Unveiling the irreversible structural evolution upon rehydration of Manganese-based Prussian White: an *in-situ* X-ray diffraction study

Supporting information

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Part I. Structural and Morphological Characterizations of MnPW-H

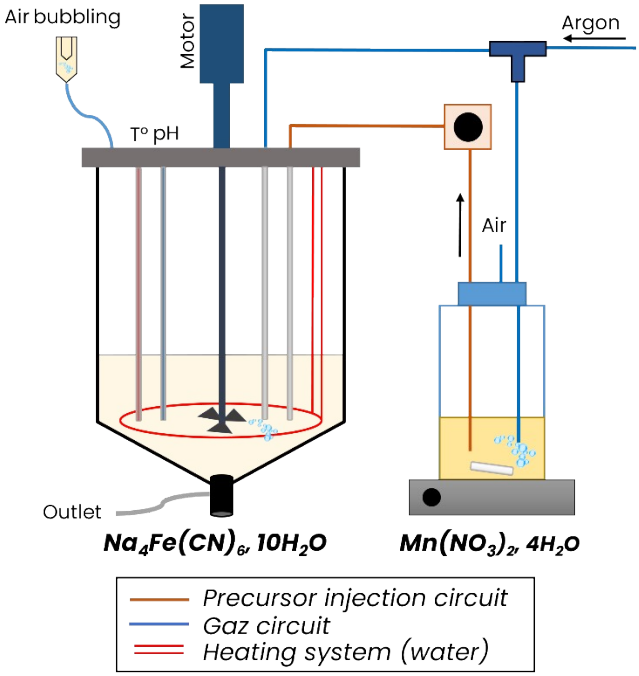

Figure S1: Scheme of the synthetis process

Table S1: Atomic coordinates for MnPW-H (R_{WP}=9.69%, R_P=10.0%, R_{exp}=0.03)

Space group $P2_1/n$ with a = 10.582(1), b = 7.555(1), c = 7.382(2) Å, α=γ=90° and β = 92.03(1) °, V=588(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.499	0.302	0.711	0.391	1.986
N	4e	0.284	0.508	0.488	0.391	1.986
N	4e	0.508	0.278	0.286	0.391	1.986
C	4e	0.502	0.206	0.815	0.646	1.986
C	4e	0.170	0.501	0.519	0.646	1.986
C	4e	0.506	0.183	0.177	0.646	1.986
O	4e	0.247	0.230	0.273	0.564	1.876
Na	4e	0.253	0.437	0.029	0.84	1.661

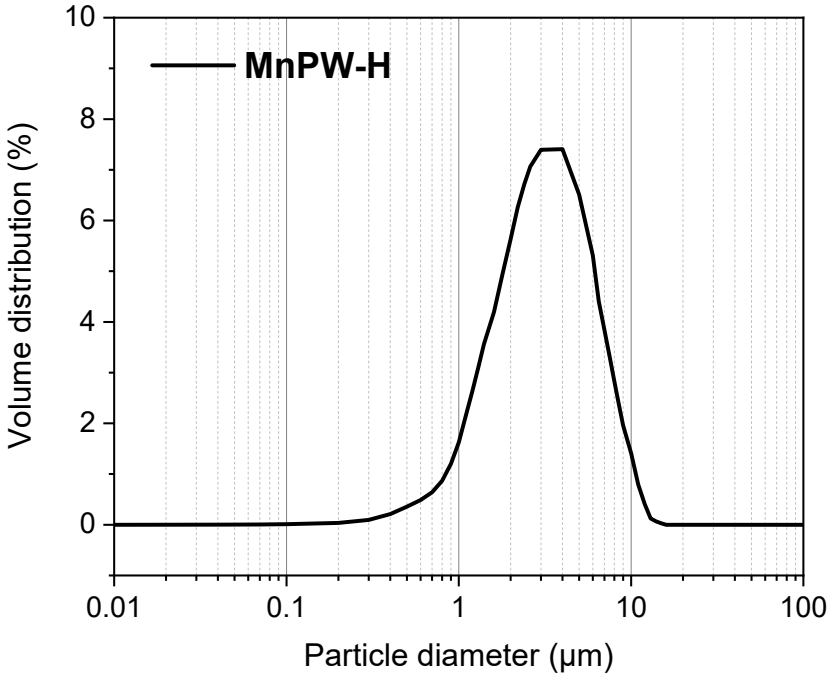

Figure S2: Comparison of the *a*, *b*, *c* and *beta* parameters of MnPW-H (purple) and MnPW-R (green) (a),

Table S2: Distribution particle value by volume of D_{10}, D_{50}, D_{90} and the mean particle size of MnPW-H

MnPW-H	D_{10}	D_{50}	D_{90}	Mean size
Mean value (μm)	1.1917	2.962	6.474	3.737

Table S3: The ICP analysis of MnPW-H

MnPW-H	Na	Fe	Mn
%wt	14.800	16.600	11.600
Ratio	0.877	1.000	1.668

Part II. Method and Tables presenting compositional and structural data

Rietveld refinement method

The Rietveld refinements were performed between 1.3° and 4.3° using FullProf Suite software. First, the hydrated (MnPW-H) and the dehydrated (MnPW-D) samples were refined with atomic positions, occupancies and lattice parameters. In order to have accurate values of atom occupancy, Manganese occupancy was fixed to 1, and Fe, Na, C and N occupancies were refined. The SXRD patterns of MnPW-H and MnPW-D were indexed in the $P2_1/n$ and the R-3 space group, respectively. Their occupancies were used as references. Indeed, the occupancies for monoclinic and rhombohedral phases were set to the reference values for all refined scans during the rehydration experiment of MnPW-D, considering the hypothesis that the rehydration process does not influence the Atom ratio. The influence of the atomic positions of all atoms was highlighted. Finally, all atomic positions were refined by fixing these previous parameters.

A constant background was used for all scans during the rehydration, and Biso parameter were not refined. It is impossible to find the accurate hydrogen position based on powder diffraction data, but the oxygen position and occupancy was refined.

