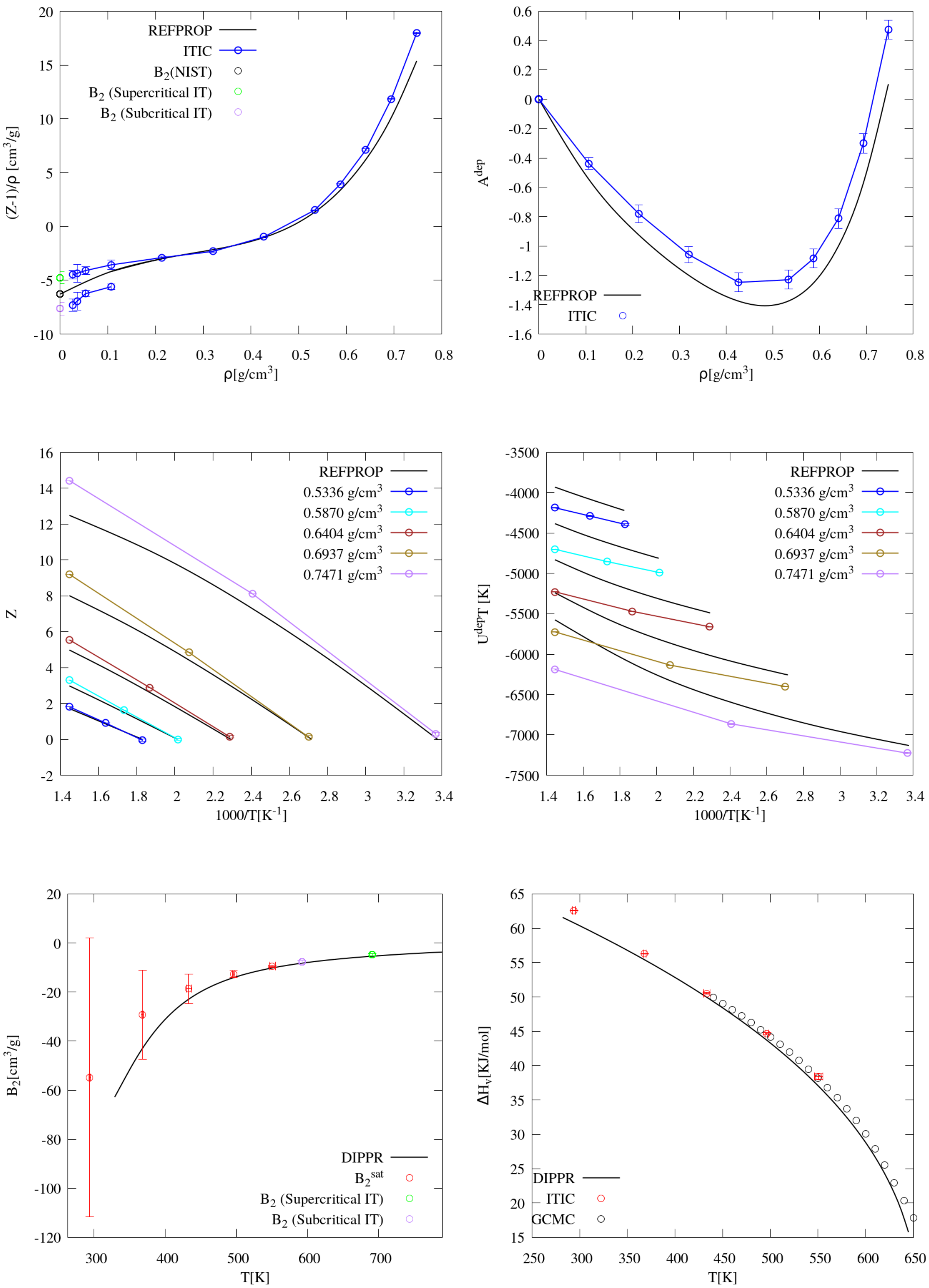

FIG. 1: Mie-UA n-dodecane

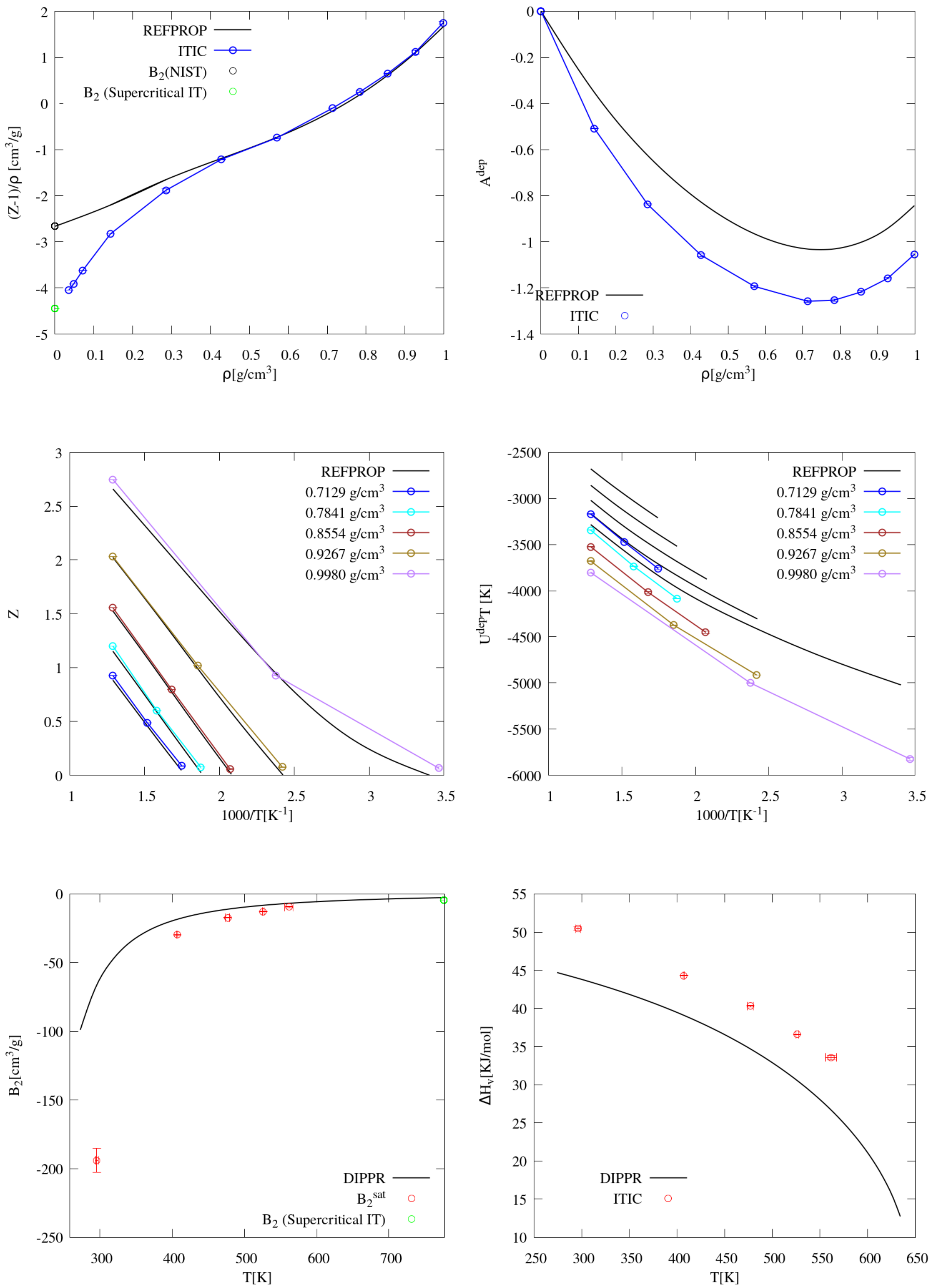

FIG. 2: TIP4P/2005 water

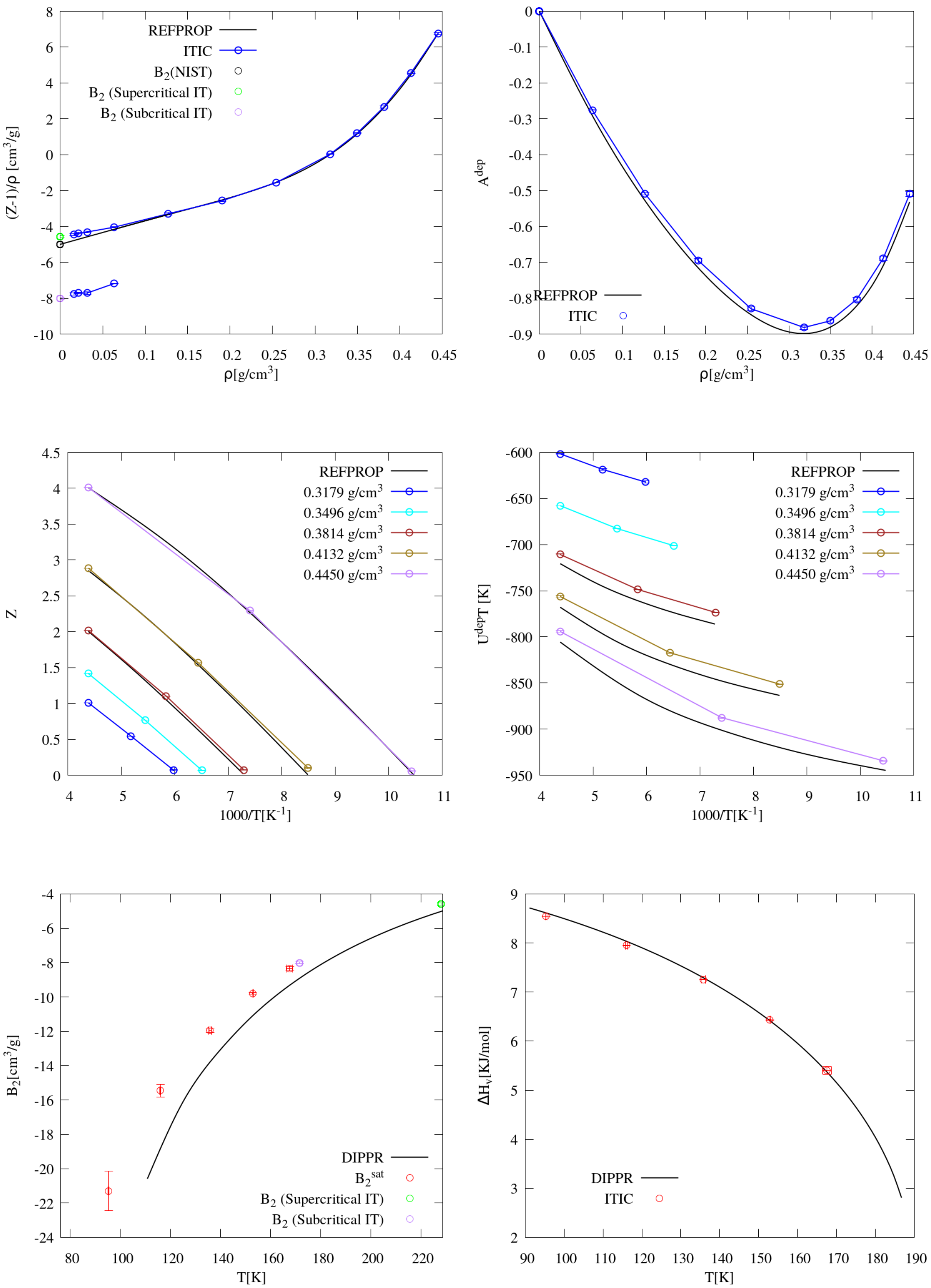

