Supporting Information for *Nuclear Quantum Effects from the Analysis of Smoothed Trajectories: Pilot Study for Water*

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1 Calculated data

1.1 BOMD

Table 1: Isobaric heat capacities for one water molecule obtained from BOMD simulations. The data is depicted as Figure 5. in the main text.

	c_p / J·K^{-1}mol^{-1}					
T / K	experimental	class. HO	quant. HO	class. sim.	1PT	GSTA
25	-	58.201	33.257	58.202	33.2951±0.0005	33.2690±0.0004
100	33.30086±0.00001	58.201	33.257	58.242	33.2674±0.0054	33.3012±0.0018
200	33.35053±0.00001	58.201	33.269	58.314	33.289±0.011	33.3815±0.0053
300	33.59584±0.00001	58.201	33.490	58.373	33.504±0.021	33.696±0.011
400	34.26208±0.00001	58.201	34.153	58.410	34.148±0.054	34.435±0.023
500	35.22593±0.00001	58.201	35.122	58.413	35.09±0.11	35.438±0.037
600	36.32471±0.00001	58.201	36.219	58.474	36.16±0.18	36.647±0.047
700	37.49627±0.00001	58.201	37.376	58.496	37.27±0.27	37.680±0.090
800	38.72398±0.00001	58.201	38.575	58.660	38.40±0.32	39.26±0.12
900	39.99172±0.00001	58.201	39.800	58.660	39.56±0.35	40.46±0.12
1000	41.27527±0.00001	58.201	41.029	58.660	40.72±0.36	41.66±0.13
1250	44.37821±0.00005	58.201	43.959	58.895	43.83±0.58	45.13±0.16
1500	47.14441±0.00007	58.201	46.494	58.895	46.30±0.54	47.54±0.14
1750	49.4397±0.0003	58.201	48.563	58.997	48.30±0.49	49.32±0.17
2000	51.3787±0.0003	58.201	50.210	58.997	49.96±0.42	50.93±0.15
2500	54.255±0.0001	58.201	52.549	59.311	52.38±0.30	53.617±0.096
3000	56.337±0.0001	58.201	54.043	59.311	53.90±0.22	55.53±0.15
4000	58.98±0.07	58.201	55.719	60.802	55.73±0.24	58.41±0.18
5000	59.5±0.6	58.201	56.566	61.350	56.61±0.20	59.83±0.20

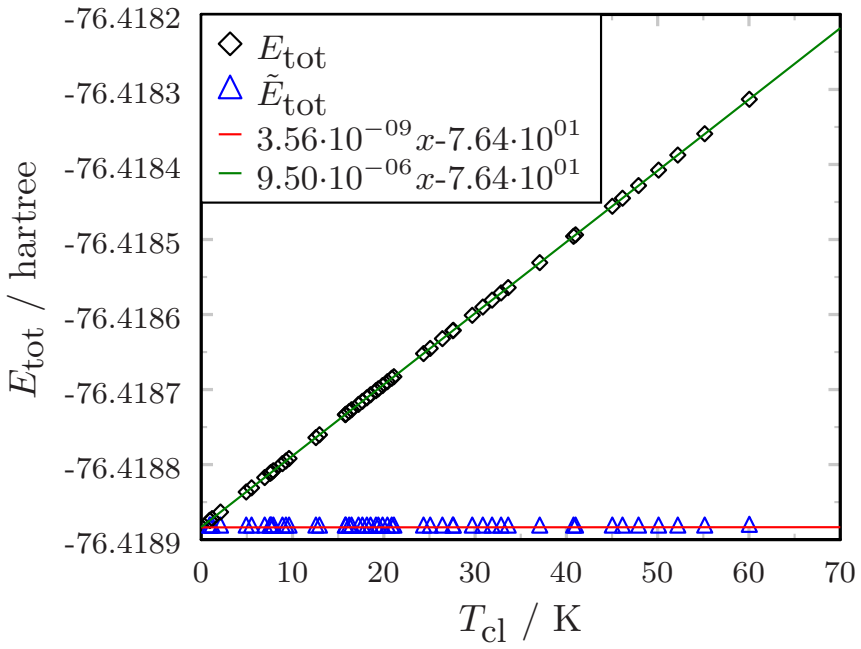

Figure 1: Classic and smoothed total energies (at 25 K) as a function of simulation temperature.

Table 2: Simulation temperature, total average energy and smoothed average energy components of trajectories associated to the calculation at 25 K.

trajectory #	$T_{\mathrm{simul.}}$ / K	$\langle E_{tot} \rangle$ / $\mathrm{E_h}$	$\langle \tilde{E}_{kin} \rangle$ / $\mathrm{E_h}$	$\langle \tilde{E}_{pot} \rangle$ / $\mathrm{E_h}$	$\langle \tilde{E}_{tot} \rangle$ / $\mathrm{E_h}$
1	19.866912	-76.418695	0.000000	-76.418883	-76.418884
2	18.551783	-76.418707	0.000000	-76.418883	-76.418884
3	37.082071	-76.418531	0.000000	-76.418883	-76.418884
4	6.952979	-76.418817	0.000000	-76.418883	-76.418884
5	46.151819	-76.418445	0.000000	-76.418883	-76.418884
6	20.393037	-76.418690	0.000000	-76.418883	-76.418884
7	20.871646	-76.418685	0.000000	-76.418883	-76.418884
8	24.353105	-76.418652	0.000000	-76.418883	-76.418884
9	7.900259	-76.418808	0.000000	-76.418883	-76.418884
10	47.907274	-76.418428	0.000000	-76.418883	-76.418884
11	17.230258	-76.418720	0.000000	-76.418883	-76.418884
12	25.086490	-76.418645	0.000000	-76.418883	-76.418884
13	45.035018	-76.418456	0.000000	-76.418883	-76.418884
14	7.539762	-76.418812	0.000000	-76.418883	-76.418884
15	12.951782	-76.418760	0.000000	-76.418883	-76.418884
16	41.008626	-76.418494	0.000000	-76.418883	-76.418884
17	21.107462	-76.418683	0.000000	-76.418883	-76.418884
18	32.849149	-76.418571	0.000000	-76.418883	-76.418884
19	16.464054	-76.418727	0.000000	-76.418883	-76.418884
20	33.628363	-76.418564	0.000000	-76.418883	-76.418884
21	29.691422	-76.418601	0.000000	-76.418883	-76.418884
22	7.615798	-76.418811	0.000000	-76.418883	-76.418884
23	30.846664	-76.418590	0.000000	-76.418883	-76.418884
24	19.399638	-76.418699	0.000000	-76.418883	-76.418884
25	27.616980	-76.418621	0.000000	-76.418883	-76.418884

26	16.204073	-76.418729	0.000000	-76.418883	-76.418884
27	60.044792	-76.418313	0.000000	-76.418883	-76.418883
28	0.930725	-76.418875	0.000000	-76.418883	-76.418884
29	40.787429	-76.418496	0.000000	-76.418883	-76.418884
30	12.561501	-76.418764	0.000000	-76.418883	-76.418884
31	27.561041	-76.418622	0.000000	-76.418883	-76.418884
32	55.157337	-76.418359	0.000000	-76.418883	-76.418884
33	9.277765	-76.418795	0.000000	-76.418883	-76.418884
34	4.928422	-76.418837	0.000000	-76.418883	-76.418884
35	52.208174	-76.418387	0.000000	-76.418883	-76.418884
36	50.102161	-76.418407	0.000000	-76.418883	-76.418884
37	7.690415	-76.418810	0.000000	-76.418883	-76.418884
38	15.842267	-76.418733	0.000000	-76.418883	-76.418884
39	8.897298	-76.418799	0.000000	-76.418883	-76.418884
40	9.620797	-76.418792	0.000000	-76.418883	-76.418884
41	18.146198	-76.418711	0.000000	-76.418883	-76.418884
42	1.189822	-76.418872	0.000000	-76.418883	-76.418884
43	17.653120	-76.418716	0.000000	-76.418883	-76.418884
44	15.779474	-76.418734	0.000000	-76.418883	-76.418884
45	0.952940	-76.418874	0.000000	-76.418883	-76.418884
46	31.862410	-76.418581	0.000000	-76.418883	-76.418884
47	2.115710	-76.418863	0.000000	-76.418883	-76.418884
48	5.514108	-76.418831	0.000000	-76.418883	-76.418884
49	26.421039	-76.418632	0.000000	-76.418883	-76.418884
50	19.142372	-76.418701	0.000000	-76.418883	-76.418884