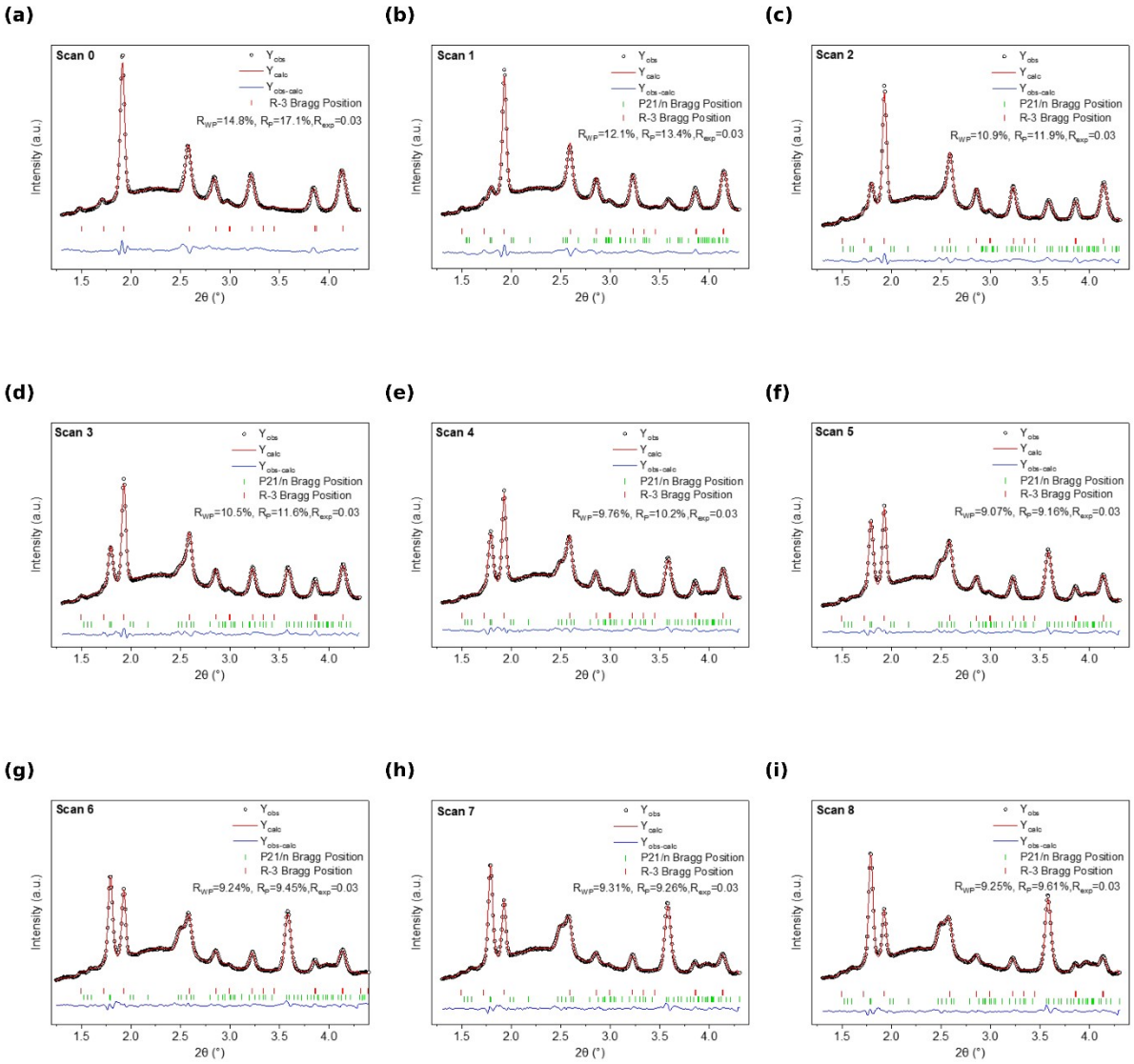

Figure S3. Rietveld refinement of the Scan 0 to Scan 8 (a-i). The black dots show observed data, the red lines correspond to the calculated patterns, and the blue lines are the difference between the observed and calculated patterns. The vertical green bars are the expected positions of Bragg reflections.

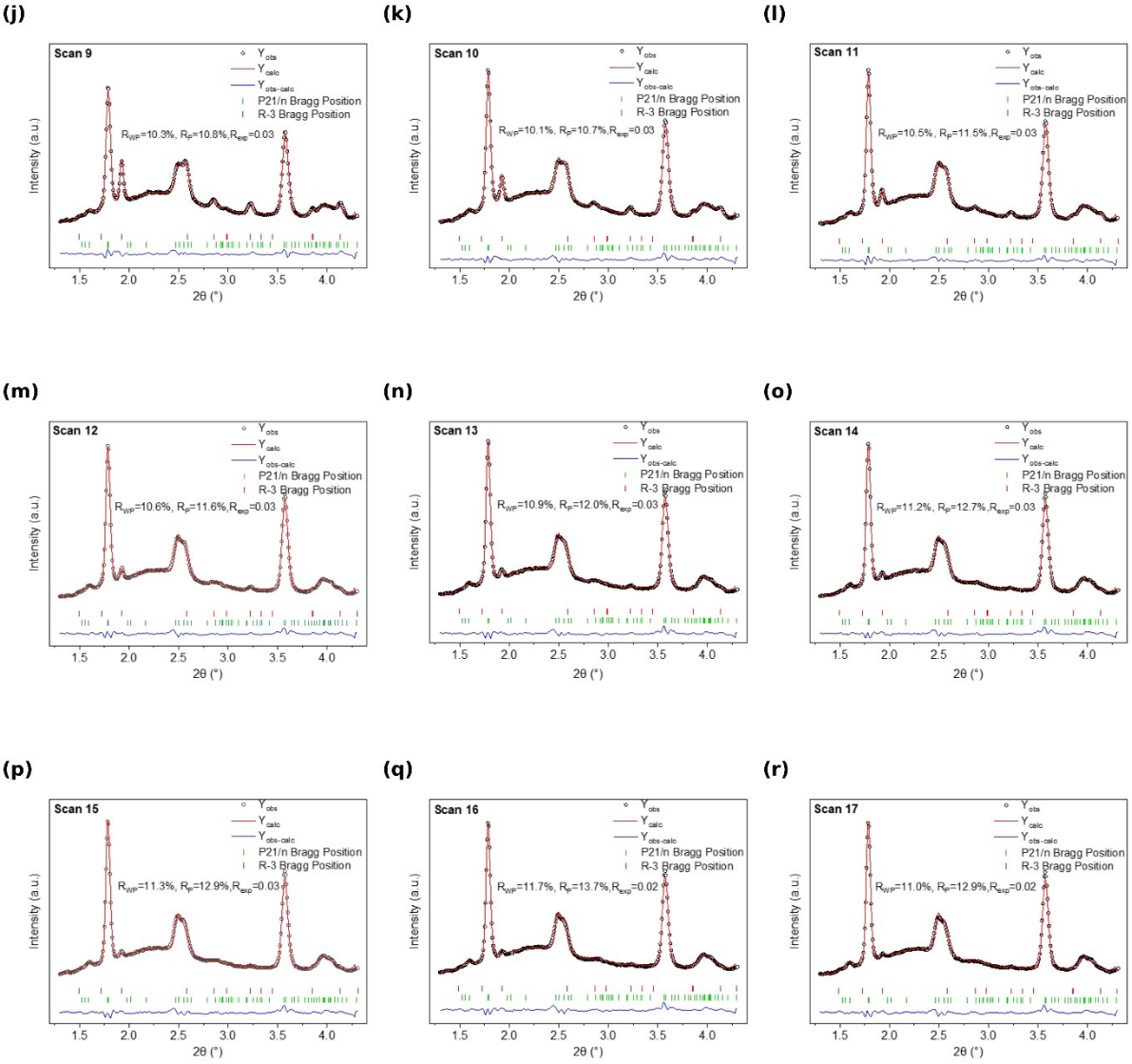

Figure S4. Rietveld refinement of the Scan 9 to Scan 17 (j-r). The black dots show observed data, the red lines correspond to the calculated patterns, and the blue lines are the difference between the observed and calculated patterns. The vertical green bars are the expected positions of Bragg reflections.

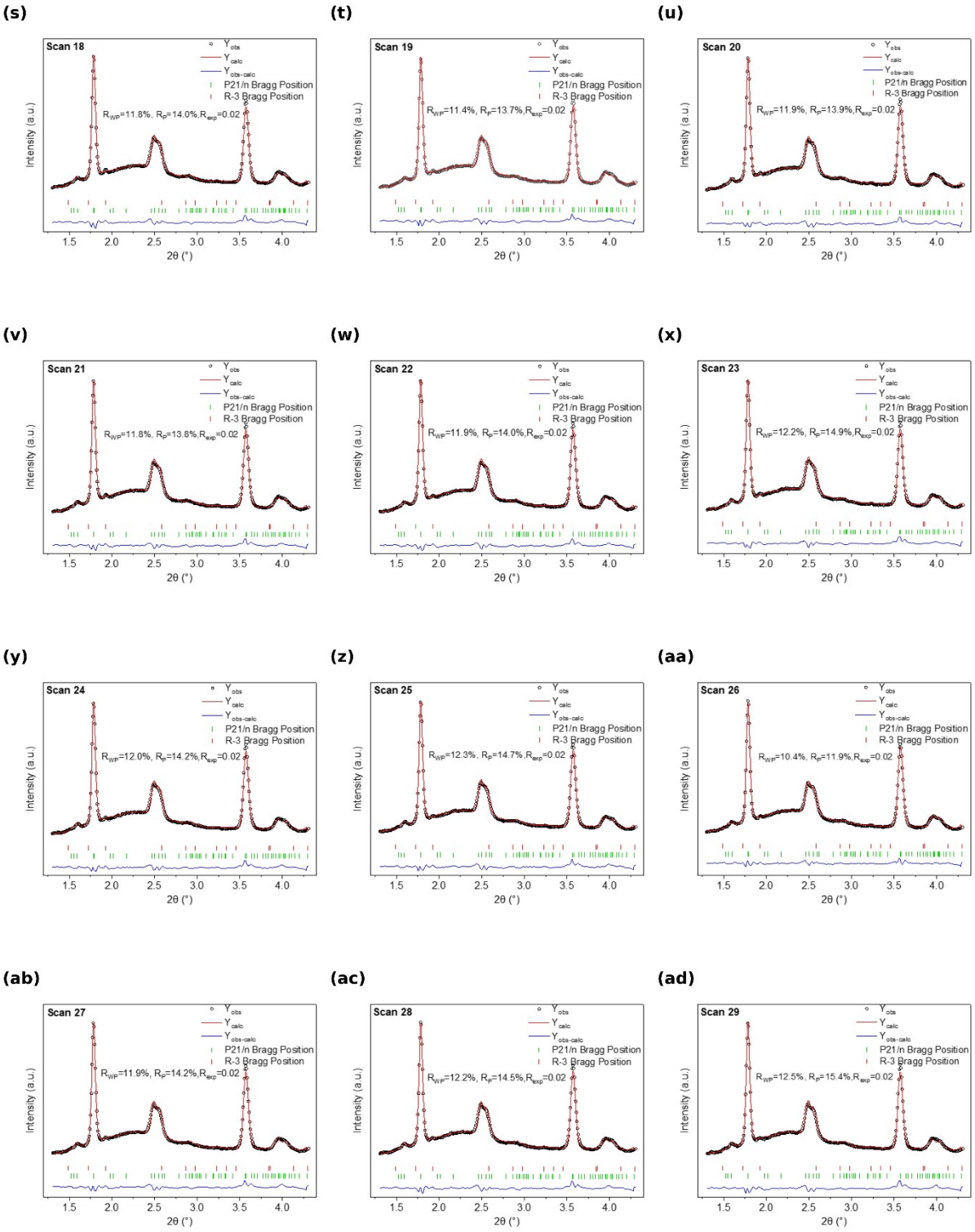

Figure S5. Rietveld refinement of the Scan 18 to Scan 29 (s-ad). The black dots show observed data, the red lines correspond to the calculated patterns, and the blue lines are the difference between the observed and calculated patterns. The vertical green bars are the expected positions of Bragg reflections.

