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Supplementary Materials for

Evidence for the charge disproportionation of iron in extraterrestrial bridgmanite

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This PDF file includes:

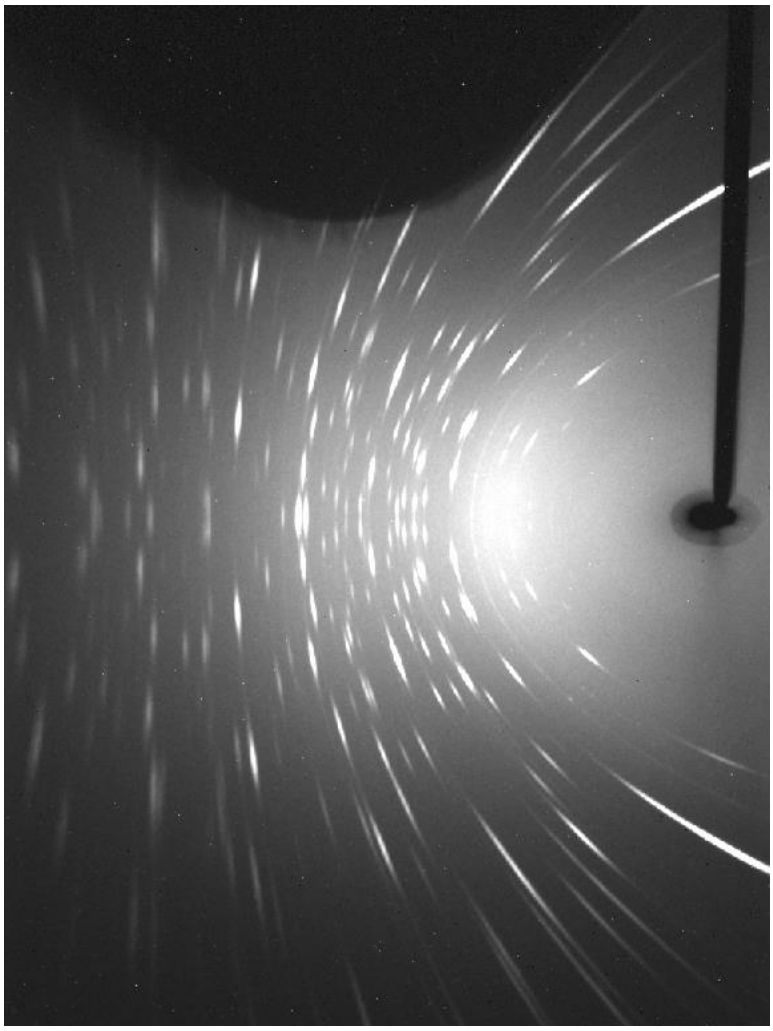

Fig. S1. Experimental x-ray diffraction image of hiroseite. The diffraction quality is intermediate between that of a single crystal (broad single spots) and that of a powder (powder rings).

