This file is the proof for the simulation time determination. It has two different type simulations, called **liquid phase simulation** and **gas phase simulation**, respectively. In order for solid verification, two systems are chosen, **BPYR_NTF2** and **BPYR_BF4**.

The starting point of those simulation is from the already equilibrated state's box, but only with the charge changes.

For these two-type simulations, the corresponding **mdp** file output control settings are;

For liquid:

```
; RUN CONTROL PARAMETERS =

integrator = md        ; md integrator
tinit = 0              ; [ps] starting time for run
dt = 0.001             ; [ps] time step for integration
nsteps = 1000000       ; maximum number of steps to integrate
comm-mode = Linear     ; Remove center of mass translation


; OUTPUT CONTROL OPTIONS =

nstxout = 100000         ; [steps] freq to write coordinates to trajectory
nstlog = 100000          ; [steps] freq to write coordinates to log file
nstenergy = 5000         ; group(s) to write to energy file
```

For gas:

```
; RUN CONTROL PARAMETERS =

integrator = md         ; md integrator
tinit = 0               ; [ps] starting time for run
dt = 0.001              ; [ps] time step for integration
nsteps = 2000000        ; maximum number of steps to integrate
comm-mode = angular     ; Remove center of mass translation


; OUTPUT CONTROL OPTIONS =

nstxout = 200000          ; [steps] freq to write coordinates to trajectory
nstlog = 200000           ; [steps] freq to write energies to log file
nstenergy = 20000         ; group(s) to write to energy file
```

For analyses, what we should do is checking and comparing the **Average** and **RMSD** values.

For the column name **Tot-Drift**, which means, for a series of data points, using the linear least-square-fitted method to get the fitted-trend-line's slope, and then use this number multiply the difference of the first data point and last data point. Therefore, it doesn't have any real-statistical meanings for the data convergence properties. As long as the average and RMSD values are similar or comparable, then we can safely come to the conclusion that the compared two data-sets both are valid and workable.

System BPYR_BF4_Liquid 40ns VS 1ns

Statistics over 40000001 steps [0.0000 through 40000.0000 ps], 41 data sets
All statistics are over 400001 points

Energy	Average	Err.Est.	RMSD	Tot-Drift	
Bond	8875.53	1.7	148.953	9.31768	(kJ/mol)
Angle	22252.1	11	238.079	-79.5197	(kJ/mol)
Fr.Dih	8241.05	13	147.801	-71.8993	(kJ/mol)
LJ (SR)	-20772.3	30	215.026	-103.612	(kJ/mol)
Cl. (SR)	-338508	160	511.91	-1136.51	(kJ/mol)
Cl. Recip.	573.444	2.8	32.4333	-14.9263	(kJ/mol)
LJ. Recip	-8171.25	4.3	28.2416	-20.2467	(kJ/mol)
Ptial	-327509	210	701.404	-1417.39	(kJ/mol)
K. En.	45188.8	5	337.504	0.49649	(kJ/mol)
Total.En	-282320	210	800.037	-1416.9	(kJ/mol)
Temp.	297.829	0.033	2.22441	0.00327312	(K)
Pressure	1.50121	0.46	310.239	-1.72098	(bar)
Cstr.rmsd	2.00E-12	2.00E-12	1.27E-09	-1.20E-11	()
Box-X	5.28766	0.00095	0.00430897	-0.00419589	(nm)
Box-Y	5.28766	0.00095	0.00430897	-0.00419589	(nm)
Box-Z	5.28766	0.00095	0.00430897	-0.00419589	(nm)
Volume	147.84	0.079	0.362754	-0.352724	(nm^3)
Density	1252.5	0.67	3.04066	2.9686	(kg/m^3)
pV	8.9031	0.0048	0.0218455	-0.0212416	(kJ/mol)
Enthalpy	-282312	210	800.052	-1416.92	(kJ/mol)
Vir-XX	15089.4	130	2485.97	650.951	(kJ/mol)
Vir-XY	218.928	97	1772.67	581.523	(kJ/mol)
Vir-XZ	288.085	13	1778.81	2.22143	(kJ/mol)
Vir-YX	218.928	97	1772.67	581.523	(kJ/mol)
Vir-YY	14967.7	110	2481.67	-26.8294	(kJ/mol)
Vir-YZ	426.818	67	1780.04	328.538	(kJ/mol)
Vir-ZX	288.085	13	1778.81	2.22136	(kJ/mol)
Vir-ZY	426.818	67	1780.04	328.538	(kJ/mol)
Vir-ZZ	15112.2	100	2474.4	-600.746	(kJ/mol)
Pres-XX	0.352786	29	559.052	-145.851	(bar)
Pres-XY	-45.078	21	399.451	-126.396	(bar)
Pres-XZ	-65.2869	2.2	400.969	1.01694	(bar)
Pres-YX	-45.078	21	399.451	-126.396	(bar)
Pres-YY	24.9615	24	557.942	4.71514	(bar)
Pres-YZ	-90.5877	15	401.343	-77.3527	(bar)
Pres-ZX	-65.2868	2.2	400.969	1.01695	(bar)
Pres-ZY	-90.5877	15	401.343	-77.3527	(bar)
Pres-ZZ	-20.8106	23	556.455	135.973	(bar)
#SurfTen	-177.045	180	3672.56	1092.28	(bar nm)
T-System	297.829	0.033	2.22441	0.00327312	(K)
Lamb-Sys	1	0	0	0	()