FIG. 3: TraPPE-UA methane

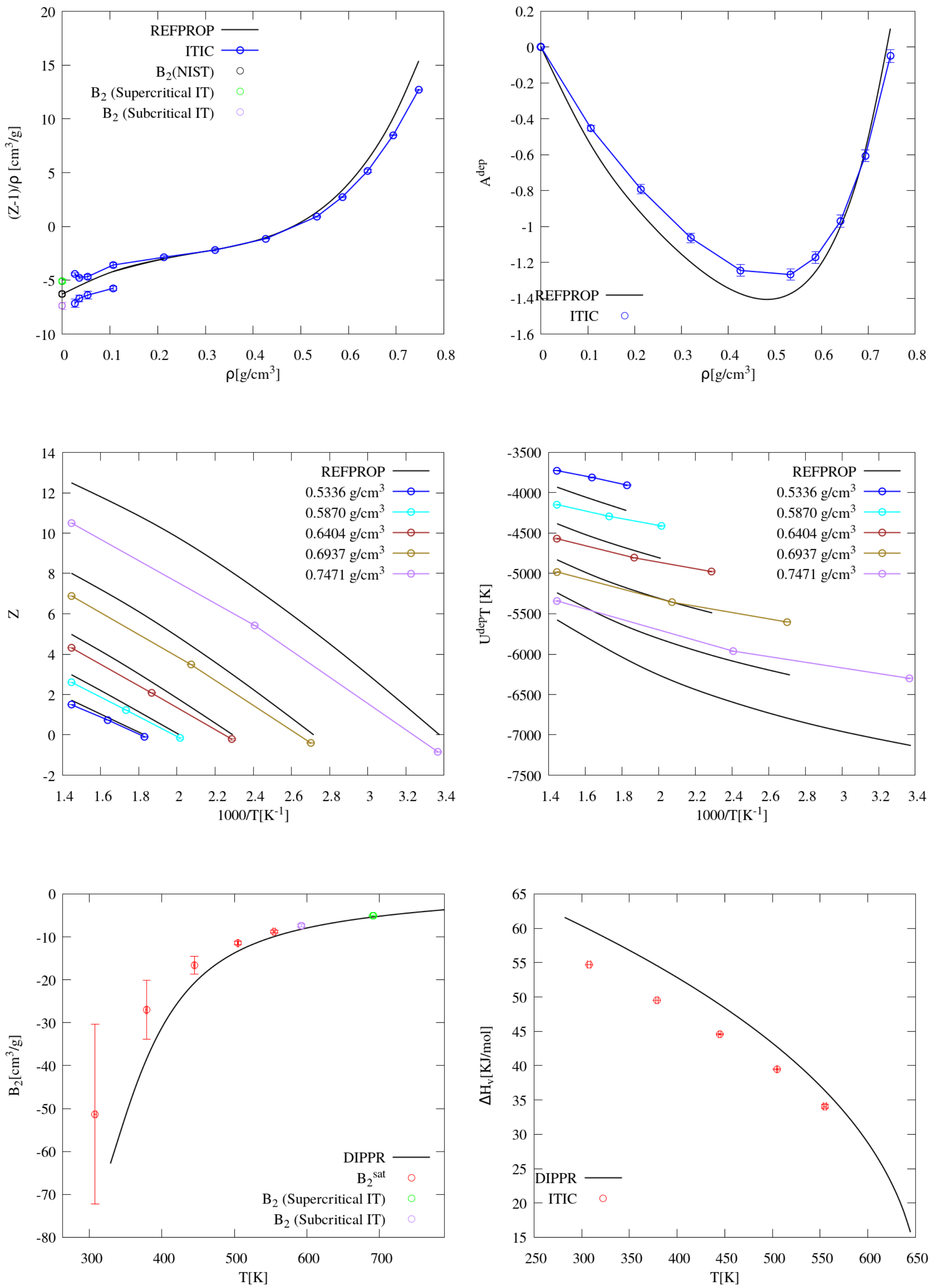

FIG. 4: TraPPE-UA *n*-dodecane

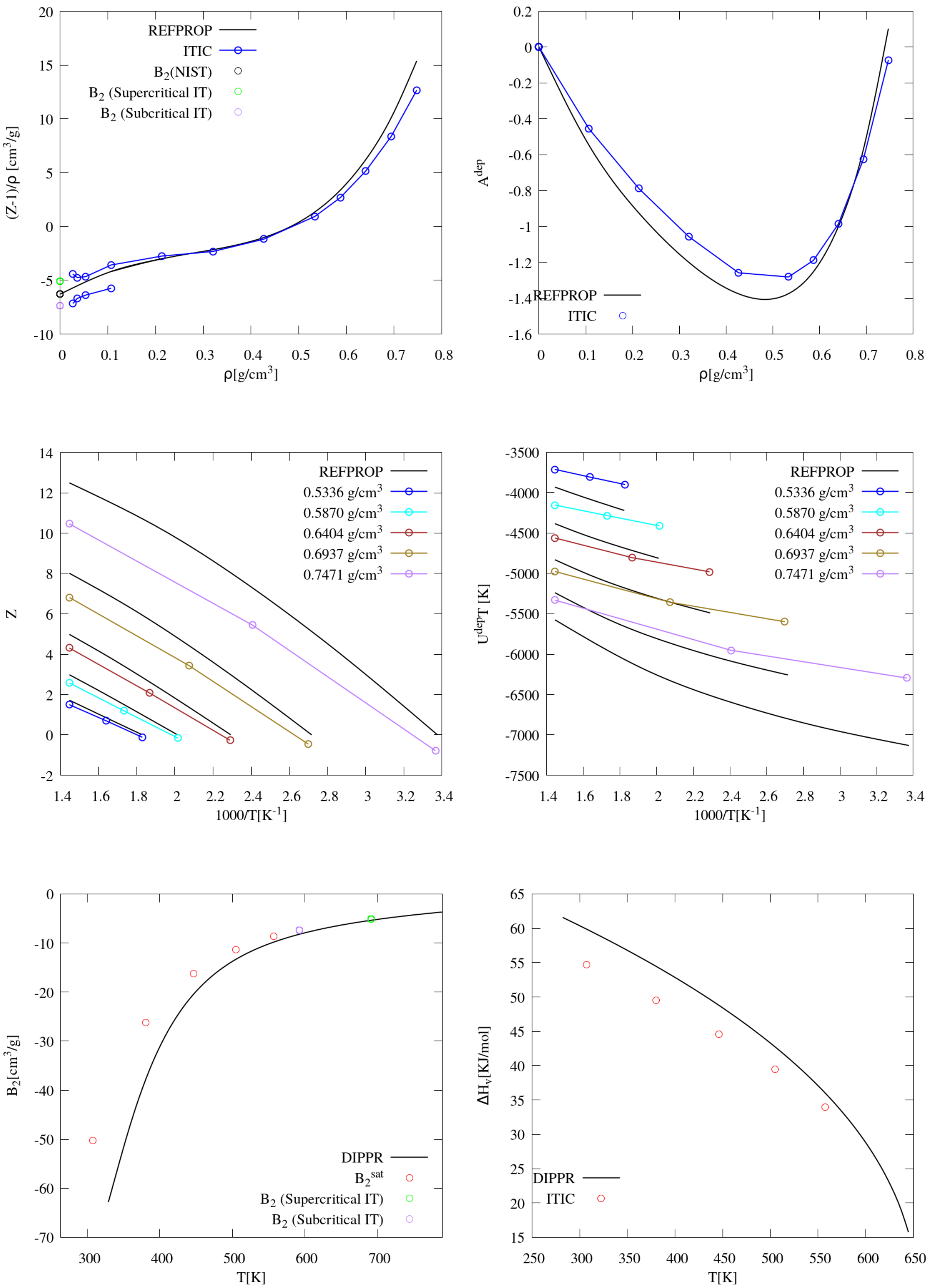

FIG. 5: TraPPE-UA n-dodecane (Gromacs)

