Electronic Supplementary Information for

Magnetic Anisotropy in a spin 1/2 Quasi-One-Dimensional Antiferromagnetic Copper(II) Complex $CuCl_2$(pdz) with a Staggered g-tensor

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ESR spectra

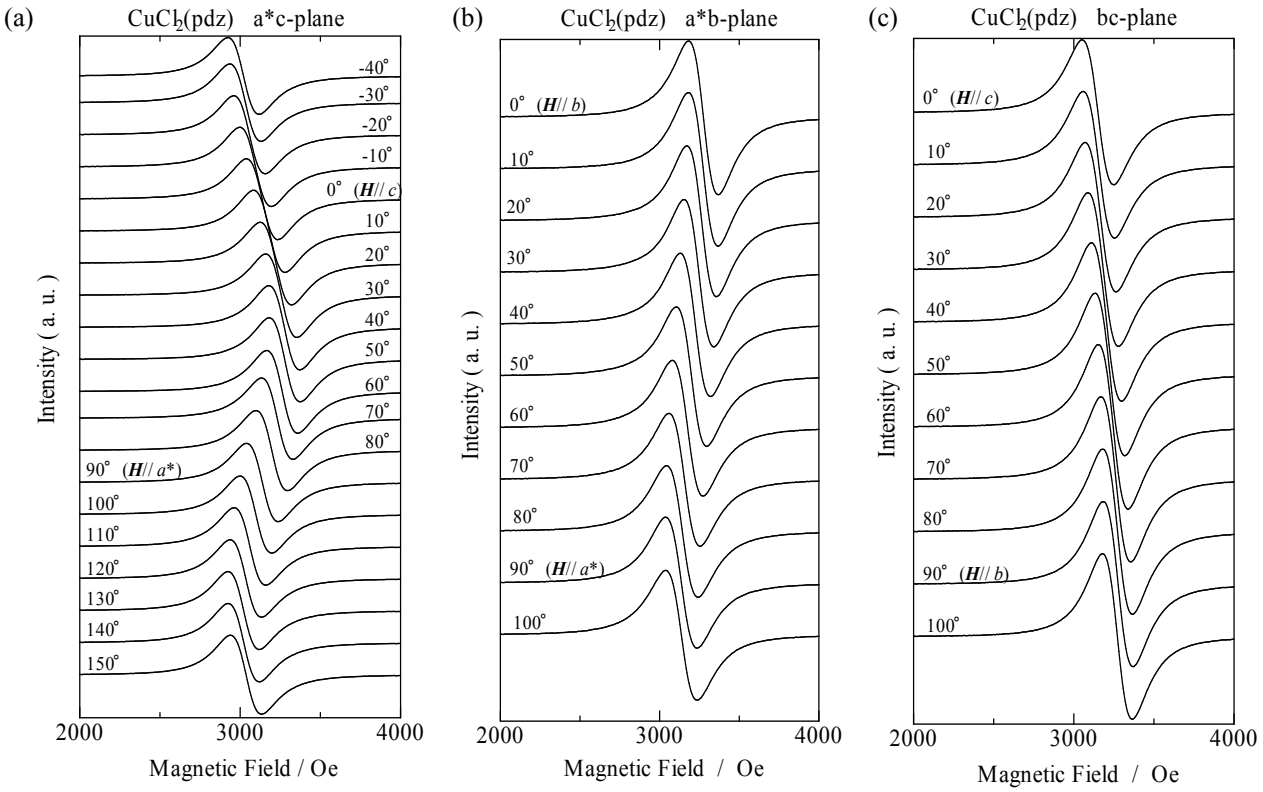


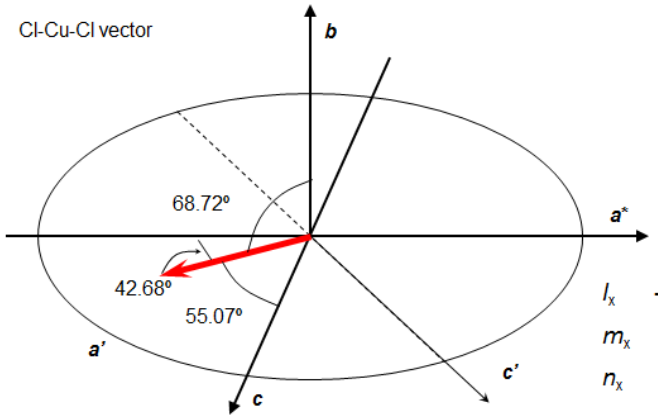
Figure S1 Orientation dependence of ESR spectra at room temperature.

