

Supplementary Material

Synthesis and Characterization of $\text{LaNi}_{0.5}\text{Ti}_{0.5}\text{O}_3$ and $\text{La}_2\text{NiTiO}_6$ Double Perovskite Nanoparticles

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Table S1. Structural parameters, average crystallite size, together with conventional discrepancy factors from Rietveld refinement of XRD data for Sample 1, Sample 2, and Sample 3.

	Sample 1 ^{a,c}	Sample 2 ^{a,d}	Sample 3 ^{a,e}	$\text{LaNi}_{0.5}\text{Ti}_{0.5}\text{O}_3$ (ICSD: 88851) ^b	$\text{La}_2\text{NiTiO}_6$ (ICSD: 95977) ^b
La_2O_3 (wt%)	66.67	67.55	66.75		
NiO (wt%)	16.79	16.41	16.58		
TiO_2 (wt%)	16.54	16.04	16.67		
Sycos (°)	−0.00685	0.00454	0.06828		
Average crystallite size (nm) ^f	27.1	32.4	39.8		
X-ray density (g cm^{-3})	6.643	6.640	6.681	6.631	6.605
Space group ^g	<i>Pbnm</i>	<i>Pbnm</i>	<i>P2₁/n</i>	<i>Pbnm</i>	<i>P2₁/n</i>
a/(Å)	5.540(2)	5.539(2)	5.541(1)	5.517	5.5545
b/(Å)	5.533(2)	5.538(1)	5.534(1)	5.551	5.5512
c/(Å)	7.834(3)	7.832(3)	7.823(2)	7.856	7.8341
β /(°)			90.053(35)		90.08
V(Å ³)	240.2(1)	240.3(1)	239.9(1)	240.6	241.6
A Position	4c	4c	4e	4c	4e
x	−0.00456(41)	0.00378(82)	0.50438(75)	−0.0048	0.5080
y	0.01976(27)	0.02238(21)	0.52603(19)	0.0206	0.5303
z	0.25	0.25	0.24973(172)	0.25	0.2586
Occ	0.5	0.5	1	0.5	1
B' Position	4b	4b	2d	4b	2d
Occ ^h	0.25	0.25	0.433(1)/ 0.077(2)	0.25	0.43/0.07
B'' Position	4b	4b	2c	4b	2c
Occ ⁱ	0.25	0.25	0.433(1)/ 0.077(2)	0.25	0.43/0.07
O(1) Position	8d	8d	4e	8d	4e
x	0.25306(317)	0.25763(292)	0.25902(734)	0.281	0.2286
y	0.29214(227)	0.28780(231)	0.22762(541)	0.249	0.2173
z	0.04430(117)	0.04495(173)	−0.02690	0.036	−0.0269
Occ	1	1	1	1	1
O(2) Position	4c	4c	4e	4c	4e
x	0.02	−0.04730(325)	0.29993(869)	0.02	0.2945
y	0.478(2)	0.48236(184)	0.69223(750)	0.499	0.7106
z	0.25	0.25	−0.03767(437)	0.25	−0.0376
Occ	0.5	0.5	1	0.5	1
O(3) Position			4e		4e
x			0.42628(714)		0.4266
y			0.97984(193)		0.9928
z			0.24110		0.2411

Occ	1		1
Chi-square (χ^2)	1.68	1.59	1.64
Rp/Rwp/R _B	12.7/14.6/4.3	12.1/13.9/3.7	11/14.1/3.14

^aTheoretical chemical composition for La₂O₃ (wt%) / NiO (wt%) / TiO₂ (wt%): 67.82 % / 15.55 % / 16.63 %. ^bReference: ICSD [1]. ^cF(20) = 20.04 (0.0082, 122) [2]. ^dF(20) = 29.82 (0.0058, 115) [2]. ^eF(20) = 16.73 (0.0137, 98) [2]. ^fThe (1 $\bar{1}$ 2) and (112) planes were selected for the Sample 3 and the other perovskites, respectively. ^gP2₁/n: 4e(x y z), 2d(0.5 0 0), 2c(0 0.5 0). ^hPbmm: 4c(x y 0.25), 4b(0.5 0 0), 8d(x y z). P2₁/n: Occ^h is mainly Ti, and Occⁱ is mostly Ni; Pbmm: Occ^h and Occⁱ are Occ Ni/Ti.