Table S4: Correlation table between the scan number and the time in minute

Scan number	Time (minute)	Scan number	Time (minute)
0	0	**15**	26.1
1	2	**16**	28.5
2	3.2	**17**	30.9
3	4.4	**18**	33.3
4	5.6	**19**	35.7
5	6.8	**20**	38.1
6	8.0	**21**	40.5
7	9.2	**22**	42.9
8	10.4	**23**	45.3
9	11.6	**24**	47.7
10	14.1	**25**	50.1
11	16.5	**26**	52.5
12	18.9	**27**	54.9
13	21.3	**28**	57.3
14	23.7	**29**	59.8

Table S5: Atomic coordinates for Scan 0 (R_{WP}=14.8%, R_P=17.1%, R_{exp}=0.03)

Space group $R\bar{3}$ with $a = b$ = 6.630 (4), c = 18.92(1) Å, α= β =90° and γ = 120°, V= 720(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.200	0.834	1.557
N	18f	0.295	0.378	0.100	0.305	5.838
C	18f	0.249	0.243	0.058	0.305	5.838

Table S6: Atomic coordinates for Scan 1 (R_{WP}=12.1%, R_P=13.4%, R_{exp}=0.03)

Space group $R\bar{3}$ with $a = b$ = 6.620(2), c = 18.917(7) Å, α= β =90° and γ = 120°, V= 719(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.200	0.834	1.557
N	18f	0.306	0.399	0.100	0.305	5.838
C	18f	0.259	0.250	0.057	0.305	5.838

Space group $P2_1/n$ with a = 10.59(2), b = 7.50(5), c = 7.37(4) Å, α=γ=90° and β = 91.0(5) °, V=590(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965

N	4e	0.499	0.302	0.711	0.391	1.986
N	4e	0.284	0.508	0.488	0.391	1.986
N	4e	0.508	0.278	0.286	0.391	1.986
C	4e	0.502	0.206	0.815	0.646	1.986
C	4e	0.170	0.501	0.519	0.646	1.986
C	4e	0.506	0.183	0.177	0.646	1.986
O	4e	0.247	0.230	0.274	0.564	1.876
Na	4e	0.253	0.437	0.029	0.84	1.661

Table S7: Atomic coordinates for Scan 2 (R_{WP}=10.9%, R_P=11.9%, R_{exp}=0.03)

Space group $R\bar{3}$ with $a = b$ = 6.616(2), c = 18.927(6) Å, α= β =90° and γ = 120°, V= 717(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.200	0.834	1.557
N	18f	0.308	0.399	0.101	0.305	5.838
C	18f	0.260	0.250	0.056	0.305	5.838

Space group $P2_1/n$ with a = 10.583(9), b = 7.74(2), c = 7.15(1) Å, α=γ=90° and β = 88.8(1) °, V=587(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.454	0.312	0.678	0.391	1.986
N	4e	0.281	0.476	0.578	0.391	1.986
N	4e	0.512	0.253	0.343	0.391	1.986
C	4e	0.502	0.217	0.814	0.646	1.986
C	4e	0.187	0.501	0.476	0.646	1.986
C	4e	0.506	0.210	0.186	0.646	1.986
O	4e	0.262	0.228	0.267	0.564	1.858
Na	4e	0.253	0.501	0.029	0.84	1.661

Table S8: Atomic coordinates for Scan 3 (R_{WP}=10.5%, R_P=11.6%, R_{exp}=0.03)

Space group $R\bar{3}$ with $a = b$ = 6.618(2), c = 18.925(7) Å, α= β =90° and γ = 120°, V= 717(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.200	0.834	1.557
N	18f	0.306	0.393	0.103	0.305	5.838
C	18f	0.259	0.246	0.057	0.305	5.838

Space group $P2_1/n$ with a = 10.581(7), b = 7.64(1), c = 7.26(1) Å, α=γ=90° and β = 88.68(9) °, V=586(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ

Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.506	0.311	0.681	0.391	1.986
N	4e	0.286	0.535	0.557	0.391	1.986
N	4e	0.552	0.300	0.292	0.391	1.986
C	4e	0.485	0.211	0.790	0.646	1.986
C	4e	0.209	0.474	0.499	0.646	1.986
C	4e	0.492	0.186	0.203	0.646	1.986
O	4e	0.260	0.216	0.244	0.564	1.750
Na	4e	0.253	0.489	0.029	0.84	1.661

Table S9: Atomic coordinates for Scan 4 (R_{WP}=9.76%, R_P=10.2%, R_{exp}=0.03)

Space group $R\bar{3}$ with $a = b$ = 6.623(2), c = 18.929(7) Å, α= β =90° and γ = 120°, V= 718(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.199	0.834	1.557
N	18f	0.299	0.390	0.100	0.305	5.838
C	18f	0.259	0.245	0.057	0.305	5.838

Space group $P2_1/n$ with a = 10.588(5), b = 7.627(8), c = 7.269(8) Å, α=γ=90° and β = 91.48(6) °, V=586(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.509	0.339	0.710	0.391	1.986
N	4e	0.278	0.554	0.545	0.391	1.986
N	4e	0.542	0.308	0.282	0.391	1.986
C	4e	0.491	0.172	0.780	0.646	1.986
C	4e	0.210	0.493	0.503	0.646	1.986
C	4e	0.490	0.176	0.214	0.646	1.986
O	4e	0.248	0.206	0.251	0.564	1.738
Na	4e	0.253	0.489	0.004	0.84	1.661

Table S10: Atomic coordinates for Scan 5 (R_{WP}=9.07%, R_P=9.16%, R_{exp}=0.03)

Space group $R\bar{3}$ with $a = b$ = 6.622(2), c = 18.939(7) Å, α= β =90° and γ = 120°, V= 720(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.199	0.834	1.557
N	18f	0.300	0.391	0.101	0.305	5.838
C	18f	0.259	0.246	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.593(3), b = 7.629(6), c = 7.269(6) Å, α=γ=90° and β = 91.53(5) °, V=587(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.497	0.332	0.715	0.391	1.986
N	4e	0.273	0.541	0.536	0.391	1.986
N	4e	0.522	0.318	0.276	0.391	1.986
C	4e	0.495	0.170	0.791	0.646	1.986
C	4e	0.212	0.495	0.505	0.646	1.986
C	4e	0.497	0.175	0.216	0.646	1.986
O	4e	0.263	0.203	0.258	0.564	1.760
Na	4e	0.249	0.512	0.004	0.84	1.661

Table S11: Atomic coordinates for Scan 6 (R_{WP}=9.24%, R_P=9.45%, R_{exp}=0.03)

Space group $R\bar{3}$ with $a = b$ = 6.623(2), c = 18.949(9) Å, α= β =90° and γ = 120°, V= 720(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.199	0.834	1.557
N	18f	0.300	0.395	0.101	0.305	5.838
C	18f	0.259	0.246	0.059	0.305	5.838

Space group $P2_1/n$ with a = 10.594(3), b = 7.639(5), c = 7.266(5) Å, α=γ=90° and β = 91.51(4) °, V=588(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.503	0.328	0.715	0.391	1.986
N	4e	0.277	0.531	0.518	0.391	1.986
N	4e	0.516	0.321	0.278	0.391	1.986
C	4e	0.494	0.177	0.809	0.646	1.986
C	4e	0.212	0.511	0.509	0.646	1.986
C	4e	0.498	0.175	0.211	0.646	1.986
O	4e	0.257	0.204	0.253	0.564	1.771
Na	4e	0.254	0.530	-0.006	0.84	1.661

Table S12: Atomic coordinates for Scan 7 (R_{WP}=9.31%, R_P=9.26%, R_{exp}=0.03)

Space group $R\bar{3}$ with $a = b$ = 6.626(3), c = 18.958(9) Å, α= β =90° and γ = 120°, V= 719(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.202	0.834	1.557
N	18f	0.301	0.396	0.101	0.305	5.838
C	18f	0.260	0.246	0.059	0.305	5.838

