Electronic Supplementary Information for the article "Thermodynamics, dynamics, and structure of supercritical water at extreme conditions"

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This Electronic Supplementary Information (ESI) provides (1) the number of hydrogen bonds (HBs) per molecule from a single distance criterion ($r_{\mathrm{O...H}} < 2.2$ Å); (2) the timestep validation results; (3) the influence of the bond flexibility on the dynamic behavior of supercritical water; and (4) numerical data obtained from the two-phase thermodynamic (2PT) model and structural parameters of the TIP4P/2005 water model.

A. The number of hydrogen bonds (HBs) from a single distance criterion

Fig. S1 shows that the number of HBs per molecule from a single distance criterion ($r_{\mathrm{O...H}} < 2.2$ Å) is almost identical to that obtained from the electron structure criterion. This result suggests that the normal vector criterion used to define $\langle n^{\mathrm{E}}_{\mathrm{HB}} \rangle$ does not readily reflect the orientational changes in the supercritical region.

B. Effect of the simulation timestep

We additionally perform a set of TIP4P/2005 simulations along an isotherm ($T_{\mathrm{r}} = 1.0$ and $\rho_{\mathrm{r}} = 0.1 - 6.1$) to validate that the timestep of $\Delta t = 1.0$ fs is sufficiently short to keep track of the dynamic behavior of supercritical water. Table S1 shows that both fluidicity data ($f^{\mathrm{t}}_{\mathrm{g}}$ and $f^{\mathrm{r}}_{\mathrm{g}}$) from $\Delta t = 1$ fs simulations agree well with those from $\Delta t = 0.5$ fs ($f'^{\mathrm{t}}_{\mathrm{g}}$ and $f'^{\mathrm{r}}_{\mathrm{g}}$). Moreover, it should be noted that the Frenkel line (FL) from the $Z(t)$ criterion obtained in this work agrees well with that proposed by Yang et al. and Fomin et al. Since Fomin et al. used the timestep of $\Delta t =$ 0.1 fs, the consistency of the FL indicates that the simulation timestep of $\Delta t = 1$ fs is sufficiently short to obtain a variety of thermodynamic properties as well as to locate the dynamic crossover within the studied thermodynamic conditions.

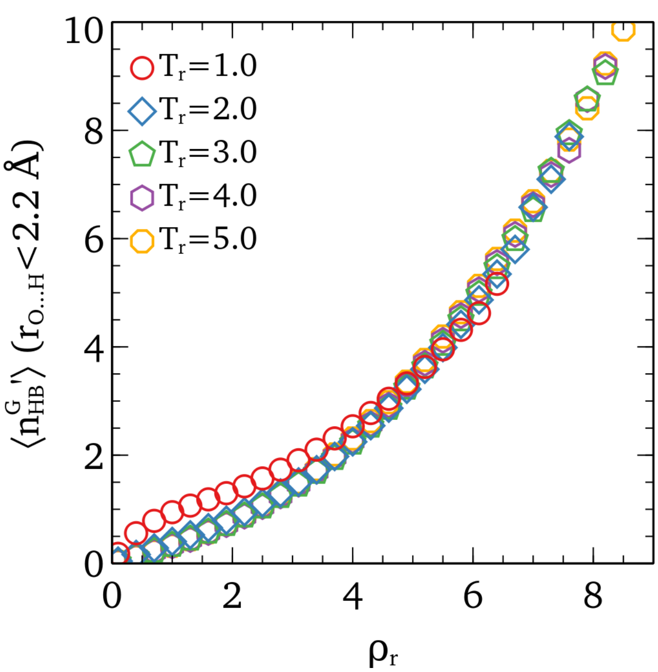

FIG. S1. The numbers of hydrogen bonds per molecule ($\langle n_{\mathrm{HB}} \rangle$) using only the OH distance criterion ($r_{\mathrm{O...H}} < 2.2$ Å). For all temperatures, it is almost identical to that obtained from the electron energy criterion [Fig. 7 (a) in the main article].

TABLE S1. Influence of the timestep selection in the TIP4P/2005 simulations at $T_{\mathrm{r}} = 1.0$. The symbols $f^{\mathrm{m}}_{\mathrm{g}}$ and $f'^{\mathrm{m}}_{\mathrm{g}}$ indicate the fluidicity data obtained from $\Delta t = 1.0$ fs and $\Delta t = 0.5$ fs, respectively. No significant discrepancy of the fluidicity data is observed.

ρ	f^t_g	f'^t_g	f^r_g	f'^r_g
28.423	0.938	0.942	0.716	0.711
198.961	0.792	0.792	0.332	0.331
369.499	0.738	0.740	0.255	0.254
540.037	0.697	0.695	0.217	0.216
710.575	0.647	0.643	0.193	0.192
881.113	0.580	0.589	0.180	0.177
1051.651	0.505	0.509	0.167	0.166
1222.189	0.421	0.422	0.158	0.155
1392.727	0.311	0.320	0.148	0.151
1563.265	0.208	0.209	0.141	0.144
1733.803	0.015	0.014	0.158	0.161

TABLE S2. Comparison of absolute entropy and fluidicity data at 298.15 K and 1,000 kg/m^3 calculated from the 2PT method for the TIP4P/2005 and the SPC/Fw water models. The intramolecular vibrational entropy cannot be calculated for the TIP4P/2005 model since it is treated as a rigid body in the simulations.

Property	TIP4P/2005	SPC/Fw
$f^{\mathrm{t}}_{\mathrm{g}}$	0.227	0.236
$f^{\mathrm{r}}_{\mathrm{g}}$	0.044	0.052
S^{t} [J/mol K]	52.312	46.014
S^{r} [J/mol K]	6.835	12.321
S^{v} [J/mol K]	n/a	0.110
S [J/mol K]	59.147	58.445

TABLE S3. Symbols and their description used in Table S4 and S5.

