Equivariant Symmetry Breaking Sets

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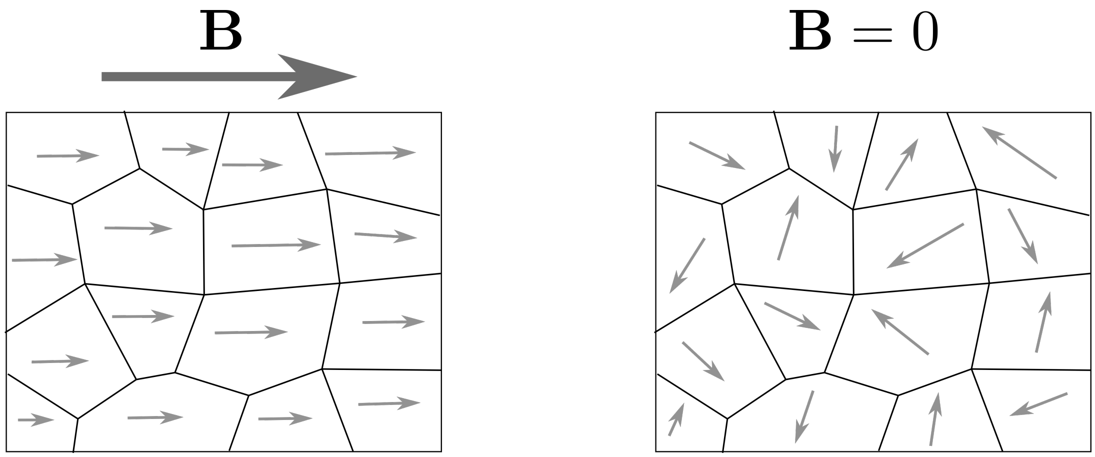
Abstract

Equivariant neural networks (ENNs) have been shown to be extremely effective in applications involving underlying symmetries. By construction ENNs cannot produce lower symmetry outputs given a higher symmetry input. However, symmetry breaking occurs in many physical systems and we may obtain a less symmetric stable state from an initial highly symmetric one. Hence, it is imperative that we understand how to systematically break symmetry in ENNs. In this work, we propose a novel symmetry breaking framework that is fully equivariant and is the first which fully addresses spontaneous symmetry breaking. We emphasize that our approach is general and applicable to equivariance under any group. To achieve this, we introduce the idea of symmetry breaking sets (SBS). Rather than redesign existing networks, we design sets of symmetry breaking objects which we feed into our network based on the symmetry of our inputs and outputs. We show there is a natural way to define equivariance on these sets, which gives an additional constraint. Minimizing the size of these sets equates to data efficiency. We prove that minimizing these sets translates to a well studied group theory problem, and tabulate solutions to this problem for the point groups. Finally, we provide some examples of symmetry breaking to demonstrate how our approach works in practice.

1 Introduction

Equivariant neural networks have emerged as a promising class of models for domains with latent symmetry (Wang et al., 2022a). This is especially useful for scientific and geometric data, where the underlying symmetries are often well known. For example, the coordinates of a molecule may be different under rotations and translations, but the molecule remains the same. Traditional neural networks must learn this symmetry through data augmentation or other training schemes. In contrast, equivariant neural networks already incorporate these symmetries and can focus on the underlying physics. ENNs have achieved state-of-the-art results on numerous tasks including molecular dynamics, molecular generation, and protein folding (Batatia et al., 2022; Batzner et al., 2022; Daigavane et al., 2023; Ganea et al., 2021; Hoogeboom et al., 2022; Jia et al., 2020; Jumper et al., 2021; Liao & Smidt, 2022).

A consequence of the symmetries built-in to ENNs is that their outputs must have equal or higher symmetry than their inputs (Smidt et al., 2021). However, many physical systems exhibit symmetry breaking. In physics, these are classified into two types: explicit symmetry breaking and spontaneous symmetry breaking (Castellani et al., 2003). In explicit symmetry breaking, the governing laws are manifestly asymmetric while in spontaneous symmetry breaking the laws are symmetric but we observe asymmetry in individual data samples. For example consider ferromagnetic materials Aharoni (2000). Suppose we have a heated ferromagnetic material which we then cool in the presence and absence of a magnetic field as shown in Figure 1. In the presence of a strong external magnetic field, we observe a magnetic moment aligned along that field in each magnetic domain. This is an example of explicit symmetry breaking since the external field explicitly breaks rotational symmetry. However, if there is no external field, we still observe a magnetic moment due to ferromagneticity which breaks rotational symmetry. However, the direction of the moment is uniformly random for each domain. This is an example of spontaneous symmetry breaking, the governing laws are symmetric yet we observe asymmetry in individual samples. We define explicit and spontaneous symmetry breaking more formally in Section 2.



(a) Explicit symmetry breaking

(b) Spontaneous symmetry breaking

Figure 1: (a) Example of explicit symmetry breaking. Magnetic moment in domains align with a strong external field. The external field explicitly breaks symmetry of the system. (b) Example of spontaneous symmetry breaking. Presence of a moment in each domain breaks rotational symmetry. However, there is no magnetic field so governing laws of the system are symmetric. Consequently the moments are uniformly random in orientation.

One class of approaches conducive for explicit symmetry breaking is learning to break symmetry. For example, Smidt et al. (2021) showed that the gradients of the loss function can be used to learn a symmetry breaking order parameter, identifying what type of missing asymmetry is needed to correctly model the results. Another related approach is approximate and relaxed equivariant networks (Huang et al., 2023; van der Ouderaa et al., 2022; Wang et al., 2023; 2022b). These networks have similar architectures to equivariant models, but allow nontrivial weights in the layers to break equivariance. Hence, they can learn how much symmetry to preserve to fit the data distribution. However, since these methods break equivariance, they are not appropriate for spontaneous symmetry breaking. If all symmetrically related lower symmetry outputs are equally likely in the data, then relaxed networks will see the distribution as symmetric and fail to break symmetry. Further, since equivariance is broken, the method is not guaranteed to behave properly when shown data transformed under the group.

In the case of spontaneous symmetry breaking, there exist some works which partially solve the problem. Balachandar et al. (2022) design a symmetry detection algorithm and an orientation aware linear layer for mirror plane symmetries. However, the scope of their methods are specific to that type of symmetry and point cloud data. Finally, Kaba & Ravanbakhsh (2023) take the approach of defining a relaxed version of equivariance which takes input symmetry into account. They derive modified constraints linear layers would need to satisfy for this relaxed equivariance and argue such models can give lower symmetry outputs. However, they mention these conditions do not reduce as easily as for the usual equivariant linear layers. Further this method still does not provide a mechanism to sample all possible outputs.

Our work focuses on the spontaneous symmetry breaking case. This case is extremely important as spontaneous symmetry breaking occurs in many physical phenomena (Beekman et al., 2019). Hence the widespread adoption of machine learning techniques for scientific applications will inevitably run into symmetry breaking issues. Examples of existing applications which may run into difficulties include crystal distortion, predicting ground state solutions from Hamiltonians, and solving PDEs (Jafary-Zadeh et al., 2019; Lewis et al., 2024; Lino et al., 2022). In the crystal distortion case, there are distortions from high symmetry to low symmetry structures (Kay & Vousden, 1949). The lowest energy states of physical systems (ground states of the Hamiltonian) are often low symmetry and famously explains the Higgs mechanism for giving particles mass (Higgs, 1964). Finally, Karman vortex sheets are a well known example of symmetry breaking in fluid simulations (Tang & Aubry, 1997).

In this work, we provide the first general solution for the spontaneous symmetry breaking problem in equivariant networks. We identify that the key difficulty is how to allow equivariant networks to output a set of valid lower symmetry outputs. Our approach is similar to Smidt et al. (2021) in that we provide symmetry breaking parameters as input to the model. However, rather than learning these parameters, we show that we can sample them from a symmetry breaking set (SBS) that we design based only on the input and output symmetries. In particular, we prove that optimizing equivariant SBSs is equivalent to a fundamental group theory question. We emphasize that this fully characterizes how to efficiently break symmetry with equivariant SBSs for any group. Counter-intuitively, we find that it is sometimes beneficial to break more symmetry than needed.

Compared to existing methods, our approach has the following advantages:

1. **Equivariance:** Our framework guarantees equivariance. That we can achieve this is a key point of this work and allows simulation of spontaneous symmetry breaking.
2. **Simple to implement:** Our approach only requires a designing a set of additional inputs into an equivariant network. We have fully characterized such sets.
3. **Generalizability:** We emphasize that our characterization of SBSs applies to any groups.

We would like to point out that to achieve our results, we assume we can detect the symmetry of our input and outputs. Further, there is the more general problem of treating symmetrically related outputs as the same in our loss. We discuss these limitations in Appendix D.

The rest of this paper is organized as follows. In Section 2 we formalize the symmetry breaking problem and the type of task performed in the spontaneous symmetry breaking setting. In Section 3, we examine the case where we break all symmetries of our input. We motivate the idea of a SBS and show that imposing equivariance leads to an additional constraint of closure under the normalizer. The intuition is that the normalizer characterizes all orientations of our data which do not change its symmetry. Next, we translate bounds on the size of the equivariant SBSs into the purely group theoretical problem of finding complements. We have tabulated these complements in Appendix F for the point groups. In Section 4, we generalize to the case where we may still share some symmetries with our input. In Section 5 we describe how to construct SBSs in an actual implementation. Finally, in Section 6, we introduce examples of symmetry breaking and demonstrate how our method works in practice.

Notation and background: An overview of the notation and common symbols used can be found in Appendix A. A brief overview of mathematical concepts needed in the paper can be found in Appendix B and an overview of ENNs can be found in Appendix C.

2 Symmetry breaking problem

Here, we make precise what we mean by a symmetry breaking and the issue it poses for equivariant neural networks. We begin with the following observation first made in Smidt et al. (2021).

Lemma 2.1. *Let $f : X \to Y$ be an G-equivariant function. We can choose f such that $f(x) = y$ only if* $\mathrm{Stab}_G(y) \geq \mathrm{Stab}_G(x)$.

See Appendix E.1 for a generalization of this lemma and a proof.

Hence, the output of an equivariant function must have at least the symmetry of the input. This motivates the following definition of symmetry breaking at the individual sample level.

