Estimation of Muon Sites in La_2CuO_4 and A New Vanadium Cluster Compound, $V_4S_9Br_4$, using Electronic and Nuclear Dipole Field Calculations

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Introduction:

We are going to report a way to estimate muon stopping positions from both of electronic and nuclear dipole field simulations. In order to verify our way, we have applied our developed method to La2CuO4 (LCO) using well known parameters obtained in the paramagnetic and magnetically ordered states. We also tested our way to investigate a spin structure in a magnetically ordered state of the new vanadium cluster compound, V4S9Br4.

The antiferromagnetic ordered state of LCO has been already provided by Vaknin *et al*. (1987). We used the value of the saturated internal field at the muon site obtained by Uemura *et al.* (1987: 410-425 G) in this study. We also tried to estimate the mangetic moment of the Cu spin in order to satisfy both results on internal fields caused from electronic and nuclear dipoles at the moun site. Previous studies suggest the magnetic moment of the Cu-spin to be 0.5 μB (Brockhouse, 1954), 0.65±0.03 μB (Forsyth et al, 1988), and 0.69±0.05 μB (Yang et al, 1989). Our current study shows the optimized magnetic moment of the Cu-spin to be 0.66 μB. We also suggest a new muon-stopping position which is on a triangle plane formed by one apical and two in-plane oxygen atoms.

The spin structure of V4S9Br4 is unclear at this moment. In order to achieve values of internal fields at the muon site in both of the paramagnetic and the magnetically ordered states, we have carried out zero-field (ZF) μSR experiments down to 5 K in the ALC are of Paul-Scherrer Institute (PSI) in Switzerland using a dc muon beam. We are going to report the experimental results and our simulation ones on the basis of some models of spin structures.

Discussions:

La2CuO4 :

1) In our simulations, we varied the value of the magnetic moment of the Cu-spin from 0.5 μB to 0.7 μB in a step of 0.01 μB(Figure 2). In the case of 0.66 μB, we found that our simulation well explained both internal fields caused from the electronic and nuclear dipole fields at one muon site. This value is between values obtain by Forsyth *et al.* and Yang *et al.*

2) Our simulation suggests one new muon site where is on a triangle plane of the CuO6octahedra formed by the apical and two in-plane oxygen atoms (Figure 3 and 4). This position is a bit far away from oxygen sites but could satisfy all magnetic parameters measured in the paramagnetic and magnetically ordered states.

V4S9Br4 :

1) We have found four components of the muon-spin precession frequency in a magnetically ordered state below about 14K(Figure 7 and 8), showing the appearance of a long-range magnetically ordered state.

2) In order to estimate muon sites, we tested some models of spin structure (Figure 6). At this moment, we have not yet achieved a reasonable model. More simulation efforts are in progress.

Methods:

We simulated both of the electronic and nuclear dipole fields and tried to find out good muon positions which can well explain both fields.

We developed our program using the MATLAB language.

We used the following equation to calculate the electronic dipole fields.

$$H_{dip}=\sum_i \frac{1}{r_i^3}\left[3\frac{(\mu_i\cdot\hat{r}_i)\hat{r}_i}{r_i^2}-\mu_i\right]$$

An for the calculation of the nuclear dipole field, we used the following equation (Schenck, 1985), wi

$$M_2^{ZF,Q,I=\text{odd}\frac{1}{2}}=\frac{1}{3}I(I+1)(\hbar\gamma_\mu\gamma_N)^2\frac{8}{3}\left[1+\frac{3}{8}\frac{I+\frac{1}{2}}{I(I+1)}\right]\sum_i\frac{1}{r_i^6}$$

We calculated both the electronic and nuclear dipole fields in the area with the 50Å radius.

For the vanadium cluster, we used the value of 1.77 μB for the magnetic moment of the V spin to find out muon positions to explain the experimental results

Result:

La_2CuO_4

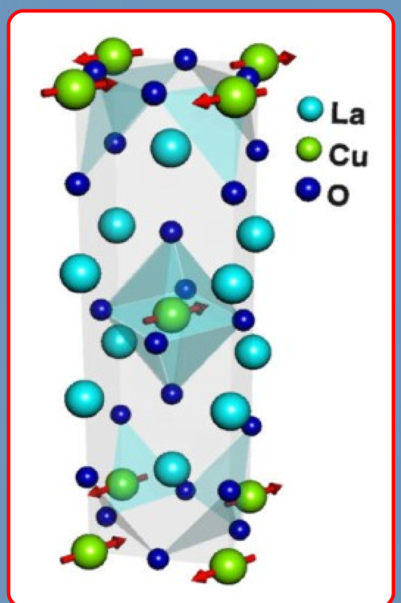


Figure.1, Antiferromagnetic spin structure proposed by Vaknin *et al*. (1987)

