Supporting Information

Magnetic Properties of the distorted kagomé lattice $Mn_3(1,2,4\text{-}(O_2C)_3C_6H_3)_2$

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1.1 Spin Wave calculations using spinW

Below is an annotated script to calculate the spin wave spectrum of $Mn_3(1,2,4\text{-}(O_2C)_3C_6H_3)_2$. The script can be run using the freely available spinW software. This can be downloaded from: https://www.psi.ch/spinw/

The calculations presented in this manuscript were performed using matlab 2014b.

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

clear all

%We create a lattice with space group "P 21/c" with just the Mn atoms.  Note the crystal structure

%is reported in P 21/n but we have transformed this to P 21/c as only standard space group settings are allowed in spinW.   The Mn atoms are defined as having

% S=5/2.

AF33kagome = sw;

AF33kagome.fileid(0)

AF33kagome.genlattice('lat_const',[11.321 6.552 10.85],'angled',[90 145.704 90],'sym','P 21/c')

AF33kagome.addatom('r',[0.09563 0.28603 0.3225],'S', 5/2,'label','MMn1','color','r')
```

```
AF33kagome.addatom('r',[0 0 0],'S', 5/2,'label','MMn2','color','g')
%%
% Next generate the list of nearest neightbours (spinW calls these bonds) and lists them.
AF33kagome.gencoupling('maxDistance',7)
display('Rows: dlx, dly, dlz, at1, at2, idx, ma1, ma2, ma3')
AF33kagome.couplingtable.table
display('Bond vectors (first three rows) and bond distances')
AF33kagome.couplingtable.bondv
%%
%Hamiltonian: we next define the exchange interactions and if required anisotropies.
%Note that “eye(3)” is just the matlab identification of the identity matrix.  The units are in meV
AF33kagome.addmatrix('label','J1','color',[255 0 0]','mat',0.4*eye(3))
AF33kagome.addmatrix('label','J2','color',[0 255 0]','mat',0.4*eye(3))
AF33kagome.addmatrix('label','J3','color',[0 0 255]','mat',0.1*eye(3))
%associated the exchange couplings defined above, with the nearest neighbour distances defined in
%the second step.
AF33kagome.addcoupling('J1',1)
AF33kagome.addcoupling('J2',2)
AF33kagome.addcoupling('J3',3)
%Plot this to show that the exchange topology and structure is correct (fig S1).
AF33kagome.plot('range', [0.5 1.5;0 3;0 2]);
%% Next optimise the magnetic structure.  This takes a little time.  As defined below the structure is
%completely free to vary and not restricted by symmetry.
opt_par.nRun = 10;
opt_par.xmin = [0     0      0  0   0    0     0];
opt_par.xmax = [2*pi   2*pi    0  0    0    pi     2*pi];
opt_par.func = @gm_planar;
```

```
AF33kagome.optmagstr(opt_par);

% Next replot the structure to show that the magnetic structure is correct.          (Fig S2)

AF33kagome.plot('range', [0.5 1.5;0 3;0 2], 'sSpin', 0.5);

%

%sw_plotspec(AF33Pow,'axLim',[0 4],'colormap', jet,'colorbar',true, 'dE',0.135)

%

%Calculate spin wave dispersion I.

%We plot the real and imaginary part of the dispersion.  We do this for the high symmetry directions
% of the reciprocal lattice.

AF33Spec = AF33kagome.spinwave({[0 0 0]  [1/2 0 0] [1/2 0 1/2] [0 0 1/2]  [0 0 0] [0 1/2 0] [0 1/2
1/2]  [0 0 1/2] [0 0 0] [1/2 0 0] [1/2 1/2 0] [0 1/2 0] [0 0 0] 100},'hermit',true, 'T', 5);

AF33Spec = sw_egrid(AF33Spec,'component','Sxx+Syy+Szz');

figure

sw_plotspec(AF33Spec,'mode',1,'axLim',[0
3],'colorbar',false,'imag',true,'sortMode',true,'dashed',true)

sw_plotspec(AF33Spec,'mode',3,'dE',0.5,'axLim',[0 7],'dashed',true)

colormap jet

%Next calculate the powder averaged spectrum, Q range is set for 0 to 4 ang-1 with 150 slices.  The
energy range 0 to 5 meV with 250 slices.