Definition 2.2 (Symmetry breaking sample)**.** Let G be a group. A sample with input x and output y is symmetry breaking with respect to G if $\mathrm{Stab}_G(x) > \mathrm{Stab}_G(y)$.

Lemma 2.1 tells us a symmetry breaking sample with respect to G can never be perfectly modeled by a G-equivariant function. In experimental samples, we may have random noise in our observations of our outputs which causes samples to be symmetry breaking. In such cases equivariance is beneficial since it can help remove the noise. However, in some cases we truly have a symmetry breaking sample even if there is no noise. In physics this is classified into two cases: explicit symmetry breaking and spontaneous symmetry breaking. In the following discussion, it is useful to view the underlying model as a set valued function. A typical function $h : X \to Y$ can be thought of as a set valued function $f : X \to \mathcal{P}(Y)$ defined as $f(x) = \{g(x)\}$. Note that if there is an action of G on Y, one can naturally define an action on $\mathcal{P}(Y)$ such that $U \subseteq Y$ transforms as $gU = \{gu : u \in U\}$. Hence there is a natural way to define equivariance of set valued functions.

In explicit symmetry breaking, the underlying physics of the system is asymmetric. For example, there may be an unknown electric field which breaks rotation symmetry.

Definition 2.3 (Explicit symmetry breaking)**.** Let G be a group. A function $f : X \to \mathcal{P}(Y)$ which is not G-equivariant explicitly symmetry breaks G.

In such cases using an equivariant function actually prevents us from learning the true function.

In spontaneous symmetry breaking, the underlying physics of the system is symmetric, however there is a set of stable lower symmetry outputs which occur with equal probability.

Definition 2.4 (Spontaneous symmetry breaking (SSB) function)**.** Let G be a group with actions defined on spaces X, Y. Let $f : X \to \mathcal{P}(Y)$ be G-equivariant. We say f spontaneous symmetry breaks at x if there is some $y \in f(x)$ such that $\mathrm{Stab}_G(x) > \mathrm{Stab}_G(y)$.

The key things here are that the set valued function f is equivariant even though individual observed samples (x, y) for $y \in f(x)$ may be symmetry breaking. Hence, our problem becomes the following.

Problem: How does one create an equivariant architecture which can output a set of possibly lower symmetry outputs?

3 Fully broken symmetry

First, we consider the case where we break all symmetry of our input. Here, our desired outputs y share no symmetry with x. In other words $\mathrm{Stab}_S(y) = \{e\}$. This will lay the foundation for analyzing the general case of partially broken symmetry. Let the symmetry group of our data x be S.

3.1 Symmetry breaking set (SBS)

When there is symmetry breaking there are multiple equally valid symmetrically related outputs. The purpose of a symmetry breaking object is to allow an equivariant network to pick one of them. In principle, we want all symmetrically related outputs to be equally likely so it makes sense to think of a set B of symmetry breaking objects we sample from.

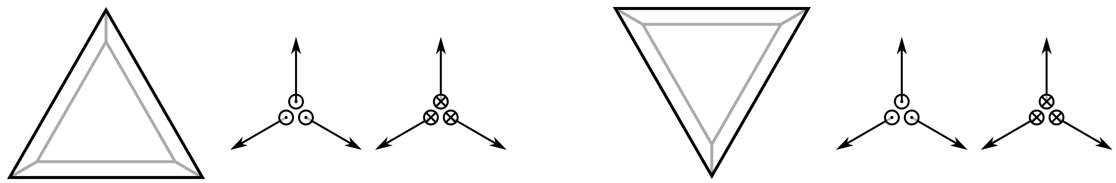
For any $s \in S$ and $b \in B$, since sb is symmetrically related to b it is natural to also include it in B. Hence, acting with s on the elements of B should leave the set unchanged. Further, for any $b \in B$, the stabilizer $\mathrm{Stab}_S(b)$ must be trivial since we want to break all symmetries of our input. This is exactly the definition of a free group action of S on B. Hence, we define a symmetry breaking set as follows.

Definition 3.1 (Symmetry breaking set)**.** Let S be a symmetry group. Let B be a set of elements which S acts on. Then B is a symmetry breaking set (SBS) if the action of S on B is a free action.

3.2 Equivariant SBS

However, the above definition of an SBS is insufficient when considering equivariance. Here, we show that we need the stronger constraint of closure under the normalizer.

To illustrate the problem, consider a network which is $SO(3)$ equivariant and a triangular prism aligned so that the triangular faces are parallel to the xy plane. Suppose our task was just to pick a point of the prism. A naive way to break the symmetry is to have an ordered pair of unit vectors. The first vector is in



(a) (b)

Figure 2: (a) Naive way to break symmetry in a triangular prism where one vector points to a vertex of a triangle and a second vector points to the lower or outer triangle. (b) A rotated version of the triangular prism in. Note that the same symmetry breaking objects now point to edges of the triangle rather than vertices. However, both prisms have the exact same symmetry elements.

the xy plane and points towards one of the triangle vertices. The second vector points up or down in the z direction, corresponding to the upper or lower triangle.

However, consider the same prism but rotated 180° around z. We can check that the symmetry groups are exactly the same so we want the same SBS. But the symmetry breaking objects are related differently. In the second prism, the first vector points to an edge rather than a vertex. For equivariance, our symmetry breaking objects should be related to both prisms in the same way. So our choice of SBS was not equivariant.

Here, one may simply choose a canonical orientation and decide that we will rotate the original SBS by 180° in the latter case. However, our input may be arbitrarily complicated, and it may be hard to decide on a canonicalization. Further, canonicalization may introduce discontinuities. Hence, we would like to construct SBSs to be only dependent on the symmetry of our data, not how our data is represented. To understand exactly what additional condition is necessary, we need to carefully investigate how the symmetry breaking scheme works.

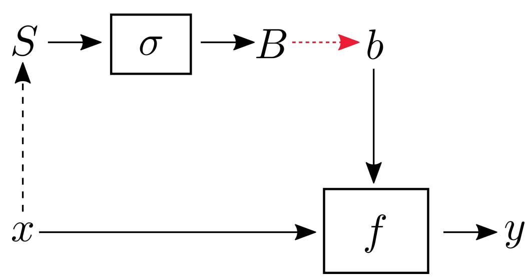


Figure 3: Diagram of how we might structure our symmetry breaking scheme. From our data x, we may obtain its symmetry S. This S is then fed into a function σ which gives us the set of symmetry breaking objects needed. We sample a b from this set breaking the symmetry of our input and feed this b along with the input x into our equivariant function f. Finally we obtain an output y which has lower symmetry than the input x.

Let f be our G-equivariant function and x be our input data. Suppose we know the symmetry S of our input. Let $\mathbf{B}$ be some set with a group action of G defined on it. We would like to obtain our set of symmetry breaking objects based on just information about the input symmetry. So suppose we have a function $\sigma : \mathrm{Sub}(G) \to \mathcal{P}(\mathbf{B})$ that does so. This function takes in a subgroup symmetry and gives a SBS composed of elements from $\mathbf{B}$. Then the symmetry breaking step happens when we take a random sample b from the SBS. This symmetry breaking object is then fed into our equivariant function, allowing it to break symmetry. A diagram of this process is shown in Figure 3.

Certainly, since we break the symmetry of our input data, we break equivariance. However, imagine we give our function all possible symmetry breaking objects and collect at the end the set Y of all outputs our model gives. This process shown in Figure 4 would then not need to break any symmetry. This is because all outputs as a set has the same symmetry as the input. Hence we can impose equivariance on our process.

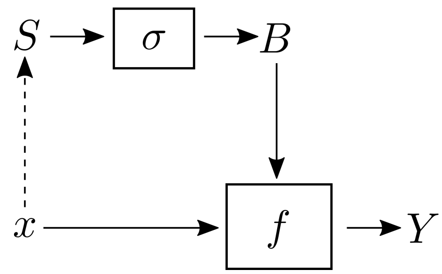


Figure 4: Diagram of how we break symmetry, but now we keep all possible outputs.

It is well known that the composition of equivariant functions remains equivariant. Hence, we just need to impose equivariance on σ. In order to do so, we must understand how the input and output transform. Suppose we act on our data with some group element $g \in G$. Then it becomes gx. Since S is the symmetry of our original data, we find $gx = gsx = (gsg^{-1})(gx)$ for any $s \in S$. So the symmetry of the transformed data is gSg^{-1}. Hence, the input of σ transforms as conjugation. Next, recall the output of σ is some subset B of elements of $\mathbf{B}$. Since there is a group action for G defined on $\mathbf{B}$, we can define an action on B by just acting on its elements and forming a new set. Figure 5 shows how our procedure would change if it were equivariant, and we act on our input by some group element g.

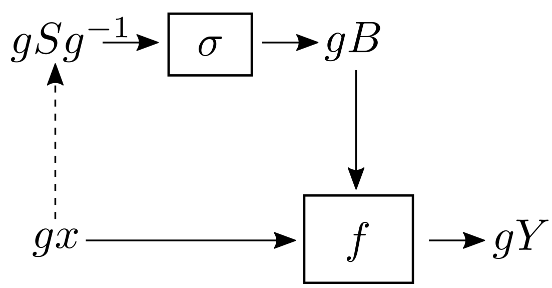


Figure 5: Diagram of what happens when we act on the input with some group element g.

We can now clearly see the issue. The input into σ transforms under conjugation, and the stabilizer of a subgroup under conjugation is precisely the definition of the normalizer $N_G(S)$. However, in many cases $N_G(S)$ is a supergroup of S. Therefore by Lemma E.1, our SBS not only needs to be invariant under S, but also be invariant under $N_G(S)$. See Appendix E.2 for a more formal justification.

With this intuition, we can now provide a proper definition for equivariant SBSs.

Definition 3.2 (Equivariant symmetry breaking sets)**.** Let S be a subgroup symmetry of a group G and $\mathbf{B}$ be a set with an action of G defined on it. Let $B \subset \mathbf{B}$ be a SBS. Then B is G-equivariant if $\forall g \in N_G(S)$ we have $B = gB$.