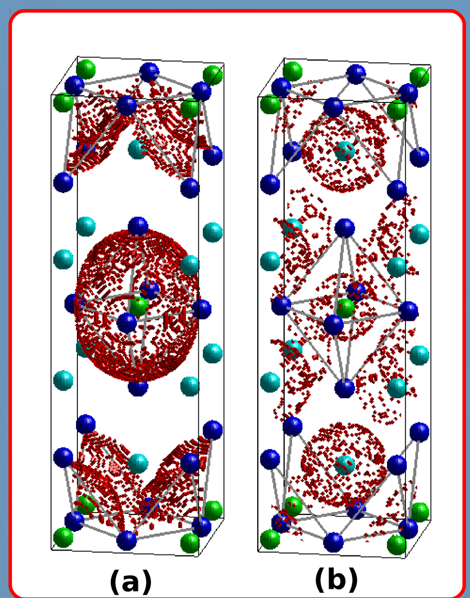


Figure.2, Internal-field mapping of (a) the electronic dipoles (410-425 G) and (b) the nuclear dipoles (1.65-1.70 G) calculated in the spherical area with the radius of 50Å. The magnetic moment of the Cu-spin was fixed to be 0.69 μB and the resolution of the mapping along each crystal axis was

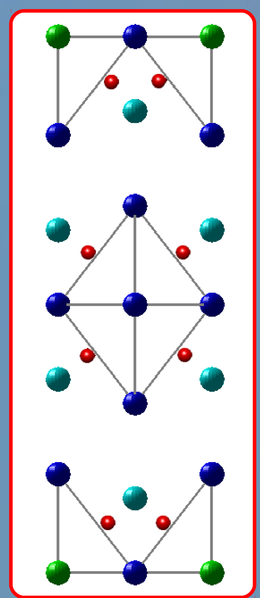
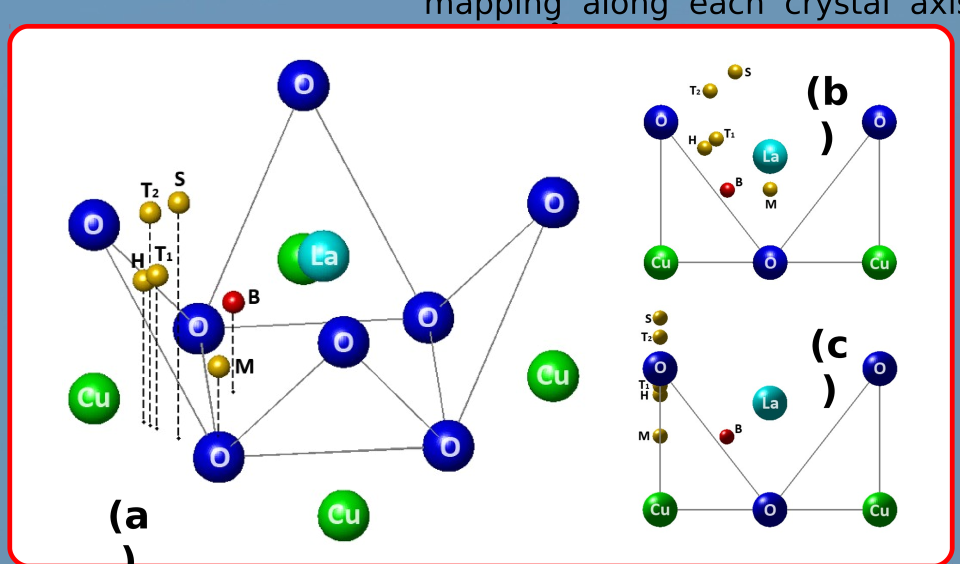


Figure.3, Red marks show suggested points which satisfy both experimental data of the electronic and nuclear dipole fields.



H : Hitti et al (1990)
T1,T2 : Torikai et al (1993)
S : Saito et al (1991)
M : McMullen et al (1991)
B : our result

Figure.4, Muon positions viewed in (a) 3D, (b) from the a-c plane, (c) from the b-c plane. Yellow marks have been suggested from previous studies. Red marks are our current study.

