

the temperature dependence of the thermal displacement of the copper ions along the [111] directions, with the average density of copper ions being mostly distributed at the center of tetrahedrally-coordinated I ions. As the ionic conductivity increases in the  $\alpha$ -phase, we found local Cu-Cu correlation evolves with the correlation lengths of 2.47 and 2.72 Å (Fig. 1) rather than the average density distribution shown by the MEM result. These two Cu-Cu correlation lengths roughly correspond to distances between neighboring Cu atoms at the tetrahedral 32f-32f sites and 8c-32f sites in the split-atom model of Fm-3m. We will discuss our results in detail of the high ionic conductivity of  $\alpha$ -phase CuI.

Keywords: superionic conductor, split-atom model, copper iodide

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**Hysteretic magnetic and dielectric properties in  $\text{Eu}_{1-x}\text{Y}_x\text{MnO}_3$**

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Magnetolectric effects in multiferroics showing both magnetic and ferroelectric orders have been of great interest in recent years. Rare-earth manganites  $\text{RMnO}_3$  with small ionic radii ( $r_R$ ) of R (e.g. R=Tb and Dy) are typical multiferroics, and their ferroelectricity is attributed to magnetic order.  $\text{EuMnO}_3$  with relatively large  $r_R$  shows (weak)-ferromagnetic and paraelectric properties. By doping yttrium into Eu site, however, the ferromagnetic nature disappears while antiferromagnetic ferroelectric feature emerges. Such evolutions of magnetic and electric properties can be tuned by changing the ratio of Eu to Y [1]. In  $\text{Eu}_{1-x}\text{Y}_x\text{MnO}_3$  with  $x \sim 0.2$ , the ferromagnetic paraelectric state competes keenly with the antiferromagnetic ferroelectric state. To examine the competition between the two phases in more detail, we performed measurements of magnetization and electric polarization in various conditions for single crystals of  $\text{Eu}_{1-x}\text{Y}_x\text{MnO}_3$  ( $x \sim 0.2$ ). In this presentation, we will present the observation of characteristic hysteretic behaviors in magnetic and dielectric properties, and discuss the observed results in terms of spatial coexistence of ferromagnetic and ferroelectric phases.

Keywords: magnetic perovskite materials, magnetolectricity, structural and magnetic phase transitions

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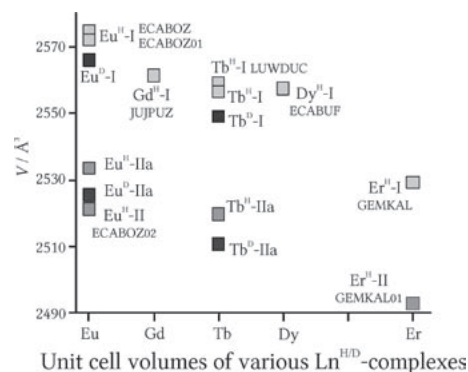
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**Subtle structural differences in the system  $[\text{Ln}(\text{phen}/\text{phen-d}_8)_2(\text{NO}_3)_3]$  ( $\text{Ln}=\text{Eu}^{3+}, \text{Tb}^{3+}$ )**

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Recently we compared the structural and electronic behaviour of  $[\text{Pr}(\text{bathophen})_2(\text{NO}_3)_3]$  (bathophen...4,7-diphenyl-1,10-phenanthroline) with those of its parent phase  $[\text{Pr}(\text{phen})_2(\text{NO}_3)_3]$

[1]. In continuation of this study the effect of phen-d<sub>8</sub> (deuterated 1,10-phenanthroline) on the syntheses of the corresponding europium and terbium complexes, for which two ( $\text{Eu}^{\text{II}}$ -I and II) and one ( $\text{Tb}^{\text{II}}$ -I) modification are described in the literature, is reported here. Precipitation from ethanol and ethanol-d<sub>6</sub> yielded powdery samples with unprecedented compositions. Instead of the expected pure modification I in all four cases, phase mixtures of I and a new modification, IIa, were obtained with preference for IIa when hydrogenated phen was used. Although the modifications' II and IIa crystal structures are very similar, it was possible to elaborate on the differences of II/IIa with the help of synchrotron powder data. Additional measurements of the optical emission properties showed a considerable decrease of the quantum yield in the case of the deuterated terbium complex whereas that of the europium complex is slightly increased. [1] Ishii, A. *et al.* (2007), *ChemPhysChem* **8**(9), 1345-1351



Keywords: modification, deuterium effect, luminescence

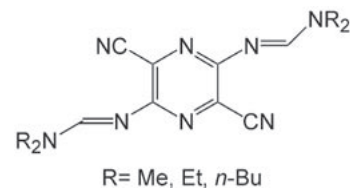
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**Structure-colour relationship of diaminodicyanopyrazine derivatives having azomethine groups**

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Three diaminodicyanopyrazine dyes with azomethine groups (Figure), which show the same colour in solution, were found to exhibit different colours in single crystals depending on the substituents on the amino groups. In this study, structure-colour relationship in the crystals of these pyrazine dyes was investigated in terms of molecular deformation and an exciton interaction. The difference in molecular conformation was found in the dihedral angles between the pyrazine ring and the azomethine groups. This geometrical feature is well-correlated with the calculated absorption band. This result indicates that the present colour difference in a crystalline state can be ascribed to the influence of molecular deformation. An exciton interaction was also estimated by using an extended-dipole model, but its influence was found to be smaller than the energy shift due to the molecular deformation.



Keywords: functional dyes and polymers, structure-colour relationships, intermolecular interactions