

THE MUSIC OF MOLECULES: NOVEL APPROACHES FOR STEM EDUCATION

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Abstract

A wide range of teaching strategies have been employed to improve the effectiveness of STEM education. In some studies, music has been used as a tool to help memorizing scientific concepts. However, music (without lyrics) can also be considered in itself as an interesting way to explore and explain the complexity of both natural and artificial structures, and a way to guide learners of every age towards the deep understanding of the difficult concept of molecular order. For this purpose, we developed a scientifically based “decryption” method to assign a given sound to single atoms within crystals. All sound parameters (pitch, duration, timbre, and dynamics) are based on physical and chemical properties of the atoms involved in the structure. The “crystal soundtrack” is accompanied by animations highlighting the position of each atom considered in its context. Possible applications of this novel educational approach range from chemistry (atomic structures, the periodic table, the octet rule), to Earth sciences (the structure of natural crystals), material sciences (artificial structures), and biology (macromolecules such as sugars and nucleic acids). Musical examples will be presented and discussed.

Keywords: STEM education; Music; Molecules; Crystals.

1 INTRODUCTION

Implementing STEM education is widely considered a priority for today's society [1; 2] Rocard et al. 2007; Kearney 2016). Every effort must be undertaken to change the die-hard students' view that science is just a dull sequence of facts and formulas. Novel, stimulating approaches involving different levels of perception can help in increasing learners' interest in several aspects of science. In science education the expression “seeing is believing” is especially meaningful, and consequently many laboratory activities are oriented at showing natural phenomena. However, basic aspects of science, such as the molecular structure of matter, are quite hard to visualize. The usual representations of chemical structures, namely molecular and structural formulas, appear difficult to memorize. Even worse, the actual significance of atom arrangements within large molecules and crystals remains vague. Hence the necessity of experimenting novel approaches supporting the understanding of concepts as complex as molecular order/disorder, and crystal symmetry.

Being the “universal language of mankind” (H.W. Longfellow), music has the potential to provide an effective support to science communication. Historically, music and mathematics have always been strongly related, from Pythagoras to Milton Babbitt and beyond [3]. Indeed, music is an art of time, since a musical piece develops with a temporal order. Some contemporary composers (e.g. Steve Coleman, Miles Okazaki) organized their music using time-dependent phenomena of natural or artificial origin. The French composer Edgar Varése (1883-1965) used the crystals as a symbolic model for musical composition [4]: “There is an idea, the basis of an internal structure, expanded and split into different shapes or groups of sound constantly changing in shape, direction, and speed, attracted and repulsed by various forces. The form of the work is a consequence of this interaction. Possible musical forms are as limitless as the exterior forms of crystals.” He was aware and stimulated by the existing relations between the structure and the forms of crystals where, despite the few elements and the point symmetry present in the unit cell, the possible forms are unlimited.

Interestingly, the British chemist John Newlands (1837-1898), in his pioneer studies on the periodic properties of elements (about four years before the first publication of Mendeleev's hypotheses) suggested a theory called Law of Octaves: “members of the same group stand to each other in the same relation as the extremities of one or more octaves in music” [5]. Unfortunately, Newland's theories were not taken too seriously by his contemporaries. Nowadays, we lack a scientifically-based system of musical representation of elements and their spatial relationship within crystals. Aim of the

present work is to set a method to describe crystal structures in musical form, in order to obtain a new and attractive teaching tool for science education.

2 THE WORLD OF CRYSTALS

2.1 Chemistry

All matter is composed of atoms. Each atom's nucleus is composed of proton(s) and neutron(s). Electron(s) placed in orbitals with different energy levels complete the atomic structure. The number of protons in the nucleus (atomic number, Z) defines an element. As noticed by Newlands and later by Mendeleev, the elements placed horizontally (periods) according to their atomic number show recursive properties in their vertical arrangements (groups). In the simplified table in Fig. 1, lacking transition elements, periods and groups are showed. As an example, all elements of group seven (halogens) share similar chemical reactivity, related to the presence of seven electrons in their outer s and p orbitals.