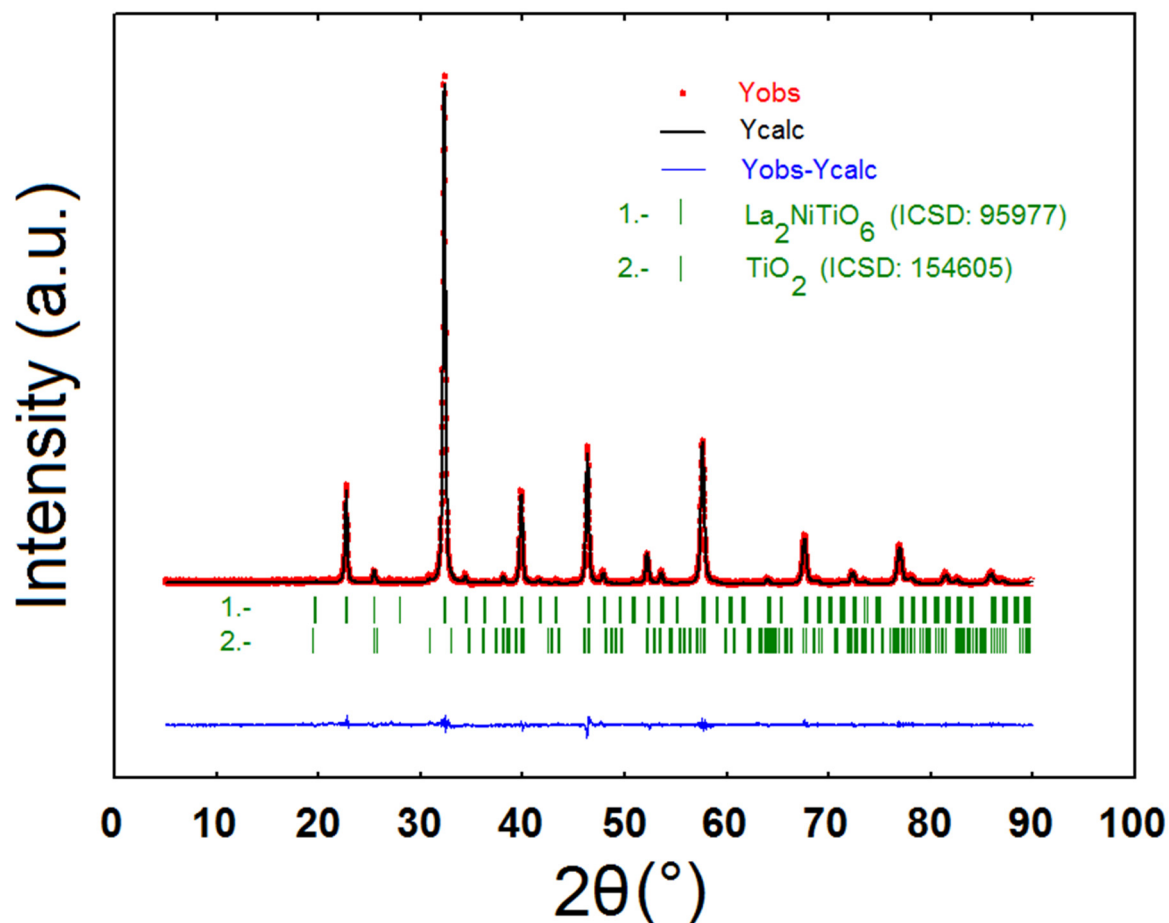


Figure S1. Observed (red symbols), calculated (black line), and difference (blue line) XRD profiles of Sample 3.

Table S2. Structural parameters, results of phase analysis together with conventional discrepancy factors from Rietveld refinement of XRD pattern for Sample 3.