3.3 Ideal case and complement of normal subgroups

Now that we know how to equivariantly break a symmetry, we would like to understand how to do so efficiently. Intuitively, we expect a smaller SBS to be better and this is indeed true. If we have a larger SBS, multiple symmetry breaking objects map to the same output so the network needs to learn that these are the same. Reducing the SBS would decrease the equivalences our network needs to learn. In the ideal case, exactly one symmetry breaking parameter corresponds to each output. Since our outputs are related by symmetry transformations (transitive) under S, this corresponds to the equivariant SBS being transitive under S. It turns out, we can equate constructing ideal equivariant SBSs to the constructing complements of normal subgroups. The intuition is that we want to maximize the symmetries of the symmetry breaking objects but only in the directions “orthogonal" to S. The complement is essentially this “orthogonal" symmetry we need. A slightly weaker version of this statement can be found in Theorem 3.1.4 of Kurzweil & Stellmacher (2004).

Theorem 3.3. *Let G be a group and S a subgroup. Let B be a G-equivariant SBS for S. Then it is possible to choose an ideal B if and only if S has a complement in $N_G(S)$.*

If b is an element where $\mathrm{Stab}_{N_G(S)}(b)$ is a complement of S in $N_G(S)$, then $\mathrm{Orb}_S(b)$ is an ideal G-equivariant SBS.

Remark 3.4. It turns out the complement if it exists is isomorphic to $N_G(S)/S$. We can intuitively think of $N_G(S)/S$ as giving all possible orientations of our data such that its symmetry remains unchanged.

The proof of this theorem is in Appendix E.3. Finding complements of normal subgroups is a well studied group theory problem Kurzweil & Stellmacher (2004). For the point groups, which are the finite subgroups of $O(3)$, we have tabulated the complements if they exist in Appendix F.

3.4 Nonideal equivariant SBSs

In the case where we cannot achieve an ideal equivariant SBS, we would still like to characterize how efficient it is. To do this, we define what we call the degeneracy of an equivariant SBS. In general, each orbit under S gives us one SBS which can be matched one to one to our outputs.

Definition 3.5 (Degeneracy)**.** Let B be a G-equivariant SBS for S. We define the degeneracy to be

$$\mathrm{Deg}_S(B) = |B/S|.$$

Note that an ideal equivariant SBS B_{ideal} (if it exists) has exactly 1 orbit of S, so $\mathrm{Deg}_S(B_{ideal}) = 1$. We would also like to understand how small we can make the degeneracy if we cannot make it 1. It turns out Theorem 3.3 allows us to convert this to a group theory problem.

Corollary 3.6. *Let G be a group and S a subgroup. Let M be such that $S \leq M \leq N_G(S)$. Let B be a G-equivariant SBS for S which is transitive under $N_G(S)$. Then it is possible to choose B such that every S-orbit is also a M-orbit if and only if S has a complement in M. In particular,*

$$\mathrm{Deg}_S(B) \leq |N_G(S)/M|.$$

See Appendix E.4 for a proof. In the ideal case we can make M to be $N_G(S)$ so the above formula gives an degeneracy of 1 as expected.

4 Partially broken symmetry

We can now use our framework for full symmetry breaking to understand the case of partial symmetry breaking. In this case, our desired output may share some nontrivial subgroup symmetry $K \leq S$ with our input. Note the case of $K = \mathbf{1}$ corresponds to full symmetry breaking and $K = S$ corresponds to no symmetry breaking.

4.1 Partial SBS

Similar to the full symmetry breaking case, we would like to create a set of objects which we can use to break our symmetry. Now we can relax the restriction of free action. Intuitively, we can allow our symmetry breaking objects to share symmetry with our input, as long as it is lower symmetry than our outputs. However, the symmetrically related outputs may be invariant under different subgroups of S. Recall that if some element y gets transformed to sy, its stabilizer K gets transformed to sKs^{-1}. Hence, the stabilizers of the outputs are the subgroups conjugate to K under S denoted as $\mathrm{Cl}_S(K)$. Based on this intuition, we can define partial SBS as follows.

Definition 4.1 (Partial SBSs)**.** Let S be a symmetry group and K a subgroup of S. Let P be a set of elements with an action by S. Then P is a K-partial SBS if for any $p \in P$, there exists some $K' \in \mathrm{Cl}_S(K)$ such that $K' \geq \mathrm{Stab}_S(p)$.

Certainly, a full SBS is a partial one as well since the stabilizers of all its elements under S is the trivial group. In general, we can always break more symmetry than needed and still obtain our desired output. However, it is useful to consider the case where we only break the necessary symmetries. Counter-intuitively, we discuss in Section 4.5 that this turns out to not always be optimal.

Definition 4.2 (Exact partial SBS)**.** Let S be a group and K a subgroup of S. Let P be a K-partial SBS for S. We say P is exact if for all $p \in P$, we have $\mathrm{Stab}_S(p) \in \mathrm{Cl}_S(K)$.

4.2 Equivariant partial SBS

Similar to before, we define equivariant partial SBSs. The idea is the same, but now we need to identify the symmetry of the input and the set of conjugate symmetries for the output. Define

$$\mathrm{SubCl}(G) = \{(S, \mathrm{Cl}_S(K)) : S \in \mathrm{Sub}(G), K \leq S\}.$$

Let $\mathbf{P}$ be a set with a group action of G defined on it. As before, the idea is that we have an function $\pi : \mathrm{SubCl}(G) \to \mathcal{P}(\mathbf{P})$ which outputs our partial SBS. The condition of equivariance for our partial SBS is imposing equivariance on π.

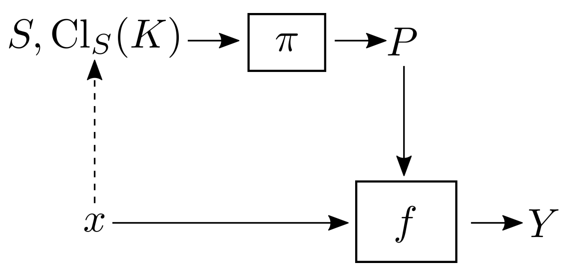


Figure 6: Diagram of how we perform partial symmetry breaking. Here, we need to specify not just the symmetry of our input but also the symmetries of our output. Since any of our outputs are equally valid, it only makes sense to specify the set of conjugate subgroups $\mathrm{Cl}_S(K)$ our outputs are symmetric under.

The symmetry breaking scheme is depicted in Figure 6. As before, we can impose equivariance on this diagram. We need to know how $\mathrm{Cl}_S(K)$ transforms. Note that if our input gets acted by g, we expect the outputs to also get acted by g. Since K is the stabilizer of one of the outputs, we expect K to transform to gKg^{-1}. Hence we have the transformation

$$\mathrm{Cl}_S(K) \to \mathrm{Cl}_{gSg^{-1}}(gKg^{-1}).$$

Similar to before, by Lemma E.1 we need the output of π to also be invariant under the stabilizer of the input. Noting that the normalizer is defined as the stabilizer of S under conjugation, we can define a generalized normalizer as the stabilizer of $S, \mathrm{Cl}_S(K)$.

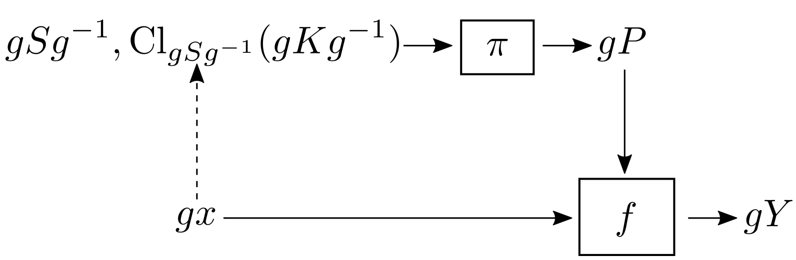


Figure 7: Diagram of how our symmetry scheme changes when we transform our input by some group element $g \in G$.

Definition 4.3 (Generalized normalizer)**.** Define the generalized normalizer $N_G(S, K)$ to be

$$N_G(S, K) = \{g : gKg^{-1} \in \mathrm{Cl}_S(K), g \in N_G(S)\}.$$

We can now define equivariant partial SBSs using closure under this generalized normalizer. See Appendix E.5 for a more formal justification.

Definition 4.4 (Equivariant partial SBSs)**.** Let S be a subgroup symmetry of a group G. Let P be a K-partial SBS. Then P breaks the symmetry G-equivariantly if $\forall g \in N_G(S, K)$ we have $P = gP$.

Note that closure under $N_G(S, K)$ is a weaker condition than closure under $N_G(S)$. Hence any equivariant full SBS is also an equivariant K-partial SBS for any K.

4.3 Ideal equivariant partial SBS

Similar to the full symmetry breaking case, we ideally would like to have a one to one correspondence between elements in our equivariant SBS and our symmetrically related outputs. For this to happen, we clearly need our SBS to be exact and for our SBS to be transitive under S. We can generalize Theorem 3.3 to obtain a necessary and sufficient condition to have an ideal equivariant partial SBS.

Theorem 4.5. *Let G be a group and S and K be subgroups $K \leq S \leq G$. Let P be a G-equivariant K-partial SBS. Then we can choose an ideal P (exact and transitive under S) if and only if $N_S(K)/K$ has a complement in $N_{N_G(S,K)}(K)/K$.*

If p is an element such that $\mathrm{Stab}_{N_G(S,K)}(p)/K$ is a complement of $N_S(K)/K$ in $N_{N_G(S,K)}(K)/K$, then $\mathrm{Orb}_S(p)$ is an ideal G-equivariant K-partial SBS

See Appendix E.6 for a proof.

4.4 Nonideal equivariant partial SBS

Similar to the full symmetry breaking case, when we cannot achieve an ideal equivariant partial SBS we want to characterize how efficient our nonideal partial SBS is. Again, the idea is that in the nonideal case, our network needs to map multiple symmetry breaking objects to the same output. We define the degeneracy of P to quantify this multiplicity.

Definition 4.6 (Degeneracy)**.** Let G be a group, S be a subgroup, and K a subgroup of S. Let P be a G-equivariant K-partial SBS for S. Let T be a transversal of S/K. Let P_t be such that every $p \in P$ is uniquely written as $p = tp_t$ for some $t \in T$ and $p_t \in P_t$. Then we define

$$\mathrm{Deg}_{S,K}(P) = |P_t|.$$

The intuition for this definition is that P_t is the set of objects which together with our input may get mapped to some output y by our equivariant network. In other words, we have $f(x, P_t) = \{y\}$ for equivariant f and all other P get mapped to different symmetrically related outputs. Without loss of generality assume y has $\mathrm{Stab}_S(y) = K$. Then for any symmetrically related output ty (where $t \in T$), we can see from equivariance of f that $f(x, tP_t) = \{ty\}$. It is now clear that the size of P_t counts how many symmetry breaking objects must be mapped to the same output.

