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ArtScience

Molecular Symmetry and Art: Visualizing the Near-Symmetry of Molecules in Piet Mondrian's De Stijl

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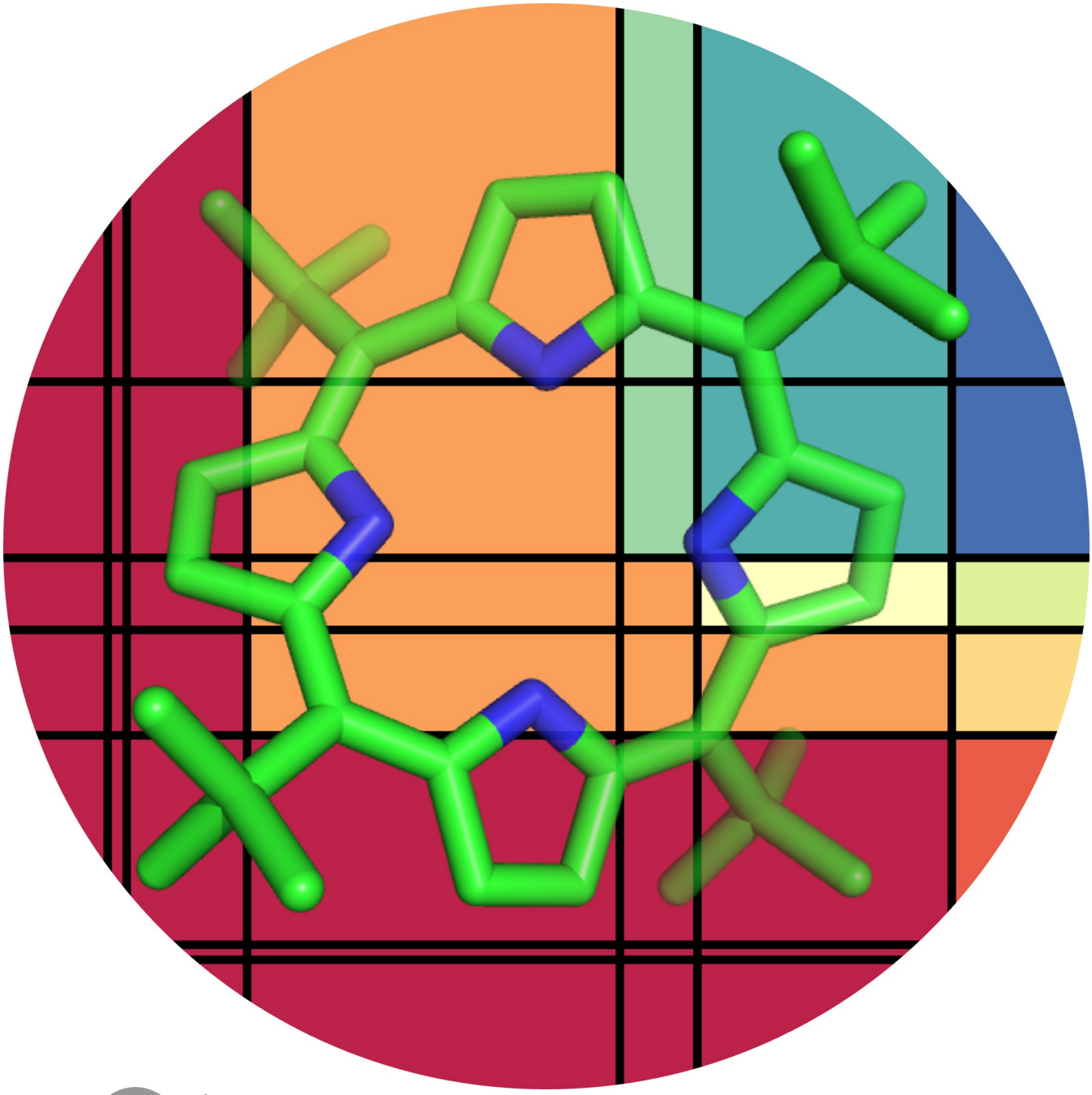

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Abstract: Symmetry and shape are essential aspects of molecular structure and how we interpret molecules and their properties. We, as chemists, are comfortable with pictorial representations of structure, in which some nuance is lost—investigating molecular shape numerically by looking at how closely it fits a reference, such as a plane, or a set of vectors or coordinates, is informative, though far from engaging. Often relationships between chemical structure and derived values are obscured. Taking our inspiration from Piet Mondrian's Compositions, we have depicted the symmetry information encoded within 3D data as blocks of color, to show clearly how chemical arguments and resultant molecular distortion may contribute to symmetry. Great art gives us a new perspective on the world; as a pastiche, this art may allow us to look at familiar molecules, such as porphyrins, in a new light, understanding how their shape and properties are intertwined.

1. Introduction

The shape of molecules and molecular aggregates is of principal importance in biochemistry, organic chemistry, and materials science.[1] In medicine and biochemistry, the shape of a molecule of interest is key in understanding its interactions with targets, as understood by shape-based drug design, and for enzyme-substrate interactions as per the lock-and-key principle.[2] Often the molecular shape can influence how the molecule interacts with light and with other molecules.[3] Exemplified here for porphyrins,[4] different shapes and arrangements of components can create vividly different optical, conductive, (organo)catalytic and receptor, biological, and adsorption properties.[5] Shape is controlled by internal bonding and peripheral or intermolecular conflict, altered by external factors such as pressure and temperature, resulting in chemical change from this impetus.[6]

The shape of an individual molecule can be thought to comprise two components. Firstly, the set of connections between atoms comprise its identity, and can be equivalently represented in a formula (e.g., Figure 1), a structured encoding (e.g., SMILES)[7] or a systematic (IUPAC) name (i.e., porphyrin).[8] Secondly, one can consider how these atoms arrange themselves in three-dimensional space when constrained by their connections and other forces as a measured or computationally estimated property, responsive to changing molecular environment—for example, the "chair" and "boat" conformations of cyclohexane.[9] The practice of structural chemistry ties these two concepts, and uses principally X-ray crystallography, a method of determining atom-scale structure with diffraction data. Theoretical chemistry approaches are becoming increasingly accurate as well.[10]

The result of a successful crystal structure determination is a three-dimensional representation of atom probability tensors from which one can determine both connectivity and conformation. The visualization of this three-dimensional data is often represented by multiple 2D views in static publications, relying on the careful language and the intuition of a familiar scientist to combine these views into a three-dimensional representation in the mind. Lightweight interactive software,[11] alongside methods such as 3D printing, offer a way to engage audiences with molecules in the native 3D environment. Other methods of crystal structure depiction, such as Hirshfeld analysis,[12] highlight a specific component of the crystal structure analysis such as intermolecular interactions.