Space group $P2_1/n$ with a = 10.601(3), b = 7.651(5), c = 7.262(5) Å, α=γ=90° and β = 91.54(4) °, V=589(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.502	0.318	0.712	0.391	1.986
N	4e	0.277	0.519	0.524	0.391	1.986
N	4e	0.508	0.317	0.282	0.391	1.986
C	4e	0.493	0.175	0.810	0.646	1.986
C	4e	0.212	0.506	0.508	0.646	1.986
C	4e	0.501	0.173	0.209	0.646	1.986
O	4e	0.257	0.204	0.254	0.564	1.795
Na	4e	0.257	0.512	-0.004	0.84	1.661

Table S13: Atomic coordinates for Scan 8 (R_{WP}=9.25%, R_P=9.61%, R_{exp}=0.03)

Space group $R\bar{3}$ with a = b = 6.625(3), c = 18.97(1) Å, α= β =90° and γ = 120°, V= 721(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.202	0.834	1.557
N	18f	0.298	0.390	0.104	0.305	5.838
C	18f	0.262	0.244	0.059	0.305	5.838

Space group $P2_1/n$ with a = 10.603(3), b = 7.652(5), c = 7.270(5) Å, α=γ=90° and β = 91.57(3) °, V=590(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.499	0.312	0.707	0.391	1.986
N	4e	0.277	0.513	0.526	0.391	1.986
N	4e	0.504	0.313	0.287	0.391	1.986
C	4e	0.494	0.179	0.817	0.646	1.986
C	4e	0.212	0.506	0.501	0.646	1.986
C	4e	0.507	0.178	0.201	0.646	1.986
O	4e	0.255	0.199	0.253	0.564	1.821
Na	4e	0.255	0.518	-0.005	0.84	1.661

Table S14: Atomic coordinates for Scan 9 (R_{WP}=10.3%, R_P=10.8%, R_{exp}=0.03)

Space group $R\bar{3}$ with a = b = 6.626(3), c = 18.98(1) Å, α= β =90° and γ = 120°, V= 721(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.206	0.834	1.557
N	18f	0.319	0.402	0.103	0.305	5.838
C	18f	0.242	0.231	0.055	0.305	5.838

Space group $P2_1/n$ with a = 10.610(3), b = 7.650(4), c = 7.278(4) Å, α=γ=90° and β = 91.51(4) °, V=590(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.490	0.317	0.734	0.391	1.986
N	4e	0.276	0.519	0.516	0.391	1.986
N	4e	0.498	0.298	0.276	0.391	1.986
C	4e	0.502	0.158	0.775	0.646	1.986
C	4e	0.202	0.514	0.500	0.646	1.986
C	4e	0.511	0.191	0.200	0.646	1.986
O	4e	0.241	0.195	0.243	0.564	1.707
Na	4e	0.248	0.524	-6e-05	0.84	1.661

Table S15: Atomic coordinates for Scan 10 (R_{WP}=10.1%, R_P=10.7%, R_{exp}=0.03)

Space group $R\bar{3}$ with a = b = 6.626(5), c = 18.97(2) Å, α= β =90° and γ = 120°, V= 721(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.211	0.834	1.557
N	18f	0.303	0.391	0.110	0.305	5.838
C	18f	0.260	0.215	0.056	0.305	5.838

Space group $P2_1/n$ with a = 10.613(3), b = 7.660(4), c = 7.280(4) Å, α=γ=90° and β = 91.57(3) °, V=591(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.493	0.318	0.719	0.391	1.986
N	4e	0.276	0.513	0.513	0.391	1.986
N	4e	0.49	0.299	0.275	0.391	1.986
C	4e	0.515	0.170	0.801	0.646	1.986
C	4e	0.201	0.506	0.506	0.646	1.986
C	4e	0.520	0.186	0.205	0.646	1.986
O	4e	0.233	0.202	0.246	0.564	1.747
Na	4e	0.253	0.527	-0.004	0.84	1.661

Table S16: Atomic coordinates for Scan 11 (R_{WP}=10.5%, R_P=11.5%, R_{exp}=0.03)

Space group $R\bar{3}$ with a = b = 6.617(7), c = 19.01(3) Å, α= β =90° and γ = 120°, V= 721(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.212	0.834	1.557
N	18f	0.318	0.396	0.111	0.305	5.838
C	18f	0.274	0.216	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.612(3), b = 7.656(4), c = 7.286(4) Å, α=γ=90° and β = 91.60(3) °, V=592(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.493	0.318	0.719	0.391	1.986
N	4e	0.272	0.513	0.516	0.391	1.986
N	4e	0.49	0.299	0.275	0.391	1.986
C	4e	0.515	0.170	0.801	0.646	1.986
C	4e	0.210	0.512	0.506	0.646	1.986
C	4e	0.520	0.186	0.205	0.646	1.986
O	4e	0.252	0.198	0.247	0.564	1.706
Na	4e	0.250	0.529	-0.004	0.84	1.661

Table S17: Atomic coordinates for Scan 12 (R_{WP}=10.6%, R_P=11.6%, R_{exp}=0.03)

Space group $R\bar{3}$ with a = b = 6.62(1), c = 19.02(5) Å, α= β =90° and γ = 120°, V= 720(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.214	0.834	1.557
N	18f	0.327	0.416	0.114	0.305	5.838
C	18f	0.276	0.207	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.608(4), b = 7.662(4), c = 7.297(5) Å, α=γ=90° and β = 91.66(3) °, V=592(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.493	0.315	0.717	0.391	1.986
N	4e	0.280	0.512	0.513	0.391	1.986
N	4e	0.484	0.300	0.280	0.391	1.986
C	4e	0.514	0.167	0.801	0.646	1.986
C	4e	0.203	0.520	0.510	0.646	1.986
C	4e	0.522	0.187	0.200	0.646	1.986
O	4e	0.231	0.203	0.250	0.564	1.871
Na	4e	0.254	0.529	-0.002	0.84	1.661

Table S18: Atomic coordinates for Scan 13 (R_{WP}=10.9%, R_P=12.0%, R_{exp}=0.03)

Space group $R\bar{3}$ with a = b = 6.623(7), c = 18.99(7) Å, α= β =90° and γ = 120°, V= 721(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.214	0.834	1.557
N	18f	0.327	0.416	0.114	0.305	5.838
C	18f	0.276	0.207	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.608(4), b = 7.664(4), c = 7.294(5) Å, α=γ=90° and β = 91.66(3) °, V=592(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.495	0.315	0.712	0.391	1.986
N	4e	0.280	0.511	0.513	0.391	1.986
N	4e	0.481	0.302	0.282	0.391	1.986
C	4e	0.515	0.169	0.809	0.646	1.986
C	4e	0.203	0.520	0.498	0.646	1.986
C	4e	0.523	0.186	0.200	0.646	1.986
O	4e	0.250	0.207	0.249	0.564	1.834
Na	4e	0.254	0.534	-0.007	0.84	1.661

Table S19: Atomic coordinates for Scan 14 (R_{WP}=11.2%, R_P=12.7%, R_{exp}=0.03)

Space group $R\bar{3}$ with a = b = 6.620(2), c = 19.0(1) Å, α= β =90° and γ = 120°, V= 720(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.214	0.834	1.557
N	18f	0.327	0.416	0.114	0.305	5.838
C	18f	0.276	0.207	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.605(4), b = 7.668(5), c = 7.297(5) Å, α=γ=90° and β = 91.68(3) °, V=593(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.493	0.314	0.714	0.391	1.986
N	4e	0.280	0.518	0.515	0.391	1.986
N	4e	0.479	0.307	0.288	0.391	1.986
C	4e	0.511	0.168	0.809	0.646	1.986
C	4e	0.203	0.517	0.496	0.646	1.986
C	4e	0.522	0.184	0.195	0.646	1.986
O	4e	0.261	0.215	0.252	0.564	1.837
Na	4e	0.254	0.534	-0.005	0.84	1.661

Table S20: Atomic coordinates for Scan 15 (R_{WP}=11.3%, R_P=12.9%, R_{exp}=0.03)

Space group $R\bar{3}$ with a = b = 6.62(3), c = 19.0(1) Å, α= β =90° and γ = 120°, V= 721(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.214	0.834	1.557
N	18f	0.327	0.416	0.114	0.305	5.838
C	18f	0.276	0.207	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.608(4), b = 7.662(5), c = 7.300(5) Å, α=γ=90° and β = 91.70(3) °, V=593(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.492	0.312	0.711	0.391	1.986
N	4e	0.280	0.518	0.518	0.391	1.986
N	4e	0.483	0.304	0.290	0.391	1.986
C	4e	0.512	0.170	0.799	0.646	1.986
C	4e	0.203	0.517	0.489	0.646	1.986
C	4e	0.526	0.182	0.194	0.646	1.986
O	4e	0.256	0.201	0.232	0.564	1.869
Na	4e	0.255	0.530	-0.003	0.84	1.661