Parameter	Sample 3	ICSD [1]
La₂NiTiO₆^a		
a	5.541(1)	5.5545
b	5.534(1)	5.5512
c	7.823(1)	7.8341
β (°)	90.06(3)	90.08
La: x	0.50494(76)	0.508
y	0.52553(19)	0.5303
z	0.25141(137)	0.2586
B(Å ²)	0.5	0.53
Occ	1	1
Ni: x	0.5	0.5
y	0	0
z	0	0

B(\AA^2)	0.5	1.8
Occ	0.076(2)	0.07
Ti1: x	0.5	0.5
y	0	0
z	0	0
B(\AA^2)	0.5	1.8
Occ	0.434(1)	0.43
Ni2: x	0	0
y	0.5	0.5
z	0	0
B(\AA^2)	0.5	1.39
Occ	0.434(1)	0.43
Ti2: x	0	0
y	0.5	0.5
z	0	0
B(\AA^2)	0.5	1.39
Occ	0.076(2)	0.07
O1: x	0.25699(594)	0.2286
y	0.22996(535)	0.2173
z	-0.0269	-0.0269
B(\AA^2)	0.5	2.5
Occ	1	1
O2: x	0.31358(731)	0.2945
y	0.69316(641)	0.7106
z	-0.04578(408)	-0.0376
B(\AA^2)	0.5	0.66
Occ	1	1
O3: x	0.44120(644)	0.4266
y	0.98731(177)	0.9928
z	0.24110	0.2411
B(\AA^2)	0.5	0.69
Occ	1	1
Scale factor(1×10^4)	3.09024 (950)	
Composition (wt.%)	97.28(0.42)	
Rbragg (%)	3.07	
TiO₂^b		
a	9.167(2)	9.18
b	5.438(1)	5.43
c	5.1649(3)	5.164
Ti: x	0.1289	0.1289
y	0.0992	0.0992
z	0.8628	0.8628
B(\AA^2)	0.5	0.93
Occ	1	1
O1: x	0.0098	0.0098
y	0.148	0.148
z	0.1838	0.1838
B(\AA^2)	0.5	1.08
Occ	1	1
O2: x	0.2312	0.2312
y	0.1116	0.1116
z	0.5362	0.5362
B(\AA^2)	0.5	1.13
Occ	1	1
Scale factor (1×10^5)	1.2182(70)	
Composition (wt.%)	2.72(0.02)	
Rbragg (%)	17.2	
Rp (%)	11	

Rwp (%)	14
χ^2	1.63

a: La₂NiTiO₆(ICSD: 95977). b: TiO₂(ICSD: 154605).

Table S3. Bond distances and bond angles for Sample 1, Sample 2, and Sample 3.

	Sample 1	Sample 2	Sample 3	LaNi _{0.5} Ti _{0.5} O ₃ (ICSD: 88851) ^a	La ₂ NiTiO ₆ (ICSD: 95977) ^a
Ni/Ti—O1	2.146(14) × 2 1.847(14) × 2	2.113(14) × 2 1.883(15) × 2		2.10348 × 2 1.85749 × 2	
Ni/Ti—O2	1.9654(10) × 2	1.978(2) × 2		1.96711 × 2	
Ti—O1			1.85(3) × 2		1.94195 × 2
Ti—O2			2.05(5) × 2		1.99239 × 2
Ti—O3			1.934(8) × 2		1.93327 × 2
Ni—O1			2.09(3) × 2		2.02983 × 2
Ni—O2			2.00(5) × 2		2.03241 × 2
Ni—O3			2.069(8) × 2		2.06865 × 2
Ni/Ti—O1—Ni/Ti	157.4(6)	157.1(6)	167.3(14)	162.1	162.668
Ni/Ti—O2—Ni/Ti	170.4(1)	163.84 (13)	150.4(19)	173.6	154.614
Ni/Ti—O3—Ni/Ti			155.5(3)		156.345

^aReference: ICSD [1].