Symmetry plays an important role in the molecules that chemists choose to study as well (see S.I. 1, Excursus).[13–20] The abundance of symmetric molecules is owed, in our view, primarily to two factors—namely the simplicity of multiple additions of the same unit (i.e., (cyclo)oligomerization)[21] and the coplanarity induced by π-systems.[22] A case in point are the porphyrins,[4,23] where the most studied types—the

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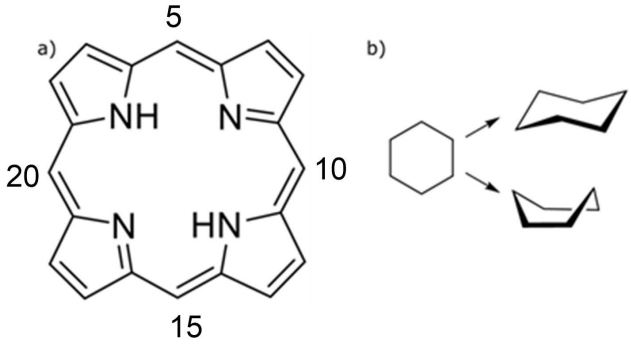

Figure 1. a) The symmetric porphyrin core as a simple skeletal representation; this form of idealized representation eschews any reference to the conformational shape of the molecule (see also Figure S1); b) the cyclohexane diagram encodes no conformation (D_{6h}) but is known to adopt chair (D_{3d}) and boat (C_{2v}) archetypes, among others.

A_4 type (5,10,15,20-tetrasubstituted)[24]—are examples of both effects occurring synergistically to develop an ideally highly-symmetric core.

But what about an artistic visualization of symmetry? Some of the most emotive artistic installations for scientists are those which involve their field of work. Examples are artworks evoking elements of symmetry such as those by R. Buckminster Fuller, Ai Weiwei, and M. C. Escher with their approximation of symmetry and disorder, transformative inclusions, and near-repeating patterns.[25] Using art, symmetry can appear as an artistic plaything, rather than an exact set of rules. On the other hand, can scientific rules be used to inform art as well?

Being introduced to using normal coordinates, one of us (CJK) found that the 'nearness' of symmetry operations could be represented mathematically, and was curious how these principles could inform art. Moreover, the practice of structural chemistry is conceptually linked to human-scale structure, architecture, and Vitruvius' ancient concepts of structure[26] (see Figure S2),[27] with beauty, symmetry and strength being necessarily interrelated. That these design principles appear in many cultures is indicative of a deeper connection.

Herein we present "Neoplastic" plots, an example of which is shown in Figure 2,[28] as an attempt to represent molecular shape and symmetry through an artistic lens perpendicular to a conventional structure depiction, demonstrating distortion in an abstract but useful manner. The artistic and informative aspects of these plots are discussed below.

Often as how we approach symmetric objects in the real world, or indeed art, upon closer inspection we see small fluctuations which can alter our perception of an object's symmetry. In general, a semantic or intuitive line is drawn depending on our method of interrogation and the descriptive usefulness of smaller features. As a macro-scale example, with an icosahedral symmetrical view, a soccer ball has I_h symmetry, from the patterning of the black and white segments and stitching, it rolls like a sphere, resulting in 60 rotational symmetries and 60 orientation-reversing symmetries; compare with the ellipsoidal Australian Rules football, which does not roll smoothly on all axes and therefore

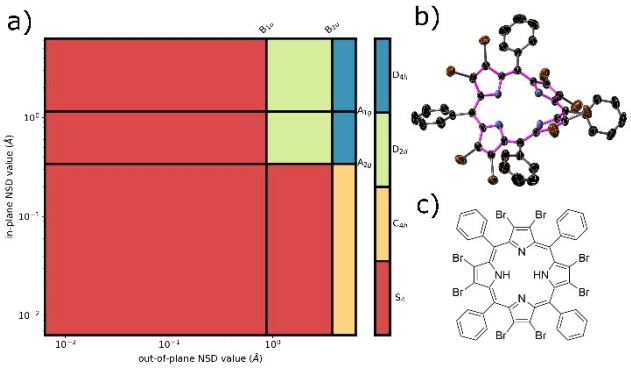

Figure 2. a) "Neoplastic" diagram of the porphyrin core of the classic nonplanar 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenylporphyrin (CCDC: RONROB), alongside two representations of this same molecule—b) the crystal structure thermal ellipsoid plot and (c) skeletal model.[28] This porphyrin shape is primarily *saddled* and a little *ruffled*, resulting in S_4 symmetry (see below).

results in a different symmetry This can be related to the architectural ideas of Buckminster Fuller and their relation to the fullerenes in chemistry; the construction of approximately spherical elements as a geometrically iterative limit rather than an idealized monolith.[29]

Much like this macroscopic example, in chemistry, it is useful to have an immediately accessible manner of displaying which shape distortions are measurable and contribute to the canonical 'shape', and which are transient minutiae arising from crystallization. This concept of increasing abstraction by removal of minor details and trying to present a general form is mimicked by the early work of Piet Mondrian in his "Trees" artworks (Figure S3)[30] which highlight elements of life through abstract shapes. In some senses, this is what we perform intuitively as scientists, the reduction of complex phenomena to the underlying *truth.*

The "Neoplastic" representation presented here is a method of displaying small and large deviations from ideal symmetry, such that a level of symmetric approximation can be imagined as a position on a plot. We have co-opted the style of Mondrian's *Compositions* to achieve this, as the non-representational artistic style allows a scientific repre-

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sentation to be supplanted retroactively as pastiche. This device allows us to understand the role of symmetry in our molecules and encodes deep information which ties artistic and scientific rationales around this core concept.

2. Piet Mondrian and De Stijl

Piet Mondrian (1872–1944) was a Dutch painter of the Modern era,[31] most famous for his "Compositions"; an early example is the *Composition II in Red, Blue and Yellow*,[32] shown in Figure 3.[33] Mondrian's work is exceptionally mimeographed within modern culture, and is a foundational portfolio of non-representational art. This artistic movement, with the intention to spurn representation of the banal world and find beauty in pure abstraction, explores aesthetic qualities divorced from the necessity of representing objects and tests the limits of minor variation and the use of restricted palettes.

