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Supporting information for article:

Pressure-dependent X-ray diffraction of the multiferroics *R*Mn_2O_5

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Supplemental Materials
Pressure-dependent x-ray diffraction of multiferroic RMn_2O_5

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REFINED PARAMETERS OF RMN_2O_5 (R = PR, SM, ND, TB AND DY)

We have refined the X-ray diffraction of RMn_2O_5 (R = Pr, Sm, Nd, Tb and Dy) at different pressure (up to ~ 8 GPa). The refined lattice parameters of RMn_2O_5 (R = Pr, Sm, Nd, Tb and Dy) are listed in Tables I to V while their refined atomic parameters are given in Tables VI to VIII. As we mentioned in the article, for the compounds with R = Dy, Tb and Nd, the refinements were difficult, especially at high pressure. The peak intensities at medium-high angles of their high pressure diffractograms were not correctly fitted. So the analysis of the atomic position are limited below 4 GPa for which the refinements were of good quality and reliable.

TABLE I: Refined parameters of $PrMn_2O_5$ at different pressures. $\lambda = 0.71$ Å

Pressure (GPa)	0	1.11	1.88	3.01	4.03	4.96	6.30	7.05	8.28
lattice parameters									
a (Å)	7.566(6)	7.535(6)	7.527(0)	7.508(6)	7.491(4)	7.473(0)	7.457(3)5	7.446(5)	7.436(3)
b (Å)	8.654(4)	8.639(3)	8.634(4)7	8.626(6)	8.618(7)	8.610(3)	8.606(5)	8.603(2)	8.599(4)
c (Å)	5.715(4)	5.703(1)	5.699(9)	5.693(6)	5.688(2)	5.683(2)	5.680(4)	5.678(5)	5.678(1)
Refinement									
χ^2	0.071	0.078	0.078	0.081	0.098	0.146	0.205	0.273	0.438
R_p (%)	4.47	4.79	4.68	4.93	5.48	6.87	8.43	9.50	13.0
R_{wp}(%)	4.84	5.03	5.08	5.32	5.96	7.54	9.19	10.80	14.1
R_{exp}(%)	18.16	17.94	18.19	18.74	19.01	19.73	20.30	20.59	21.37
R_{bragg}(%)	2.76	2.55	2.78	3.22	3.81	4.38	5.52	6.35	10.04

TABLE II: Refined parameters of $SmMn_2O_5$ at different pressures. $\lambda = 0.71$ Å

Pressure (GPa)	0	1.19	2.15	3.25	4.11	5.55	6.37
lattice parameters							
a (Å)	7.439(2)	7.410(4)	7.396(2)	7.380(0)	7.364(2)	7.347(5)	7.329(4)
b (Å)	8.584(3)	8.569(5)	8.562(1)	8.555(7)	8.549(0)	8.544(1)	8.537(1)
c (Å)	5.694(6)	5.683(9)	5.678(1)	5.672(1)	5.667(3)	5.664(0)	5.660(2)
Refinement							
χ^2	0.029	0.031	0.017	0.017	0.016	0.026	0.023
R_p (%)	7.04	7.60	5.48	5.18	5.10	4.87	4.59
R_{wp}(%)	6.46	7.14	5.33	5.33	5.25	5.39	5.10
R_{exp}(%)	37.88	40.79	40.40	40.08	41.62	33.80	33.88
R_{bragg}(%)	5.41	4.39	1.64	1.76	1.55	1.67	1.39

TABLE III: Refined parameters of $NdMn_2O_5$ at different pressures. $\lambda = 0.71$ Å