Note that in the case $K = \mathbf{1}$, $S/K = S$ so P_t just consists of representatives from P/S. So this reduces to the degeneracy defined for full SBS. Also, note that in the ideal case, there is exactly one symmetry breaking object for each output. So degeneracy is 1 in that case.

We would like to derive bounds on the degeneracy of our equivariant partial SBSs. Similar to the full SBS case, we use Theorem 4.5 to convert this into a group theory question.

Corollary 4.7. *Let G be a group, S a subgroup, and K a subgroup of S. Let K' be a subgroup of K and M a subgroup of $N_G(S, K) \cap N_G(S, K')$ which contains S. Suppose P is a G-equivariant K-partial SBS for S which is transitive under $N_G(S, K)$. We can choose P such that $\mathrm{Stab}_S(p) \in \mathrm{Cl}_{N_G(S,K)}(K')$ for all p and all S-orbits in P are also M-orbits if and only if $N_S(K')/K'$ has a complement in $N_M(K')/K'$. Further, such a P has*

$$\mathrm{Deg}_{S,K}(P) \leq |K/K'| \cdot |N_G(S, K)/M|.$$

See Appendix E.7 for a proof.

4.5 Optimality of exact partial symmetry breaking

Note that in the previous section, we have been very careful to allow our partial SBS to break more symmetry than needed. Intuitively, we would like to say that it is always optimal to break down exactly to the symmetry of our output. That is, we only need to consider exact partial SBSs.

Certainly, ignoring any equivariance constraints, given any non-exact K-partial SBS, we can construct an exact K-partial SBS by picking an element b with $\mathrm{Stab}_S(b) \leq K$ and identifying its orbit under K together as one partial symmetry breaking object $p = Kb$. We construct the orbit of p under action by S as our K-partial SBS.

We might expect that some modification of this construction can convert any non-exact equivariant K-partial SBS into an exact equivariant K-partial symmetry breaking one. Naively, we just take the orbit of the elements in the construction above under $N_G(S, K)$ to obtain G-equivariance. However, in Appendix G we come up with an explicit example where no exact equivariant K-partial SBS is smaller than the best equivariant full SBS.

5 Constructing SBSs

Now that we have fully characterized what equivariant symmetry breaking sets are, we show how to construct them.

5.1 Expressing subgroups

First, it is important to have a way of expressing subgroup of G, the group we want to be equivariant under. We focus on $G = O(3)$ in this section though the ideas here are applicable for other groups as well.

The subgroups of $O(3)$ are well studied and have been completely classified Hahn et al. (1983). In particular, there are 7 infinite axial families of finite point groups and 7 additional finite ones. There are only 5 infinite subgroups which are closed. However, the names of these subgroups do not specify how they are "oriented" in $O(3)$. Hence, we propose to represent the subgroups in the following way. We first choose a canonical orientation of the classified point groups.

Figure 8: Two identical triangular prisms differing by a rotation. Both have symmetry D_{6h} by name, however the actual symmetry axes differ.

A standard choice is inspired by the Hermann-Mauguin naming scheme for point groups. For the 7 infinite series of axial groups, we choose to align the high order symmetry axis along the z-axis. If in addition there are 2-fold rotations, we choose one of them to be along the x-axis. If there are no 2-fold rotations but there are mirror plane parallel to the z-axis, we choose the yz-plane to be in the group. Of the remaining 7 point groups, 5 are cubic groups. For these we can choose the cube they leave invariant to have sides perpendicular to one of the x, y, z axes. Finally, the remaining 2 point groups are the icosahedral groups with and without inversion. For these we can choose to align a 5-fold axis with the z-axis and a 3-fold axis with the x-axis.

Next, for any point group S with arbitrary alignment, there is always some $g \in SO(3)$ such that $g^{-1}Sg$ brings it to the canonical orientations defined above. Hence, we can always express an arbitrary point group S as a pair $g, \texttt{name}(S)$ of a rotation and the name of the group.

5.2 Representing a set of conjugate subgroups

In the partial symnmetry breaking case, we also provide a set of conjugate subgroups. Similar to our notation $\mathrm{Cl}_S(K)$, we can specify a set of conjugate subgroups with (S, K), where subgroups S and K are represented in the way described previously.

5.3 Representing a SBS

The idea is very simple. We start with some object which breaks enough symmetry for our task. To satisfy the equivariance condition of closure under the normalizer or generalized normalized, we can simply take the orbit as our SBS or partial SBS. In principle a SBS can consist of multiple such orbits, but we can always only use one orbit as a SBS and multiple orbits increase the degeneracy. Hence we assume all our SBSs consist of one orbit and we can fully specify a SBS as a pair (b, N) where b is a symmetry breaking object and N is a group over which we take the orbit of b.

In the case of finite group N, we can explicitly compute the elements in the orbit. However, if N is infinite then this does not work. In practice, it is usually enough that we can sample lower symmetry outputs. Hence, it suffices to be able to sample the SBS which we can do by sampling an element from N.

5.4 Constructing an equivariant full SBS

We would like to construct a full SBS given an input symmetry $S = (g, \texttt{name}(S))$. However, we want to do so in an equivariant way. One way to achieve this is to first consider only any input group in its canonical orientation and construct a SBS B for it. Then simply returning gB would guarantee that our construction is equivariant. Hence, we just need to construct a canonical SBS for each possible point group.

Note an equivariant full SBS needs closure under a normalizer. If we work with $O(3)$ equivariance, we simply look up the normalizer $N_{O(3)}(S)$ from Table 4. If we are equivariant under some subgroup $G \subset O(3)$ then we note that $N_G(S) = N_{O(3)}(S) \cap G$ which can be used to compute the desired normalizer. All that remains is how to specify a canonical symmetry breaking object for each point group in canonical orientation. If we have such an object, then we obtain the following algorithm for creating equivariant full SBSs. Let `Normalizers` be a function which takes in a name of a point group and gives the corresponding normalizer classified in Table 4.

Algorithm 1 Equivariant full SBS

Input
- S — Symmetry of input expressed as pair $(g, \texttt{name}(S))$
- b — Canonical symmetry breaking object

Output
- B — Symmetry breaking set expressed as a pair (b', N)

$(n, \texttt{name}(N_{O(3)}(S))) \leftarrow \texttt{Normalizers}[\texttt{name}(S)]$
$N \leftarrow (gn, \texttt{name}(N_{O(3)}(S)))$
return (gb, N)

In general, the choice of a canonical symmetry breaking object is flexible. To satisfy the definition, one just needs the corresponding object for $\texttt{name}(S)$ to not share any symmetries with $S = (e, \texttt{name}(S))$. However, as discussed in Section 3.3, an ideal SBS should be more efficient than a nonideal one. Hence, if possible we would like to pick such an object so that it generates an ideal SBS. Theorem 3.3 tells us exactly the conditions needed to choose an ideal SBS. In particular, we would need the additional condition that b have the symmetry of a complement H while not having the symmetry of S. We fully characterized the relevant cases in Appendix F.

5.5 Constructing equivariant partial SBS

In the partial symmetry breaking case, we want to obtain a partial SBS from the symmetry of the input and the set of conjugate subgroup symmetries of the outputs. Importantly, note that we want closure under $N_G(S,K)$ rather than under $N_G(S)$. To compute $N_G(S,K)$, we use the following fact.

Lemma 5.1. *We have the following formula*

$$N_G(S,K) = S(N_G(S) \cap N_G(K)).$$

See Appendix E.8 for a proof.

Thus we get the following algorithm for computing an equivariant partial SBS.

Algorithm 2 Equivariant partial SBS from object

Input

S — Symmetry of input expressed as pair $(g_S, \texttt{name}(S))$

$\mathrm{Cl}_S(K)$ — Set of conjugate subgroups expressed as $(S,K) = ((g_S, \texttt{name}(S)), (g_K, \texttt{name}(K)))$

p — Canonical partial symmetry breaking object

Output

P — Symmetry breaking set expressed as a pair (p', N)

$N_1 \leftarrow \texttt{Normalizers}[\texttt{name}(S)]$
$(n, \texttt{name}(N_2)) \leftarrow \texttt{Normalizers}[\texttt{name}(K)]$
$N_2 \leftarrow (g_S^{-1} g_K n, \texttt{name}(N_2))$
$N \leftarrow N_1 \cap N_2$
$N \leftarrow (e, \texttt{name}(S))N$
$N \leftarrow g_S N g_S^{-1}$
return $(g_S p, N)$

We emphasize that for any $K' < K$, a K'-partial SBS can also serve as a K-partial SBS since we can always break more symmetry than needed. In particular, a full SBS often suffices for simplicity.

Similar to the full SBS case, we have flexibility in choosing our canonical object used to generate the partial SBS. To satisfy the definition, all we need is for $\mathrm{Stab}_G(p) \leq K'$ for some $K' \in \mathrm{Cl}_S(K)$. An ideal partial SBS is desirable, especially if we wish to ensure we do not break any extra symmetry. The condition given by Theorem 4.5 is more complicated. However, if we have a `FindComplement` function, we can automate the process of finding a symmetry an object which generates an ideal partial SBS should have. Here, let `Quotient` be a function which returns a quotient group and a mapping from cosets to elements of the quotient group. We have the following algorithm which returns a pair of subgroups (H,K) such that if p has $H \leq \mathrm{Stab}_{O(3)}(p)$ and $\mathrm{Stab}_S(p) = K$ then p generates an ideal partial SBS.

6 Experiments

Here, we provide some example tasks where we apply our framework to full symmetry breaking and partial symmetry breaking cases. We consider the cases where we can find an ideal equivariant SBS or partial SBS. We explicitly work through how to obtain the ideal equivariant SBS in each case. This section serves primarily as a proof of concept for how our approach works in practice.

For each of our tasks, we trained an equivariant convolutional message-passing graph neural network (GNN) to output a vector pointing to a vertex of the prism. We use a modified version of the predefined network from the `e3nn` library Geiger & Smidt (2022). Each layer consists of the equivariant 3D steerable convolutions followed by gated nonlinearities described in Weiler et al. (2018). We use a gaussian basis for our radial network.

