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Structure of Molecular Water and the 3D Pythagoras Theorem

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Abstract

Water ice crystals inherently embed in their shape complex hexagonal structures, emerging mostly due to the O-H bond angle 104.5 degrees being close to the 120 degrees found in hexagons. This article explores the possible integration of water molecules into a recently published mathematical architecture called the Universal Gear model. Already published in a mathematics peer-reviewed journal, the Universal Gear is an orthogonally-intertwined construct of Pythagoras theorem driven planes, that all together provide a perfect balance in terms of the three main equations governing three-dimensional existence: zero net sum of lengths, zero net sum of areas and zero net sum of volumes. Computer-aided Design shows how a group of (simplified and realistic) water molecules successfully integrate into the (regular and irregular) version of the Universal Gear. Interestingly the geometric pattern that emerges from the projected field of water molecules integrated into the Universal Gear is a structure already observed in monuments of ancient civilizations. The ambient conditions, in terms of pressure and temperature, where such a structure could appear is not yet known, requiring further research preferably using computational molecular dynamics.

Keywords: water, molecule, geometry, model, universal gear, pythagoras, theorem

Hexagons have always been associated with the shape of water ice cristals (Natterer et al 2017, Pradzynski et al 2021). An important reason for this association is attributed to the fact that the internal angle 104.5 degree formed between the O-H bonds of a water molecule (Sharp and Vanderkooi, 2010) [Figure a] is (in a general sense) compatible to the internal angle 120 degrees of an hexagon (Figure b). Despite the discrepancy between these two angles (which results in a question mark concerning the adequacy of integrating water molecules into planar hexagonal grids by other researches [Huang et al 2023, Tang et al 2020, Pradzynski et al 2012, Plummer 1978]), the interrelation is there. The fact hexagons form the 2D backbone of three dimensional geometrical models — like the Universal Gear, already published in this article (Teia 2019) — suggests an affinity between water and such geometrical models exists.

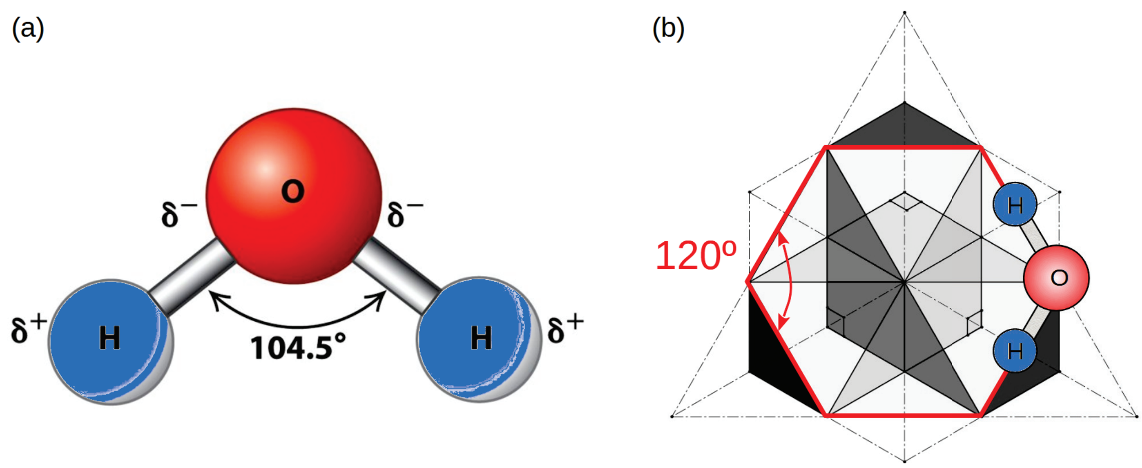

Figure 1: Synchronicity between internal angles formed by: (a) O-H bonds in a water molecule and (b) within hexagons of the Universal Gear model

1. Hypothesis

It is the thesis of this article that the fact that hexagons are present in the (already published) theory of the 3D equivalent Pythagoras theorem — the Universal Gear model — suggests that this theory can provide a template (due to its malleability to adapt its angular relationships, in particular the hexagon internal angle of 120 degrees, whilst maintaining its validity) for spatial organization of water molecules that are aligned to each other (in terms of their intermolecular forces), forming a force-balanced molecular grid that exists in quasi-static equilibrium.

2. Theory

Geometrically speaking, the Universal Gear model comprises of three-dimensional infinite interlaced 2D Pythagoras Theorems embedded in planes along all three orthogonal directions that are constantly connected and in perfect balance. In so doing, this concept governs information exchange in one-dimension (lines), two-dimensions (areas) and three-dimensions (volume) throughout the grid. This theory has already been published in a journal focused on mathematics research, and hence only the key aspects of most relevance to this article will be highlighted here. Functionally speaking, the Universal Gear is a three-dimensional network of information that is fundamentally governed by three sum equations: the sum of two lengths equals a third length, the sum of two areas equals a third area (Teia, 2018a) and the sum of two volumes equals a third (Teia, 2018b). The mathematical mechanism that interconnects all these three sums is the Pythagoras Theorem, that is weaved in intertwined orthogonal (to each other) two-dimensional planes. The corner stone that constitute the three dimensional Universal Gear is the truncated octahedron, which in its regular form has a surface composed of squares and hexagons, holding within the later the 120 degree inner angle (Teia 2019). This will be explained later in further detail. In the irregular form of the truncated octahedron, the hexagonal surface morphs with its internal angle changing from 120 degrees into any value from 0-180 degrees, including the internal angle 104.5 degrees formed in between the O-H bonds of a water molecule. Thus, as we shall see later on, the Universal Gear (of which the case $x = y$ is a special case named the three-dimensional Pythagorean Gear, already extensively discussed in the following article [Teia 2018a, Teia 2018b]) can accommodate and be populated by arrays of water molecules possessing its central internal 104.5 degree angle. At this point, it is unknown at which pressure and temperature combination does this H2O geometrical construct occurs. However, this is not the focus of the present article, which is indeed to determine on how the H2O molecules fit in an intramolecular force-balanced geometric grid.

