Discovery of elgoresyite, $(Mg,Fe)_5Si_2O_9$: Implications for novel iron-magnesium silicates in rocky planetary interiors

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Table ST1.
Analytical data (in wt%) for the new magnesium silicate.

Constituent	Mean	Range	SD	Probe Standard
SiO_2	31.36	30.95 – 31.56	0.75	forsterite
Al_2O_3	0.68	0.50 – 0.81	0.15	albite
FeO	30.72	29.92 – 31.08	0.68	fayalite
MgO	36.43	35.88 – 36.94	0.79	forsterite
CaO	0.31	0.22 – 0.46	0.07	plagioclase
Na_2O	0.26	0.14 – 0.53	0.06	albite
Total	99.76	99.08 – 100.33		

Table ST2.

X-ray powder diffraction data (d in Å) for the new magnesium silicate.

h	k	l	d_{calc}	I	d_{obs}	I
0	0	1	11.057	5	-	-
2	0	1	4.2038	15	4.21	15
-2	0	2	3.7128	6	-	-
2	0	2	3.4506	6	-	-
2	0	3	2.7979	100	2.801	100
-1	1	1	2.5895	13	2.591	10
1	1	1	2.5651	30	2.563	35
-2	0	4	2.4621	76	2.460	70
-1	1	2	2.4096	9	-	-
1	1	2	2.3705	13	2.372	5
-4	0	1	2.3271	24	2.325	30
2	0	4	2.3072	40	2.308	40
0	0	5	2.2115	6	-	-
3	1	0	2.0696	28	2.070	35
-2	0	5	2.0597	16	2.060	20
-3	1	1	2.0526	9	2.054	10
3	1	1	2.0164	61	2.017	55
-3	1	2	1.9703	67	1.968	65
2	0	5	1.9451	5	-	-
3	1	2	1.9077	35	1.909	30
-3	1	3	1.8436	62	1.845	60
-1	1	5	1.7158	12	1.716	10
1	1	5	1.6807	21	1.678	25
3	1	4	1.6190	12	1.618	10
0	0	7	1.5796	23	1.578	20
5	1	0	1.5511	7	-	-
-3	1	5	1.5495	5	-	-
-1	1	6	1.5281	23	1.529	25
5	1	1	1.5232	23	1.520	20
1	1	6	1.4984	18	1.496	15
3	1	5	1.4754	11	-	-
6	0	2	1.4747	26	1.476	35
5	1	2	1.4701	10	1.471	10
-5	1	3	1.4620	8	-	-
-3	1	6	1.4112	6	-	-
4	0	6	1.3990	9	-	-
-5	1	4	1.3895	10	1.390	10
0	2	0	1.3815	31	1.380	35
-1	1	7	1.3696	5	-	-
-6	0	5	1.3228	19	1.321	25
5	1	4	1.3186	5	-	-
-3	1	7	1.2865	4	-	-
2	2	3	1.2387	13	1.240	15
-4	0	8	1.2310	7	-	-
-2	2	4	1.2048	13	1.206	10
-4	2	1	1.1879	6	-	-
2	2	4	1.1853	4	-	-
-8	0	2	1.1636	7	-	-
0	2	7	1.0399	9	-	-
6	2	2	1.0082	12	-	-

The calculated diffraction pattern was obtained with the atom coordinates reported in Table S3 (only reflections with $I_{rel} \geq 4$ are listed).

Table ST3.

Atoms, Wyckoff positions, mean electron numbers, proposed site populations, fractional coordinates of atoms, and isotropic displacement parameters in the structure of the new magnesium silicate.

atom	Wyckoff	s.o.f.	site population	x	y	z	U_{iso}
*M*1	2*d*	14.90	$(Mg_{0.45}Si_{0.40}Fe_{0.15})$	0	½	½	0.0015(5)
*M*2	4*i*	15.90	$(Mg_{0.43}Si_{0.34}Fe_{0.23})$	0.2668(3)	0	0.62338(15)	0.0031(4)
*M*3	4*i*	13.98	$(Mg_{0.55}Si_{0.36}Fe_{0.09})$	0.3528(3)	0	0.93433(14)	0.0018(3)
*M*4	4*i*	17.80	$(Mg_{0.50}Fe_{0.40}Si_{0.10})$	0.06772(19)	0	0.78787(9)	0.0023(3)
O1	4*i*		$O_{1.00}$	0.4125(6)	0	0.7784(3)	0.0047(8)
O2	2*a*		$O_{1.00}$	0	0	0	0.0084(15)
O3	4*i*		$O_{1.00}$	0.1318(5)	0	0.4483(3)	0.0085(8)
O4	4*i*		$O_{1.00}$	0.3660(5)	0	0.3411(3)	0.0104(9)
O5	4*i*		$O_{1.00}$	0.3064(7)	0	0.1011(4)	0.0056(10)

Table ST4.

Selected bond distances (Å) in the structure of the new magnesium silicate.

*M*1	O3	1.969(4) (×4)
	O4	2.089(4) (×2)
*M*2	O3	1.887(4) (×2)
	O4	1.921(4) (×2)
	O1	2.117(5)
	O3	2.239(4)
*M*3	O1	1.857(5)
	O5	1.930(5)
	O2	2.050(2) (×2)
	O5	2.053(5) (×2)
*M*4	O1	2.006(5) (×2)
	O4	2.115(3) (×2)
	O5	2.147(4) (×2)
	O2	2.482(1)

Table ST5.

Bond valence sums calculated with the site populations reported in Table ST3 and according to the parameters of Brese and O'Keeffe (*56*).

	***M*1**	***M*2**	***M*3**	***M*4**	**ΣO**
O1		0.312	0.618	$0.443^{\times 2\downarrow}$	1.816
O2			$0.367^{\times 2\downarrow}$	0.123	1.714
O3	$0.457^{\times 4\downarrow}$	0.223 $0.581^{\times 2\downarrow}$			2.299
O4	$0.330^{\times 2\downarrow}$	$0.530^{\times 2\downarrow}$		$0.331^{\times 2\downarrow}$	2.052
O5			0.507 $0.364^{\times 2\downarrow}$	$0.303^{\times 2\downarrow}$	1.841
	2.488	2.757	2.587	2.277	

References

56. N. Brese, M. O'keeffe, Bond-valence parameters for solids. *Acta Crystallographica Section B: Structural Science* **47**, 192-197 (1991).