Algorithm 3 Ideal partial SBS generating object symmetry

Input
- S — Symmetry of input expressed as pair $(g_S, \texttt{name}(S))$
- $\text{Cl}_S(K)$ — Set of conjugate subgroups expressed as $(S, K) = ((g_S, \texttt{name}(S)), (g_K, \texttt{name}(K)))$

Output
- H — Symmetry needed for object p to generate ideal partial SBS

$N_1 \leftarrow \texttt{Normalizers}[\texttt{name}(S)]$
$(n, \texttt{name}(N_2)) \leftarrow \texttt{Normalizers}[\texttt{name}(K)]$
$N_2 \leftarrow (g_S^{-1} g_K n, \texttt{name}(N_2))$
$N \leftarrow N_1 \cap N_2$
$N' \leftarrow (e, \texttt{name}(S)) \cap N_2$
$(Q_1, \phi) \leftarrow \texttt{Quotient}[N, (g_S^{-1} g_K, K)]$
$Q_2 \leftarrow \phi(N')$
$C \leftarrow \texttt{FindComplement}[Q_1, Q_2]$
if C exists **then**
  $(h, \texttt{name}(H)) \leftarrow \phi^{-1}(C)$
  return $((g_S h, \texttt{name}(H)), K)$
else
  return None
end if

6.1 Full symmetry breaking: triangular prism

For an example of full symmetry breaking, we consider the task of pointing to a vertex of a triangular prism, similar to that described in Section 3.2. Our input is a graph with 6 nodes with edges given by the edges of the prism. We have position features at the nodes corresponding to the positions of the vertices. Since we want this to be a full-symmetry breaking task, we require chirality in our prism. In order to make it chiral, we also have shared pseudoscalar features of value 1 at all the vertices.

For this task, the hidden features in our model are up to $l = 2$ of both parities and our convolutional filters use up to $l = 4$ spherical harmonics. For our radial network, we use a 3 layer fully connected network with 16 hidden features in each layer. We add our symmetry breaking object as an additional feature to all nodes of the graph. We output vectors (odd parity $l = 1$) at each node and take the sum as our output.

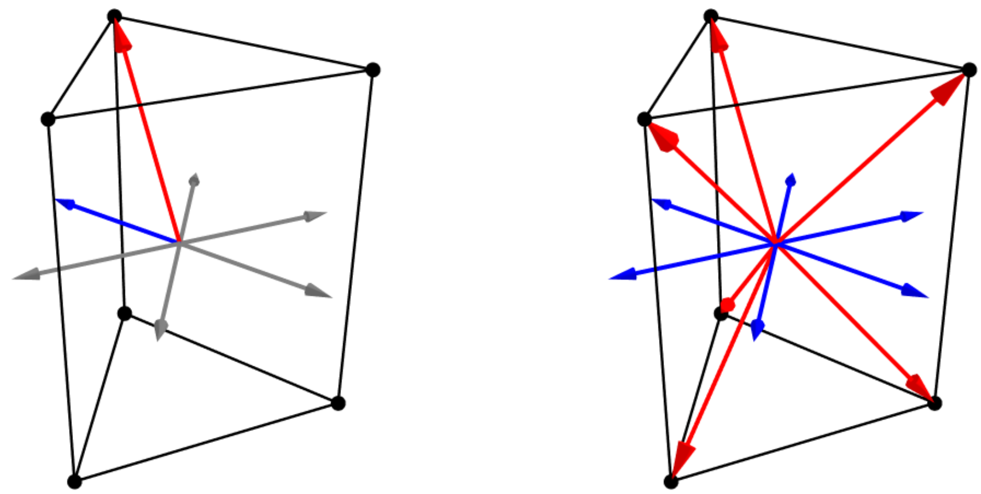
In this case, it turns out a choice of ideal equivariant SBS is the set of unit vectors parallel to an edge of the triangular faces of the prism. See Appendix H.1.1 for details on why this choice works.

We first fix a choice of one symmetry breaking object from our equivariant SBS and one of the vertices of the triangular prism. We then give the chosen symmetry breaking object as an additional input to our equivariant GNN and train it to output a vector (odd $l = 1$) feature pointing to our chosen point from the center. An example of the result of this training is shown in Figure 9a. We also observe that no matter which choices of vertex and symmetry breaking object we pick, our equivariant network is able to learn to output the vector pointing that that vertex. In practice, this means that we can choose any of our symmetry breaking objects as additional input.

Once trained on one pair of symmetry breaking object and vertex, the equivariance of our GNN means that inputting the other symmetry breaking objects in our SBS gives the other symmetrically related outputs. This is shown in Figure 9b.

Further, rather than picking one vertex, we also tried modifying our loss so that we compute the loss for all choices of vertex and take the minimum. Hence, our network can learn which vertex to pair with each symmetry breaking object. In this prism example, our pairing is random. This method of taking the minimum loss is especially useful when we have multiple instances of symmetry breaking in our data.

Finally, in Appendix H.1.2 we demonstrate that a non-equivariant SBS fails as described in Section 3.2 and in Appendix H.1.3 we show that a nonideal SBS is less efficient than an ideal one.



(a) (b)

Figure 9: (a) Output (red) generated by our model and symmetry breaking object (blue) given. (b) The set of all the outputs generated by our model if we feed in all symmetry breaking objects.

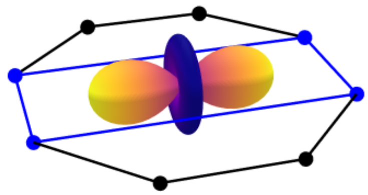
6.2 Partial symmetry breaking: octagon to rectangle

For an example of partial symmetry breaking, we consider the task of deforming an octagon to a rectangle. We choose to make our octagon chiral and impose chirality on our octagon by adding pseudoscalar features of value 1 to all vertices. We select this example because the construction of the stabilizer for a single symmetry breaking object illustrates the general procedure. The nodes of the input graph are just the vertices of the octagon and the edges are just the sides.

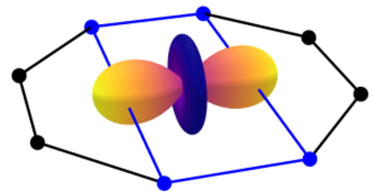
We use the exact same architecture as for the triangular prism experiment. Here, we output vector (odd parity $l = 1$) features on each vertex which represents the distortion of that vertex. As shown in Appendix H.2.1, one choice of ideal equivariant SBS for this case consists of $l = 2$ objects aligned to be parallel to an edge of the octagon.

Similar to the prism case, we try training by matching a specific symmetry breaking object to a rectangle. When the symmetry breaking object and rectangle are compatible (share the same symmetries), then our model has no problem learning to deform the octagon into the rectangle. This is shown in Figures 10a and 10b. An interesting failure case occurs when we try to match a symmetry breaking object and rectangle with incompatible symmetries. This is shown in Figure 10c. Here, the D_2 symmetry of the rectangle and of the symmetry breaking object are misaligned. As a result, our model predicts an output which has symmetry of D_4 which is the group generated when we include the symmetry elements of both the target rectangle and the symmetry breaking object. Hence, the resulting shape is a square.

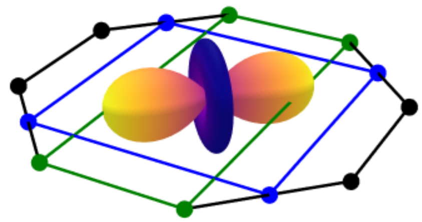
As with the triangular prism case, we also tried letting the model choose which rectangle to deform to given a symmetry breaking object. In this case, our model computes loss separately for all 4 possible rectangles and takes the minimum. We note that for a given symmetry breaking object, 2 of the possible rectangles are symmetrically compatible while 2 are not. Over 200 random initializations, we find roughly 30% of the time our model attempts to match symmetrically incompatible symmetry breaking objects to a rectangle. This is better than the 50% we would expect if it matches pairs randomly.



(a)



(b)



(c)

Figure 10: (a) Output (blue) of our model when we match a symmetry breaking object with a compatible rectangle. (b) Output (blue) of our model when we match a symmetry breaking object with a different compatible rectangle. (c) Output (blue) when we match a symmetry breaking object with an incompatible rectangle (green). Note the square has symmetries of both the symmetry breaking object and the target rectangle.

6.3 $BaTiO_3$ phase transitions

Finally, we demonstrate our framework on a more realistic example. For this, we examine the crystal structure of barium titanate ($BaTiO_3$). Specifically, as we decrease temperature, there is a phase transition from a high space-group symmetry $P_{m\bar{3}m}$ state to a lower space-group symmetry P_{4mm} state at 403K Kay & Vousden (1949); Oliveira et al. (2020); Woodward (1997). The high and low symmetry states are shown in Figures 11a and 11b respectively. Note that the real distortions are rather small and hard to see visually. Table 1 provides some numerical quantities which help distinguish the two. In particular, there are 3 distinct Ti-O-Ti bond angles in a primitive cell, 2 of which are distorted equally to 171.80° in the low symmetry structure. This bent angle is shown more clearly in the schematic in Figure 11b.

For this task, we seek to deform a high symmetry state into the lower symmetry one. Data for the high and low symmetry $BaTiO_3$ crystals are obtained from materials project database Jain et al. (2013). For our demonstration, we focus on breaking point group symmetries which are O_h and C_{4v} for $P_{m\bar{3}m}$ and P_{4mm} respectively, leaving translational symmetry for future work. Hence, we set the unit cell of both crystals to be a cube with side length 4Å, which is close to the real unit cells.

The model used for this task has a similar architecture as the previous ones, with the modification of incorporating periodic boundary conditions because we are modelling a crystal. Similar to the octagon distortion task, we output vector ($l = 1$) features at each node which tells us how much to distort the corresponding atom.

It turns out that any object sharing C_{4v} symmetry works for generating an ideal equivariant partial SBS. This is because O_h has itself as normalizer in $O(3)$ so the symmetry completely determines orientation. A simple choice consists of vectors (odd parity $l = 1$ object) pointing along the 4-fold rotation axes. As shown in Figure 12 and Table 1, our model is able to learn to distort the crystal structure appropriately when given an appropriate symmetry breaking object. Without such an input the model cannot provide any distortions.