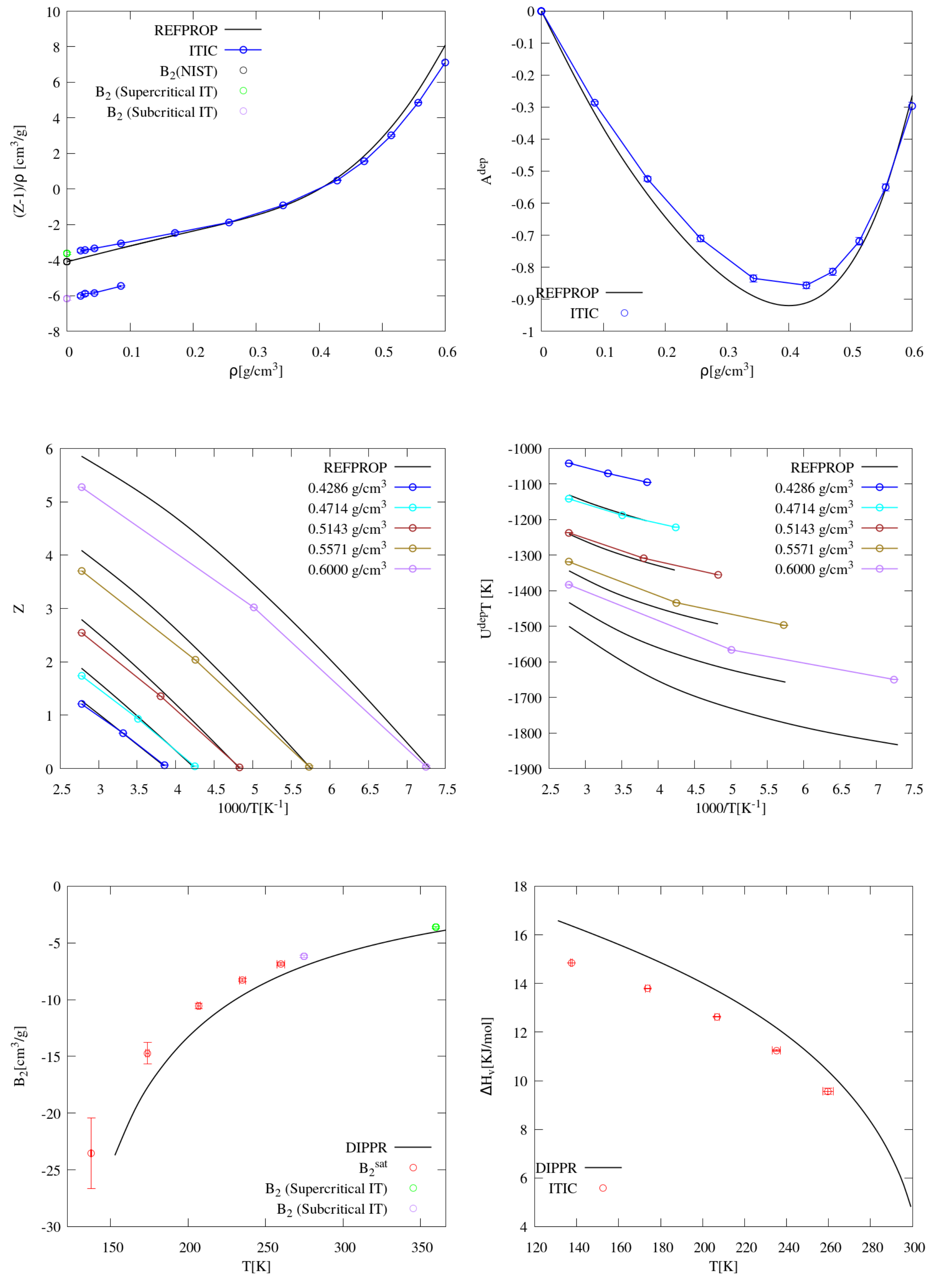

FIG. 6: TraPPE-UA ethane

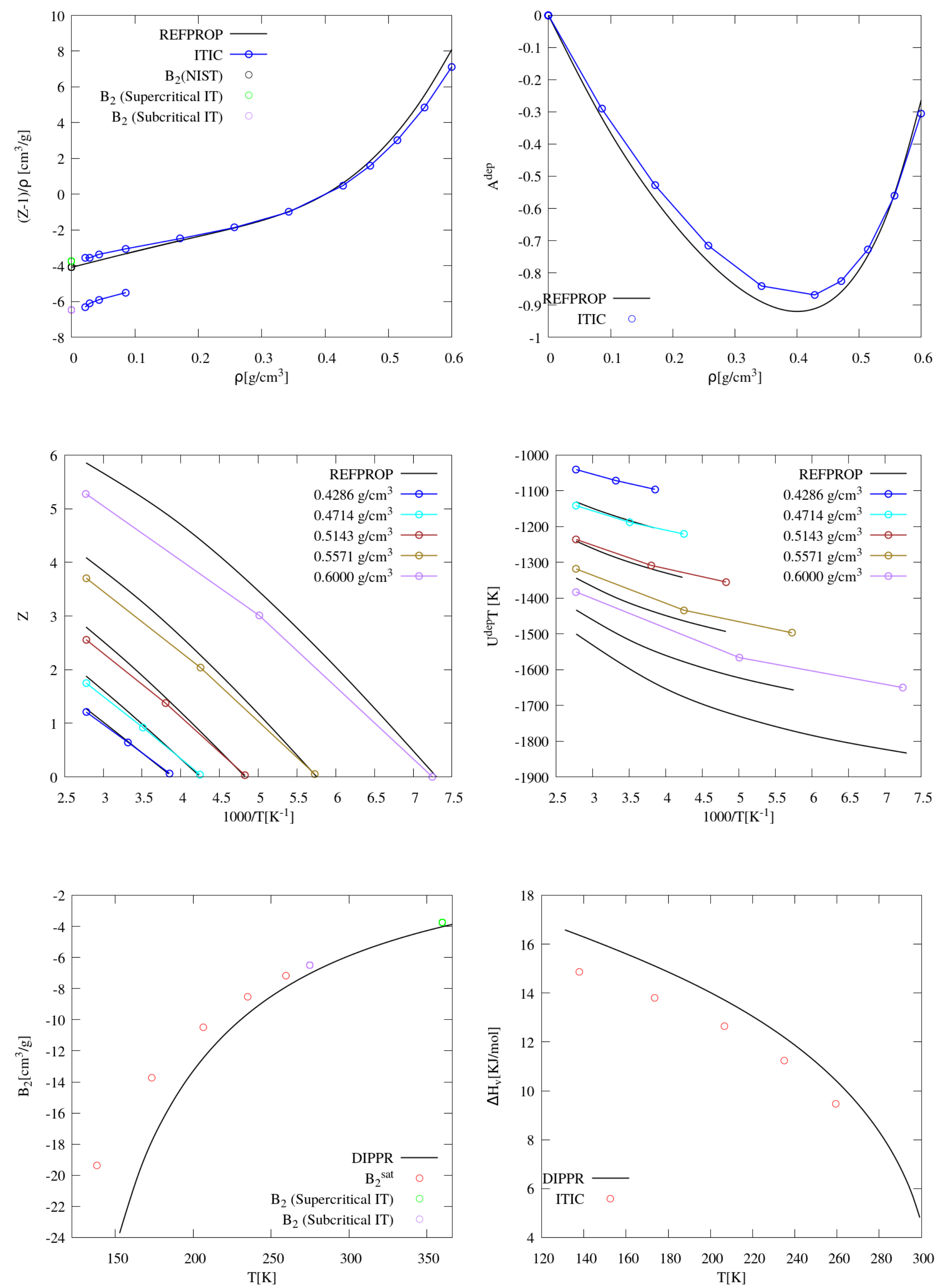

FIG. 7: TraPPE-UA ethane (Gromacs)