Table S21: Atomic coordinates for Scan 16 (R_{WP}=11.7%, R_P=13.7%, R_{exp}=0.02)

Space group $R\bar{3}$ with a = b = 6.60(4), c = 19.0(2) Å, α= β =90° and γ = 120°, V= 721(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.214	0.834	1.557
N	18f	0.327	0.416	0.114	0.305	5.838
C	18f	0.276	0.207	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.610(4), b = 7.663(5), c = 7.296(5) Å, α=γ=90° and β = 91.71(3) °, V=593(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.491	0.316	0.714	0.391	1.986
N	4e	0.280	0.513	0.514	0.391	1.986
N	4e	0.483	0.303	0.304	0.391	1.986
C	4e	0.511	0.173	0.807	0.646	1.986
C	4e	0.203	0.518	0.495	0.646	1.986
C	4e	0.537	0.203	0.179	0.646	1.986
O	4e	0.251	0.204	0.254	0.564	1.972
Na	4e	0.256	0.527	-0.006	0.84	1.661

Table S22: Atomic coordinates for Scan 17 (R_{WP}=11.0%, R_P=12.9%, R_{exp}=0.02)

Space group $R\bar{3}$ with a = b = 6.60(4), c = 19.0(2) Å, α= β =90° and γ = 120°, V= 720(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.214	0.834	1.557
N	18f	0.327	0.416	0.114	0.305	5.838
C	18f	0.276	0.207	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.602(4), b = 7.669(5), c = 7.298(6) Å, α=γ=90° and β = 91.70(3) °, V=592(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.497	0.324	0.720	0.391	1.986
N	4e	0.280	0.512	0.516	0.391	1.986
N	4e	0.480	0.305	0.299	0.391	1.986
C	4e	0.511	0.174	0.814	0.646	1.986
C	4e	0.203	0.511	0.496	0.646	1.986
C	4e	0.527	0.187	0.188	0.646	1.986
O	4e	0.245	0.207	0.262	0.564	1.921
Na	4e	0.258	0.532	-0.007	0.84	1.661

Table S23: Atomic coordinates for Scan 18 (R_{WP}=11.8%, R_P=14.0%, R_{exp}=0.02)

Space group $R\bar{3}$ with a = b = 6.60(4), c = 19.0(2) Å, α= β =90° and γ = 120°, V= 720(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.214	0.834	1.557
N	18f	0.327	0.416	0.114	0.305	5.838
C	18f	0.276	0.207	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.606(4), b = 7.667(5), c = 7.297(5) Å, α=γ=90° and β = 91.71(3) °, V=593(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.492	0.317	0.715	0.391	1.986
N	4e	0.280	0.514	0.520	0.391	1.986
N	4e	0.479	0.308	0.296	0.391	1.986
C	4e	0.514	0.169	0.815	0.646	1.986
C	4e	0.203	0.522	0.492	0.646	1.986
C	4e	0.525	0.181	0.192	0.646	1.986
O	4e	0.226	0.217	0.228	0.564	1.965
Na	4e	0.256	0.532	-0.009	0.84	1.661

Table S24: Atomic coordinates for Scan 19 (R_{WP}=11.4%, R_P=13.7%, R_{exp}=0.02)

Space group $R\bar{3}$ with a = b = 6.60(4), c = 19.0(2) Å, α= β =90° and γ = 120°, V= 720(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.214	0.834	1.557
N	18f	0.327	0.416	0.114	0.305	5.838
C	18f	0.276	0.207	0.0586	0.305	5.838

Space group $P2_1/n$ with a = 10.605(4), b = 7.670(5), c = 7.299(5) Å, α=γ=90° and β = 91.69(3) °, V=593(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.492	0.310	0.710	0.391	1.986
N	4e	0.280	0.514	0.515	0.391	1.986
N	4e	0.481	0.309	0.300	0.391	1.986
C	4e	0.512	0.172	0.817	0.646	1.986
C	4e	0.203	0.513	0.499	0.646	1.986
C	4e	0.522	0.180	0.190	0.646	1.986
O	4e	0.250	0.210	0.262	0.564	1.936
Na	4e	0.256	0.531	-0.005	0.84	1.661

Table S25: Atomic coordinates for Scan 20 (R_{WP}=11.9%, R_P=13.9%, R_{exp}=0.02)

Space group $R\bar{3}$ with a = b = 6.60(4), c = 19.0(2) Å, α= β =90° and γ = 120°, V= 720(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.214	0.834	1.557
N	18f	0.327	0.416	0.114	0.305	5.838
C	18f	0.276	0.207	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.604(4), b = 7.668(5), c = 7.299(5) Å, α=γ=90° and β = 91.72(3) °, V=593(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.490	0.309	0.715	0.391	1.986
N	4e	0.280	0.516	0.518	0.391	1.986
N	4e	0.482	0.321	0.304	0.391	1.986
C	4e	0.513	0.178	0.826	0.646	1.986
C	4e	0.203	0.521	0.493	0.646	1.986
C	4e	0.522	0.209	0.190	0.646	1.986
O	4e	0.233	0.206	0.269	0.564	1.933
Na	4e	0.258	0.528	-0.007	0.84	1.661

Table S26: Atomic coordinates for Scan 21 (R_{WP}=11.8%, R_P=13.8%, R_{exp}=0.02)

Space group $R\bar{3}$ with a = b = 6.60(4), c = 19.0(2) Å, α= β =90° and γ = 120°, V= 720(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.214	0.834	1.557
N	18f	0.327	0.416	0.114	0.305	5.838
C	18f	0.276	0.207	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.601(4), b = 7.673(5), c = 7.300(6) Å, α=γ=90° and β = 91.71(3) °, V=593(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.495	0.316	0.717	0.391	1.986
N	4e	0.280	0.513	0.517	0.391	1.986
N	4e	0.477	0.317	0.305	0.391	1.986
C	4e	0.510	0.171	0.818	0.646	1.986
C	4e	0.203	0.508	0.498	0.646	1.986
C	4e	0.520	0.189	0.201	0.646	1.986
O	4e	0.239	0.205	0.253	0.564	1.955
Na	4e	0.258	0.529	-0.005	0.84	1.661

Table S27: Atomic coordinates for Scan 22 (R_{WP}=11.9%, R_P=14.0%, R_{exp}=0.02)

Space group $R\bar{3}$ with $a = b$ = 6.60(4), c = 19.0(2) Å, α= β =90° and γ = 120°, V= 720(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.214	0.834	1.557
N	18f	0.327	0.416	0.114	0.305	5.838
C	18f	0.276	0.207	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.601(4), b = 7.673(5), c = 7.304(6) Å, α=γ=90° and β = 91.71(3) °, V=593(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.492	0.316	0.717	0.391	1.986
N	4e	0.280	0.514	0.519	0.391	1.986
N	4e	0.478	0.317	0.305	0.391	1.986
C	4e	0.512	0.173	0.821	0.646	1.986
C	4e	0.203	0.509	0.496	0.646	1.986
C	4e	0.521	0.182	0.198	0.646	1.986
O	4e	0.238	0.206	0.253	0.564	1.972
Na	4e	0.255	0.533	-0.007	0.84	1.661

Table S28: Atomic coordinates for Scan 23 (R_{WP}=12.2%, R_P=14.9% ,R_{exp}=0.02)

Space group $R\bar{3}$ with $a = b$ = 6.60(4), c = 19.0(2) Å, α= β =90° and γ = 120°, V= 720(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.214	0.834	1.557
N	18f	0.327	0.416	0.114	0.305	5.838

C	18f	0.276	0.207	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.602(5), b = 7.674(6), c = 7.304(6) Å, α=γ=90° and β = 91.71(3) °, V=593(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.490	0.313	0.718	0.391	1.986
N	4e	0.280	0.514	0.517	0.391	1.986
N	4e	0.480	0.315	0.302	0.391	1.986
C	4e	0.512	0.172	0.821	0.646	1.986
C	4e	0.203	0.520	0.496	0.646	1.986
C	4e	0.523	0.179	0.198	0.646	1.986
O	4e	0.222	0.211	0.260	0.564	1.972
Na	4e	0.256	0.532	-0.006	0.84	1.661

Table S29: Atomic coordinates for Scan 24 (R_{WP}=12.0%, R_P=14.2%, R_{exp}=0.02)

