Ж У Р Н А Л С Т Р У К Т У Р Н О Й Х И М И И

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ДОПОЛНИТЕЛЬНЫЕ МАТЕРИАЛЫ К СТАТЬЕ

ВЛИЯНИЕ ДАВЛЕНИЯ НА СТРУКТУРНЫЕ, ЭЛЕКТРОННЫЕ И ОПТИЧЕСКИЕ СВОЙСТВА ИОДИДА ХОЛИНА

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Table S1. Atom coordinates in primitive cell of choline iodide obtained with PBE-D3 full geometry optimization with (P = 3 GPa) and without pressure (P = 0 GPa)

Atom	P=0 GPa: a=5.8302 Å, b=7.9816 Å, c=8.9134 Å, β=92.677°			P=3 GPa: a= 5.6958 Å, b= 7.3539 Å, c= 8.4724 Å, β= 94.541°		
	x/a	*y/b*	*z/c*	*x/a*	*y/b*	*z/c*
I	0.1441	-0.4707	0.2208	0.1349	-0.4739	0.2050
O	0.0555	0.1896	0.4191	0.0491	0.0580	0.4333
N	-0.4822	0.0472	0.2215	-0.4818	0.0427	0.2287
C1	0.3054	0.0460	0.1186	0.3001	0.0343	0.1173
C2	-0.3554	-0.1164	0.2069	-0.3479	-0.1332	0.2227
C3	-0.3261	0.1881	0.1778	-0.3273	0.1949	0.1797
C4	0.4596	0.0787	0.3838	0.4627	0.0844	0.3967
C5	0.2845	-0.0384	0.4497	0.2713	-0.0286	0.4629
H1	0.3591	0.0339	0.0026	0.3561	0.2165	-0.0030
H2	0.2126	0.1644	0.1327	0.1999	0.1603	0.1284
H3	0.1977	-0.0612	0.1471	0.1951	-0.0848	0.1452
H4	-0.3007	-0.1254	0.0908	-0.2908	-0.1482	0.1026
H5	-0.2039	-0.1145	0.2852	-0.1935	-0.1244	0.3083
H6	-0.4716	-0.2206	0.2305	-0.4649	-0.2462	0.2487
H7	-0.4204	0.3067	0.1873	-0.4289	0.3215	0.1830
H8	-0.2768	0.1674	0.0617	-0.2776	0.1674	0.0595
H9	-0.1728	0.1864	0.2543	-0.1697	0.1989	0.2624
H10	-0.3759	0.0708	0.4489	-0.3702	0.0685	0.4689
H11	0.3934	0.2078	0.3877	0.4060	0.2273	0.3973
H12	0.3241	-0.0406	-0.4278	0.3156	-0.0394	-0.4083
H13	0.3025	-0.1680	0.4079	0.2652	-0.1680	0.4139
H14	-0.0113	0.0333	-0.4817	-0.0192	0.0610	-0.4627

Table S2. Bond length (Å) and bond angles (°) in choline iodide crystal obtained using PBE-D3 with (P = 3 GPa) and without pressure (P = 0 GPa)

P=0				P=3 GPa			
Bond length, Å							
N-C1	1.5059	C1-H1	1.0982	N-C1	1.5007	C1-H1	1.0956
N-C2	1.5095	C2-H4	1.0992	N-C2	1.5049	C2-H4	1.0982
N-C3	1.5093	C3-H7	1.0996	N-C3	1.5023	C3-H7	1.0977
N-C4	1.5223	C4-H10	1.0993	N-C4	1.5132	C4-H10	1.0964
C4-C5	1.5222	C5-H12	1.1059	C4-C5	1.5132	C5-H12	1.1037
C5-O	1.4252	O-H14	0.9896	C5-O	1.4213	O-H14	0.9918
I-O	3.4664	I-H14	2.4856	I-O	3.3249	I-H14	2.3438
Bond angles, °							
C1-N-C2	109.5	H1-C1-H2	110.279	C1-N-C2	109.8	H1-C1-H2	110.096
C2-N-C3	108.6	H4-C2-H5	109.823	C2-N-C3	108.7	H4-C2-H5	109.749
C3-N-C4	106.6	H7-C3-H8	110.795	C3-N-C4	106.3	H7-C3-H8	110.8
C4-N-C5	31.7	H10-C4-H11	109.589	C4-N-C5	31.7	H10-C4-H11	109.951
C1-C2-C3	36.1	H12-C5-H13	107.383	C1-C2-C3	35.9	H12-C5-H13	107.621
O-H14-I	170.961	C5-O-H14	105.673	O-H14-I	169.955	C5-O-H14	105.048