GROUPS									
		I	II	III	IV	V	VI	VII	VIII
PERIODS	1	H						He	
	2	Li	Be	B	C	N	O	F	Ne
	3	Na	Mg	Al	Si	P	S	Cl	Ar
	4	K	Ca	Ga	Ge	As	Se	Br	Kr
	5	Rb	Sr	In	Sn	Sb	Te	I	Xe
	6	Cs	Ba	Ti	Pb	Bi	Po	At	Rn

Fig. 1 The Periodic Table of Elements (partial)

2.2 Crystallography

The solid state is a form of condensed matter where the atoms are in close proximity to each other and are characterized by both a well-defined volume and a well-defined shape. The solids can be classified as function of their atomic-scale structure in two main classes: crystalline and amorphous. Atomic positions in crystalline materials exhibit a property called "long-range order" or "translational periodicity"; i.e. the atomic positions are repeated in space in a regular array. In amorphous solids, translational periodicity is absent, i.e. they only have a "short-range order", consequence of the chemical bonding between atoms holding the solid together. As a consequence of the lack of translational symmetry in the amorphous solids, their properties are isotropic, i.e. independent of the direction in which they are measured. Contrarily, in general, crystals are anisotropic, meaning that their properties will be affected by the observation direction. The latter can be defined on the basis of a unit cell, which represents the smallest volume of the crystal having the same rational properties of the crystal. The unit cell is the smallest building block of a crystal, whose geometric arrangement defines the crystal's characteristic symmetry and whose repetition in space produces the crystal lattice of the solid. The unit cell is an expression of the ordered internal arrangement of atoms in the crystal and contains all the symmetry elements operating into the crystal structure. Indeed, in addition to the translational symmetry, also symmetry operations such as rotation- and screw-axes, reflection- and

glide-mirrors, inversion centers or a combination of these can be present in the crystal structure and therefore operate also inside its unit cell (Table 1).

Table 1. Symmetry operators compatible with the crystalline state.

Symmetry Element	Point elements	Elements with translation
Proper	Rotational axes 1 2 3 4 6	Screw axes $2_1 3_1 3_2 4_1 4_2 4_3 6_1 6_2 6_3 6_4 6_5$
Improper	Inversion axes $\bar{1} \bar{2} \bar{3} \bar{4} \bar{6}$	Glide planes $a b c n d$

When a crystal forms without impediments to its growth, crystal faces form as smooth planar boundaries that make up the surface of the crystal. These crystal faces are expression of the ordered internal arrangement of atoms and reflect the symmetry of the crystal lattice stripped of any translational components. Therefore, the study of the morphology of the crystal allows the derivation only of the set of symmetry elements without translations, called "symmetry class" or "point group" of the crystal. This symmetry, however, will not be the same of the crystal, if screw axes or glide planes operate in it (Fig. 2).