Symbol	Unit	Description
n_{HB}	-	Average number of HBs per molecule
$n_{\mathrm{HB}}^{\mathrm{E}}$	-	n_{HB} from the Kumar criterion
$n_{\mathrm{HB}}^{\mathrm{G}}$	-	n_{HB} from the distance-angle criterion
$n_{\mathrm{HB}}^{\mathrm{G}'}$	-	n_{HB} from the distance criterion
$\langle q \rangle$	-	Average orientational tetrahedral order
$f_{\mathrm{FCC-HCP}}$	-	The fraction of FCC and HCP types
$f_{\mathrm{g}}^{\mathrm{t}}$	-	Translational fluidicity
$f_{\mathrm{g}}^{\mathrm{r}}$	-	Rotational fluidicity
T_{r}	-	Reduced temperature ($= T/T_{\mathrm{c}}$)
T_{c}	K	Critical temperature (TIP4P/2005)
ρ	$\mathrm{kg/m^3}$	Bulk density
p	bar	Pressure
E	kJ/mol	Internal energy
H	kJ/mol	Enthalpy
S	kJ/mol K	Entropy
A	kJ/mol	Helmholtz free energy
G	kJ/mol	Gibbs free energy
D_{t}	$\mathrm{m/s^2}$	Translational diffusivity
D_{r}	$\mathrm{rad/ps^2}$	Rotational diffusivity

C. Influence of the bond flexibility on the dynamic crossover

The TIP4P/2005 water model is one of the best rigid nonpolarizable water models that can represent a variety of thermophysical properties well.[1] However, the model does not reflect the high polarizability of water as well as the charge transfer effect, which are important in aqueous electrolyte solutions. The polarizability of a molecule can be implicitly reflected in a water model by introducing bond and angle flexibility. To examine the influence of bond flexibility on the dynamic behavior of water, we perform a series of MD simulations using the SPC/Fw water model under different conditions.[2] Table S2 compares the fluidicity and thermodynamic data obtained from the TIP4P/2005 model to those from the SPC/Fw model at ambient condition (1,000 $\mathrm{kg/m^3}$ and 298.15 K). The translational and rotational fluidicity are not significantly affected by the intramolecular vibration at 298.15 K and 1,000 $\mathrm{kg/m^3}$. The thermodynamic contribution of the intramolecular vibration is quite small compared to the translational and rotational contributions as shown by Pascal et al.[3] and Lin et al.[4] The absolute entropy data are slightly different from Pascal et al.,[3] which could arise from the fact that this work uses the weighting function corrected by Sun et al.[5]

We also conduct simulations at $T = 654.1 - 2616.4$ K ($T_{\mathrm{r}} = 1.0 - 4.0$ for the TIP4P/2005 model). Fig. S2 shows that both fluidicity values are slightly higher than those from the TIP4P/2005 model but the overall behavior agrees well. Interestingly, the rotational fluidicity of the flexible water model also does not converge to zero, which suggests that the plastic crystal would also exist in the SPC/Fw model. All these results suggest that the intramolecular vibration would affect thermophysical properties only when the molecular polarizability becomes important but would not have a significant effect on the overall thermodynamic behavior considered in this work.

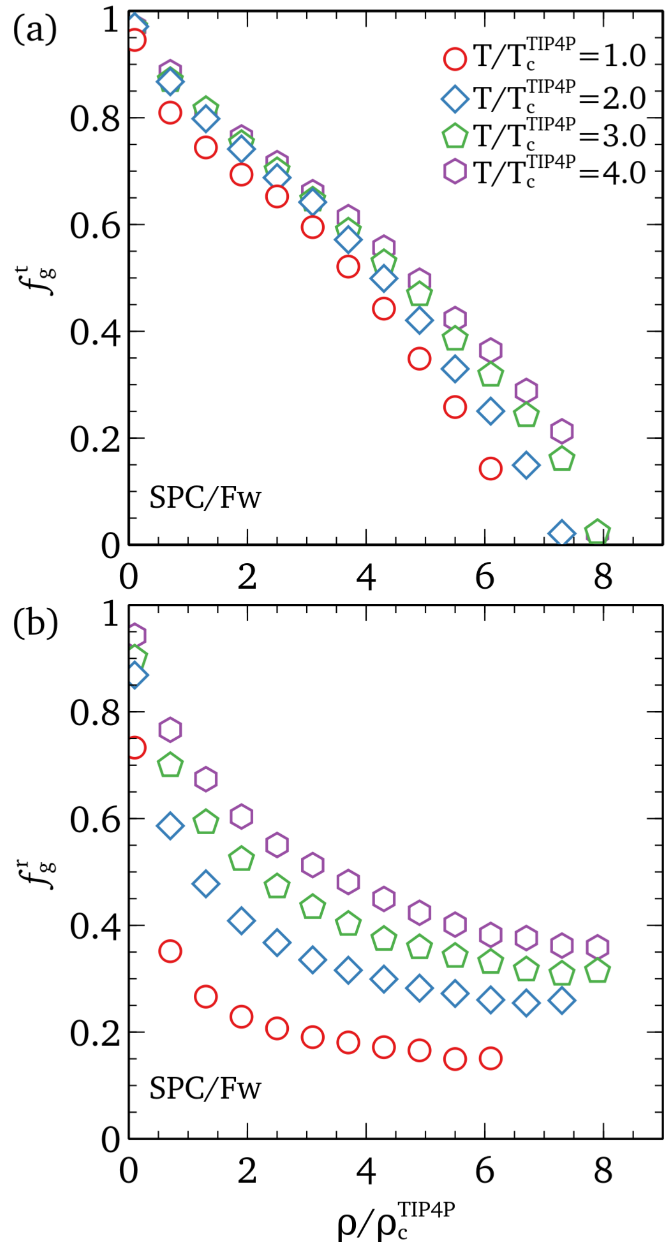

FIG. S2. (a) Translational fluidicity ($f_{\mathrm{g}}^{\mathrm{t}}$) and (b) rotational fluidicity (f_g^r) of the SPC/Fw model along isotherms. These fluidicity values are plotted against the reduced density based on the critical density of the TIP4P/2005 model for the direct comparison. The fluidicity data are slightly higher than that obtained from the TIP4P/2005 model (see Fig. 2 in the main article), but the overall behavior does not change despite the change in the model parameters.