Pressure (GPa)	0	0.76	1.43	2.37	3.05	3.84	4.62	5.64	6.54	7.28
lattice parameters										
a (Å)	7.524(5)	7.510(9)	7.505(7)	7.497(0)	7.477(6)	7.461(2)	7.441(9)	7.425(6)	7.409(0)	7.397(6)
b (Å)	8.624(8)	8.620(3)	8.616(2)	8.608(7)	8.601(9)	8.595(6)	8.593(0)	8.590(2)	8.588(3)	8.586(0)
c (Å)	5.708(1)	5.703(6)	5.701(1)	5.696(5)	5.692(1)	5.688(0)	5.683(8)	5.683(4)	5.681(5)	5.683(7)
Refinement										
χ^2	0.107	0.256	0.216	0.259	0.265	0.285	0.327	0.365	0.423	0.419
R_p (%)	8.21	12.0	11.3	11.5	11.3	12.4	13.5	15.1	16.7	20.2
R_{wp}(%)	8.79	13.3	12.6	12.4	13.5	14.6	15.9	17.1	18.8	21.6
R_{exp}(%)	26.84	26.361	27.08	24.36	26.18	27.35	27.74	28.33	28.93	33.37
R_{bragg}(%)	6.42	8.83	9.25	8.88	9.06	9.58	9.96	11.42	11.41	15.93

TABLE IV: Refined parameters of $TbMn_2O_5$ at different pressures. $\lambda = 0.71$ Å

Pressure (GPa)	0	0.81	1.96	2.66	3.61	4.69	5.96	6.88	7.80	8.60
lattice parameters										
a (Å)	7.354(1)	7.338(1)	7.318(7)	7.301(7)	7.284(3)	7.267(3)	7.251(9)	7.240(2)	7.225(3)	7.203(5)
b (Å)	8.545(1)	8.539(7)	8.533(5)	8.526(2)	8.519(5)	8.513(4)	8.508(7)	8.504(2)	8.496(8)	8.479(9)
c (Å)	5.692(7)	5.688(9)	5.681(9)	5.676(3)	5.671(3)	5.666(9)	5.662(8)	5.660(1)	5.655(6)	5.643(9)
Refinement										
χ^2	0.067	0.055	0.083	0.146	0.229	0.294	0.329	0.419	0.492	0.513
R_p (%)	5.47	4.36	5.46	7.71	10.0	11.6	12.9	14.2	16.4	16.8
R_{wp}(%)	5.42	4.71	5.88	8.12	10.5	12.3	13.3	15.40	17.0	17.7
R_{exp}(%)	20.88	20.03	20.42	21.23	21.97	22.71	23.22	23.73	24.31	24.77
R_{bragg}(%)	3.54	2.37	3.64	5.37	7.66	8.78	9.25	11.72	12.67	12.63

TABLE V: Refined parameters of $DyMn_2O_5$ at different pressures. $\lambda = 0.71$ Å

Pressure (GPa)	0	0.85	1.23	2.11	3.06	3.62	4.84	5.74	6.75	7.72
lattice parameters										
a (Å)	7.299(3)	7.276(7)	7.261(3)	7.243(5)	7.221(1)	7.209(5)	7.190(0)	7.178(3)	7.164(7)	7.156(4)
b (Å)	8.523(9)	8.509(8)	8.501(5)	8.492(3)	8.481(6)	8.476(5)	8.468(8)	8.464(7)	8.459(1)	8.455(9)
c (Å)	5.679(9)	5.672(5)	5.668(2)	5.662(5)	5.655(9)	5.652(2)	5.646(5)	5.644(3)	5.639(8)	5.637(3)
Refinement										
χ^2	0.192	0.188	0.239	0.218	0.253	0.263	0.275	0.308	0.340	0.418
R_p (%)	10.7	10.6	12.6	11.8	13.1	13.1	13.5	13.6	14.2	15.3
R_{wp}(%)	10.5	10.6	12.2	12.0	13.1	13.3	13.8	14.6	15.5	17.0
R_{exp}(%)	23.97	24.49	24.98	25.66	25.98	26.04	26.27	26.36	26.52	26.32
R_{bragg}(%)	8.06	8.13	10.54	9.16	10.73	10.66	10.99	10.27	10.63	10.83

TABLE VI: Refined atomic parameters and isotropic displacement (temperature) parameter (in $Å^2$) of $PrMn_2O_5$ (left) and $SmMn_2O_5$ (right) at different pressures.