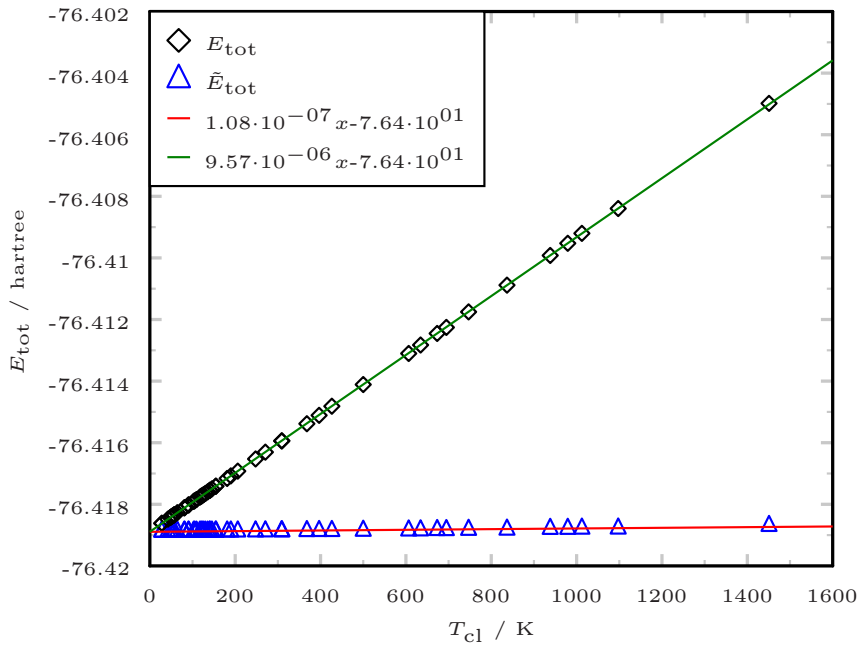

Figure 2: Classic and smoothed total energies (at 300 K) as a function of simulation temperature.

Table 3: Simulation temperature, total average energy and smoothed average energy components of trajectories associated to the calculation at 300 K.

trajectory #	$T_{\text{simul.}}$ / K	$\langle E_{tot} \rangle$ / E_h	$\langle \tilde{E}_{kin} \rangle$ / E_h	$\langle \tilde{E}_{pot} \rangle$ / E_h	$\langle \tilde{E}_{tot} \rangle$ / E_h
1	47.771430	-76.418420	0.000001	-76.418882	-76.418882
2	51.736343	-76.418392	0.000001	-76.418882	-76.418881
3	57.199859	-76.418330	0.000001	-76.418882	-76.418881
4	64.431401	-76.418271	0.000001	-76.418882	-76.418880
5	80.493234	-76.418118	0.000001	-76.418882	-76.418880
6	91.234938	-76.418016	0.000001	-76.418881	-76.418880
7	102.817529	-76.417906	0.000003	-76.418881	-76.418879
8	105.107134	-76.417884	0.000003	-76.418881	-76.418879
9	120.166742	-76.417741	0.000002	-76.418880	-76.418879
10	122.772521	-76.417716	0.000003	-76.418881	-76.418877
11	126.177977	-76.417684	0.000003	-76.418880	-76.418878
12	140.687295	-76.417546	0.000003	-76.418880	-76.418878
13	145.455027	-76.417499	0.000003	-76.418879	-76.418877
14	154.985656	-76.417409	0.000003	-76.418879	-76.418877
15	189.806466	-76.417077	0.000003	-76.418878	-76.418875
16	309.464605	-76.415939	0.000007	-76.418874	-76.418867
17	27.935496	-76.418618	0.000001	-76.418883	-76.418882
18	28.249487	-76.418615	0.000000	-76.418883	-76.418882
19	42.342384	-76.418481	0.000001	-76.418883	-76.418882
20	49.724228	-76.418411	0.000001	-76.418883	-76.418881
21	55.024174	-76.418361	0.000001	-76.418882	-76.418882
22	57.232434	-76.418339	0.000001	-76.418882	-76.418882
23	81.602441	-76.418108	0.000002	-76.418882	-76.418880
24	90.299678	-76.418024	0.000002	-76.418882	-76.418879
25	109.325354	-76.417845	0.000003	-76.418881	-76.418879
26	117.332536	-76.417768	0.000003	-76.418881	-76.418878
27	130.175509	-76.417645	0.000002	-76.418880	-76.418879
28	135.572848	-76.417595	0.000002	-76.418880	-76.418878
29	140.428636	-76.417548	0.000003	-76.418880	-76.418877
30	154.305208	-76.417416	0.000003	-76.418879	-76.418877
31	181.146542	-76.417161	0.000005	-76.418879	-76.418874
32	206.026005	-76.416923	0.000004	-76.418878	-76.418874
33	247.740147	-76.416527	0.000006	-76.418876	-76.418871
34	270.718106	-76.416307	0.000005	-76.418875	-76.418870
35	308.915773	-76.415943	0.000006	-76.418872	-76.418866
36	367.968859	-76.415384	0.000009	-76.418870	-76.418860
37	396.643958	-76.415112	0.000010	-76.418868	-76.418858
38	426.520818	-76.414816	0.000008	-76.418866	-76.418857
39	500.065127	-76.414112	0.000011	-76.418860	-76.418850
40	606.577917	-76.413103	0.000012	-76.418853	-76.418841
41	634.429189	-76.412828	0.000014	-76.418851	-76.418838
42	673.297040	-76.412453	0.000016	-76.418843	-76.418826
43	694.843623	-76.412257	0.000015	-76.418844	-76.418828
44	746.962952	-76.411753	0.000017	-76.418837	-76.418819
45	836.906759	-76.410884	0.000017	-76.418830	-76.418814
46	938.225161	-76.409920	0.000022	-76.418811	-76.418789
47	979.341762	-76.409526	0.000023	-76.418810	-76.418787
48	1012.447338	-76.409203	0.000022	-76.418803	-76.418781
49	1097.556042	-76.408397	0.000023	-76.418801	-76.418778

50	1451.022386	-76.404983	0.000030	-76.418723	-76.418693

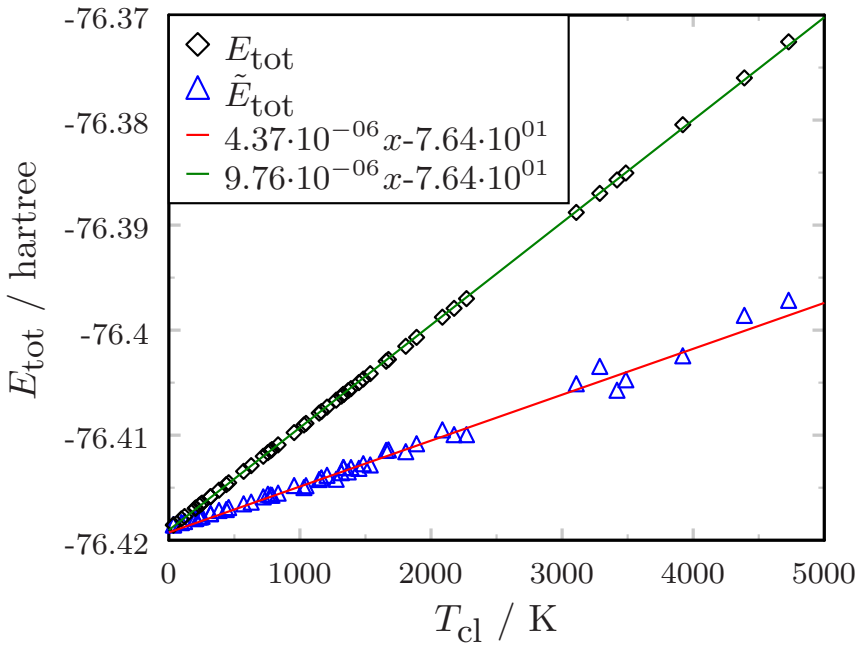

Figure 3: Classic and smoothed total energies (at 1250 K) as a function of simulation temperature.