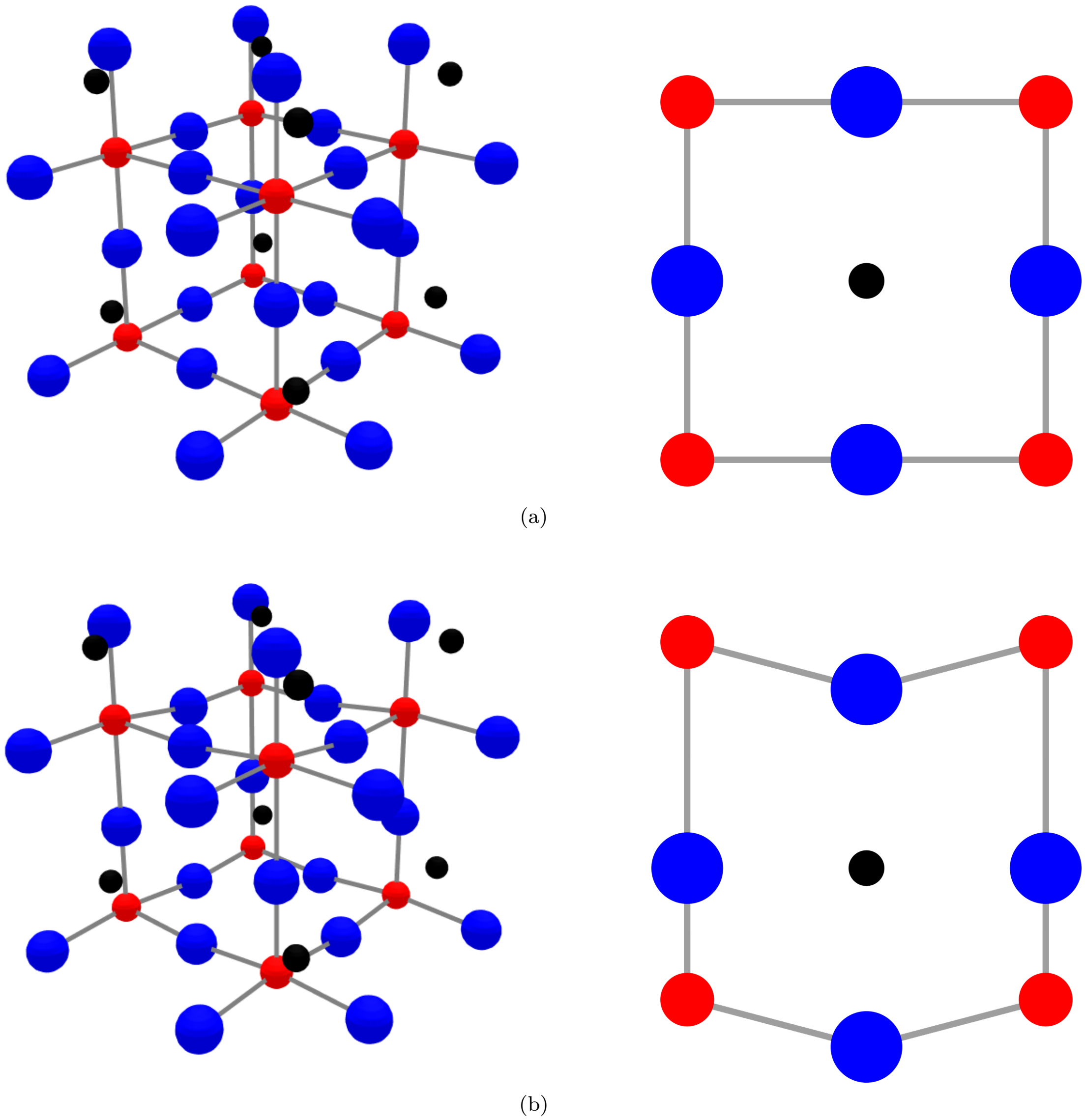


Figure 11: (a) Initial high symmetry crystal structure of $BaTiO_3$. Left is an actual plot of the crystal structure and right is a side-on schematic. (b) Target low symmetry crystal structure of $BaTiO_3$. Left is an actual plot of the distorted crystal structure and right is a side-on schematic with exaggerated distortion. The angle of the bent bond is 171.80°.

Table 1: Values of various quantities which help distinguish the high symmetry and low symmetry structures. Our models here try to distort the high symmetry structure to the low symmetry one.

Structure	Bond length average	Bond length variance	Ti-O-Ti
High symmetry	2	0	180°
Low symmetry	2.003417	0.01392	171.80°
Model (no SBS)	2	0	180°
Model (SB object $(1, 0, 0)$)	2.003417	0.01392	171.80°

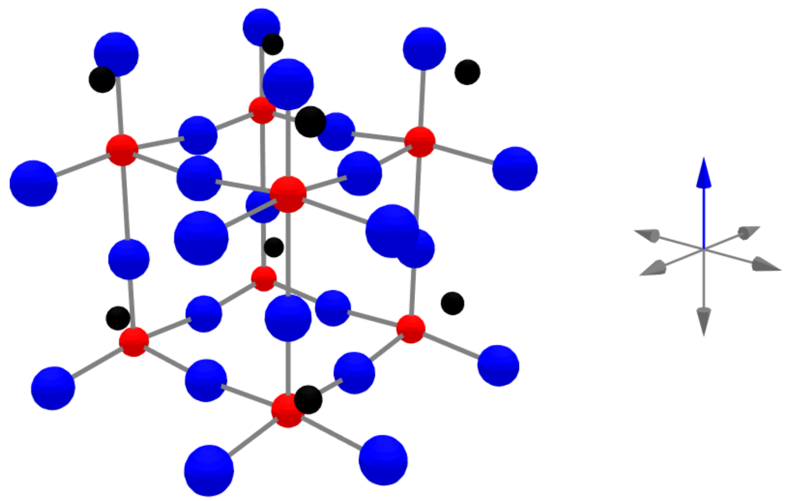


Figure 12: Distorted crystal structure generated by our model when given a symmetry breaking object shown on the right in blue.

7 Conclusion

We formalize the problem equivariant neural networks face in the spontaneous symmetry breaking setting. We propose the idea of equivariant symmetry breaking sets which allows ENNs to sample or generate all possible symmetrically related outputs given a highly symmetric input. Importantly, we show that minimizing these sets is intimately connected to a well studied group theory problem, and tabulate solutions for the ideal case for the point groups. We then demonstrate how our symmetry breaking framework works in practice on example problems.

One future direction is to include translations and tabulate complements for the space groups in their respective normalizers. This would be particularly useful for crystallography applications. Another direction is to automate finding stabilizers for partial symmetry breaking objects. In addition, our method assumes we can efficiently detect the symmetry of our input and outputs. Designing fast symmetry detection algorithms would also be extremely beneficial. Finally, designing efficient loss functions which do not punish symmetrically related outputs would be useful for any network dealing with spontaneous symmetry breaking.

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A Notation and commonly used symbols

Here, we present the notation we use throughout this paper and the typical variable names.

Table 2: Notation used throughout this paper

$\mathrm{Stab}_G(x)$	Stabilizer of an element x under a group G
$N_G(S)$	Normalizer of group S in group G
$\mathrm{Cl}_G(S)$	Set of groups obtained by conjugating group S with elements in G
$\mathrm{Orb}_G(x)$	Orbit of an element x under action by elements of group G
$\mathcal{P}(X)$	Set of all subsets of X
G/S	When G is a group, this is the set of left cosets. If S is a normal subgroup, this also denotes the quotient group
X/S	When X is a set, this is the equivalence classes induced by action of S on X
$S \leq G$	If S and G are groups, this denotes that S is a subgroup of G
$f\|_X$	Function f with domain restricted to X

Table 3: Commonly used symbols

G	Group our network is equivariant under
$\mathbf{1}$	Used to denote the trivial group
e	Identity element of a group
x	Input
y	Output
S	Symmetry of our input, more precisely $\mathrm{Stab}_G(x)$
K	Symmetry of our output, more precisely $\mathrm{Stab}_S(y)$
B	Full symmetry breaking set
P	Partial symmetry breaking set

B Group theory

Group theory is the mathematical language used to describe symmetries. Here, we present a brief overview of concepts from group theory we need to both define equivariance, and to understand our proposed symmetry breaking scheme. For a more comprehensive treatment of group theory, we refer to standard textbooks Dresselhaus et al. (2007); Dummit & Foote (2004); Kurzweil & Stellmacher (2004). We begin by defining what a group is.

Definition B.1 (Group)**.** Let G be a nonempty set equipped with a binary operator $\cdot : G \times G \to G$. This is a group if the follwing group axioms are satsfied

1. Associativity: For all $a, b, c \in G$, we have $(a \cdot b) \cdot c = a \cdot (b \cdot c)$
2. Identity element: There is an element $e \in G$ such that for all $g \in G$ we have $e \cdot g = g \cdot e = g$
3. Inverse element: For all $g \in G$, there is an inverse $g^{-1} \in G$ such that $g \cdot g^{-1} = g^{-1} \cdot g = e$ for identity e.

Some examples of groups include the group of rotation matrices with matrix multiplication as the group operation, the group of integers under addition, and the group of positive reals under multiplication. One very important group is the group of automorphisms on a vector space. This group is denoted $GL(V)$ and we can think of it as the group of invertible matrices.

While abstractly groups are interesting on their own, we care about using them to describe symmetries. Intuitively, the group elements abstractly represent the symmetry operations. In order to understand what these actions are, we need to define a group action.

Definition B.2 (Group action)**.** Let G be a group and Ω a set. A group action is a function $\alpha : G \times \Omega \to \Omega$ such that $\alpha(e, x) = x$ and $\alpha(g, \alpha(h, x)) = \alpha(gh, x)$ for all $g, h \in G$ and $x \in \Omega$.

Often, we may want to relate two groups to each other. This is done using group homomorphisms, a mapping which preserves the group structure.

Definition B.3 (Group homomorphism and isomorphism)**.** Let G and H be groups. A group homomorphism is a function $f : G \to H$ such that $f(u \cdot v) = f(u) \cdot f(v)$ for all $u, v \in G$. A group homomorphism is an isomorphism if f is a bijection.

Because there are many linear algebra tools for working with matrices, it is particular useful to relate arbitrary groups to groups consisting of matrices. Such a homomorphism together with the vector space the matrices act on is a group representation.

Definition B.4 (Group representation)**.** Let G be a group and V a vector space over a field F. A group representation is a homomorphism $\rho : G \to GL(V)$ taking elements of G to autmorphisms of V.