Atom	x	y	z	B
0 GPa				
Pr	0.1457(5)	0.1735(2)	0	0.0062(1)
Mn1	0	0.5	0.2544(5)	0.0070(9)
Mn2	0.4113(5)	0.3531(2)	0.5	0.0057(8)
O1	0	0	0.2690(5)	0.005
O2	0.1656(5)	0.4454(4)	0	0.005
O3	0.1337(3)	0.4377(0)	0.5	0.005
O4	0.4046(3)	0.2028(7)	0.2550(7)	0.005
1.11 GPa				
Pr	0.1480(0)	0.1742(2)	0	0.0061(6)
Mn1	0	0.5	0.25497	0.0068(4)
Mn2	0.41091	0.35138	0.5	0.0052(4)
1.88 GPa				
Pr	0.1474(9)	0.1741(2)	0	0.0089(1)
Mn1	0	0.5	0.2550(2)	0.0096(2)
Mn2	0.4118(4)	0.3507(2)	0.5	0.0089(0)
3.01 GPa				
Pr	0.1475(4)	0.1746(2)	0	0.0117(2)
Mn1	0	0.5	0.25389	0.0120(8)
Mn2	0.41217	0.35152	0.5	0.0135(3)
4.03 GPa				
Pr	0.1472(8)	0.1745(5)	0	0.0138(3)
Mn1	0	0.5	0.2536(2)	0.0172(3)
Mn2	0.4122(4)	0.3510(4)	0.5	0.0147(7)
4.96 GPa				
Pr	0.1482(4)	0.1751(2)	0	0.0153(2)
Mn1	0	0.5	0.2520(6)	0.0182(3)
Mn2	0.4126(8)	0.3514(8)	0.5	0.0181(7)
6.30 GPa				
Pr	0.1480(7)	0.1755(6)	0	0.0192(1)
Mn1	0	0.5	0.2508(1)	0.0212(7)
Mn2	0.41322(2)	0.3523(6)	0.5	0.0225(8)
7.05 GPa				
Pr	0.1485(1)	0.1752(7)	0	0.0242(1)
Mn1	0	0.5	0.2502(6)	0.0252(4)
Mn2	0.4125(7)	0.3529(3)	0.5	0.0252(1)
8.28 GPa				
Pr	0.1484(4)	0.1755(9)	0	0.0282(3)
Mn1	0	0.5	0.2508(4)	0.0312(6)
Mn2	0.41173	0.331(2)	0.5	0.0352(5)

Atom	x	y	z	B
0 GPa				
Sm	0.1411(7)	0.1748(5)	0	0.0079(9)
Mn1	0	0.5	0.2556(2)	0.0063(7)
Mn2	0.4131(7)	0.3542(1)	0.5	0.0081(2)
O1	0	0	0.2527(1)	0.005
O2	0.1760(5)	0.4694(6)	0	0.005
O3	0.1429(7)	0.4339(5)	0.5	0.005
O4	0.4016(3)	0.2054(6)	0.2522(0)	0.005
1.19 GPa				
Sm	0.1412(6)	0.1754(3)	0	0.0070(1)
Mn1	0	0.5	0.2510(7)	0.0052(7)
Mn2	0.4149(1)	0.3558(8)	0.5	0.0083(1)
2.15 GPa				
Sm	0.1415(7)	0.1756(4)	0	0.0059(8)
Mn1	0	0.5	0.2503(9)	0.0056(2)
Mn2	0.4143(5)	0.3564(0)	0.5	0.0064(1)
3.25 GPa				
Sm	0.1416(0)	0.1754(6)	0	0.0057(8)
Mn1	0	0.5	0.2503(2)	0.0050(4)
Mn2	0.4136(0)	0.3561(2)	0.5	0.0055(8)
4.11 GPa				
Sm	0.1415(8)	0.1754(2)	0	0.0098(6)
Mn1	0	0.5	0.2502(3)	0.0087(5)
Mn2	0.4138(7)	0.3559(0)	0.5	0.0094(7)
5.55 GPa				
Sm	0.1413(2)	0.1751(8)	0	0.0123(2)
Mn1	0	0.5	0.2495(0)	0.015(4)
Mn2	0.4136(0)	0.3565(1)	0.5	0.0011(3)
6.37 GPa				
Sm	0.1411(2)	0.1750(2)	0	0.0172(8)
Mn1	0	0.5	0.2493(7)	0.0192(3)
Mn2	0.4135(6)	0.3566(0)	0.5	0.0152(5)

