

Supporting Information:

# A Polarizable Water Model Derived from a Model Electron Density

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**Table S1.** Force Field Parameters for the HIPPO Water Model

TERM	PARAMETER	UNIT	VALUE
Bond	O-H Bond Length	Å	0.9572
	Bond Force Constant	$kcal \cdot mol^{-1} \cdot \text{Å}^{-2}$	551.108
Angle	H-O-H Angle Value	degree (°)	104.52
	Angle Force Constant	$kcal \cdot mol^{-1} \cdot rad^{-2}$	47.8253
Atomic Multipole	O Monopole	$e$	-0.374842
	O Dipole Z	$e \cdot bohr$	0.054116
	O Quadrupole XX	$e \cdot bohr^2$	0.680265
	O Quadrupole YY	$e \cdot bohr^2$	-0.611121
	O Quadrupole ZZ	$e \cdot bohr^2$	-0.069144
	H Monopole	$e$	0.187421
	H Dipole X	$e \cdot bohr$	0.008106
	H Dipole Z	$e \cdot bohr$	-0.200116
	H Quadrupole XX	$e \cdot bohr^2$	0.066936
	H Quadrupole YY	$e \cdot bohr^2$	0.043814
	H Quadrupole ZZ	$e \cdot bohr^2$	-0.11075
	H Quadrupole XZ	$e \cdot bohr^2$	0.007338
Pauli Repulsion	O Size	$\sqrt{kcal \cdot mol^{-1} \cdot \text{Å}}$	23.0592
	O $\alpha$ Damping	Å <sup>-1</sup>	4.41372
	O Valence	$e$	3.37829
	H Size	$\sqrt{kcal \cdot mol^{-1} \cdot \text{Å}}$	16.023
	H $\alpha$ Damping	Å <sup>-1</sup>	4.92152
	H Valence	$e$	0.63308
Charge Penetration	O # Core Electrons	None	6
	O $\alpha$ Damping	Å <sup>-1</sup>	4.28982
	H # Core Electrons	None	1
	H $\alpha$ Damping	Å <sup>-1</sup>	5.21764
Dispersion	O C <sub>6</sub> Coefficient	$\sqrt{kcal \cdot mol^{-1} \cdot \text{Å}^6}$	16.1193
	O $\alpha$ Damping	Å <sup>-1</sup>	4.28982
	H C <sub>6</sub> Coefficient	$\sqrt{kcal \cdot mol^{-1} \cdot \text{Å}^6}$	3.6813
	H $\alpha$ Damping	Å <sup>-1</sup>	5.21764
Polarization	O Polarizability	Å	0.725918
	H Polarizability	Å	0.359954
Charge Transfer	O Prefactor	$e^2 \cdot \text{Å}^{-1}$	3.63984
	O $\alpha$ Damping	Å <sup>-1</sup>	0
	H Prefactor	$e^2 \cdot \text{Å}^{-1}$	0
	H $\alpha$ Damping	Å <sup>-1</sup>	3.2776
Charge Flux (CF)	CF Bond Length	Å	0.9572
	CF Bond Force Constant	$e \cdot \text{Å}^{-1}$	-0.027265
	CF Angle Value	degree (°)	104.52
	CF Angle Force Constant	$e \cdot rad^{-1}$	0.102621
	CF Bond-Angle Constant	$e \cdot \text{Å}^{-1}$	-0.039303

**Table S2.** Smith Dimer CCSD(T) CBS Energies vs. HIPPO and Selected Water Models.  
All energy values are in kcal/mol.

DIMER	CCSD(T) /CBS	HIPPO (Single)	HIPPO (Opt)	AMOEBA+ ChgFlux	AMOEBA 14	AMOEBA 03	iAMOEBA	TIP3P
1	-4.967	-4.917	-4.957	-4.854	-4.644	-4.956	-5.092	-6.024
2	-4.459	-4.330	-4.339	-4.247	-4.144	-4.389	-4.478	-5.510
3	-4.410	-4.232	-4.238	-4.122	-4.118	-4.314	-4.474	-5.752
4	-4.281	-4.378	-4.574	-4.221	-3.848	-3.724	-3.856	-4.251
5	-4.034	-3.994	-4.193	-3.701	-3.498	-3.401	-3.460	-3.587
6	-3.991	-3.823	-3.913	-3.431	-3.360	-3.248	-3.298	-3.684
7	-3.168	-3.090	-3.121	-2.886	-2.352	-2.794	-2.863	-3.693
8	-1.425	-1.354	-1.377	-1.416	-0.989	-1.462	-1.414	-1.388
9	-3.208	-3.169	-3.184	-2.965	-2.420	-2.932	-3.427	-4.605
10	-2.286	-2.278	-2.295	-2.164	-1.779	-2.122	-2.728	-4.040
RMS		0.101	0.129	0.269	0.538	0.390	0.367	1.016

