Supplementary information to the paper

The mineralogy of the historical Mochalin Log *REE* deposit, South Urals, Russia. Part I. New gatelite-group minerals ferriperbøeite-(La), $(CaLa_3)(Fe^{3+}Al_2Fe^{2+})[Si_2O_7][SiO_4]_3O(OH)_2$, and perbøeite-(La), $(CaLa_3)(Al_3Fe^{2+})[Si_2O_7][SiO_4]_3O(OH)_2$

by Anatoly V. Kasatkin, Natalia V. Zubkova, Igor V. Pekov, Nikita V. Chukanov, Radek Škoda, Yury S. Polekhovsky, Atali A. Agakhanov, Dmitriy I. Belakovskiy, Aleksey M. Kuznetsov, Sergey N. Britvin and Dmitry Y. Pushcharovsky

Table S1. Non-*REE* minerals found in *REE* nodules of the Mochalin Log deposit and their distribution (based on our data).

Mineral species	Simplified formula*	Distribution
Sulfides		
Chalcopyrite**	$CuFeS_2$	X
Galena**	PbS	X
Molybdenite**	MoS_2	X
Pyrite	FeS_2	XX
Sphalerite**	ZnS	X
Oxides		
Baddeleyite**	ZrO_2	XX
Chromite**	$Fe^{2+}Cr_2O_4$	XX
Columbite-(Fe)**	$Fe^{2+}Nb_2O_6$	XXX
Columbite-(Mn)**	$Mn^{2+}Nb_2O_6$	X
Corundum	Al_2O_3	XX
Cryptomelane**	$K(Mn^{4+}{}_7Mn^{3+})O_{16}$	XX
Goethite	FeO(OH)	X
Hercynite**	$Fe^{2+}Al_2O_4$	XX
Hollandite**[1]	$Ba(Mn^{4+}{}_6Mn^{3+}{}_2)O_{16}$	XXX
Ilmenite	$Fe^{2+}Ti^{4+}O_3$	XXXX
Magnetite[1]	$Fe^{2+}Fe^{3+}{}_2O_4$	XXXX
Pyrochlore group minerals[2]	$A_2Nb_2(O,OH)_6Z$	XX
Quartz[1]	SiO_2	XXXXX
Rutile[1]	TiO_2	XXX
Spinel**	$MgAl_2O_4$	XX
Stefanweissite**	$(Ca,REE)_2Zr_2(Nb,Ti)(Ti,Nb)_2Fe^{2+}O_{14}$	XX
Thorianite**	ThO_2	XXXX
Todorokite**	$(Na,Ca,K,Ba,Sr)_{1-x}(Mn,Mg,Al)_6O_{12}\cdot 3\text{-}4H_2O$	XX
Ulvöspinel**	$Fe^{2+}{}_2TiO_4$	XX
Vernadite**	$(Mn,Fe,Ca,Na)(O,OH)_2\cdot nH_2O$	X
Zirconolite**	$(Ca,Y)Zr(Ti,Mg,Al)_2O_7$	X
Carbonates		
Calcite	$CaCO_3$	XX
Sulfates		
Baryte**[1]	$BaSO_4$	XXX
Phosphates		
Cheralite**	$CaTh(PO_4)_2$	X
Fluorapatite[1]	$Ca_5(PO_4)_3F$	XXXX
Silicates		
Aegirine	$NaFe^{3+}Si_2O_6$	X
Albite[1]	$Na(AlSi_3O_8)$	XXXX
Almandine	$Fe^{2+}{}_3Al_2(SiO_4)_3$	XX
Annite[1]	$KFe^{2+}{}_3(AlSi_3O_{10})(OH)_2$	XXX
Anorthite	$Ca(Al_2Si_2O_8)$	XX
Augite	$(Ca,Mg,Fe)_2Si_2O_6$	X
Chamosite**[1]	$(Fe^{2+},Mg,Al,Fe^{3+})_6(Si,Al)_4O_{10}(OH,O)_8$	XX
Clinochlore[1]	$Mg_5Al(AlSi_3O_{10})(OH)_8$	XX
Diopside	$CaMgSi_2O_6$	X
Epidote	$Ca_2(Al_2Fe^{3+})[Si_2O_7][SiO_4]O(OH)$	XXX
Ferri-winchite**	$\square(NaCa)(Mg_4Fe^{3+})Si_8O_{22}(OH)_2$	X
Ferro-edenite**	$NaCa_2Fe^{2+}{}_5(Si_7Al)O_{22}(OH)_2$	X

