

## **Supplemental Material**

### **Keplerite, $\text{Ca}_9(\text{Ca}_{0.5}\square_{0.5})\text{Mg}(\text{PO}_4)_7$ , a new meteoritic and terrestrial phosphate isomorphous with merrillite, $\text{Ca}_9\text{NaMg}(\text{PO}_4)_7$**

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**Table S1.** Chemical composition of holotype keplerite from the Marjalahti meteorite

Analysis #	Constituent, wt. %					Formula amounts, <i>apfu</i> (O = 28)			
	CaO	MgO	FeO	P <sub>2</sub> O <sub>5</sub>	Total	Mg	P	Ca	Fe
1	48.86	3.88	1.17	46.06	99.97	1.03	6.97	9.36	0.17
2	49.03	4.00	1.11	46.54	100.68	1.06	6.99	9.31	0.16
3	49.00	3.85	1.33	46.67	100.85	1.02	7.00	9.30	0.20
4	49.21	3.81	1.31	46.56	100.89	1.01	6.98	9.34	0.19
5	48.93	3.90	1.39	46.10	100.32	1.04	6.96	9.35	0.21
6	49.10	3.78	1.36	46.49	100.73	1.00	6.98	9.34	0.20
7	48.64	3.91	1.47	46.01	100.03	1.04	6.97	9.32	0.22
8	48.71	4.00	1.34	45.87	99.92	1.07	6.95	9.35	0.20
9	48.31	3.93	1.45	45.83	99.52	1.05	6.97	9.30	0.22
Average	48.87	3.90	1.33	46.24	100.34	1.04	6.97	9.33	0.20

**Table S2.** Crystal parameters, data collection and structure refinement details for holotype keplerite

<b>Crystal Data</b>	
Formula	$\text{Ca}_9(\text{Ca}_{0.33}\text{Fe}_{0.20}\square_{0.47})_{1.00}\text{Mg}(\text{PO}_4)_7$
Crystal size (mm)	$0.02 \times 0.02 \times 0.02$
Crystal system	Trigonal
Space group	$R\bar{3}c$
$a$ (Å)	10.3330(4)
$c$ (Å)	37.0668(24)
$V$ (Å <sup>3</sup> )	3427.4(3)
$Z$	6
$D_x$ (g cm <sup>-3</sup> )	3.123
<b>Data collection and refinement</b>	
Radiation	MoK $\alpha$ ( $\lambda = 0.71073$ Å)
Temperature (K)	296
$2\Theta$ range (°)	4.00 – 54.00
Total reflections collected	8921
No. unique reflections	1798
No. unique observed, $I > 2\sigma(I)$	1577
$h, k, l$ range	$-13 \rightarrow 13, -13 \rightarrow 13, -48 \rightarrow 43$
$F(000)$	3197
$\mu$ (mm <sup>-1</sup> )	2.92
No. refined parameters	139
$R_{\text{int.}}$	0.076
$R_\sigma$	0.046
$R_1 [F \geq 4\sigma(F)]$	0.039
$R_1$ (all data)	0.047
$wR_2$	0.082
$S = GoF$	1.053
Absolute structure parameter	0.10(6)
Residual density (e Å <sup>-3</sup> ) (min, max)	-1.05, 0.72