D. NVT Simulation Results (TIP4P/2005)

Table S3 describes the variables used in Table S4 and S5. Table S4 shows the structural analysis results including the number of hydrogen bonds following different criteria, the orientational tetrahedral order, and the fraction of face-centered cubic or hexagonal close packed topological types. Table S5 shows the thermodynamic and dynamic data obtained from the 2PT model.

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[2] Y. Wu, H. L. Tepper, and G. A. Voth, The Journal of chemical physics **124**, 024503 (2006).
[3] T. A. Pascal, D. Schärf, Y. Jung, and T. D. Kühne, The Journal of chemical physics **137**, 244507 (2012).
[4] S.-T. Lin, P. K. Maiti, and W. A. Goddard III, The Journal of Physical Chemistry B **114**, 8191 (2010).
[5] T. Sun, J. Xian, H. Zhang, Z. Zhang, and Y. Zhang, The Journal of chemical physics **147**, 194505 (2017).

TABLE S4: Structural properties from the *NVT* simulations.

ρ	$n_{\mathrm{HB}}^{\mathrm{E}}$	$n_{\mathrm{HB}}^{\mathrm{G}}$	$n_{\mathrm{HB}}^{\mathrm{G'}}$	$\langle q\rangle$	$f_{\mathrm{FCC-HCP}}$
		$T_r = 1.0$			
28.423	0.174	0.188	0.177	-0.267	0.018
113.692	0.549	0.618	0.558	-0.178	0.021
198.961	0.777	0.886	0.786	-0.053	0.026
284.23	0.938	1.070	0.946	0.022	0.030
369.499	1.060	1.212	1.068	0.073	0.034
454.768	1.176	1.345	1.184	0.113	0.038
540.037	1.291	1.473	1.297	0.143	0.043
625.306	1.420	1.619	1.425	0.169	0.049
710.575	1.567	1.771	1.570	0.189	0.058
795.844	1.733	1.928	1.732	0.205	0.069
881.113	1.909	2.085	1.906	0.214	0.083
966.382	2.108	2.233	2.101	0.220	0.101
1051.651	2.320	2.376	2.309	0.222	0.126
1136.92	2.548	2.500	2.533	0.222	0.156
1222.189	2.798	2.611	2.779	0.219	0.196
1307.458	3.062	2.691	3.042	0.215	0.245
1392.727	3.347	2.742	3.325	0.206	0.302
1477.996	3.651	2.771	3.629	0.201	0.369
1563.265	3.978	2.757	3.955	0.193	0.442
1648.534	4.337	2.727	4.315	0.186	0.513
1733.803	4.644	2.673	4.623	0.128	0.992
1819.072	5.177	2.647	5.165	0.116	0.996
		$T_r = 2.0$			
28.423	0.042	0.029	0.043	-0.133	0.023
113.692	0.163	0.116	0.165	-0.067	0.026
198.961	0.281	0.204	0.285	-0.004	0.031
284.23	0.400	0.293	0.405	0.043	0.036
369.499	0.521	0.381	0.528	0.079	0.042
454.768	0.651	0.475	0.659	0.107	0.048
540.037	0.790	0.576	0.797	0.129	0.056
625.306	0.942	0.682	0.951	0.146	0.066
710.575	1.108	0.788	1.117	0.158	0.076
795.844	1.291	0.906	1.300	0.168	0.090
881.113	1.497	1.028	1.505	0.176	0.105
966.382	1.719	1.149	1.730	0.180	0.123
1051.651	1.966	1.275	1.976	0.183	0.145
1136.92	2.236	1.395	2.246	0.184	0.170
1222.189	2.533	1.509	2.545	0.185	0.199
1307.458	2.852	1.615	2.868	0.183	0.233
1392.727	3.199	1.705	3.217	0.181	0.273
1477.996	3.562	1.774	3.586	0.177	0.318
1563.265	3.960	1.823	3.987	0.173	0.368
1648.534	4.374	1.834	4.416	0.171	0.419
1733.803	4.813	1.844	4.868	0.167	0.477
1819.072	5.279	1.817	5.345	0.162	0.536
1904.341	5.723	1.995	5.801	0.129	0.996
1989.61	6.471	2.007	6.579	0.093	0.997
2074.879	6.961	1.861	7.097	0.076	0.999
2160.148	7.698	1.762	7.883	0.064	0.994
		$T_r = 3.0$			
28.423	0.031	0.017	0.032	-0.115	0.023
113.692	0.126	0.071	0.129	-0.046	0.028
198.961	0.227	0.127	0.231	0.010	0.033
284.23	0.334	0.187	0.340	0.053	0.038
369.499	0.447	0.251	0.455	0.083	0.044
454.768	0.575	0.320	0.584	0.108	0.050
540.037	0.713	0.395	0.725	0.126	0.058
625.306	0.867	0.477	0.881	0.142	0.067
710.575	1.033	0.557	1.049	0.153	0.077
795.844	1.222	0.649	1.242	0.162	0.089
881.113	1.431	0.746	1.452	0.168	0.103
966.382	1.662	0.845	1.688	0.172	0.119
1051.651	1.916	0.945	1.944	0.176	0.138
1136.92	2.196	1.045	2.228	0.178	0.158
1222.189	2.506	1.141	2.542	0.178	0.183
1307.458	2.827	1.230	2.871	0.179	0.210
1392.727	3.190	1.316	3.243	0.176	0.244
1477.996	3.573	1.388	3.636	0.176	0.278
1563.265	3.983	1.439	4.054	0.173	0.319
1648.534	4.415	1.481	4.506	0.171	0.360
1733.803	4.870	1.506	4.976	0.166	0.407
1819.072	5.341	1.499	5.469	0.162	0.454
1904.341	5.835	1.477	5.989	0.158	0.505
1989.61	6.342	1.428	6.524	0.155	0.558
2074.879	7.046	1.671	7.249	0.101	0.996
2160.148	7.699	1.577	7.944	0.092	0.995
2245.417	8.268	1.453	8.567	0.074	0.999
2330.686	8.698	1.239	9.052	0.055	0.993
		$T_r = 4.0$			
28.423	0.028	0.014	0.029	-0.108	0.024
113.692	0.117	0.056	0.121	-0.039	0.028
198.961	0.214	0.102	0.219	0.013	0.033
284.23	0.318	0.150	0.326	0.053	0.038
369.499	0.433	0.203	0.443	0.084	0.043
454.768	0.560	0.261	0.573	0.107	0.050
540.037	0.702	0.322	0.718	0.125	0.057
625.306	0.855	0.391	0.874	0.138	0.065
710.575	1.028	0.462	1.051	0.149	0.075