Table 4: Simulation temperature, total average energy and smoothed average energy components of trajectories associated to the calculation at 1250 K.

trajectory #	$T_{\mathrm{simul.}}$ / K	$\langle E_{tot} \rangle$ / $\mathrm{E_h}$	$\langle \tilde{E}_{kin} \rangle$ / $\mathrm{E_h}$	$\langle \tilde{E}_{pot} \rangle$ / $\mathrm{E_h}$	$\langle \tilde{E}_{tot} \rangle$ / $\mathrm{E_h}$
1	1333.712780	-76.406120	0.002742	-76.416044	-76.413302
2	4390.608111	-76.375986	0.009447	-76.408255	-76.398810
3	3920.875781	-76.380442	0.007521	-76.410177	-76.402658
4	318.963531	-76.415850	0.000600	-76.418283	-76.417684
5	1316.959622	-76.406279	0.002502	-76.416287	-76.413786
6	3287.607896	-76.386981	0.007297	-76.410963	-76.403668
7	201.064587	-76.416972	0.000363	-76.418519	-76.418156
8	833.676272	-76.410921	0.001556	-76.417287	-76.415732
9	119.952866	-76.417744	0.000224	-76.418659	-76.418434
10	1675.450639	-76.402794	0.003559	-76.415176	-76.411617
11	3419.041133	-76.385700	0.006125	-76.412059	-76.405935
12	1163.992933	-76.407751	0.002264	-76.416543	-76.414279
13	2086.883121	-76.398765	0.004439	-76.414146	-76.409709
14	775.597843	-76.411476	0.001466	-76.417374	-76.415909
15	570.587407	-76.413443	0.001058	-76.417807	-76.416749
16	1449.906882	-76.404994	0.002698	-76.416070	-76.413372
17	1368.644295	-76.405759	0.002524	-76.416233	-76.413710
18	3486.513693	-76.385039	0.006606	-76.411545	-76.404940
19	438.271156	-76.414706	0.000787	-76.418079	-76.417292
20	253.740096	-76.416469	0.000470	-76.418408	-76.417939
21	2270.896377	-76.396998	0.004219	-76.414382	-76.410165
22	1147.048718	-76.407899	0.002182	-76.416615	-76.414434

23	786.716463	-76.411371	0.001461	-76.417393	-76.415933
24	1483.558337	-76.404656	0.002914	-76.415843	-76.412930
25	1657.986969	-76.402961	0.003534	-76.415195	-76.411661
26	1389.552737	-76.405570	0.002741	-76.416038	-76.413298
27	720.395718	-76.412007	0.001381	-76.417469	-76.416089
28	755.823636	-76.411661	0.001504	-76.417339	-76.415836
29	3108.433250	-76.388792	0.006522	-76.411837	-76.405317
30	318.042130	-76.415853	0.000594	-76.418277	-76.417682
31	1807.519706	-76.401536	0.003447	-76.415230	-76.411784
32	1046.303525	-76.408878	0.001895	-76.416917	-76.415022
33	1030.810745	-76.409026	0.001806	-76.417009	-76.415203
34	956.005693	-76.409750	0.001909	-76.416919	-76.415010
35	1206.747793	-76.407327	0.002378	-76.416412	-76.414034
36	37.096872	-76.418531	0.000069	-76.418814	-76.418746
37	1330.512774	-76.406116	0.002735	-76.416023	-76.413288
38	456.468694	-76.414531	0.000880	-76.417984	-76.417104
39	4728.359660	-76.372550	0.010030	-76.407403	-76.397376
40	232.310763	-76.416672	0.000436	-76.418442	-76.418007
41	382.688870	-76.415236	0.000743	-76.418125	-76.417383
42	628.172103	-76.412899	0.001140	-76.417731	-76.416590
43	205.860126	-76.416926	0.000369	-76.418513	-76.418144
44	1890.097622	-76.400688	0.003801	-76.414829	-76.411030
45	244.924500	-76.416553	0.000444	-76.418435	-76.417992
46	34.152788	-76.418559	0.000063	-76.418820	-76.418758
47	95.924918	-76.417972	0.000172	-76.418710	-76.418538
48	2176.243159	-76.397924	0.004227	-76.414390	-76.410163
49	1276.579412	-76.406664	0.002191	-76.416600	-76.414410
50	1536.470085	-76.404141	0.002842	-76.415890	-76.413048

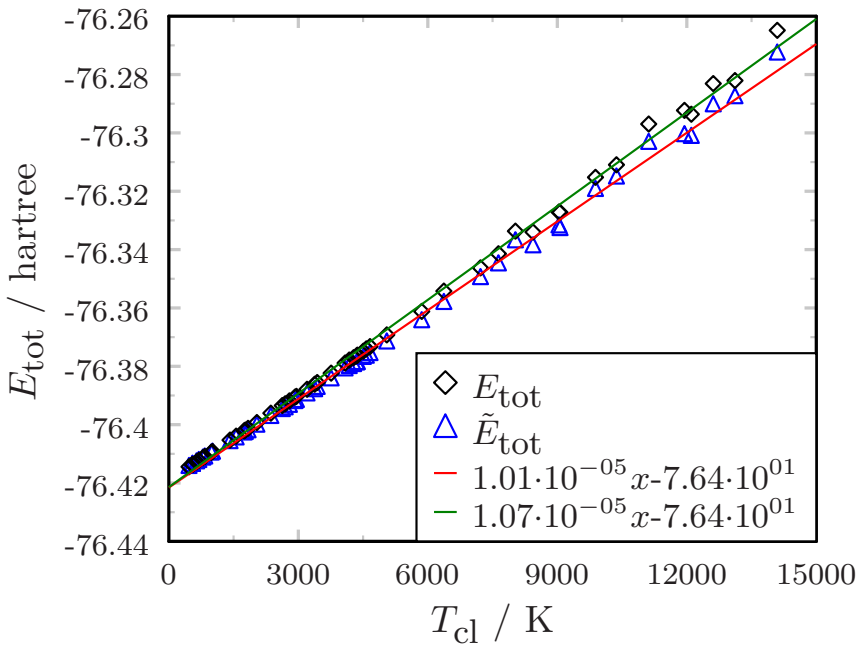

Figure 4: Classic and smoothed total energies (at 5000 K) as a function of simulation temperature.

Table 5: Simulation temperature, total average energy and smoothed average energy components of trajectories associated to the calculation at 5000 K.

