molecules

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Supplementary Materials

Effect of transitional metals (Mn and Ni) substitution in$LiCoPO_4$olivines

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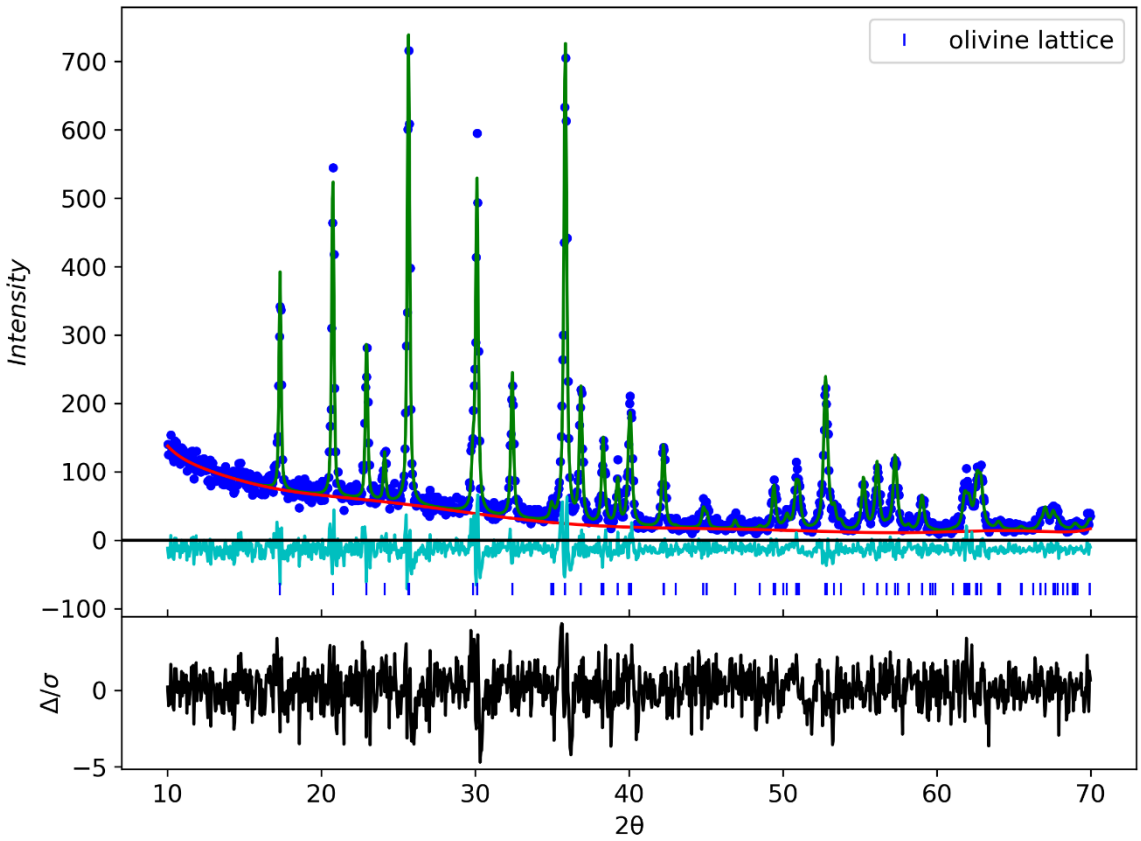

Figure S1. Rietveld refinement plot obtained for the LCmP samples.