3. Idealized Molecular Model (120º)

To understand how real H2O molecules (i.e., holding an O-H internal angle of 104.5 degree) fit into the three-dimensional geometric model, it is easier to start with a simplified approach. Hence, firstly we assume a simplified angle between the O-H bonds of 120 degrees, which allows the integration of our (simplified or ideal) water molecule into the particular case of the Universal Gear (right angle): to start simple, the special case where the two sides of the right triangle are equal (having both length x) will be firstly considered. From a two dimensional perspective, this means that a plane can be subdivided into infinite equal isosceles triangles AOB, where their hypotenuse lines form the diagonal grid and the sides form the orthogonal grid (Figure 2a). Such Computer-Aided Design (CAD) work [that in Figure 2] can be done with open source software, such as Geogebra for 2D drawings (Feng 2013) and FreeCAD for 3D constructs (Havre 2021). Now imagine that you have three such planes perpendicular to each other, and you take an isosceles triangle from each plane (i.e., A_1OB_1, A_2OB_2 and A_3OB_3) and align them such that they form the structure previously shown in Figure b. From a three dimensional perspective, this means that the isosceles triangles A_1OB_1, A_2OB_2 and A_3OB_3 form a volumetric structure, and that this structure is in fact a one-eighth section quadrant of a truncated octahedron (TO) [shown in Figure 2b]. Extrapolating to infinity, this alignment means that intersecting several parallel 2D isosceles-triangle grids or planes in one direction (for example, perpendicular to the x-direction, here assumed in an arbitrary direction) with several parallel 2D grids in the y-direction, and likewise with several parallel 2D grids in the z-direction (all linked at their junction nodes), the result is the volumetric grid in Figure 2b formed by several truncated octahedrons.

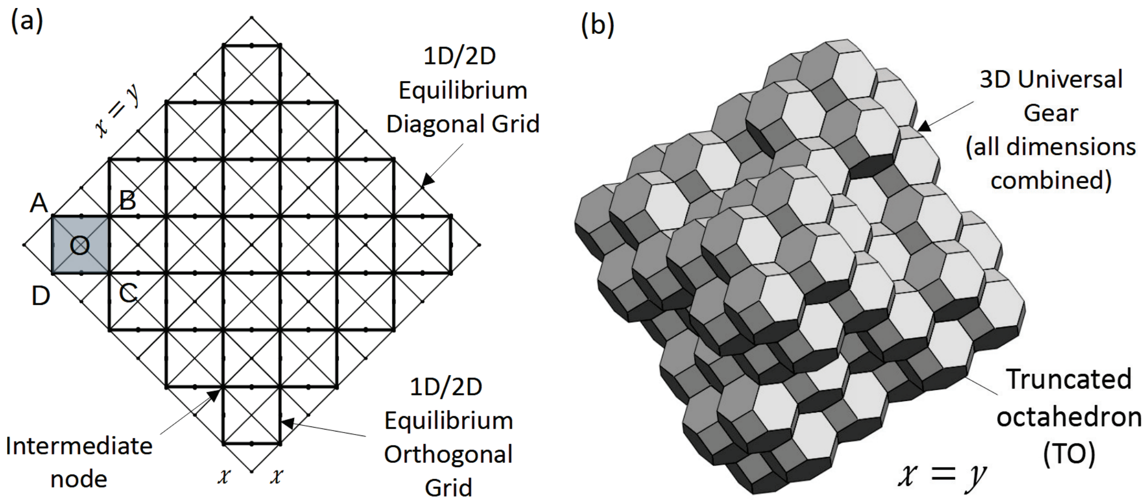

Figure 2: Universal Gear model ($x = y$): (a) 2D plane of isosceles triangles and (b) 3D grid of regular TOs

Figure 3a shows the 2D fundamental building block of Figure 2a, and in turn Figure 3b shows the 3D fundamental building block (in itself built from the 2D element) of Figure 2b. Figure 3a shows how the orthogonal and diagonal lines in Figure 3a form squares within squares (like for instance ABCD), that are in turn composed of right triangles of equal leg lengths x and hypotenuse length $z = \sqrt{2}x$. These 2D building blocks like square ABCD (in Figure 3a) interconnect orthogonaly to form a 3D fundamental block that is the truncated octahedron in Figure 3b. The surface of a truncated octahedron (TO) is composed of both squares and hexagons, and the diagonal AB of the hexagon (in Figure 3b) is the same as the diagonal AB of the triangle (in Figure 3a). As mentioned before, the core of the Universal Gear is the orthogonal interconnection of triangles such that they form a three-dimensional equivalent, i.e. forming in essence the drawing shown initially in Figure b. This geometric construct (Figure b) is applicable to the particular case when $x = y$, but a general equivalent with $x \neq y$ is possible, and indeed will be discussed later in the next section.

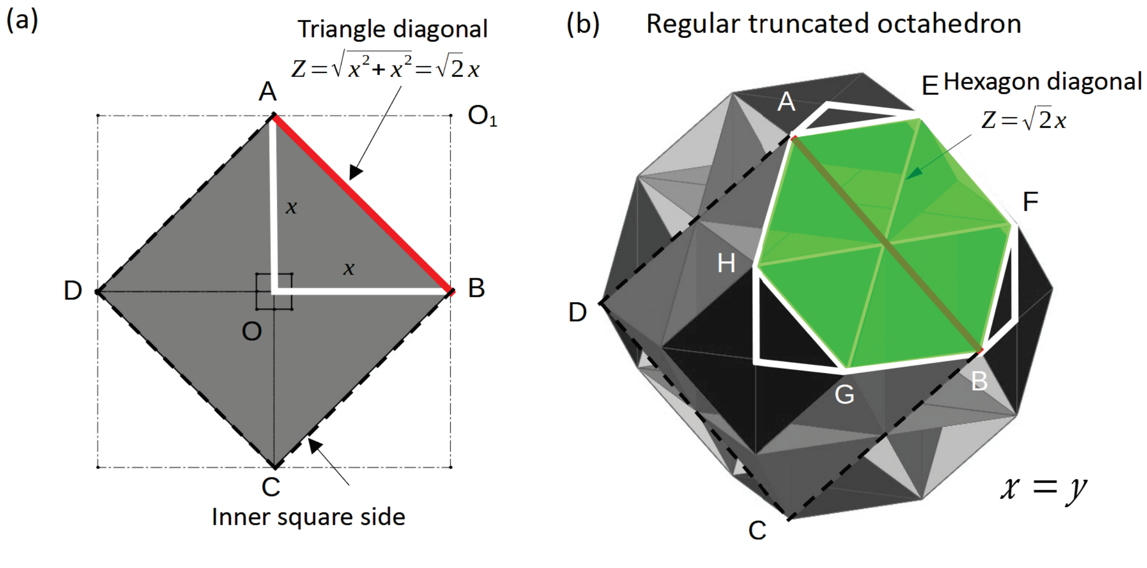

Figure 3: Elements composing the Universal Grid [$x = y$]: (a) square from isosceles triangles in 2D and (b) a TO in 3D

Figure 4a shows how each oxygen atom places itself (by means of the repulsive action to the surrounding oxygen atoms) at the corners of an octahedron. This alignment occurs because the strongest (electrically-speaking) atom in a water molecule is the oxygen. And while its electric field is omnidirectional, the O-O repulsion between oxygen atoms occurs along the path linking the centre of both atoms, resulting (in terms of intermolecular forces) in the oxygen atoms repelling each other and forming a tightly-packed grid with a fundamental octahedral disposition (Figure 4b).

