

Supplementary Material (ESI) for *Physical Chemistry Chemical Physics*
This journal is © The Owner Societies 2008

Coexistence lines for the SPC/E model

Temperatures (T) are given in K,
pressures (p) in bar,
internal energies (U) in kcal/mol, and
densities (rho) in g/cm³

T	p	U_1	U_2	rho_1	rho_2
Liquid-Ih					
209.8	500	-12.51	-13.286	1.042	0.9553
210.8	400	-12.61	-13.272	1.022	0.9546
212.8	200	-12.57	-13.244	1.031	0.9533
213.7	100	-12.59	-13.248	1.014	0.9519
214.6	1	-12.53	-13.225	1.010	0.9512
216.3	-200	-12.53	-13.197	1.009	0.9493
226.4	-2000	-12.34	-13.089	0.951	0.9284
215.6	-5000	-11.84	-13.035	0.793	0.8987

Liquid-II

215.7	1	-12.46	-13.402	1.033	1.2121
226.7	1000	-12.27	-13.333	1.076	1.2163
234.8	2000	-12.11	-13.294	1.108	1.2212
241.1	3000	-12.06	-13.261	1.120	1.2266
245.9	4000	-11.97	-13.241	1.159	1.2324
249.8	5000	-11.90	-13.228	1.193	1.2394
254.9	7500	-11.94	-13.216	1.236	1.2551
256.4	10000	-11.82	-13.219	1.283	1.2708
253.8	13000	-11.89	-13.235	1.324	1.2895
247.7	16000	-11.83	-13.261	1.356	1.3081
239.7	19000	-11.94	-13.291	1.385	1.3258
228.3	22000	-12.005	-13.322	1.423	1.3426
213.6	25000	-12.01	-13.362	1.454	1.3597

Liquid-VI

225.0	20690	-12.02	-12.501	1.421	1.4538
234.2	25000	-11.90	-12.408	1.448	1.4714
242.3	31500	-11.73	-12.285	1.486	1.4972
245.3	37000	-11.58	-12.187	1.519	1.5175
242.5	43000	-11.43	-12.098	1.551	1.5397
235.5	49000	-11.36	-12.028	1.581	1.5606
224.4	55000	-11.25	-11.966	1.606	1.5815
211.4	61000	-11.21	-11.891	1.629	1.6011
193.9	67000	-11.14	-11.842	1.654	1.6204

Supplementary Material (ESI) for *Physical Chemistry Chemical Physics*
This journal is © The Owner Societies 2008

Triple points and coexistence lines for the TIP4P/2005 model

Temperatures (T) are given in K,
pressures (p) in bar,
internal energies (U) in kcal/mol, and
densities (rho) in g/cm³

Triple points

Liquid-Ih-III triple point

T	p	U(liq)	U(Ih)	U(III)	rho(liq)	rho(Ih)	rho(III)
213.1	3060	-12.68	-13.660	-13.349	1.121	0.9515	1.1740

Liquid-III-V triple point

T	p	U(liq)	U(III)	U(V)	rho(liq)	rho(III)	rho(V)
215.3	3690	-12.65	-13.336	-13.249	1.152	1.1814	1.2625

Liquid-V-VI triple point

T	p	U(liq)	U(V)	U(VI)	rho(liq)	rho(V)	rho(VI)
241.6	8060	-12.24	-13.086	-12.980	1.239	1.2859	1.3575

Ih-II-III triple point

T	p	U(Ih)	U(II)	U(III)	rho(Ih)	rho(II)	rho(III)
195.9	3110	-13.784	-13.603	-13.474	0.9535	1.1996	1.1793

II-III-V triple point

T	p	U(II)	U(III)	U(V)	rho(II)	rho(III)	rho(V)
200.0	3690	-13.577	-13.445	-13.358	1.2024	1.1859	1.2670

