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Supporting information for article:

Structure change of monoclinic ZrO2 baddeleyite involving softenings of bulk modulus and atom vibrations

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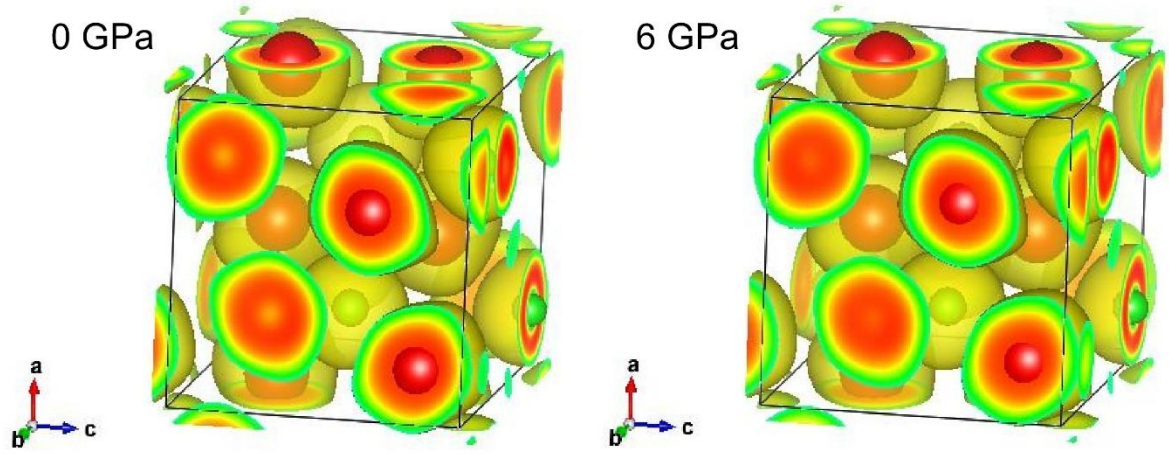

Figure S1. Calculated isosurface of electron localization functions = 0.3 at 0 and 6 GPa with the crystal structures.

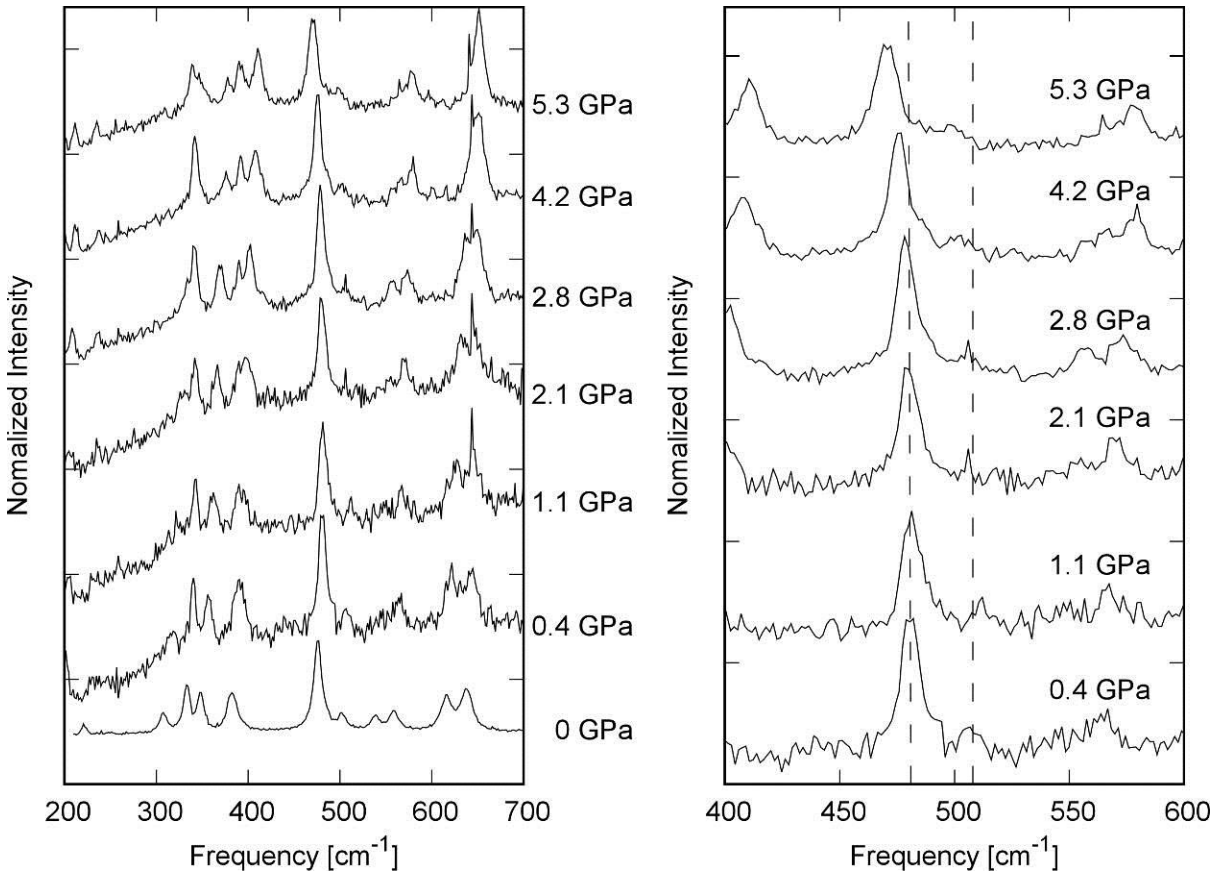

Figure S2. Raman spectra of baddeleyite at various pressures. (Right) A close-up figure to two softening modes. Vertical dashed lines are guides for eyes.

Table S1. Calculated Γ-point phonon frequencies of baddeleyite together with the previous data. Fadda LDA is the results with the DFPT methods under LDA by Fadda et al. (2010). Luo is the results with the finite displacement method under LDA by Luo et al. (2009).

A_g modes [cm^{-1}]			B_g modes [cm^{-1}]		
This study	Fadda LDA	Luo	This study	Fadda LDA	Luo
634.95	634.7	629.71	751.10	750.1	747.8
551.23	552.1	552.22	611.06	610.6	612.9
468.17	467.8	453.88	541.27	539.9	538.11
384.65	383.6	388.41	489.91	488.2	481.38
354.71	353.9	359.19	391.09	390.3	389.1
324.53	324.9	334.09	332.50	332.1	331.95
192.86	193.2	194.39	320.28	320.7	319.09
183.58	183.2	184.32	224.55	225.3	224.11
116.13	116.9	133.46	175.97	177.5	176.3

A_u modes [cm^{-1}]			B_u modes [cm^{-1}]		
This study	Fadda LDA	Luo	This study	Fadda LDA	Luo
643.77	642.0	643.32	720.31	720.0	712.15
580.65	580.0	574.12	491.61	491.3	493.73
475.95	475.7	475.86	420.68	420.5	429.79
402.36	403.1	404.31	364.29	363.1	370.26
360.47	359.4	364.68	320.44	320.1	326.87
261.36	261.2	264.1	312.52	313.1	321.73
240.03	239.7	234.53	230.24	230.7	232.14
183.70	183.8	182.73			