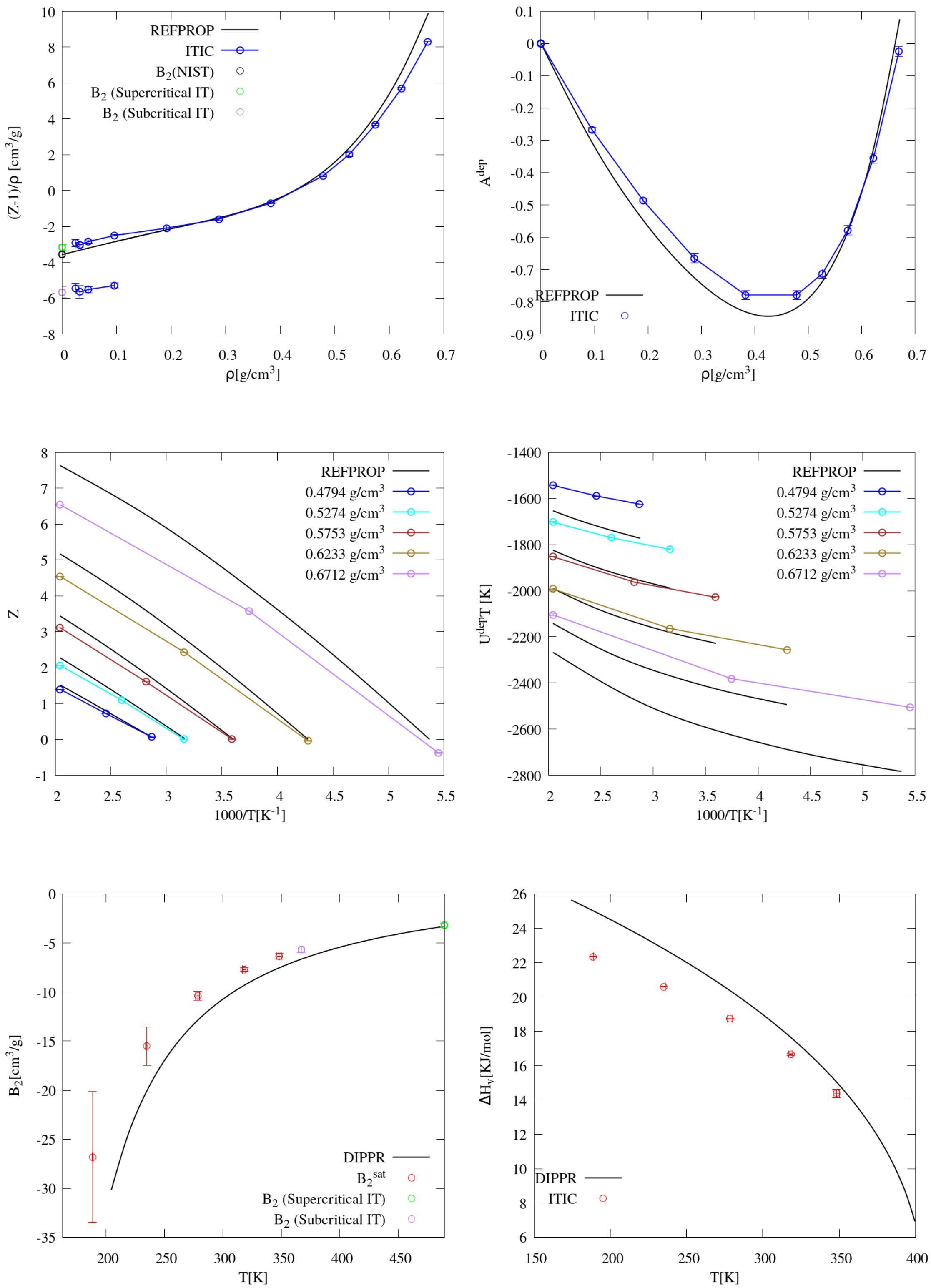

FIG. 8: TraPPE-UA isobutane

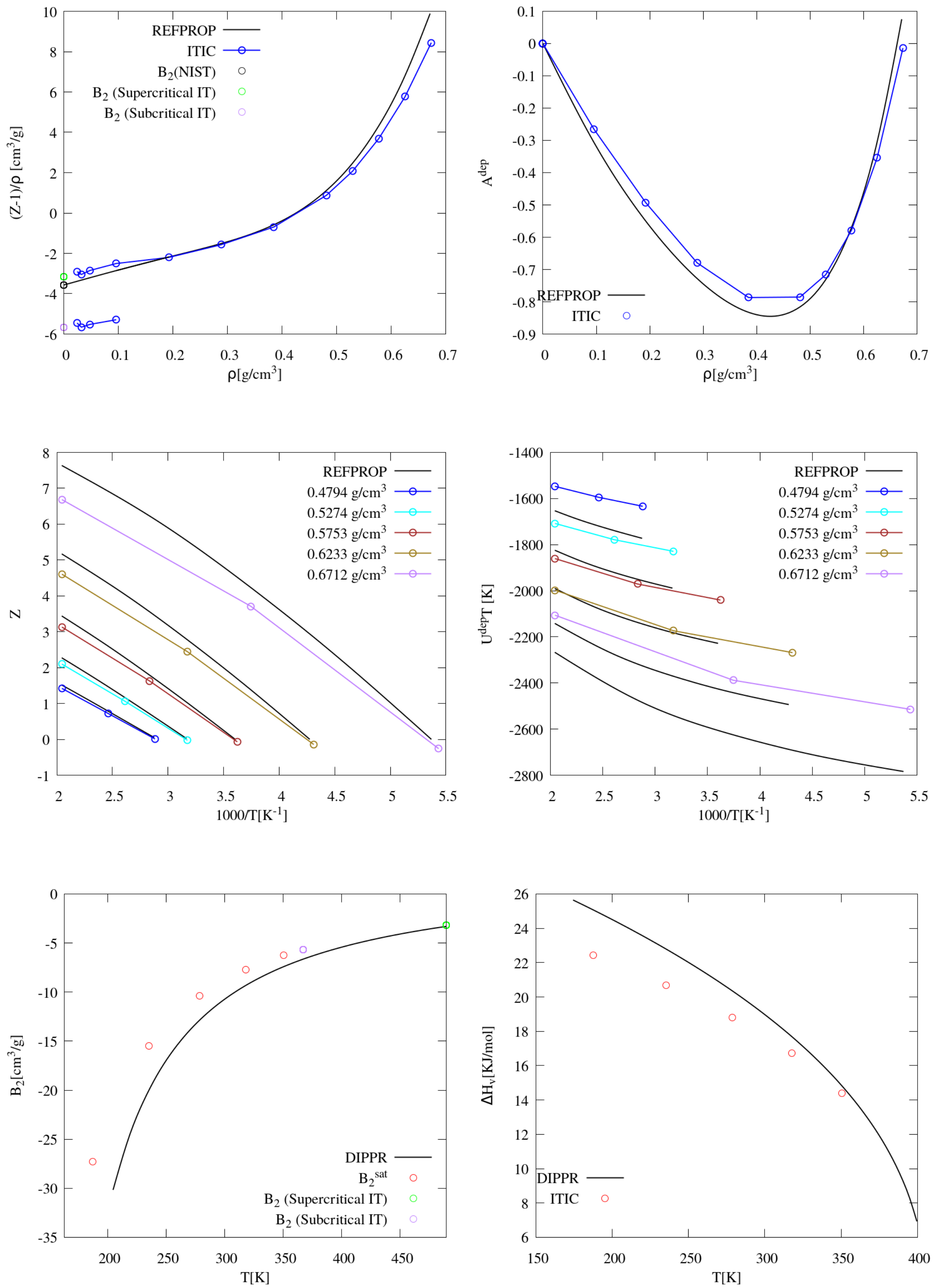

FIG. 9: TraPPE-UA isobutane (Gromacs)