**Table S3.** Smith Dimer Stationary Point Coordinates Optimized at MP2/aug-cc-pV5Z (Å)

## Water Dimer 1

1	O	0.867811	0.000000	-1.203650
2	H	0.324645	0.000000	-1.990082
3	H	0.240169	0.000000	-0.471356
4	O	-0.824511	0.000000	1.145226
5	H	-0.626009	0.759085	1.694337
6	H	-0.626009	-0.759085	1.694337

## Water Dimer 2

1	O	0.789087	-0.092190	-1.267117
2	H	0.224701	0.014459	-2.030818
3	H	0.188557	-0.098628	-0.513676
4	O	-0.698068	0.045728	1.224131
5	H	-1.622580	0.146691	1.448936
6	H	-0.235228	0.674859	1.777784

## Water Dimer 3

1	O	-0.777272	-1.287171	0.000000
2	H	-0.198888	-2.047722	0.000000
3	H	-0.185961	-0.527199	0.000000
4	O	0.695025	1.224519	0.000000
5	H	0.110214	1.981948	0.000000
6	H	1.579959	1.587303	0.000000

## Water Dimer 4

1	O	-0.091509	-0.685060	-1.217748
2	H	-0.682702	-0.634116	-1.967731
3	H	-0.660630	-0.651495	-0.445365
4	O	0.091509	0.685060	1.217748
5	H	0.682702	0.634116	1.967731
6	H	0.660630	0.651495	0.445365

## Water Dimer 5

1	O	-0.283054	0.357940	-1.308251
2	H	-0.875503	0.262511	-2.052579
3	H	-0.845473	0.329558	-0.531050
4	O	0.300075	-0.308066	1.317241
5	H	0.639378	-0.960931	1.927788
6	H	0.811455	-0.422669	0.513166

## Water Dimer 6

1	O	0.339146	-1.331260	0.000002
2	H	0.928501	-2.083902	-0.000031
3	H	0.909760	-0.559894	0.000006
4	O	-0.339146	1.331260	0.000002
5	H	-0.928501	2.083902	-0.000031
6	H	-0.909760	0.559894	0.000006

Water Dimer 7

1	O	-0.785836	0.000024	1.181640
2	H	-1.574007	-0.003265	0.637789
3	H	-1.109620	0.000454	2.082238
4	O	0.863223	0.000463	-1.267227
5	H	0.731698	-0.747337	-0.683651
6	H	0.723746	0.742424	-0.678047

Water Dimer 8

1	O	1.053603	1.285792	0.000191
2	H	0.467832	1.360914	-0.753108
3	H	0.463133	1.358092	0.750088
4	O	-1.053603	-1.285792	0.000191
5	H	-0.467832	-1.360914	-0.753108
6	H	-0.463133	-1.358092	0.750088

Water Dimer 9

1	O	1.575300	0.000000	-0.013799
2	H	0.938355	-0.000034	-0.728916
3	H	1.006338	0.000092	0.756168
4	O	-1.442383	-0.000006	0.011432
5	H	-2.027063	0.757805	0.005212
6	H	-2.027120	-0.757772	0.005097

Water Dimer 10

1	O	-0.002641	-1.517670	-0.000005
2	H	-0.754700	-2.109631	-0.000027
3	H	0.757286	-2.099507	0.000047
4	O	0.002535	1.650701	0.000003
5	H	0.743716	1.045225	-0.000030
6	H	-0.744615	1.052616	0.000046