trajectory #	$T_{\text{simul.}}$ / K	$\langle E_{tot} \rangle$ / E_h	$\langle \tilde{E}_{kin} \rangle$ / E_h	$\langle \tilde{E}_{pot} \rangle$ / E_h	$\langle \tilde{E}_{tot} \rangle$ / E_h
1	694.597252	-76.412247	0.003077	-76.415765	-76.412689
2	832.494556	-76.410929	0.003666	-76.415165	-76.411500
3	4506.500275	-76.374828	0.020136	-76.397496	-76.377361
4	7636.440400	-76.341424	0.034297	-76.379610	-76.345316
5	9063.468751	-76.327251	0.040026	-76.373233	-76.333212
6	2040.201700	-76.399266	0.009020	-76.409619	-76.400600
7	4368.340222	-76.376170	0.019263	-76.398386	-76.379124
8	644.151392	-76.412745	0.002850	-76.416009	-76.413159
9	9038.999319	-76.327107	0.040314	-76.372607	-76.332297
10	982.043308	-76.409507	0.004338	-76.414492	-76.410155
11	3760.138562	-76.382341	0.016661	-76.401379	-76.384720
12	11946.573497	-76.292284	0.052342	-76.353364	-76.301028
13	8030.156058	-76.333672	0.036247	-76.373648	-76.337404
14	5859.544865	-76.361192	0.026000	-76.390802	-76.364806
15	4083.537327	-76.378875	0.018182	-76.399481	-76.381301
16	4575.501891	-76.374025	0.020265	-76.397210	-76.376947
17	12614.085664	-76.283101	0.056049	-76.346836	-76.290793
18	8437.617711	-76.333970	0.037476	-76.376591	-76.339119
19	13117.096906	-76.282069	0.059287	-76.347298	-76.288017
20	12105.297308	-76.293607	0.053473	-76.355082	-76.301615
21	2922.968254	-76.390565	0.012912	-76.405411	-76.392501
22	549.589885	-76.413649	0.002423	-76.416443	-76.414020
23	2695.951150	-76.392856	0.011907	-76.406547	-76.394641
24	1559.022966	-76.403924	0.006884	-76.411842	-76.404960
25	467.747909	-76.414429	0.002061	-76.416808	-76.414748
26	1012.207299	-76.409205	0.004488	-76.414329	-76.409841
27	3201.477583	-76.387872	0.014196	-76.404076	-76.389881
28	789.298853	-76.411345	0.003481	-76.415358	-76.411878
29	4661.383275	-76.373232	0.020727	-76.396772	-76.376046
30	6372.270967	-76.354221	0.028101	-76.386633	-76.358535
31	1418.049310	-76.405286	0.006257	-76.412493	-76.406237
32	4281.244289	-76.377042	0.018939	-76.398760	-76.379822
33	5049.506397	-76.369229	0.022547	-76.394627	-76.372083
34	4179.721979	-76.377850	0.018527	-76.399019	-76.380493
35	547.907468	-76.413660	0.002417	-76.416446	-76.414029
36	3379.384684	-76.386144	0.014892	-76.403321	-76.388431
37	7220.628161	-76.346267	0.032399	-76.382415	-76.350019
38	2955.958697	-76.390300	0.013120	-76.405242	-76.392124
39	4352.087788	-76.376417	0.019231	-76.398494	-76.379265
40	3437.303508	-76.385556	0.015274	-76.402920	-76.387648
41	10370.950675	-76.310926	0.046938	-76.362483	-76.315549
42	1772.759492	-76.401867	0.007819	-76.410877	-76.403059
43	2629.017172	-76.393449	0.011586	-76.406822	-76.395238
44	1745.959868	-76.402125	0.007716	-76.410984	-76.403270
45	1835.608640	-76.401258	0.008085	-76.410599	-76.402515
46	14096.703269	-76.264856	0.062834	-76.335880	-76.273052
47	2363.561500	-76.396067	0.010451	-76.408058	-76.397608
48	9885.165643	-76.315232	0.044663	-76.364461	-76.319803
49	11118.135359	-76.296954	0.049428	-76.353086	-76.303663

50	2793.732543	-76.391847	0.012290	-76.406080	-76.393791

1.2 SPC/Fw

Table 6: Isobaric heat capacities for bulk water. The data is depicted as Figure 6. in the main text.

	c_p / J·K^{-1}mol^{-1}					
T / K	exp.	class HO	quant. HO	class. sim.	1PT	GSTA
25	3.079	74.826	2.768	75.321±0.044	0.7187±0.0078	3.80±0.15
50	7.875	74.826	6.992	75.961±0.058	1.579±0.013	8.38±0.25
100	15.735	74.826	13.667	77.438±0.086	3.170±0.022	17.28±0.35
150	22.071	74.826	19.303	79.10±0.10	5.783±0.031	24.53±0.33
200	28.230	74.826	24.429	81.30±0.16	10.314±0.058	33.61±0.46
273.15	75.917	74.826	31.020	110.35±0.74	20.689±0.090	72.3±1.0
298.15	75.375	74.826	32.964	109.27±0.42	23.097±0.077	72.64±0.57
323.15	75.277	74.826	34.752	107.31±0.61	25.206±0.076	72.19±0.82
348.15	75.521	74.826	36.392	107.05±0.57	27.162±0.083	73.65±0.79
373.15	75.993	74.826	37.895	105.98±0.45	28.641±0.080	72.74±0.67
400	35.982	58.198	34.742	56.93±0.30	50.85±0.21	40.46±0.42
500	35.699	58.198	35.912	55.77±0.32	50.58±0.21	38.16±0.19
600	36.521	58.198	37.086	54.94±0.20	52.93±0.18	39.73±0.21
700	37.596	58.198	38.250	54.88±0.20	54.20±0.16	41.12±0.23
800	38.780	58.198	39.424	55.19±0.16	55.08±0.16	41.85±0.12
900	40.023	58.198	40.613	54.59±0.24	56.89±0.18	42.61±0.20
1000	41.292	58.198	41.801	55.04±0.17	57.72±0.16	43.60±0.14

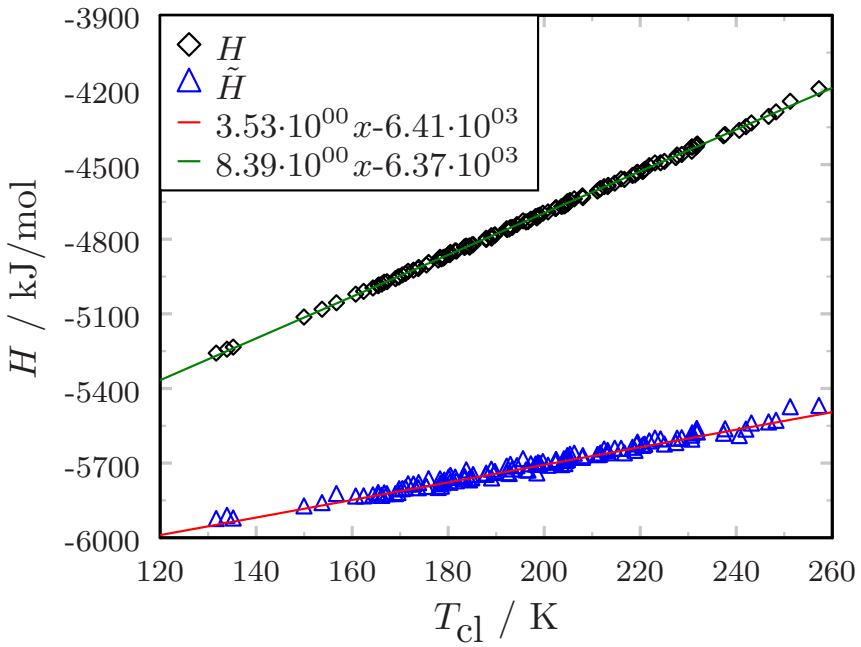

Figure 5: Classic and smoothed enthalpy (for ice at 200 K) as a function of simulation temperature.

Table 7: Simulation temperature, average enthalpy and smoothed average enthalpy components of trajectories associated to the calculation of ice at 200 K.

trajectory #	$T_{\text{simul.}}$ K	$\langle H \rangle$	$\langle \tilde{E}_{kin} \rangle$	$\langle \tilde{E}_{pot} \rangle$ kJ/mol	pV	$\langle \tilde{H} \rangle$
1	173.842	-4913.473	227.832	-6027.933	0.193	-5799.908
2	184.449	-4831.896	233.174	-6022.647	0.192	-5789.281
3	173.763	-4918.117	219.663	-6039.935	0.193	-5820.079
4	193.329	-4752.560	248.973	-5994.896	0.195	-5745.728
5	192.273	-4760.814	241.639	-6002.849	0.195	-5761.015
6	196.202	-4730.455	246.145	-5996.196	0.195	-5749.856
7	204.301	-4665.358	258.060	-5983.364	0.194	-5725.109
8	189.735	-4782.629	245.219	-6001.752	0.195	-5756.339
9	160.733	-5020.859	203.668	-6056.820	0.194	-5852.957
10	220.502	-4527.844	288.196	-5940.972	0.194	-5652.582
11	207.945	-4625.961	266.207	-5966.443	0.196	-5700.039
12	199.714	-4695.534	259.964	-5976.727	0.195	-5716.568
13	204.817	-4649.202	267.705	-5960.787	0.197	-5692.886
14	180.458	-4853.180	237.208	-6008.922	0.196	-5771.518
15	211.478	-4600.041	270.936	-5960.328	0.195	-5689.198
16	169.536	-4951.608	210.091	-6049.478	0.194	-5839.194
17	169.024	-4958.438	209.301	-6053.234	0.193	-5843.739
18	227.669	-4461.696	296.819	-5921.762	0.195	-5624.747
19	208.047	-4632.879	272.554	-5965.743	0.194	-5692.996
20	231.780	-4419.462	310.041	-5896.269	0.196	-5586.032
21	218.392	-4543.676	284.791	-5945.442	0.194	-5660.458
22	183.757	-4827.546	248.419	-5997.894	0.194	-5749.281
23	212.472	-4588.847	280.090	-5947.439	0.196	-5667.153
24	241.995	-4347.725	313.277	-5901.816	0.194	-5588.345
25	153.714	-5081.492	194.098	-6073.278	0.192	-5878.988
26	221.883	-4504.345	290.824	-5926.221	0.196	-5635.201
27	243.152	-4332.782	322.169	-5887.016	0.195	-5564.653
28	187.900	-4796.274	238.826	-6006.627	0.195	-5767.605
29	196.612	-4729.209	247.894	-5998.826	0.194	-5750.738
30	169.782	-4951.332	218.476	-6042.503	0.193	-5823.833
31	216.016	-4557.299	279.596	-5944.660	0.196	-5664.868
32	177.919	-4883.655	217.808	-6037.644	0.194	-5819.642
33	230.806	-4429.462	304.364	-5907.117	0.197	-5602.556
34	167.240	-4970.872	208.400	-6052.801	0.193	-5844.207
35	248.285	-4288.396	325.834	-5879.812	0.196	-5553.783
36	185.186	-4821.460	240.896	-6009.187	0.194	-5768.097
37	218.908	-4541.521	278.748	-5951.506	0.195	-5672.563
38	192.705	-4758.877	241.096	-6005.770	0.194	-5764.481
39	251.238	-4245.656	342.735	-5841.832	0.198	-5498.899
40	189.650	-4784.185	244.361	-6003.627	0.194	-5759.072
41	220.683	-4524.924	288.473	-5939.768	0.194	-5651.101
42	178.578	-4878.558	221.297	-6035.381	0.194	-5813.890
43	230.733	-4446.264	298.431	-5927.487	0.193	-5628.863
44	184.923	-4823.348	234.557	-6015.973	0.194	-5781.222
45	206.254	-4637.905	271.867	-5955.603	0.196	-5683.540
46	198.686	-4706.071	258.170	-5980.023	0.195	-5721.658
47	187.917	-4801.263	244.382	-6006.927	0.193	-5762.352
48	171.125	-4937.463	217.736	-6038.504	0.194	-5820.575