Analyzing detail of deconvolution of the local g-tensor

When considering the direction cosines (l, m, n) of the external field (***H***) with respect to the principal axes of the local g-tensor (g_x, g_y, g_z), observed g-value is given by

$$g^2 = {g_x}^2 l^2 + {g_y}^2 m^2 + {g_z}^2 n^2$$

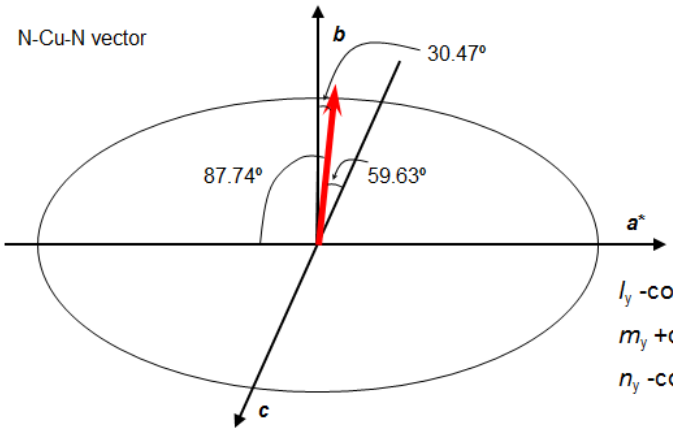
where x, y and z shows the Cl-Cu-Cl, N-Cu-N, and normal to the square plane directions. Meanwhile, we can evaluate the direction cosines of the principal axes of the local g-tensor (l_i, m_i, n_i), where $i = x, y, z$, with respect to the crystallographic axes (a^*, b, c) from the geometry of the local crystal field as shown in Figure S2and S3.



l_x -cos(42.68)= -0.73515, $\cos^2(42.68)$=0.540448

m_x +cos(68.72)= 0.362925, $\cos^2(68.72)$=0.131715

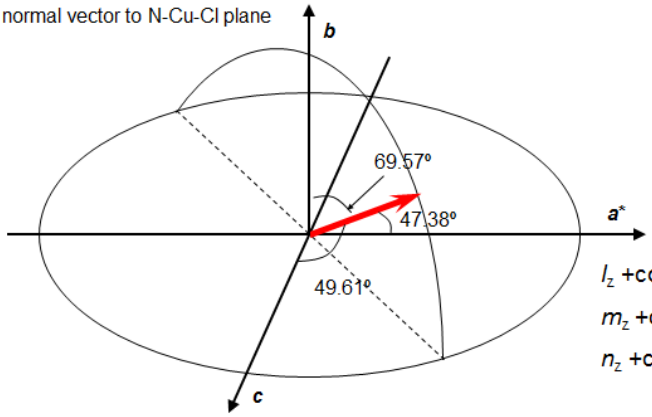
n_x +cos(55.07)= 0.572575, $\cos^2(55.07)$=0.327843