Coexistence lines

T	p	U_1	U_2	rho_1	rho_2
---	---	-----	-----	-------	-------

Liquid-Ih

252.1	1	-12.17	-13.327	0.996	0.9208
248.0	500	-12.36	-13.368	0.996	0.9261
243.8	1000	-12.29	-13.416	1.039	0.9307
236.8	1600	-12.35	-13.477	1.074	0.9367
225.0	2400	-12.51	-13.569	1.116	0.9455
210.5	3200	-12.66	-13.679	1.133	0.9526

liquid-III

212.8	3000	-12.68	-13.354	1.125	1.1732
214.7	3500	-12.60	-13.342	1.143	1.1786

liquid-V

Supplementary Material (ESI) for *Physical Chemistry Chemical Physics*
This journal is © The Owner Societies 2008

210.7	3200	-12.67	-13.279	1.141	1.2599
218.1	4000	-12.61	-13.233	1.168	1.2641
225.6	5000	-12.47	-13.187	1.187	1.2694
232.6	6000	-12.35	-13.137	1.203	1.2745
237.5	7000	-12.31	-13.112	1.219	1.2802
241.5	8000	-12.31	-13.086	1.235	1.2859

liquid-VI

245.0	8540	-12.23	-12.962	1.245	1.3590
254.4	10000	-12.02	-12.907	1.265	1.3651
265.1	12000	-11.97	-12.836	1.286	1.3728
278.3	15000	-11.77	-12.756	1.316	1.3853
293.7	20000	-11.55	-12.640	1.365	1.4064
303.4	25000	-11.38	-12.547	1.396	1.4271

Ih-II

195.9	3107	-13.786	-13.606	0.9536	1.1996
180.0	3016	-13.895	-13.712	0.9550	1.2031
160.0	2902	-14.035	-13.847	0.9558	1.2080

Ih-III

195.0	3000	-13.610	-13.475	1.1988	1.1791
200.0	3097	-13.755	-13.444	0.9530	1.1782
200.1	3700	-13.578	-13.438	1.2021	1.1857
213.1	3064	-13.663	-13.352	0.9512	1.1748

II-V

200.0	3690	-13.577	-13.358	1.2024	1.2670
185.0	4270	-13.681	-13.471	1.2100	1.2755
170.0	4870	-13.788	-13.576	1.2179	1.2841
152.0	5580	-13.910	-13.700	1.2270	1.2939
134.0	6280	-14.026	-13.816	1.2353	1.3031
116.0	7000	-14.134	-13.925	1.2438	1.3117

III-V

215.3	3690	-13.335	-13.249	1.1816	1.2621
200.0	3687	-13.447	-13.361	1.1857	1.2672

V-VI

241.6	8060	-13.086	-12.980	1.2859	1.3575
215.0	7820	-13.276	-13.168	1.2920	1.3650
190.0	7620	-13.449	-13.339	1.2970	1.3717
165.0	7430	-13.616	-13.499	1.3026	1.3783
140.0	7270	-13.776	-13.657	1.3079	1.3847
115.0	7130	-13.931	-13.813	1.3130	1.3909

Supplementary Material (ESI) for *Physical Chemistry Chemical Physics*
This journal is © The Owner Societies 2008

Triple points and coexistence lines for the TIP4P/Ice model

Temperatures (T) are given in K,
pressures (p) in bar,
internal energies (U) in kcal/mol, and
densities (rho) in g/cm³

Triple points

Liquid-Ih-III triple point

T	p	U(Liq)	U(Ih)	U(III)	rho(liq)	rho(Ih)	rho(III)
231.8	2955	-13.90	-14.940	-14.624	1.112	0.9335	1.1541

Liquid-III-V triple point

T	p	U(Liq)	U(III)	U(V)	rho(liq)	rho(III)	rho(V)
232.6	3270	-13.93	-14.620	-14.536	1.1205	1.1579	1.2387

Liquid-V-VI triple point

T	p	U(Liq)	U(V)	U(VI)	rho(liq)	rho(V)	rho(VI)
258.4	7630	-13.525	-14.385	-14.275	1.211	1.2608	1.3323