The composition shown in Figure 3 consists of blocks of color separated by vertical and horizontal black lines of variable widths. They are a sustained motif of Mondrian, with many compositions finished in the period 1916–1944, his intent through this series was to explore how small variations in elements which were relatively devoid of emotive characteristics could evoke an artistic balance. Between bold colors and subtle variation within the severe style, the deceptive simplicity of the neoplastic movement was also its greatest strength in appealing to a wide audience, widely influencing art, fashion,[34] music,[35] design,[36] and science[37] (Figure 4 and Figure S4).

Mondrian's artworks were conceived to be divorced from any representational element of the world or nature, which consisted of curves and shades, by using modern shapes. Many scientists have been fascinated by these deceptively simple artworks, and Mondrian's stylistic elements have emerged in statistics and in mathematics, each preserving elements from art while introducing scientific concepts. Among these are: the *Mondrian Process*, a novel solution for the generation of decision tree-like objects by division of a product space,[39] with the related *Mondrian Forest* finding application in physics.[40] The *Mondrian*

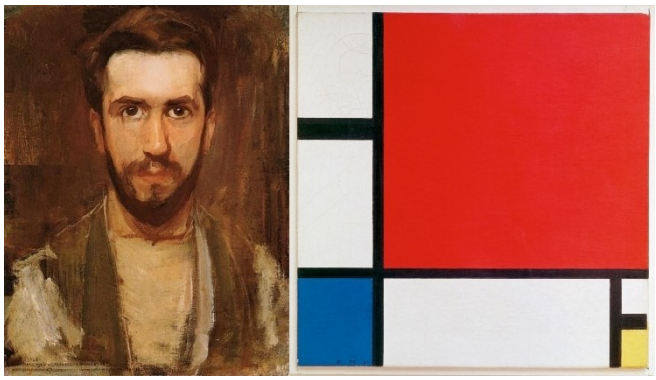

Figure 3. Piet Mondrian[33a] and his *Composition II in Red, Blue and Yellow*, emblematic of his characteristic style.[33b]

Figure 4. Representative uses of Mondrian's De Stijl. Top) Models wearing Mondrian Collection by Yves Saint Laurent in the Gemeentemuseum at The Hague, 1966.[38] Bottom) Spanish postage stamp released by Correos in 2007. Reprinted with permission from ref. [37]. Copyright 2007 American Chemical Society.

Problem involves finding the minimum solution to the volume disparity of unique divisions of a regular grid.[41] In each case, the striking imagery involved is a key component of translating scientific concepts to audiences. The similarity between the crystal precipitation patterns of titanium carbide and these artworks is termed *Mondrian Patterning*.[42] Finally, Mondrian's work has allowed a test-case in procedural generation of artworks, formalizing insight into aesthetic perception.[43]

Mondrian's approach to representation and involvement of symmetric elements in his work, painting with rectilinear elements on square canvasses, is highly reminiscent of scientific plots which often take the same basic form. The *Neoplastic* movement, or *De Stijl*, in its simplest form, was the rejection of the modernist fascination with abstract representation of the real, and movement towards the ideal of pure abstraction based on a set of defined principles.[44]

The naming of this artistic movement as *Neoplastic*[45a] generally refers to the concept developed by Theo van Doesburg (Figure S5) and Mondrian in 1917 and outlined in a series of contributions to the Dutch artist journal 'De Stijl' (Figure 5).[45b] Infused by many ideas, the principles outlined in De Stijl were also an attempt to counteract the destructive chaos of World War I by creating art of universal

Figure 5. De Stijl, Vol. 1, no. 1, Delft, October 1917. Design by Vilmos Huszár. Image in the public domain.[45]

fundamental simplicity achieving harmony through reduction.

While 'plastic art' refers to all visual art forms, as a chemist one is tempted to also relate this break with past art forms to the optimism surrounding early twentieth century synthetic materials, such as Bakelite,[46] to break with traditional product forms and manufacturing methods constrained by natural materials, and to emulate this synthesis in art. This name belies an intrinsic link between art and chemistry, that the materials we use first informs products, then ideas and broader culture (Figure S6).[47] The other common meaning of plastic—as pliable—is shown by the plots described in this contribution; in demonstrating the bending and twisting of a molecule,[5a] we are using the *Neoplastic* ideas to demonstrate plasticity.

The intention of this new plotting device is to demonstrate symmetry and its limits in near-symmetric molecules, with porphyrins used as an example. A procession may be inferred through the progression from the perfectly abstract symmetry, as denoted by the upper right corner of each plot (see below, Figure 7), to the real measured crystallographic fragment symmetry, on the lower left. this is emblematic of the interplay between the two representations imbued in each molecule, the real and the ideal, standing at antipodes —the demonstration of which was one of Mondrian's artistic themes.[48] In a way, the scientific use of this concept described here as a method of representing abstraction of porphyrins, the "Colors of Life",[49] is a thought provoking juxtaposition, encoding an abstract representation intended to be impossible with the constraints of the form.

3. Depicting Porphyrins in De Stijl

Porphyrins are perfect for the investigation of symmetry-breaking molecular conformations. As we have previously reviewed, the patterning and modification of a porphyrin molecule can alter its shape and symmetry in a predictable manner.[14] Normal-coordinate or symmetric-coordinate studies allow one to quantify these movements in terms of symmetric class, such that determining resultant symmetry is reduced to series of matrix operations.[50] Additionally, there is a wealth of information on the effect of these symmetry-breaking movements on the resultant properties of the photoactive core and how this conformational flexibility is used in nature to control porphyrinoid cofactor functions.[3a,5a,f]

3.1. Technical Aspects of Plot Generation

The Normal-coordinate Structural Decomposition (NSD) program—the standard means to analyze and describe porphyrin macrocycle conformations—has been previously described and recently reviewed.[3a,14,50] This program is a computational method of decomposing the distortion of a substituted porphyrin molecule into a normal-coordinate space, where representations of atomic coordinates have an idealized symmetry, for example, a *Ruffled* (B_{1g}) or *Dome* (A_{2u}) shape. From the crystallographically (or computationally) identified positions of the 24-atom porphyrin macrocycle, we can obtain the magnitude attributable to 66 orthogonal modes (i.e., 3n–6), classed by their irreducible representations in the D_{4h} symmetry group.[51]

The result is a set of numbers which relate the magnitude of distortion in real space classed by symmetric terms. By knowing the magnitude of the symmetric distortions, one can determine the approximate symmetry of a distorted molecule by, for example, ignoring small movements and considering only large deviations. While this distortion can be represented in numerical terms, it is difficult to conceptualize the symmetry of the summation of multiple disorder modes, therefore a pictographic representation is highly desirable, and speaks to our motivation for this work.