l_y -cos(87.74)= -0.0394342, $\cos^2(87.74)$=0.00156

m_y +cos(30.47)= 0.861895, $\cos^2(30.47)$=0.74286

n_y -cos(59.63)= -0.505582, $\cos^2(59.63)$=0.255613

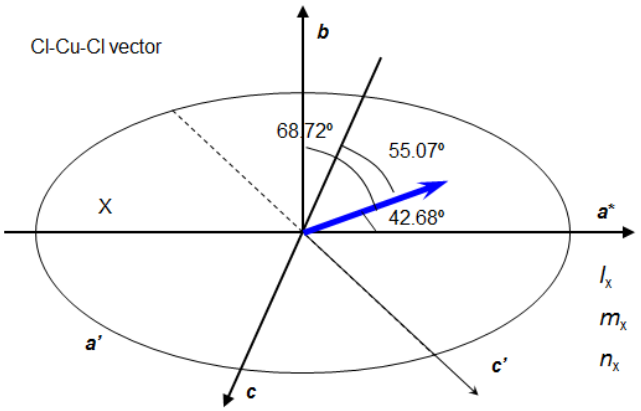


l_z +cos(47.38)= 0.677133, $\cos^2(47.38)$=0.458509

m_z +cos(69.57)= 0.3490628, $\cos^2(69.57)$=0.1218448

n_z +cos(49.61)= 0.6479870, $\cos^2(49.61)$=0.419887

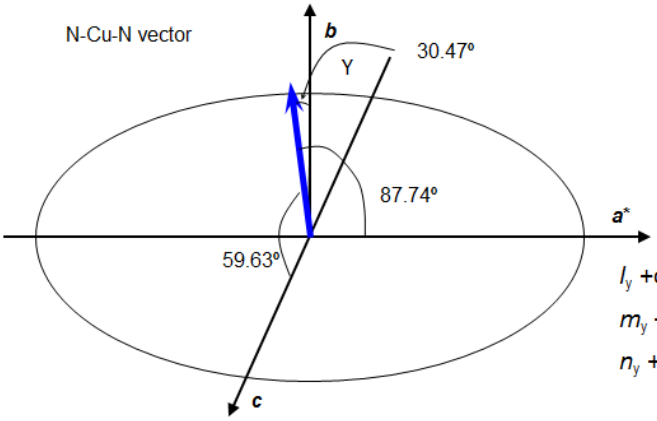
Figure S2 The direction cosines the principal axes of the local *g*-tensor (l_i, m_i, n_i), where $i = x, y, z$, for one sublattice (α-sublattice) with respect to the crystallographic axes.



l_x +cos(42.68)= +0.73515, $\cos^2$(42.68)=0.540448

m_x +cos(68.72)= 0.362925, $\cos^2$(68.72)=0.131715

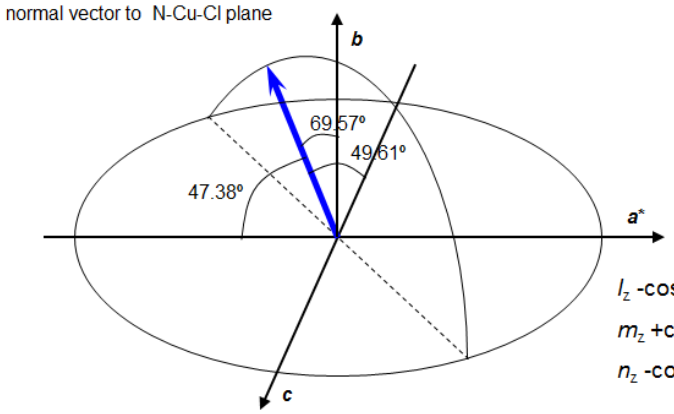
n_x -cos(55.07)= 0.572575, $\cos^2$(55.07)=0.327843



l_y +cos(87.74)= +0.0394342, $\cos^2$(87.74)=0.00156

m_y +cos(30.47)= 0.861895, $\cos^2$(30.47)=0.74286

n_y +cos(59.63)= +0.505582, $\cos^2$(59.63)=0.255613



l_z -cos(47.38)= 0.677133, $\cos^2$(47.38)=0.458509

m_z +cos(69.57)= 0.3490628, $\cos^2$(69.57)=0.1218448

n_z -cos(49.61)= 0.6479870, $\cos^2$(49.61)=0.419887

Figure S3 The direction cosines the principal axes of the local *g*-tensor (l_i, m_i, n_i), where $i = x, y, z$, for other sublattice (β-sublattice) with respect to the crystallographic axes.

When defined the direction cosines of ***H*** with respect to the crystallographic axes (a^*, b, c) as L, M and N, respectively, those are directly given by experiments, l, m and n are shown by the following equations,

$$l = Ll_x + Mm_x + Nn_x$$
$$m = Ll_y + Mm_y + Nn_y$$
$$n = Ll_z + Mm_z + Nn_z$$

Therefore, because observed g-value is average of magnetically inequivalent g-tensor, diagonal elements of the local g-tensor (g_x, g_y, g_z) can be evaluated by fitting the following equation to the orientation dependence of g-value.

$$g = \sqrt{\frac{\left(g_x{}^2 l_\alpha{}^2 + g_y{}^2 m_\alpha{}^2 + g_z{}^2 n_\alpha{}^2\right) + \left(g_x{}^2 l_\beta{}^2 + g_y{}^2 m_\beta{}^2 + g_z{}^2 n_\beta{}^2\right)}{2}}$$

where α and β shows the two magnetically inequivalent sublattices,

We used the following value for the fitting of data on a^*b-plane, bc-plane, and a^*c-plane, respectively.