Given any representation, there are often orthogonal subspaces which do not interact with each other. If this is the case, we can break our representation down into smaller pieces by restricting to these subspaces. Hence, it is useful to consider the representations which cannot be broken down. These are known as the irreducible representations (irreps) and often form the building blocks of more complex representations.

Definition B.5 (Irreducible representation)**.** Let G be a group, V a vector space, and $\rho : G \to GL(V)$ a representation. A representation is irreducible if there is no nontrivial proper subspace $W \subset V$ such that $\rho|_W$ is a representation of G over space W.

There has been much work on understanding the irreps of various groups and many equivariant neural network designs use this knowledge.

One natural question is whether there is a subset of group elements which themselves form a group under the same group operation. Such a subset is a called a subgroup.

Definition B.6 (Subgroup)**.** Let G be a group and $S \subseteq G$. If S together with the group operation of G $\cdot$ satisfy the group axioms, then S is a subgroup of G which we denote as $S \leq G$.

One particular feature of a subgroup is that we can use them to decompose our group into disjoint chunks called cosets.

Definition B.7 (Cosets)**.** Let G be a group and S a subgroup. The left cosets are sets obtained by multiplying S with some fixed element of G on the left. That is, the left cosets are for all $g \in G$

$$gS = \{gs : s \in S\}.$$

We denote the set of left cosets as G/S. The right cosets are defined similarly except we multiply with a fixed element of G on the right. That is, the right cosets are for all $g \in G$

$$Sg = \{sg : s \in S\}.$$

We denote the set of right cosets as $G\backslash S$.

In general, the left and right cosets are not the same. However, for some subgroups they are the same. Those subgroups are called normal subgroups.

Definition B.8 (Normal subgroup)**.** Let G be a group and N a subgroup. Then N is a normal subgroup if for all $g \in G$, we have $gNg^{-1} = N$.

It turns out that given a normal subgroup, one can construct a group operation on the cosets. The resulting group is called a quotient group.

Definition B.9 (Quotient group)**.** Let G be a group and N a normal subgroup. One can define a group operation on the cosets as $aN \cdot bN = (a \cdot b)N$. The resulting group is called the quotient group and is denoted G/N.

For subgroups S which are not normal in G, it is often useful to consider a subgroup of G containing S where S is in fact normal. The largest such subgroup is called the normalizer.

Definition B.10 (Normalizer)**.** Let G be a group and S a subgroup. The normalizer of S in G is

$$N_G(S) = \{g : gSg^{-1} = S\}.$$

Similar to orthogonal vector spaces, one can imagine an analogous notion for groups. These are called complement subgroups.

Definition B.11 (Complement)**.** Let G be a group and S a subgroup. A subgroup H is a complement of S if for all $g \in G$, we have $g = sh$ for some $s \in S$ and $h \in H$ and $S \cap H = \{e\}$.

It turns out that if S is a normal subgroup of G and H is a complement, then H is isomorphic to the quotient group.

Finally, it is useful to define what we mean by symmetry of an object. These are all group elements which leave the object unchanged and is called the stabilizer.

Definition B.12 (Stabilizer)**.** Let G be a group, Ω some set with an action of G defined on it, and $u \in \Omega$. The stabilizer of u is all elements of G which leave u invariant. That is

$$\mathrm{Stab}_G(u) = \{g : gu = u, g \in G\}.$$

One can check that the stabilizer is indeed a subgroup. Closely related to the stabilizer is the orbit. This is all the values we get when we act with our group on some object.

Definition B.13 (Orbit)**.** Let G be a group, Ω some set with an action of G defined on it, and $u \in \Omega$. The orbit of u is the set of all values obtained when we act with all elements of G on it. That is,

$$\mathrm{Orb}_G(u) = \{gu : g \in G\} = Gu.$$

It turns out one can show that the stabilizer of elements in the orbit are related. This relation turns out to be conjugation which we define below.

Definition B.14 (Conjugate subgroups)**.** Let S and S' be subgroups of G. We say S and S' are conjugate in G if there is some $g \in G$ such that $S = gS'g^{-1}$. We denote the set of all conjugate subgroups by

$$\mathrm{Cl}_G(S) = \{gSg^{-1} : g \in G\}.$$

C Equivariant neural networks

Here, we give a brief overview of equivariant neural networks. For a more in depth coverage of the general theory and construction of equivariance, we refer to works such as Cohen et al. (2019); Finzi et al. (2020); Kondor & Trivedi (2018). We emphasize that the symmetry breaking techniques presented in the paper apply to any equivariant architecture.

We first define equivariance.

Definition C.1 (Equivariance)**.** Let G be a group with actions on spaces X and Y. A function $f : X \to Y$ is said to be equivariant if for all $x \in X$ and $g \in G$ we have

$$f(gx) = gf(x).$$

Intuitively, we can interpret this as rotating the input giving the same result as just rotating the output. It is easy to check that the composition of equivariant functions is still an equivariant function. Hence, equivariant neural networks are designed using a composition of equivariant layers.

There has been considerable study into how one should design equivariant layers. One approach is to modify convolutional filters by transforming them with the elements of our group Cohen & Welling (2016a). This approach is known as group convolution and is based on the intuition that convolutional filters are translation equivariant. In group convolution, one interprets our data as a signal over some domain. The first layer is a lifting convolution which transforms our data into a signal over the group. The remaining layers then just convolve this signal with filters which are also signals over the group.

One can further use group theory tools to break down the convolutional filters into irreps. This leads to steerable convolutional networks Cohen & Welling (2016b). These can be extended and used to parameterize continuous filters which can be used for infinite groups Cohen et al. (2018). It turns out the irreps of the group are natural data types for equivariant networks. Further, we can express the convolutions as tensor products of irreps. We can think of equivariant operations as being composed of tensor products of irreps, linear mixing of irreps, and scaling by invariant quantities. Combining these, we get tensorfield networks which works on point clouds and is rotation equivariant Thomas et al. (2018). In this paper, we demonstrate our method using networks built from the `e3nn` framework for $O(3)$ equivariance Geiger & Smidt (2022).

D Limitations

D.1 Symmetry detection

To use our procedure, we do assume knowledge of the symmetries of the inputs and outputs to our network. In the full symmetry breaking framework, we only need the symmetry of the input. In the partial symmetry breaking framework, we need the symmetry of both the input and the output. However, we argue that this is not a major concern.

First, symmetry detection is a well studied problem and there are many algorithms exist for various types of data Bokeloh et al. (2009); Keller & Shkolnisky (2004); Largent et al. (2012); Mitra et al. (2006). Further, sometimes the symmetries of the inputs and outputs are already known. This is especially true for crystallographic data Jain et al. (2013). In addition, because we only need the symmetry to design equivariant SBSs, we only need to perform symmetry detection once. This can simply be incorporated as a preprocessing step for our data.

Further, we want to emphasize that our framework can be used to prove whether knowledge of input symmetry is beneficial. We prove in Lemma F.1 that no finite subgroups of $SO(2)$ have complement in their normalizer (which is also just $SO(2)$). Combined with Corollary 3.6 this actually implies the degeneracy of any $SO(2)$-equivariant SBS for cyclic groups is infinite. Hence, we cannot do much better than a something like noise injection, which introduces asymmetry without knowledge of input symmetry.

D.2 Loss functions

While this work focuses on allowing equivariant networks to produce a set of lower symmetry outcomes, it turns out another important problem is designing appropriate loss functions. Suppose we only have one example input output pair x, y where y shares no symmetries with x. In this case there is no problem. We can fix any $b \in B$ and train to minimize a simple MAE loss $||f(x, b) - y||^2$ for example.

However, suppose we observe x, y and x, y' in the data where $y' = sy$ and $s \in S = \mathrm{Stab}_G(x)$. Then suppose we try to minimize MSE loss $||f(x, b) - y||^2 + ||f(x, b') - y'||^2$, where $b' = s'b$. Then by equivariance, the second term in the loss is

$$||f(x, b') - y'||^2 = ||f(x, s'b) - y'||^2 = ||s'f(x, b) - sy||^2 = ||f(x, b) - s'^{-1}sy||^2.$$

So in fact we see we must choose $s' = s$. So with multiple input output pairs and a simple loss directly comparing outputs such as MSE, we have a problem pairing symmetry breaking objects with outputs.

However, suppose instead our loss was chosen such that $\texttt{loss}(y, y') = \texttt{loss}(y, y)$ is small if $y' = sy$ for any $s \in S$. Then even if our network outputs sy instead of y when given some symmetry breaking object b, we do not punish it. Hence, this pairing problem would not exist. A simple version of such a loss would be to compute the MSE for all possible symmetrically related outputs and take the closest one

$$\texttt{loss}(f(x, b), y) = \min_{s \in S}(||f(x, b) - sy||^2).$$

This is what we use for our experimental examples in this work. However, this can be inefficient for large or infinite S and designing appropriate loss functions in such cases remains an open question.

E Proofs

E.1 Proof of Lemma 2.1

Lemma E.1. *Let X be a space with a transitive group action by G defined on it. Let Y be some space with a group action of G defined on it. Let $f : X \to Y$ be an G-equivariant function. We can choose f such that $f(u) = y$ if and only if $\mathrm{Stab}_G(y) \geq \mathrm{Stab}_G(u)$. Further this uniquely defines $f|_{\mathrm{Orb}_G(x)}$.*

Proof. First suppose we did have $f(u) = y$. For any $g \in \mathrm{Stab}_G(u)$, we have by equivariance of f that

$$gy = f(gu) = f(u) = y.$$

So $g \in \mathrm{Stab}_G(y)$.

Next, suppose $\mathrm{Stab}_G(y) \geq \mathrm{Stab}_G(u)$. For any $x \in X$, there is some $r \in G$ so that $x = ru$. Let us pick exactly one such r for each X and form a set R. Hence any x is uniquely written as $x = ru$ for $r \in R$. Define

$$f(x) = f(ru) = ry.$$

We claim f is equivariant. For any $g \in G$ and $x \in X$, let $x = ru$ and $gx = r'u$ for some $r, r' \in R$. Then,

$$f(gx) = f(gru) = f(r'u) = r'y.$$

But note that $gx = r'u$ implies $r'^{-1}gx = r'^{-1}gru = u$. So $r'^{-1}gr \in \mathrm{Stab}_G(u) \leq \mathrm{Stab}_G(y)$. Hence, we also have $r'^{-1}gry = y$. So,

$$f(gx) = r'y = r'(r'^{-1}gry) = gry = gf(x).$$

Hence, f is equivariant.