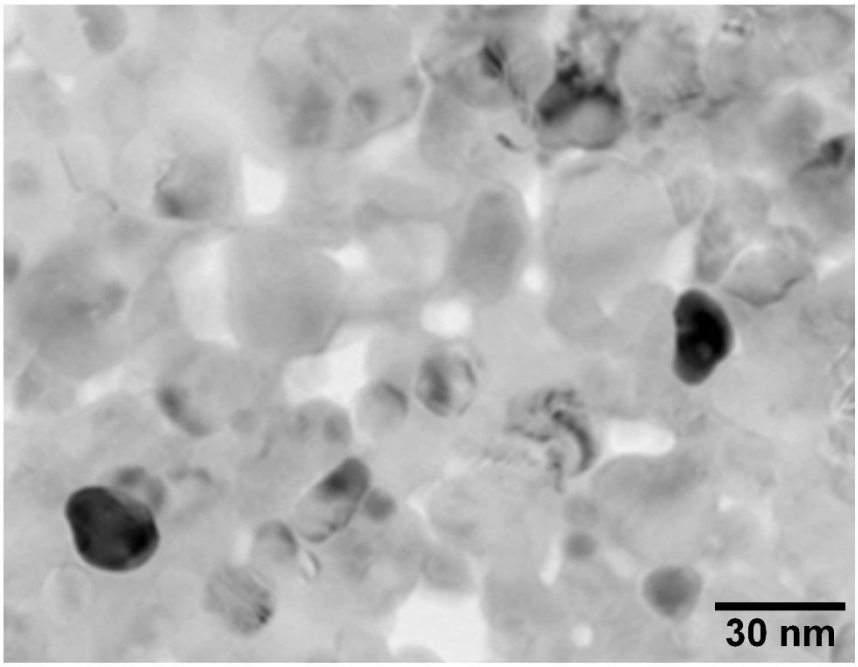

Fig. S2. TEM image of hiroseite. The Fe nanoparticles (black material) are isolated and there are not Fe-rich veins connecting the hiroseite-bearing portion.

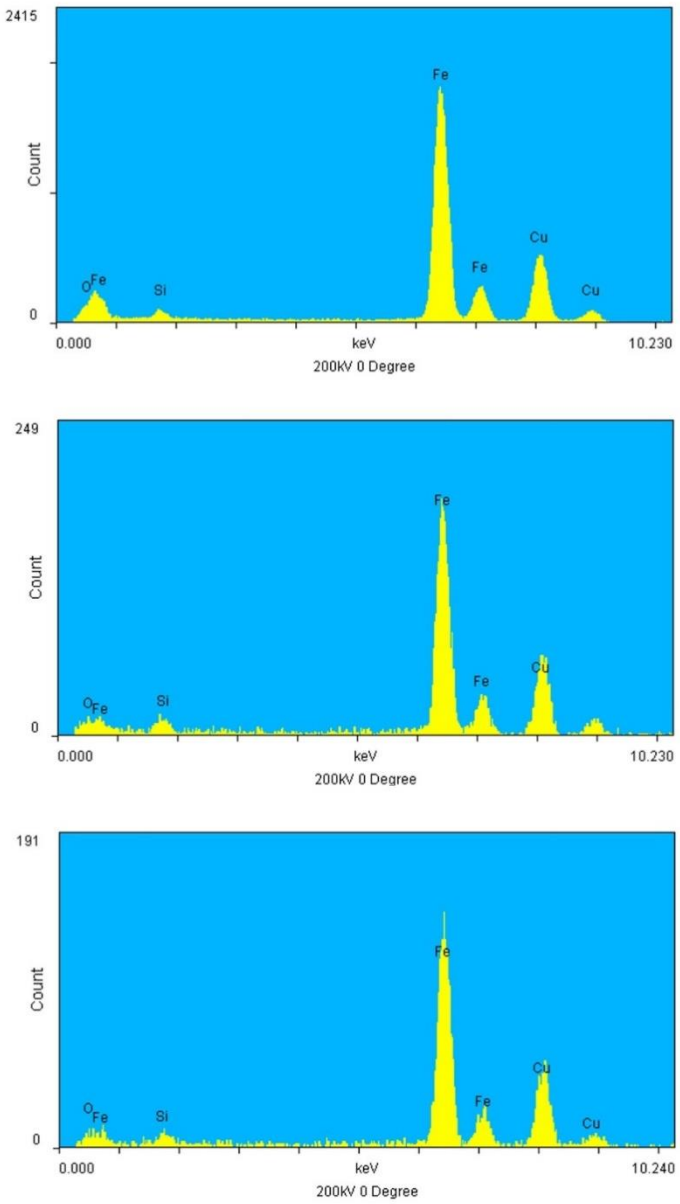

Fig. S3. TEM-EDS spectra collected on the Fe nanofragments embedded in hiroseite. Copper peaks are due to the sample holder.