TABLE VII: Refined atomic parameters and isotropic displacement (temperature) parameter (in Å^2) of $NdMn_2O_5$ (left) and $TbMn_2O_5$ (right) at different pressures.

Atom	x	y	z	B
0 GPa				
Nd	0.1422(9)	0.1745(3)	0	0.0089(1)
Mn1	0	0.5	0.2570(9)	0.0072(7)
Mn2	0.4165(5)	0.3661(5)	0.5	0.0095(3)
O1	0	0	0.2349(7)	0.005
O2	0.1571(6)	0.4469(4)	0	0.005
O3	0.1524(6)	0.4374(4)	0.5	0.005
O4	0.4009(3)	0.2067(3)	0.2515(6)	0.005
0.76 GPa				
Nd	0.1399(2)	0.1739(9)	0	0.0076(5)
Mn1	0	0.5	0.2664(6)	0.0068(3)
Mn2	0.4161(9)	0.3677(9)	0.5	0.0085(1)
1.43 GPa				
Nd	0.1386(7)	0.1733(5)	0	0.0127(5)
Mn1	0	0.5	0.2648(1)	0.0146(4)
Mn2	0.4190(2)	0.3711(3)	0.5	0.0175(3)
2.37 GPa				
Nd	0.1385(0)	0.1732(5)	0	0.0247(4)
Mn1	0	0.5	0.2658(4)	0.0314(8)
Mn2	0.4187(4)	0.3721(3)	0.5	0.0294(2)
3.05 GPa				
Nd	0.1432(9)	0.1769(1)	0	0.0328(6)
Mn1	0	0.5	0.2637(0)	0.0307(4)
Mn2	0.4268(5)	0.3661(2)	0.5	0.0344(5)

Atom	x	y	z	B
0 GPa				
Tb	0.1404(4)	0.1719(9)	0	0.0089(8)
Mn1	0	0.5	0.25024	0.0075(7)
Mn2	0.4101(9)	0.3536(3)	0.5	0.0135(1)
O1	0	0	0.2598(4)	0.005
O2	0.1693(1)	0.4431(6)	0	0.005
O3	0.1429(3)	0.4322(5)	0.5	0.005
O4	0.3988(1)	0.2017(8)	0.2473(5)	0.005
0.81 GPa				
Tb	0.1407(8)	0.1725(1)	0	0.0067(2)
Mn1	0	0.5	0.2498(3)	0.0060(5)
Mn2	0.4109(1)	0.3550(9)	0.5	0.0083(7)
1.96 GPa				
Tb	0.1413(5)	0.1732(9)	0	0.0043(9)
Mn1	0	0.5	0.2488(6)	0.0051(2)
Mn2	0.4116(7)	0.3584(4)	0.5	0.0065(7)
2.66 GPa				
Tb	0.1425(2)	0.1742(4)	0	0.0038(1)
Mn1	0	0.5	0.24644	0.0029(7)
Mn2	0.41116	0.35908	0.5	0.0064(3)
3.61 GPa				
Tb	0.1428(3)	0.1747(9)	0	0.0018(9)
Mn1	0	0.5	0.2449(7)	0.0027(3)
Mn2	0.4116(5)	0.3584(3)	0.5	0.0058(9)

TABLE VIII: Refined atomic parameters and isotropic displacement (temperature) parameter (in Å^2) of $DyMn_2O_5$ at different pressures.