**Table S3.** Calculated X-ray powder diffraction pattern for holotype keplerite <sup>a</sup>

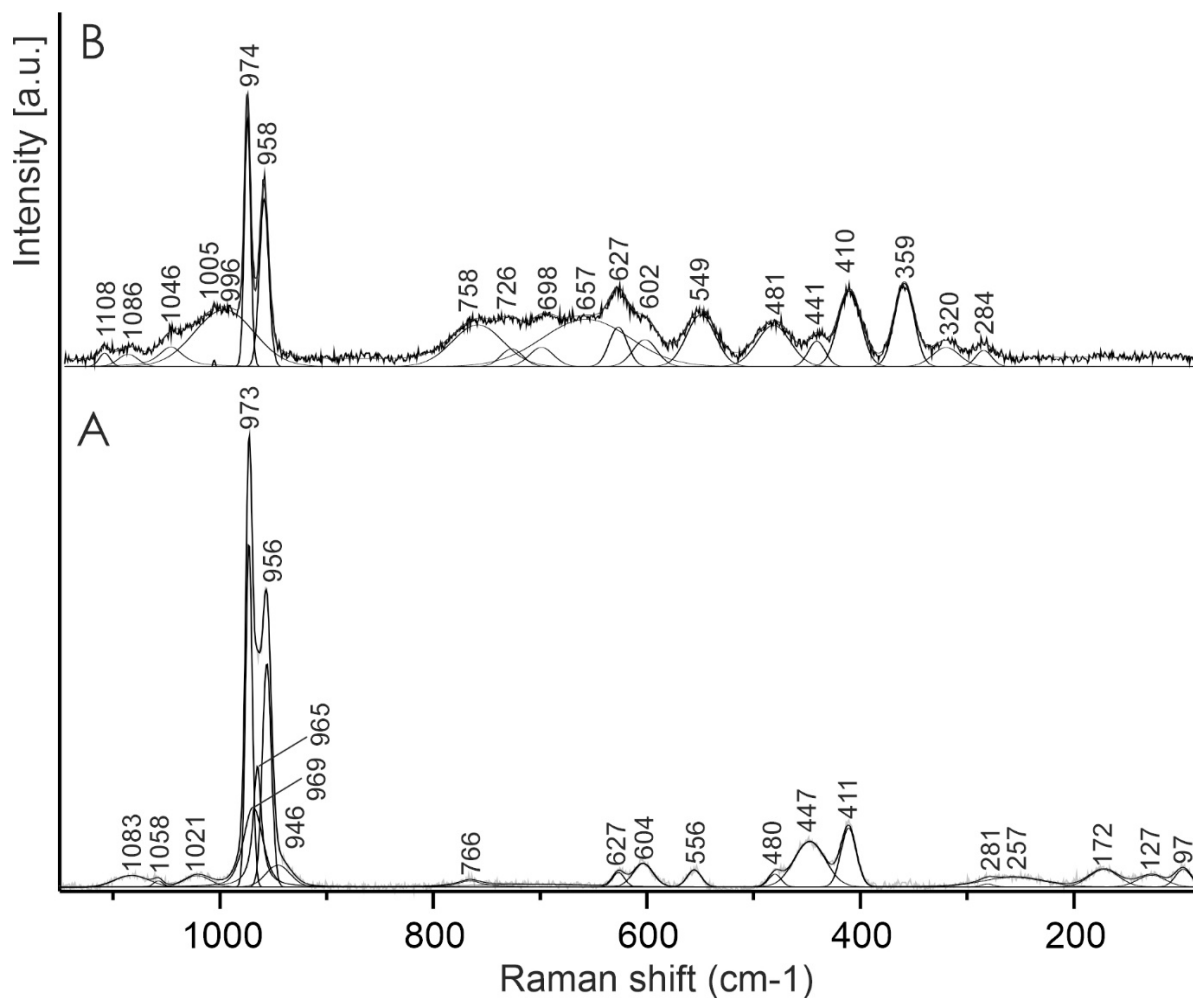
<i>I</i> <sub>calc</sub>	<i>d</i> <sub>calc</sub>	<i>hkl</i>	<i>I</i> <sub>calc</sub>	<i>d</i> <sub>calc</sub>	<i>hkl</i>
6	8.0585	102	2	1.9288	413
16	6.4372	104	22	1.9153	4.0.10
3	6.1778	006	19	1.8770	328
25	5.1665	110	14	1.8620	416
8	4.3494	202	5	1.8148	1.0.20
8	4.0292	204	6	1.7959	3.2.10
24	3.4245	1.0.10	6	1.7814	502
4	3.3683	211	5	1.7645	419
11	3.3273	212	8	1.7573	504
4	3.2205	119	3	1.7222	330
3	3.2186	208	28	1.7123	2.0.20
46	3.1772	214	7	1.6947	3.0.18
13	2.9829	300	2	1.6935	3.1.16
100	2.8544	2.0.10	5	1.6695	508
17	2.7318	218	2	1.6637	424
8	2.6862	306	3	1.6506	4.1.12
5	2.6512	1.1.12	2	1.6253	2.1.20
64	2.5833	220	3	1.6224	3.2.14
5	2.5388	1.0.14	2	1.6117	5.0.10
6	2.5286	223	2	1.6093	4.0.16
14	2.4985	2.1.10	3	1.5889	339
3	2.4764	311	4	1.5886	428
2	2.3872	2.1.11	2	1.5836	514
6	2.3833	226	8	1.5386	4.2.10
4	2.3535	315	8	1.5365	3.2.16
8	2.2427	1.0.16	3	1.5185	518
3	2.2293	1.1.15	3	1.5081	2.1.22
2	2.2210	402	4	1.4914	600
11	2.1747	404	4	1.4530	434
16	2.1457	3.0.12	2	1.4329	520
2	2.0848	2.1.14	3	1.4272	4.0.20
3	2.0623	3.1.10	2	1.4170	4.1.18
2	2.0593	0.0.18	3	1.4022	438
2	2.0498	321	5	1.3959	526
4	2.0405	322	5	1.3757	3.2.20
7	2.0146	408	2	1.3637	611
4	2.0044	324	2	1.3256	2.2.24
3	1.9816	2.2.12	2	1.3137	2.1.26