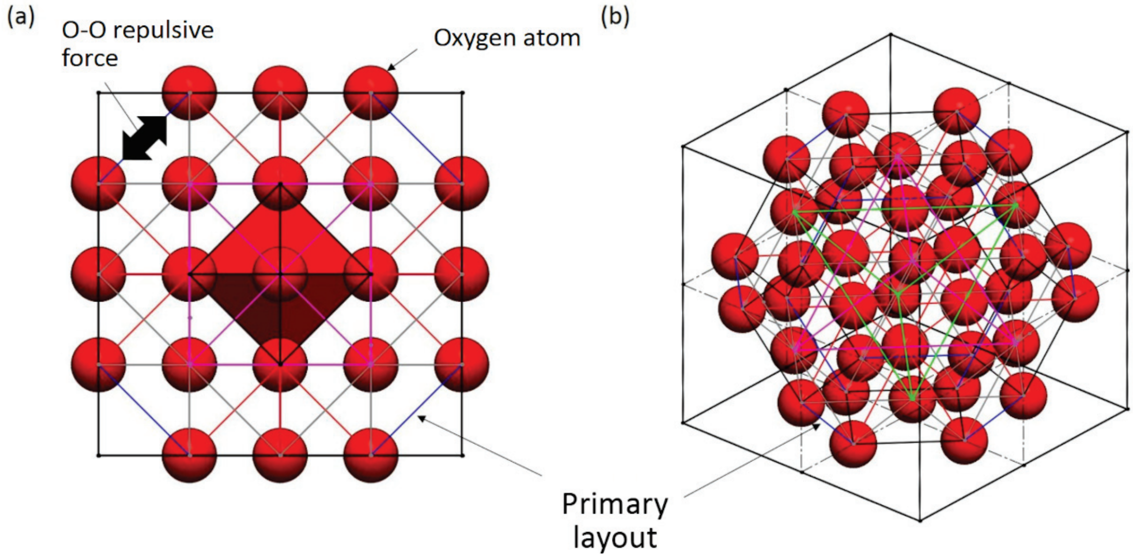

Figure 4: Primary layout of oxygen atoms onto the Universal Gear [$x = y$]: (a) side view and (b) perspective view

When clustered in a confined volume, a grid populated by equal atomic elements will repel each other and tend to organize themselves such that two rules are met: (1) their relative position yields the shortest distance between them, and (2) that distance is equal in between all of them. The result is seen in Figure 5a from the side, and is seen in Figure 5b from an isometric view. Figure 4a is a 2D image, and thus shows an apparent variation in proximity of oxygen atoms in 3D that does not exist, as these are projections. Indeed Figure 4b shows the distance between all oxygen atoms to be all equal. In group, these octahedrons cluster to form larger geometrical constructs composed of a number of organized oxygen atoms (as will be shown later). This O-O alignment constitutes the primary layout of the water molecules disposition with the Universal Gear ($x = y$). The secondary layout constitutes the alignment of the O-H bonds with neighbouring oxygen atoms. To understand the construction of the secondary layout, it is best to start with the most fundamental flat geometrical structure on the surface of the truncated octahedron, which is the square face (Figure 5a). In the most simplistic construction, it is plausible to assume that oxygen atoms occupy the corners of the square (satisfying the nodes of the octahedrons defined in the previous primary layout in Figure 5), whilst the hydrogen bonds align along the edges of the square.

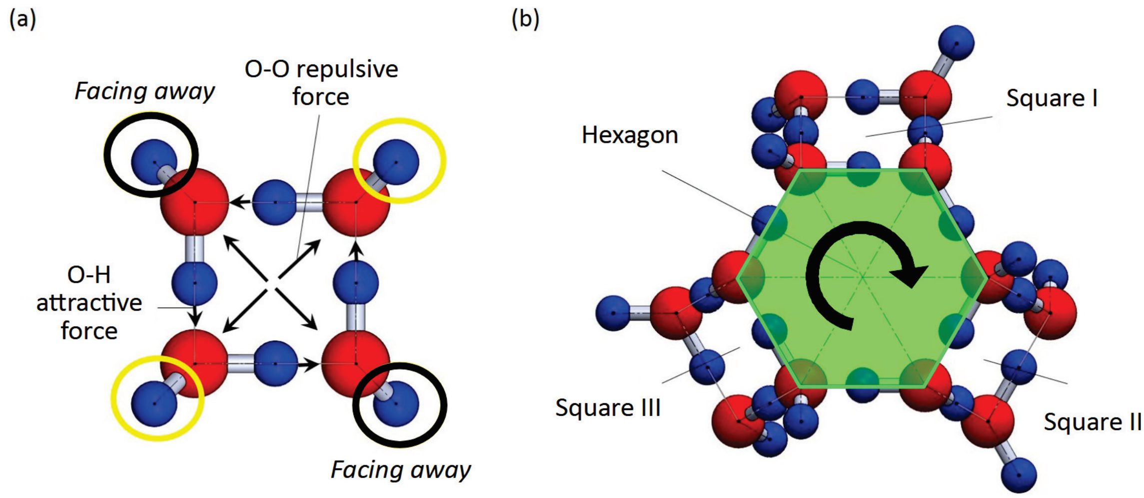

Figure 5: Integrating water molecules with aligned O-H bonds into a (a) square-shape and (b) hexagonal-shape