Table S3. Anisotropy properties of elastic modules in the absence of pressure (P = 0) and at a pressure of P = 3 GPa [From: R. Gaillac, P. Pullumbi, F. Coudert. J. Phys. Condens. Matter, 2016, 28, 275201]

Pressure	Bulk modulus, GPa		Shear modulus, GPa		Young's modulus, GPa		Poisson's ratio	
	B_{min}	B_{max}	G_{min}	G_{max}	E_{min}	E_{max}	ν_{min}	ν_{max}
0	95.28	21.16	2.89	7.70	8.75	22.18	0.081	0.729
3 GPa	173.35	56.22	9.45	17.68	25.22	43.35	0.043	0.569

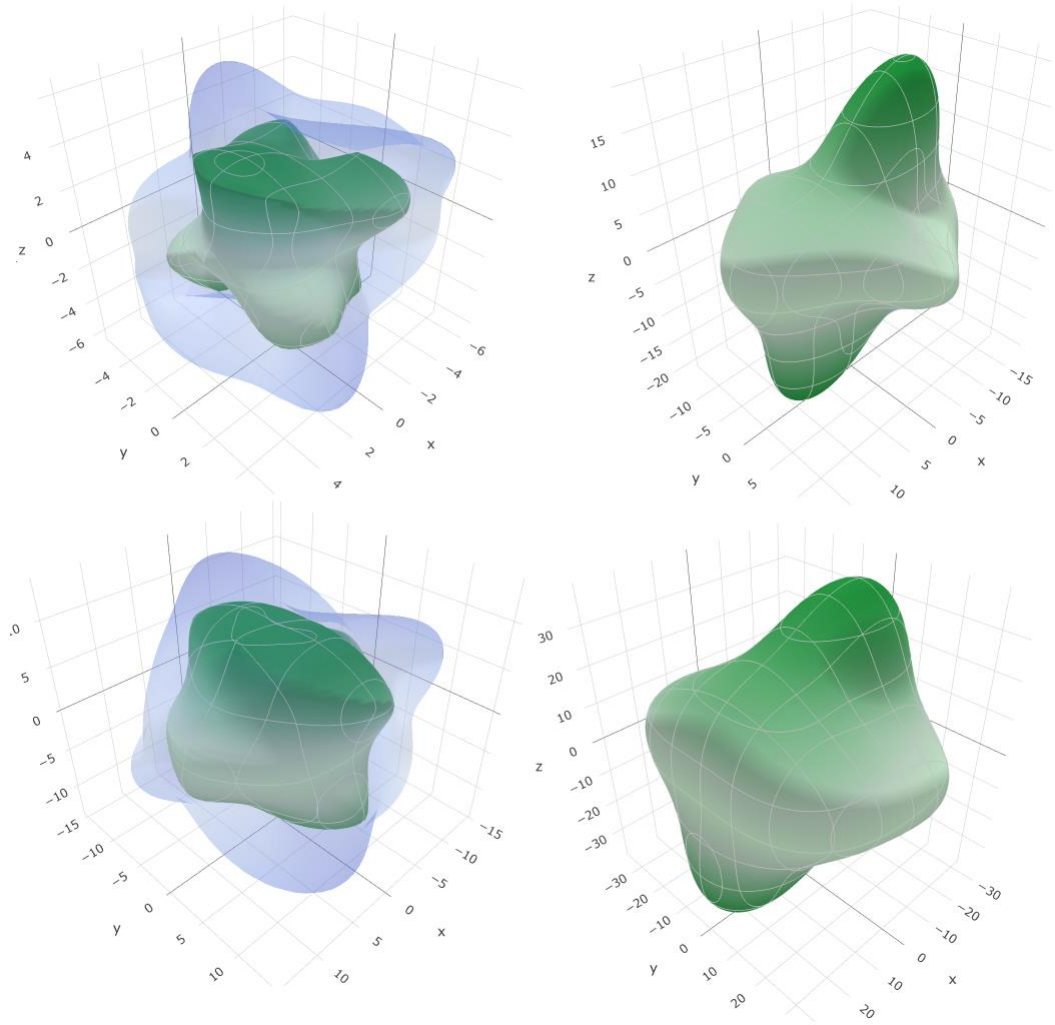

Fig. S1. Spatial dependence of the shear modulus G_H (left) and Young's modulus E_H (right) in the absence of pressure (top) and under pressure 3 GPa (bottom)

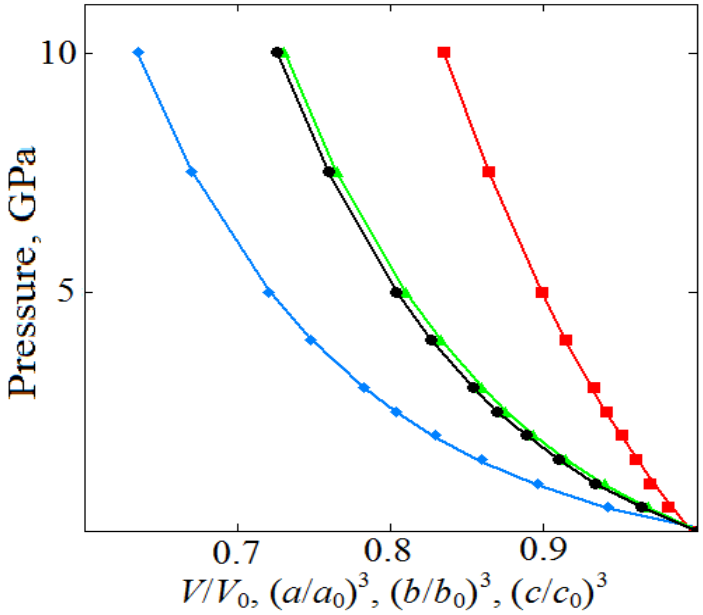

Fig. S2. Dependences of pressure P on the relative change in volume V / V0 (line color black, circles), lattice constant $(a/a_0)^3$ (red, squares), lattice constant $(b/b_0)^3$ (blue, rhombus), lattice constant $(c/c_0)^3$ (green, triangle) obtained using the equation of state $P(V) = \frac{3B_0}{2}(x^{-7} - x^{-5})\left(1 + \frac{3}{4}(B_1 - 4)(x^{-2} - 1)\right)$, where $x = (V/V_0)^{1/3}$, $B_0 = -V(\partial P/\partial V)_T$ is the isothermal bulk compression module, and B_1 is its first derivative with respect to pressure at x = 1. Parameters of the equation: for the volume V_{0V}= 414.601 Å^3, B_{0V}=11.5 GPa, B_{1V}=6.33; for the lattice constant $(a/a_0)^3$ = 197.377 Å^3, B_{0a}= 38.27 GPa, B_{1a}=4.43; for the lattice constant $(b/b_0)^3$ = 515.639 Å^3, B_{0b}= 5.31 GPa, B_{1b}= 6.04; for the lattice constant $(c/c_0)^3$ = 709.324 Å^3, B_{0c}= 12.47 GPa, B_{1c}= 5.98.