The concerted movement of atoms can be considered as the adoption of an altered shape from the symmetric version, with each symmetric irreducible representation term representing a different mode of stretching or bending. This can be understood by envisioning the differences between folding, stretching, fluting, or wringing a sheet of paper; while each is similar in that they distort the original shape, they are distinct patterns which can be easily identified (Figure 6). In this sense, the design of distortion—away from symmetry—can be compared to a molecular origami—taking a symmetrical molecule (or paper,[52] in our analogy) and manipulating its shape to craft a new form.

Similarly, the measured magnitude of each mode is important, as small movements are conceptually eclipsed by larger deviations. The NSD method is one way of quantifying the different component shapes that make up a molecule. This analysis relays distortion magnitudes encoding this information in the NSD table (Figure S7); analogous to the "nutritional information" on processed foods, it relays important quantitative, obscured information which complements descriptive features.

The magnitudes of distortion described for porphyrins are the NSD "comp." value, a combination (sum-of-squares) of extent of the many predefined modes which share each symmetric basis. This measurement is the real-space devia-

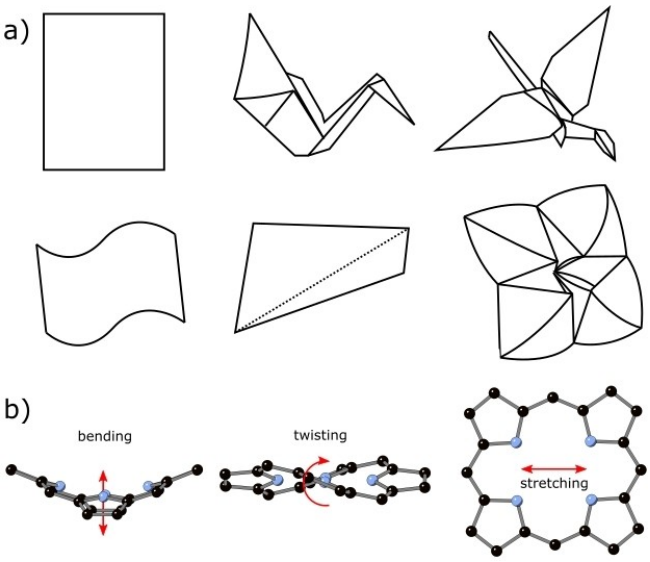

Figure 6. a) Origami involves the folding of symmetrical paper into lower symmetry forms. b) Bending, stretching, and twisting of porphyrin macrocycles.[5a]

tion of the atoms of each pyrrole component from ideal along its calculated vibrational modes, approximating that same movement in real space. For other molecules which can be investigated through our related Symmetry-Coordinate Structural Decomposition (SCSD) method program,[51] the deviation described is the sum movement of all atoms along the symmetric basis, or the symmetry displacement coordinates. In practice, we have found that asymmetric distortions of rigid groups, such as anthracene or 4,4-difluoro-4-bora-3a,4a-diaza-*s*-indacene (BODIPY) are dominated by an individual principal component per symmetry basis.

Symmetry in each case is determined by a predefined lookup table of point groups. A, B and E operations (B_{1g}, B_{2g}, etc.) are assigned to a precomputed binary representation of the point group table, based on whether the symmetry operations are present (1) or absent (0) under this distortion. A multiplication (i.e., AND operation) yields a string which represents the symmetry of the total group which is compared with another precomputed lookup table. These tables are presented for the point groups C_{2v}, C_{2h}, D_{2h} and D_{4h} (Table S1). For technical details see S.I. 2.

A static plot is generated using matplotlib[53] (pyplot.contourf), in Python. These methods are available through an online interface at www.sengegroup.eu/nsd (extended output, for porphyrins) and www.sengegroup.eu/scsd, with source code available (S.I. 2.2.). Representation of the axes as logarithmic allows interesting features at different scales to be highlighted; in some cases, a large element appears in the center of a plot, demonstrating a compromise between the two representational demands.

3.2. Motivation Behind the Present Work

The most common feedback to the NSD program we encountered was that the display of unadorned numerical values for representing molecular shape and symmetry was unapproachable and inscrutable (see Figures S7, S9, S10). The utility of being immediately understood—or at least approachable—is greatly increased as these techniques can inform general chemistry. The present method of data display is intended to intrigue the viewer and draw attention from that intrigue, to allow NSD and the related SCSD method[51] to be more visual and presentable. Additionally, this presentation opens an avenue for discussion on artistic representations of scientific conceptions of symmetry, similar to Heilbronner and Dunitz' delightful *Reflections on Symmetry*,[54] allowing an agreeable crosstalk. For the scientist, this plot is intended to act as a tool to rapidly assess and demonstrate the emergent symmetry of near-symmetric molecular moieties, allowing for deeper insight into crystallographic data beyond initial inspection, to be discussed simultaneously with the numeric values. For the artist, this plot can provide a visually pleasing representation of contrasting (scientific and artistic) interpretations of symmetry, and hopefully provide inspiration for the incorporation of scientific ideas into artwork.

Diagrams such as the one shown in Figure 2 can be considered as a conceptual counterpart to the commonly encountered phase diagrams, with phase boundaries replaced by increasingly closer scrutiny of atom positions in the crystallographically determined solid state. Similarly, this diagram can be used for calculated molecules to assess the correct assignment of a symmetry point group from spectroscopic studies—should the hierarchy of distortional modes persist, the correct point group under any investigation should be demonstrated on this plot at some level.

3.3. Description of the Diagram

A Neoplastic plot in Mondrian's style is an abstract representation of the symmetry of an individual molecule, split by the thresholds across which additional distortion is considered. In a Neoplastic plot pertaining to a porphyrinoid molecule, vertical and horizontal lines are co-opted to represent the magnitude of symmetric distortions along the primary (out of plane, z_{3D}) and secondary (in plane, x_{3D} and y_{3D}) axes of the porphyrin molecule in three dimensions. The point groups pertaining to the molecule are represented as large blocks of color, divided by indicators of the symmetric distortions which alter the symmetric representation of the chromophore core. Both x and y axes are placed on logarithmic scales.