Statistics over 1000001 steps [0.0000 through 1000.0000 ps], 41 data sets
All statistics are over 10001 points

Energy	Average	Err.Est.	RMSD	Tot-Drift	
Bond	8840.92	16	158.932	92.0558	(kJ/mol)
Angle	22357.2	29	250.785	-162.182	(kJ/mol)
Fr.Dih	8377.28	30	162.907	-147.26	(kJ/mol)
LJ (SR)	-20461	64	297.102	-403.701	(kJ/mol)
Cl. (SR)	-336684	400	1259.11	-2655	(kJ/mol)
Cl. Recip.	617.806	10	149.841	-61.5599	(kJ/mol)
LJ. Recip	-8117.37	13	109.944	-85.0174	(kJ/mol)
Ptial	-325069	530	1681.72	-3422.67	(kJ/mol)
K. En.	45220.5	43	527.149	-205.199	(kJ/mol)
Total.En	-279849	560	2039.97	-3627.87	(kJ/mol)
Temp.	298.038	0.29	3.47432	-1.35242	(K)
Pressure	0.34765	0.69	316.382	-1.90628	(bar)
Cstr.rmsd	7.93E-11	7.90E-11	7.93E-09	-4.76E-10	()
Box-X	5.29992	0.0034	0.0111779	-0.0211178	(nm)
Box-Y	5.29992	0.0034	0.0111779	-0.0211178	(nm)
Box-Z	5.29992	0.0034	0.0111779	-0.0211178	(nm)
Volume	148.872	0.28	0.954155	-1.78873	(nm^3)
Density	1243.86	2.3	7.67534	14.7198	(kg/m^3)
pV	8.96528	0.017	0.0574605	-0.10772	(kJ/mol)
Enthalpy	-279840	560	2040.02	-3627.98	(kJ/mol)
Vir-XX	14731.3	110	2481.43	-90.3864	(kJ/mol)
Vir-XY	93.1238	130	1781.23	649.995	(kJ/mol)
Vir-XZ	93.5501	64	1773.99	-272.271	(kJ/mol)
Vir-YX	93.1238	130	1781.23	649.995	(kJ/mol)
Vir-YY	15739.8	76	2495.45	-91.8323	(kJ/mol)
Vir-YZ	-379.293	130	1775.71	-332.695	(kJ/mol)
Vir-ZX	93.55	64	1773.99	-272.271	(kJ/mol)
Vir-ZY	-379.293	130	1775.71	-332.696	(kJ/mol)
Vir-ZZ	14746.2	33	2475.57	-1.93436	(kJ/mol)
Pres-XX	81.0959	23	552.79	0.767831	(bar)
Pres-XY	-16.2445	28	398.873	-145.092	(bar)
Pres-XZ	-30.4735	14	397.446	62.3093	(bar)
Pres-YX	-16.2445	28	398.873	-145.092	(bar)
Pres-YY	-142.297	21	557.81	9.44757	(bar)
Pres-YZ	78.5162	28	397.655	73.6825	(bar)
Pres-ZX	-30.4735	14	397.446	62.3092	(bar)
Pres-ZY	78.5163	28	397.655	73.6826	(bar)
Pres-ZZ	62.2443	7.7	551.282	-15.9342	(bar)
#SurfTen	491.743	64	3596.89	-111.756	(bar nm)
T-System	298.038	0.29	3.47432	-1.35242	(K)
Lamb-Sys	1	0	0	0	()

