

Table S1. Crystal data, measurement and structural refinement parameters of the studied $\text{La}_3\text{Fe}(\text{MoO}_4)_6$

$\text{La}_3\text{Fe}(\text{MoO}_4)_6$	
Crystal data	
Crys. symmetry	orthorhombic
space group	Pbca
a (Å)	19.3164(11)
b (Å)	10.4143(5)
c (Å)	22.0594(12)
V (Å³)	4437.6(4)
Z	8
Dx (g/cm³)	4.4415
μ (mm⁻¹) (for λ Kα=0.7107 Å)	10.105
Appearance	orange-red
Data collection	
λ(Mo Kα) (Å)	0.71073
Scan mode	ω and ϕ
θ(min–max) (°)	1.85–36.79
R(int) (%)	0.032
Recording reciprocal space	-24 ≤ h ≤ 32 -17 ≤ k ≤ 17 -33 ≤ l ≤ 28
Refinement	
Measured, independent obs.*refl.	10170
No. of Refined parameters	307
Refin. method,	F²
R1(F²)(obs) / R1(F²)(all)	0.0218/0.0315
wR2(F²)(obs) /wR2(F²)(all)	0.0283/0.0307
GOF(obs) / GOF(all)	1.41/1.44
$\Delta\rho_{\text{max}} / \Delta\rho_{\text{min}}$ (e Å⁻³)	1.37/-3.95

Table S2. Atomic coordinates and equivalent isotropic displacement parameters (\AA^2) for $\text{La}_3\text{Fe}(\text{MoO}_4)_6$

Atom	Wyckoff position	x	y	z	U_{eq}	BVS sum
La1	8c	0.393987(8)	0.050598(14)	0.231741(7)	0.01029(4)	3.005(7)
La2	8c	0.615154(8)	-0.059983(14)	0.269137(7)	0.01022(4)	3.263(8)
La3	8c	0.214111(8)	0.246231(13)	0.488597(7)	0.00994(4)	3.272(9)
Mo1	8c	0.612449(11)	-0.04103(2)	0.458071(11)	0.00894(6)	6.06(2)
Mo2	8c	0.271712(11)	-0.23992(2)	0.178052(11)	0.00895(5)	5.93(2)
Mo3	8c	0.390481(11)	0.04171(2)	0.039843(11)	0.00930(6)	5.99(2)
Mo4	8c	0.255757(11)	0.00466(2)	0.358563(11)	0.01136(6)	6.10(2)
Mo5	8c	0.502167(12)	-0.27166(2)	0.164048(11)	0.01020(6)	6.02(2)
Mo6	8c	0.449273(12)	-0.26686(2)	0.338072(11)	0.01096(6)	5.91(2)
Fe1	8c	0.46960(2)	-0.25449(4)	0.00152(2)	0.01019(11)	3.473(10)
O1	8c	0.44205(13)	-0.26288(19)	0.41844(10)	0.0220(7)	2.051(11)
O2	8c	0.45806(11)	0.12574(19)	0.00373(10)	0.0204(6)	2.076(11)
O3	8c	0.39636(10)	-0.12787(17)	0.02237(9)	0.0140(5)	2.158(9)
O4	8c	0.58375(11)	-0.2265(2)	0.18965(11)	0.0216(6)	2.080(11)
O5	8c	0.29158(11)	-0.1032(2)	0.41095(10)	0.0233(6)	2.173(12)
O6	8c	0.53370(11)	-0.1151(2)	0.47415(10)	0.0233(6)	2.165(11)
O7	8c	0.30967(11)	0.0913(2)	0.01416(11)	0.0253(7)	1.917(11)
O8	8c	0.39685(12)	0.0638(2)	0.11675(9)	0.0236(7)	2.028(12)
O9	8c	0.60892(9)	0.12141(17)	0.48614(9)	0.0128(5)	2.213(9)
O10	8c	0.50953(10)	0.07526(18)	0.29926(9)	0.0165(5)	1.908(9)
O11	8c	0.42767(12)	-0.4220(2)	0.31327(10)	0.0256(7)	1.956(11)
O12	8c	0.68031(11)	-0.1196(2)	0.49415(11)	0.0262(7)	2.036(12)
O13	8c	0.20740(11)	0.1173(2)	0.40067(10)	0.0234(6)	2.071(12)
O14	8c	0.31678(10)	0.23831(16)	0.20170(9)	0.0127(5)	2.054(9)
O15	8c	0.46486(11)	0.25880(18)	0.18965(10)	0.0177(6)	1.925(10)
O16	8c	0.49737(12)	-0.2872(2)	0.08465(9)	0.0227(6)	2.088(11)
O17	8c	0.32420(11)	-0.35567(19)	0.21158(10)	0.0213(6)	2.025(11)
O18	8c	0.32102(12)	0.08161(19)	0.31713(10)	0.0235(6)	2.092(12)
O19	8c	0.20244(11)	-0.0755(2)	0.30788(10)	0.0218(6)	2.140(12)
O20	8c	0.29561(10)	-0.08266(18)	0.19850(10)	0.0173(6)	1.938(10)
O21	8c	0.62742(13)	-0.0424(2)	0.38083(10)	0.0276(7)	2.044(12)
O22	8c	0.27829(13)	-0.25366(19)	0.09970(11)	0.0241(7)	2.008(13)
O23	8c	0.39729(11)	-0.1502(2)	0.30569(10)	0.0248(7)	1.838(12)
O24	8c	0.44542(11)	-0.1537(2)	0.18821(10)	0.0254(7)	1.988(12)