In the abstract sense, porphyrins have D_{4h} symmetry, which is assigned to the top right corner of each plot—the symmetry elements of which as applied to an ideal porphyrin molecule are shown in Figure S1. As the eye moves left or down, it crosses thresholds beyond which we consider a new distortion of out-of-plane or in-plane motion. Beyond that threshold, the mental image of, e.g., a *saddled*

porphyrin, the accepted atom positions (closer now to the measured atom positions) and the point group (i.e., D_{2d}) are changed, as represented by a change in plot color. In a plot describing a porphyrinoid more distorted from the reference (5,10,15,20-tetraphenylporphyrinato)copper(II) [Cu-(II)TPP],[3a] these thresholds would appear closer to the upper right; consequently, more of the plot would be taken up by colors representing lower point groups. A simple example is the macrocyclic unit of the recently published 5,15-bis(pent-3-yl)porphyrin demonstrated in Figure 7.[55]

The porphyrin core has the initial assumption of D_{4h} symmetry, as indicated at the upper right limit of Figure 7a. As we progress away from the upper right in a diagonal manner down and then left (in plane and then out-of-plane), we encounter the measured distortional aspects of the porphyrin core in order from most, to least, prominent which relays an important narrative about a crystal structure. 5,15-Bis(pent-3-yl)porphyrin has different substitution at the 5,15- and 10,20-positions; the stretching of the dialkyl axis yields a B_{2g} distortion of 0.6 Å, reducing the symmetry to D_{2h}. An A_{1g} (totally symmetric expansion) distortion compared to the idealized model has no effect on the symmetry, and thus transiting this line will retain D_{2h} symmetry. The different positioning of the pyrroles (i.e., amine vs. imine) yields a minor B_{1g} distortion of around 0.1 Å, which reduces the symmetry to C_{2h}; although localized here, these protons will not show a significant barrier to isomerization through prototropism. While this molecule is mostly planar, a small non-planar component is indicated as

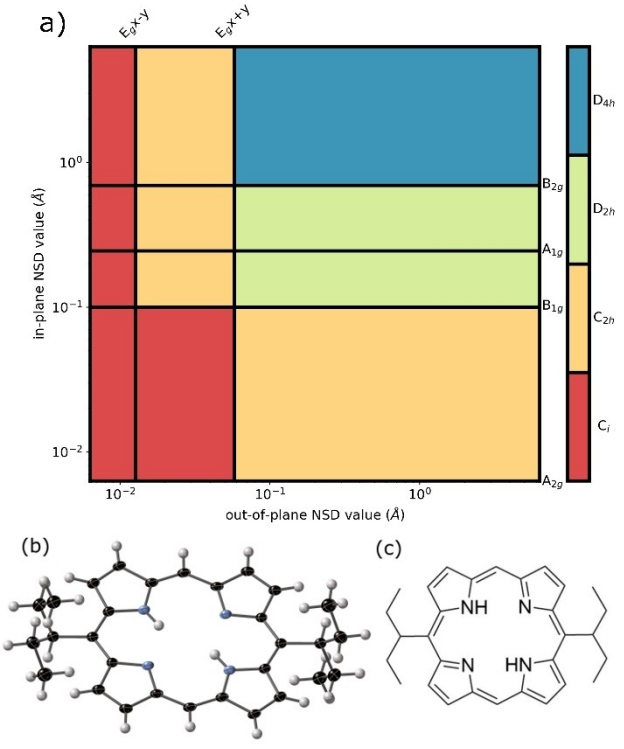

Figure 7. (a) The Mondrian diagram and (b) view of the molecular structure of 5,15-bis(pent-3-yl)porphyrin (c) in the crystal [CCDC: TUSROR].[55]

the $E_g(x)$ which reduces symmetry to that indicated by the crystal structure, of C_i. As shown above, the reading of this plot alongside a diagram of the relevant symmetry modes tells a story about the structure not evident from a simple diagram, such as that in Figure 7b.

Different spectroscopic and diffraction techniques operate on the same molecule at different timescales and temperatures, and therefore will probe the same molecule with different apparent point group symmetries. One could logically surmise that the largest distortion components will be the most resistant to thermal inversion, and the symmetry derived from techniques such as NMR (nuclear magnetic resonance) should be represented somewhere on a Mondrian plot, at coordinates approximately consistent between similar analytes.[23b]

Symmetry and chirality are often approached as Boolean (i.e., True or False) concepts, with a defined point group being an abstract concept attributable to any molecule, and either chiral-or-achiral based on the presence of a single stereocenter. The experience of a crystallographer is the idealized symmetry of a molecule and the symmetry imposed by the space group are often related but not identical. In the solid state, small perturbations based on steric environment alter the molecules in small but measurable ways (not necessarily indicated by spectroscopic techniques), and disorder can overlap chemically distinct environments. While more apt measures may be available which meld these concepts, depicting molecules in more intuitive terms is imperative.

This representation is essential when considering the drive for asymmetric molecules. For example, in attempting to engage porphyrin molecules as antennae in visible light circular dichroic (CD) spectroscopy, it is crucial that under the ambient conditions and measurement timescales these molecules have an induced chirality, and in turn an achiral point group.[56] As demonstrated in Mondrian plots, the introduction of both *gerade* and *ungerade* distortions into a porphyrin is an approachable method to access chiral point groups.[57]

Skeletal representations (i.e., simple 2D illustrations, see Figure 1) of porphyrins are considered by the right-hand border of the Neoplastic plot—by concerning only the in-plane deviations of a molecule in a planar depiction. Similarly, a skeletal plot[58] of molecular deviations from coplanarity, also a common representation of porphyrin molecules for publication (Figure S9), is represented by the upper-left quadrant. In crystallography, the accuracy of three-dimensional determination allows for symmetric determination in the lower left quadrant, although a crystallographically confined molecule is not necessarily indicative of its structure in solution. The conformation in the solid state is not representative of the molecule in solution or gas phase where it is most often encountered.[59] The solution state can be probed with data-rich spectroscopic techniques such as NMR studies.[23] Often the symmetry information revealed through these investigations is one of the point groups represented in the center to upper right quadrant of a Mondrian plot. Variable temperature NMR can often probe the same molecule in a variety of point groups,[59] allowing

averaged symmetry to appear due to time-scale constraints; this can be represented as crossing thresholds on this plot, where additional energy can cause a molecule to racemize over an energy barrier on NMR timescales.

