Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

DEEPENING THE SHEAR STRUCTURE $FeNb_{11}O_{29}$: INFLUENCE OF POLYMORPHISM AND DOPING ON STRUCTURAL, SPECTROSCOPIC AND MAGNETIC PROPERTIES

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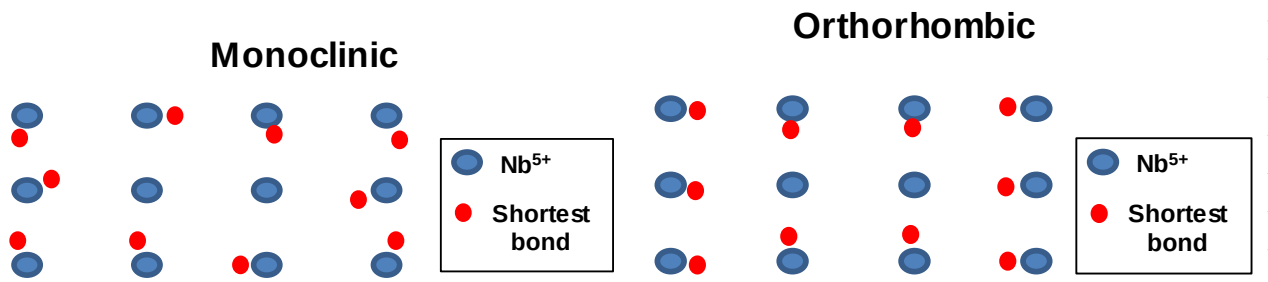

Figure S1 (a, b) Scheme showing the Nb displacement (red) with respect to an ideal situation of regular octahedra (blue) in the monoclinic and orthorhombic phases respectively.

Table S1 – Nb-O bond lengths for the six niobium sites in the undoped and doped monoclinic samples.

			Monoclinic samples		
		Bond multiplicity	Undoped	Mn doped	V doped
Nb1	O6	1x	1.739	1.7595	1.7419
	O7	1x	1.8417	1.8304	1.8415
	O4	2x	1.9983	1.9967	1.9978
			1.9983	1.9967	1.9978
	O2	1x	2.1713	2.1581	2.1688
	O6	1x	2.4493	2.4623	2.4483
Nb2	O5	1x	1.7101	1.7191	1.6908
	O8	1x	1.8294	1.8518	1.8395
	O2	2x	2.0345	2.0275	2.038
			2.0345	2.0275	2.038
	O4	1x	2.192	2.1778	2.2092
	O3	1x	2.2675	2.2437	2.261
Nb3	O9	1x	1.6172	1.5968	1.629
	O3	2x	1.9942	2.002	1.9924
			1.9942	2.002	1.9924
	O5	1x	2.0572	2.036	2.0098
	O6	1x	2.2562	2.289	2.3017
	O2	1x	2.4102	2.4367	2.4057
Nb4	O15	1x	1.7471	1.7444	1.7683
	O10	1x	1.869	1.8591	1.8702
	O13	2x	1.9583	1.9619	1.9562
			1.9583	1.9619	1.9562
	O7	1x	2.0997	2.1043	2.0774
	O11	1x	2.2171	2.2298	2.2129
Nb5	O14	1x	1.8625	1.8747	1.8902
	O11	2x	1.9632	1.9629	1.9595
			1.9632	1.9629	1.9595
	O15	1x	2.0095	1.9739	1.9546
	O8	1x	2.0388	2.0749	2.0906
	O13	1x	2.2638	2.2551	2.2393
Nb6	O12	2x	1.9138	1.9136	1.913
			1.9138	1.9136	1.913
	O14	1x	1.9601	1.9617	1.9761
	O10	1x	1.9663	1.9677	1.9514
	O1	1x	1.992	2.0232	2.0104
	O9	1x	2.1398	2.1099	2.1197

*1 In the V doped sample, Nb5-O15 is shorter than Nb5-O11

*2 In the V doped sample, Nb6-O10 is shorter than Nb6-O14

Table S2 – Nb-O bond lengths for the six niobium sites in the undoped and doped orthorhombic samples.