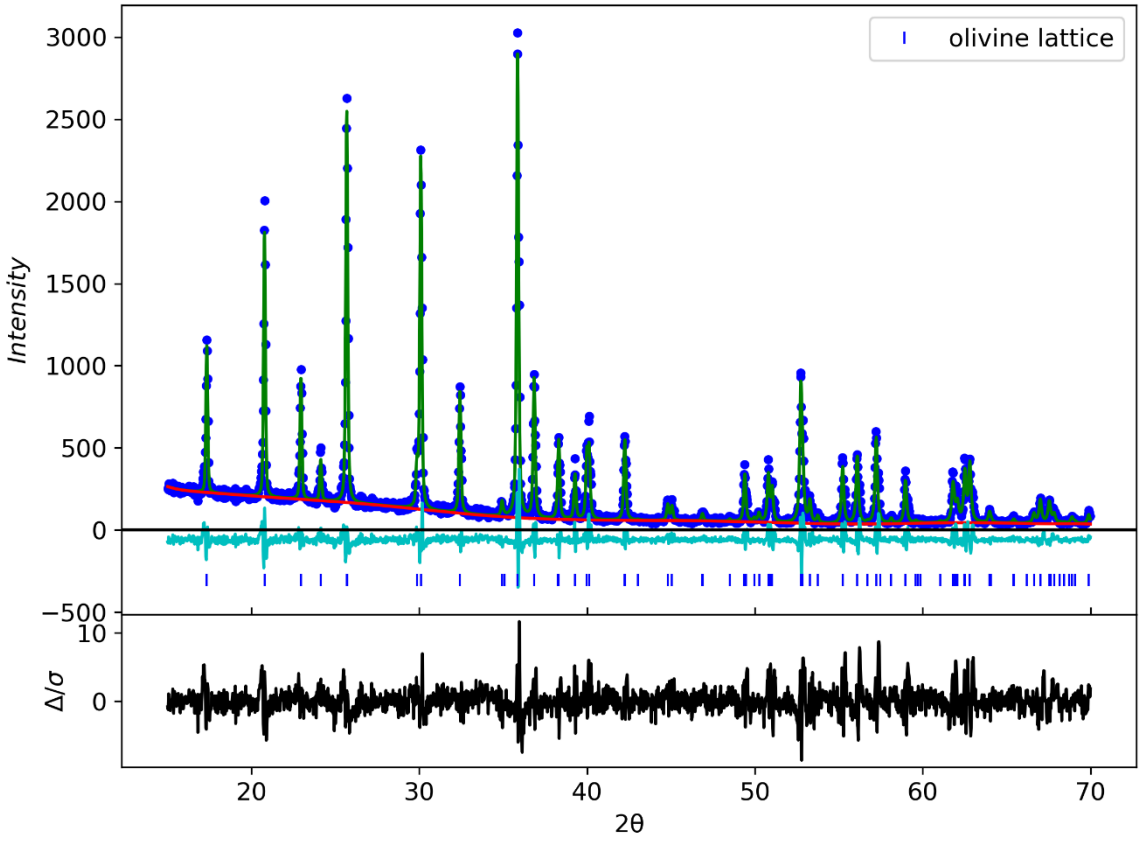

Figure S2. Rietveld refinement plot obtained for the LCmP@Ar samples.