System BPYR_BF4_Gas 20ns VS 2ns

Statistics over 20000001 steps [0.0000 through 20000.0000 ps], 33 data sets
All statistics are over 200001 points

Energy	Average	Err.Est.	RMSD	Tot-Drift	
Bond	17.3646	0.15	6.599	0.19934	(kJ/mol)
Angle	47.5912	0.1	11.1984	-0.618173	(kJ/mol)
Fr.Dih	18.0398	0.081	6.45502	-0.349075	(kJ/mol)
LJ (SR)	9.08815	0.038	9.09419	-0.146577	(kJ/mol)
Cl. (SR)	-562.545	0.25	12.4192	0.414292	(kJ/mol)
Ptial	-470.461	0.31	14.9349	-0.500195	(kJ/mol)
K. En.	82.9123	0.19	14.269	-0.751073	(kJ/mol)
Total.En	-387.549	0.47	20.8345	-1.25127	(kJ/mol)
Conserved	-248.352	30	60.8324	209.963	(kJ/mol)
Temp.	297.672	0.69	51.2287	-2.6965	(K)
Pressure	0	0	0	0	(bar)
Constr.	1.89E-12	1.90E-12	8.47E-10	-1.14E-11	()
Vir-XX	29.0206	0.2	113.044	-0.143336	(kJ/mol)
Vir-XY	-1.05035	0.6	78.7578	-3.50914	(kJ/mol)
Vir-XZ	-0.126562	0.61	77.9138	2.07751	(kJ/mol)
Vir-YX	-1.05035	0.6	78.7578	-3.50914	(kJ/mol)
Vir-YY	27.4034	0.2	129.232	0.597388	(kJ/mol)
Vir-YZ	-0.498017	0.26	82.6322	0.260398	(kJ/mol)
Vir-ZX	-0.126563	0.61	77.9138	2.07752	(kJ/mol)
Vir-ZY	-0.498018	0.26	82.6322	0.260402	(kJ/mol)
Vir-ZZ	27.2991	0.33	131.073	-0.101725	(kJ/mol)
Pres-XX	0	0	0	0	(bar)
Pres-XY	0	0	0	0	(bar)
Pres-XZ	0	0	0	0	(bar)
Pres-YX	0	0	0	0	(bar)
Pres-YY	0	0	0	0	(bar)
Pres-YZ	0	0	0	0	(bar)
Pres-ZX	0	0	0	0	(bar)
Pres-ZY	0	0	0	0	(bar)
Pres-ZZ	0	0	0	0	(bar)
#SurfTen	0	0	0	0	(bar nm)
T-System	297.672	0.69	51.2287	-2.6965	(K)
Lamb-Sys	1	0	0	0	()

Statistics over 2000001 steps [0.0000 through 2000.0000 ps], 33 data sets
All statistics are over 20001 points

Energy	Average	Err.Est.	RMSD	Tot-Drift	
Bond	18.0059	0.28	6.70376	0.435287	(kJ/mol)
Angle	47.6028	0.32	11.1589	-0.291137	(kJ/mol)
Fr.Dih	18.2576	0.33	6.51916	0.633273	(kJ/mol)
LJ (SR)	8.99484	0.08	8.97942	-0.107981	(kJ/mol)
Cl. (SR)	-562.747	0.47	12.2943	-2.51183	(kJ/mol)
Ptial	-469.886	0.84	14.854	-1.84239	(kJ/mol)
K. En.	83.3292	0.6	14.0245	-1.915	(kJ/mol)
Total.En	-386.557	1.4	20.3272	-3.75738	(kJ/mol)
Conserved	-341.678	3.7	7.63938	25.134	(kJ/mol)
Temp.	299.168	2.2	50.3506	-6.87522	(K)
Pressure	0	0	0	0	(bar)
Constr.	1.89E-11	1.90E-11	2.68E-09	-1.14E-10	()
Vir-XX	28.1617	0.75	119.317	-5.08013	(kJ/mol)
Vir-XY	1.22776	0.28	80.5173	-0.346208	(kJ/mol)
Vir-XZ	-1.7566	0.39	82.2793	0.97979	(kJ/mol)
Vir-YX	1.22776	0.28	80.5173	-0.346216	(kJ/mol)
Vir-YY	26.562	0.42	132.031	0.465	(kJ/mol)
Vir-YZ	-1.06163	0.44	81.5313	-1.28325	(kJ/mol)
Vir-ZX	-1.7566	0.39	82.2793	0.979838	(kJ/mol)
Vir-ZY	-1.06163	0.44	81.5313	-1.28322	(kJ/mol)
Vir-ZZ	28.7419	0.32	117.781	1.61798	(kJ/mol)
Pres-XX	0	0	0	0	(bar)
Pres-XY	0	0	0	0	(bar)
Pres-XZ	0	0	0	0	(bar)
Pres-YX	0	0	0	0	(bar)
Pres-YY	0	0	0	0	(bar)
Pres-YZ	0	0	0	0	(bar)
Pres-ZX	0	0	0	0	(bar)
Pres-ZY	0	0	0	0	(bar)
Pres-ZZ	0	0	0	0	(bar)
#SurfTen	0	0	0	0	(bar nm)
T-System	299.168	2.2	50.3506	-6.87522	(K)
Lamb-Sys	1	0	0	0	()