Atom	x	y	z	B
0 GPa				
Dy	0.1417(6)	0.1790(6)	0	0.0126(3)
Mn1	0	0.5	0.2384(0)	0.0137(2)
Mn2	0.4135(8)	0.3476(8)	0.5	0.0145(8)
O1	0	0	0.2893(5)	0.005
O2	0.2406(9)	0.4459(2)	0	0.005
O3	0.1562(5)	0.4421(7)	0.5	0.005
O4	0.3951(0)	0.2082(3)	0.2414(1)	0.005
0.85 GPa				
Dy	0.1424(4)	0.1798(9)	0	0.0101(2)
Mn1	0	0.5	0.2387(7)	0.0140(1)
Mn2	0.4169(5)	0.3452(4)	0.5	0.0155(2)

Atom	x	y	z	B
1.23 GPa				
Dy	0.1424(7)	0.1798(5)	0	0.0097(8)
Mn1	0	0.5	0.23856	0.0132(0)
Mn2	0.41926	0.34441	0.5	0.0123(7)
2.11 GPa				
Dy	0.1414(5)	0.1798(3)	0	0.0073(8)
Mn1	0	0.5	0.2345(8)	0.0104(3)
Mn2	0.4149(4)	0.3412(2)	0.5	0.0114(2)
3.06 GPa				
Dy	0.1407(9)	0.1801(7)	0	0.0087(5)
Mn1	0	0.5	0.2317(1)	0.0078(1)
Mn2	0.4161(2)	0.3363(2)	0.5	0.00142(7)

DFT OPTIMIZED GEOMETRIES

All the DFT optimized geometries can be found in the cif archives provided as supplementary independent files.

$DyMn_2O_5$: cif_DyMn2O5_Pm_AFM.tar.gz

$GdMn_2O_5$: cif_gdMn2O5_Pm_AFM.tar.gz

MICROSCOPIC CONTENT OF EFFECTIVE MAGNETIC EXCHANGES : GENERAL DESCRIPTION

The effective exchange integrals between two magnetic sites bridged by a ligand can be expressed as the singlet-triplet energy difference when each magnetic site support one electron. Let us call d and d' the magnetic orbitals of the M and M' magnetic sites and p the ligand orbital bridging the interaction. The other electrons will be supposed to be in doubly occupied orbitals and ignored in the present representation.

The effective exchange integral can be calculated in a quasi-degenerate perturbative scheme in which the model space is restricted to the two main configurations of the two spin states, namely $|p\bar{p}\,d\bar{d}'\rangle$ and $|p\bar{p}\,d'\bar{d}\rangle$. In our notations the overligned orbitals support down spins and the unbarred ones up spins, d refers to the fist magnetic atom while d' to the second. One thus have

$$J = J_d + J_{sd} + J_{sb} \tag{1}$$

where $J_d = \langle d\bar{d}'|\hat{V}|d'\bar{d}\rangle$ is the first order term of the perturbation series, it corresponds to the direct Pauli exchange between the two magnetic orbitals

As well known from the 3rd Hund's rule this term is always ferromagnetic.

This term is small, but not always negligible

$J_{sd} = -4\,\dfrac{\left|\langle d|\hat{F}|d'\rangle\right|^2}{U}$ is the second order term, it corresponds to the direct or Anderson's super-exchange and may also be found under the name of through-space super-exchange

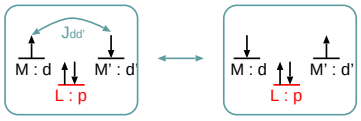
When symmetry allowed, this term is always antiferromagnetic.