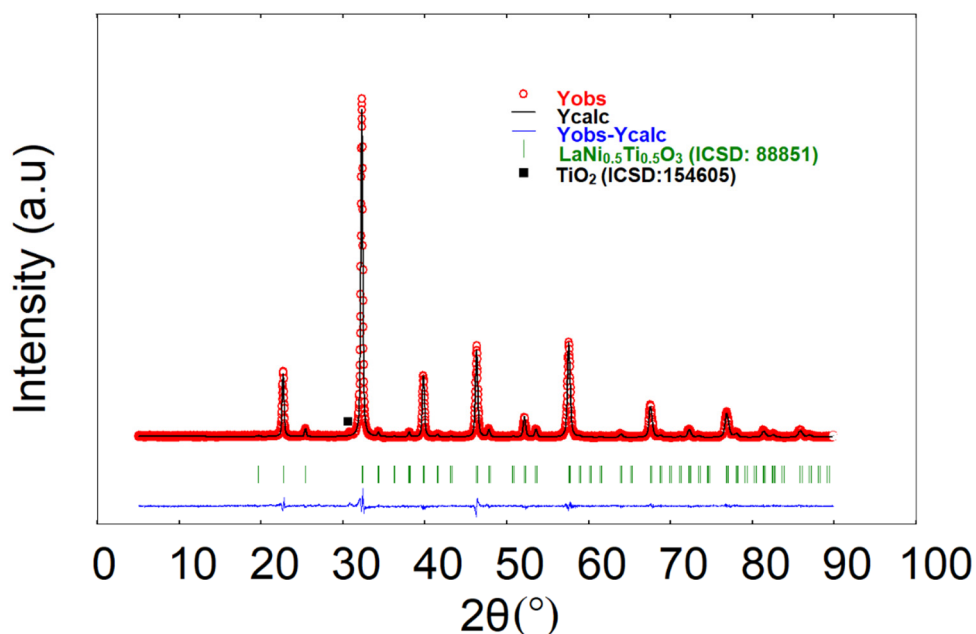


Figure S2. Observed (red symbols), calculated (black line) and difference (blue line) X-ray diffraction profile of Sample 3 using *Pbmm* space group (ICSD: 88851, [1]).

Table S4. Structural parameters, average crystallite size, together with conventional discrepancy factors from Rietveld refinement of XRD data for Sample 3.

	Sample 3 ^a	LaNi _{0.5} Ti _{0.5} O ₃ (ICSD: 88851) ^b
La ₂ O ₃ (wt%)	66.75	
NiO (wt%)	16.58	
TiO ₂ (wt%)	16.67	
Syco _s (°)	0.12418	
Average crystallite size (nm) ^c	39.8	
X-ray density (g cm ⁻³)	6.622	6.631
Space group ^d	<i>Pbnm</i>	<i>Pbnm</i>
a/(Å)	5.5448(14)	5.517
b/(Å)	5.5428(7)	5.551
c/(Å)	7.8391(19)	7.856
V(Å ³)	240.9(1)	240.6
A Position	4c	4c
x	0.0052(6)	-0.0048
y	0.02633(18)	0.0206
z	0.25000	0.25
Occ	0.5	0.5
B' Position	4b	4b
Occ Ni/Ti	0.25	0.25
B'' Position	4b	4b
Occ Ni/Ti	0.25	0.25
O(1) Position	8d	8d
x	0.266(3)	0.281
y	0.288(2)	0.249
z	0.0463(16)	0.036
Occ	1	1
O(2) Position	4c	4c
x	-0.056(3)	0.02
y	0.4821(17)	0.499
z	0.25	0.25
Occ	0.5	0.5
O(3) Position		
x		
y		
z		
Occ		
Chi-square (χ^2)	1.82	
Rp/Rwp/R _B	12.3/14.8/3.89	