Note that the other hydrogen bonds in Figure 5a (highlighted with circles) automatically point away from the square, with only two possibilities: either above (yellow circles) or below (black circles) of the plane of the square. The result is two opposing corners with an O-H bond above, and the other two opposing O-H bonds below the square plane. Now that the squares have been populated with spacially-orientated water molecules, it is simple to place them on the surface of the truncated octahedron (as shown in Figure 5b), where care must be taken to make sure the O-H bonds in between the squares align (forming here a clockwise rotation). As a general rule, the O-H bond of the square that falls on the side of the hexagon must match the sense of rotation of all the hydrogen bonds in that hexagon, which in this case are pointing clockwise. By doing so, the three-dimensional orientation of all the water molecules in the square is completely constraint and locked in place. Thus, the structure in Figure 5b becomes the building block for the construction of the entire truncated octahedron (by overlapping it to Figure 3b). From here onwards, everything automatically falls into place, where the result is each of the hexagonal faces holds the same structure shown in Figure 5b, and fit together naturally by design as shown in Figure 6 (i.e., Figure 6a shows a side view, while Figure 6b a perspective view). Here, the peripheral H2O-filled squares of a hexagonal structure are shared with other neighbouring hexagonal structures with the H-O bond orientations matching inherently and synchronously. Figure 6b highlights in a perspective view the original octahedron, and the aligned primary layout of the oxygen atoms (located at the vertices of the truncated octahedron), and secondary layout of the O-H bonds perfectly aligned with a neighbouring oxygen atom (along the lines of the truncated octahedron). The outer pointing O-H bonds (highlighted with yellow circles) interface and belong to neighbouring truncated octahedrons. For example, the outer pointing O-H bonds on the top square of the truncated octahedron 1 or TO1 (in Figure 7a) are aligned with the sides of the hexagonal faces of the truncated octahedron 2 or TO2 (sitting on top of the truncated octahedron 1). Figure 7a is the building block to create larger constructs. When several truncated octahedrons are interconnected together, they form the grid in Figure 7b, which can extend indefinitely occupying and defining the one-, two- and three-dimensions. As such, the water molecular arrangement for one truncated octahedron, as shown in Figure 6b, can be iteratively and symbiotically integrated in the truncated octahedron's grid, such that all peripheral outward pointing H-O bonds in any given truncated octahedron become part of the neighbouring truncated octahedrons, yielding a perfectly interconnected and intramolecularly force-balanced grid.

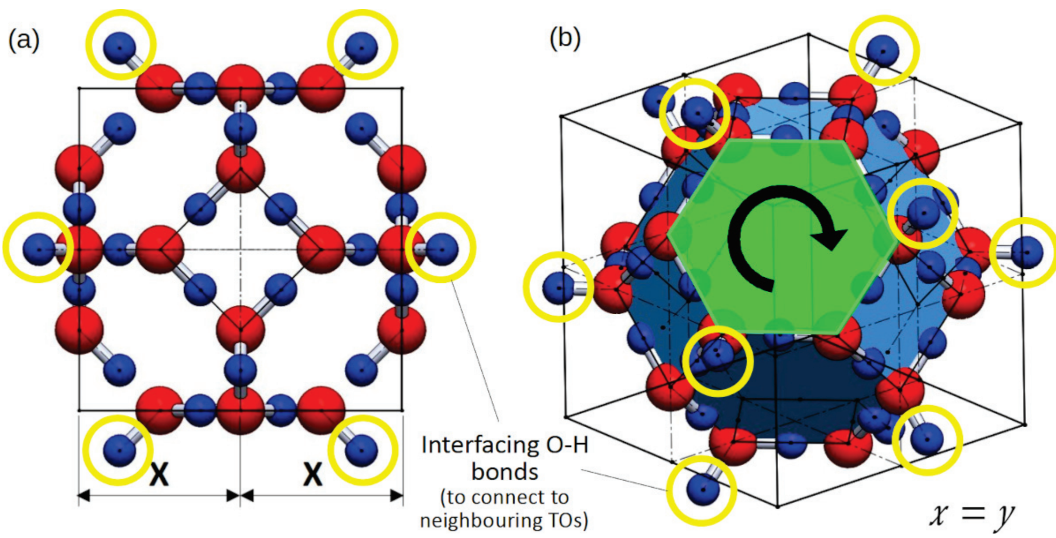

Figure 6: Secondary layout of O-H bonds onto the Universal Gear [$x = y$]: (a) side view and (b) perspective view

Note that from this perspective, Figure 7b appears to be a hexagonal grid, one must always remember that it is in fact a three dimensional construction, even in the formation of an ice crystal. The reason why an ice crystal appears bidimensional and hexagonal-shaped is because the growth is primarily governed by the influence of the flat surface that promotes lateral growth in favour of vertical growth, however it is still a three-dimensional structure, and the lateral and vertical growth (despite occurring at different rates) still follow the fundamental rule of a three-dimensional truncated octahedron grid. In a nutshell, compressing the 3D grid in one direction highlights the hexagonal shape, however compression does not remove the growth in the transverse direction, that the model needs to account for in order to be three-dimensionally valid.

The pattern shown in Figure 7b of a hexagon surrounded by triangles interconnected by rectangles is not uncommon, and indeed is found in geometrically meaningful structures from ancient times (like for example the dragon statues at the entrance of the forbidden city of China shown in Figure 8a). Curiously, one of these dragons holds under their paw a representation of the sphere of knowledge (including a complex geometrical pattern engraved in its surface). The explanation of the fractal construction of this pattern (and how it morphs into the pattern highlighted in the sphere) is explained in full at this open-source article. For the sake of the present article, a brief explanation is now given. The

