Supplementary material for

New insights into the zircon-reidite phase transition

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Contains:

- Tables S1 and S2
- Captions for figures S1 and S2

Additional files:

- 3 crystallographic information files, cif's, for the three phases calculated at various pressures, including the frequencies of the Raman-active phonon modes:
  - zircon_hydro.cif
  - nphase_hydro.cif
  - reidite_hydro.cif
- Two gif files with animations illustrating the atomic motions associated with two phonon modes in zircon:
  - Figure_S1_197_Eg_1.gif
  - Figure_S2_250_B2g.gif

Table S1. Calculated wavenumbers ω (cm^{-1}) symmetry and relative intensity *I* in arbitrary units (normalized to 1000 for the most intense peak) according to the scattering geometry polarizations for a polycrystalline powder and a single crystal of zircon at *P* = 0 and *P* = 19.5 GPa.

Zircon P = 0 GPa

mode		polycrystalline powder			single crystal					
ω (cm^{-1})	**symmetry**	***I* tot**	***I* par**	***I* perp**	**xx**	**xy**	**xz**	**yy**	**yz**	**zz**
439	A_{1g} (1)	1000	623	377	633	0	0	633	0	744
970	A_{1g} (2)	234	231	3	146	0	0	146	0	55
216	B_{1g} (1)	22	12	9	23	0	0	23	0	0
387	B_{1g} (2)	49	28	21	51	0	0	51	0	0
636	B_{1g} (3)	4	2	2	4	0	0	4	0	0
1015	B_{1g} (4)	959	548	411	1000	0	0	1000	0	0
250	B_{2g} (1)	21	12	9	0	22	0	0	0	0
197	E_g (1)	30	17	13	0	0	16	0	16	0
225	E_g (2)	120	69	51	0	0	63	0	63	0
341	E_g (3)	552	315	237	0	0	288	0	288	0
542	E_g (4)	24	14	10	0	0	12	0	12	0
922	E_g (5)	2	1	1	0	0	1	0	1	0

Zircon P = 19.5 GPa

mode		polycrystalline powder			single crystal					
ω (cm^{-1})	**symmetry**	**tot**	**par**	**perp**	**xx**	**xy**	**xz**	**yy**	**yz**	**zz**
468	A_{1g} (1)	212	137	75	140	0	0	140	0	121
1062	A_{1g} (2)	140	127	13	107	0	0	107	0	1
239	B_{1g} (1)	12	7	5	12	0	0	12	0	0
427	B_{1g} (2)	5	3	2	5	0	0	5	0	0
675	B_{1g} (3)	0	0	0	0	0	0	0	0	0
1115	B_{1g} (4)	1000	571	429	1000	0	0	1000	0	0
217	B_{2g} (1)	1	1	0	0	1	0	0	0	0
178	E_g (1)	25	14	11	0	0	12	0	12	0
226	E_g (2)	22	13	10	0	0	11	0	11	0
429	E_g (3)	205	117	88	0	0	102	0	102	0
555	E_g (4)	3	2	1	0	0	2	0	2	0
1015	E_g (5)	2	1	1	0	0	1	0	1	0

Table S2. Calculated wavenumbers ω (cm^{-1}) symmetry and relative intensity *I* in arbitrary units (normalized to 1000 for the most intense peak) according to the scattering geometry polarizations for a polycrystalline powder and a single crystal of the new phase HPLS $ZrSiO_4$ at P = 20

HPLS $ZrSiO_4$ at P = 20 GPa										
mode		**polycrystalline powder**			**single crystal**					
ω (cm^{-1})	**symmetry**	**tot**	**par**	**perp**	**xx**	**xy**	**xz**	**yy**	**yz**	**zz**
94	A_1 (1)	538	523	14	144	0	0	144	0	486
467	A_1 (2)	664	433	231	443	0	0	443	0	367
1054	A_1 (3)	149	135	14	114	0	0	114	0	1
239	B_1 (1)	95	54	41	95	0	0	95	0	0
410	B_1 (2)	18	10	8	18	0	0	18	0	0
427	B_1 (3)	18	10	8	18	0	0	18	0	0
674	B_1 (4)	0	0	0	0	0	0	0	0	0
1109	B_1 (5)	1000	571	429	1000	0	0	1000	0	0
236	B_2 (1)	7	4	3	0	7	0	0	0	0
371	B_2 (2)	1	1	1	0	1	0	0	0	0
637	B_2 (3)	0	0	0	0	0	0	0	0	0
1074	B_2 (4)	1	1	1	0	1	0	0	0	0
196	E (1)	204	117	87	0	0	102	0	102	0
230	E (2)	263	150	113	0	0	131	0	131	0
293	E (3)	9	5	4	0	0	4	0	4	0
403	E (4)	75	43	32	0	0	38	0	38	0
422	E (5)	475	271	203	0	0	237	0	237	0
450	E (6)	165	94	71	0	0	82	0	82	0
560	E (7)	5	3	2	0	0	2	0	2	0
955	E (8)	0	0	0	0	0	0	0	0	0
1010	E (9)	1	1	0	0	0	1	0	1	0

Table S3. Calculated wavenumbers ω (cm^{-1}) symmetry and relative intensity *I* in arbitrary units (normalized to 1000 for the most intense peak) according to the scattering geometry polarizations for a polycrystalline powder and a single crystal of reidite at P = 0.

Reidite										
mode		polycrystalline powder			single crystal					
ω (cm^{-1})	symmetry	tot	par	perp	xx	xy	xz	yy	yz	zz
326	A_g (1)	193	114	79	55	0	0	55	0	104
409	A_g (2)	1000	731	269	1	0	0	1	0	1000
861	A_g (3)	27	26	1	10	0	0	10	0	2
242	B_g (1)	16	9	7	0	8	0	0	0	0
350	B_g (2)	435	249	186	18	227	0	18	0	0
465	B_g (3)	328	188	141	9	176	0	9	0	0
608	B_g (4)	59	34	25	9	25	0	9	0	0
852	B_g (5)	427	244	183	45	196	0	45	0	0
209	E_g (1)	79	45	34	0	0	22	0	22	0
300	E_g (2)	152	87	65	0	0	43	0	43	0
458	E_g (3)	327	187	140	0	0	92	0	92	0
558	E_g (4)	457	261	196	0	0	129	0	129	0
891	E_g (5)	426	243	183	0	0	120	0	120	0

Figure Captions

Figure S1. Graphical representation of the direct inspection of the eigenvectors of the calculated mode Eg (1) at 197 cm^{-1} by means of the graphic interface software Moldraw (http://www.moldraw.unito.it/_sgg/f10000.htm).

Figure S2. Graphical representation of the direct inspection of the eigenvectors of the calculated mode B_{2g} at 247.8 cm^{-1} by means of the graphic interface software Moldraw (http://www.moldraw.unito.it/_sgg/f10000.htm).