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ρ	$n_{\mathrm{HB}}^{\mathrm{E}}$	$n_{\mathrm{HB}}^{\mathrm{G}}$	$n_{\mathrm{HB}}^{\mathrm{G}'}$	$\langle q \rangle$	$f_{\mathrm{FCC-HCP}}$
795.844	1.220	0.537	1.248	0.158	0.086
881.113	1.433	0.620	1.465	0.165	0.098
966.382	1.669	0.700	1.705	0.169	0.112
1051.651	1.928	0.789	1.971	0.174	0.129
1136.92	2.212	0.875	2.264	0.175	0.147
1222.189	2.519	0.963	2.577	0.178	0.167
1307.458	2.855	1.044	2.923	0.176	0.192
1392.727	3.214	1.120	3.296	0.176	0.220
1477.996	3.607	1.187	3.698	0.174	0.250
1563.265	4.012	1.240	4.121	0.174	0.283
1648.534	4.450	1.280	4.577	0.169	0.320
1733.803	4.910	1.310	5.056	0.167	0.359
1819.072	5.378	1.317	5.555	0.164	0.401
1904.341	5.875	1.317	6.078	0.161	0.446
1989.61	6.387	1.292	6.628	0.158	0.492
2074.879	6.906	1.247	7.184	0.154	0.537
2160.148	7.342	1.374	7.631	0.144	0.992
2245.417	8.223	1.339	8.570	0.100	0.993
2330.686	8.772	1.189	9.180	0.094	0.982
			$T_{\mathrm{r}} = 5.0$		
28.423	0.028	0.012	0.028	-0.108	0.024
113.692	0.115	0.047	0.119	-0.037	0.028
198.961	0.213	0.089	0.219	0.014	0.033
284.23	0.318	0.133	0.327	0.054	0.037
369.499	0.435	0.180	0.447	0.083	0.044
454.768	0.563	0.230	0.578	0.107	0.049
540.037	0.708	0.287	0.728	0.122	0.056
625.306	0.866	0.343	0.891	0.135	0.064
710.575	1.044	0.410	1.074	0.147	0.073
795.844	1.239	0.477	1.274	0.156	0.082
881.113	1.456	0.551	1.498	0.163	0.094
966.382	1.693	0.625	1.742	0.168	0.107
1051.651	1.956	0.702	2.013	0.172	0.122
1136.92	2.242	0.776	2.308	0.173	0.138
1222.189	2.554	0.850	2.629	0.176	0.158
1307.458	2.888	0.927	2.977	0.176	0.178
1392.727	3.256	0.997	3.357	0.176	0.202
1477.996	3.639	1.056	3.759	0.176	0.228
1563.265	4.055	1.108	4.191	0.174	0.257
1648.534	4.481	1.156	4.640	0.172	0.289
1733.803	4.944	1.179	5.127	0.169	0.324
1819.072	5.417	1.201	5.625	0.167	0.361
1904.341	5.905	1.205	6.148	0.164	0.403
1989.61	6.413	1.191	6.689	0.161	0.444
2074.879	6.928	1.163	7.251	0.156	0.486
2160.148	7.460	1.118	7.829	0.154	0.530
2245.417	7.985	1.060	8.407	0.150	0.578
2330.686	8.794	1.188	9.234	0.083	0.997
2415.955	9.353	1.045	9.863	0.080	0.990
2501.224	9.869	0.912	10.460	0.077	0.988

TABLE S5: Thermodynamic and dynamic properties from the NVT simulations.