^aTheoretical chemical composition for La₂O₃ (wt%) / NiO (wt%) / TiO₂ (wt%): 67.82 % / 15.55 % / 16.63 %. ^bReference: ICSD [1]. ^cIt was selected the (112) plane. ^d*Pbnm*: 4c(x y 0.25), 4b(0.5 0 0), 8d(x y z).

```

! wavelength, zeropoint, Ngrid
1.540600 0.0000 0
! Codes for symmetry
0 0 0 1 0 0
! w, Nind
0.300 3
!Pmin, Pmax, Vmin, Vmax, Rmin, Rmax, Rmaxref
-2. 50. 8. 125000. 0.05 0.15 0.50
5.540,5.540,5.5334,5.5334,7.834,7.834,90,90,90,90,90
! Ntests, Nruns
-100 20
! 2-theta Intensity
22.729 1165.66077
25.483 166.01009
32.332 6113.91406
34.264 134.48129
37.955 124.73923
39.884 1151.93445
41.602 113.57584
43.135 112.58904
46.398 1674.59241
47.800 171.24411
52.237 371.15247
57.677 1591.25061
67.655 570.33246
72.260 193.13924
72.433 182.96774
77.018 469.38516
78.087 132.52876
78.214 137.56558
81.350 161.02144
81.456 160.85553
85.987 173.49216

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Figure S3. Both unit-cell parameters and corrected observed 2-theta values based on the Rietveld Refinement of XRD data of the Sample 1 to perform the indexation of the corresponding XRD pattern.

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! wavelength, zeropoint, Ngrid
1.540600 0.0000 0
! Codes for symmetry
0 0 0 1 0 0
! w, Nind
0.300 3
!Pmin, Pmax, Vmin, Vmax, Rmin, Rmax, Rmaxref
-2. 50. 8. 125000. 0.05 0.15 0.50
5.539,5.539,5.538,5.538,7.832,7.832,90,90,90,90,90,90
! Ntests, Nruns
-100 20
! 2-theta Intensity
19.491 111.19807
22.721 1377.63684
25.372 168.81578
27.908 102.65396
32.329 7107.37012
34.405 127.2098
38.002 140.27457
38.125 140.02853
39.866 1307.08606
41.621 107.36599
46.396 1903.33923
47.747 167.05431
47.87 175.30615
50.784 96.97334
52.206 436.61438
53.68 152.98846
57.655 1882.16492
64.005 127.13898
67.657 709.97998
68.749 121.28933
71.118 91.8567
72.355 215.15233
77.005 586.34283
81.562 170.39136
83.776 80.01309
85.897 183.95049

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Figure S4. Both unit-cell parameters and corrected observed 2-theta values based on the Rietveld Refinement of XRD data of the Sample 2 to perform the indexation of the corresponding XRD pattern.