Some aspects of Mondrian's original works and style, notably the restricted color palette, had to be abandoned for pragmatic terms.[60,61]

4. Using Mondrian Representations—Test Cases for the Chemists

The Mondrian representations allow detailed interpretations of molecular structures and symmetry relationships. To illustrate this we have compiled a series of 'test cases' and give detailed analyses in the S.I. (see section 3.):

- The classics: 2,3,7,8,12,13,17,18-octaethylporphyrin (H_2OEP) and 5,10,15,20-tetraphenylporphyrin (H_2TPP) (Figure S11–S13).[62–66]
- Bisaquo(5,10,15,20-tetraphenylporphyrinato)zinc(II) [Zn(II)TPP(OH_2)$_2$] as an example of a compounds with multiple reported crystal structures, illustrating the impact of different refinement strategies (Figure S14).[67]
- Oxygenated and deoxygenated heme as example for the use of Mondrian plots in biological chemistry (Figure S15).[68,69]
- Chirality in porphyrin dication salts (Figure S16, S17).[55,70,71] and
- nonplanar atropisomeric porphyrins (Figure S18)[72–74] as illustrations of current studies in our group.

The artistic appeal of some of the associated Mondrian plots is highlighted in Figure 8.

Further simple examples of Mondrian plots are available in the S.I. as a guide to navigating and narrating the near-symmetry nuance of novel compounds (Figure 9). These include: (unsubstituted) porphyrin PORPIN02 (Figure S19),[75] planar Zn(II)OEP ALOKOB (Figure S20),[76] *sad* distorted Zn(II)OETPP·MeOH JICNIS (Figure S21),[77] *ruf* distorted (pyridine)(5,10,15,20-tetra(*tert*-butyl)porphyrinato)zinc(II) ZIJDAX (Figure S22),[78] (5,10,15,20-tetrakis(1-ethylpropyl)porphyrinato)nickel(II) DOWDUO (Figure S23),[79] [N^{21},N^{22}-B(−$OBCl_3$)$_2$B-N^{23},N^{24}]-tetrakis(4-chlorophenyl)porphyrin NOLYES (Figure S24) as an example of a 'stretched' porphyrin,[80] and a series of free base and nickel(II) complexes of 2,3,7,8,12,13,17,18-octaethylporphyrins with various degrees of nonplanarity induced by different numbers of meso-alkyl residues—QAKJER (Figure S25),[81] QAKJAN (Figure S26),[81] QAKKES (Figure S27),[81] QAKKIW (Figure S28),[81] NOLXUH (Figure S29),[82] CUBZII (Figure S30).[83]

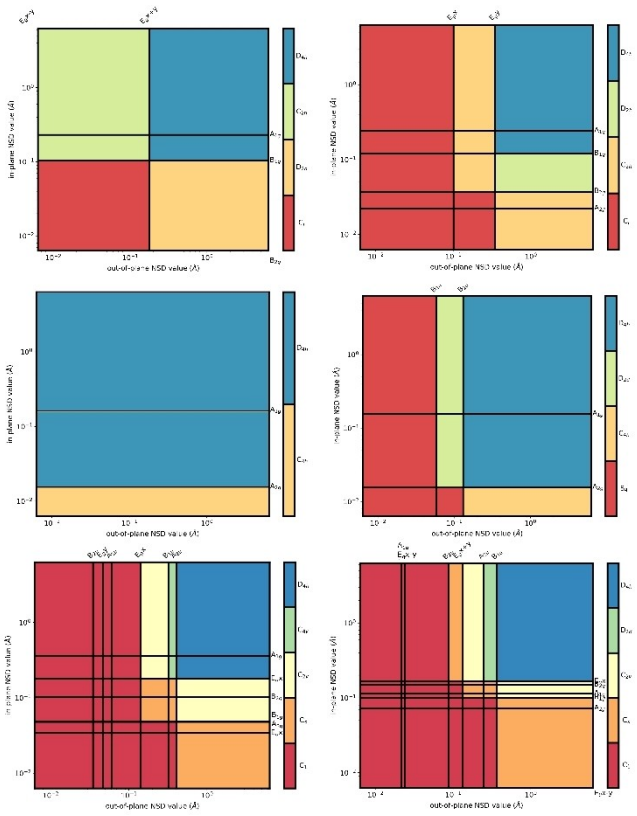

Figure 8. Vernissage—A portrait gallery of various porphyrins in Neoplastic style. For discussion see S.I. From left to right by row: OETPOR10,[63] TPHPOR15,[64] ZNTPOR05,[67c] ZNTPOR06,[67d] deoxy-heme (PDB: 2dn2 and oxy-heme (PDB: 2dn1).[69]

5. Discussion

5.1. Art and Science Interplay

The interplay between artistic and scientific notions of symmetry has a long history, with architecture featuring prominently, as described above.[84] As explained, the fundamental operations of symmetry we have enumerated, in both crystallographic space-group and molecular point group terms, such as reflection, rotation and inversion have both strict mathematical definitions and malleable, intuitive artistic definitions in parallel. Exploration of symmetric operations and concepts is found in the visual work of M. C. Escher and the sculptural work of Ai Weiwei, and in the illustrations accompanying C. S. Lewis' work, among many others.[25] This notion of artistic and scientific interplay is similarly expressed in the Pulitzer Prize-winning *Gödel, Escher, Bach* in which Hofstadter uses artistic representations as a device for the expression of complex ideas around self-reference in logical systems.[85]

Naturally, there are many more examples of cross-pollination between the arts and science which go beyond '#SciArt'.[86] A full discussion of the many classic and contemporary cases linking science, visual arts, music, poetry, literature, and design is for another time, but we note that mankind's advances often entail periods of