ρ	p	E	H	S	A	G	f_g^t	f_g^r	D_t	D_r
					$T_r = 1.0$					
28.423	0.068	12.369	16.683	0.198	-117.048	-112.734	0.942	0.711	840.858	497.178
113.692	0.153	4.496	6.924	0.167	-104.436	-102.007	0.84	0.421	218.852	73.398
198.961	0.175	0.013	1.594	0.153	-100.016	-98.435	0.792	0.331	136.603	33.848
284.23	0.179	-2.942	-1.805	0.145	-97.906	-96.769	0.762	0.285	103.651	22.674
369.499	0.184	-5.147	-4.25	0.139	-96.347	-95.449	0.74	0.254	84.539	16.852
454.768	0.206	-7.098	-6.283	0.135	-95.582	-94.767	0.715	0.232	69.755	12.62
540.037	0.284	-8.958	-8.011	0.131	-94.74	-93.793	0.695	0.216	59.966	10.517
625.306	0.497	-10.822	-9.389	0.127	-94.218	-92.785	0.668	0.204	49.998	9.024
710.575	0.97	-12.676	-10.217	0.124	-93.617	-91.158	0.643	0.192	42.534	7.68
795.844	1.865	-14.463	-10.241	0.12	-92.856	-88.635	0.614	0.183	35.826	6.712
881.113	3.393	-16.122	-9.185	0.116	-91.974	-85.037	0.589	0.177	30.728	5.962
966.382	5.815	-17.571	-6.731	0.112	-91.056	-80.216	0.546	0.17	24.225	5.42
1051.651	9.428	-18.76	-2.61	0.109	-89.832	-73.682	0.509	0.166	19.686	4.909
1136.92	14.586	-19.628	3.484	0.105	-88.224	-65.112	0.465	0.162	15.356	4.698
1222.189	21.728	-20.113	11.915	0.101	-86.055	-54.027	0.422	0.155	11.964	4.254
1307.458	31.323	-20.147	23.013	0.097	-83.423	-40.263	0.372	0.153	8.792	4.083
1392.727	43.965	-19.643	37.227	0.093	-80.148	-23.278	0.32	0.151	6.216	3.881
1477.996	60.303	-18.535	54.968	0.088	-76.057	-2.554	0.264	0.146	4.079	3.578
1563.265	81.093	-16.735	76.718	0.083	-71.204	22.25	0.209	0.144	2.504	3.388
1648.534	107.348	-14.115	103.196	0.078	-65.252	52.059	0.149	0.138	1.292	2.982
1733.803	120.114	-12.246	112.561	0.074	-60.677	64.129	0.014	0.161	0.019	4.088
1819.072	158.676	-7.941	149.205	0.071	-54.056	103.091	0.016	0.156	0.024	3.722
					$T_r = 1.1$					
28.423	0.08	14.858	19.925	0.206	-133.203	-128.136	0.948	0.736	970.15	597.504
113.692	0.214	8.267	11.655	0.176	-118.441	-115.052	0.864	0.46	269.577	89.523
198.961	0.283	4.086	6.647	0.163	-113.079	-110.518	0.815	0.361	163.899	45.076
284.23	0.334	1.033	3.153	0.154	-109.955	-107.835	0.782	0.312	120.545	28.745
369.499	0.397	-1.422	0.512	0.148	-107.947	-106.013	0.756	0.281	96.462	21.225
454.768	0.495	-3.591	-1.629	0.143	-106.501	-104.539	0.732	0.257	79.508	16.355
540.037	0.679	-5.635	-3.37	0.138	-105.204	-102.938	0.707	0.237	66.497	13.338
625.306	1.032	-7.612	-4.639	0.134	-104.256	-101.282	0.679	0.222	55.414	11.345
710.575	1.674	-9.518	-5.273	0.13	-103.372	-99.127	0.646	0.211	45.2	9.608
795.844	2.767	-11.321	-5.058	0.126	-102.218	-95.955	0.619	0.205	38.42	8.568
881.113	4.526	-12.981	-3.727	0.122	-100.958	-91.704	0.591	0.194	32.505	7.548
966.382	7.203	-14.429	-1.002	0.118	-99.631	-86.203	0.558	0.19	26.939	6.916
1051.651	11.117	-15.601	3.443	0.115	-97.998	-78.953	0.517	0.184	21.438	6.403
1136.92	16.615	-16.46	9.867	0.111	-95.981	-69.653	0.474	0.176	16.887	5.737
1222.189	24.138	-16.911	18.67	0.107	-93.576	-57.996	0.432	0.174	13.222	5.555
1307.458	34.192	-16.893	30.22	0.102	-90.571	-43.457	0.382	0.169	9.769	5.006
1392.727	47.336	-16.348	44.883	0.098	-86.88	-25.649	0.336	0.162	7.239	4.666
1477.996	64.235	-15.169	63.128	0.094	-82.572	-4.275	0.281	0.161	4.875	4.452
1563.265	85.659	-13.278	85.437	0.089	-77.343	21.372	0.226	0.158	3.087	4.318
1648.534	112.579	-10.565	112.462	0.084	-71.049	51.979	0.166	0.154	1.663	3.855
1733.803	146.048	-6.908	144.845	0.079	-63.745	88.008	0.109	0.149	0.735	3.594
					$T_r = 1.3$					
28.423	0.101	19.03	25.455	0.216	-164.485	-158.059	0.957	0.789	1205.485	821.342
113.692	0.324	13.923	19.064	0.191	-148.709	-143.568	0.88	0.524	329.128	138.663
198.961	0.493	10.181	14.647	0.177	-140.633	-136.167	0.835	0.424	201.526	70.649
284.23	0.656	7.21	11.366	0.168	-135.743	-131.588	0.802	0.362	146.708	42.735
369.499	0.849	4.666	8.804	0.161	-132.427	-128.289	0.773	0.325	114.771	31.884
454.768	1.116	2.371	6.79	0.155	-129.391	-124.972	0.751	0.303	95.331	24.711
540.037	1.513	0.232	5.28	0.15	-127.361	-122.312	0.722	0.278	77.745	19.454

