

Table S1. Spherical harmonic coefficients for the pPv phase obtained from Rietveld refinements.

Data	A036	A038	A042	B017	B018	B019	B020	B038	B040	B041
P (GPa)	105.4	109.3	100.2	92.1	93.6	87.8	89.5	85.0	79.2	78.2
T (K)	300	300	300	1740	1420	300	300	300	300	300
(2,0,0)	0.3040	0.3879	0.3484	0.0352	-0.0201	-0.0073	-0.0477	-0.0560	-0.0226	-0.0171
(2,0,2)	1.0730	1.1355	1.0452	0.9971	0.9853	1.2852	1.2067	1.1130	1.0927	1.0994
(4,0,0)				-0.5044	-0.3821	-0.2759	-0.3178	-0.3457	-0.2960	-0.3507
(4,0,2)				0.7635	0.7724	0.5268	0.6138	0.7187	0.6137	0.6256
(4,0,4)				-0.1474	-0.0976	-0.5569	-0.3435	-0.2239	-0.4347	-0.3332