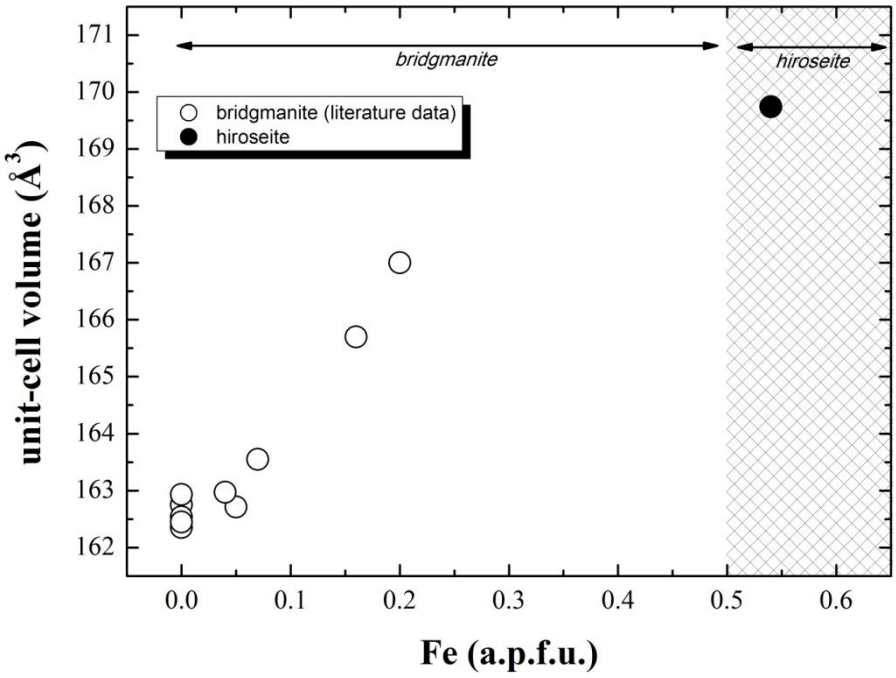

Fig. S4. Bridgmanite-hiroseite series. Iron in atoms per formula unit (a.p.f.u.) plotted against the unit-cell volume for members of the bridgmanite-hiroseite series (*41-45*). The shaded region indicates the field of hiroseite.

Table S1. Electron microprobe analyses of minerals of the Suizhou meteorite. Chemical formulae were calculated on the basis of one (Fe-bearing periclase), three (hiroseite, glass) and four (olivine, ringwoodite and ahrensite) oxygen atoms.

	hiroseite	*Fe-bearing periclase*	*olivine*	*ringwoodite*	*ahrensite*	*glass*
SiO_2	45.34	0.00	40.89	35.66	35.93	56.38
Al_2O_3	6.49	0.01	0.00	2.16	1.91	0.23
Cr_2O_3	0.01	0.00	0.02	0.46	0.24	0.13
Fe_2O_3	6.65	0.00	0.00	0.00	0.00	0.00
FeO	26.91	58.37	9.26	18.66	38.26	2.76
MgO	12.64	41.68	48.85	40.62	19.92	38.94
CaO	0.95	0.00	0.08	2.15	2.01	0.85
MnO	0.01	0.00	0.02	0.06	0.05	0.44
Na_2O	0.80	0.00	0.00	1.03	0.88	0.09
Total	99.80	100.05	99.12	100.80	99.20	99.82
Si	0.89	0.00	1.01	0.92	1.02	0.97
Al	0.15	0.00	0.00	0.07	0.06	0.00
Cr^{3+}	0.00	0.00	0.00	0.01	0.01	0.00
Fe^{3+}	0.10	0.00	0.00	0.00	0.00	0.00
Fe^{2+}	0.44	0.44	0.19	0.40	0.91	0.04
Mg	0.37	0.56	1.79	1.56	0.85	0.99
Ca	0.02	0.00	0.00	0.06	0.06	0.02
Mn	0.00	0.00	0.00	0.00	0.00	0.01
Na	0.03	0.00	0.00	0.05	0.05	0.00
Σ*cat*	2.00	1.00	2.99	3.07	2.96	2.03

Table S2. X-ray powder diffraction data (*d* in angstroms) for hiroseite. Strongest diffraction peaks are given in bold.