Space group $R\bar{3}$ with a = b = 6.60(4), c = 19.0(2) Å, α= β =90° and γ = 120°, V= 720(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.214	0.834	1.557
N	18f	0.327	0.416	0.114	0.305	5.838
C	18f	0.276	0.207	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.602(4), b = 7.665(5), c = 7.302(6) Å, α=γ=90° and β = 91.72(3) °, V=593(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.490	0.305	0.718	0.391	1.986
N	4e	0.280	0.515	0.517	0.391	1.986
N	4e	0.488	0.322	0.305	0.391	1.986
C	4e	0.513	0.179	0.824	0.646	1.986
C	4e	0.203	0.519	0.492	0.646	1.986
C	4e	0.524	0.180	0.199	0.646	1.986
O	4e	0.238	0.203	0.252	0.564	2.000
Na	4e	0.256	0.529	-0.008	0.84	1.661

Table S30: Atomic coordinates for Scan 25 (R_{WP}=12.3%, R_P=14.7%, R_{exp}=0.02)

Space group $R\bar{3}$ with a = b = 6.60(4), c = 19.0(2) Å, α= β =90° and γ = 120°, V= 720(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.214	0.834	1.557
N	18f	0.327	0.416	0.114	0.305	5.838

C	18f	0.276	0.207	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.604(4), b = 7.669(5), c = 7.302(6) Å, α=γ=90° and β = 91.73(3) °, V=593(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.495	0.309	0.720	0.391	1.986
N	4e	0.280	0.515	0.518	0.391	1.986
N	4e	0.485	0.317	0.305	0.391	1.986
C	4e	0.514	0.177	0.824	0.646	1.986
C	4e	0.203	0.511	0.495	0.646	1.986
C	4e	0.525	0.177	0.194	0.646	1.986
O	4e	0.247	0.207	0.255	0.564	1.969
Na	4e	0.255	0.533	-0.006	0.84	1.661

Table S31: Atomic coordinates for Scan 26 (R_{WP}=10.4%, R_P=11.9%, R_{exp}=0.02)

Space group $R\bar{3}$ with a = b = 6.60(4), c = 19.0(2) Å, α= β =90° and γ = 120°, V= 720(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.214	0.834	1.557
N	18f	0.327	0.416	0.114	0.305	5.838
C	18f	0.276	0.207	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.601(3), b = 7.666(5), c = 7.295(5) Å, α=γ=90° and β = 91.70(3) °, V=593(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.494	0.306	0.719	0.391	1.986
N	4e	0.257	0.522	0.524	0.391	1.986
N	4e	0.483	0.314	0.303	0.391	1.986
C	4e	0.516	0.174	0.822	0.646	1.986
C	4e	0.238	0.515	0.487	0.646	1.986
C	4e	0.524	0.175	0.191	0.646	1.986
O	4e	0.240	0.217	0.258	0.564	1.778
Na	4e	0.255	0.525	0.001	0.84	1.661

Table S32: Atomic coordinates for Scan 27 (R_{WP}=11.9%, R_P=14.2%, R_{exp}=0.02)

Space group $R\bar{3}$ with a = b = 6.60(4), c = 19.0(2) Å, α= β =90° and γ = 120°, V= 720(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.214	0.834	1.557
N	18f	0.327	0.416	0.114	0.305	5.838

C	18f	0.276	0.207	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.604(4), b = 7.670(5), c = 7.304(6) Å, α=γ=90° and β = 91.74(3) °, V=594(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.492	0.306	0.718	0.391	1.986
N	4e	0.280	0.513	0.515	0.391	1.986
N	4e	0.483	0.312	0.304	0.391	1.986
C	4e	0.517	0.175	0.819	0.646	1.986
C	4e	0.203	0.512	0.495	0.646	1.986
C	4e	0.522	0.173	0.190	0.646	1.986
O	4e	0.236	0.213	0.269	0.564	1.978
Na	4e	0.254	0.532	-0.007	0.84	1.661

Table S33: Atomic coordinates for Scan 28 (R_{WP}=12.2%, R_P=14.5%, R_{exp}=0.02)

Space group $R\bar{3}$ with a = b = 6.60(4), c = 19.0(2) Å, α= β =90° and γ = 120°, V= 720(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.214	0.834	1.557
N	18f	0.327	0.416	0.114	0.305	5.838
C	18f	0.276	0.207	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.603(5), b = 7.670(6), c = 7.304(6) Å, α=γ=90° and β = 91.73(3) °, V=593(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.490	0.304	0.718	0.391	1.986
N	4e	0.280	0.515	0.524	0.391	1.986
N	4e	0.483	0.312	0.301	0.391	1.986
C	4e	0.516	0.175	0.819	0.646	1.986
C	4e	0.203	0.512	0.497	0.646	1.986
C	4e	0.524	0.172	0.189	0.646	1.986
O	4e	0.236	0.208	0.250	0.564	1.996
Na	4e	0.255	0.532	-0.006	0.84	1.661

Table S34: Atomic coordinates for Scan 29 (R_{WP}=12.5%, R_P=15.4%, R_{exp}=0.02)

Space group $R\bar{3}$ with a = b = 6.60(4), c = 19.0(2) Å, α= β =90° and γ = 120°, V= 720(1) Å^3

Atom	Wyck	X	Y	Z	Biso	Occ
Fe	3a	0.0	0.0	0.0	0.684	0.967
Mn	3b	0.333	0.667	0.167	0.688	1.0
Na	6c	0.0	0.0	0.214	0.834	1.557
N	18f	0.327	0.416	0.114	0.305	5.838

C	18f	0.276	0.207	0.058	0.305	5.838

Space group $P2_1/n$ with a = 10.601(5), b = 7.669(6), c = 7.307(6) Å, α=γ=90° and β = 91.76(3) °, V=593(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.492	0.309	0.719	0.391	1.986
N	4e	0.280	0.522	0.526	0.391	1.986
N	4e	0.481	0.312	0.297	0.391	1.986
C	4e	0.514	0.171	0.817	0.646	1.986
C	4e	0.203	0.514	0.486	0.646	1.986
C	4e	0.525	0.171	0.189	0.646	1.986
O	4e	0.227	0.215	0.269	0.564	1.912
Na	4e	0.253	0.531	-0.007	0.84	1.661

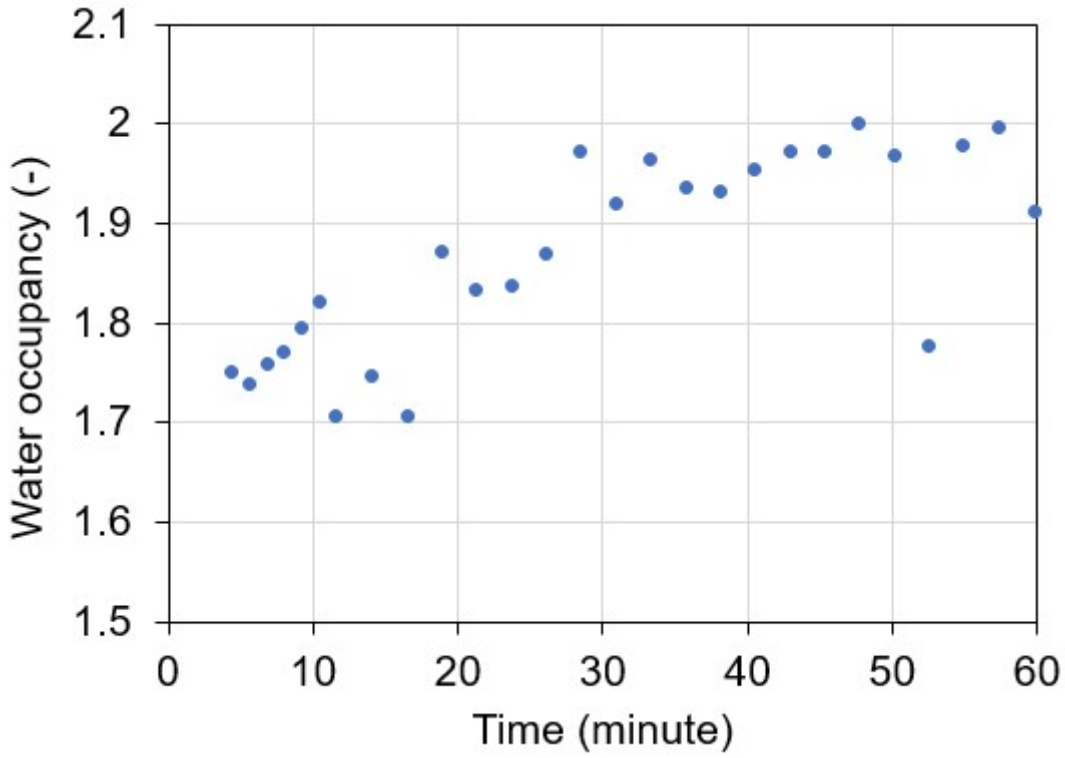

Figure S6: Evolution of the water occupancy in the monoclinic phase during the rehydration *in-situ* experiment

