**MS28-P4** **Isolated Heptanuclear Bi-capped Dicubane SBUs in a Lanthanide-MOF Series : Structural, Topological, and Luminescent Behavior.** Enrique Gutiérrez-Puebla, Richard D´Vries, Susana Álvarez-García, Alicia de Andrés, Natalia Snejko, and Angeles Monge. *Instituto de Ciencias de Materiales de Madrid, CSIC, Cantoblanco 28049 (Madrid) Spain.*
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A new family of isostructural compounds with formula **$[Ln_7(3,5\text{-}DSB)_4(OH)_9(H_2O)_{15}]\cdot 4H_2O$ (RPF-17**-Ln, where Ln = Y, Sm, Eu, Gd, Tb, Dy, Ho, Er and Yb) is presented. By combining the lanthanide cations with the 3,5-DSB ligand the formation ofsingular hepta-nuclear $[Ln_7(OH)_9]^{+12}$ metallic core SBUhas been promoted. This new core has been defined as a bi-capped dicubane SBU, and acts as a 4-connected node in a bidimensional net with $(4^4{\cdot}6^2)$ topology. The 3,5-DSB ligand acts as a di-topic linker in the 2D net, and contributes to the 3D, UO3 type supramolecular network through the non coordinatedsulfonate oxygen atoms, *via* hydrogen bonds. The analysis of the Raman and infrared vibrational modes along the series compared to the DSB-Na salt evidencesthe stabilization of the aromatic rings in the **RPF-17**-Ln compounds and a reduced symmetrization of the carboxylic bonds in spite of its bidentate bridging coordination. A competition between a broad emission band related to the ligand and the narrow rare-earth transitions leads to the disappearance of the ligand emission for the most efficient f-f transitions observed in Tb and Eu compounds (green and red emissions, respectively)[1],[2].

[1] Rocha, J.; Carlos, L. D.; Paz, F. A. A.; Ananias, D. (2011).*Chem. Soc. Rev.40*, 926

[2] D'Vries, R. F.; Iglesias, M.; Snejko, N.; Alvarez-Garcia, S.; Gutierrez-Puebla, E.; Monge, M. A.(2012) *J. Mater. Chem.22*, 1191.

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**MS28-P5** **Gapless Dispersion Surfacesin Diffraction Physics.** Tetso Nakajima, *Adv. Sci. Res. Lab., SIT, Fusaiji 1690, Saitama 369-0293, Japan.*
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It is significant for constructing gapless dispersion surfaces (GDS) that the diagonal elements in the secular equations in the diffraction physics of the two wave approximation could be formulated from the *quadratic forms of wave numbers* by the *central proper simultaneous linear equations with two unknowns* in following script, by using $h^2/8\pi^2 m = 1$ by atomic units:

$$\begin{vmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{vmatrix} = \begin{vmatrix} (k^2 - \boldsymbol{k}_0^2) & S_{12} \\ S_{21} & (k^2 - \boldsymbol{k}_g^2) \end{vmatrix} =$$
$$k^4 - (\boldsymbol{k}_0^2 + \boldsymbol{k}_g^2)k^2 + \boldsymbol{k}_0^2 \boldsymbol{k}_g^2 - |S_{12} \cdot S_{21}| = 0, \qquad (1)$$

where $\boldsymbol{k_O}$ is the refracted *O*-wave and $\boldsymbol{k}_g$ the reflected *G*-wave, which satisfy the Bragg condition $\boldsymbol{k_O} + \boldsymbol{k}_g = \boldsymbol{K}_g$, where $|\boldsymbol{k_O}| \cong |\boldsymbol{k}_g|$ only in an ε -neighborhood of the Brillouin zone boundary (BZB). Then, two roots of $X(= k^2)$ in eq. (1) could be given by:

$$X = (1/2) \cdot \left[ (\boldsymbol{k}_0^2 + \boldsymbol{k}_g^2) \pm \left\{ (\boldsymbol{k}_0^2 - \boldsymbol{k}_g^2)^2 + 4|S_{12} \cdot S_{21}| \right\}^{1/2} \right], \quad (2)$$