System BPYR_NTF2_Liquid 40ns VS 1ns

Statistics over 40000001 steps [0.0000 through 40000.0000 ps], 41 data sets
All statistics are over 400001 points

Energy	Average	Err.Est.	RMSD	Tot-Drift	
Bond	15186.1	2.6	194.97	-5.12847	(kJ/mol)
Angle	36440.7	9.1	309.23	17.3577	(kJ/mol)
Fr.Dih	20167.1	37	277.006	20.6846	(kJ/mol)
LJ (SR)	-48441.5	78	281.059	-548.645	(kJ/mol)
Cl. (SR)	-188604	230	670.259	-1300.25	(kJ/mol)
Cl. Recip.	738.763	13	36.0025	-87.1899	(kJ/mol)
LJ. Recip	-14699.9	11	45.1372	-82.423	(kJ/mol)
Ptial	-179213	310	860	-1985.59	(kJ/mol)
K. En.	63769.5	1.9	394.18	6.58644	(kJ/mol)
Total.En	-115444	300	954.907	-1979.01	(kJ/mol)
Temp.	297.868	0.0087	1.84122	0.030764	(K)
Pressure	0.891308	0.32	299.28	0.82824	(bar)
Cstr.rmsd	2.17E-12	2.20E-12	1.37E-09	-1.30E-11	()
Box-X	6.04521	0.0016	0.00502035	-0.0117898	(nm)
Box-Y	6.04521	0.0016	0.00502035	-0.0117898	(nm)
Box-Z	6.04521	0.0016	0.00502035	-0.0117898	(nm)
Volume	220.92	0.18	0.551047	-1.29343	(nm^3)
Density	1564.78	1.3	3.88944	9.14297	(kg/m^3)
pV	13.3041	0.011	0.0331848	-0.0778922	(kJ/mol)
Enthalpy	-115430	300	954.931	-1979.08	(kJ/mol)
Vir-XX	21633.3	60	3421.05	259.951	(kJ/mol)
Vir-XY	13.8325	46	2403.26	106.589	(kJ/mol)
Vir-XZ	-17.818	54	2405.07	-335.495	(kJ/mol)
Vir-YX	13.8325	46	2403.26	106.589	(kJ/mol)
Vir-YY	21175.9	85	3421.61	129.377	(kJ/mol)
Vir-YZ	-256.254	73	2409.59	-269.35	(kJ/mol)
Vir-ZX	-17.8179	54	2405.07	-335.495	(kJ/mol)
Vir-ZY	-256.254	73	2409.59	-269.35	(kJ/mol)
Vir-ZZ	20943.2	81	3419.48	-399.223	(kJ/mol)
Pres-XX	-55.9149	9.6	514.794	-43.2366	(bar)
Pres-XY	-2.18226	6.2	362.11	-14.219	(bar)
Pres-XZ	1.96665	7.8	362.476	44.9176	(bar)
Pres-YX	-2.18227	6.2	362.11	-14.219	(bar)
Pres-YY	4.1701	12	514.599	-18.484	(bar)
Pres-YZ	35.1232	11	363.093	40.5604	(bar)
Pres-ZX	1.96664	7.8	362.476	44.9176	(bar)
Pres-ZY	35.1232	11	363.093	40.5604	(bar)
Pres-ZZ	54.4187	12	514.423	64.2053	(bar)
#SurfTen	485.288	110	3793.45	573.826	(bar nm)
T-System	297.868	0.0087	1.84122	0.030764	(K)
Lamb-Sys	1	0	0	0	()