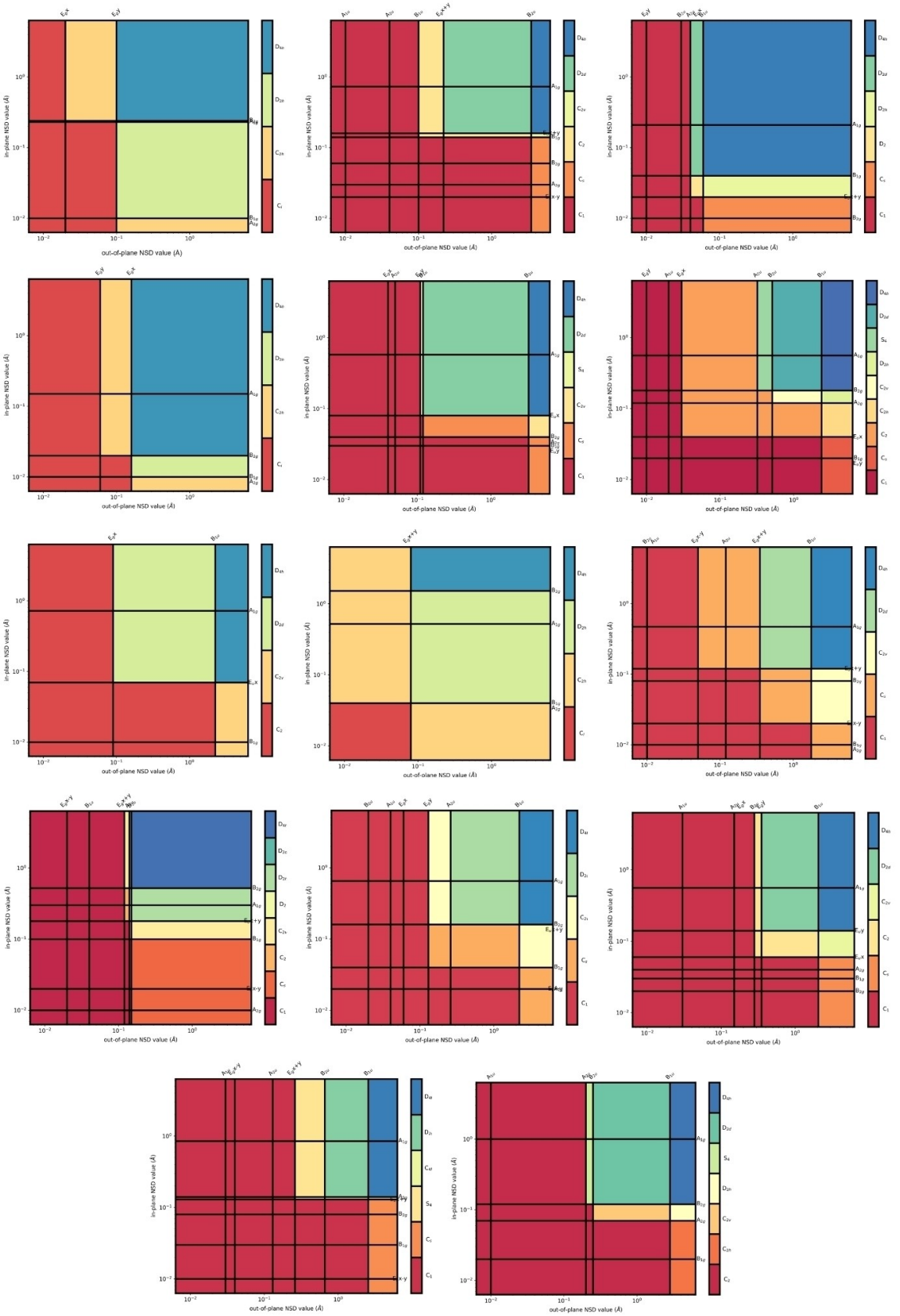

Figure 9. Vernissage—A portrait gallery of various porphyrins in Neoplastic style. For discussion see S.I. From left to right by row: OKOQUA,[65] SATQOU,[66] PORPIN02,[75] ALOKOB,[76] JICNIS,[77] ZIJDAX,[78] DOWDUO,[79] NOLYES,[80] QAKJER,[81] QAKJAN,[81] QAKKES,[81] QAKKIW,[81] NOLXUH,[82] CUBZII.[83]

convergence where artistic and scientific revolutions coincide.[87a] Mondrian's De Stijl grew out of the advent of cubism—a turning point in occidental art—which coincided with Einstein's *Annus mirabilis* papers which transformed our concepts of space, time, mass, and energy.[87b]

In chemistry the art, symmetry, and science interplay can be traced back to the Platonic bodies (see also Figure S6) and Archimedian solids, culminating in van't Hoff's tetrahedral carbon[88]—all entailing the use of imagination as essential in science.[86] Intriguing contemporary examples are Cernak and co-worker's "*Molecular Sonification for Molecule to Music Information Transfer*", i.e., the representation of molecular structure as a musical composition and Neumann, Schnurr, and Wegner's "*Perspective Isomorphs*" as a means to classify molecular structures.[89]

The art-science interface is increasingly seen as a necessary focus for future developments in both areas, requiring a *"more inclusive understanding of the subtle interplay between science and art, and the belief that as individuals and cultural agents we all blend both aspects in our respective fields of endeavor"*.[90] In fact, contemporary initiatives in 'Art and Science' require a transformative break of discipline boundaries and merger to 'ArtScience'.[91]

In the present case, the interplay between artistic representations and scientific data can expand the thinking of the scientist into more abstract notions, more pleasing visual representations, or engaging teaching materials. Similarly, this can expand the artist's rigor towards the conveyance of increasingly complex and nonintuitive notions, placing a deeper truth to abstract forms and allowing for quantified notions of aesthetic appeal.

5.2. Top-down and Bottom-up Approaches to Symmetry

We have discussed the Neoplastic diagrams above with reference to the normal coordinate structural decomposition of the molecule, due to how this device is constructed and interpreted. A related approach of describing symmetry, the continuous symmetry measure, can also be imagined using this plot. With symmetry coordinates, one adds symmetric distortion modes (from molecular design) to an ideal frame to arrive at the 'compromise' symmetry (i.e., the top-down approach, from highest symmetry). This is contrasted with the bottom-up approach of CSM[19] or SYMMOL,[92] which effectively subtracts minor deformations from the dissymmetric structure to arrive at this same atomic positions, and therefore symmetry. An equivalent interpretation of neoplastic diagrams can be found. With a bottom-up approach, one would begin at the lower left corner of this diagram and eliminate the smallest orthogonal vectors to arrive at a compromise symmetry—usually the spatially closest corner of a block to that bottom left corner. In light of this nomenclature, one may desire to present this diagram as a diamond—another common motif of Mondrian[93] (see Figure S31)—which would relate symmetry and gravity and emphasize the dichotomy of approaches. Each panel in this system will have a Continuous Symmetry Measure value, which can be calculated by simple matrix operations—an indication of the magnitude of this measure can be approximated by distance to the bottom corner.