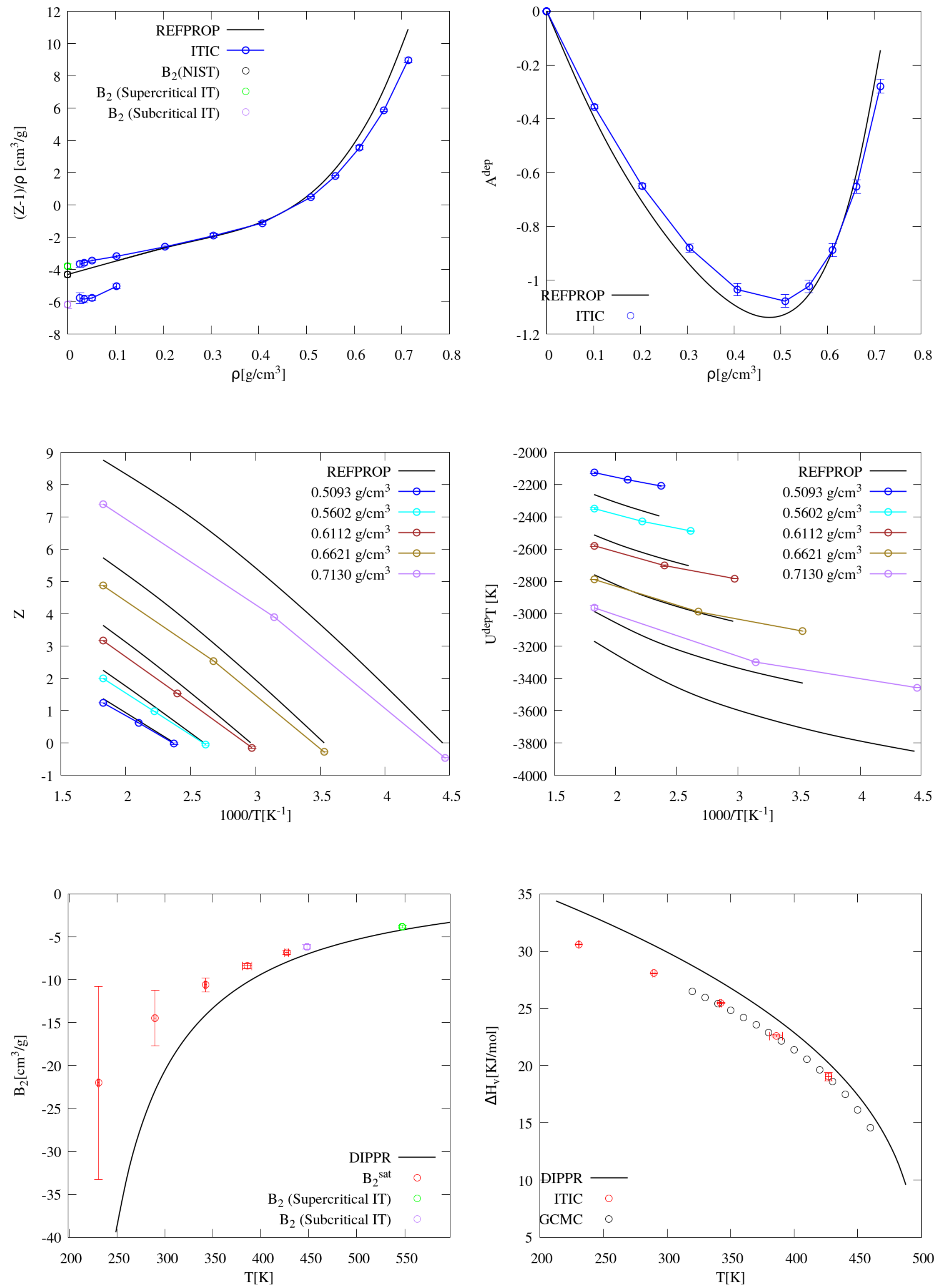

FIG. 10: TraPPE-UA isohexane (Gromacs)

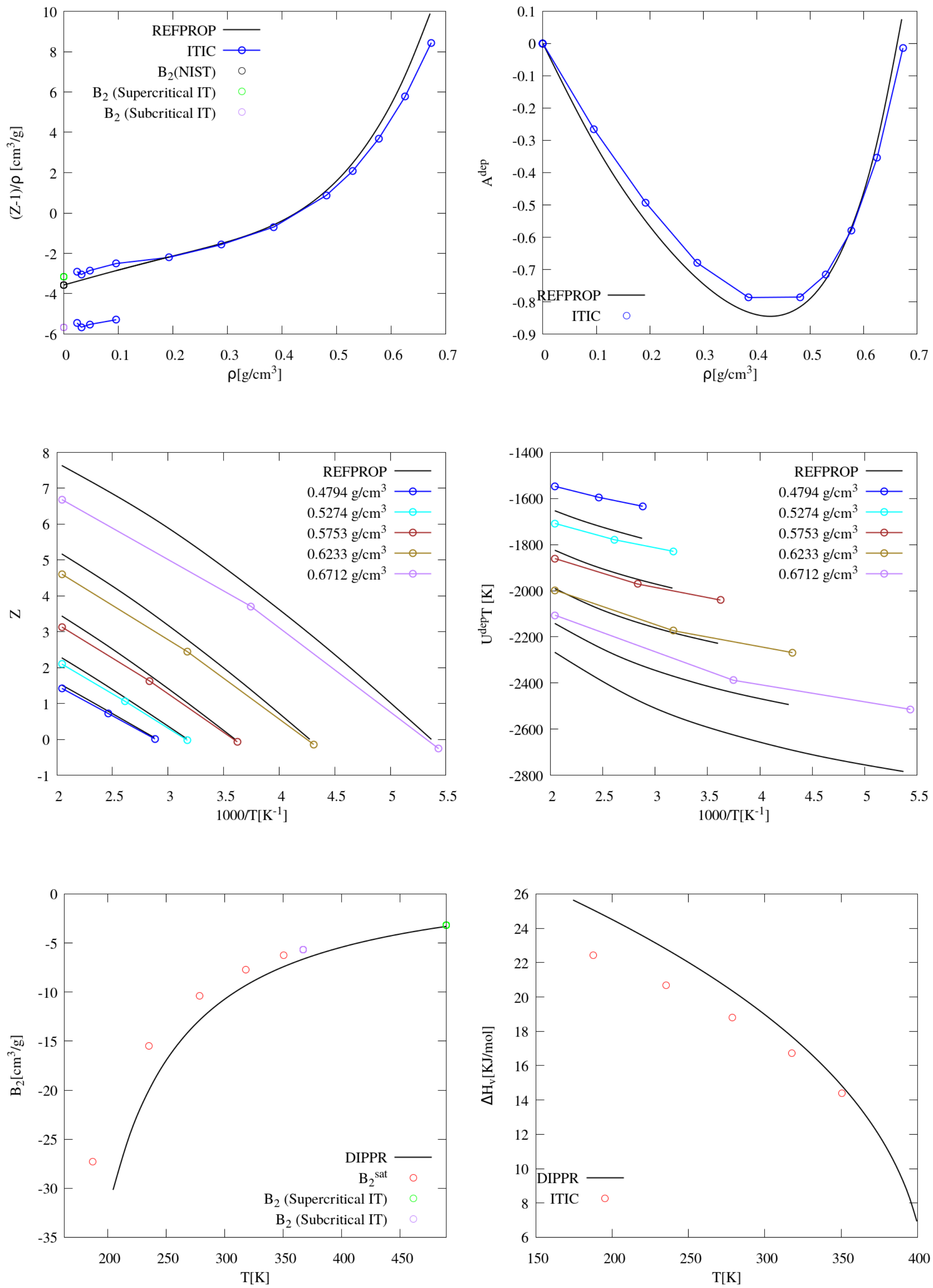

FIG. 11: TraPPE-UA isobutane (Gromacs)