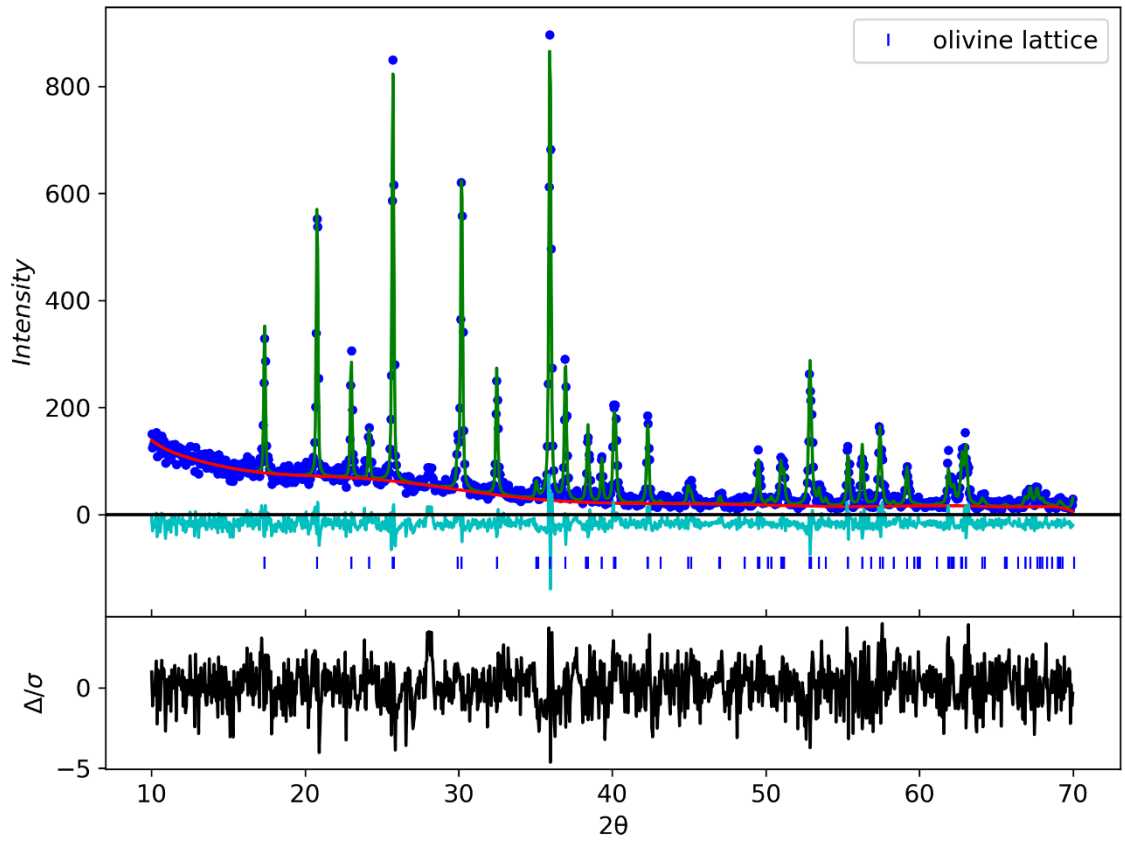

Figure S3. Rietveld refinement plot obtained for the LCnP samples.