Table S3: Atomic displacement parameters (\AA^2) for $\text{La}_3\text{Fe}(\text{MoO}_4)_6$

Atom	U11	U22	U33	U12	U13	U23
La1	0.01101(6)	0.00935(6)	0.01051(8)	-0.00017(5)	-0.00149(5)	0.00023(5)
La2	0.01335(7)	0.00787(6)	0.00943(7)	0.00008(5)	-0.00026(5)	0.00039(5)
La3	0.00899(6)	0.01190(7)	0.00893(8)	0.00126(5)	0.00068(5)	-0.00002(5)
Mo1	0.00905(9)	0.00785(9)	0.00991(11)	-0.00047(7)	-0.00042(8)	-0.00065(8)
Mo2	0.00831(9)	0.00984(9)	0.00870(10)	0.00042(7)	0.00053(8)	-0.00044(7)
Mo3	0.01020(9)	0.00726(9)	0.01045(11)	-0.00012(7)	-0.00049(8)	-0.00089(8)
Mo4	0.01470(10)	0.01096(10)	0.00842(11)	0.00096(8)	-0.00019(8)	-0.00058(8)
Mo5	0.01061(9)	0.01120(10)	0.00880(11)	0.00092(7)	-0.00087(8)	0.00026(8)
Mo6	0.01263(10)	0.01293(10)	0.00732(11)	-0.00119(7)	-0.00044(8)	-0.00031(8)
Fe1	0.01072(18)	0.01056(18)	0.0093(2)	0.00061(14)	0.00016(16)	0.00024(14)
O1	0.0335(13)	0.0249(11)	0.0077(10)	-0.0020(9)	-0.0033(9)	-0.0020(8)
O2	0.0205(10)	0.0157(10)	0.0251(12)	-0.0072(8)	0.0024(9)	0.0020(9)
O3	0.0142(9)	0.0088(8)	0.0190(10)	-0.0001(7)	0.0028(8)	-0.0018(7)
O4	0.0149(9)	0.0273(11)	0.0226(12)	-0.0048(8)	-0.0038(9)	-0.0074(9)
O5	0.0291(11)	0.0228(11)	0.0178(11)	0.0052(9)	0.0003(9)	0.0090(9)
O6	0.0181(10)	0.0171(10)	0.0347(13)	-0.0083(8)	0.0072(10)	-0.0009(9)
O7	0.0170(10)	0.0277(12)	0.0313(13)	0.0102(9)	-0.0036(9)	-0.0033(10)
O8	0.0387(13)	0.0227(11)	0.0094(10)	-0.0008(9)	0.0000(9)	-0.0041(8)
O9	0.0124(8)	0.0087(8)	0.0174(10)	-0.0003(6)	-0.0001(7)	-0.0020(7)
O10	0.0195(9)	0.0116(8)	0.0183(10)	0.0024(7)	0.0013(8)	-0.0021(8)
O11	0.0405(13)	0.0216(11)	0.0146(11)	-0.0131(10)	0.0016(10)	-0.0070(9)
O12	0.0226(11)	0.0252(11)	0.0308(13)	0.0134(9)	-0.0082(10)	-0.0050(10)
O13	0.0251(11)	0.0249(11)	0.0203(11)	0.0076(9)	-0.0007(9)	-0.0097(9)
O14	0.0104(8)	0.0124(8)	0.0151(10)	0.0004(6)	-0.0023(8)	-0.0002(7)
O15	0.0144(9)	0.0198(10)	0.0190(11)	0.0016(7)	0.0012(9)	-0.0033(8)
O16	0.0267(11)	0.0311(12)	0.0104(10)	-0.0026(9)	-0.0080(9)	0.0026(9)
O17	0.0205(10)	0.0168(10)	0.0265(12)	0.0055(8)	-0.0067(9)	0.0018(9)
O18	0.0321(12)	0.0171(10)	0.0215(12)	-0.0045(9)	0.0127(10)	-0.0015(9)
O19	0.0230(10)	0.0229(11)	0.0193(11)	0.0003(8)	-0.0062(9)	-0.0067(9)
O20	0.0166(9)	0.0129(9)	0.0223(11)	-0.0035(7)	-0.0026(8)	-0.0024(8)
O21	0.0435(14)	0.0281(12)	0.0111(11)	-0.0036(10)	0.0039(10)	-0.0034(9)
O22	0.0270(12)	0.0346(14)	0.0108(11)	-0.0018(9)	0.0029(9)	-0.0020(9)
O23	0.0220(10)	0.0331(13)	0.0192(11)	0.0085(9)	0.0007(9)	0.0072(10)
O24	0.0270(11)	0.0220(11)	0.0272(12)	0.0107(9)	0.0076(10)	0.0033(9)

Table S4: Evolution of the specific surface area as a function of the attrition time for 20 g of $\text{La}_3\text{Fe}(\text{MoO}_4)_6$

Attrition time (h)	Specific surface area (m^2/g)
0	0.4
1	2.1
2	2.9
3	3.2
4	5.6