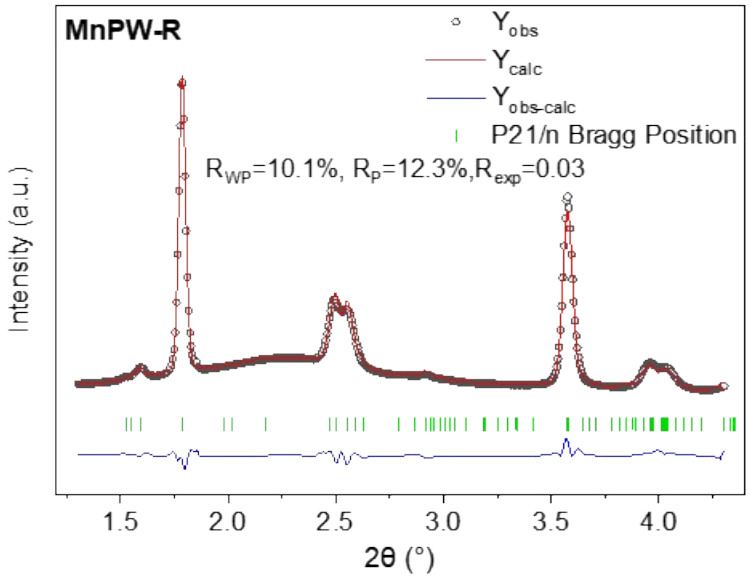

Figure S7: Rietveld refinement of MnPW-R exposed 24 hours at ambient air

Table S35: Atomic coordinates for MnPW-R (R_{WP}=10.1%, R_P=12.3%, R_{exp}=0.03)

Space group $P2_1/n$ with a = 10.584(2), b = 7.643(3), c = 7.304(3) Å, α=γ=90° and β = 91.60(2) °, V=590(1) Å^3

Atom	Wyck.	X	Y	Z	Biso	Occ
Mn	2a	0.5	0.5	0.5	0.846	1.0
Fe	2d	0.5	0.0	1.0	0.988	0.965
N	4e	0.497	0.304	0.722	0.391	1.986
N	4e	0.277	0.528	0.521	0.391	1.986
N	4e	0.487	0.287	0.301	0.391	1.986
C	4e	0.514	0.147	0.831	0.646	1.986
C	4e	0.210	0.517	0.499	0.646	1.986
C	4e	0.520	0.188	0.192	0.646	1.986
O	4e	0.246	0.206	0.256	0.564	1.838
Na	4e	0.251	0.509	0.001	0.84	1.661

Part III. Comparison of Structural, Morphological and Electochemical Characterization of MnPW-H, MnPW-D and MnPW-R

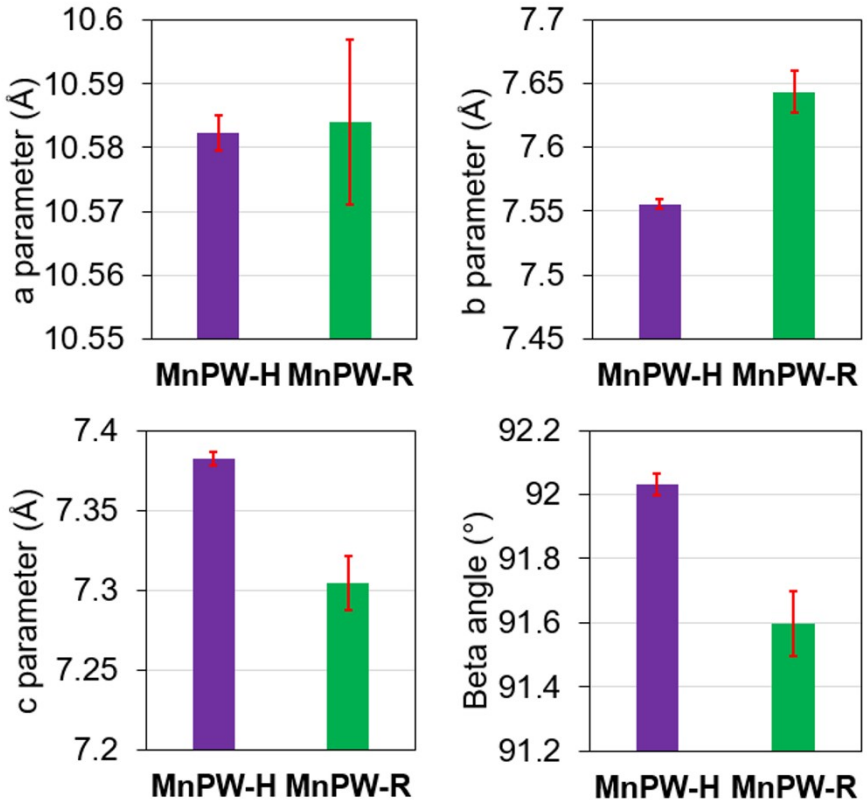

Figure S8: Comparison of the *a*, *b*, *c* and *beta* parameters of MnPW-H (purple) and MnPW-R (green) (a)