%1000 random orientations are taken to calculate the spin wave dispersion.  The resolution is set at
0.135 meV.  (fig s4)

AF33Pow =
AF33kagome.powspec(linspace(0,4,150),'Evect',linspace(0,5,250),'nRand',1000,'hermit',false);

figure;

sw_plotspec(AF33Pow,'axLim',[0 2],'colorbar',true, 'dE',0.135)

colormap jet

%
```

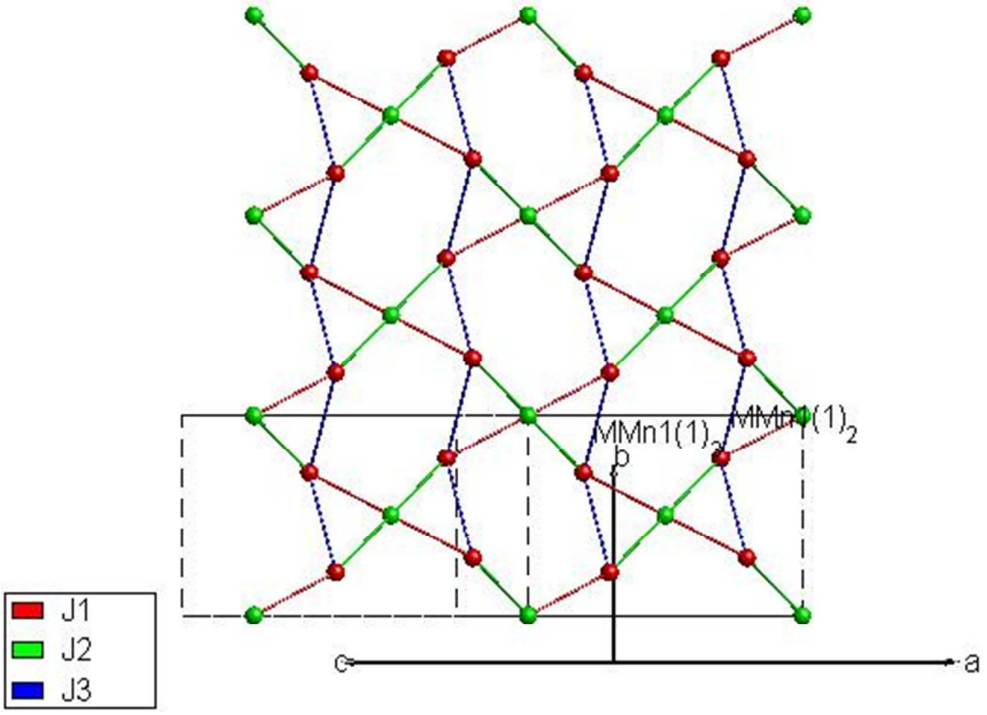

Fig S1. Structure of **1** with the exchange interactions highlighted. Mn1 are shown in green and Mn2 in red.