```

! wavelength, zeropoint, Ngrid
1.540600 0.0000 0
! Codes for symmetry
0 0 0 0 1 0
! w, Nind
0.300 3
!Pmin, Pmax, Vmin, Vmax, Rmin, Rmax, Rmaxref
-2. 50. 8. 125000. 0.05 0.15 0.50
5.541,5.541,5.534,5.534,7.823,7.832,90,90,90.053,90.053,90,90
! Ntests, Nruns
-100 20
! 2-theta Intensity
19.646 98.55988
22.755 1594.68848
25.448 252.16383
27.835 84.39839
32.352 7990.29395
34.397 182.82043
38.139 180.88072
39.875 1483.26709
41.56 110.71102
41.648 112.81496
43.223 98.07073
46.389 2156.59546
47.872 219.73148
49.311 67.40535
50.846 102.5596
52.214 515.2486
53.581 237.08159
57.629 2281.96021
60.398 77.94698
61.405 79.21719
61.638 64.80818
63.942 145.94818
67.594 811.90674
68.822 106.70824
70.053 68.18274
72.284 223.97472
73.432 100.66191
76.924 590.33081
78.027 173.95406
78.275 145.45277
81.38 208.30444
81.459 192.9984
82.484 120.6182
82.603 136.0921
82.725 102.89496
85.819 212.56348
85.964 225.44009
86.918 107.56834
87.033 108.12737
87.233 103.72082

```

Figure S5. Both unit-cell parameters and corrected observed 2-theta values based on the Rietveld Refinement of XRD data of the Sample 3 to perform the indexation of the corresponding XRD pattern.

FINAL VALUES : (STANDARD DEVIATIONS : 2nd LINE)							
ZERO	LAMBDA	A	B	C	ALPHA	BETA	GAMMA
0.000	1.5406	5.5279	5.5345	7.8414	90.000	90.000	90.000
0.011	0.0000	0.0010	0.0010	0.0014	0.000	0.000	0.000
RECIPROCAL CELL :		0.18090	0.18068	0.12753	90.000	90.000	90.000
VOLUME (A**3) :		239.904					
H	K	L	TH(OBS)	TH-ZERO	TH(CALC)	DIFF.	
1	1	0	22.729	22.729	22.717	0.012	
0	2	0	32.332	32.332	32.325	0.007	
0	0	3	34.264	34.264	34.280	-0.016	
2	0	2	39.884	39.884	39.874	0.010	
2	2	0	46.398	46.398	46.394	0.003	
0	2	3	47.800	47.800	47.830	-0.031	
1	3	0	52.237	52.237	52.231	0.006	
3	1	2	57.677	57.677	57.687	-0.010	
0	4	0	67.655	67.655	67.659	-0.004	
0	0	6	72.260	72.260	72.230	0.030	
3	3	0	72.433	72.433	72.434	-0.001	