49	179.183	-4872.211	232.478	-6022.377	0.194	-5789.705
50	204.541	-4659.813	262.731	-5975.440	0.195	-5712.514
51	171.649	-4929.086	224.265	-6029.028	0.194	-5804.569
52	178.301	-4872.906	231.389	-6016.706	0.195	-5785.122
53	199.056	-4703.465	257.548	-5981.840	0.195	-5724.098
54	203.631	-4668.380	254.712	-5984.038	0.195	-5729.131
55	183.393	-4833.188	236.777	-6012.333	0.194	-5775.362
56	198.206	-4708.919	255.197	-5982.400	0.195	-5727.008
57	237.671	-4378.996	312.302	-5900.383	0.195	-5587.886
58	181.712	-4847.912	228.959	-6022.077	0.195	-5792.923
59	194.313	-4741.177	253.778	-5986.408	0.195	-5732.435
60	213.210	-4588.502	279.880	-5952.474	0.194	-5672.399
61	228.642	-4459.312	300.915	-5922.985	0.195	-5621.875
62	149.953	-5112.827	188.800	-6081.280	0.192	-5892.287
63	198.625	-4709.528	257.289	-5985.248	0.193	-5727.765
64	213.331	-4583.615	273.460	-5955.454	0.196	-5681.799
65	204.109	-4666.069	267.928	-5973.561	0.194	-5705.439
66	257.219	-4195.108	341.719	-5835.916	0.199	-5493.999
67	135.210	-5233.710	168.533	-6108.522	0.192	-5939.797
68	166.159	-4980.467	206.200	-6057.118	0.193	-5850.725
69	224.225	-4492.610	297.014	-5924.505	0.195	-5627.296
70	192.953	-4753.579	257.633	-5985.221	0.194	-5727.395
71	180.342	-4862.024	227.303	-6026.411	0.195	-5798.913
72	202.326	-4676.215	260.469	-5976.732	0.196	-5716.068
73	156.716	-5055.534	210.774	-6053.276	0.193	-5842.309
74	216.691	-4559.759	274.018	-5957.169	0.194	-5682.957
75	227.412	-4471.872	292.022	-5934.019	0.194	-5641.802
76	246.734	-4306.325	325.113	-5885.298	0.194	-5559.990
77	181.454	-4846.683	233.744	-6012.503	0.195	-5778.563
78	204.838	-4657.430	265.080	-5974.613	0.195	-5709.338
79	195.580	-4726.201	265.763	-5970.628	0.195	-5704.670
80	184.404	-4827.283	232.189	-6018.044	0.194	-5785.660
81	231.892	-4417.414	302.887	-5903.221	0.197	-5600.137
82	175.461	-4903.691	220.946	-6037.237	0.193	-5816.098
83	166.666	-4972.944	209.303	-6050.079	0.194	-5840.582
84	175.910	-4893.599	233.477	-6017.788	0.194	-5784.117
85	165.404	-4986.973	211.962	-6051.573	0.193	-5839.419
86	197.210	-4719.583	257.383	-5983.477	0.195	-5725.899
87	231.659	-4428.782	309.614	-5906.593	0.195	-5596.784
88	219.428	-4530.818	291.724	-5931.867	0.195	-5639.948
89	214.684	-4574.651	283.370	-5947.756	0.194	-5664.191
90	170.458	-4943.366	217.458	-6041.331	0.194	-5823.679
91	192.177	-4758.126	252.575	-5987.621	0.195	-5734.851
92	237.349	-4384.282	303.662	-5909.641	0.195	-5605.784
93	179.017	-4875.121	228.891	-6025.732	0.193	-5796.648
94	219.278	-4532.268	288.972	-5935.730	0.195	-5646.563
95	198.455	-4714.443	241.146	-6003.828	0.194	-5762.488
96	205.027	-4653.779	270.054	-5966.441	0.195	-5696.192
97	133.918	-5242.103	173.289	-6101.924	0.192	-5928.444
98	172.755	-4924.445	226.293	-6031.909	0.193	-5805.423
99	178.369	-4877.307	224.884	-6028.564	0.194	-5803.486
100	164.315	-4996.013	207.272	-6056.070	0.193	-5848.606
101	225.031	-4487.208	287.618	-5935.935	0.196	-5648.121
102	189.030	-4795.656	236.058	-6017.589	0.193	-5781.338

103	205.363	-4644.404	269.895	-5958.323	0.196	-5688.232
104	211.079	-4606.193	272.965	-5962.373	0.194	-5689.213
105	204.864	-4654.241	266.285	-5969.756	0.195	-5703.277
106	188.985	-4785.932	248.459	-5995.523	0.194	-5746.869
107	165.526	-4983.896	205.750	-6055.202	0.194	-5849.258
108	230.712	-4429.675	298.431	-5910.660	0.197	-5612.032
109	220.931	-4519.250	287.248	-5936.258	0.195	-5648.815
110	183.412	-4831.074	230.599	-6014.892	0.196	-5784.097
111	200.792	-4690.299	254.053	-5986.179	0.195	-5731.931
112	162.376	-5009.690	204.030	-6057.817	0.193	-5853.594
113	178.898	-4875.414	227.168	-6028.666	0.194	-5801.305
114	202.465	-4673.128	263.949	-5972.474	0.195	-5708.330
115	211.703	-4596.578	273.718	-5956.762	0.195	-5682.849
116	180.079	-4860.881	236.251	-6014.022	0.194	-5777.577
117	131.675	-5257.700	166.486	-6108.163	0.193	-5941.484
118	202.380	-4676.373	259.174	-5979.102	0.195	-5719.733
119	223.067	-4493.392	296.262	-5920.230	0.196	-5623.771
120	240.626	-4362.442	302.307	-5917.661	0.195	-5615.159

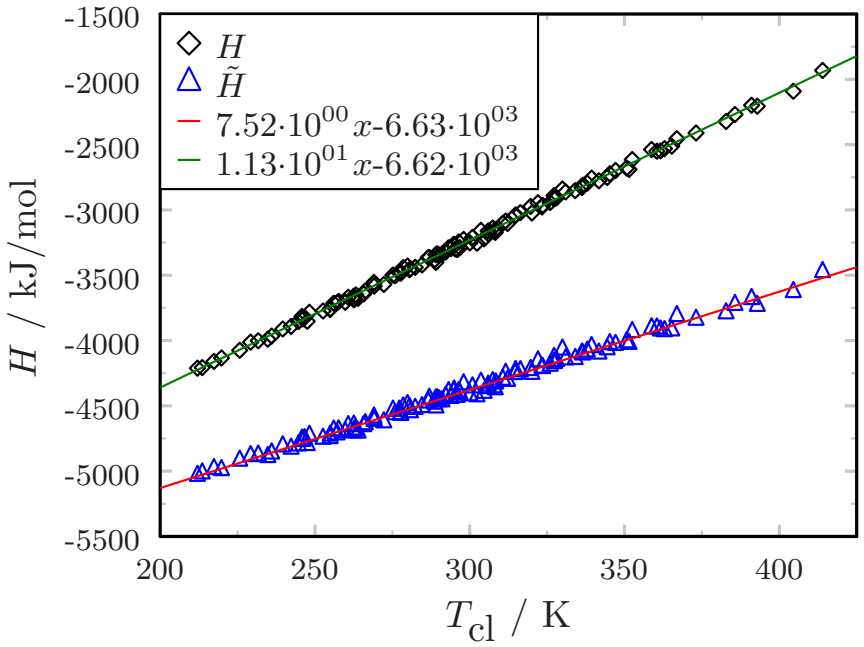

Figure 6: Classic and smoothed enthalpy (for water at 298 K) as a function of simulation temperature.