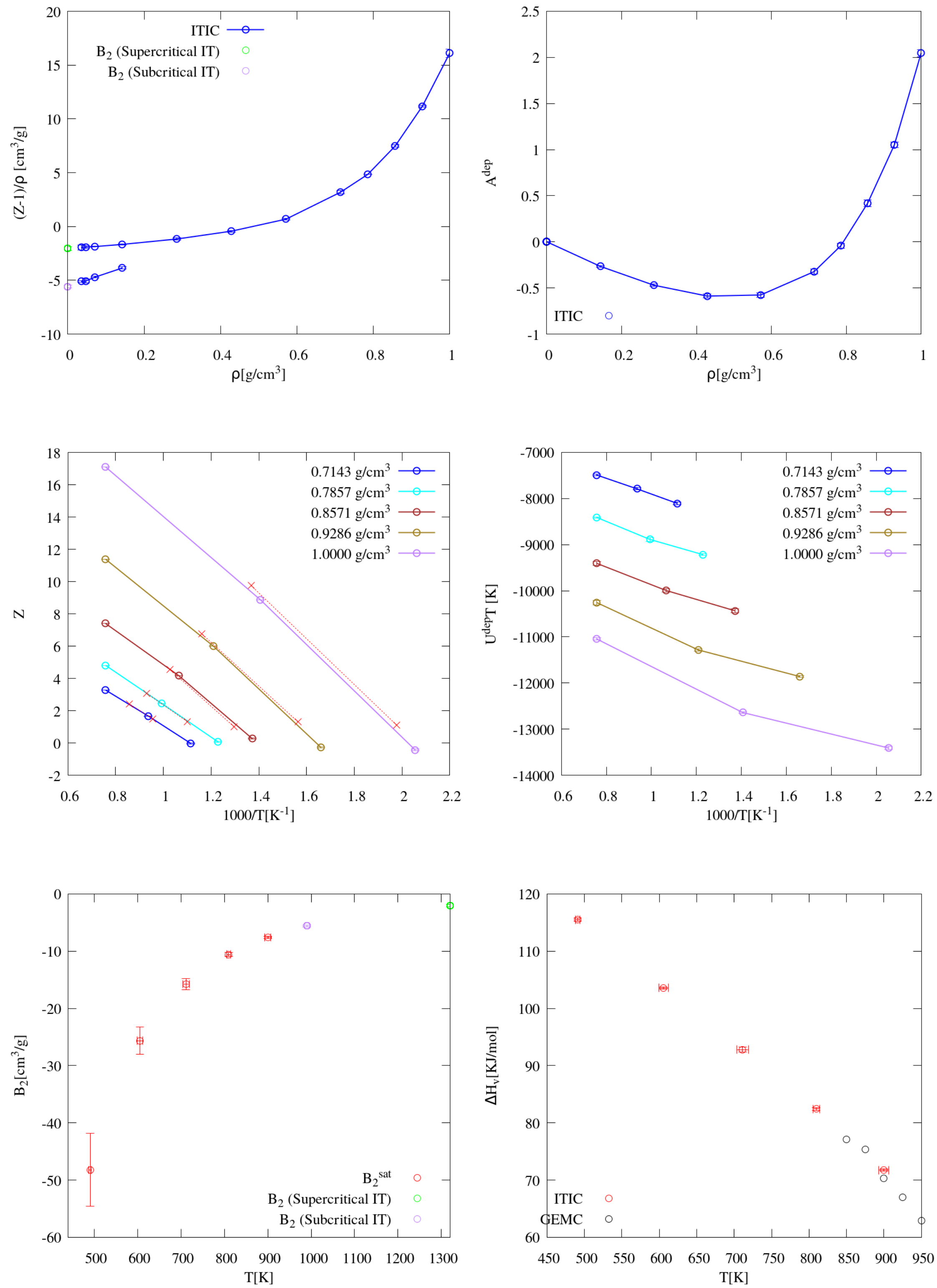

FIG. 12: TraPPE-UA 1-naphthalenyl,4-phenanthrenyl butane (GOMC). Linear extrapolation of red (X) symbols in Z vs. $1000/T$ plot were used to obtain initial T^{sat} values at each isochore.

IV. OTHER FIGURES AND TABLES

TABLE XXIII: Accuracy of the ITIC method for n-dodecane when third virial coefficient is used. Deviations are calculated using $\frac{\text{ITIC}-\text{REFPROP}}{\text{REFPROP}} \times 100$

[K] $T_{\text{est}}^{\text{sat}}$	$T_{\text{r}}^{\text{sat}}$	[K] T^{sat}	[MPa] P^{sat}	% Dev.	[g/cm^3] ρ_{liq}	% Dev.	[g/cm^3] ρ_{vap}	% Dev.	[kJ/mol] ΔH_{v}	% Dev.
657.25	0.99	649.9	1.5262975	-6.22	0.3202	-6.50	0.078805	-35.14	15.53	19.29
647.87	0.97	640.99	1.3893581	-3.77	0.3736	-0.39	0.072524	-23.21	18.87	11.45
632.18	0.94	619.68	1.0590791	-1.53	0.4269	-0.05	0.054218	-8.35	24.14	3.98
606.45	0.90	588.97	0.6797089	-0.30	0.4803	0.05	0.032526	-1.60	30.45	2.19
602.79	0.83	548.84	0.3474356	-0.01	0.5336	0.19	0.015668	-0.19	36.80	1.59
546.57	0.76	497.84	0.1233584	0.10	0.5870	0.16	0.005536	0.10	42.94	1.15
479.80	0.67	437.25	0.0242641	0.08	0.6404	0.14	0.001167	0.09	48.85	0.76
404.91	0.56	369.29	0.0016902	0.36	0.6937	0.13	0.000094	0.36	54.83	0.47
325.82	0.45	297.52	0.0000171	0.83	0.7471	0.13	0.000001	1.02	61.34	0.19

TABLE XXIV: Accuracy of the ITIC method for n-dodecane when third virial coefficient is not used. For $T_{\text{r}}^{\text{sat}} > 0.9$ the fixed-point iteration does not converge.

[K] $T_{\text{est}}^{\text{sat}}$	$T_{\text{r}}^{\text{sat}}$	[K] T^{sat}	[MPa] P^{sat}	% Dev.	[g/cm^3] ρ_{liq}	% Dev.	[g/cm^3] ρ_{vap}	% Dev.	[kJ/mol] ΔH_{v}	% Dev.
606.45	0.90	589.18	0.7107295	4.25	0.4803	0.05	0.040963	23.92	28.88	-3.08
602.79	0.83	548.85	0.3501108	0.76	0.5336	0.19	0.016114	2.65	36.67	1.22
546.57	0.76	497.84	0.1234819	0.20	0.5870	0.16	0.005554	0.43	42.93	1.12
479.80	0.67	437.25	0.0242654	0.09	0.6404	0.14	0.001167	0.10	48.85	0.76
404.91	0.56	369.29	0.0016902	0.36	0.6937	0.13	0.000094	0.36	54.83	0.47
325.82	0.45	297.52	0.0000171	0.83	0.7471	0.13	0.000001	1.02	61.34	0.19

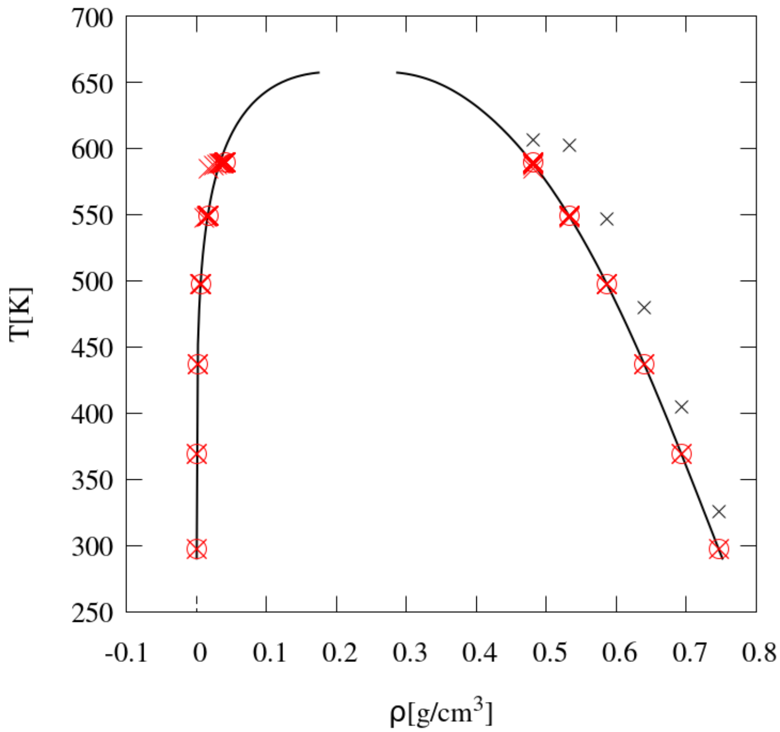

FIG. 13: The $T^{\rm sat}$ iteration compared to n-Dodecane coexistence curves. ITIC results (circles) are obtained using NIST REFPROP[1] values for $U^{\rm dep}$ and Z, when virial expansion in is truncated at B_2. Solid line represents true NIST REFPROP VLE data. The inital estimate of saturation temperature $T^{\rm sat}_{\rm est}$ is represented by black X symbols and red X symbols are the ($T^{\rm sat}$,ρ) points showing the converegence path. The ITIC method generally converges fast especilly at low temperatures.

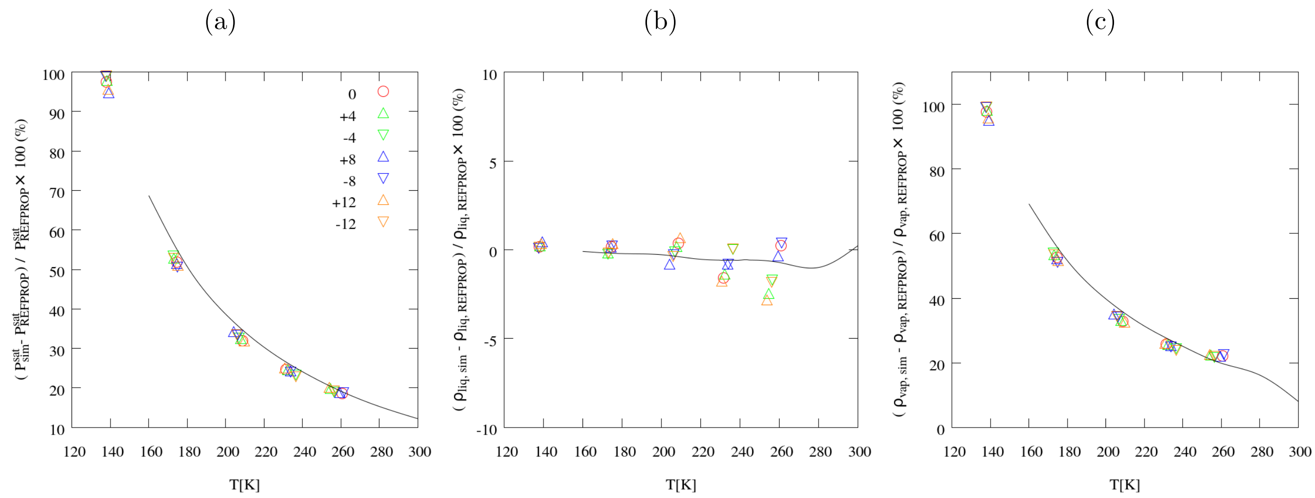

FIG. 14: In Section 3, the sensitivity of the ITIC method to $T^{\mathrm{sat}}_{\mathrm{est}}$ was investigated using REFPROP data. This figure investigates this sensitivity by applying simulation data for TraPPE ethane. The y-axis represents deviations from REFPROP data. Lines are GCMC results[2] and circles are ITIC results when $T^{\mathrm{sat}}_{\mathrm{est}}$ are taken from REFPROP. Triangles pointing up or down represent ITIC results when $T^{\mathrm{sat}}_{\mathrm{est}}$ is increased or decreased by the percentage shown in the legend, respectively. Accuracy of ITIC saturation properties does not significantly depend on $T^{\mathrm{sat}}_{\mathrm{est}}$ deviations.