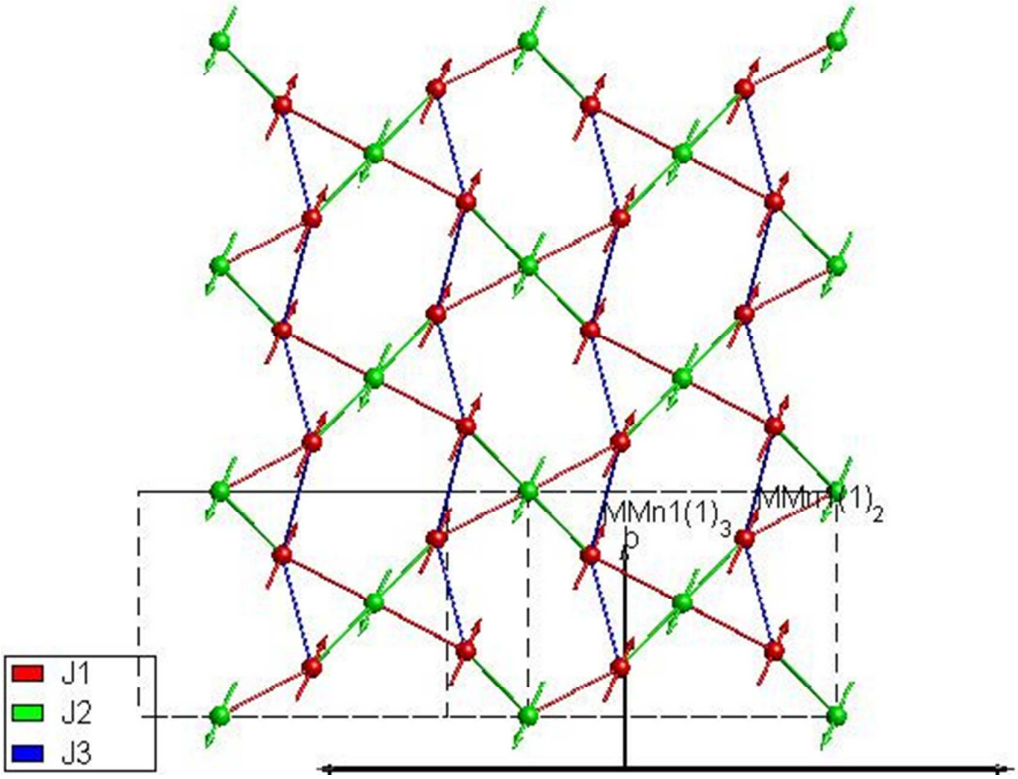

Fig S2: Magnetic structure as calculated with spinW and used in the spin wave calculation

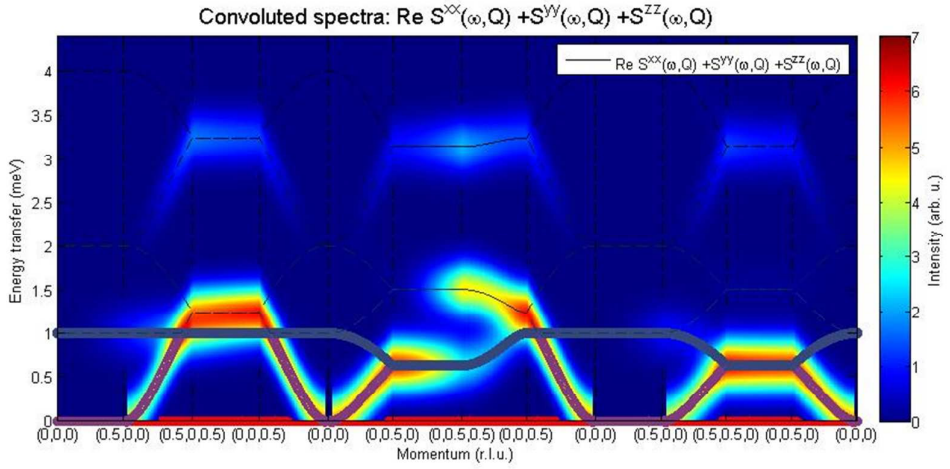

Fig S3: Spin wave dispersion of **1** plotted in the high symmetry directions. The Color scale is proportional to the predicted intensity.

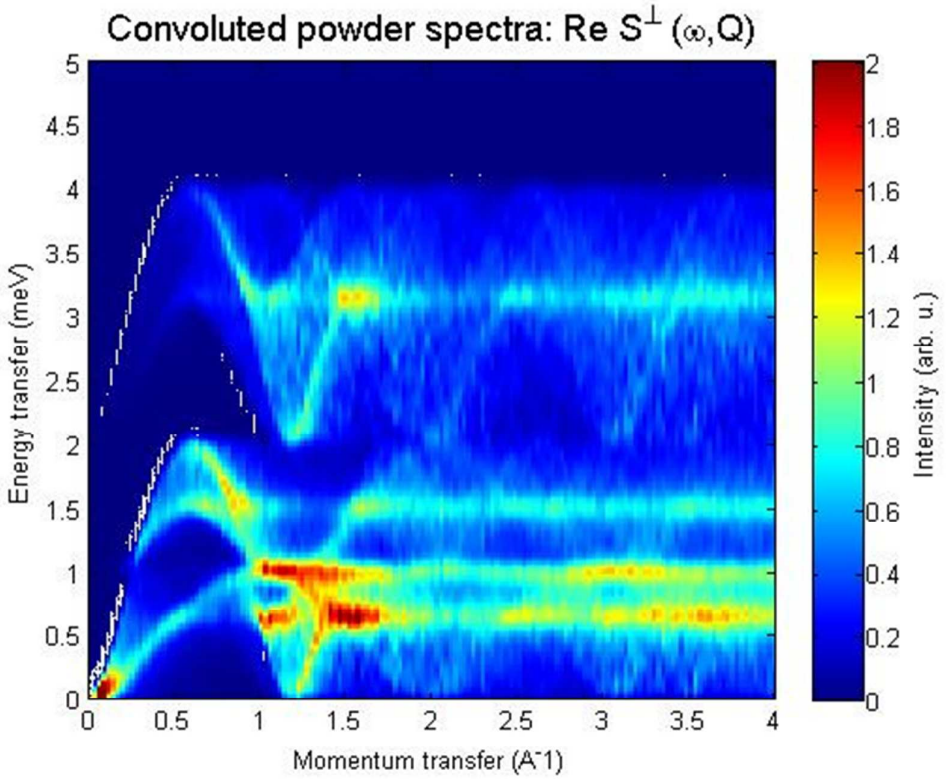

Fig S4: Powder averaged spectrum for **1**.