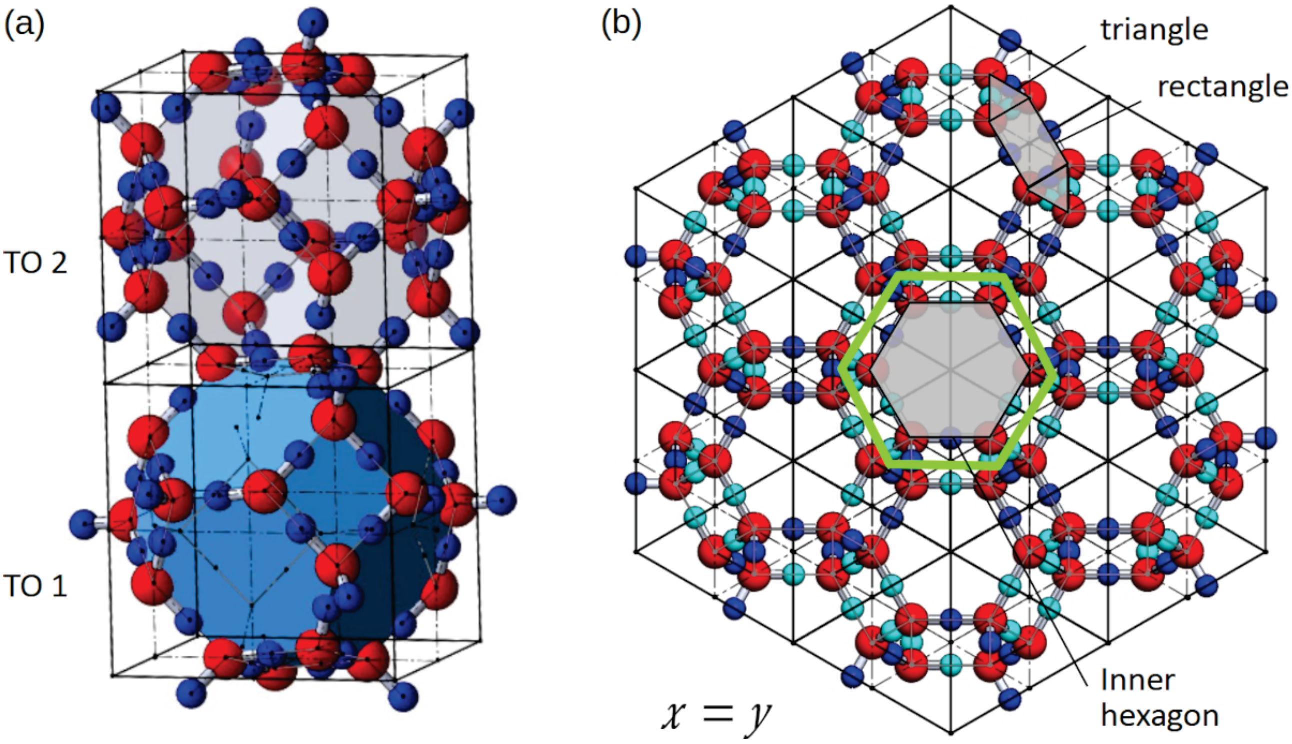

Figure 7: Connecting H2O surface-filled truncated octahedrons: (a) two together and (b) a cluster of eight

key geometrical structure to bear in mind is: a triangle followed by a rectangle and then a triangle (where in the surface of the sphere this is drawn as two arcs forming an oval, which represents the fractal case of a triangle-rectangle-triangle at infinity). This sequence of triangle-rectangle-triangle is seen following the periphery of each hexagon in Figure 7b. Note that this is in fact a 2D perspective surface view of a 3D structure. Hence, this pattern has both a two- and three-dimensional meaning. A chain of such geometrical keys is seen in Figure 8a disposed in a hexagonal sphere (coloured in green), around an inner hexagon formed only by triangles (coloured in red), that the sphere marks equivalently as a flower. In Figure 8b, the fundamental pattern with two levels down in fractal definition. It has at its centre a red circle to highlight where in Figure 8a it is located, and each corner of the green hexagon has such a fundamental pattern. Such structure migrates, and copies itself all around the sphere. In an infinitely defined fractal the straight lines transform into arcs, resulting in the pattern of the sphere. Considering the small nature of water molecules, from a macro view the higher fractal expression of the grid in Figure 7b would also be perfectly curvilinear. This suggests that the pattern and its meaning may have been known to these ancient civilizations.

Now that the hydrogen O-H bonds have been defined on the surface of the truncated octahedron, it is necessary to remember that the interior of the truncated octahedron also has water molecules. It was shown previously in Figure 4 that the oxygen atoms at the interior are locked in place via intermolecular O-O repulsion. These also have O-H bonds to surrounding water molecules that need to be defined. In fact, these oxygen atoms assume a disposition of an octahedron (as shown in Figure 9a), with O-H bonds in between them in the disposition of a zigzag, with the other O-H bonds pointing outwards. The integration of this internal H2O structure within the truncated octahedron is shown in Figure 9b. The main point to notice is that, while the O-H bonds alignment with Oxygen atoms is strong and well defined within this interior octahedron, and also within the surface of the outer truncated octahedron, there is no exact alignment for the outer pointing O-H bonds (that connect to the oxygen atoms on the surface of the outer truncated octahedron). The lack of preferred orientation to these outward pointing O-H bonds introduces a certain flexibility to their disposition, which can be influenced and even imprinted by an external influence (e.g., electric field or vibration). This relates to the idea that water has a memory (Liu et al 2018). Indeed this degree of freedom at the interior of the outer irregular truncated octahedron can be seen as analogous to the binary state of atoms when storing information on hard drives (Gibney 2017, Natterer et al 2017).

Figure 10 shows a truncated octahedron (highlighted in solid grey) surrounded by three integrated regular truncated octahedron with (holding in themselves) inner octahedrons (being the later highlighted in green). The O-H bond pointing outwards for each of the three interior octahedrons do not have a preferred alignment to any oxygen atom (on the outer

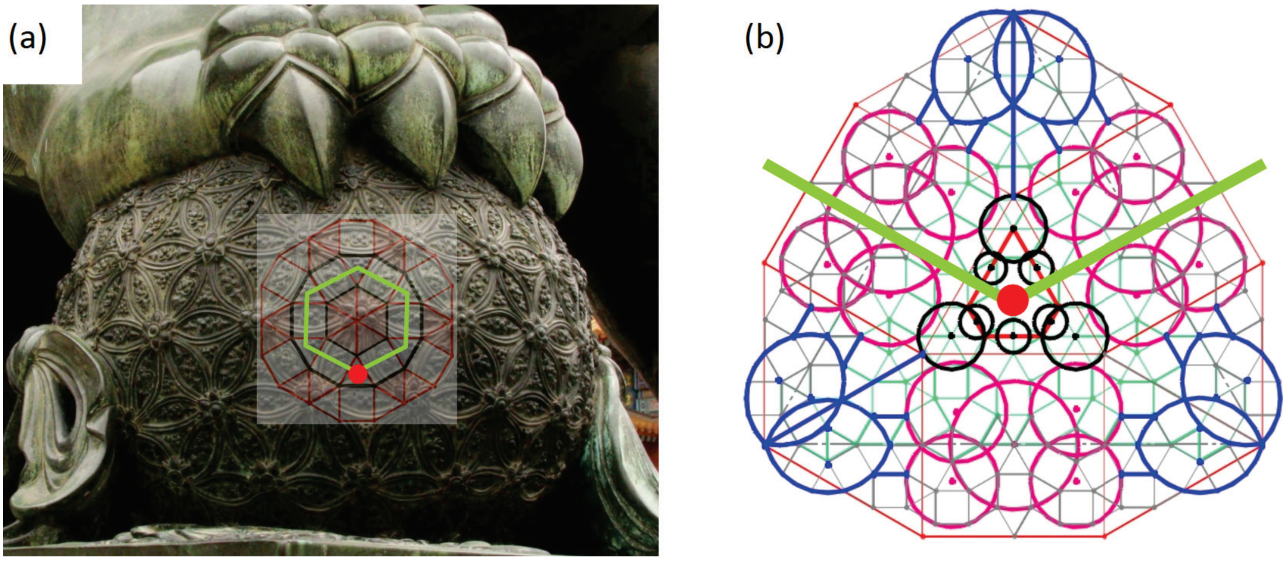

Figure 8: The H2O geometrical pattern: (a) identified in the sphere of knowledge and (b) expressed with 3 fractal levels