Fluorcalciobritholite**	$(Ca,REE)_5(SiO_4,PO_4)_3F$	X
Hastingsite**	$NaCa_2(Fe^{2+}_4Fe^{3+})(Si_6Al_2)O_{22}(OH)_2$	X
Heulandite-Ca**[1]	$(Ca,Na,K)_5(Si_{27}Al_9)O_{72}\cdot 26H_2O$	XX
Heulandite-Sr**	$(Sr,Ca,Na)_5(Si_{27}Al_9)O_{72}\cdot 24H_2O$	X
Huttonite	$Th(SiO_4)$	XX
Magnesio-hastingsite**	$NaCa_2(Mg_4Fe^{3+})(Si_6Al_2)O_{22}(OH)_2$	XX
Meionite**	$Ca_4Al_6Si_6O_{24}(CO_3)$	X
Microcline[1]	$K(AlSi_3O_8)$	XXXX
Montmorillonite**[1]	$(Na,Ca)_{0.3}(Al,Mg)_2Si_4O_{10}(OH)_2\cdot nH_2O$	XX
Muscovite[1]	$KAl_2(Si_3Al)O_{10}(OH)_2$	XX
Nontronite**[1]	$Na_{0.3}Fe^{3+}_2(Si,Al)_4O_{10}(OH)_2\cdot nH_2O$	XXX
Pargasite**	$NaCa_2(Mg_4Al)(Si_6Al_2)O_{22}(OH)_2$	XX
Phlogopite**	$KMg_3(AlSi_3O_{10})(OH)_2$	X
Potassic-hastingsite**	$KCa_2(Fe^{2+}_4Fe^{3+})(Si_6Al_2)O_{22}(OH)_2$	XX
Pyrophyllite**	$Al_2Si_4O_{10}(OH)_2$	X
Rhodonite**	$CaMn_3Mn(Si_5O_{15})$	XX
Saponite**[1]	$(Ca,Na)_{0.3}(Mg,Fe)_3(Si,Al)_4O_{10}(OH)_2\cdot 4H_2O$	XX
Spessartine**	$Mn^{2+}_3Al_2(SiO_4)_3$	XX
Thorite**[1]	$Th(SiO_4)$	XXXX
Titanite	$Ca(TiSiO_4)O$	XXX
Zircon[1]	$Zr(SiO_4)$	XXXX

Distribution of minerals: XXXXX – abundant, XXXX – common, XXX – subordinate, XX – rare, X – very rare.

*Formulae are given in accordance with the New IMA List of Minerals published at CNMNC website.

**Minerals identified by the authors for the first time at the deposit.

[1]Minerals associated with ferriperboeite-(La) and perboeite-(La).

[2]Identified by EMPA as ‘calciopyrochlore’ and ‘kenopyrochlore’.

Table S2. Powder X-ray diffraction data (*d* in Å) of ferriperbøeite-(La).

