

The external perturbations can be temperature, light irradiation, pressure, and pulsed magnetic fields all may change the magnetic coupling interaction in transition metal systems. Here, we use pressure as external force to study magneto-structural correlation.

We report here the structure and magnetic behavior of one 1-D helical chain iron complex $[\text{FeII}(\mu\text{-bpt})(\mu\text{-COOC}_5\text{H}_4\text{N}) \cdot 1/2 \text{H}_2\text{O}]_n$ (bpt=3,5-bis (pyrid-2-yl)-1,2,4-triazole), [1], in ambient conditions and under hydrostatic pressure. The complex was crystallized in a tetragonal space group $I4_1/a$ at ambient pressure, each iron atoms linked by one bpt and one isonicotinic acid legend, which form an infinite helical chain along the screw axis 4_1 at c-axis direction. The iron atoms are iron (2+) high spin state with distorted N_4O_2 coordinated shell.

High-pressure powder X-ray diffraction experiments from 0.03GPa to 2.79GPa pressure were carried out to understand precisely the correlation between the structure and magnetic behavior. The careful analysis of a series high pressure structures showing a pressure-induced shrinking more than 10% along the chain direction, which can describe as spring compressed 10%. This make the iron-iron distance from 4.445(2) Å at ambient pressure change significantly to 4.083(6) Å at around 2GPa. Magneto-structural correlation will be discussed. The coordinated shells of Iron (N_4O_2) also decrease 0.11 Å about averagely. The spin state of iron and magnetic property of title compound also will be shown in this report

[1] S-M Chen, *Structure and Magnetic Properties of Dinuclear metal Complexes with a Tetradentate bpt Ligand*. Ph. D. Thesis, 2009, National Taiwan University, Taipei, Taiwan. R.O.C.

Keywords: high pressure XRD, molecular magnetic materials, high pressure magnetism

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Structure and OD character of $5M_3$ ferriphlogopite from Ruiz Peak

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The first finding of a non-MDO mica polytype where two types of layers coexist is here reported. The sample is a 5-layer ferriphlogopite from Ruiz Peak, New Mexico, crystallizing in $C2$, $a = 5.3146(2)$ Å, $b = 9.2063(3)$ Å, $c = 49.730(2)$ Å, $\beta = 92.031(4)^\circ$. Data collection was performed on a Mar345 equipped with image plate detector, with completeness of 99.4% up to resolution 0.8 Å, 5049 unique reflections of which 3195 observed, and redundancy 13.6. The homo-octahedral stacking sequence was determined by PID analysis [1] and corresponds to the $5M_3$ polytype [2]. The structure model was obtained from the atomic coordinates of the $1M$ polytype by applying the stacking vectors, and refined with Jana2006 [3], to $R_{\text{(obs)}} = 7.03\%$. A reliable model for the distribution of the octahedral cations (Mg^{2+} , Al^{3+} , Fe^{3+} , Ti^{4+}) in the 9 independent sites cannot be obtained by structure refinement; the occupation of these sites has instead been estimated by exploiting the OD nature of mica polytypes [4]. An iterative computation of the Fourier map from a hybrid data set including computed family diffractions ($k = 3n$), which correspond to the family structure in which all octahedral site have the same content, and observed non-family diffractions, followed by adjustment of the model to reproduce the computed map, has been performed; this unambiguously resulted in two layers out of three having a prominent peak in a *cis* site, all the layers being meso-octahedral. The OD symbol for this polytype is $|1.5\ 5.3\ 5.5\ 1.1\ 3.1|$.

The $5M_3$ polytype with all layer of type $M1$ (origin of the octahedral sheet in the *trans* site) belongs to the $3T$ structural series. In this

case, however, the presence of $M2$ layers testifies the occurrence of structural adjustments at the polytype formations stage [5]. The original components could have been a two equal basic structures ($1M$ or $2M_1$) differently oriented, or two different basic structures ($1M$ or $2M_1$ or $3T$). The possible formation mechanism is currently under investigation.

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Euclidean groups in spaces of arbitrary dimensions

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Different categories of Euclidean groups are established according to an analysis of the Fundamental theorem on Euclidean groups which is formulated and proved. The first division is into the *space*, *subperiodic* and *site point groups*. According to the character of the translation subgroup, the groups with the *discrete*, *continuous* and *semicontinuous* lattice are distinguished. The groups are classified as the *crystallographic*, *noncrystallographic* and *partially crystallographic* groups. In this connection, the concepts of crystallographic and space groups are amended.

Geometric classes and their splitting into arithmetic classes are defined as usual. Arithmetic classes are the natural classification units and the groups of such a class are distinguished by systems of nonprimitive translations in Seitz symbols for Euclidean operators. If the geometric class is reducible (irreducible) then the arithmetic class is either reducible or decomposable (irreducible). The factorization of the groups of decomposable or reducible classes by partial translation subgroups leads to groups of lower dimensions of the translation subgroup.

The class of the systems of nonprimitive translations which differ only by shift functions define an *extension class* within which the groups differ only by their location. Groups of the extension class have the same Hermann-Mauguin symbol and the same symmetry diagram. It is shown how to take the group location into consideration which is not done in Vol. A of IT. As a result, the data about subgroups are incomplete. The location of groups has been first considered in Vol. E of IT and in a software attachment GI * KoBo-1 to Vol. D of IT.