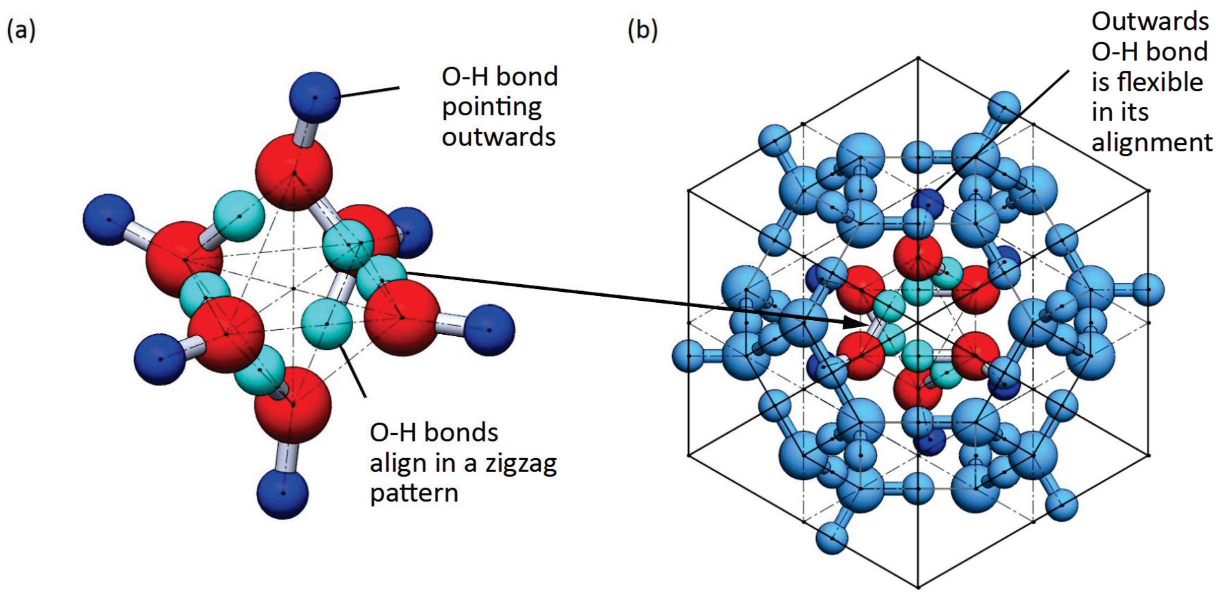

Figure 9: Interior of H2O-filled truncated octahedrons: (a) general view and (b) integrated within a TO

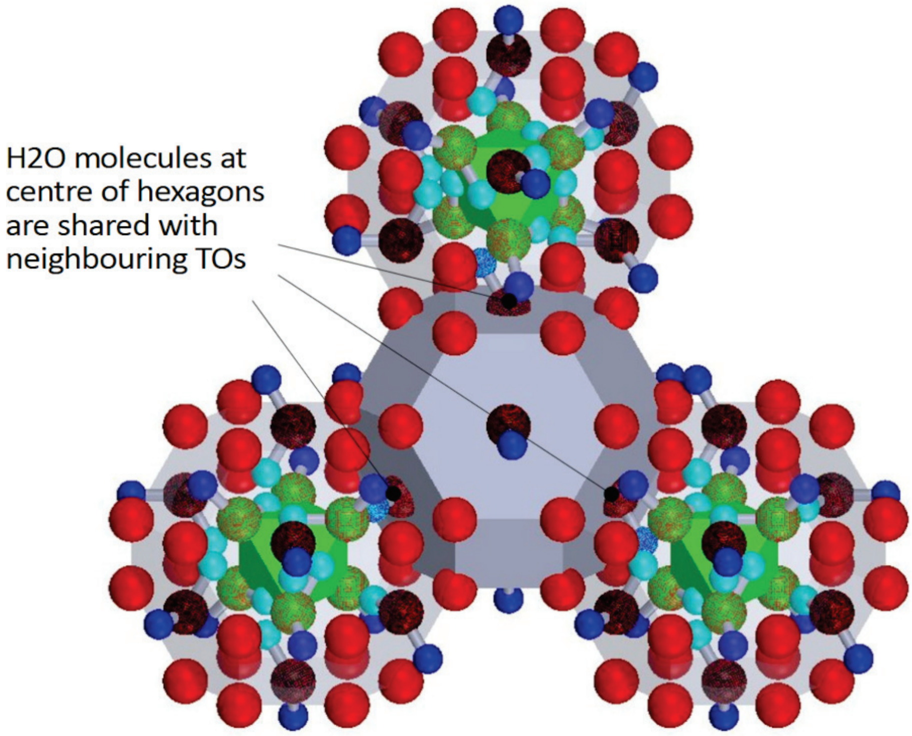

Figure 10: Water molecules shared between several TOs, and the flexible orientated inner tetrahedrons (in green)

TO), and have flexibility towards where they can point, providing the means to store information. Moreover, note that there is also an oxygen atom at the centre of each hexagon shared in between the neighbouring outer truncated octahedrons. Similarly as before, the H-O bond have no preferred direction of alignment to surrounding oxygen atoms. In all these cases, the degree of freedom of the O-H bonds of these oxygen atoms (which they themselves are locked in place) attribute to water a certain memory effect, within a grid that is otherwise all defined by intermolecular forces both in terms of the O-O repulsion, as well as the O-H bond alignment (due to the hydrogen attraction to surrounding oxygen atoms).

4. Realistic Molecular Model (104.5º)

Finally, we will now discuss the implications of having a water molecule with a 104.5 degrees between the two O-H bonds, instead of the previous 120 degrees. It is logical to infer that if $x = y$ gives 120º, then $x \neq y$ gives all other angles (including 104.5 degrees). This means that the Universal Gear moves from its special case (right triangles with $x = y$) shown previously in Figure 3 into the general case (scalene triangles with $x \neq y$), which is now discussed. Graphically, this translates into the original balanced grid in Figure 2a (where $x = y$) distorting into the unbalanced grid shown in Figure 11a (where $x \neq y$). What this means is that from a two dimensional perspective, the infinitely subdivided plane changes its shape as the isosceles triangles are replaced by scalene triangles. All three orthogonal (perpendicular to the x, y and z-axis) planes change in such a way that their interface points remain the same, and all triangles remain connected via these points in a harmonious way. The details of this geometric process is beyond the scope of this article, and is already previously explained in detail (Teia 2019). It is critical to highlight that these identical scalene triangles result in the construction of two types of quadrilaterals within the grid, one is a square (i.e., formed by four scalene triangles revolving around each other such that they form an outer square and an inner square) or the other a diamond (i.e., formed by four scalene triangles aligned with their short and long legs matched). From a three dimensional perspective, this means that some regular truncated octahedrons will contract (i.e., governed by the diamond), and others will expand (i.e., governed by the square). As the junction or intermediate nodes of the various perpendicular planes displace, the field composed of truncated octahedrons contracts and expands in an alternating manner such that the net is zero (that is, the volume increase of an expanding irregular truncated octahedron [ITO] is matched by the volume reduction of the surrounding contracting irregular truncated octahedrons [ITO]), with the end result shown in Figure 11b.