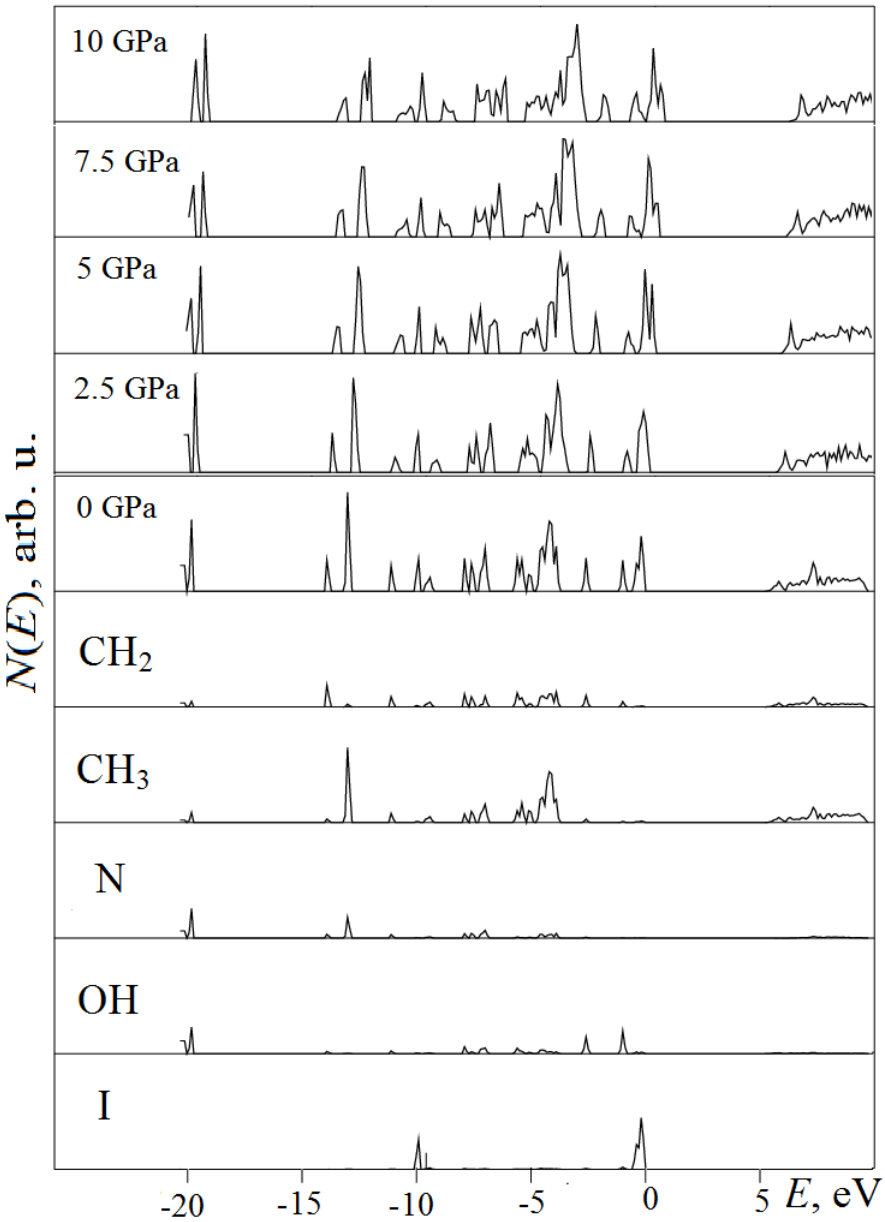

Fig. S3. The density of electronic states of N (E) choline iodide in the absence of pressure (P = 0) and under pressure 2.5, 5.0, 7.5, 10 GPa (above). Partial density from the states of iodine (I), hydroxyl group (OH), nitrogen (N), methyl (-CH_3) and methylene (-CH_2) groups in the absence of pressure (bottom)