where omitted $U_0$, since the average value of $U(\mathbf{r})$, which only translates the origin of *X*. The indefinite refracted states $k$ as unknown are characterized by lifting both degenerated states of $\boldsymbol{k_O}$ and $\boldsymbol{k_G}$ due to the perturbations of off-diagonals $S_{12}$ and $S_{21}$ and contributing to the momentum GDS. Both of $S_{12}$ and $S_{21}$ in eq. (1) are given by the $g$th Fourier components of the periodic potential energy $U(\mathbf{r})$ in the crystal in electron and neutron diffractions and similarly by $g$th Fourier components of the electric susceptibility $\chi(\mathbf{r})$ in X-ray diffraction. (Here, when absorption can be neglected, $|S_{12} \cdot S_{21}|$ should be $|S_{12}|^2$, since $S_{12} \cdot S_{21}$ could be real.) It can be considered that the magnitudes of $\boldsymbol{k_O}$ and $\boldsymbol{k_G}$ are so different that the term $4|S_{12}|^2$ under the radical sign in eq. (2) can be neglected compared with the first term. Then, $X$ takes the value $\boldsymbol{k}_0^2$ or $\boldsymbol{k}_g^2$ and either the amplitudes of $\chi_\mathbf{O}$ or $\boldsymbol{d}_0$ of *O*-wave or those of $\chi_{\boldsymbol{g}}$ or $\boldsymbol{d}_g$ of *G*-wave, which could be determined from the ratio of the elements in a row of eq. (1), becomes zero. Consequently, the solution is a plain wave of $\boldsymbol{k_O}$ or $\boldsymbol{k_g}$. If the magnitudes of $\boldsymbol{k_O}$ and $\boldsymbol{k_g}$ are close each other, then $4|S_{12}|^2$ cannot be neglected. Thus the amplitude of neither plane wave is negligible. When $|\boldsymbol{k_O}| = |\boldsymbol{k}_g|$, we have $\boldsymbol{k^2} = 1/2\,(\boldsymbol{k_0^2} + \boldsymbol{k_g^2}) \pm |S_{12}|$ and hence the ratio of $\chi_\mathbf{O}{:}\chi_{\boldsymbol{g}}$ and $\boldsymbol{d}_0{:}\boldsymbol{d}_g$, determined from eq. (1) is $S_{21}{:}\pm|S_{12}|$. Therefore, $\chi_\mathbf{O}{:}\chi_{\boldsymbol{g}}$ and $\boldsymbol{d}_0{:}\boldsymbol{d}_g$ are $1{:}1$. In case of $|\boldsymbol{k_O}| \approx |\boldsymbol{k}_g|$, assuming that $4|S_{12}|$ is larger compared with the first term under the radical sign in eq. (2), the roots *X* can be expanded in the following series,:

$$X = (1/2) \cdot (\boldsymbol{k}_0^2 + \boldsymbol{k}_g^2) \pm |S_{12}| \pm (\boldsymbol{k}_0^2 - \boldsymbol{k}_g^2)^2 / 8|S_{12}| \pm \cdots \quad (3)$$

If we translate the origin of $\boldsymbol{k_O}$ by $-\boldsymbol{K}_g/\boldsymbol{2}$ and consider the vector $\boldsymbol{k_O} + \boldsymbol{K}_g/\boldsymbol{2}$, and if we denote by $\boldsymbol{x}$ the component of $\boldsymbol{k_O} + \boldsymbol{K}_g/\boldsymbol{2}$ parallel to $-\boldsymbol{K}_g$ and by $z$ the normal component, then eq. (3) can be written as $X = \boldsymbol{z^2} + \boldsymbol{x}^2 + \boldsymbol{K}_g^2/4 \pm |S_{12}| \pm \boldsymbol{x}^2/(2|S_{12}|/\boldsymbol{K}_g^2) \pm \cdots$, by using the following relations: $\boldsymbol{k}_g^2 = \boldsymbol{k}_0^2 + 2\boldsymbol{k_O}\boldsymbol{K}_g + \boldsymbol{K}_g^2 = \boldsymbol{k}_0^2 + 2\boldsymbol{x}|\boldsymbol{K}_g|$ and $\boldsymbol{k}_0^2 = \boldsymbol{z}^2 + \boldsymbol{x}^2 + \boldsymbol{x}|\boldsymbol{K}_g| + |\boldsymbol{K}_g|^2/4$. The result of the solutions of the coupled ellipse and hyperbola as a new universal GDS from the 4th and 5th terms in eq.(3) in an ε -neighborhood of BZB could be represented as:

$$X(\perp \boldsymbol{x}\,\&\,z) = k^2(\perp \boldsymbol{x}\,\&\,z) = \boldsymbol{y}^2$$
$$= \pm|S_{12}| \pm \boldsymbol{x}^2/(2|S_{12}|/\boldsymbol{K}_g^2) = \pm b^2 \pm (\mathrm{b}/a)^2\boldsymbol{x}^2, \qquad (4)$$

where $a^2 = (\sqrt{2}|S_{12}|/K_g)^2$ and $b^2 = |S_{12}|, (b \gg a)$ in the canonical form of $(y/b)^2 \pm (x/a)^2 = \pm 1$ from which reasonable GDS from eq. (4) could be determined. Detailed discussion on the new universal GDS will be given.