This term is negligible in bridged systems, due to the large M-M' bond length.

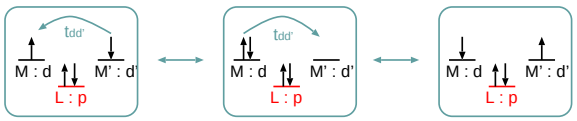
$J_{sb} = = -4\,\dfrac{\left|\langle d|\hat{F}|p\rangle\right|^2\left|\langle d'|\hat{F}|p\rangle\right|^2}{(U+\varepsilon_d-\varepsilon_p)^2\,U} - 8\,\dfrac{\left|\langle d|\hat{F}|p\rangle\right|^2\left|\langle d'|\hat{F}|p\rangle\right|^2}{2\,(U+\varepsilon_d-\varepsilon_p)^3}$ is the fourth order term, it corresponds to the through-bridge or through-ligands super-exchange

When symmetry allowed, this term is always antiferromagnetic and usually dominant.

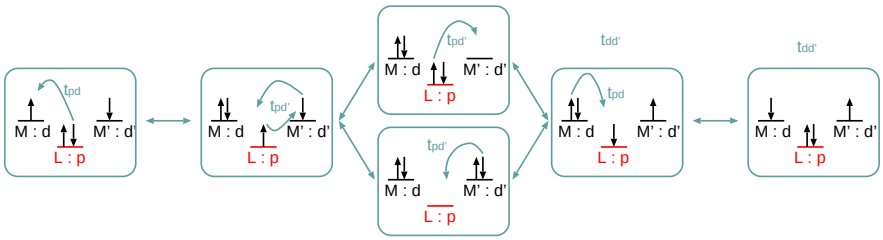
In the above formula $\hat{V}$ is the electron-electron repulsion operator and U its integral when two electrons are in the same magnetic orbital, $\hat{F}$ is the Fock operator which diagonal part can be associated with the orbital energies (ε) and the extradiagonal part to the hopping integrals. A graphical representation of the J_d, J_{sd} and J_{sb} terms can be found in Figure 1a, Figure 1b and Figure 1c.



(a) The direct exchange term, J_d. $J_{dd'} = \langle d\bar{d}'|\hat{V}|d'\bar{d}\rangle$



(b) The direct super-exchange term.



(c) The ligand mediated super-exchange term.

FIG. 1: Schematic representation of the different terms in an effective exchange integral between 2 sites, each supporting one magnetic electron.

When there are more than one electron and one magnetic orbital per magnetic site, the exchange integral is composed of all possible different terms of the above kinds. The latters should be summed up with appropriate coefficients (that depend on the number of magnetic electrons and orbitals on each magnetic atoms).

THE J_1 AND J_2 EFFECTIVE MAGNETIC INTEGRALS IN THE RMn_2O_5 COMPOUNDS

The J_1 and J_2 magnetic integrals couple the Mn^{4+} ions along the **c** direction. The through-bridge super-exchange terms are mediated by two O3 atoms for J_2 and two O2 oxygens for J_1. The super-exchange paths are pictured in Figure 2.

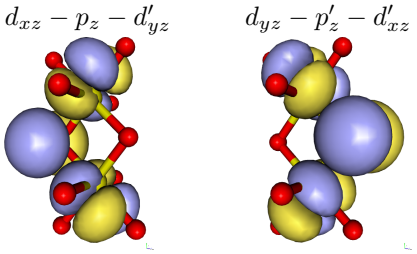


FIG. 2: Schematic representation of super-exchange path for the J_1 and J_2 magnetic integrals.