Ih-II-III triple point

T	p	U(Ih)	U(II)	U(III)	rho(Ih)	rho(II)	rho(III)
219.4	2990	-15.033	-14.861	-14.714	0.9348	1.1773	1.1577

II-III-V triple point

T	p	U(II)	U(III)	U(V)	rho(II)	rho(III)	rho(V)
221.6	3280	-14.849	-14.702	-14.616	1.1786	1.1604	1.2422

Coexistence lines

T	p	U_1	U_2	rho_1	rho_2
---	---	-----	-----	-------	-------

Liquid-Ih

272.2	1	-13.33	-14.607	0.992	0.9061
267.4	500	-13.33	-14.651	1.024	0.9107
262.2	1000	-13.47	-14.703	1.025	0.9157
255.9	1500	-13.61	-14.755	1.063	0.9204
248.2	2000	-13.69	-14.823	1.075	0.9246
240.3	2500	-13.75	-14.883	1.098	0.9294
230.9	3000	-13.85	-14.945	1.1162	0.9345

Liquid-III

231.9	3000	-13.855	-14.625	1.115	1.1539
232.9	3400	-13.855	-14.619	1.124	1.1593

Liquid-V

Supplementary Material (ESI) for *Physical Chemistry Chemical Physics*
This journal is © The Owner Societies 2008

235.1	3500	-13.82	-14.521	1.125	1.2397
239.5	4000	-13.78	-14.493	1.148	1.2426
245.9	5000	-13.69	-14.452	1.182	1.2471
253.5	6500	-13.57	-14.409	1.195	1.2550
259.6	8000	-13.53	-14.381	1.223	1.2631

Liquid-VI

265.6	8540	-13.44	-14.232	1.224	1.3349
297.2	14000	-13.00	-14.043	1.276	1.3549
321.0	21000	-12.69	-13.879	1.335	1.3819
337.0	30000	-12.44	-13.709	1.394	1.4157
340.5	40000	-12.21	-13.567	1.458	1.4510
334.9	50000	-12.10	-13.450	1.502	1.4838

Ih-II

219.4	2990	-15.039	-14.859	0.9348	1.1774
210.0	2943	-15.105	-14.923	0.9351	1.1792
200.0	2893	-15.173	-14.994	0.9360	1.1815

Ih-III

231.8	2955	-14.938	-14.612	0.9340	1.1530
220.0	2988	-15.022	-14.711	0.9356	1.1563

II-III

219.5	3000	-14.863	-14.711	1.1773	1.1563
222.5	3400	-14.846	-14.693	1.1788	1.1616

II-V

221.6	3280	-14.852	-14.617	1.1785	1.2430
210.0	3740	-14.936	-14.703	1.1841	1.2488
200.0	4130	-15.005	-14.778	1.1886	1.2543

III-V

232.6	3270	-14.620	-14.538	1.1579	1.2391
222.0	3280	-14.698	-14.622	1.1607	1.2428

V-VI

258.4	7631	-14.389	-14.273	1.2612	1.3321
240.0	7510	-14.524	-14.404	1.2645	1.3372
220.0	7420	-14.657	-14.544	1.2696	1.3426
200.0	7331	-14.790	-14.673	1.2732	1.3474

Supplementary Material (ESI) for *Physical Chemistry Chemical Physics*
This journal is © The Owner Societies 2008

Coexistence lines for the TIP4P model

Temperatures (T) are given in K,
pressures (p) in bar,
internal energies (U) in kcal/mol, and
densities (rho) in g/cm³

T	p	U_1	U_2	rho_1	rho_2
Liquid-Ih					
232.4	1	-10.90	-12.023	1.012	0.9409
231.9	100	-10.96	-12.031	1.006	0.9416
230.4	300	-10.91	-12.052	1.028	0.9439
228.8	500	-10.97	-12.075	1.030	0.9458
219.9	1500	-11.07	-12.153	1.071	0.9572
207.7	2500	-11.27	-12.256	1.123	0.9678
199.2	3000	-11.38	-12.315	1.141	0.9737
193.4	3300	-11.46	-12.360	1.161	0.9771