2	4	0	77.018	77.018	77.010	0.008	
0	4	3	78.087	78.087	78.088	-0.001	
4	2	1	78.214	78.214	78.207	0.006	
0	2	6	81.350	81.350	81.360	-0.010	
4	0	4	85.987	85.987	85.995	-0.008	
M(20) = 31.06							
F(20) = 20.04 (0.0082, 122)							
Final Rp on the .prf = 0.1734906							

Figure S6. Unit-cell parameters, the corrected observed and calculated peak positions, and the respective difference obtained from the McMaille software for the case of the Sample 1.

FINAL VALUES : (STANDARD DEVIATIONS : 2nd LINE)							
ZERO	LAMBDA	A	B	C	ALPHA	BETA	GAMMA
0.006	1.5406	5.5338	5.5261	7.8293	90.000	90.000	90.000
0.010	0.0000	0.0008	0.0017	0.0016	0.000	0.000	0.000
RECIPROCAL CELL :		0.18071	0.18096	0.12772	90.000	90.000	90.000
VOLUME (A**3) :		239.425					
H	K	L	TH(OBS)	TH-ZERO	TH(CALC)	DIFF.	
1	1	0	22.721	22.727	22.722	0.004	
1	1	2	32.329	32.335	32.334	0.001	
0	2	1	34.405	34.411	34.391	0.019	
1	2	1	38.125	38.131	38.145	-0.015	
2	0	2	39.866	39.872	39.866	0.006	
2	2	0	46.396	46.402	46.406	-0.004	
2	0	3	47.870	47.876	47.875	0.001	
1	1	4	52.206	52.212	52.220	-0.008	
1	3	1	53.680	53.686	53.691	-0.005	
3	1	2	57.655	57.661	57.661	0.000	
3	1	3	64.005	64.011	64.015	-0.005	
4	0	0	67.657	67.663	67.669	-0.006	
0	0	6	72.355	72.361	72.359	0.001	
4	2	0	77.005	77.011	77.026	-0.015	
4	2	2	81.562	81.568	81.542	0.025	
M(20) = 46.44							
F(20) = 29.82 (0.0058, 115)							
Final Rp on the .prf = 0.1901640							

Figure S7. Unit-cell parameters, the corrected observed and calculated peak positions, and the respective difference obtained from the McMaille software for the case of the Sample 2.

FINAL VALUES : (STANDARD DEVIATIONS : 2nd LINE)							
ZERO	LAMBDA	A	B	C	ALPHA	BETA	GAMMA
-0.015	1.5406	5.5405	5.5367	7.8243	90.000	90.134	90.000
0.008	0.0000	0.0007	0.0008	0.0015	0.000	0.009	0.000
RECIPROCAL CELL :		0.18049	0.18061	0.12781	90.000	89.866	90.000
VOLUME (A**3) :		240.021					