<sup>a</sup> Calculated using STOE WinXPOW v. 2.02 for CuK $\alpha_1$  radiation, based on atomic coordinates and unit-cell parameters obtained from structure refinement. Reflections with the relative intensity less than 2 have been omitted.

**Table S4.** Chemical composition of pyroxene from symplectites and adjacent olivine <sup>a</sup>

Constituent, wt. %					Formula amounts, <i>apfu</i>			
MgO	FeO	MnO	SiO <sub>2</sub>	Total	Mg	Fe	Mn	Si
<b>Orthopyroxene</b>								
34.41	57.26	0.38	8.23	100.28	1.78	0.24	0.01	1.99
34.29	57.28	0.32	8.18	100.07	1.78	0.24	0.01	1.99
34.39	57.21	0.24	8.35	100.19	1.78	0.24	0.01	1.99
34.04	57.74	0.31	8.43	100.52	1.75	0.24	0.01	2.00
<b>34.28</b>	<b>57.37</b>	<b>0.31</b>	<b>8.30</b>	<b>100.27</b>	<b>1.77</b>	<b>0.24</b>	<b>0.01</b>	<b>1.99</b>
<b>Olivine</b>								
47.97	11.42	0.25	40.95	100.59	1.75	0.23	0.01	1.00
48.17	11.49	0.19	40.69	100.54	1.76	0.24	0.00	1.00
48.22	11.38	0.27	40.67	100.54	1.76	0.23	0.01	1.00
47.81	11.36	0.26	40.52	99.95	1.76	0.23	0.01	1.00
47.47	11.41	0.24	40.72	99.84	1.75	0.24	0.01	1.01
<b>47.93</b>	<b>11.41</b>	<b>0.24</b>	<b>40.71</b>	<b>100.29</b>	<b>1.76</b>	<b>0.23</b>	<b>0.01</b>	<b>1.00</b>

<sup>a</sup> Average values are typed in bold.



**Figure S1.** Raman spectra of terrestrial keplerite from the Hatturim Basin. (A) *REE*-free keplerite. (B) *REE*-bearing keplerite (B). Spectrum of *REE*-bearing keplerite has low quality (intensity) and high background caused by luminescence of *REE*.