Liquid-III					
196.6	5000	-11.39	-12.024	1.207	1.2233
196.2	4500	-11.34	-12.025	1.208	1.2168
195.9	4000	-11.36	-12.028	1.195	1.2112
195.0	3500	-11.36	-12.034	1.175	1.2046
193.4	3000	-11.41	-12.042	1.160	1.1978
191.6	2500	-11.46	-12.054	1.147	1.1899

Liquid-V					
196.0	3820	-11.37	-11.936	1.192	1.2909
199.5	4300	-11.36	-11.915	1.202	1.2934
204.3	5000	-11.32	-11.885	1.216	1.2969
213.6	6500	-11.18	-11.828	1.235	1.3058
218.8	7660	-11.04	-11.794	1.276	1.3133
220.0	8000	-11.01	-11.788	1.274	1.3156
224.4	10000	-10.95	-11.754	1.295	1.3290
227.8	12000	-10.93	-11.722	1.318	1.3420
229.5	15000	-10.93	-11.691	1.360	1.3615
225.9	20000	-10.87	-11.646	1.415	1.3935
216.8	25000	-10.85	-11.634	1.456	1.4238

Liquid-VI					
201.4	6000	-11.28	-11.784	1.236	1.3819
210.3	7000	-11.17	-11.728	1.250	1.3855
225.0	8940	-10.98	-11.634	1.283	1.3928
251.7	14000	-10.61	-11.465	1.337	1.4147
272.6	21000	-10.34	-11.301	1.405	1.4468
284.6	30000	-10.04	-11.143	1.470	1.4864
287.4	40000	-9.81	-10.992	1.534	1.5266
280.6	50000	-9.69	-10.848	1.590	1.5643
264.1	60000	-9.55	-10.723	1.638	1.5992

Ih-II					
120.0	2910	-12.87	-12.654	0.981	1.243
150.0	3040	-12.67	-12.456	0.979	1.234
180.0	3170	-12.46	-12.248	0.977	1.226

Supplementary Material (ESI) for *Physical Chemistry Chemical Physics*
This journal is © The Owner Societies 2008

II-III

180.3	5000	-12.261	-12.141	1.2396	1.2275
177.9	4500	-12.275	-12.161	1.2366	1.2215
174.9	4000	-12.295	-12.180	1.2340	1.2167
171.3	3500	-12.314	-12.204	1.2310	1.2095
167.1	3000	-12.339	-12.237	1.2288	1.2058
162.1	2500	-12.371	-12.269	1.2265	1.1966

II-V

75.0	8180	-12.917	-12.721	1.2875	1.3579
100.0	7170	-12.772	-12.578	1.2756	1.3447
125.0	6140	-12.622	-12.425	1.2627	1.3303
152.6	5000	-12.441	-12.245	1.2475	1.3139
165.0	4470	-12.356	-12.162	1.2400	1.3063
180.0	3848	-12.252	-12.051	1.2308	1.2962

II-VI

150.0	6210	-12.461	-12.121	1.2564	1.4013
120.0	6890	-12.651	-12.312	1.2690	1.4155
90.0	7570	-12.831	-12.496	1.2803	1.4291
70.0	8010	-12.947	-12.613	1.2875	1.4378

III-V

175.2	4046	-12.177	-12.085	1.2168	1.2994
200.0	4047	-11.997	-11.903	1.2079	1.2910

V-VI

220.8	8390	-11.784	-11.656	1.3177	1.3905
190.0	8190	-11.992	-11.868	1.3252	1.4005
160.0	8030	-12.197	-12.070	1.3337	1.4100
125.0	7840	-12.417	-12.293	1.3424	1.4205
90.0	7670	-12.636	-12.507	1.3504	1.4307