		Orthorhombic samples			
		Bond multiplicity	Undoped	Mn doped	V doped
Nb1	O9	1x	1.7598	1.8022	1.7776
	O4	2x	1.9719	1.9624	1.969
			1.9719	1.9624	1.969
	O8	1x	2.002	2.0002	1.9978
	O8	1x	2.2782	2.2309	2.2564
	O5	1x	2.3261	2.3004	2.3176
Nb2	O10	1x	1.8229	1.8229	1.8105
	O6	1x	1.8453	1.8728	1.884
	O5	2x	1.9754	1.9671	1.9704
			1.9754	1.9671	1.9704
	O4	1x	2.1717	2.1376	2.132
	O7	1x	2.35	2.34	2.3523
Nb3	O11	1x	1.7828	1.7897	1.7642
	O7	2x	1.9539	1.9484	1.9563
			1.9539	1.9484	1.9563
	O6	1x	1.9922	1.9299	1.9759
	O8	1x	2.067	2.1215	2.0878
	O5	1x	2.354	2.3475	2.3699
Nb4	O16	1x	1.8383	1.857	1.8233
	O1	1x	1.9619	1.9334	1.9557
	O12	2x	1.9734	1.9665	1.9765
			1.9734	1.9665	1.9765
	O9	1x	2.0042	2.0277	2.0071
	O13	1x	2.2152	2.1904	2.2274
Nb5	O14	1x	1.817	1.7858	1.8265
	O10	1x	1.964	2.0393	2.0551
	O13	2x	1.9818	1.9889	1.9813
			1.9818	1.9889	1.9813
	O2	1x	2.0063	1.9296	1.911
	O12	1x	2.2521	2.2859	2.2506
Nb6	O3	1x	1.8253	1.906	1.8887
	O15	2x	1.919	1.9105	1.914
			1.919	1.9105	1.914
	O16	1x	1.9486	1.9422	1.9562
	O14	1x	1.9881	1.9787	1.969
	O11	1x	2.2311	2.1485	2.1647

*3 In the Mn doped sample, Nb3-O6 is shorter than Nb3-O7

*4 In both doped samples, from the shortest bond, the order is: Nb5-O2, Nb5-O13, Nb5-O10

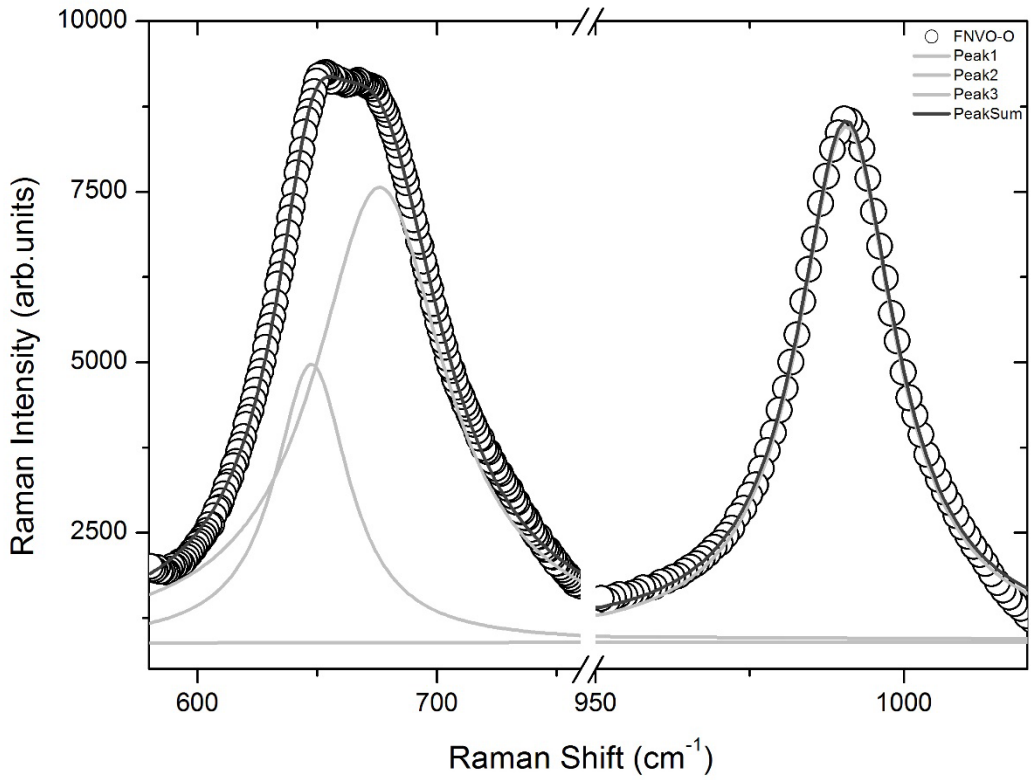

Figure S2 - Example of a best-fit procedure performed on the Raman data from FNVO-O sample in two different regions: 580-760 cm^{-1} and 950-1040 cm^{-1} (see text).