Diagrams of the Young type are suggested for a rough classification of groups in arbitrary dimensions. The groups up to three dimensions are considered in detail as the groups of material physics and a unique system of Hermann-Mauguin symbols for them is developed.

Keywords: seitz symbols, extension class, group location

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3D space groups 2D hyperbolic orbifolds and “sponge” groups

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Crystallographic patterns in three-dimensional euclidean space (E3) can be generated via orbits of motifs under the action of certain two-dimensional discrete groups acting in hyperbolic space (H2) followed by “wrapping” of the hyperbolic planar pattern onto three-periodic hyperbolic surfaces (e.g. minimal surfaces). This approach underlies the EPINET project [1] described in detail elsewhere [3], [4], [5].

We describe an explicit mapping between H2 and E3, mediated by three-periodic hyperbolic surfaces embedded in E3, that allows unique identification of a discrete hyperbolic group plus a surface with a space group.

The approach leads to the following concepts. First, point and plane groups describe isometries of the 2D sphere and euclidean plane respectively. Orbifolds offer a single coherent concept for point, plane and “saddle” groups, where the latter are isometries of H2. Second, we present a simple taxonomy of these groups into 8 classes via orbifolds, based on the generic topological and conformal structure of the orbifold. Third, we define crystallographic saddle groups (“sponge groups”) -- analogous to crystallographic point groups. These include those hyperbolic orbifolds whose orbits on embedded surfaces induce space groups in E3. We present a number of sponge groups within all eight classes, including the most symmetric example. These results allow many of the 230 space groups to be described in a concise manner, combining 2D isometries with surface topology.

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Crystal planes in Clifford geometric algebra

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Clifford’s geometric algebra [1] efficiently encodes geometric information in terms of compact algebraic expressions. These expressions allow to easily retrieve all geometric properties (radius, position, center, normal directions, orientation, distances, angles, ...), and one can simultaneously use these expressions as operators for transformations like reflections, rotations, roto-reflections, inversions (at points and spheres), roto-reflections, glide and screw transformations, etc. Products allow to combine objects, to intersect them, to compute their relative location and angles, etc. Thus geometric algebra has already been successfully applied to the description of crystallographic symmetry [2], [3]. We now extend this treatment by studying the description of offset subspaces in the geometric algebra of projective space $Cl(R^{n+1})$ and in the conformal model of Euclidean geometry, i.e. in $Cl(R^{n+1,1})$, see e.g. [4]. In particular, crystal planes in any dimension are such offset subspaces. The problem of defining a kD plane in terms of $k+1$ points on the plane is easily solved by taking the *outer* product of these points. Reciprocal vectors appear as support vectors of crystal planes, identical to the Euclidean parts of dual vectors describing hyperplanes in the above model algebras [5].

We mainly address crystallographers, who want to know how to successfully express their problems in the new comprehensive mathematical language of Clifford geometric algebra. We see a need for this, because so far many mainstream crystallographers are relatively unfamiliar with Clifford geometric algebra [6]. We focus on expressing key notions in standard crystallography, which clearly demonstrate how to employ the powerful invariant and dimension-

independent tools of Clifford geometric algebra. Thus we explain e.g. how to turn crystallographic *Miller indexes* into multivector expressions for crystallographic planes, and based on this how to directly compute crystal plane d -spacing, phase angles of structure factors, reflection conditions for the occurrence of Bragg reflections, interfacial angles, and the like.

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Symmetry relations and phase stability of magnesium borohydride $Mg(BH_4)_2$

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We studied the phase stability of $Mg(BH_4)_2$ by means of symmetry analysis of different structures optimized via first-principles methods [1]. In particular, we focused on the symmetry relations between space groups I41/amd (IT 141), I-4m2(IT 119) and F222 (IT 22) as one chain of subgroups and groups I41/amd (IT 141), Fddd (IT 70) and F222 (IT 22) as the second chain of subgroups. By that analysis, based on the theory of space groups and their representations (symmetry analysis method –SAM [2]) we found all transformations from the parent structure, described by the high symmetry group, to the structures with symmetries belonging to the appropriate subgroups. The main interesting result of the symmetry transformation provided the displacements of the atoms from their initial positions (by polar vector type SAM), and the ordering of clusters localized on given positions (by second rank tensor type SAM). The deformations of BH_4 clusters have been investigated by these two ways. Both vector and tensor type methods lead to the same description of ordering of deformed clusters, with the number of free parameters reduced to the same necessary minimum. Moreover this minimal number of free parameters has been used in the procedure of finding the lowest total energy for each proposed model of $Mg(BH_4)_2$ structure as follows. For every transformation from parent group to it subgroup, from symmetry point of view, each atom is allowed to move only in a strictly given direction (a displacement vector). This permits us to reduce the number of parameters we have to consider when looking for the minimum energy of the system under investigation. For example: the transition between groups (IT 141) and (IT 119) for $Mg(BH_4)_2$ in general is described by 264 free, independent parameters (88 atoms in the unit cell, each can move along x,y,z axis). Using the symmetry analysis this number is reduced to only 9 coefficients and in the case of transition between (IT 119) and (IT 22) this number becomes 12