H	K	L	TH(OBS)	TH-ZERO	TH(CALC)	DIFF.	
1	0	1	19.646	19.631	19.639	-0.008	
0	0	2	22.755	22.740	22.712	0.029	
1	1	1	25.448	25.433	25.429	0.004	
1	0	-2	27.835	27.820	27.864	-0.044	
1	1	2	32.352	32.337	32.346	-0.009	
0	0	3	34.397	34.382	34.357	0.025	
1	0	3	38.139	38.124	38.141	-0.017	
0	2	2	39.875	39.860	39.860	0.000	
1	1	-3	41.560	41.545	41.535	0.010	
1	1	3	41.648	41.633	41.601	0.032	
1	2	2	43.223	43.208	43.222	-0.014	
0	0	4	46.389	46.374	46.382	-0.008	
2	2	1	47.872	47.857	47.865	-0.008	
3	0	0	49.311	49.296	49.302	-0.006	
1	2	3	50.846	50.831	50.828	0.003	
1	3	0	52.214	52.199	52.198	0.001	
1	3	-1	53.581	53.566	53.581	-0.015	
1	3	-2	57.629	57.614	57.612	0.002	
3	0	-3	61.405	61.390	61.396	-0.006	
3	1	-3	63.942	63.927	63.893	0.034	
2	2	-4	67.594	67.579	67.581	-0.002	
4	0	1	68.822	68.807	68.804	0.003	
0	3	4	70.053	70.038	70.036	0.003	
3	1	-4	72.284	72.269	72.258	0.011	
4	2	0	76.924	76.909	76.902	0.007	
4	2	-1	78.027	78.012	78.010	0.002	
4	2	-2	81.380	81.365	81.368	-0.002	
2	4	-2	81.459	81.444	81.434	0.010	
3	1	-5	82.484	82.469	82.493	-0.024	
1	3	-5	82.603	82.588	82.591	-0.003	
3	1	5	82.725	82.710	82.714	-0.004	
4	0	-4	85.819	85.804	85.794	0.010	
0	4	4	85.964	85.949	85.960	-0.011	
4	2	-3	86.918	86.903	86.923	-0.020	
2	4	-3	87.033	87.018	87.003	0.015	
M(20) =	19.95						
F(20) =	16.73	(0.0137,	98)			
Final Rp on the .prf = 0.2305329							

Figure S8. Unit-cell parameters, the corrected observed and calculated peak positions, and the respective difference obtained from the McMaille software for the case of the Sample 3.

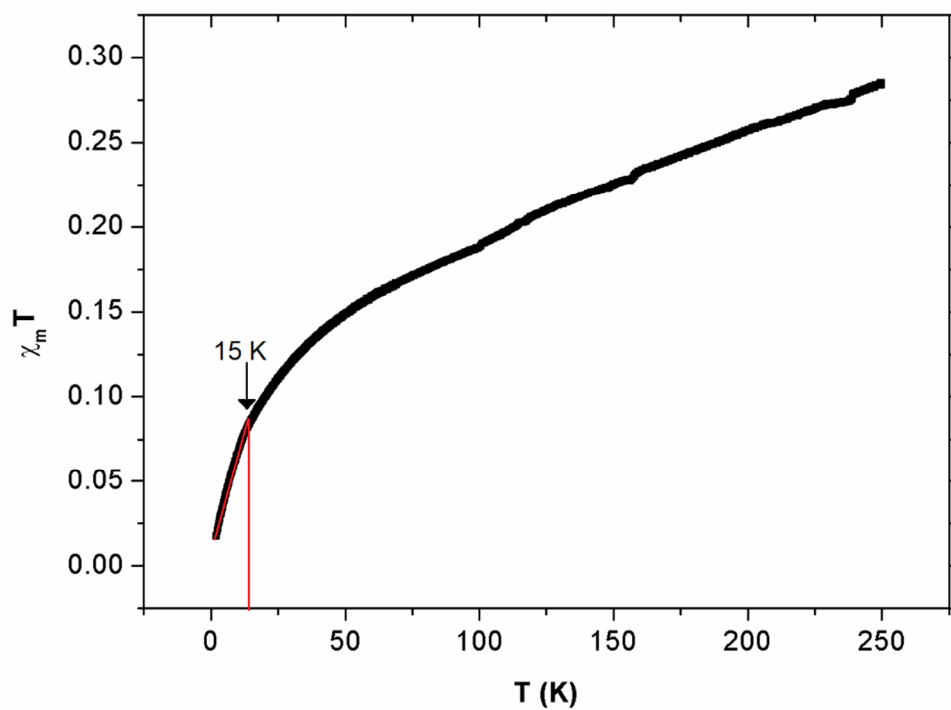


Figure S9. $\chi_m T$ vs. T curve showing the Néel temperature for the Sample 1.

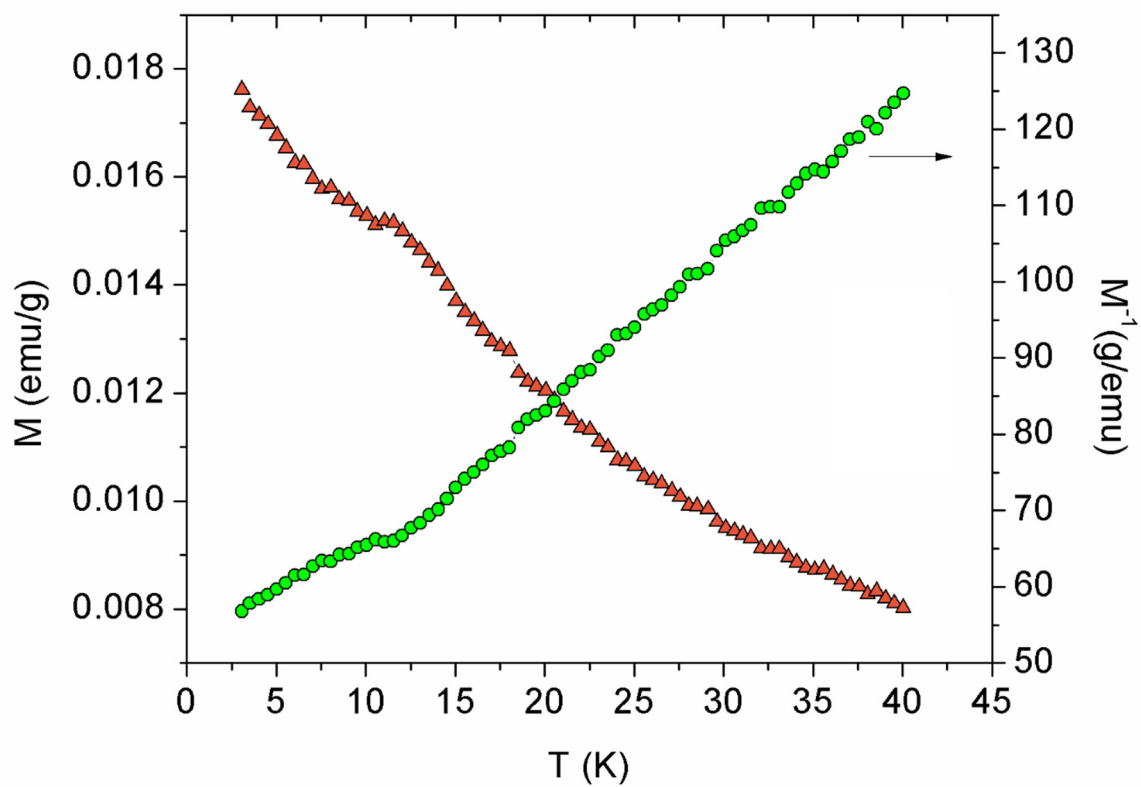


Figure S10. Variation of M along with M^{-1} vs. temperature for Sample 2 from 2 to 40 K.

References

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