5.3. Expansion of the Concept

The use of a neoplastic symmetry representation can be expanded to other simple and well-studied symmetric molecules easily. One requires the highest symmetry achievable, the 3D positions of these atoms and, optionally, a totally symmetric molecule for comparison. This practical symmetric-coordinate structural decomposition for crystallographic analysis will be described in a future publication, but yields values comparable with those described for porphyrins, using a matrix version of previous symmetry-coordinate calculations.[51] As an example, the D_{2h}-symmetric anthracene core can be distorted in the "twistacene" series[94] whose Mondrian plots shown in Figures S32 and S33 are enlightening as to the symmetric character and its influence. Similarly, we have applied this concept to distorted dipyrromethene ligands such as that in the recently reported photosensitizer Ir(Cp*)(Me_4DPM)$Cl^{[95]-}$which primarily displays a B_2—"flap" conformational mode, exacerbated by steric bulk (Figure S34), a triphenylhexabenzo-BODIPY (Figure S35),[96] and chair and boat conformations of cyclohexane (Figure 1b, Figures S36 and S37).[97] Detailed plots are included alongside a brief commentary on structural symmetry in the S.I., as a guide to using these devices in publications of crystallographic data (Figure 10).

This concept can similarly be applied to macroscopic objects by analogy, though no programmatic display yet exists. Dunitz highlighted potatoes as an example of a chiral object that is difficult to assign handedness[98]—though the common stackable pressed potato chip can be analogous to porphyrin distortion. In D_{4h}—an out-of-plane "bending" of this chip ($A_{2u}+B_{2u}+(A_{2u}\times B_{2u}=$in-plane B_{1g})) reduces this symmetry to C_{2v}; the magnitudes of these bends may vary between manufacturers (around 0.7–1.3 cm) but the identities are fixed for that idiographic shape, so hypothetical Mondrian plots would therefore appear similar.[99]

Although the representation is dependent on the relation of points, this display methodology could be expanded to relations of fields, functions, or into multi-dimensional space, dependent on the framing of the data reduction. An evolutionary form of this plot, abandoning straight lines or using animation, can be imagined for displaying the molecular dynamics of, e.g., time-resolved crystallographic series.

6. Conclusions

The Mondrian plot presented here is a simple tool for the analysis of molecular symmetry, which can be used for structural discussion and display. We believe the use of this artistic form helps to show an important aspect of structural chemistry as an appealing visual device. The contrasting views of symmetry between artistic and scientific commun-

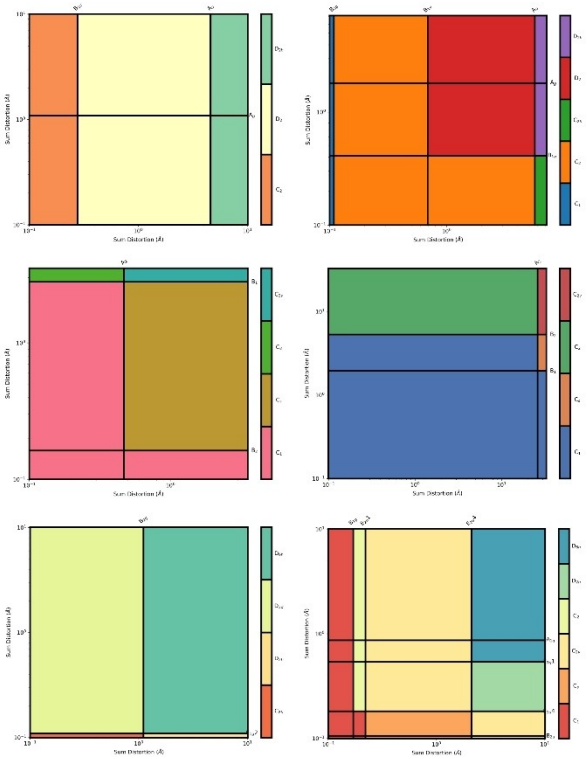

Figure 10. Vernissage—A portrait gallery of SCSD parameters of non-porphyrinoid compounds in Neoplastic style. For discussion see S.I. From left to right by row: ZOPJUJ,[94a] JEZXOE,[94b] OLOTAN,[95] HEDMAH,[96] CYCHEX06,[97a] DIYNUV.[97b]

ities, as discussed, can be unified somewhat by cross-pollination of ideas, and we would welcome any additional collaboration in this area. Similarly, this display-oriented approach invites scientists to think more about the assumptions that they are using in the modelling and discussion of molecular symmetry, and perhaps, to formalize insights around observed structural minutiae. Likewise, this visual device is a useful tool in the storytelling aspect of structural description, ordering the importance of crystal features to their effects on the primary component.

Our continuing work will focus on using this and similar representations to show and communicate the shape intricacies of molecules, as well as to integrate this shape analysis into popular crystallography programs. This plot, as part of the NSD and SCSD programs,[51] is available at www.sengegroup.eu/nsd and www.sengegroup.eu/scsd to run on molecular components of interest to the reader, given an appropriate set of coordinates.

Supporting Information

See footnote on the first page of this article: Excursus—Symmetry in Chemistry; supplementary illustrations and Mondrian plot descriptions; technical aspects of plot generation. The authors have cited additional references within the Supporting Information.[100,101,102]

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

Data are available in the supplementary material.

The software is freely available on the internet (see links in paper)

Keywords: Piet Mondrian · symmetry · ArtScience · porphyrinoids · De Stijl

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[60] a) Four colors cannot represent the 26 possible sub-point-groups of D_{4h} without confusion (see S. I. 3.4. for color palettes). Additionally, by representing thresholds, the black lines must span the entire plot,[60b] although these lose meaning when dividing two areas of equal symmetry due to being representable as a combination of already accessed symmetry terms.[60b,61] The colormaps used in the Mondrian plot are to be decided by the user, though perceptual uniformity and maximum contrast are encouraged. We believe that this participation model is similar to that encouraged by the *Compositions'* simplicity showing that artistic contributions can be made accessible by constrained criteria making something appealing.[61]; b) The boundaries of the plot are decided as the bounds imposed by crystallography—distortion for a porphyrin molecule rarely exceeds 5 Å in NSD terms, and atoms in a standard X-ray experiment cannot usually be meaningfully positionally identified to a greater accuracy than 0.01 Å.

[61] A uniform representation of the "Red, Yellow and Blue" color Scheme of Mondrian is accessible, under the name "RdYlBu". Variations on the cubehelix pattern are good choices if the plot is likely to be printed, and "Spectral" is very visually approachable in color. The Supporting Information provides a visual gallery.

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