**Table S4.** Water Dimer HIPPO and SAPT Energy Components (kcal/mol)

DIMER	ELECTROSTATICS		REPULSION		INDUCTION		DISPERSION	
	HIPPO	SAPT	HIPPO	SAPT	HIPPO	SAPT	HIPPO	SAPT
1	-8.633	-8.624	8.373	8.340	-3.167	-2.115	-1.522	-1.820
2	-7.389	-7.289	7.351	7.142	-2.890	-1.924	-1.433	-1.707
3	-6.949	-6.741	6.865	6.506	-2.786	-1.855	-1.394	-1.660
4	-7.191	-6.790	6.318	5.557	-1.977	-0.701	-1.553	-1.707
5	-6.588	-5.915	6.043	4.801	-1.927	-0.710	-1.550	-1.665
6	-6.311	-5.419	5.901	4.265	-1.890	-0.784	-1.554	-1.652
7	-4.640	-4.577	3.442	3.398	-0.993	-0.577	-0.987	-1.184
8	-1.668	-1.913	1.033	1.454	-0.245	-0.242	-0.506	-0.655
9	-4.435	-4.437	3.014	3.136	-0.990	-0.593	-0.867	-1.074
10	-2.777	-2.786	1.700	1.918	-0.645	-0.486	-0.646	-0.812

DIMER	TOTAL ENERGY		
	HIPPO	SAPT	CCSD(T)
1	-4.917	-4.219	-4.967
2	-4.330	-3.778	-4.459
3	-4.232	-3.750	-4.410
4	-4.378	-3.641	-4.281
5	-3.994	-3.489	-4.034
6	-3.823	-3.590	-3.991
7	-3.090	-2.940	-3.168
8	-1.354	-1.356	-1.425
9	-3.169	-2.968	-3.208
10	-2.278	-2.167	-2.286

MEAN ABSOLUTE DEVIATION FROM SAPT	
Electrostatics	0.260
Repulsion	0.504
Induction	0.752
Dispersion	0.192
Total	0.367

**Table S5.** Liquid Water Density (kg/m<sup>3</sup>) vs. Temperature (K)

<b>TEMP</b>	<b>HIPPO</b>	<b>EXPT</b>	<b>% Error</b>
248.15	989.78	989.59	0.02
250.15	991.09	991.17	-0.01
253.15	992.88	993.55	-0.07
258.15	995.39	996.28	-0.09
260.15	996.39	997.02	-0.06
263.15	997.29	998.12	-0.08
268.15	998.49	999.26	-0.08
270.15	998.76	999.55	-0.08
273.15	999.13	999.84	-0.07
277.15	999.37	999.97	-0.06
280.15	999.38	999.90	-0.05
283.15	999.18	999.70	-0.05
288.15	998.63	999.10	-0.05
290.15	998.37	998.77	-0.04
293.15	997.70	998.20	-0.05
298.15	996.49	997.04	-0.05
300.15	995.98	996.51	-0.05
303.15	994.93	995.65	-0.07
308.15	993.23	994.03	-0.08
310.15	992.37	993.33	-0.10
313.15	991.21	992.22	-0.10
318.15	989.04	990.21	-0.12
320.15	987.96	989.36	-0.14
323.15	986.51	988.04	-0.15
328.15	983.94	985.70	-0.18
330.15	982.65	984.71	-0.21
333.15	980.98	983.20	-0.23
336.15	979.18	981.63	-0.25
338.15	978.01	980.55	-0.26
340.15	976.64	979.46	-0.29
343.15	974.89	977.77	-0.29
348.15	971.48	974.85	-0.35
350.15	969.91	973.64	-0.38
353.15	967.86	971.80	-0.41
358.15	964.20	968.62	-0.46
360.15	962.48	967.31	-0.50
363.15	960.32	965.32	-0.52
368.15	956.26	961.90	-0.59
370.15	954.58	960.50	-0.62
373.15	952.01	958.36	-0.66