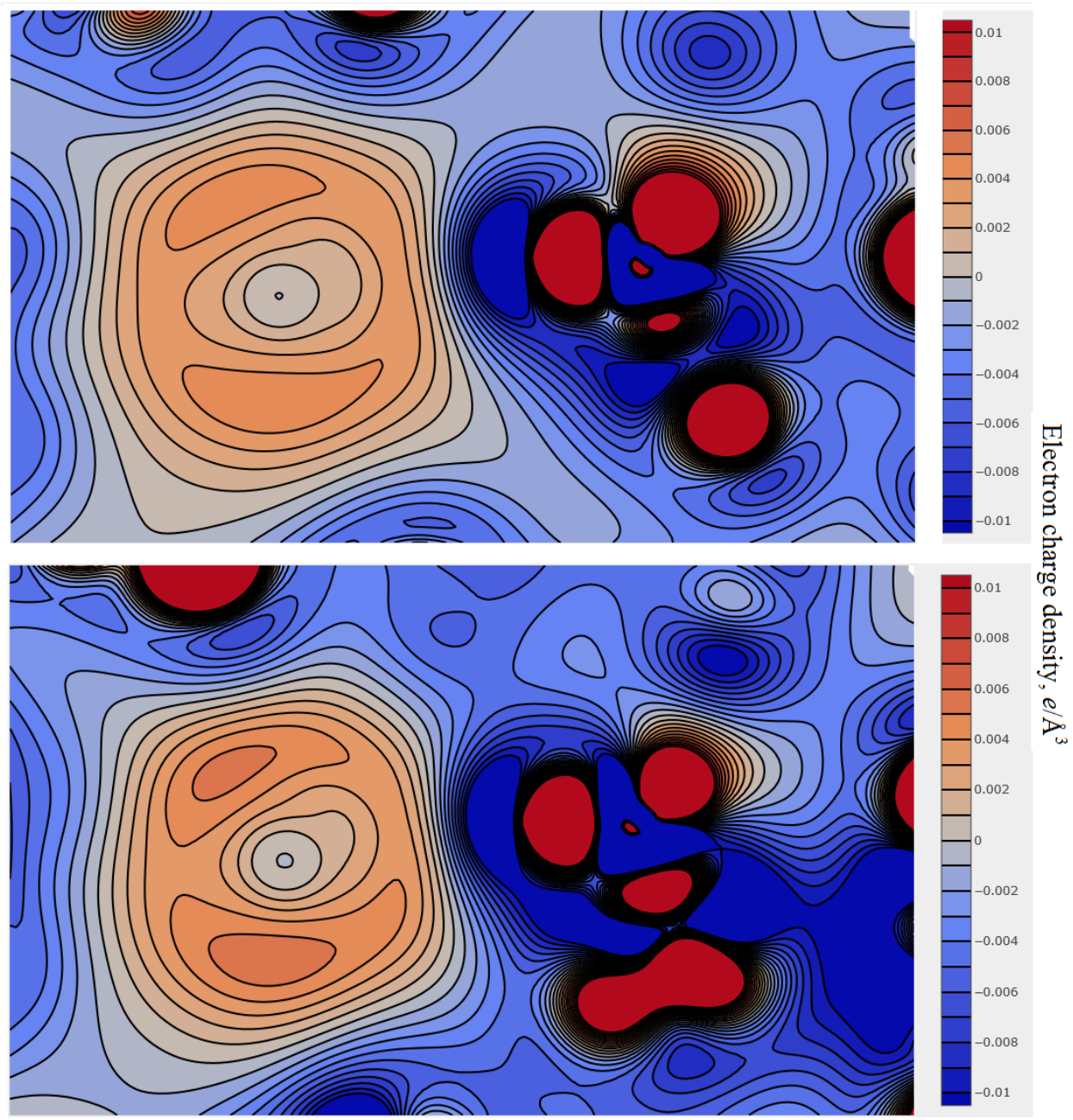

Fig. S4. Distribution of deformation electron density in a projection with the shortest O-H ••• I distances in the absence of pressure (above) and under a pressure of 5 GPa (below)

Table S4. The frequencies of normal long-wavelength oscillations ω_0 of choline iodide calculated in the absence of pressure P calculated by the PBE + D3 method, the baric shift $d\omega/dP$, and the Gruneisen mode parameter $\gamma_i = (B_0/\omega_{0i})/(\partial\omega_i/\partial P)$. In the case of a nonlinear dependence of $\omega(P)$, the values of $d\omega_i/dP$ and γ_i are absent.