Table 8: Simulation temperature, average enthalpy and smoothed average enthalpy components of trajectories associated to the calculation of liquid water at 298 K.

trajectory #	$T_{\text{simul.}}$ K	$\langle H \rangle$	$\langle \tilde{E}_{kin} \rangle$	$\langle \tilde{E}_{pot} \rangle$ kJ/mol	pV	$\langle \tilde{H} \rangle$
1	307.835	-3162.206	585.343	-4952.010	0.188	-4366.478
2	308.359	-3150.129	596.075	-4933.913	0.189	-4337.649
3	336.268	-2828.335	657.556	-4765.978	0.188	-4108.234
4	252.611	-3774.111	481.489	-5241.123	0.182	-4759.451

5	254.891	-3762.387	486.578	-5242.027	0.190	-4755.259
6	300.893	-3210.106	582.781	-4950.254	0.190	-4367.283
7	350.688	-2678.919	680.624	-4703.671	0.192	-4022.855
8	289.539	-3335.833	555.239	-5014.808	0.188	-4459.381
9	263.933	-3676.990	499.797	-5212.503	0.186	-4712.521
10	361.633	-2547.799	703.618	-4636.248	0.192	-3932.438
11	265.754	-3643.048	515.082	-5178.171	0.187	-4662.902
12	344.391	-2751.782	666.863	-4743.147	0.190	-4076.094
13	290.074	-3348.092	558.160	-5031.509	0.188	-4473.161
14	323.558	-2965.447	619.414	-4839.269	0.190	-4219.665
15	231.684	-4001.624	451.602	-5338.506	0.185	-4886.719
16	277.288	-3481.563	538.139	-5082.920	0.188	-4544.593
17	262.668	-3682.517	504.367	-5203.037	0.184	-4698.486
18	293.973	-3296.012	558.088	-5006.240	0.188	-4447.964
19	284.579	-3421.314	550.258	-5068.183	0.184	-4517.740
20	319.668	-2973.247	602.726	-4837.727	0.189	-4234.812
21	300.042	-3251.965	569.161	-4996.838	0.185	-4427.492
22	234.765	-3989.659	451.195	-5350.427	0.186	-4899.047
23	362.919	-2531.071	697.656	-4635.031	0.195	-3937.180
24	327.360	-2912.130	628.244	-4809.492	0.189	-4181.059
25	347.112	-2697.667	665.988	-4709.437	0.196	-4043.253
26	382.803	-2323.245	738.289	-4539.802	0.195	-3801.317
27	391.047	-2198.610	761.245	-4454.012	0.201	-3692.567
28	280.525	-3457.837	548.607	-5073.731	0.187	-4524.937
29	345.234	-2723.579	674.812	-4711.616	0.192	-4036.611
30	373.104	-2410.959	720.999	-4571.880	0.201	-3850.679
31	311.603	-3085.598	613.618	-4877.283	0.191	-4263.474
32	294.841	-3263.700	568.115	-4970.209	0.186	-4401.909
33	282.390	-3439.643	544.094	-5075.115	0.184	-4530.836
34	358.733	-2537.651	694.208	-4610.384	0.193	-3915.983
35	229.218	-4012.390	444.432	-5336.507	0.188	-4891.888
36	327.218	-2890.250	636.638	-4779.120	0.191	-4142.291
37	323.331	-2977.951	628.081	-4844.779	0.190	-4216.507
38	279.914	-3429.180	542.443	-5045.081	0.187	-4502.451
39	310.674	-3101.978	593.333	-4902.530	0.187	-4309.009
40	262.606	-3687.930	501.409	-5212.057	0.182	-4710.467
41	272.241	-3570.714	516.931	-5151.669	0.188	-4634.551
42	296.806	-3288.956	580.214	-4998.905	0.186	-4418.504
43	292.237	-3322.292	570.858	-5009.462	0.184	-4438.419
44	306.025	-3183.820	586.305	-4959.520	0.188	-4373.026
45	336.532	-2810.442	645.044	-4761.459	0.194	-4116.221
46	385.676	-2269.316	754.037	-4491.604	0.202	-3737.365
47	298.024	-3226.023	591.540	-4934.824	0.184	-4343.100
48	236.017	-3966.202	456.784	-5329.615	0.183	-4872.648
49	366.900	-2454.715	731.412	-4553.786	0.196	-3822.178
50	225.697	-4074.793	444.188	-5371.311	0.181	-4926.942
51	329.944	-2840.122	652.065	-4730.311	0.193	-4078.053
52	239.603	-3911.605	471.412	-5289.374	0.187	-4817.775
53	289.085	-3401.692	556.117	-5077.030	0.188	-4520.726
54	269.068	-3561.347	520.426	-5117.766	0.187	-4597.153
55	308.237	-3172.430	583.683	-4965.588	0.187	-4381.718
56	278.519	-3441.538	534.097	-5055.249	0.186	-4520.966
57	325.969	-2943.607	628.248	-4830.639	0.187	-4202.203
58	334.071	-2852.193	639.959	-4790.690	0.192	-4150.540