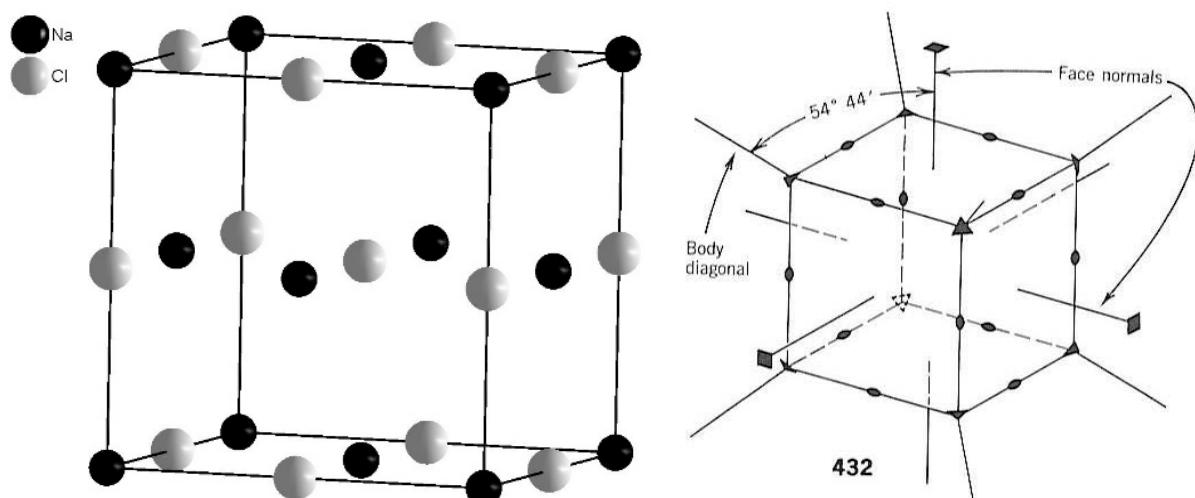


Figure 2. Unit cell of sodium chloride (NaCl) and its point rotational axes

In addition, crystals can also exhibit phenomena of polymorphism; i.e. two or more minerals have identical chemical content but different crystal structures. For example, two polymorphs of C very known are graphite and diamond. Graphite structure is composed of sheets of six-member rings of C atoms, where each carbon atom has three neighboring atoms positioned at the vertices of an equilateral triangle. Diamond crystal structure, differently, has each carbon atom bond to four others located to the apices of a regular tetrahedron. In spite of their identical chemical composition, the different crystal structures give to the diamond a stronger lattice if compared to that of the graphite (Fig. 3).



Fig.3 Diamond crystal (left) and graphite sample (right)

3 METHODOLOGY

Our method of translation of crystalline structures into music tries to give aural images of crystals in order to strengthen the message of traditional educational approaches to mineralogy/crystallography or substitute it for unsighted persons. Such translation needs a formalized algorithm to convert chemical compositions and crystal structures in organized sounds. Crystals, as anisotropic entities, need directional tools to be described using the music. Preferred directions in the crystal related to symmetry operators determine the families of crystallographic planes perpendicular to them, which is scanned to translate the crystal structure into music. This approach tries to highlight the anisotropies of the crystal structures according to the observation direction (§ 2.2).

Each crystal phase is defined by a fixed stoichiometry and a specific symmetry (i.e. space group). Our approach considers both aspects in order to determine the rhythm and timbre (position of a given element in the periodic table), and the pitch and intensity (atomic polar coordinates in the unit cell) of notes. The musical composition algorithm is not used with aesthetic end, although the translation into music of crystal chemical composition and symmetry was not mechanical, but compositional skills have been used to improve both the musicality and the educational potential of the outputs.

The starting point of the algorithm is to determine the duration and the instruments of the notes corresponding to the elements in a given crystal. The position of each element in the periodic table gives unique correspondence with the duration and the timbre of the related notes in the score. The duration of notes was inspired by the octet rule introduced in 1916 by Lewis [6] and Kossel [7] in separate publications.

Just as we have semitone as interval unit in pitch determination, we used the quaver () as a rhythmic unit for duration. The duration of each note is thus determined after the following equation:

note duration = \times group (Fig. 4). The durations originated form a geometric progression.

The music originated has a pulsed tempo, which can be regular or irregular, according to the sequence of duration obtained from the “scanning” of the crystallographic plains. The music originated is ametric (i.e. music not depending on metric organization), but in analogy to the octet rule, within the melody some durations of notes will sum up to 8/8 more or less regularly, giving a sense of metre.

The tempo (i.e. speed of musical execution) it is not predetermined after the crystal structure, but is fixed *a posteriori* to facilitate the understanding of the structure.

To assign the instruments to the elements, we associate the periods of the periodic table with different families of instruments (Fig. 4). As an example, since the elements of the second period include those typical of organic compounds (i.e. Carbon, Nitrogen, Oxygen), we associate them to voices, symbolizing life. The pitched percussions are the instruments of the third period, assigned to the different elements according to the sound decay, and so on.