I_{obs}	d_{obs}	I_{calc}*	d_{calc}**	*h k l*
72	**15.81**	53	15.84	001
4	8.91	2	8.919	-101
23	8.03	18	8.044	100
12	7.53	10	7.526	-102
4	6.17	3	6.165	101
2	5.706	1	5.706	-103
2	5.285	1	5.281	003
8	4.824	6	4.821	-111
43	**4.700**	9, 29, 8	4.707, 4.667, 4.643	102, 110, 012
14	4.202	4, 8	4.208, 4.197	-203, 111
5	4.025	3	4.022	200
7	3.963	6	3.961	004
7	3.884	4	3.883	013
53	**3.521**	3, 43, 19	3.520, 3.519, 3.488	-105, -212, -114
7	3.397	6	3.392	-213
15	3.292	10, 6	3.292, 3.284	210, -205
5	3.257	4	3.258	014
5	3.126	6	3.125	113
17	3.084	19	3.083	202
100	**3.003**	3, 100, 8	3.015, 2.999, 2.973	211, -115, -303
39	**2.868**	7, 42, 3	2.882, 2.865, 2.857	-304, 020, -301
4	2.825	4	2.819	021
28	**2.775**	30	2.773	015
14	2.720	11	2.715	212
24	2.705	20	2.699	120
33	**2.687**	28	2.683	203
60	**2.636**	2, 8, 57	2.640, 2.639, 2.633	006, -313, -312
4	2.564	5	2.560	-123
5	2.521	5	2.518	023
11	2.456	13	2.453	-315
3	2.412	1	2.410	-222
3	2.362	1, 3	2.368, 2.358	-223, 115
14	2.281	4, 13, 1, 4	2.286, 2.279, 2.276, 2.272	-217, -224, -117, 123
3	2.228	1, 1	2.230, 2.228	-404, 221
17	2.193	16	2.191	-402
17	2.162	25	2.159	-225
7	2.128	10	2.125	025
17	2.102	5, 2, 6, 19	2.105, 2.104, 2.100, 2.099	017, -406, 312, 222
14	1.961	20, 5	1.958, 1.958	223, -209
7	1.936	11	1.934	313
3	1.924	4	1.920	125
5	1.898	2, 3	1.902, 1.897	-109, 410
7	1.885	4, 7	1.888, 1.881	-417, -227
14	1.862	15	1.859	117
1	1.826	1	1.824	131
3	1.807	4	1.805	-319
6	1.792	1, 3, 4, 2	1.798, 1.790, 1.788, 1.788	411, -327, -504, -418
5	1.778	5	1.776	027

8	1.760	2, 1, 6, 2, 7	1.761, 1.760, 1.760, 1.760, 1.756	-423, -409, -2.0.10, -424, -232
5	1.743	6, 1	1.740, 1.739	-422, -233
4	1.705	1, 9	1.707, 1.702	-514, -1.0.10
14	1.681	3, 3, 2, 14, 9	1.683, 1.683, 1.682, 1.679, 1.676	207, -419, -2.1.10, -135, 118
8	1.659	3, 7	1.662, 1.657	-3.1.10, -512
10	1.609	3, 2, 2, 13	1.614, 1.609, 1.607, 1.605	217, 500, -333, -332
4	1.591	5	1.589	413
2	1.566	1, 1, 2	1.567, 1.563, 1.562	324, 226, -335
2	1.551	3	1.549	510
1	1.534	1	1.534	501
2	1.502	7	1.500	-2.2.10
5	1.483	1, 2, 1, 4, 2	1.485, 1.482, 1.482, 1.479, 1.478	-3.2.10, 511, -522, 218, -4.1.11
4	1.472	4, 4	1.470, 1.469	-527, -607
16	1.435	4, 3, 16, 8	1.437, 1.435, 1.432, 1.432	405, -614, 040, 423
3	1.387	1, 1, 1, 1, 5	1.386, 1.386, 1.385, 1.385, 1.384	0.2.10, -612, -5.1.11, 430, 129

*For the calculated pattern, only reflections with intensities ≥1 are given; **for the unit-cell parameters calculated from single-crystal data.

Table S3. Powder X-ray diffraction data (*d* in Å) of perbøeite-(La).