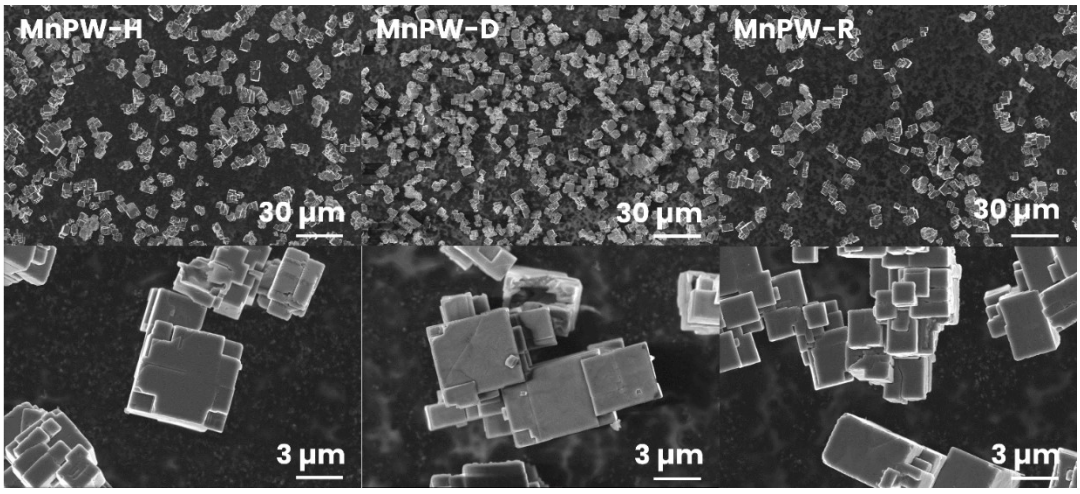

Figure S9: SEM observations of MnPW-H; MnPW-D and MnPW-R

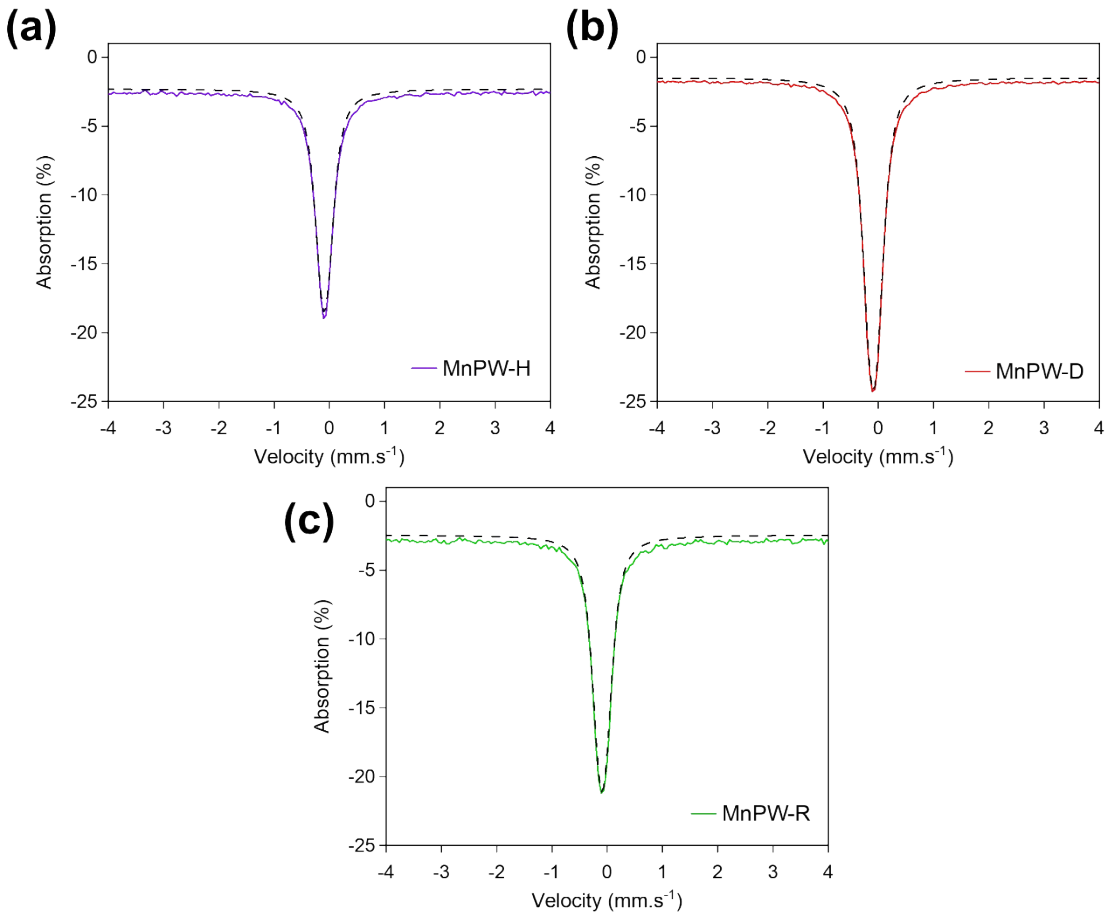

Figure S10: Mössbauer spectra of samples MnPW-H (a), MnPW-D (b), and MnPW-R (c)

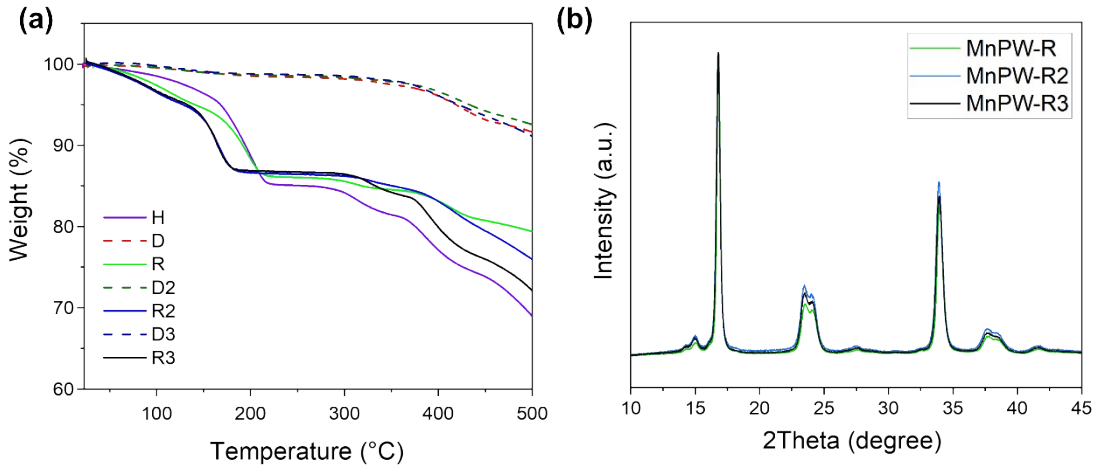

Figure S11: TGA measurements (a) of MnPW-H, D, R1, D2, R2, D3, and R3 under Argon at 10°C.min^{-1} and laboratory XRD measurements of MnPW-R, MnPW-R2 and MnPW-R3 (b)

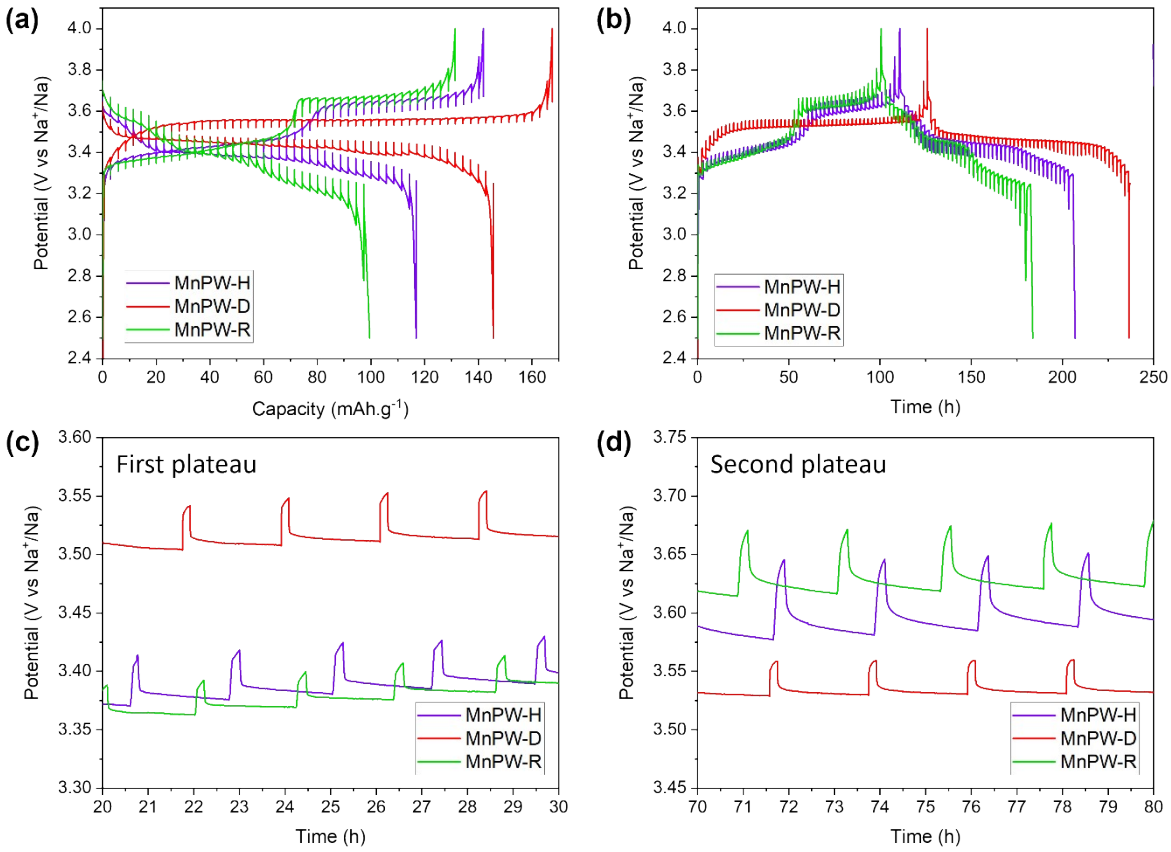

Figure S12: GITT curves of MnPW-H, D, R at 20 mA.g^{-1} with a relaxation time of 120 minutes : GITT curves depending on the capacity (a), and the time (b), and zoom on alternating phase of current pulse and relaxation on the first plateau (c) and the second plateau (d) during the charge

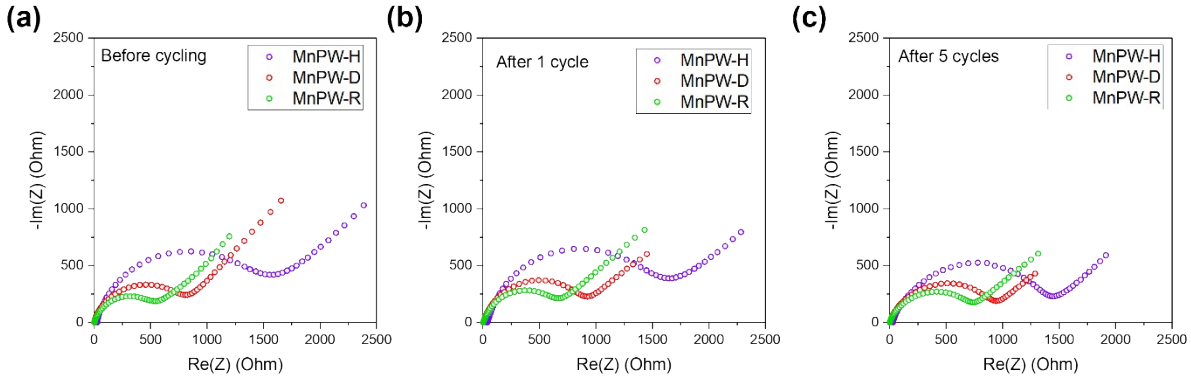

Figure S13: EIS measurements of MnPW-H, D, R before cycling (a), after one cycle (b), and after 5 cycles (c) from 1000 MHz to 10000 mHz, with an applied amplitude of 20 mV.