h	*k*	*l*	d_{obs}	*I*
0	1	1	3.98	1
0	2	0	3.50	2
1	0	1	3.480	2
1	1	1	3.117	1
2	0	0	2.501	16
1	**2**	**1**	**2.468**	**56**
0	0	2	2.423	18
2	1	0	2.355	1
2	0	1	2.222	2
1	0	2	2.181	2
2	1	1	2.118	3
0	3	1	2.103	5
1	1	2	2.082	9
2	2	0	2.035	3
0	2	2	1.9925	3
1	3	1	1.9387	5
2	2	1	1.8763	4
1	2	2	1.8510	1
0	**4**	**0**	**1.7508**	**68**
2	**0**	**2**	**1.7402**	**100**
2	3	0	1.7064	1
2	1	2	1.6888	4
2	3	1	1.6096	2
1	3	2	1.5935	1
3	0	1	1.5765	1
0	1	3	1.5740	3
1	4	1	1.5640	1
2	2	2	1.5583	5
3	1	1	1.5380	1
1	0	3	1.5372	10
1	1	3	1.5014	2
3	2	1	1.4375	1
2	**4**	**0**	**1.4342**	**26**
0	4	2	1.4191	11
1	**2**	**3**	**1.4075**	**33**
2	3	2	1.3952	3
2	4	1	1.3753	1
3	0	2	1.3735	1
1	4	2	1.3652	1
2	0	3	1.3569	1
3	1	2	1.3478	1
0	5	1	1.3455	3
2	1	3	1.3321	1
0	3	3	1.3283	1
3	3	1	1.3065	4
1	5	1	1.2993	2
1	3	3	1.2838	1
3	2	2	1.2786	1
2	2	3	1.2652	1
4	0	0	1.2504	1
2	4	2	1.2342	7
4	**1**	**0**	**1.2309**	**27**
2	5	0	1.2220	1
0	0	4	1.2115	1
4	0	1	1.2107	3
4	1	1	1.1930	1
2	5	1	1.1849	1
3	3	2	1.1838	3
1	5	2	1.1785	1
4	2	0	1.1776	1
1	0	4	1.1775	1
2	3	3	1.1731	1
3	4	1	1.1715	1
0	6	0	1.1672	3
1	1	4	1.1612	1
3	0	3	1.1601	1
1	4	3	1.1551	1
0	2	4	1.1449	1
3	1	3	1.1445	1
4	2	1	1.1443	3
1	2	4	1.1160	1
4	0	2	1.1112	1
1	6	1	1.1066	4
4	3	0	1.1022	13
3	2	3	1.1012	1
4	1	2	1.0974	2
2	5	2	1.0911	1
2	0	4	1.0903	5
3	4	2	1.0806	1
2	1	4	1.0773	1
4	3	1	1.0748	1
2	4	3	1.0725	1
4	2	2	1.0591	1
0	5	3	1.0582	1
2	6	0	1.0577	3
0	6	2	1.0515	3
1	3	4	1.0513	1
3	5	1	1.0471	10
2	2	4	1.0410	9
3	3	3	1.0389	1
1	5	3	1.0353	11
2	6	1	1.0333	3
1	6	2	1.0290	5
4	4	0	1.0175	1
1	0	1		

Table S3. Atoms, site occupancy factors (s.o.f.), fractional coordinates of atoms, and B_{eq} in the structure of hiroseite.

Atoms	s.o.f.	*x*/*a*	*y*/*b*	*z*/*c*	B_{eq}
A	$[Fe_{0.55(2)}Mg_{0.45}]$	0.5288(10)	0.25	0.5111(9)	3.8(3)
B	$[Si_{1.00}]$	0	0	0.5	3.5(3)
O1	$[O_{1.00}]$	0.993(5)	0.25	0.397(5)	5.9(1)
O2	$[O_{1.00}]$	0.208(4)	0.544(2)	0.198(3)	5.9(1)

Table S4. Selected bond distances (in angstroms) in the structure of hiroseite.

A	O1	1.99(2)
	O2	2.075(16) (×2)
	O1	2.38(3)
	O2	2.408(15) (×2)
	O2	2.464(15) (×2)
B	O2	1.776(17) (×2)
	O2	1.820(16) (×2)
	O1	1.821(6) (×2)