Looking more in particular at each individual element, the alteration of the lengths of the sides of the right triangle $x \neq y$ created an unbalance that distorted the 2D square previously shown in Figure 3a into that shown in Figure 12a. In particular, not only did the outer square expanded with hypotenuse length $z = \sqrt{x^2 + y^2}$, but a new small square emerged

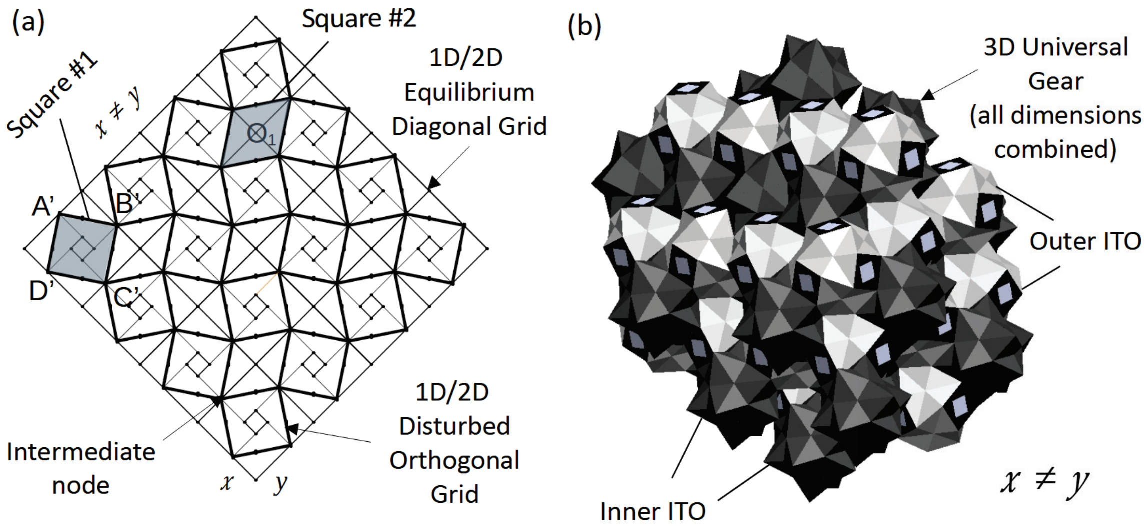

Figure 11: Universal Gear model ($x \neq y$): (a) 2D plane of scalene triangles and (b) 3D grid of irregular TOs

at the centre. From a fractal perspective, this geometrical construct of a square formed within a square links directly to the already published central square theory article #1 (Teia 2015, Teia 2016), where infinite families of right triangles governed Pythagorean triples are found propagating fractally both inwardly and outwardly towards infinity (Teia, 2016). Note that previous publications (namely article #2 and article #3) have proven the existence of other Pythagoras Theorems governed by other regular polygons that revolve around (angle-matched) scalene triangles, like for instance the regular triangles (Teia, 2021a) and regular hexagons (Teia, 2021b), respectively. This alteration of $x = y$ into $x \neq y$ migrates into the 3D domain, where the regular truncated octahedron now also morphs into an irregular shape, keeping the balanced of all three equation (i.e., sum of lengths, sum of areas and sum of volumes), resulting in two types: those who expand (i.e., the expanded irregular truncated octahedron in Figure 12b), and those who contract (i.e., the contracted irregular truncated octahedron Figure 12c). The main difference between the two ITOs is in their 2D building blocks, where the expanded ITO in Figure 12b has in its interior the modified $A'B'C'D'$ (including at its centre the smaller square), while the contracted ITO in Figure 12c has four right triangles (no smaller square at the centre). Note that the diagonal of the square $z = \sqrt{x^2 + y^2}$ in Figure 3a is the same as the diagonal found interconnecting the morphing hexagons in Figure 3b and Figure 3c.

In order to adapt the Universal Gear to accommodate the reality of the water molecules, the relative value between x and y was changed iteratively, until the internal angle of the morphing hexagon matched the required 104.5 degrees for the water molecule to align perfectly within its geometrical structure. When populated by real H2O molecules (as done before for Figure 6) results in the construct in Figure 7. Note that this resulted in a new central square in Figure 13a that is smaller than that shown in Figure 12a (where a larger difference between x and y was shown intentionally for the purpose of a clearer illustration). While now slightly more complex, the alignment and interfacing between asymmetrical neighbouring truncated octahedrons is done in the same manner as in Figure 7, except that now the directions of the O-H bonds have changed slightly. Nonetheless, it is relatively straightforward to see how the asymmetrical truncated octahedron in Figure 13b can replace the symmetric one in Figure 6b, in producing the (now slightly different, but still very similar) water grid in Figure 7b.

5. Conclusion

Human's inquisitive fascination for water comes from its tremendous flexibility to accommodate geometrical patterns — being the most visible and noteworthy, the beautiful complex hexagonal structures formed in ice crystals (no two are alike). The already peer-reviewed published geometrical model Universal Gear accommodates inherently in its construction a certain affinity with hexagons. This article proves that real water molecules (with an internal O-H bond angle of 104.5 degrees, instead of the idealized 120 degrees in other researches) can be integrated in the Universal Gear, such that they are in perfect balance in terms of their O-O repulsion and O-H bond alignment to neighbouring oxygen atoms. Moreover, the flexibility of this model provided as a result the integration of the reality of the H2O internal angle of 104.5 degrees, rather than trying to force fit the H2O molecule into a 120 degree pattern to favour hexagonal integration, (as it is often done with ice crystal related molecular models). It is unclear under which pressure and temperature conditions this structure might appear, but this research shows it to be stable from a point of view of intramolecular forces. Moreover, the 2D and 3D geometric pattern has been shown to match those observed in artefacts of ancient civilizations, such as in the

