Supplementary material for

Effect of structural water on the elasticity of orthopyroxene

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The hydrous orthopyroxene crystallizes in orthorhombic structure with space group *Pbca*. We measured the elastic velocities of three samples with orientations of (-0.566, 0.675, 0.472), (0.940, -0.150, 0.307), and (-0.099, -0.558, -0.824) at ambient conditions. All the measured and calculated data are listed in Table S1-S3. In Table S4, the elastic data are presented for Al,Fe,Ca-bearing $MgSiO_3$ orthopyroxene samples from previous studies after removing Fe and Ca effect. The crystal structure of orthopyroxene was shown in Fig. S1.

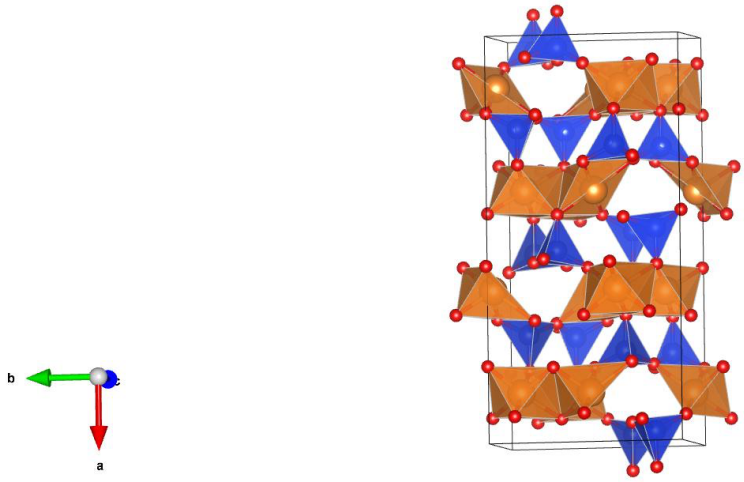

Fig. S1. The crystal structure of orthopyroxene with orange Mg-O octahedra and blue Si-O tetrahedra (Momma and Izumi 2011). The Mg, Si and O are shown as blue, orange and red spheres, respectively.

Table S1. Measured and calculated velocities of the sample with orientation (-0.566, 0.675, 0.472).

χ (°)	Measured velocities*			Calculated velocities		
	v_P (km/s)	v_{S1} (km/s)	v_{S2} (km/s)	v_P (km/s)	v_{S1} (km/s)	v_{S2} (km/s)
0	8.509	5.088	/	8.459	5.094	4.543
15	8.578	5.022	/	8.495	5.062	4.730
30	/	4.998	/	8.475	5.062	4.932
45	8.451	5.013	/	8.443	5.105	4.996
60	8.437	5.139	/	8.388	5.114	4.996
75	8.323	5.124	/	8.345	5.062	4.977
90	8.308	5.100	/	8.270	5.051	4.889
105	8.325	5.021	/	8.183	5.039	4.793
120	8.271	4.954	/	8.142	5.050	4.695
135	/	5.167	/	8.152	5.083	4.569
150	8.326	5.115	/	8.238	5.105	4.462
165	8.412	5.2	/	8.376	5.105	4.439
180	8.451	5.053	/	8.443	5.083	4.534

*: The uncertainty of the measured velocities is <0.3%.

Table S2. Measured and calculated velocities of the sample with orientation (0.940, -0.150, 0.307).

χ (°)	Measured velocities*			Calculated velocities		
	v_P (km/s)	v_{S1} (km/s)	v_{S2} (km/s)	v_P (km/s)	v_{S1} (km/s)	v_{S2} (km/s)
0	7.474	/	5.056	7.445	5.159	4.927
15	7.823	/	4.847	7.833	5.086	4.717
30	8.031	/	4.727	8.111	5.060	4.669
45	8.241	/	4.868	8.276	5.049	4.801
60	8.242	/	5.002	8.331	5.066	4.992
75	8.310	/	5.168	8.331	5.153	5.027
90	8.237	/	5.047	8.320	5.097	5.024
105	8.285	/	4.867	8.272	5.046	4.895
120	8.092	/	4.728	8.128	5.043	4.756
135	7.843	/	4.77	7.870	5.039	4.790
150	7.500	/	4.955	7.567	5.045	4.962
165	7.388	/	5.112	7.401	5.156	4.973
180	7.484	/	5.033	7.530	5.138	4.876

*: The uncertainty of the measured velocities is <0.3%.

Table S3. Measured and calculated velocities of the sample with orientation (-0.099, -0.558, -0.824).