I_{obs}	d_{obs}	I_{calc}*	d_{calc}**	*h k l*
83	**15.85**	53	15.881	001
10	9.01	1	8.940	-101
41	**8.03**	18	8.054	100
18	7.54	8	7.551	-102
7	6.20	3	6.172	101
20	4.828	6	4.824	-111
68	**4.665**	9, 30, 8	4.713, 4.669, 4.646	102, 110, 012
16	4.205	4, 7	4.220, 4.200	-203, 111
8	3.961	6	3.970	004
7	3.888	4	3.888	013
99	**3.523**	3, 42, 19	3.531, 3.524, 3.485	-105, -212, -114
18	3.397	6	3.398	-213
32	3.291	15, 4	3.295, 3.264	210, 014
56	**3.116**	6, 19	3.129, 3.086	113, 202
100	**3.009**	3, 100, 9	3.018, 3.006, 2.980	211, -115, -303
55	**2.874**	7, 42, 3	2.890, 2.865, 2.862	-304, 020, -301
20	2.780	30	2.778	015
27	2.705	20	2.700	120
35	2.691	27, 4	2.687, 2.685	203, 300
54	**2.640**	2, 7, 55	2.647, 2.644, 2.637	006, -313, -312
6	2.568	1, 5	2.580, 2.562	-314, -123
11	2.520	5	2.519	023
21	2.455	13	2.460	-315
6	2.414	1	2.412	-222
5	2.366	1, 2	2.371, 2.361	-223, 115
15	2.303	8	2.301	-307
25	2.282	12, 1, 4	2.282, 2.282, 2.273	-224, -117, 123
11	2.227	1, 3	2.230, 2.225	221, -125
36	2.195	16, 2	2.195, 2.190	-402, -405
34	2.164	25	2.162	-225
14	2.130	10	2.127	025
28	2.101	2, 5, 6, 19	2.110, 2.109, 2.102, 2.100	-406, 017, 312, 222
11	1.961	4, 19	1.964, 1.960	-209, 223
7	1.934	11	1.936	313
12	1.895	3, 3	1.900, 1.893	410, -417
23	1.864	14, 4	1.863, 1.859	117, 130
1	1.826	1	1.824	131
14	1.796	1, 3, 2, 4	1.800, 1.794, 1.793, 1.792	411, -327, -418, -504
13	1.761	1, 6, 2, 2, 6	1.766, 1.766, 1.763, 1.762, 1.757	-409, -2.0.10, -423, -424, -232
12	1.744	6, 1	1.742, 1.740	-422, -233
21	1.683	3, 3, 3, 13, 8	1.687, 1.687, 1.685, 1.680, 1.679	-419, 225, 207, -135, 118
23	1.644	6, 4, 16, 6	1.647, 1.645, 1.643, 1.637	420, -517, -427, 035
13	1.616	3, 3	1.620, 1.617	-229, 217
17	1.609	2, 1, 12	1.611, 1.608, 1.607	500, -333, -332
6	1.484	2, 1, 2, 4	1.484, 1.484, 1.483, 1.481	511, -522, -4.1.11, 218
10	1.435	4, 2, 7, 15	1.439, 1.437, 1.433, 1.433	405, -614, 423, 040
6	1.373	6	1.371	137

*For the calculated pattern, only reflections with intensities ≥1 are given; **for the unit-cell parameters calculated from single-crystal data.

Table S4. Bond-valence calculations for ferriperbøeite-(La) (first line of each row) and perbøeite-(La) (second line of each row).