59	413.978	-1932.194	820.104	-4305.999	0.207	-3485.688
60	260.753	-3668.719	508.466	-5171.045	0.186	-4662.394
61	352.505	-2614.502	694.709	-4639.476	0.198	-3944.569
62	293.179	-3289.878	572.701	-4976.575	0.186	-4403.688
63	213.589	-4207.351	415.773	-5439.783	0.186	-5023.824
64	360.451	-2550.450	708.576	-4626.063	0.193	-3917.294
65	290.120	-3345.797	557.847	-5024.998	0.183	-4466.969
66	266.255	-3620.086	511.693	-5160.538	0.189	-4648.655
67	275.198	-3498.754	538.279	-5082.928	0.187	-4544.462
68	256.068	-3714.749	495.478	-5192.975	0.185	-4697.312
69	302.339	-3255.285	576.991	-5012.846	0.188	-4435.667
70	351.457	-2690.077	683.063	-4718.210	0.191	-4034.956
71	246.662	-3823.014	480.477	-5243.169	0.188	-4762.505
72	259.778	-3707.525	500.555	-5211.279	0.190	-4710.533
73	288.714	-3381.062	557.396	-5049.434	0.183	-4491.855
74	262.550	-3660.815	514.830	-5173.714	0.185	-4658.699
75	269.057	-3555.452	509.078	-5121.315	0.187	-4612.049
76	339.368	-2756.469	657.300	-4717.087	0.192	-4059.594
77	330.980	-2862.197	630.987	-4785.183	0.186	-4154.011
78	280.842	-3451.061	531.118	-5088.009	0.190	-4556.700
79	392.882	-2206.087	746.141	-4491.388	0.200	-3745.048
80	365.248	-2512.240	698.473	-4631.337	0.195	-3932.670
81	246.087	-3834.301	479.147	-5254.933	0.186	-4775.600
82	303.619	-3156.364	582.576	-4914.733	0.193	-4331.964
83	248.214	-3783.578	481.302	-5217.825	0.188	-4736.335
84	295.377	-3299.316	570.356	-5008.410	0.188	-4437.866
85	316.366	-3020.682	607.998	-4852.092	0.189	-4243.905
86	277.716	-3484.891	525.534	-5103.411	0.185	-4577.692
87	242.294	-3892.281	462.352	-5298.135	0.185	-4835.597
88	327.161	-2915.198	630.387	-4810.928	0.190	-4180.350
89	312.211	-3104.108	596.860	-4914.191	0.189	-4317.142
90	296.471	-3245.336	564.962	-4967.096	0.187	-4401.947
91	257.159	-3709.188	483.348	-5209.772	0.190	-4726.234
92	263.227	-3650.907	496.396	-5186.025	0.184	-4689.444
93	404.535	-2091.519	786.877	-4425.802	0.199	-3638.727
94	307.432	-3138.813	592.024	-4919.075	0.186	-4326.865
95	254.938	-3757.612	494.066	-5229.749	0.185	-4735.498
96	296.004	-3303.243	572.277	-5012.106	0.189	-4439.640
97	322.040	-2944.745	630.644	-4798.483	0.189	-4167.650
98	294.966	-3264.629	575.211	-4966.393	0.188	-4390.995
99	314.822	-3037.854	613.243	-4854.649	0.192	-4241.215
100	269.144	-3583.120	517.330	-5141.535	0.189	-4624.016
101	320.083	-3023.590	615.110	-4879.130	0.191	-4263.830
102	212.032	-4211.474	401.948	-5445.229	0.180	-5043.101
103	247.507	-3852.922	477.722	-5285.764	0.187	-4807.855
104	341.725	-2776.979	652.345	-4761.522	0.191	-4108.985
105	275.912	-3504.185	530.195	-5102.918	0.186	-4572.536
106	244.661	-3855.208	465.800	-5276.958	0.187	-4810.970
107	219.800	-4133.563	414.879	-5413.956	0.184	-4998.892
108	291.045	-3337.710	553.617	-5028.078	0.184	-4474.278
109	277.612	-3474.493	521.786	-5094.717	0.186	-4572.745
110	245.806	-3815.481	471.820	-5238.946	0.185	-4766.941
111	304.641	-3221.322	580.791	-4990.218	0.185	-4409.241
112	314.713	-3043.357	601.856	-4867.148	0.189	-4265.103

113	217.377	-4159.517	422.876	-5413.482	0.186	-4990.420
114	286.934	-3363.963	561.047	-5014.981	0.188	-4453.746
115	257.654	-3700.400	496.470	-5192.483	0.188	-4695.825
116	286.634	-3363.781	546.274	-5029.739	0.186	-4483.279
117	289.030	-3342.901	557.636	-5016.137	0.188	-4458.313
118	337.971	-2795.042	654.691	-4748.510	0.192	-4093.627
119	305.955	-3161.124	583.363	-4938.036	0.188	-4354.485
120	328.022	-2907.402	634.853	-4800.676	0.192	-4165.631

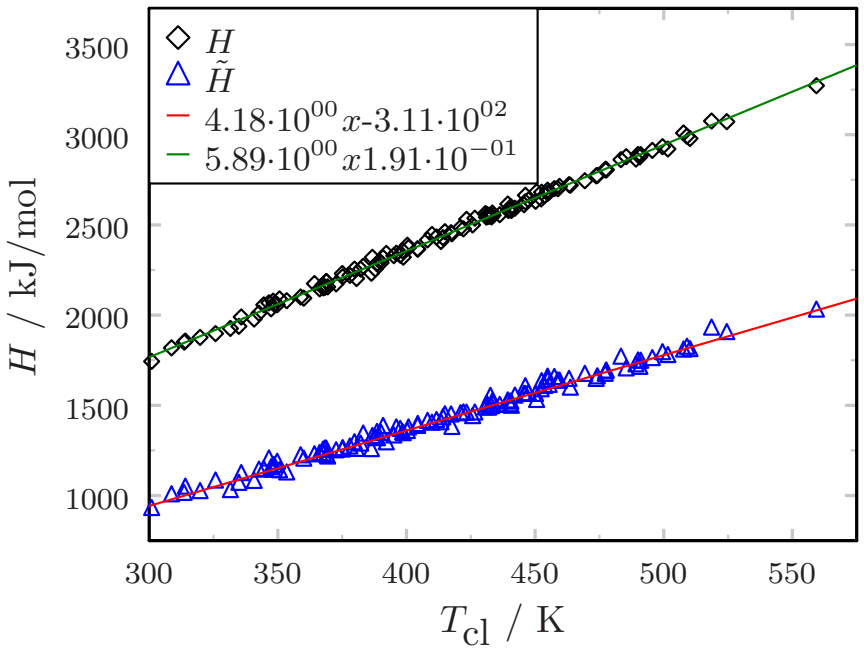

Figure 7: Classic and smoothed enthalpy (for water vapor at 400 K) as a function of simulation temperature.

Table 9: Simulation temperature, average enthalpy and smoothed average enthalpy components of trajectories associated to the calculation of water vapor at 400 K.

trajectory #	$T_{\mathrm{simul.}}$ K	$\langle H \rangle$	$\langle \tilde{E}_{kin} \rangle$	$\langle \tilde{E}_{pot} \rangle$ kJ/mol	pV	$\langle \tilde{H} \rangle$
1	450.577	2683.102	1156.667	-8.783	372.381	1520.265
2	392.149	2341.960	984.321	-18.530	319.522	1285.313
3	350.634	2089.687	873.282	-24.908	282.107	1130.481
4	417.642	2450.733	1070.968	-43.776	343.303	1370.495
5	353.438	2079.775	882.256	-47.938	284.038	1118.356
6	331.555	1926.185	826.437	-70.258	264.345	1020.525
7	446.243	2664.062	1166.286	-9.319	396.949	1553.915
8	364.224	2174.816	926.726	-20.158	312.284	1218.851
9	344.542	2056.985	869.001	-26.173	294.901	1137.730
10	386.744	2320.359	991.524	-9.036	337.856	1320.343
11	507.707	3009.540	1353.512	-18.021	464.042	1799.534
12	430.679	2562.673	1119.515	-21.719	381.199	1478.995
13	439.389	2615.586	1145.944	-17.361	389.036	1517.619
14	485.406	2878.289	1280.496	-17.770	432.307	1695.034

15	423.349	2530.748	1092.405	-10.722	367.677	1449.360
16	400.341	2387.217	1024.390	-21.162	344.761	1347.990
17	426.580	2537.161	1101.880	-18.694	367.403	1450.590
18	348.182	2077.480	870.901	-27.988	290.094	1133.007
19	409.907	2447.155	1054.808	-19.209	358.461	1394.060
20	375.062	2230.499	954.345	-23.002	314.113	1245.456
21	368.930	2185.615	938.018	-27.102	304.991	1215.908
22	340.793	1978.023	861.035	-58.659	269.079	1071.455
23	386.366	2232.058	997.930	-60.165	309.949	1247.714
24	334.850	1937.806	853.091	-63.051	270.716	1060.756
25	380.588	2202.845	991.215	-61.422	319.170	1248.963
26	372.650	2173.082	971.203	-46.126	316.054	1241.131
27	398.760	2321.011	1045.703	-52.616	343.009	1336.097
28	474.185	2773.785	1267.904	-40.840	423.906	1650.970
29	433.690	2553.415	1146.470	-30.041	383.692	1500.121
30	422.148	2478.056	1114.604	-34.955	371.147	1450.796
31	413.416	2407.988	1089.043	-50.613	358.034	1396.465
32	360.084	2094.057	938.664	-50.481	306.493	1194.676
33	387.869	2255.563	1023.366	-51.393	338.055	1310.028
34	458.859	2699.992	1233.744	-25.004	419.238	1627.977
35	366.246	2145.623	952.635	-37.983	311.098	1225.751
36	442.155	2592.439	1181.489	-28.385	391.165	1544.269
37	367.543	2166.461	956.655	-27.035	314.438	1244.059
38	453.775	2663.448	1217.201	-22.313	402.941	1597.829
39	367.662	2151.077	953.828	-37.828	306.854	1222.854
40	559.340	3271.460	1532.201	-14.954	503.616	2020.862
41	509.011	2991.274	1375.543	-9.714	449.425	1815.253
42	433.361	2565.508	1144.752	-3.022	370.535	1512.266
43	490.012	2890.286	1314.307	-5.853	430.682	1739.135
44	379.796	2254.963	980.401	-2.899	308.096	1285.598
45	431.396	2557.608	1132.338	1.715	360.420	1494.473
46	411.685	2432.926	1075.864	-11.936	344.701	1408.629
47	447.449	2638.388	1185.644	-10.579	382.424	1557.489
48	414.931	2462.304	1089.676	-1.971	352.861	1440.566
49	495.559	2912.997	1330.945	-11.812	432.991	1752.124
50	375.213	2212.094	967.656	-17.418	302.869	1253.107
51	436.259	2556.563	1150.858	-19.689	361.338	1492.507
52	477.232	2805.226	1270.961	-2.754	397.024	1665.231
53	408.175	2416.938	1067.931	5.705	330.264	1403.901
54	491.042	2889.286	1318.057	-0.577	420.001	1737.481
55	368.777	2186.549	954.674	-4.787	300.934	1250.820
56	417.331	2456.946	1101.286	-7.657	346.161	1439.790
57	397.571	2332.055	1047.435	-15.554	327.780	1359.660
58	501.610	2920.543	1358.977	-20.137	430.098	1768.938
59	396.042	2342.870	1040.406	-3.636	331.129	1367.899
60	335.784	1989.667	857.844	-11.364	268.307	1114.787
61	463.186	2723.136	1243.697	-5.584	398.857	1636.970
62	455.475	2682.387	1217.514	-4.520	390.501	1603.495
63	499.524	2933.522	1352.457	-3.770	436.027	1784.714
64	459.478	2713.387	1229.402	1.730	396.057	1627.190
65	314.043	1855.817	803.282	-21.483	258.084	1039.883
66	368.220	2153.389	969.030	-30.037	311.556	1250.550
67	358.862	2100.234	940.725	-33.711	306.201	1213.215
68	469.329	2744.632	1270.382	-23.182	417.540	1664.739