χ (°)	Measured velocities*			Calculated velocities		
	v_P (km/s)	v_{S1} (km/s)	v_{S2} (km/s)	v_P (km/s)	v_{S1} (km/s)	v_{S2} (km/s)
0	8.091	5.074	/	8.037	5.065	4.668
15	/	4.982	/	7.898	5.04	4.778
30	/	5.100	/	7.925	5.058	4.728
45	8.200	5.061	/	8.111	5.085	4.572
60	8.308	5.113	/	8.328	5.086	4.51
75	8.391	4.998	/	8.476	5.072	4.624
90	8.443	5.027	/	8.532	5.056	4.844
105	8.525	4.991	/	8.533	5.046	5.013
120	8.516	4.923	/	8.529	5.044	5.009
135	8.501	4.863	4.863	8.513	5.053	4.844
150	8.405	5.066	5.066	8.436	5.065	4.652
165	8.273	5.127	/	8.269	5.074	4.577
180	8.091	5.074	/	8.037	5.065	4.668

*: The uncertainty of the measured velocities is <0.3%.

Table S4. The elasticity of Al,Fe,Ca-bearing $MgSiO_3$ orthopyroxene after removing Fe and Ca effect (the bold data).

	Hydrous Al-bearing Orthopyroxene (this study)	Al,Fe,Ca -bearing Orthopyroxene (Zhang & Bass, 2016)	Al,Fe,Ca -bearing Orthopyroxene (Chai et al., 1997)	Al,Fe-bearing Orthopyroxene (Jackson et al., 2007)	Ca-bearing Orthopyroxene (Perrillat et al., 2007)	End-member Orthopyroxene(Jackson et al., 1999)
H_2O (ppm)	842-900	-	-	-	0	0
Fe#	0	8.4	9.5	0.2	0	0
Al_2O_3 (wt. %)	1.64	2.5	5.0	0.4	0	0
CaO (wt. %)	1.0	1.1	1.1	0	1.9	0
C_{11} (GPa)	235(2)	**240.6(5)**	**245.8(10)**	**236(1)**	224.1(1)	233(1)
C_{22} (GPa)	173(2)	**182.9(7)**	**188.3(8)**	**173(1)**	165.8(2)	171(1)
C_{33} (GPa)	222(2)	**236.9(6)**	**245.5(10)**	**216(1)**	202.9(1)	216(1)
C_{44} (GPa)	86(1)	**83.2(4)**	**85.4(12)**	**84(1)**	82.2(1)	83(1)
C_{55} (GPa)	82(1)	**81.6(3)**	**83.9(8)**	**79(1)**	73.8(1)	79(1)
C_{66} (GPa)	82(1)	**78.3(6)**	**80.4(12)**	**80(1)**	77.1(1)	77(1)
C_{12} (GPa)	75(3)	**81.2(9)**	**81.3(16)**	**74(1)**	71.4(1)	73(2)
C_{13} (GPa)	67(2)	**63.4(6)**	**65.4(18)**	**57(1)**	52.7(1)	56(2)
C_{23} (GPa)	49(2)	**57.3(8)**	**60.1(24)**	**50(1)**	45.2(1)	50(3)
$K_{S,\mathrm{Voigt}}$ (GPa)	112(1)	**118(1)**	**121.5(5)**	**109.5(15)**	103.5(15)	108.7(15)
$G_{S,\mathrm{Voigt}}$ (GPa)	79.1(5)	**79.1(7)**	**81.5(4)**	**78.6(7)**	74.9(11)	77.2(7)
$K_{S,\mathrm{Reuss}}$ (GPa)	110(1)	**116(1)**	**119.8(5)**	**107.4(15)**	101.5(15)	106.7(15)
$G_{S,\mathrm{Reuss}}$ (GPa)	77.7(5)	**77.8(7)**	**80.2(4)**	**77.3(7)**	73.5(11)	75.9(7)

$K_{S,\mathrm{VRH}}$ (GPa)	111(2)	**117(1)**	**120.6(5)**	**108.5(15)**	102.5(15)	107.6(15)
$G_{S,\mathrm{VRH}}$ (GPa)	78.4(1)	**78.5(7)**	**80.8(4)**	**77.9(7)**	74.2(11)	76.8(7)
V_P (km/s)	8.18(3)	**8.32(3)**	**8.43(1)**	**8.15(8)**	7.92	8.11
V_S (km/s)	4.94(2)	**4.96(2)**	**5.04(1)**	**4.94(5)**	4.81	4.90

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