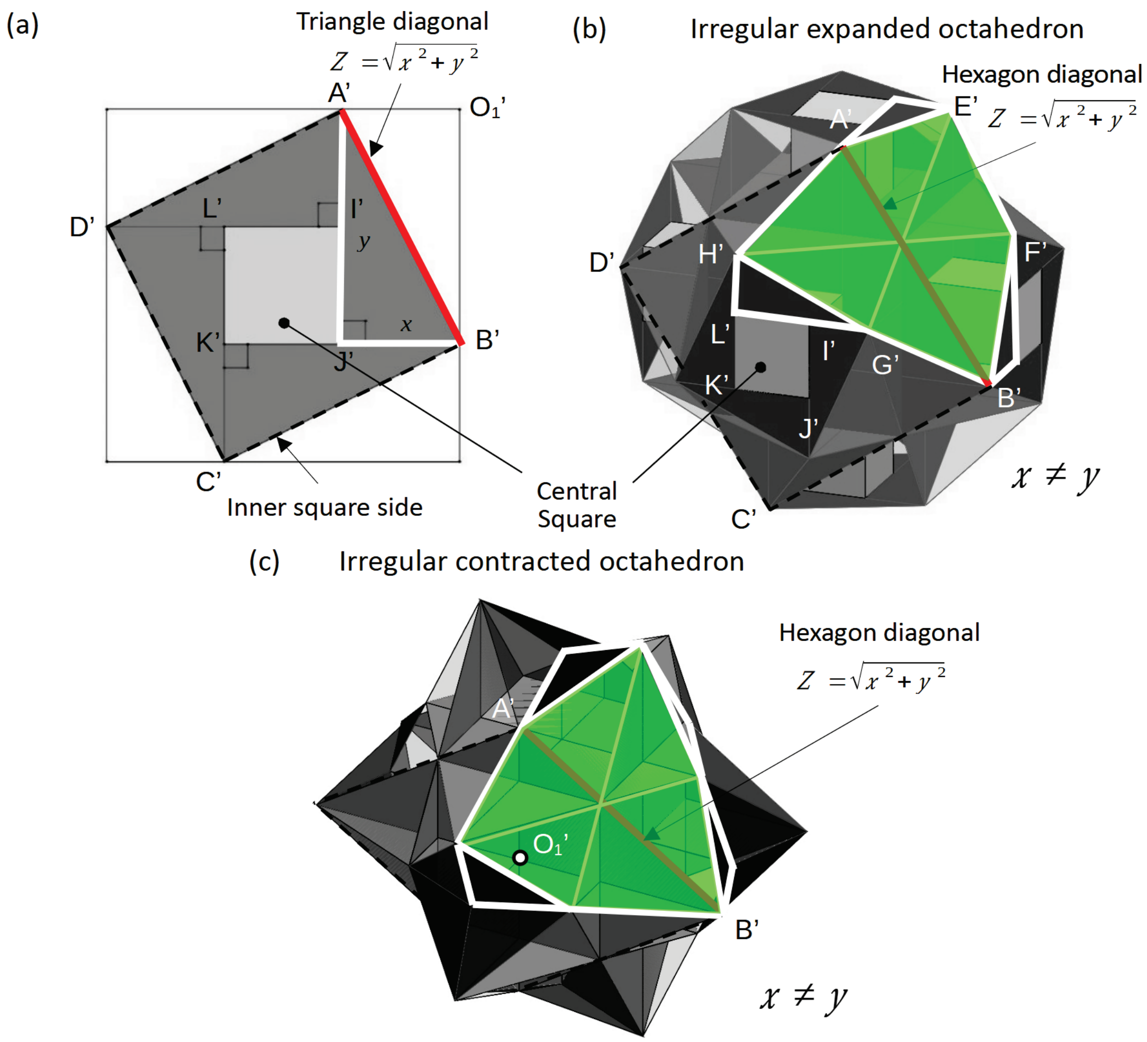

Figure 12: Fundamental elements composing the Universal Grid [$x \neq y$]: (a) square from scalene triangles in 2D, (b) expanded irregular TOin 3D and (c) contracted irregular TO in 3D

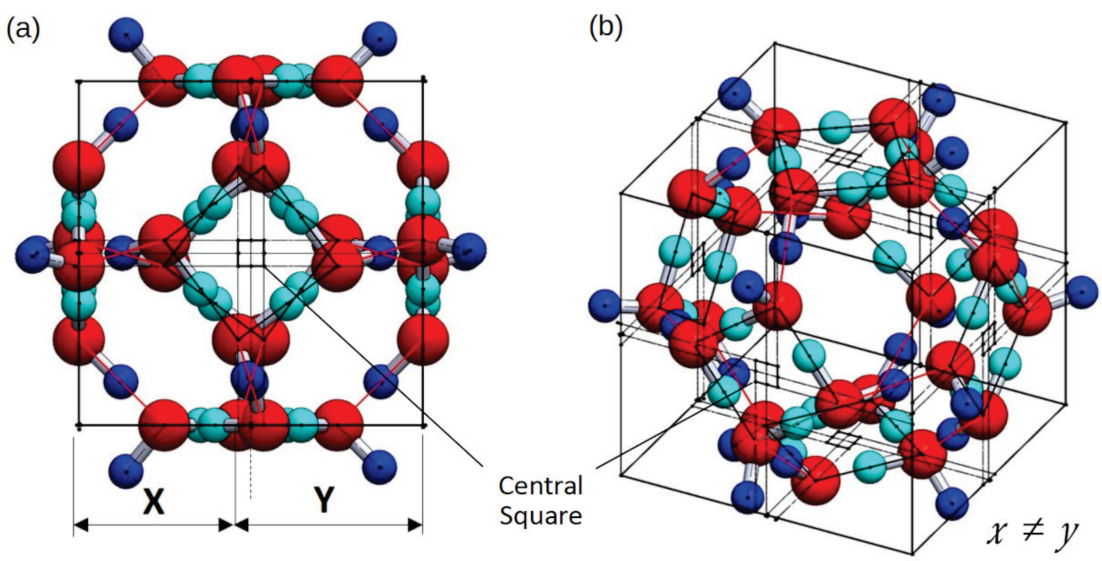

Figure 13: Integrating H2O molecules into an expanded irregular truncated octahedron: (a) side and (b) perspective view

sphere under the paw of the dragon statues at the entrance of the Forbidden City in China. Finally, a possible mechanism for information storage in water has been explained from the perspective of the Universal Gear, allowing certain water molecules in the stable overall molecular matrix to acquire certain directional properties when under external influences like an electric field (very much like hard drives store information do by orientating atoms in their atomic structure), enabling the storage of information in the molecular structure of water possible.

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