**Table S6.** Liquid Water Heat of Vaporization (kJ/mol) vs. Temperature (K)

<b>TEMP</b>	<b>HIPPO</b>	<b>HIPPO Corrected</b>	<b>EXPT</b>	<b>% Error</b>
248.15	47.01	–	46.15	1.85
250.15	46.82	46.05	46.06	1.65
253.15	46.59	45.85	45.92	1.46
258.15	46.26	45.58	45.70	1.23
260.15	46.10	45.44	45.61	1.07
263.15	45.99	45.36	45.48	1.12
268.15	45.57	44.99	45.27	0.66
270.15	45.45	44.90	45.18	0.61
273.15	45.27	44.76	45.05	0.49
277.15	44.98	44.50	44.88	0.22
280.15	44.89	44.44	44.76	0.29
283.15	44.72	44.30	44.63	0.20
288.15	44.33	43.97	44.42	-0.19
290.15	44.22	43.88	44.33	-0.24
293.15	44.03	43.71	44.20	-0.40
298.15	43.82	43.55	43.99	-0.38
300.15	43.61	43.35	43.90	-0.68
303.15	43.47	43.24	43.78	-0.71
308.15	43.23	43.05	43.56	-0.76
310.15	42.99	42.83	43.47	-1.11
313.15	42.94	42.80	43.35	-0.94
318.15	42.54	42.45	43.13	-1.36
320.15	42.43	42.36	43.04	-1.42
323.15	42.26	42.21	42.91	-1.51
328.15	41.99	41.99	42.70	-1.64
330.15	41.91	41.92	42.61	-1.63
333.15	41.67	41.70	42.48	-1.90
336.15	41.56	41.62	42.34	-1.86
338.15	41.41	41.49	42.26	-1.99
340.15	41.31	41.40	42.17	-2.03
343.15	41.12	41.23	42.03	-2.17
348.15	40.84	40.99	41.81	-2.32
350.15	40.82	40.99	41.72	-2.14
353.15	40.66	40.85	41.58	-2.22
358.15	40.30	40.53	41.35	-2.54
360.15	40.23	40.48	41.26	-2.48
363.15	40.09	40.35	41.12	-2.51
368.15	39.90	40.20	40.88	-2.41
370.15	39.70	40.02	40.79	-2.67
373.15	39.53	39.86	40.65	-2.77



**Table S7.** Liquid Water Dielectric Constant vs. Temperature (K)

<b>TEMP</b>	<b>HIPPO</b>	<b>EXPT</b>	<b>% Error</b>
248.15	98.30	99.15	-0.86
250.15	95.68	98.13	-2.49
253.15	95.09	96.58	-1.54
258.15	94.94	94.24	0.74
260.15	94.19	93.34	0.91
263.15	92.55	92.04	0.55
268.15	91.13	89.94	1.32
270.15	89.84	89.12	0.80
273.15	91.38	87.90	3.96
277.15	87.43	86.31	1.30
280.15	85.14	85.14	0.00
283.15	85.53	83.98	1.84
288.15	81.89	82.08	-0.24
290.15	79.42	81.33	-2.35
293.15	78.26	80.22	-2.44
298.15	76.88	78.41	-1.95
300.15	75.64	77.70	-2.65
303.15	74.56	76.64	-2.71
308.15	71.70	74.90	-4.27
310.15	72.43	74.22	-2.41
313.15	70.27	73.20	-4.01
318.15	68.48	71.54	-4.28
320.15	68.69	70.89	-3.10
323.15	66.34	69.92	-5.11
328.15	66.12	68.33	-3.24
330.15	65.03	67.70	-3.94
333.15	64.09	66.77	-4.02
336.15	62.97	65.86	-4.39
338.15	61.69	65.26	-5.47
340.15	60.10	64.66	-7.05
343.15	60.61	63.77	-4.96
348.15	59.30	62.32	-4.85
350.15	58.23	61.75	-5.71
353.15	56.67	60.90	-6.94
358.15	55.87	59.51	-6.11
360.15	55.40	58.96	-6.04
363.15	54.43	58.15	-6.40
368.15	52.65	56.83	-7.36
370.15	52.59	56.30	-6.58
373.15	51.25	55.52	-7.69

**Table S8.** Liquid Water Self-Diffusion Coefficient ( $\times 10^{-5}$  cm<sup>2</sup>/s) vs. Temperature (K)

<b>TEMP</b>	<b>HIPPO</b>	<b>EXPT</b>	<b>% Error</b>
248.15	0.404	0.319	26.65
253.15	0.530	0.421	25.89
258.15	0.680	0.539	26.16
263.15	0.847	0.683	24.01
268.15	1.033	0.888	16.33
273.15	1.239	1.099	12.74
277.15	1.418	1.261	12.45
278.15	1.464	1.303	12.36
283.15	1.722	1.525	12.92
288.15	1.970	1.765	11.61
293.15	2.252	2.023	11.32
298.15	2.557	2.299	11.22
303.15	2.877	2.594	10.91
308.15	3.216	2.907	10.63
313.15	3.560	3.238	9.94
318.15	3.925	3.588	9.39
328.15	4.718	4.345	8.58
336.15	5.406	5.008	7.95
338.15	5.586	5.181	7.82
343.15	6.023	5.615	7.27
348.15	6.495	6.086	6.72
353.15	6.993	6.557	6.65
358.15	7.494	7.066	6.06
363.15	7.981	7.574	5.37
368.15	8.498	8.120	4.66
373.15	9.052	8.667	4.44