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625.306	2.133	-1.798	4.347	0.146	-125.602	-119.457	0.69	0.261	63.324	16.764
710.575	3.098	-3.712	4.143	0.141	-123.589	-115.734	0.665	0.249	53.996	14.236
795.844	4.572	-5.506	4.844	0.137	-121.774	-111.423	0.633	0.236	44.696	12.617
881.113	6.772	-7.125	6.72	0.133	-119.879	-106.033	0.604	0.228	37.621	11.273
966.382	9.955	-8.528	10.03	0.129	-117.861	-99.304	0.565	0.221	30.298	10.076
1051.651	14.436	-9.647	15.083	0.124	-115.497	-90.767	0.53	0.212	24.836	9.294
1136.92	20.605	-10.412	22.239	0.12	-112.876	-80.226	0.489	0.206	19.854	8.77
1222.189	28.864	-10.785	31.761	0.116	-109.716	-67.171	0.447	0.2	15.569	8.067
1307.458	39.759	-10.662	44.121	0.112	-106.097	-51.313	0.392	0.194	11.236	7.143
1392.727	53.863	-9.985	59.688	0.108	-101.731	-32.057	0.35	0.189	8.561	6.698
1477.996	71.82	-8.673	78.868	0.103	-96.655	-9.113	0.302	0.184	6.168	6.29
1563.265	94.411	-6.621	102.181	0.099	-90.802	18	0.248	0.182	4.019	6.039
1648.534	122.579	-3.731	130.225	0.094	-83.841	50.115	0.197	0.176	2.496	5.573
1733.803	157.393	0.123	163.665	0.089	-75.852	87.69	0.142	0.172	1.313	5.119
					$T_r = 1.5$					
28.423	0.122	22.772	30.475	0.223	-196.098	-188.395	0.964	0.815	1496.19	1040.16
113.692	0.426	18.538	25.287	0.2	-177.891	-171.142	0.896	0.582	403.784	204.117
198.961	0.694	15.177	21.462	0.188	-168.803	-162.518	0.85	0.466	238.254	92.145
284.23	0.974	12.359	18.531	0.178	-162.251	-156.079	0.819	0.406	173.267	60.755
369.499	1.307	9.877	16.249	0.171	-157.976	-151.604	0.784	0.366	130.467	43.935
454.768	1.744	7.607	14.517	0.165	-154.135	-147.225	0.757	0.334	105.565	33.575
540.037	2.352	5.482	13.328	0.159	-150.909	-143.063	0.73	0.315	86.922	27.101
625.306	3.23	3.488	12.794	0.155	-148.239	-138.933	0.699	0.296	71.209	22.889
710.575	4.503	1.611	13.028	0.15	-145.531	-134.114	0.672	0.282	59.952	19.882
795.844	6.342	-0.12	14.238	0.146	-142.877	-128.52	0.641	0.266	49.727	16.856
881.113	8.964	-1.662	16.666	0.141	-140.174	-121.846	0.613	0.258	42.066	15.605
966.382	12.635	-2.983	20.572	0.137	-137.363	-113.808	0.578	0.247	34.713	13.961
1051.651	17.673	-4.005	26.27	0.133	-134.441	-104.166	0.541	0.236	28.215	12.727
1136.92	24.458	-4.686	34.07	0.129	-131.067	-92.311	0.497	0.227	22.128	10.705
1222.189	33.441	-4.938	44.355	0.125	-127.275	-77.982	0.457	0.222	17.663	10.161
1307.458	45.13	-4.693	57.491	0.121	-122.952	-60.767	0.415	0.217	13.765	9.763
1392.727	60.106	-3.893	73.856	0.116	-118.017	-40.268	0.368	0.211	10.283	9.017
1477.996	79.059	-2.42	93.945	0.112	-112.297	-15.931	0.316	0.207	7.269	8.682
1563.265	102.757	-0.207	118.211	0.108	-105.713	12.706	0.266	0.204	5.002	7.994
1648.534	132.091	2.853	147.203	0.103	-98.188	46.162	0.222	0.198	3.406	7.385
1733.803	168.192	6.902	181.665	0.098	-89.472	85.29	0.169	0.193	1.962	6.949
					$T_r = 2.0$					
28.423	0.169	31.504	42.191	0.233	-273.094	-262.407	0.97	0.873	1982.33	1781.85
113.692	0.66	28.462	38.924	0.216	-253.895	-243.433	0.913	0.669	540.806	347.862
198.961	1.166	25.796	36.35	0.205	-241.848	-231.294	0.867	0.568	307.42	183.875
284.23	1.733	23.398	34.382	0.196	-233.272	-222.288	0.828	0.503	211.617	117.525
369.499	2.413	21.196	32.959	0.19	-226.747	-214.985	0.79	0.449	156.199	78.584
454.768	3.271	19.142	32.099	0.183	-220.332	-207.376	0.763	0.417	125.855	62.411
540.037	4.389	17.212	31.853	0.177	-214.686	-200.045	0.735	0.386	103.062	50.079
625.306	5.881	15.419	32.363	0.172	-209.728	-192.783	0.707	0.367	85.544	42.794
710.575	7.88	13.748	33.727	0.167	-205.002	-185.023	0.68	0.349	71.839	36.869
795.844	10.577	12.252	36.195	0.163	-200.615	-176.671	0.648	0.33	59.354	30.596
881.113	14.19	10.958	39.972	0.158	-195.861	-166.847	0.622	0.317	50.7	27.484
966.382	19.004	9.905	45.333	0.154	-191.65	-156.222	0.583	0.305	41	24.55
1051.651	25.333	9.157	52.554	0.15	-186.645	-143.249	0.554	0.295	34.642	21.949
1136.92	33.578	8.772	61.979	0.146	-181.753	-128.546	0.513	0.287	27.734	20.575
1222.189	44.204	8.835	73.993	0.141	-176.228	-111.069	0.477	0.279	22.631	19.248
1307.458	57.736	9.408	88.963	0.137	-170.211	-90.657	0.44	0.266	18.179	16.652
1392.727	74.754	10.558	107.254	0.133	-163.672	-66.976	0.399	0.262	14.215	16.384