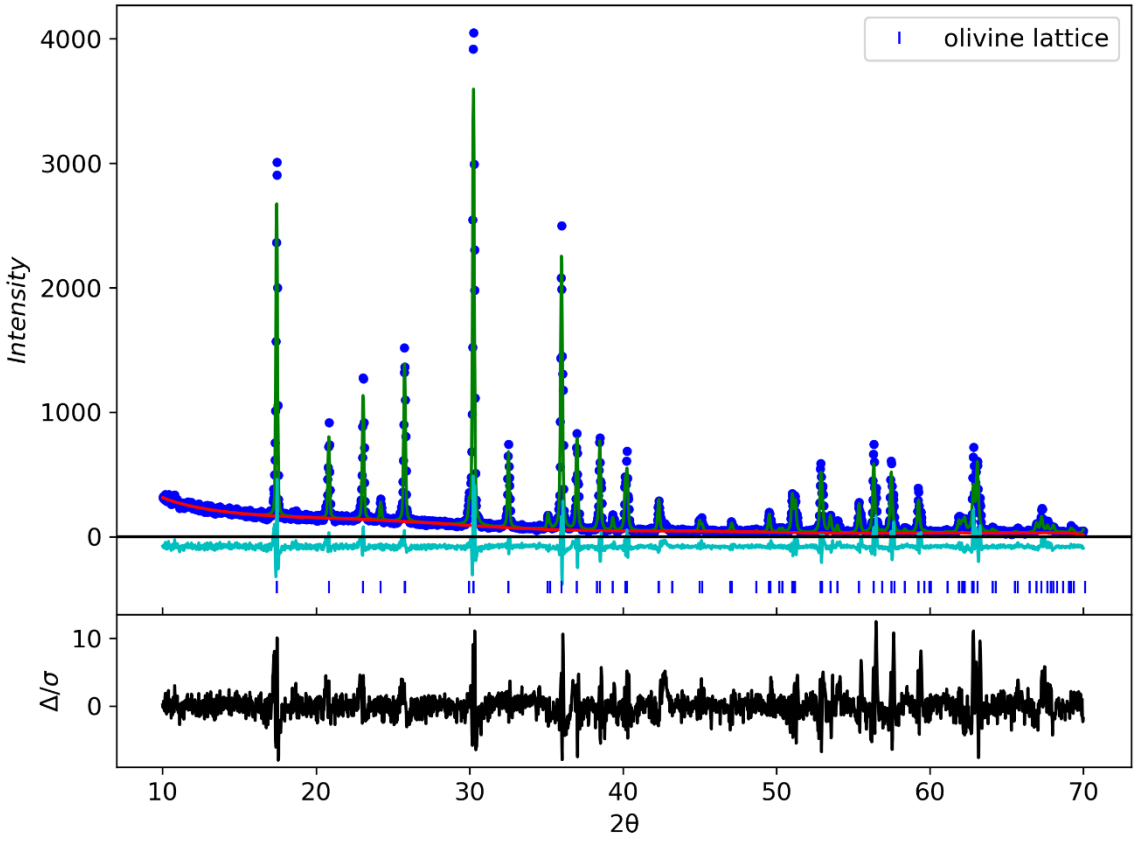

Figure S4. Rietveld refinement plot obtained for the LCnP@Ar samples.

Table S1. Mean square relative displacements in (σ^2 / 10^{-3}Å^2) obtained by best fit for LCmP based samples. CN is the coordination number; M-Z represent the central absorber (M, that is Co or Mn respectively in the Co K-edge and the Mn K-edge fits) and the scattering atom (Z, that is O, P/O or Co/Mn in the three shells considered). Statistical errors on distances are in all cases smaller than 0.2x10^{-3}Å^2

			Co K-edge		Mn K-edge	
Shell	**M-Z**	**C-N**	**LCmP**	**LCmP@Ar**	**LCmP**	**LCmP@Ar**
	M-O	2	8.9	3.2	7.7	2.8
1st shell	M-O	2	0.1	0.1	0.1	0.1
	M-O	2	1.6	2.1	1.7	0.1
	M-P	1	4.7	4.5	5.7	1.5
2nd shell	M-P	4	6.8	6.1	7.7	8.8
	M-O	6	35.7	20.6	27.9	14.5
	M-M′	4	10.6	14.1	8.4	8.5
3rd shell	M-M′	2	7.9	8.9	6.7	6.2
R factor(%)			4.9	7.9	4.8	9.7

Table S2. Mean square relative displacements in (σ^2 / 10^{-3}Å^2) obtained by best fit for LCnP based samples. CN is the coordination number; M-Z represent the central absorber (M, that is Co or Ni respectively in the Co K-edge and the Ni K-edge fits) and the scattering atom (Z, that is O, P/O or Co/Ni in the three shells considered). Statistical errors on distances are in all cases smaller than 0.2x10^{-3}Å^2

			Co K-edge		Ni K-edge	
Shell	**M-Z**	**C-N**	**LCnP**	**LCnP@Ar**	**LCnP**	**LCnP@Ar**
	M-O	2	8.1	18.8	14.8	1.2
1st shell	M-O	2	0.1	0.1	0.1	0.1
	M-O	2	0.4	2.0	0.4	0.1
	M-P	1	4.8	2.6	5.8	0.1
2nd shell	M-P	4	7.4	6.8	6.7	5.8
	M-O	6	28.7	22.4	27.6	22.8
	M-M′	4	11.4	8.4	14.9	13.0
3rd shell	M-M′	2	9.7	5.9	11.6	2.5
R factor(%)			3.9	5.9	8.6	16.8