Statistics over 1000001 steps [0.0000 through 1000.0000 ps], 41 data sets
All statistics are over 10001 points

Energy	Average	Err.Est.	RMSD	Tot-Drift	
Bond	15203.5	17	197.573	35.0517	(kJ/mol)
Angle	36497.7	20	307.27	-139.269	(kJ/mol)
Fr.Dih	19935.5	170	481.437	1148.98	(kJ/mol)
LJ (SR)	-47829.9	95	329.517	-650.832	(kJ/mol)
Cl. (SR)	-186730	600	1494.53	-3944.01	(kJ/mol)
Cl. Recip.	838.1	20	67.8138	-131.564	(kJ/mol)
LJ. Recip	-14604.8	21	185.819	-142.615	(kJ/mol)
Ptial	-176690	580	1410.46	-3824.26	(kJ/mol)
K. En.	63785.4	26	406.246	-85.9588	(kJ/mol)
Total.En	-112904	600	1527.39	-3910.22	(kJ/mol)
Temp.	297.943	0.12	1.89758	-0.401515	(K)
Pressure	0.0119758	2.2	298.879	13.2904	(bar)
Cstr.rmsd	8.49E-11	8.50E-11	8.49E-09	-5.09E-10	()
Box-X	6.05911	0.0033	0.00776157	-0.0222577	(nm)
Box-Y	6.05911	0.0033	0.00776157	-0.0222577	(nm)
Box-Z	6.05911	0.0033	0.00776157	-0.0222577	(nm)
Volume	222.448	0.36	0.856411	-2.45397	(nm^3)
Density	1554.04	2.5	5.95054	17.0909	(kg/m^3)
pV	13.3961	0.022	0.0515742	-0.147781	(kJ/mol)
Enthalpy	-112891	600	1527.43	-3910.37	(kJ/mol)
Vir-XX	21729.9	110	3424.46	354.399	(kJ/mol)
Vir-XY	-203.388	110	2410.06	-572.903	(kJ/mol)
Vir-XZ	-109.084	14	2405.69	-109.974	(kJ/mol)
Vir-YX	-203.388	110	2410.06	-572.903	(kJ/mol)
Vir-YY	20811.1	190	3450.32	-1187.9	(kJ/mol)
Vir-YZ	61.5249	68	2418.81	-108.887	(kJ/mol)
Vir-ZX	-109.084	14	2405.69	-109.974	(kJ/mol)
Vir-ZY	61.525	68	2418.81	-108.887	(kJ/mol)
Vir-ZZ	21245.6	170	3446.46	478.51	(kJ/mol)
Pres-XX	-67.4404	16	511.316	-50.8709	(bar)
Pres-XY	27.6877	16	361.031	89.0809	(bar)
Pres-XZ	24.2677	1.4	360.093	8.8355	(bar)
Pres-YX	27.6876	16	361.031	89.0809	(bar)
Pres-YY	64.0538	29	515.089	178.037	(bar)
Pres-YZ	-9.88514	10	361.92	18.1986	(bar)
Pres-ZX	24.2677	1.4	360.093	8.8355	(bar)
Pres-ZY	-9.88516	10	361.92	18.1986	(bar)
Pres-ZZ	3.42255	25	514.325	-87.2948	(bar)
#SurfTen	31.2932	240	3820.97	-914.956	(bar nm)
T-System	297.943	0.12	1.89758	-0.401515	(K)
Lamb-Sys	1	0	0	0	()

System BPYR_NTF2_Gas 20ns VS 2ns

Statistics over 40000001 steps [0.0000 through 40000.0000 ps], 41 data sets
All statistics are over 400001 points