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1477.996	95.987	12.411	129.41	0.129	-156.278	-39.28	0.352	0.254	10.596	14.91
1563.265	122.16	15.012	155.792	0.125	-148.155	-7.376	0.31	0.249	7.905	13.655
1648.534	154.181	18.495	186.985	0.12	-138.948	29.543	0.265	0.243	5.595	12.669
1733.803	193.101	22.966	223.611	0.116	-128.744	71.901	0.22	0.238	3.806	12.168
1819.072	240.195	28.587	266.466	0.111	-117.121	120.759	0.169	0.235	2.231	11.738
1904.341	258.111	29.289	273.466	0.105	-108.626	135.551	0.017	0.244	0.035	12.256
1989.61	315.385	36.091	321.664	0.102	-97.742	187.831	0.009	0.244	0.012	12.583
2074.879	395.982	46.153	389.969	0.099	-82.832	260.984	0.008	0.234	0.01	10.935
2160.148	481.074	56.507	457.716	0.096	-68.937	332.272	0.007	0.232	0.007	10.799
					$T_r = 2.5$					
28.423	0.215	39.927	53.544	0.239	-351.555	-337.938	0.973	0.907	2339.955	2655.08
113.692	0.878	37.536	51.453	0.225	-331.107	-317.19	0.92	0.736	649.371	554.427
198.961	1.608	35.338	49.894	0.216	-317.611	-303.055	0.874	0.639	361.965	274.472
284.23	2.447	33.292	48.805	0.209	-307.75	-292.237	0.834	0.568	246.257	175.793
369.499	3.46	31.385	48.256	0.202	-298.802	-281.931	0.798	0.526	181.913	131.62
454.768	4.719	29.586	48.278	0.195	-289.797	-271.104	0.773	0.482	147.966	100.012
540.037	6.319	27.898	48.979	0.19	-283.004	-261.924	0.739	0.453	117.689	79.883
625.306	8.383	26.347	50.499	0.185	-275.836	-251.684	0.713	0.43	98.26	67.293
710.575	11.066	24.94	52.995	0.18	-269.382	-241.327	0.687	0.404	82.907	58.239
795.844	14.547	23.698	56.627	0.175	-262.967	-230.038	0.658	0.384	69.577	48.836
881.113	19.074	22.669	61.668	0.171	-256.875	-217.877	0.627	0.369	58.155	42.133
966.382	24.93	21.91	68.385	0.167	-250.496	-204.02	0.599	0.355	49.426	38.3
1051.651	32.448	21.451	77.036	0.162	-244.261	-188.676	0.563	0.343	40.495	35.148
1136.92	42.044	21.396	88.017	0.158	-237.425	-170.804	0.536	0.332	34.554	31.759
1222.189	54.162	21.767	101.604	0.154	-230.452	-150.616	0.499	0.321	28.222	27.408
1307.458	69.365	22.681	118.259	0.15	-222.974	-127.397	0.458	0.31	22.365	27.203
1392.727	88.236	24.188	138.324	0.146	-214.685	-100.548	0.427	0.299	18.562	24.015
1477.996	111.503	26.403	162.315	0.142	-205.97	-70.058	0.386	0.297	14.473	22.416
1563.265	139.933	29.4	190.662	0.138	-196.206	-34.944	0.346	0.288	11.171	20.685
1648.534	174.407	33.296	223.89	0.134	-185.469	5.124	0.301	0.28	8.186	19.86
1733.803	215.959	38.181	262.578	0.13	-173.62	50.777	0.254	0.273	5.662	18.51
1819.072	265.73	44.184	307.352	0.125	-160.602	102.566	0.212	0.268	3.892	16.844
1904.341	325.105	51.475	359.03	0.121	-146.177	161.379	0.168	0.263	2.436	16.489
					$T_r = 3.0$					
28.423	0.26	48.249	64.743	0.244	-430.112	-413.618	0.976	0.928	2821.29	3480.15
113.692	1.09	46.276	63.554	0.232	-408.357	-391.08	0.923	0.788	736.053	774.001
198.961	2.029	44.424	62.794	0.224	-396.057	-377.687	0.875	0.693	400.615	397.062
284.23	3.13	42.68	62.52	0.217	-382.941	-363.101	0.841	0.629	281.293	264.978
369.499	4.461	41.024	62.775	0.21	-371.621	-349.87	0.811	0.576	215.043	183.812
454.768	6.102	39.486	63.661	0.205	-362.525	-338.351	0.777	0.538	166.151	140.844
540.037	8.156	38.036	65.245	0.2	-353.487	-326.278	0.747	0.51	133.817	117.227
625.306	10.757	36.729	67.72	0.194	-344.904	-313.914	0.721	0.482	111.956	101.858
710.575	14.071	35.573	71.248	0.19	-336.433	-300.758	0.696	0.457	95.188	83.516
795.844	18.291	34.583	75.987	0.185	-329.035	-287.631	0.667	0.437	79.589	72.396
881.113	23.675	33.84	82.247	0.181	-321.609	-273.202	0.632	0.415	65.222	59.947
966.382	30.509	33.351	90.226	0.177	-313.04	-256.165	0.615	0.4	58.242	54.791
1051.651	39.135	33.204	100.245	0.173	-305.599	-238.558	0.578	0.382	47.662	48.542
1136.92	49.966	33.434	112.61	0.169	-297.593	-218.417	0.543	0.366	39.254	42.858
1222.189	63.474	34.142	127.705	0.165	-288.954	-195.391	0.509	0.356	32.437	39.364
1307.458	80.215	35.37	145.898	0.161	-279.841	-169.313	0.477	0.35	27.059	37.151
1392.727	100.832	37.237	167.666	0.157	-270.179	-139.75	0.442	0.341	22.064	33.444
1477.996	125.956	39.792	193.32	0.153	-259.874	-106.346	0.403	0.326	17.477	30.194
1563.265	156.479	43.175	223.504	0.149	-248.547	-68.218	0.372	0.32	14.348	29.101
1648.534	193.205	47.447	258.584	0.145	-236.53	-25.393	0.327	0.318	10.651	27.045