	A(1)	*A*(2)	*A*(3)	*A*(4)	*M*(1)	*M*(2)	*M*(3)	Si(1)	Si(2)	Si(3)	Si(4)	Si(5)	Σ	H-bonding	Σ
O(1)	$0.31^{x2\downarrow}$ $0.32^{x2\downarrow}$				$0.44^{x2\downarrow}$ $0.42^{x2\downarrow}$		$0.26^{x2\downarrow}$ $0.27^{x2\downarrow}$	$0.96^{x2\downarrow}$ $0.95^{x2\downarrow}$					1.97 1.96		1.97 1.96
O(2)		$0.26^{x2\downarrow}$ $0.25^{x2\downarrow}$		$0.38^{x2\downarrow}$ $0.38^{x2\downarrow}$			$0.31^{x2\downarrow}$ $0.32^{x2\downarrow}$			$0.98^{x2\downarrow}$ $0.98^{x2\downarrow}$			1.93 1.93		1.93 1.93
O(3)	$0.34^{x2\downarrow}$ $0.36^{x2\downarrow}$	$0.20^{x2\downarrow}$ $0.20^{x2\downarrow}$				0.52 0.51			$0.98^{x2\downarrow}$ $0.99^{x2\downarrow}$				2.04 2.06		2.04 2.06
O(4)					$0.61^{x2\downarrow x2\rightarrow}$ $0.61^{x2\downarrow x2\rightarrow}$		0.46 0.45						1.68 1.67	+0.16(O(11)) +0.13(O(11))	1.84 1.80
O(5)	0.22 0.22				$0.43^{x2\downarrow x2\rightarrow}$ $0.40^{x2\downarrow x2\rightarrow}$					0.90 0.90			1.98 1.92		1.98 1.92
O(6)	0.08 0.09					$0.47^{x2\rightarrow}$ $0.47^{x2\rightarrow}$				0.94 0.94			1.96 1.97		1.96 1.97
O(7)	0.35 0.34	0.60 0.61						1.08 1.07					2.03 2.02		2.03 2.02
O(8)		$0.10^{x2\downarrow x2\rightarrow}$ $0.10^{x2\downarrow x2\rightarrow}$		0.07 0.06			0.50 0.52		1.07 1.02				1.84 1.80		1.84 1.80
O(9)	$0.05^{x2\downarrow x2\rightarrow}$ $0.06^{x2\downarrow x2\rightarrow}$							0.96 0.95	0.98 1.00				2.05 2.07		2.04 2.07
O(10)		0.24 0.23				$0.53^{x2\rightarrow}$ $0.55^{x2\rightarrow}$							1.30 1.33	–0.22(O(15) –0.21(O(15)	1.08 1.12
O(11)				0.30 0.31		$0.52^{x2\rightarrow}$ $0.54^{x2\rightarrow}$							1.34 1.39	–0.16(O(4) –0.13(O(4)	1.18 1.26
O(12)			0.18 0.18			$0.45^{x2\rightarrow}$ $0.44^{x2\rightarrow}$					0.90 0.88		1.98 1.94		1.98 1.94
O(13)			$0.34^{x2\downarrow}$ $0.34^{x2\downarrow}$	$0.20^{x2\downarrow}$ $0.19^{x2\downarrow}$		0.50 0.50						$0.96^{x2\downarrow}$ $0.95^{x2\downarrow}$	2.00 1.98		2.00 1.98
O(14)		$0.46^{x2\downarrow}$ $0.45^{x2\downarrow}$	$0.36^{x2\downarrow}$ $0.35^{x2\downarrow}$	$0.25^{x2\downarrow}$ $0.25^{x2\downarrow}$							$1.01^{x2\downarrow}$ $1.02^{x2\downarrow}$		2.08 2.07		2.08 2.07
O(15)			0.37 0.11 0.37 0.11								0.97 0.98		1.46 1.46	+0.22(O(10)) +0.21(O(10))	1.68 1.67
O(16)			0.06 $0.04^{x2\downarrow x2\rightarrow}$ 0.06 $0.04^{x2\downarrow x2\rightarrow}$	0.74 0.73								1.09 1.10	1.97 1.97		1.97 1.97
O(17)		0.09 0.08	0.51 0.50	$0.11^{x2\downarrow x2\rightarrow}$ $0.11^{x2\downarrow x2\rightarrow}$								1.06 1.10	1.88 1.90		1.88 1.90

Σ	2.05 2.13	2.97 2.92	2.71 2.68	2.99 2.96	2.96 2.86	2.99 3.01	2.10 2.15	3.96 3.92	4.01 4.00	3.80 3.80	3.89 3.90	4.07 4.10			

Parameters were taken from Gagné and Hawthorne (2015) and from Ferraris and Ivaldi (1988) for H-bonding. Values were calculated taking into account the refined occupancies for the *M*(1–3) and *A*(1) sites and the split character of the O(15) site. For Fe cations in *M*(3) site the bond-valence parameters of Fe^{2+} was used. The bond-valence parameters of La^{3+} were used for *A*(1–4) sites.

Ferraris G. and Ivaldi G. (1988) Bond valence vs. bond length in O···O hydrogen bonds. *Acta Crystallographica*, **B44**, 341-344.

Gagné O.C. and Hawthorne F.C. (2015) Comprehensive derivation of bond-valence parameters for ion pairs involving oxygen. *Acta Crystallographica*, **B71**, 562–578.

Figure S1: a – historical dump no.2 where first nodules containing ferriperbøeite-(La) and perbøeite-(La) were collected. The memorial plate says that Mochalin Log has been visited in 1912 by Academician A.E. Fersman; **b** – recently uncovered dump № 2*bis*. August 2018.

Figure S2: a – typical nodules composed of numerous *REE* minerals; **b** – biggest nodule *in situ* found by one of the authors (A.M.K.) at the dump #7. Size of the nodule is 11 x 10 x 6 cm, weight 1.1 kg.