		tone duration = $\text{note} \times \text{group}$									
		I A	II A	III A	IV A	V A	VI A	VII A	VIII A		
(1)		hydrogen H 1.0079							helium He 4.0026		
Human voices (2)		lithium Li 6.941	beryllium Be 9.0122		boron B 10.811	carbon C 12.011	nitrogen N 14.007	oxygen O 15.999	fluorine F 18.998	neon Ne 20.180	
Pitched percussions (3)		sodium Na 22.990	magnesium Mg 24.305		aluminum Al 26.982	silicon Si 28.086	phosphorus P 30.974	sulfur S 32.065	chlorine Cl 35.453	argon Ar 39.948	
Brass instruments (4)		potassium K 39.098	calcium Ca 40.078		gallium Ga 69.723	germanium Ge 72.64	arsenic As 74.922	selenium Se 78.96	bromine Br 79.904	krypton Kr 83.798	
Woodwinds (5)		rubidium Rb 85.468	strontium Sr 87.62		indium In 114.82	tin Sn 118.71	antimony Sb 121.76	tellurium Te 127.60	iodine I 126.90	xenon Xe 131.29	
Chordophone instruments (6)		caesium Cs 132.91	barium Ba 137.33		thallium Tl 204.38	lead Pb 207.2	bismuth Bi 208.98	polonium Po [209]	astatine At [210]	radon Rn [222]	
Synthesizers (7)		francium Fr [223]	radium Ra [226]								
tone duration = $(\text{note} \times \text{group}) - \text{note}$											
		III B	IV B	VB	VI B	VII B	—	VIII B	—	IB	II B
(4)		scandium Sc 44.956	titanium Ti 47.867	vanadium V 50.942	chromium Cr 51.996	manganese Mn 54.938	iron Fe 55.845	cobalt Co 58.933	nickel Ni 58.693	copper Cu 63.546	zinc Zn 65.38
(5)		yttrium Y 88.906	zirconium Zr 91.224	niobium Nb 92.906	molybdenum Mo 95.96	technetium Tc [98]	ruthenium Ru 101.07	rhodium Rh 102.91	palladium Pd 106.42	silver Ag 107.87	cadmium Cd 112.41
(6)		57-71 lanthanide series	hafnium Hf 178.49	tantalum Ta 180.95	tungsten W 183.84	rhenium Re 186.21	osmium Os 190.23	iridium Ir 192.22	platinum Pt 195.08	gold Au 196.97	mercury Hg 200.59
(7)		89-103 actinide series	rutherfordium Rf [261]	dubnium Db [262]	seaborgium Sg [266]	bohrium Bh [264]	hassium Hs [277]	meitnerium Mt [268]	darmstadtium Ds [271]	roentgenium Rg [272]	

Transition metals

Figure 4. Scheme showing how sound duration and timbre are associated to the different elements

Once the instruments and the durations of notes are set, the unit cell of the crystal should be identified to score the music. When two or more unit cells are possible, the smallest one is chosen.

The abstraction of symmetry operations is a useful key to translate crystal structures, or more generally molecular structures, into music. As explained above, the characterizing rotation axis has the precedence over polar coordinates of atoms to determine pitch and dynamics of related notes. The path along the symmetry axes is described by a melody or a counterpoint obtained after the translation of a given crystalline phase into musical language.

The pitch of each note is assigned on the basis of the angles formed by each atom in the crystal structure, conventionally assigning the starting point to an atom in the C position. The symmetry axis taken into account passes through the origin of the pitch disk, which is parallel to the plane family perpendicular to it. Therefore, an atom at 30° from the starting position becomes C#, according to the scheme in Figure 5. Angles falling in the sectors between two limit angles are represented with clusters of the two corresponding notes (e.g. 45°, D#-D). In this way, the position of each atom lying on a given plane determines an ordered pitch set used to score the music. A numeric using digits between 0 and 11 is also possible [8]. The sequence of tones is created alternating clockwise and counterclockwise scans of the piled planes.