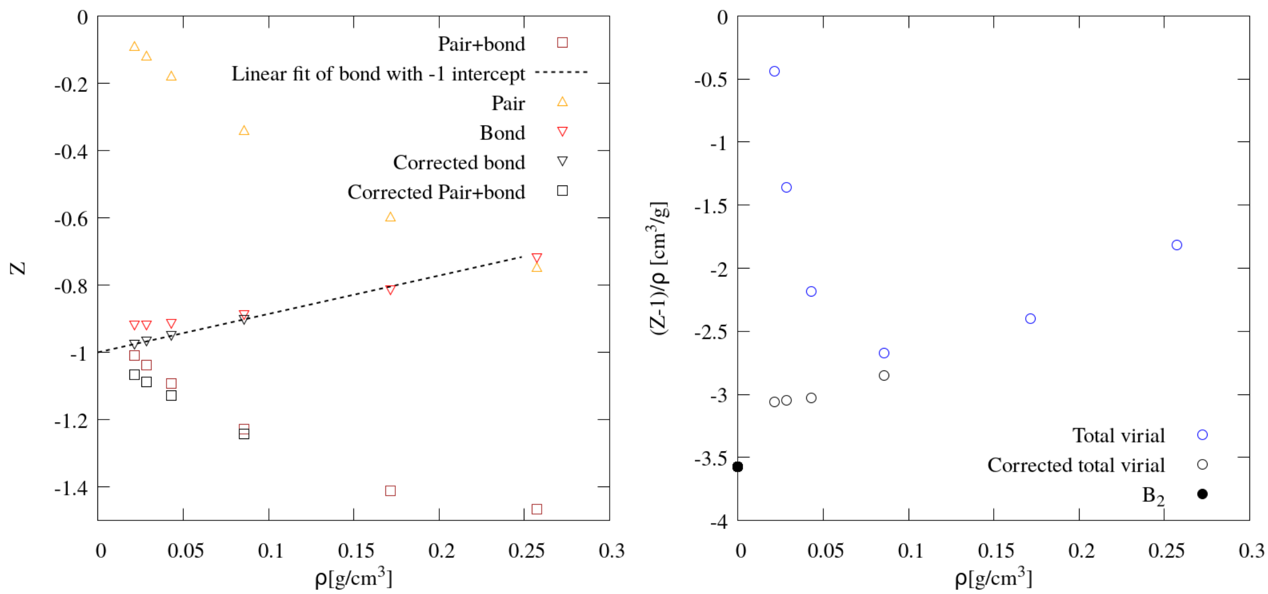

FIG. 15: Virial contributions to compressibility factor for harmonic bond TraPPE-UA ethane (N=3200). The intermolecular contribution to the virial (pair) is approaching zero as expected, but the bonded contribution deviates significantly from its steady approach to -1 as the density approaches zero. The discrepancy is magnified in the computation of $(Z-1)/\rho$ owing to the division by density. The bonded contribution to the virial is a quantity reported by LAMMPS with little recourse for user intervention. Presumably, the problem is the small number of intermolecular collisions at low density relative to the large number of intramolecular collisions, inhibiting the equilibration of the various components of momentum. To illustrate one manner of correcting for this deficiency, we used a linear extrapolation of the intramolecular virial (bond), enforcing a value of -1 at zero density. Then we corrected the total virial (pair+bond). This procedure reduces the problem, but requires considerably more effort than switching to fixed bond lengths. Note that the kinetic contribution to compressibility factor for this system (not shown in the figure) has a constant value of 2 at all densities, therefore the total Z approaches 1 at zero density.

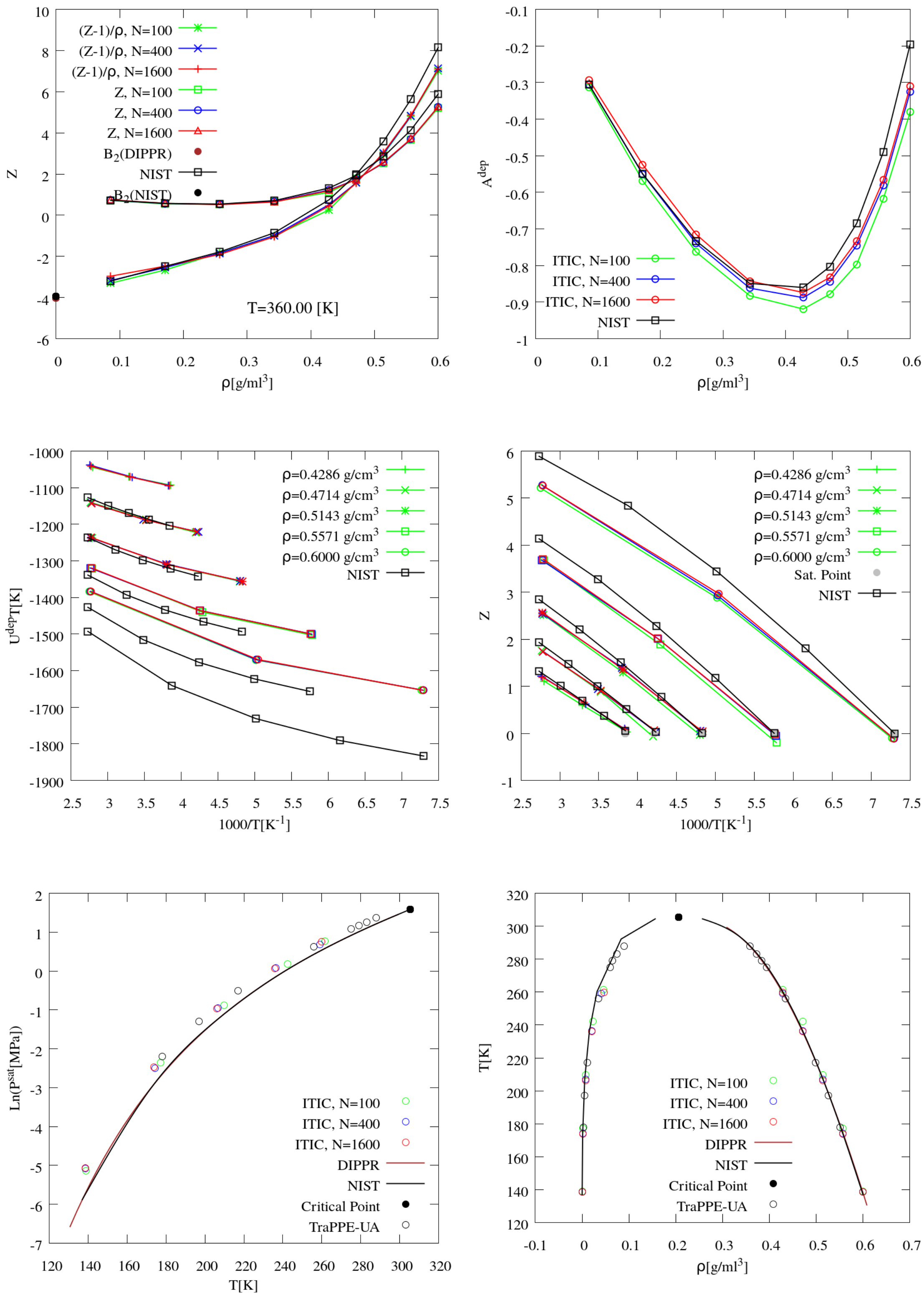

FIG. 16: Effect of number of ethane molcules on ITIC method. Simulation were performed using LAMMPS and C-C bonds are held constant using SHAKE algorithm.

V. U^{dep} CALCULATION METHODS

In this section, U^{dep} calculation from two approaches mentioned in Section 4.1 are compared and further discussed. The first approach uses Eq. (28) (single molecule approach). the second approach uses Eq. (29) (U^{intra} approach). The following figures compare the ITIC results (filled symbols) with GEMC results from the literature (open symbols). The different shapes/colors for ITIC correspond to different ways for computing U^{dep}. These figures compare deviations from REFPROP values as a baseline to make the magnitudes of the discrepancies more clear. In other words, the best ITIC method is the one that agrees with the open symbols (GEMC), not the one that has lower deviation from REFPROP.

The red filled squares (single molecule method) provide the best agreement in P^{sat} and ρ^{vap} for n-dodecane (C12). However, the green filled circles (Eq. (29)) provide indistinguishable values for smaller molecules, e.g., isobutane (iC4). The blue filled triangles (without subtracting intra method) is simply wrong and will not be discussed further.

The difference between U^{dep} calculated using the single molecule approach is on average around 1.7 % for C12. This small difference causes a significant deviation in P^{sat} and ρ_{vap} which increases with decreasing temperature, while the ρ_{liq} values are essentially the same. P^{sat} differences for C12 and iC6 are 10-15 % for $T_{\text{r}} = 0.45$ and 1-4 % for $T_{\text{r}} = 0.85$.