**Table S9.** Liquid Water Isobaric Heat Capacity (cal/mol/K) vs. Temperature (K)

<b>TEMP</b>	<b>HIPPO</b>	<b>EXPT</b>	<b>% Error</b>
248.15	23.322	19.256	21.12
250.15	23.130	19.077	21.25
253.15	22.858	18.777	21.73
258.15	22.446	18.494	21.37
260.15	22.294	18.418	21.04
263.15	22.079	18.330	20.45
268.15	21.753	18.228	19.34
270.15	21.633	18.197	18.88
273.15	21.462	18.157	18.20
277.15	21.251	18.115	17.31
280.15	21.105	18.089	16.67
283.15	20.967	18.066	16.06
288.15	20.754	18.036	15.07
290.15	20.675	18.026	14.70
293.15	20.560	18.015	14.13
298.15	20.382	18.002	13.22
300.15	20.315	17.999	12.87
303.15	20.217	17.997	12.34
308.15	20.063	17.995	11.49
310.15	20.004	17.995	11.16
313.15	19.918	17.996	10.68
318.15	19.781	18.000	9.89
320.15	19.728	18.001	9.59
323.15	19.651	18.004	9.15
328.15	19.528	18.010	8.43
330.15	19.480	18.013	8.14
333.15	19.411	18.018	7.73
336.15	19.344	18.024	7.32
338.15	19.302	18.028	7.07
340.15	19.260	18.033	6.80
343.15	19.200	18.041	6.42
348.15	19.108	18.055	5.83
350.15	19.074	18.061	5.61
353.15	19.027	18.071	5.29
358.15	18.959	18.090	4.80
360.15	18.936	18.097	4.64
363.15	18.907	18.109	4.41
368.15	18.874	18.130	4.10
370.15	18.867	18.138	4.02
373.15	18.863	18.151	3.92

**Table S10.** Liquid Water Isothermal Compressibility ( $\times 10^{-6}$  bar) vs. Temperature (K)

<b>TEMP</b>	<b>HIPPO</b>	<b>EXPT</b>	<b>% Error</b>
248.15	59.311	70.940	-16.39
250.15	63.921	68.264	-6.36
253.15	60.385	64.250	-6.02
258.15	56.026	59.440	-5.74
260.15	55.788	57.996	-3.81
263.15	55.795	55.830	-0.06
268.15	53.698	53.060	1.20
270.15	54.836	52.120	5.21
273.15	51.639	50.885	1.48
277.15	50.844	49.481	2.75
280.15	50.873	48.587	4.70
283.15	50.536	47.809	5.70
288.15	49.173	46.733	5.22
290.15	48.187	46.371	3.92
293.15	49.372	45.892	7.58
298.15	46.531	45.247	2.84
300.15	48.753	45.038	8.25
303.15	48.025	44.771	7.27
308.15	48.877	44.440	9.98
310.15	49.696	44.345	12.07
313.15	48.212	44.239	8.98
318.15	47.699	44.154	8.03
320.15	48.083	44.149	8.91
323.15	50.002	44.173	13.20
328.15	49.943	44.290	12.76
330.15	49.784	44.362	12.22
333.15	50.086	44.496	12.56
336.15	48.474	44.662	8.54
338.15	49.420	44.788	10.34
340.15	51.367	44.928	14.33
343.15	51.174	45.162	13.31
348.15	51.664	45.614	13.26
350.15	51.650	45.817	12.73
353.15	52.177	46.143	13.08
358.15	52.864	46.748	13.08
360.15	52.590	47.011	11.87
363.15	54.047	47.429	13.95
368.15	55.407	48.185	14.99
370.15	55.531	48.509	14.48
373.15	57.852	49.019	18.02