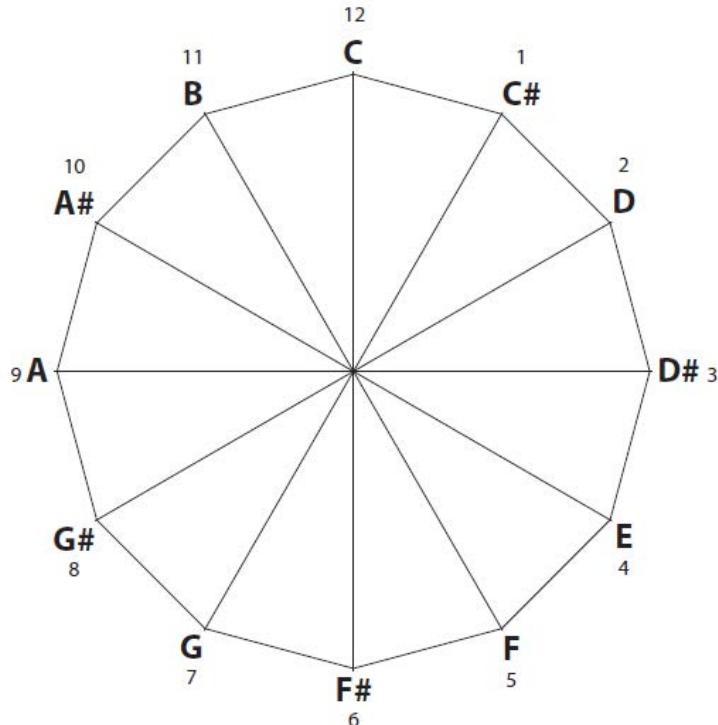


Figure 5. The Pitch Disk, representing the note pitches as a function of angles within the crystal structure. The center of the circle is placed in correspondence of a symmetry element

Some exceptions occur for those atom positions, which fall on the pitch disk center. In our method, this position is conventionally associated with C or F#(Gb) according to the previous and or following pitch in the ordered set. The end of the scan of a given rotation axis is marked by a C and F#(Gb) bichord (i.e. a chord of two tones played at the same time).

Together with each pitch defined by the pitch disk, an intensity level (i.e. dynamics) must be associated. It is established after the Western music notation, using dynamic levels between *pianissimo* (*pp*) to *fortissimo* (*ff*) inversely proportional to the distance of atoms from the rotation axis considered. A *ff* level is attributed to an atom located at the center of the pitch disk.

The final form of the music is given by the sequence of melodies/counterpoints obtained by the scan of each rotation axis of the crystal structure. In order to put in evidence the crystalline periodicity, a repetition of the music sections related to each rotation axis can be considered.

4 EXAMPLE

The musical score of the halite (NaCl) crystal structure is shown in Fig. 6. Each sodium (Na) atom is represented in the upper stave by a 1/8-long note, or quaver (Na is in the first group, see Fig. 4). Chloride (Cl) atoms, reported in the lower stave, are each represented by 7/8-long notes (Cl is in the seventh group). The scan is performed along the three-fold axis, as in the orientation shown in Fig. 6 (red spheres indicate Cl atoms; blue spheres represent Na atoms). The dynamics, ranging from *forte* (*f*) to *piano* (*p*), indicate the distance of atoms from the symmetry axis.

Each plan is scanned sequentially, alternating clockwise and counterclockwise directions. The F sharp (F#) note starting the score coincides with the symmetry axis. Our musical scores are produced as the soundtrack of animations evidencing sequentially the position of each atom within the crystal structure.