As the dependence of the $\langle d|\hat{F}|p\rangle$ factors (in the J_{sb} super-exchange term) to the geometrical parameters is similar to the dependence of the overlaps between the magnetic orbital, d, and the ligands bridging-orbital, p, it is easy to see in Figure 2 that J_1 and J_2 do not depend on the Mn^{4+}–O–Mn^{4+} angle, but only on the Mn^{4+}–O distances (J_{sb}) and to a lesser extend on the Mn^{4+}–Mn^{4+} distances (J_d).

THE J_3 EFFECTIVE MAGNETIC INTEGRALS IN THE RMn_2O_5 COMPOUNDS

The J_3 magnetic integrals couple the Mn^{4+} and Mn^{3+} ions along a direction roughly **b**. These integrals are associated to the inter-chain coupling. In a non-polar Pbam group their contribution to the magnetic energy (in and Heisenberg Hamiltonian scheme) is zero, while in the polar phase, the J_3 integrals differentiate to lift the magnetic frustration, into a J_{3FM} and J_{3AFM} according to the FM/AFM ordering of the Mn^{4+} and Mn^{3+} ions. The through-bridge super-exchange terms are mediated by a O4 oxygen. The super-exchange paths are pictured in Figure 3.

One sees from Figure 3 that while the $d'_{x'y'} - p_y - d_{yz}$ super-exchange path does not depend on the Mn_1–O4–Mn_2 angle, α_3, this is not the case for the two other ones. Indeed the $d'_{x'z'} - p_x - d_{xz}$ super-exchange path varies as $\cos^2\alpha_3$ and the $d'_{z'^2} - p_x - d_{xz}$ super-exchange path varies as $\sin^2\alpha_3$. Of course all three terms depend on the Mn–O distances, however usually the angle dependence brings larger variations of the magnetic integrals than distance ones.

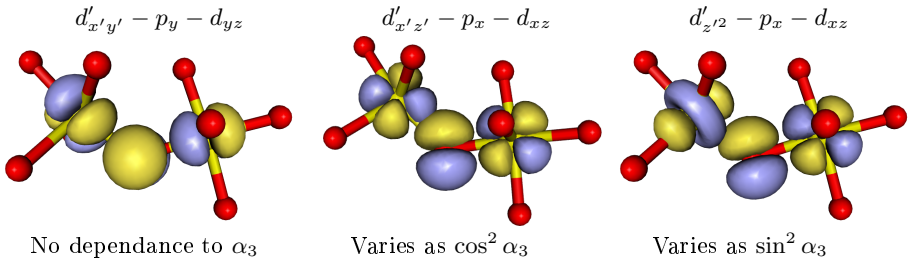


FIG. 3: Schematic representation of super-exchange paths for the J_3 magnetic integrals. The z' axis for the square-pyramid is the apical one, the x' axis being the Mn-O axis toward the bridging oxygen O4. Similarly one can name z the axis between the Mn^{4+} ion in the octahedron and the O4 oxygen, y the axis perpendicular to the figures and x the second axis within the figure.

THE J_4 EFFECTIVE MAGNETIC INTEGRALS IN THE RMn_2O_5 COMPOUNDS

The J_4 magnetic integrals couple the Mn^{4+} and Mn^{3+} ions along the chain that run along roughly **a**. This is one of the two integrals associated with the intra-chain coupling, the second largest AFM exchange in the system. The through-bridge super-exchange terms are mediated by a O3 oxygen. The super-exchange paths are pictured in Figure 4.

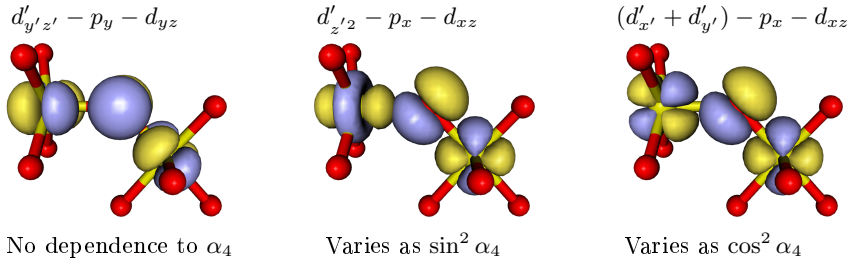


FIG. 4: Schematic representation of super-exchange paths for the J_4 magnetic integrals. The z' axis for the square-pyramid is the apical one, the x' and y' axes being along the other Mn-O bonds. Similarly one can name z the axis between the Mn^{4+} ion in the octahedron and the O3 oxygen, y the axis perpendicular to the figures and x the second axis within the figure.