Energy	Average	Err.Est.	RMSD	Tot-Drift	
Bond	30.6436	0.15	8.8271	0.261822	(kJ/mol)
Angle	75.1318	0.24	14.1099	-0.742203	(kJ/mol)
Fr.Dih	44.179	0.56	14.0166	-2.69415	(kJ/mol)
LJ (SR)	-21.3027	0.092	7.35647	-0.411736	(kJ/mol)
Cl. (SR)	-292.679	0.75	21.6484	3.59225	(kJ/mol)
Ptial	-164.028	0.16	18.2012	0.00598449	(kJ/mol)
K. En.	120.598	0.13	17.1097	-0.461029	(kJ/mol)
Total.En	-43.43	0.26	24.986	-0.455044	(kJ/mol)
Conserved	39.6634	26	53.1103	177.699	(kJ/mol)
Temp.	299.061	0.32	42.429	-1.14327	(K)
Pressure	0	0	0	0	(bar)
Constr.	4.17E-12	4.20E-12	1.86E-09	-2.50E-11	()
Vir-XX	40.5881	0.7	169.115	0.610943	(kJ/mol)
Vir-XY	0.6361	0.77	107.098	-4.56174	(kJ/mol)
Vir-XZ	-0.159533	0.5	107.432	-2.48632	(kJ/mol)
Vir-YX	0.636095	0.77	107.098	-4.56175	(kJ/mol)
Vir-YY	40.7082	0.75	168.061	-4.33325	(kJ/mol)
Vir-YZ	0.647405	0.32	106.95	0.102988	(kJ/mol)
Vir-ZX	-0.159537	0.5	107.432	-2.48632	(kJ/mol)
Vir-ZY	0.647406	0.32	106.95	0.102986	(kJ/mol)
Vir-ZZ	39.6715	1.1	172.874	1.99562	(kJ/mol)
Pres-XX	0	0	0	0	(bar)
Pres-XY	0	0	0	0	(bar)
Pres-XZ	0	0	0	0	(bar)
Pres-YX	0	0	0	0	(bar)
Pres-YY	0	0	0	0	(bar)
Pres-YZ	0	0	0	0	(bar)
Pres-ZX	0	0	0	0	(bar)
Pres-ZY	0	0	0	0	(bar)
Pres-ZZ	0	0	0	0	(bar)
#SurfTen	0	0	0	0	(bar nm)
T-System	299.061	0.32	42.429	-1.14327	(K)
Lamb-Sys	1	0	0	0	()

Statistics over 1000001 steps [0.0000 through 1000.0000 ps], 41 data sets
All statistics are over 10001 points

Energy	Average	Err.Est.	RMSD	Tot-Drift	
Bond	30.1806	0.32	8.78672	0.969229	(kJ/mol)
Angle	74.5315	0.33	14.1447	0.187802	(kJ/mol)
Fr.Dih	46.1815	0.95	13.1757	3.29109	(kJ/mol)
LJ (SR)	-21.3125	0.092	7.29696	0.384715	(kJ/mol)
Cl. (SR)	-296.434	0.81	20.0946	-1.68555	(kJ/mol)
Ptial	-166.853	0.97	18.1371	3.14728	(kJ/mol)
K. En.	118.913	0.55	17.2986	0.0465535	(kJ/mol)
Total.En	-47.94	1.5	25.5554	3.19384	(kJ/mol)
Conserved	-43.2014	2.7	5.80857	16.9188	(kJ/mol)
Temp.	294.884	1.4	42.8976	0.115447	(K)
Pressure	0	0	0	0	(bar)
Constr.	4.17E-11	4.20E-11	5.90E-09	-2.50E-10	()
Vir-XX	40.2081	1.7	159.205	9.44232	(kJ/mol)
Vir-XY	2.25343	0.24	105.231	0.817054	(kJ/mol)
Vir-XZ	1.10656	1.1	106.522	-5.36697	(kJ/mol)
Vir-YX	2.25344	0.24	105.231	0.817017	(kJ/mol)
Vir-YY	37.3755	1.4	169.609	5.62712	(kJ/mol)
Vir-YZ	0.480287	0.32	109.023	-0.354551	(kJ/mol)
Vir-ZX	1.10657	1.1	106.522	-5.36701	(kJ/mol)
Vir-ZY	0.480284	0.32	109.023	-0.354548	(kJ/mol)
Vir-ZZ	37.6855	1.3	172.591	7.43898	(kJ/mol)
Pres-XX	0	0	0	0	(bar)
Pres-XY	0	0	0	0	(bar)
Pres-XZ	0	0	0	0	(bar)
Pres-YX	0	0	0	0	(bar)
Pres-YY	0	0	0	0	(bar)
Pres-YZ	0	0	0	0	(bar)
Pres-ZX	0	0	0	0	(bar)
Pres-ZY	0	0	0	0	(bar)
Pres-ZZ	0	0	0	0	(bar)
#SurfTen	0	0	0	0	(bar nm)
T-System	294.884	1.4	42.8976	0.115448	(K)
Lamb-Sys	1	0	0	0	()