69	524.506	3072.092	1435.164	-14.253	475.436	1896.347
70	390.157	2290.483	1027.660	-30.987	339.952	1336.625
71	349.753	2057.592	909.034	-34.030	302.643	1177.646
72	452.540	2681.193	1217.014	-10.834	417.879	1624.059
73	383.191	2270.506	1009.773	-16.873	340.926	1333.826
74	457.463	2701.258	1237.379	-17.033	427.172	1647.519
75	483.369	2861.692	1313.482	-7.939	454.308	1759.851
76	390.912	2318.069	1036.820	-15.786	354.924	1375.958
77	518.582	3075.653	1423.118	-4.524	502.541	1921.135
78	346.533	2068.264	900.377	-10.946	306.400	1195.831
79	325.778	1897.561	844.713	-46.054	274.865	1073.523
80	454.840	2692.630	1232.593	-2.903	419.588	1649.278
81	446.178	2627.834	1204.845	-8.938	400.292	1596.198
82	454.920	2675.756	1231.647	-6.045	404.631	1630.233
83	432.623	2550.262	1164.951	-5.471	383.532	1543.011
84	388.538	2285.640	1027.300	-15.434	331.094	1342.960
85	404.384	2364.779	1070.936	-21.710	337.825	1387.051
86	452.362	2643.890	1212.514	-18.527	385.603	1579.590
87	445.701	2611.684	1190.075	-19.195	382.760	1553.639
88	414.172	2429.609	1095.245	-21.271	350.350	1424.325
89	404.318	2368.211	1063.486	-25.034	338.110	1376.562
90	450.183	2630.697	1197.808	-17.833	373.713	1553.688
91	378.006	2219.989	979.001	-21.012	303.985	1261.974
92	369.353	2156.389	949.952	-32.352	289.121	1206.721
93	382.180	2254.877	985.894	-15.389	307.828	1278.333
94	398.484	2356.485	1029.394	-11.505	323.329	1341.218
95	463.677	2719.589	1223.037	-13.749	379.022	1588.310
96	440.754	2579.413	1154.132	-17.908	351.907	1488.132
97	490.721	2877.102	1306.162	-6.708	404.407	1703.860
98	440.390	2585.154	1154.508	-10.091	352.314	1496.731
99	319.775	1876.444	802.987	-30.981	242.885	1014.891
100	425.708	2499.663	1107.438	-11.105	334.193	1430.526
101	440.557	2600.686	1154.697	-3.388	360.448	1511.756
102	395.086	2329.307	1020.976	-15.452	317.973	1323.498
103	431.945	2546.960	1131.610	-11.194	357.242	1477.658
104	313.587	1850.264	787.171	-28.931	246.893	1005.133
105	388.738	2286.577	1010.596	-24.444	322.268	1308.420
106	431.078	2543.082	1140.096	-12.037	369.639	1497.698
107	421.020	2485.729	1103.956	-15.180	357.547	1446.323
108	400.787	2373.665	1042.975	-13.541	338.191	1367.625
109	477.471	2808.722	1276.601	-9.679	412.025	1678.947
110	433.065	2544.046	1141.381	-14.318	359.038	1486.101
111	473.736	2771.914	1259.742	-15.960	393.019	1636.801
112	300.947	1743.588	749.755	-50.537	221.978	921.196
113	439.606	2580.151	1162.035	-16.094	367.405	1513.346
114	308.671	1818.591	779.708	-26.884	244.310	997.134
115	477.672	2804.380	1282.118	-7.235	408.443	1683.327
116	342.660	2010.698	883.386	-23.361	273.935	1133.960
117	510.199	2978.893	1379.321	-14.732	437.316	1801.905
118	348.530	2061.333	893.830	-15.359	281.333	1159.804
119	489.190	2864.839	1313.558	-13.075	417.027	1717.510
120	347.366	2034.824	896.099	-23.655	275.078	1147.522

2 PIMD simulations

The results of the N, p, T PIMD simulations with 32 beads are collected in Figure 8 and Table 10. The enthalpy changes linearly with the temperature, therefore the heat capacity is constant, 79.6 J/K/mol in this temperature range.

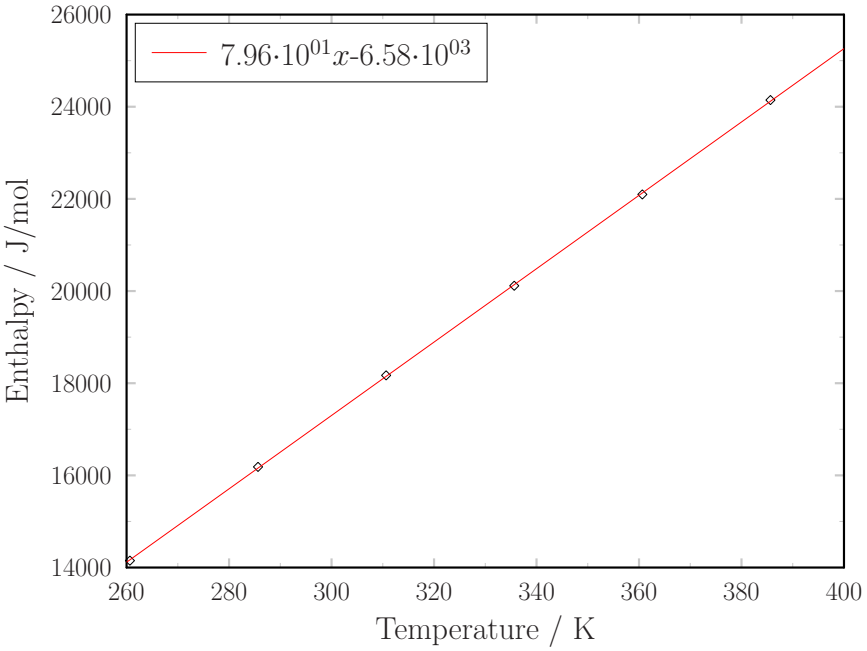

Figure 8: Enthalpy of N, p, T PIMD simulations as a function of temperature.

Table 10: Simulation temperature, density, average energy and enthalpy.

T	ρ	$\langle E \rangle$	$\langle H \rangle$
K	kg/m^3	J/mol	
260.65	1006.0	14147.7	14149.5
285.65	996.3	16182.0	16183.8
310.65	978.8	18168.5	18170.4
335.65	958.3	20112.7	20114.6
360.65	934.7	22094.7	22096.6
385.65	903.6	24142.6	24144.7