The analysis of Figure 4 shows that the $d'_{y'z'} - p_y - d_{yz}$ super-exchange path does not depend on the Mn_1–O3–Mn_2 angle, α_4, while this is not the case for the two other ones. The $d'_{z'^2} - p_x - d_{xz}$ super-exchange path is expected to be the largest term as it involves σ type of overlap ($d'_{z'^2} - p_x$), while all the other super-exchange path are associated with π type of transfer integrals. It varies as $\sin^2 \alpha_4$. Finally the $(d'_{x'} + d'_{y'}) - p_x - d_{xz}$ path varies as $\cos^2 \alpha_4$.

THE J_5 EFFECTIVE MAGNETIC INTEGRALS IN THE RMn_2O_5 COMPOUNDS

The J_5 magnetic integrals couple two Mn^{3+} ions roughly along the **b** direction. This is the other intra-chain exchange integral and the largest AFM one. The through-bridge super-exchange terms are mediated by two O1 oxygens. The super-exchange paths are pictured in Figure 5.

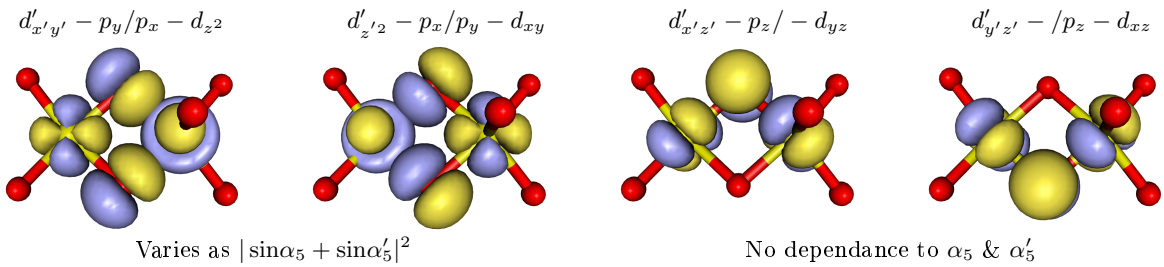


FIG. 5: Schematic representation of super-exchange paths for the J_5 magnetic integrals. The z' and z axes of the two square-pyramid are chosen as the apical ones, that are roughly perpendicular to the figure. The x' and and x axes are along the other Mn-O bonds roughly directed north-east in the figure, while the y' and y axes are along the other Mn-O bonds roughly directed south-east in the figure. α_5 will denote the Mn^{3+}–O1–Mn^{3+} angle with the top oxygen on the figure, while α'_5 is the Mn^{3+}–O1–Mn^{3+} angle with the bottom oxygen.

The J_5 effective magnetic integrals has four through-bridge super-exchange terms. As a consequence J_5 is the largest AFM magnetic coupling in the RMn_2O_5 compounds. Out of these two are independent of the Mn^{3+}–O1–Mn^{3+} angles, α_5 and α'_5, namely the $d'_{x'z'} - p_z/ - d_{yz}$ and $d'_{y'z'} - /p_z - d_{xz}$ paths (see Figure 5). The two other paths, $d'_{x'y'} - p_y/p_x - d_{z^2}$ and $d'_{z'^2} - p_x/p_y - d_{xy}$, are maximum for 90° angles and vary as $|\sin\alpha_5 + \sin\alpha'_5|^2$.