Irrep. *A*			Irrep. *B*		
ω_0, cm^{-1}	$d\omega/dP$, cm^{-1}/GPa	γ	ω_0, cm^{-1}	$d\omega/dP$, cm^{-1}/GPa	γ
33.9	2.78	0.895	33.9	4.69	1.51
40.1	5.38	1.463			
54.3	11.28	2.266	59.5	-	
69.2	-		67.6	11.81	1.907
86.0	11.87	1.507	87.3	9.73	1.216
99.3	11.25	1.235	91.8	11.53	1.372
109.9	17.87	1.774	106.3	15.91	1.632
121.4	15.02	1.35	119.5	12.98	1.186
145.5	15.00	1.124	141.1	13.59	1.051

206.7	8.51	0.449	202.2	10.03	0.541
253.5	3.43	0.148	259.2	4.48	0.189
291.5	-	-	298.6	-	-
323.5	-	-	325.5	3.58	0.12
325.7	-	-	345.4	-3.69	-0.117
357.5	-	-	365.7	-	-
370.5	4.40	0.129	375.8	4.91	0.143
384.8	4.81	0.136	403.6	6.14	0.166
433.3	-	-	436.3	4.64	0.116
447.0	4.55	0.111	450.5	6.56	0.159
467.6	3.45	0.08	471.0	6.35	0.147
527.6	1.55	0.032	529.1	-	-
706.7	6.28	0.097	707.1	6.44	0.099
855.3	5.61	0.072	857.1	6.16	0.078
890.1	5.76	0.071	885.9	5.11	0.063
934.0	4.64	0.054	932.1	4.27	0.05
949.7	4.25	0.049	951.9	4.61	0.053
998.9	6.23	0.068	996.3	5.38	0.059
1046.9	3.06	0.032	1047.8	3.31	0.035
1057.5	0.63	0.006	1059.4	1.23	0.013
1078.9	5.18	0.052	1078.9	5.32	0.054
1124.6	2.72	0.026	1118.8	2.49	0.024
1131.9	2.63	0.025	1134.0	3.01	0.029
1200.2	3.12	0.028	1200.6	3.29	0.03
1226.4	1.81	0.016	1224.4	1.32	0.012
1253.2	1.52	0.013	1254.3	2.11	0.018
1267.8	2.91	0.025	1273.4	3.23	0.028
1320.3	-	-	1321.5	0.57	0.005
1339.6	-	-	1341.1	-	-
1353.8	-1.94	-0.016	1358.8	-	-
1389.7	-2.36	-0.019	1390.7	-2.47	-0.019
1396.7	-2.62	-0.02	1396.6	-2.92	-0.023
1415.1	-	-	1412.3	-0.45	-0.003
1419.1	1.84	0.014	1418.6	1.38	0.011
1437.8	-1.66	-0.013	1439.7	-2.60	-0.02
1450.3	-1.36	-0.01	1449.6	-1.83	-0.014
1453.0	-	-	1452.3	-	
1455.1	-1.15	-0.008	1455.7	-	
1462.4	0.62	0.004	1461.6	0.77	0.005
1478.8	-1.25	-0.009	1484.6	-0.44	-0.003
1486.4	-1.09	-0.008	1489.2	-	
1496.5	-	-	1495.0	-	
2951.4	4.71	0.017	2951.5	4.70	0.017
2994.4	5.53	0.02	2994.1	5.37	0.02
2996.6	5.88	0.021	2996.1	5.42	0.02
3002.1	4.93	0.018	3000.8	5.23	0.019
3012.3	5.13	0.019	3014.1	4.65	0.017
3016.1	5.09	0.018	3015.5	4.59	0.017
3084.8	8.82	0.031	3084.8	8.65	0.031
3100.3	5.49	0.019	3100.8	5.56	0.02
3104.8	5.44	0.019	3104.6	6.04	0.021
3110.4	4.71	0.017	3111.0	4.65	0.016
3113.6	6.03	0.021	3113.1	8.42	0.029
3118.4	3.38	0.012	3118.5	5.72	0.02
3133.4	4.676	0.016	3133.5	4.74	0.017
3362.7	-20.61	-0.067	3366.3	-20.77	-0.067