$V_4S_9Br_4$

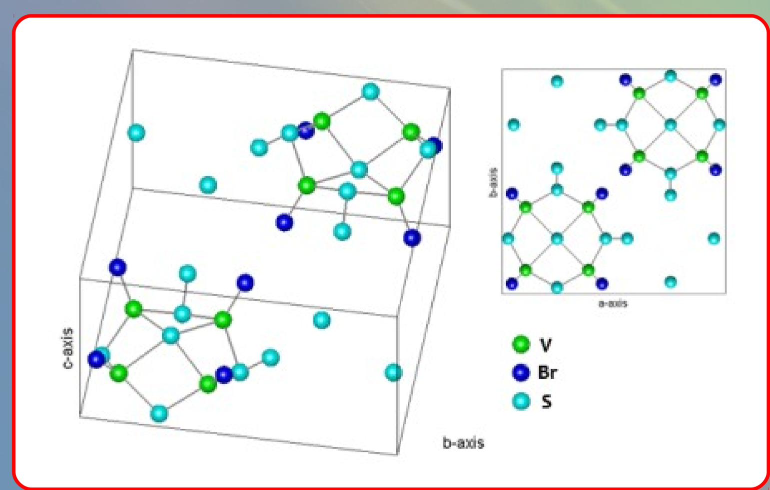


Figure.5, Vanadium cluster crystal structure

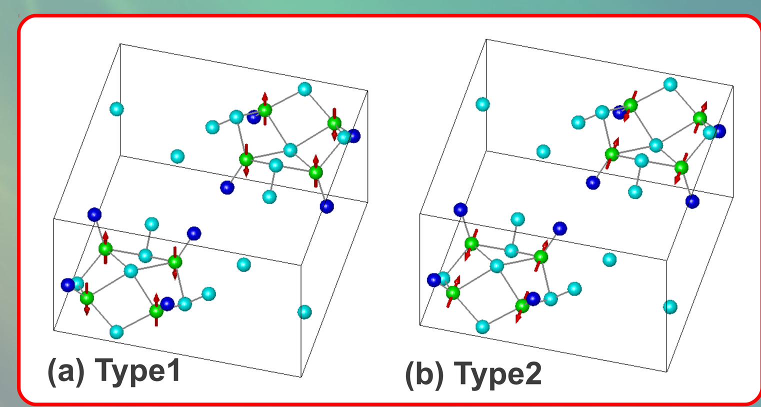
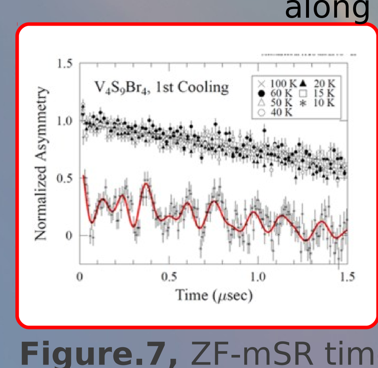


Figure.6, two tested spin structures (a) Antiferromagnetic alignment along the c-axis (Type-1) and (b) antiferromagnetic alignment along the b-axis(Type-2)



Observed frequencies are

A) 2.7 MHz
B) 5.4 MHz
C) 8.7 MHz
D) 12.3 MHz

Figure.7, ZF-mSR time spectra of V4S9Br4 measured at several temperature points. Solid lines are the best-fit results.

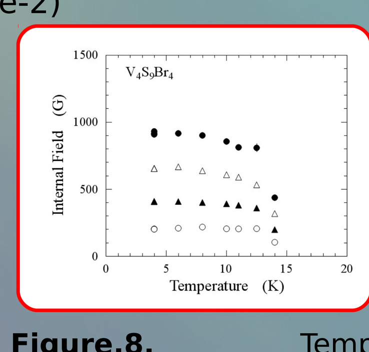


Figure.8, Temperature dependences of observed four components of the muon-spin precession frequencies. The magnetic transition temperature is estimated to be 14 K which is in good agreement with that determined from the susceptibility measurement

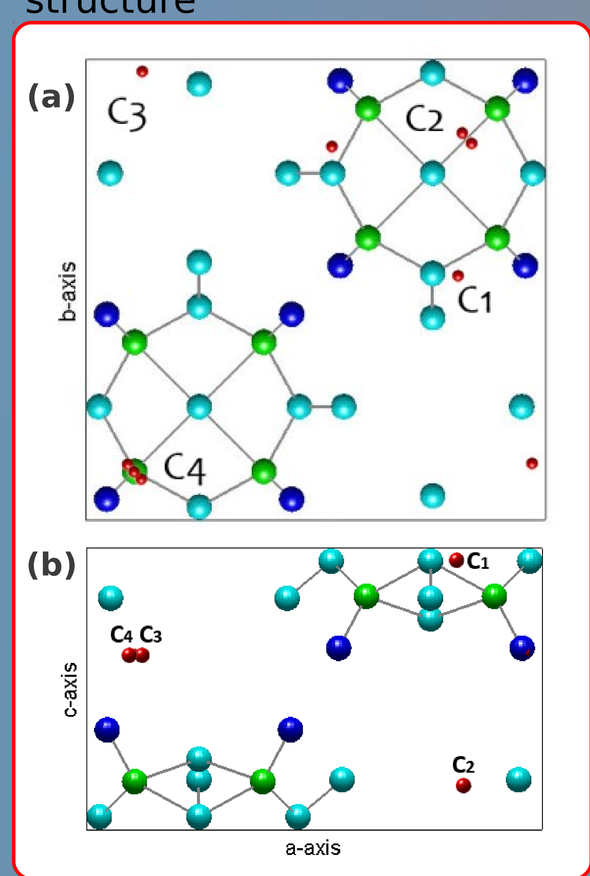


Figure.9, Possible muon sites of the C-site (8.7 MHz) suggested from our simulation of the electronic and nuclear dipole fields (C1,C2,C3, and C4) viewed (a) from the ab-plane and (b) from the ac-plane. Calculations were carried out in the spherical area with the 50 Å radius. The magnetic moment of V-spin was 1.77 μB, and the resolution of the field mapping was 0.054Å.

References:

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