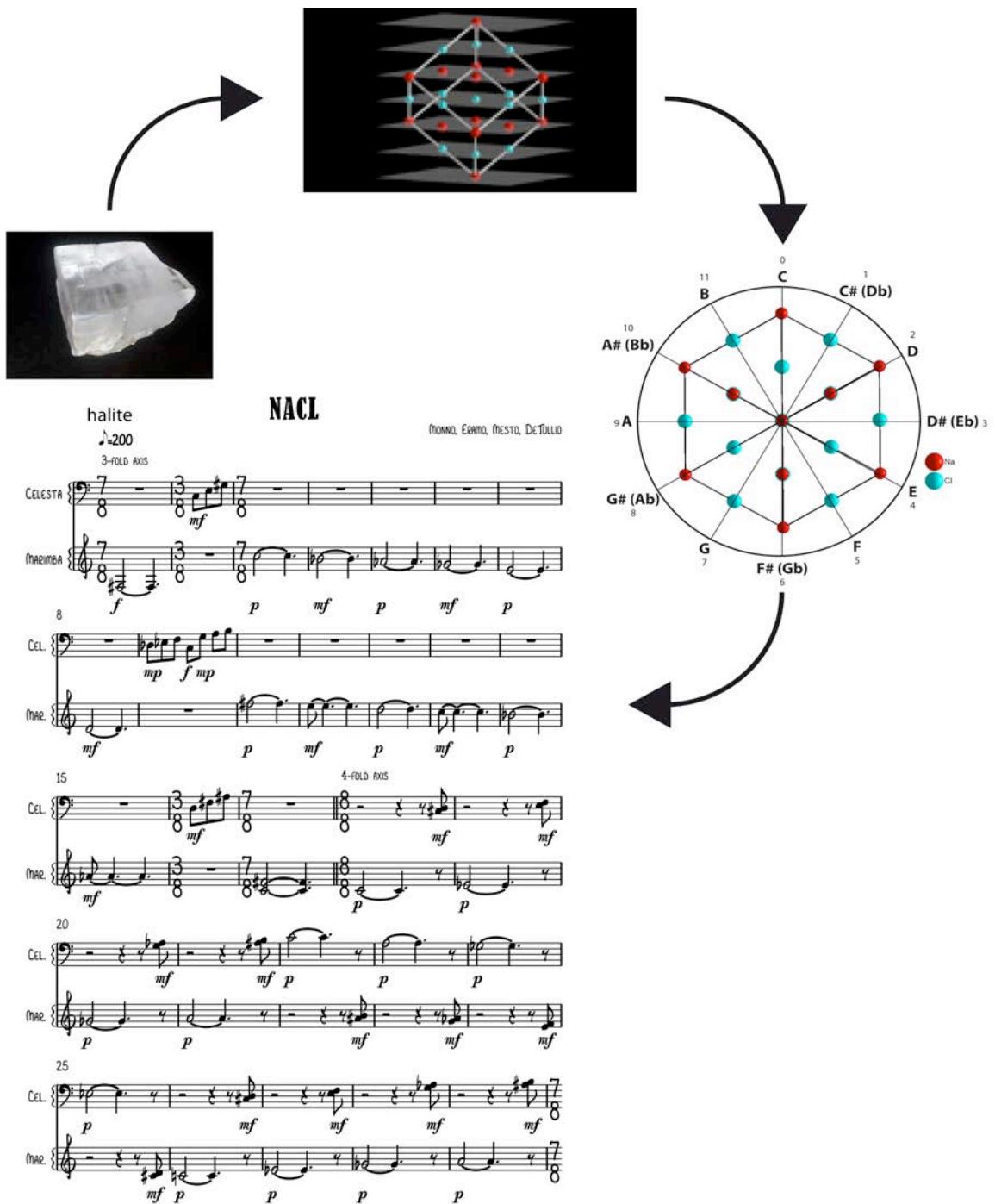


Figure 6. The halite crystal (NaCl) and its corresponding musical score

5 CONCLUSIONS AND FUTURE PERSPECTIVES

Music has been already used as an aid to memorize scientific concepts delivered through lyrics [9]. Our approach is totally different. As previously discussed, music and science have much in common. Crystals are the symbol of concreteness and music of abstraction, although music is actually science in many ways (acoustics, human physiology, mathematics).

The above-described and exemplified method for obtaining a reproducible musical form based on crystal structures has several potential advantages in science education.

In basic chemistry classes, explaining complex concepts such as the periodic properties of the elements could be troublesome, due to the difficulty in visualizing the changes occurring in the elements and corresponding chemical properties along the period. The use of the quaver (1/8 note) as

a discrete musical unit creates an interesting conceptual parallelism with the number of electrons in the orbitals. In other words, one electron can be visualized as a single quaver note, and the semibreve (whole note, with a musical value of 8/8) fulfills the completion of the period symbolizing the octet rule.

In the mineralogical sciences, the minerals are subdivided on the basis of their chemical composition and their structural features [10]. The use of a musical approach, here discussed, for the systematic study of crystal structures of all mineralogical classes can help in better highlighting the structural and chemical differences between the many mineralogical phases present in Nature.

This method can also exploit the display of museum mineral collections by means of an interactive approach. For example, single installations can be organized to illustrate the chemical and structural features of the minerals of every class, empowering the visitors' perception with audiovisual experiences that associate cognitive information to emotive feelings, with evident improvement in knowledge transfer.

Hence, the listening of music derived directly from the structures and 3D visualizations of the unit cell help the full understanding of the differences between crystalline and morphological symmetries. Similarly, they illustrate the diversity of the crystal structures, even if these have the same chemical content (polymorphism). The same approach can highlight structural disorders (atomic replacements) and or defects (ion vacancy, lattice deformations) occurring in the crystal.

Further applications could also include material sciences (novel materials), and biology (macromolecules such as sugars and nucleic acids; minerals in the human body, etc.), pharmacology (innovative drugs) and so on. In this way, a significant contribution is given to the teaching of crystallography.

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