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1733.803	237.193	52.725	299.185	0.141	-223.119	23.34	0.284	0.304	7.786	24.329
1819.072	289.578	59.141	345.928	0.137	-208.766	78.02	0.249	0.299	5.857	22.823
1904.341	351.677	66.835	399.528	0.132	-192.652	140.04	0.203	0.292	3.83	22.378
1989.61	424.9	75.944	460.679	0.128	-175.105	209.63	0.158	0.288	2.341	21.302
2074.879	444.758	75.31	461.476	0.122	-163.956	222.21	0.01	0.295	0.019	22.042
2160.148	536.641	86.517	534.069	0.119	-146.955	300.597	0.011	0.288	0.031	20.451
2245.417	648.273	100.237	620.357	0.116	-127.63	392.491	0.008	0.288	0.012	20.523
2330.686	795.981	118.925	734.191	0.113	-103.311	511.955	0.004	0.139	0.009	18.67
					$T_r = 4.0$					
28.423	0.349	64.764	86.905	0.25	-590.019	-567.878	0.979	0.953	3553.385	5988.82
113.692	1.499	63.346	87.105	0.241	-567.5	-543.74	0.929	0.848	907.827	1279.41
198.961	2.838	61.988	87.689	0.235	-552.107	-526.406	0.886	0.774	502.869	694.121
284.23	4.435	60.717	88.827	0.23	-540.194	-512.084	0.846	0.709	334.479	450.96
369.499	6.358	59.502	90.503	0.224	-526.233	-495.231	0.814	0.666	252.276	331.197
454.768	8.714	58.396	92.915	0.218	-513.224	-478.705	0.785	0.626	200.506	243.196
540.037	11.622	57.393	96.164	0.214	-502.107	-463.336	0.756	0.593	162.061	207.773
625.306	15.222	56.539	100.394	0.209	-490.827	-446.972	0.728	0.565	133.77	172.158
710.575	19.705	55.844	105.801	0.205	-479.737	-429.78	0.707	0.532	115.785	136.838
795.844	25.284	55.346	112.582	0.201	-470.376	-413.141	0.672	0.508	94.141	121.258
881.113	32.225	55.105	120.993	0.196	-458.306	-392.418	0.654	0.491	83.628	102.315
966.382	40.838	55.164	131.295	0.192	-447.754	-371.623	0.626	0.474	71.009	93.309
1051.651	51.486	55.558	143.757	0.188	-436.933	-348.734	0.603	0.453	61.834	80.544
1136.92	64.59	56.379	158.727	0.185	-426.766	-324.417	0.562	0.439	49.666	72.881
1222.189	80.646	57.678	176.553	0.181	-414.874	-295.999	0.54	0.428	43.594	68.13
1307.458	100.213	59.553	197.636	0.177	-403.223	-265.139	0.505	0.412	35.957	59.885
1392.727	123.944	62.064	222.389	0.173	-390.895	-230.57	0.473	0.399	29.919	56.146
1477.996	152.518	65.295	251.2	0.169	-377.519	-191.614	0.443	0.383	25.063	49.216
1563.265	186.796	69.366	284.634	0.165	-363.506	-148.239	0.403	0.38	19.857	47.395
1648.534	227.659	74.356	323.144	0.162	-348.596	-99.807	0.367	0.37	15.821	44.433
1733.803	276.062	80.365	367.213	0.158	-332.598	-45.75	0.331	0.357	12.377	40.059
1819.072	333.199	87.546	417.534	0.154	-315.204	14.783	0.291	0.354	9.323	38.525
1904.341	400.294	95.988	474.673	0.15	-296.406	82.278	0.254	0.347	6.958	35.862
1989.61	478.857	105.865	539.457	0.146	-276.154	157.438	0.219	0.338	5.079	33.508
2074.879	570.462	117.321	612.631	0.142	-254.157	241.154	0.177	0.334	3.298	32.96
2160.148	605.296	118.012	622.821	0.136	-237.107	267.703	0.021	0.334	0.069	32.159
2245.417	709.079	130.14	699.047	0.132	-215.347	353.559	0.016	0.329	0.043	30.689
2330.686	855.291	148.472	809.583	0.13	-190.425	470.686	0.007	0.322	0.011	28.685
					$T_r = 5.0$					
28.423	0.439	81.204	109.023	0.256	-755.434	-727.615	0.98	0.966	4091.175	8342.61
113.692	1.898	80.151	110.226	0.248	-730.616	-700.541	0.931	0.885	1039.58	1873.29
198.961	3.624	79.166	111.978	0.242	-712.043	-679.232	0.89	0.828	582.21	1036.96
284.23	5.682	78.237	114.25	0.237	-696.819	-660.806	0.853	0.778	392.704	667.842
369.499	8.166	77.401	117.214	0.232	-682.881	-643.068	0.822	0.73	296.78	508.488
454.768	11.187	76.657	120.975	0.228	-670.209	-625.891	0.79	0.691	229.97	380.999
540.037	14.879	76.045	125.68	0.224	-655.394	-605.759	0.763	0.664	187.923	316.71
625.306	19.397	75.588	131.471	0.219	-641.812	-585.929	0.741	0.631	160.052	256.802
710.575	24.957	75.316	138.591	0.216	-629.683	-566.408	0.713	0.6	133.13	216.161
795.844	31.773	75.257	147.182	0.212	-616.885	-544.961	0.685	0.583	111.738	186.291
881.113	40.132	75.466	157.52	0.208	-603.405	-521.35	0.665	0.554	98.584	161.043
966.382	50.363	76.013	169.9	0.204	-590.123	-496.236	0.64	0.537	84.816	142.293
1051.651	62.838	76.904	184.549	0.2	-577.539	-469.894	0.611	0.518	71.819	132.21
1136.92	78.007	78.271	201.879	0.196	-563.877	-440.269	0.587	0.499	62.629	113.283
1222.189	96.357	80.124	222.157	0.193	-550.348	-408.316	0.558	0.479	53.201	100.955
1307.458	118.492	82.577	245.846	0.189	-535.738	-372.469	0.531	0.466	45.651	87.723

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1392.727	145.034	85.675	273.28	0.186	-521.335	-333.729	0.493	0.452	37.091	80.649
1477.996	176.701	89.533	304.914	0.182	-505.21	-289.828	0.466	0.439	31.598	76.128
1563.265	214.39	94.244	341.311	0.178	-488.749	-241.682	0.429	0.43	25.547	71.669
1648.534	258.937	99.892	382.862	0.175	-471.031	-188.061	0.401	0.42	21.505	67.145
1733.803	311.398	106.614	430.178	0.171	-452.291	-128.728	0.37	0.406	17.636	58.563
1819.072	372.92	114.5	483.825	0.167	-432.401	-63.076	0.33	0.402	13.56	57.425
1904.341	444.61	123.633	544.241	0.163	-411.017	9.591	0.292	0.393	10.349	55.253
1989.61	528.068	134.242	612.393	0.16	-388.028	90.124	0.26	0.38	8.045	46.989
2074.879	624.844	146.432	688.961	0.156	-363.434	179.095	0.222	0.382	5.749	49.27
2160.148	736.538	160.316	774.58	0.152	-337.119	277.145	0.188	0.368	4.094	44.519
2245.417	843.118	172.294	848.742	0.147	-307.188	369.26	0.08	0.37	1.259	44.941
2330.686	889.58	173.123	860.738	0.142	-291.64	395.975	0.008	0.365	0.013	42.307
2415.955	1057.275	193.661	982.052	0.139	-261.213	527.178	0.013	0.357	0.032	39.352
2501.224	1243.47	215.794	1111.419	0.137	-230.754	664.872	0.009	0.351	0.016	37.284