The improvement with the single molecule method is most evident for the Mie-C12 results, where the single molecule method completely resolves the discrepancy between the ITIC and GCMC P^{sat} values. However, note that the single molecule method did not reduce the deviation between the ITIC and GCMC ρ_{liq} values.

It is also important that the difference between the single molecule method and the U^{intra} method for TraPPE-C12 is of a similar magnitude as the difference between GEMC and GEMC+Gibbs Duhem from the literature. Therefore, the deviations introduced by our original assumption are still less than the statistical uncertainty in the simulation data.

In brief, the single molecule method is clearly the most rigorous approach. However, the U^{intra} method is not obsolete as it has some benefits for smaller molecules compared to the single molecule method. For example, although the additional single molecule simulations are extremely fast, this adds to the complexity of the ITIC method. Furthermore, single molecule simulations are ill-suited for traditional molecular dynamics simulations where a thermostat couples many degrees of freedom to a single bath, e.g., Nos-Hoover. Stochastic

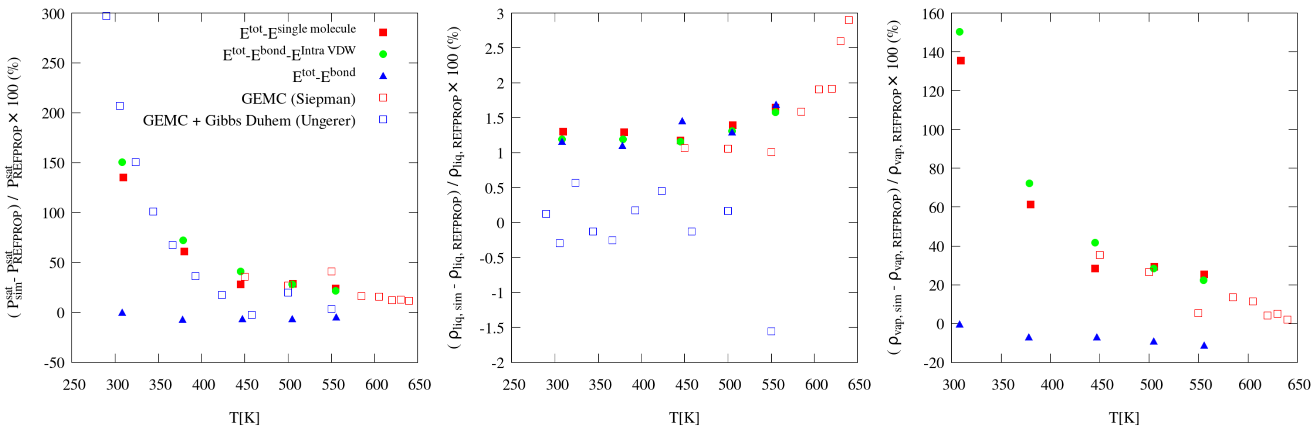

FIG. 17: TraPPE-UA n-dodecane

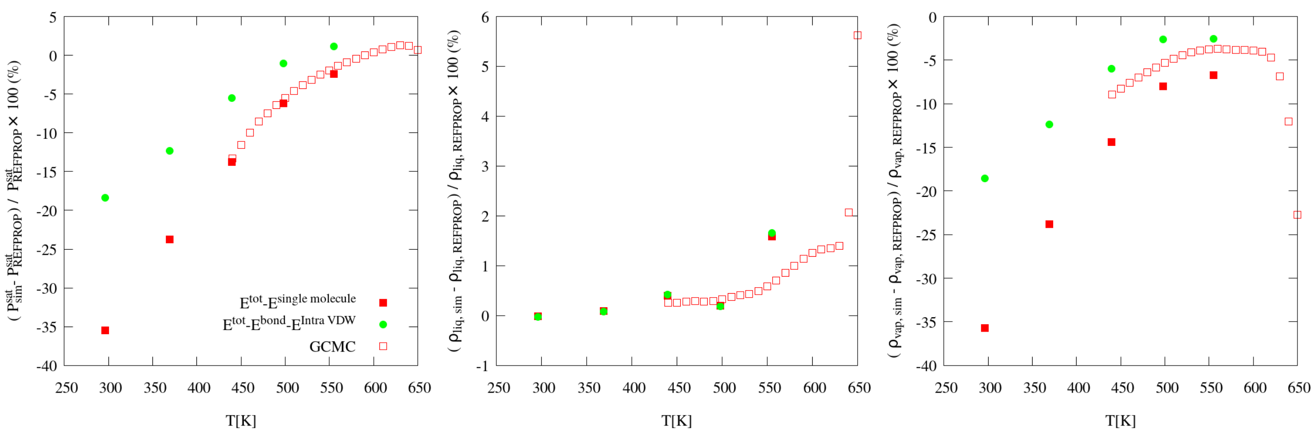

FIG. 18: Mie-UA n-dodecane

dynamics (which is available in some molecular dynamics packages, e.g., GROMACS) is better suited for single molecule simulations, but this again adds complexity that is not needed for smaller molecules.

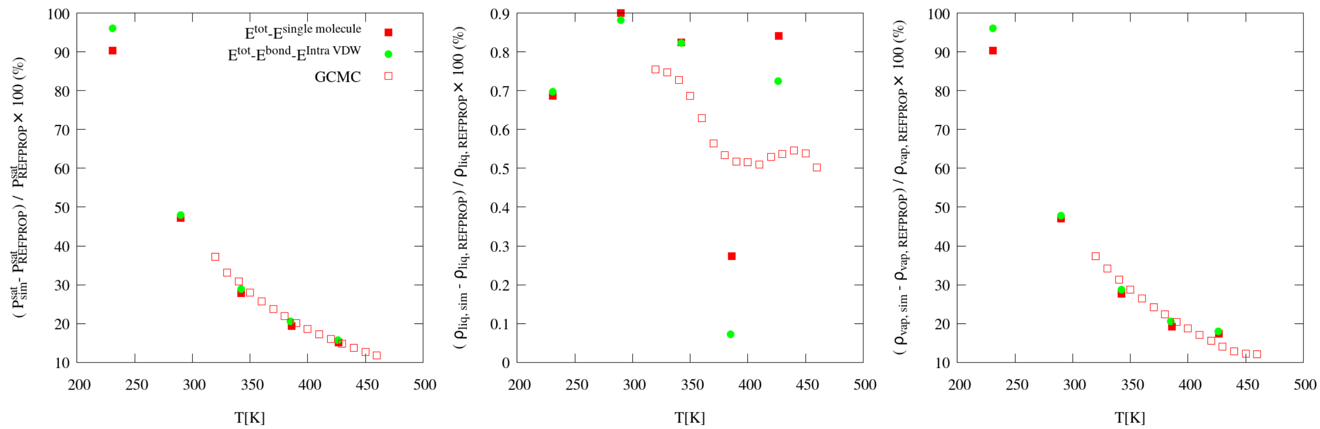

FIG. 19: TraPPE-UA isohexane

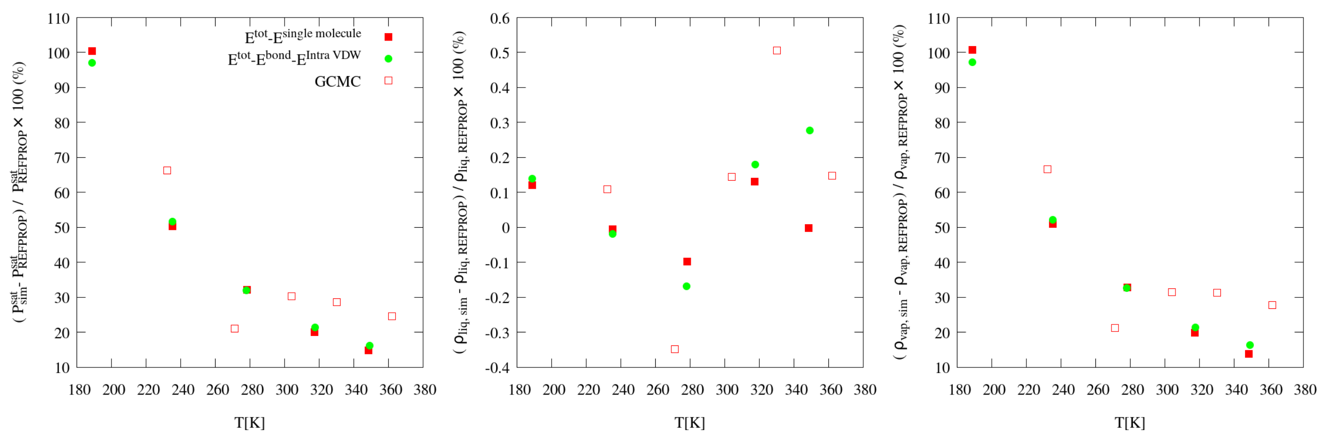

FIG. 20: TraPPE-UA isobutane

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[2]V. Shen, D. Siderius, W. Krekelberg, and H. E. Hatch, "NIST Standard Reference Simulation Website," (2008).