**Table S11.** Liquid Water Thermal Expansion Coefficient ( $\times 10^{-4}/\text{K}$ ) vs. Temperature (K)

<b>TEMP</b>	<b>HIPPO</b>	<b>EXPT</b>	<b>% Error</b>
248.15	-7.348	-9.559	-23.13
250.15	-6.673	-8.378	-20.35
253.15	-5.722	-6.606	-13.38
258.15	-4.288	-4.503	-4.77
260.15	-3.763	-3.871	-2.79
263.15	-3.021	-2.924	3.32
268.15	-1.900	-1.686	12.69
270.15	-1.487	-1.260	18.02
273.15	-0.904	-0.681	32.75
277.15	-0.186	0.003	-
280.15	0.313	0.460	-31.96
283.15	0.780	0.880	-11.36
288.15	1.499	1.509	-0.66
290.15	1.767	1.740	1.55
293.15	2.152	2.068	4.06
298.15	2.750	2.572	6.92
300.15	2.976	2.761	7.79
303.15	3.301	3.032	8.87
308.15	3.815	3.457	10.36
310.15	4.011	3.619	10.83
313.15	4.296	3.853	11.50
318.15	4.751	4.225	12.45
320.15	4.925	4.367	12.78
323.15	5.182	4.575	13.27
328.15	5.595	4.910	13.95
330.15	5.755	5.040	14.19
333.15	5.992	5.231	14.55
336.15	6.225	5.417	14.92
338.15	6.378	5.539	15.15
340.15	6.529	5.660	15.35
343.15	6.755	5.837	15.73
348.15	7.126	6.128	16.29
350.15	7.272	6.242	16.50
353.15	7.493	6.411	16.88
358.15	7.864	6.689	17.57
360.15	8.012	6.799	17.84
363.15	8.240	6.962	18.36
368.15	8.628	7.233	19.29
370.15	8.788	7.340	19.73
373.15	9.035	7.501	20.45

**Table S12.** Liquid-Vapor Interface Surface Tension (mJ/m<sup>2</sup>) vs. Temperature (K)

<b>TEMP</b>	<b>HIPPO</b>	<b>EXPT</b>	<b>% Error</b>
248.15	84.65	79.19	6.89
258.15	83.16	77.82	6.86
268.15	80.84	76.42	5.78
278.15	78.47	74.95	4.70
288.15	78.44	73.50	6.72
298.15	74.92	71.99	4.07
308.15	75.17	70.41	6.76
318.15	70.35	68.78	2.28
328.15	73.02	67.10	8.82
338.15	66.70	65.36	2.05
348.15	66.53	63.58	4.64
358.15	61.96	61.75	0.34
368.15	60.56	59.87	1.15
378.15	56.73	57.94	-2.09
388.15	55.31	55.97	-1.18
408.15	49.69	51.89	-4.24
418.15	50.07	49.80	1.01
438.15	38.16	45.49	-16.11
458.15	36.94	41.07	-10.06

**Table S13.** Liquid Water Density (kg/m<sup>3</sup>) vs. Pressure (Atm)

<b>PRESSURE</b>	<b>HIPPO</b>	<b>EXPT</b>	<b>% Error</b>
1	996.49	997.04	0.01
99	1001.36	1001.50	-0.01
495	1019.73	1016.12	0.41
1012	1040.66	1038.83	0.38
1973	1077.19	1070.66	0.70
2965	1108.49	1100.11	0.85
3967	1135.89	1126.13	0.99
4929	1159.44	1149.43	0.98
7125	1205.45	1193.32	1.12
9375	1244.37	1234.57	0.92

**Table S14.** Water Second Virial Coefficient (L/mol) vs. Temperature (K)

TEMP	EXPT	HIPPO			
		$B_{cl}(T)$	$\Delta B_{trans}$	$\Delta B_{rot}$	$B(T)$
298.15	-1.1158	-1.2911	0.0024	0.0275	-1.2612
310.15	-0.9733	-1.0549	0.0018	0.0203	-1.0328
320.15	-0.8489	-0.9038	0.0014	0.0160	-0.8863
340.15	-0.6594	-0.6850	0.0009	0.0104	-0.6736
360.15	-0.5253	-0.5378	0.0006	0.0071	-0.5301
380.15	-0.4281	-0.4344	0.0004	0.0050	-0.4289
400.15	-0.3559	-0.3590	0.0003	0.0037	-0.3550
423.15	-0.2940	-0.2951	0.0002	0.0027	-0.2922
473.15	-0.2062	-0.2057	0.0001	0.0015	-0.2041
523.15	-0.1535	-0.1528	0.0001	0.0009	-0.1518
573.15	-0.1185	-0.1185	0.0001	0.0006	-0.1179
623.15	-0.0937	-0.0949	0.0000	0.0004	-0.0945