a^*b-plane (*H* // *b* when θ = 0)

$$l_\alpha = l_{x\alpha}sin(\theta) + m_{x\alpha}cos(\theta)$$
$$m_\alpha = l_{y\alpha}sin(\theta) + m_{y\alpha}cos(\theta)$$
$$n_\alpha = l_{z\alpha}sin(\theta) + m_{z\alpha}cos(\theta)$$
$$l_\beta = l_{x\beta}sin(\theta) + m_{x\beta}cos(\theta)$$
$$m_\beta = l_{y\beta}sin(\theta) + m_{y\beta}cos(\theta)$$
$$n_\alpha = l_{z\alpha}sin(\theta) + m_{z\alpha}cos(\theta)$$

bc-plane (*H* // *c* when θ = 0)

$$l_\alpha = m_{x\alpha}sin(\theta) + n_{x\alpha}cos(\theta)$$
$$m_\alpha = m_{y\alpha}sin(\theta) + n_{y\alpha}cos(\theta)$$
$$n_\alpha = m_{z\alpha}sin(\theta) + n_{z\alpha}cos(\theta)$$
$$l_\beta = m_{x\beta}sin(\theta) + n_{x\beta}cos(\theta)$$
$$m_\beta = m_{y\beta}sin(\theta) + n_{y\beta}cos(\theta)$$
$$n_\alpha = m_{z\alpha}sin(\theta) + n_{z\alpha}cos(\theta)$$

ca^*-plane (*H* // *c* when θ = 0)

$$l = l_x sin(\theta) + n_x cos(\theta)$$
$$m = l_y sin(\theta) + n_y cos(\theta)$$
$$n = l_z sin(\theta) + n_z cos(\theta)$$

We used only l_x, l_y and l_z of α-sublattice for fitting the data on the ca^*-plane, because α and β sublattice become equivalent with respect to the magnetic field parallel to the b-axis.

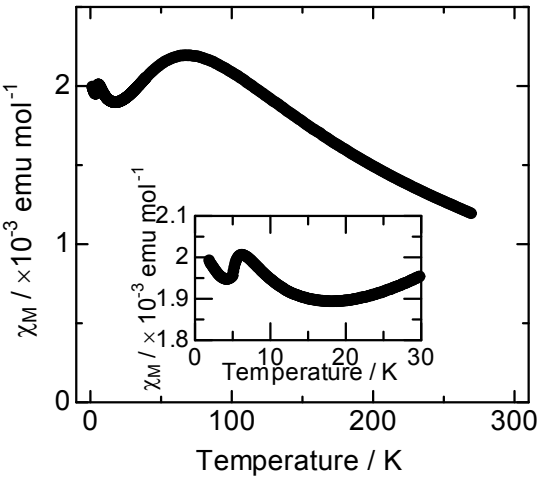


Fig. S4 Temperature dependence of magnetic susceptibility in polycrystalline sample of $CuCl_2(pdz)$ at 10000 Oe. Inset shows magnification of the data below 30 K.

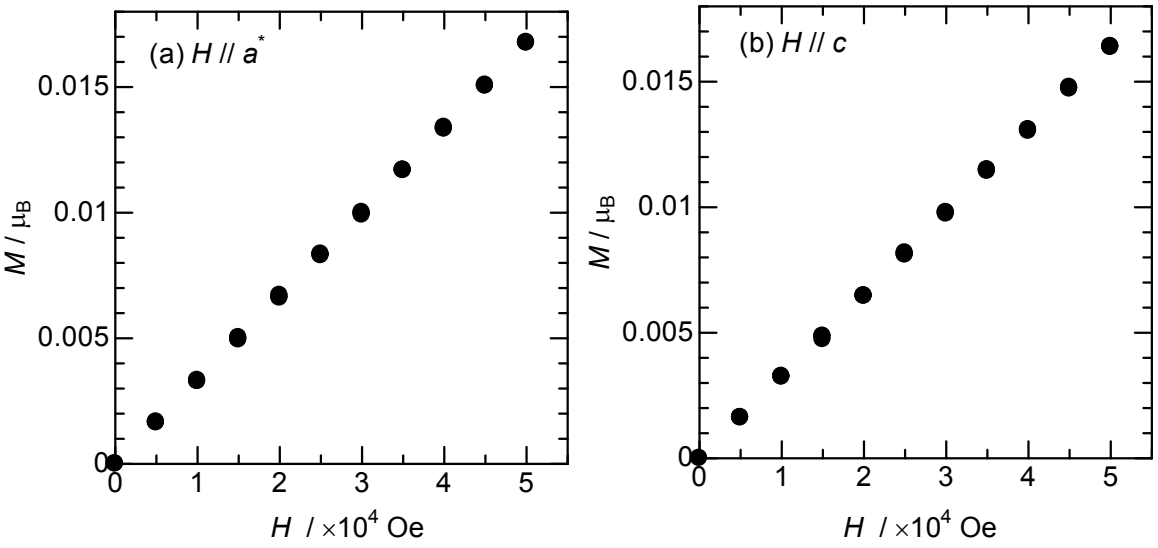


Fig. S5 Magnetization curve (per ion) of $CuCl_2(pdz)$ under (a) H // a^* and (b) H // c at 2.0 K.