Finally, for uniqueness, suppose f, f' are two equivariant functions such that $f(u) = f'(u) = y$. Then by equivariance, for any $x = gu \in X$ we have

$$f(x) = f(gu) = gy = f'(gu) = f'(x).$$

□

E.2 Formal justification of Definition 3.2

We can justify Definition 3.2 by characterizing exactly when σ can be equivariant. This leads to the following proposition.

Proposition E.2. *Let G be a group and S be a subgroup of G. Let $B \in \mathcal{P}(\mathbf{B})$ be a set where there is some group action of G defined on $\mathbf{B}$. Then there exists an equivariant $\sigma|_{\mathrm{Cl}_G(S)} : \mathrm{Cl}_G(S) \to \mathcal{P}(\mathbf{B})$ such that $\sigma|_{\mathrm{Cl}_G(S)} = B$ if and only if $nB = B$ for all $n \in N_G(S)$.*

Proof. Note that $\mathrm{Cl}_G(S)$ is a set where action by conjugation is a transitive one. Also note by definition that $\mathrm{Stab}_G(S)$ for this action is precisely the definition of a normalizer $N_G(S)$. Then by Lemma E.1, we see such a function exists if and only B is also symmetric under $N_G(S)$. □

E.3 Proof of Theorem 3.3

Theorem 3.3. *Let G be a group and S a subgroup. Let B be a G-equivariant SBS for S. Then it is possible to choose an ideal B if and only if S has a complement in $N_G(S)$.*

Proof. Suppose B is transitive under S and pick $b \in B$. Consider the stabilizer group $\mathrm{Stab}_{N_G(S)}(b)$. For any $g \in N_G(S)$, by transitivity under S we must have $gb = sb$ for some $s \in S$. So, $s^{-1}gu = u$ implying that $h = s^{-1}g \in \mathrm{Stab}_{N_G(S)}(b)$. So we find that we can write any g as $g = sh$ for some $s \in S$ and $h \in \mathrm{Stab}_{N_G(S)}(u)$ so

$$N_G(S) = S \cdot \mathrm{Stab}_{N_G(S)}(u).$$

But note that since B is symmetry breaking, $S \cap \mathrm{Stab}_{N_G(S)}(u) = \{e\}$. Hence, $\mathrm{Stab}_{N_G(S)}(u)$ is indeed a complement.

For the converse, suppose H is a complement of S in $N_G(S)$. We claim $B = N_G(S)/H$ is the equivariant SBS we desire. Note that clearly by construction, this is closed under $N_G(S)$ so we satisfy the equivariance condition. Further, note that $\mathrm{Stab}_S(H) = \mathrm{Stab}_{N_G(S)}(H) \cap S = H \cap S = \{e\}$. Since B is transitive under $N_G(S)$, stabilizers of all other elements are obtained by conjugation and hence also trivial. Hence, it is indeed symmetry breaking. Finally, any $g \in N_G(S)$ is uniquely written as sh for some $s \in S, h \in H$ so $gH = shH = sH$. So B is transitive under S as well. □

E.4 Proof of Corollary 3.6

Corollary 3.6. *Let G be a group and S a subgroup. Let M be such that $S \leq M \leq N_G(S)$. Let B be a G-equivariant SBS for S which is transitive under $N_G(S)$. Then it is possible to choose B such that every M-orbit is also transitive under S if and only if S has a complement in M. In particular, such a B has*

$$\mathrm{Deg}_S(B) \leq |N_G(S)/M|.$$

Proof. Suppose we have such a B and pick any $b \in B$. By transitivity of the orbit under S, we have $Mb = Sb$. Let $B' = Mb$. We can check that this is in fact an ideal M-equivariant SBS for S. That it is a symmetry breaker follows since B is symmetry breaking. That it is M-equivariant and transitive follows since $Mb = Sb$ and $N_M(S) = M$. By Theorem 3.3 this implies S has a complement in M.

Next, suppose we have a complement of S in M. By Theorem 3.3 we can construct B' which is an ideal M-equivariant SBS for S. We can lift this to a G-equivariant SBS for S by just taking $B = N_G(S)B'$.

Finally, to compute the order, we note that every S-orbit is also a M orbit. Since B is transitive under $N_G(S)$, there are at most $|N_G(S)/M|$ number of M-orbits and hence only that many S-orbits. So

$$\mathrm{Deg}_S(B) \leq |N_G(S)/M|.$$

□

E.5 Justification of Definition 4.4

Similar to the full SBS case, we can justify Definition 4.4 by characterizing exactly when an equivariant π can exist. This leads to the following proposition.

Proposition E.3. *Let G be a group, S a subgroup of G, and K a subgroup of S. Let $\mathbf{P}$ be a set with a group action of G defined on it and $P \subset \mathbf{P}$. There exists an equivariant $\pi|_{\mathrm{Orb}_G((S,\mathrm{Cl}_S(K)))} : \mathrm{Orb}_G((S, \mathrm{Cl}_S(K))) \to \mathcal{P}(\mathbf{P})$ such that $\pi|_{\mathrm{Orb}_G((S,\mathrm{Cl}_S(K)))}((S, \mathrm{Cl}_S(K))) = P$ if and only if $N_G(S, K)$ leaves P invariant.*

Proof. By Lemma E.1, we need P to be closed under the stabilizer of the input. But the generalized normalizer $N_G(S, K)$ is precisely this stabilizer. □

E.6 Proof of Theorem 4.5

Theorem 4.5. *Let G be a group and S and K be subgroups $K \leq S \leq G$. Let P be a G-equivariant K-partial SBS. Then we can choose an ideal P (exact and transitive under S) if and only if $N_S(K)/K$ has a complement in $N_{N_G(S,K)}(K)/K$.*

Proof. Let $P = Su$ where u has symmetry $\mathrm{Stab}_S(u) = K$. We can define an action of any coset $N_G(S, K)/K$ on u as just the action of a coset representative on u. This is consistent since u is invariant under K. In particular, note that K is a normal subgroup of $N_S(K)$ so $N_S(K)/K$ is a quotient group. Let $B' = (N_S(K)/K)u$. Since u is in a K-partial SBS, we must have $su \neq u$ for any $s \in S - K$. Hence, for any coset $gK \in N_S(K)/K$, $gu \neq u$ if $g \notin K$. Therefore, B' must be a SBS for $N_S(K)/K$.

Next, consider any coset gK in $N_{N_G(S,K)}(K)/K$. Then we know $gu \in Su$ so $gu = su$ for some $s \in S$. Since K was a symmetry of u, $gKg^{-1} = sKs^{-1}$ is a symmetry of $gu = su$. So the stabilizer of su must be $sKs^{-1} = K$. Hence, s must be in $N_S(K)$. Therefore the action of gK on u gives us an element of $B' = (N_S(K)/K)u$. Hence B' is $N_{N_G(S,K)}(K)/K$-equivariant.

By Theorem 3.3, the existence of an ideal $N_{N_G(S,K)}(K)/K$-equivariant SBS for $N_S(K)/K$ implies that $N_S(K)/K$ has a complement in $N_{N_G(S,K)}(K)/K$.

For the converse direction, suppose that A is a complement of $N_S(K)/K$ in $N_{N_G(S,K)}(K)/K$. Note the elements of A are cosets of K so we can define a set of elements of $N_G(S,K)$ as

$$H = \bigcup_{C \in A} C.$$

Define $P = \mathrm{Orb}_S(H)$. We claim that P is a transitive exact equivariant partial SBS.

We first show that P is exact K-partial symmetry breaking. Consider $s \in S$. We can write

$$sH = \bigcup_{C \in A} sC = \bigcup_{C \in sA} C.$$

Now we see if $s \in K$, then since K is the identity in the quotient group $sA = A$. Hence $sH = H$ in this case. If $s \in N_S(K) - K$, then sK is not the identity in $N_S(K)/K$. But A is a complement so $sA \neq A$ implying $sH \neq H$. Finally, if $s \notin N_S(K)$ then $sK \notin N_{N_G(S,K)}(K)/K$. So $sH \not\subset N_{N_G(S,K)}(K)$. But $H \subset N_{N_G(S,K)}(K)$ so $sH \neq H$. Hence, $\mathrm{Stab}_S(H) = K$ and since the rest of P is just the orbit of H, stabilizers of the other elements are in $\mathrm{Cl}_S(K)$. Hence, P as we constructed is an exact K-partial SBS.

For equivariance consider any $n \in N_G(S,K)$ giving a coset

$$nH = \bigcup_{C \in A} nC = \bigcup_{C \in nA} C.$$

If $n \in N_{N_G(S,K)}(K)$ then since A is a complement, $(nK) = (sK)(aK)$ for some $sK \in N_S(K)/K$ and $aK \in A$, so $nA = (nK)A = (sK)(aK)A = (sK)A = sA$ for some $s \in N_S(K) \subset S$. Hence, $nH = sH$ for some $s \in S$. If $n \notin N_{N_G(S,K)}(K)$, then there is some s so that $nKn^{-1} = sKs^{-1}$. Therefore, $s^{-1}nKn^{-1}s = K$ so $s^{-1}n \in N_{N_G(S,K)}$. But we saw before that this means there is some s' such that $s^{-1}nH = s'H$. Thus, $nH = ss'H$ and $ss' \in S$. So $nH \in P$ so P is indeed closed under action by $N_G(S,K)$. ☐

E.7 Proof of Corollary 4.7

Corollary 4.7. *Let G be a group, S a subgroup, and K a subgroup of S. Let K' be a subgroup of K and M a subgroup of $N_G(S,K) \cap N_G(S,K')$ which contains S. Suppose P is a G-equivariant K-partial SBS for S which is transitive under $N_G(S,K)$. We can choose P such that $\mathrm{Stab}_S(p) \in \mathrm{Cl}_{N_G(S,K)}(K')$ for all p and all M-orbits in P are transitive under S if and only if $N_S(K')/K'$ has a complement in $N_M(K')/K'$. Further, such a P has*

$$\mathrm{Deg}_{S,K}(P) \leq |K/K'| \cdot |N_G(S,K)/M|.$$

Proof. Suppose we had such a P. Pick some $p \in P$ such that $\mathrm{Stab}_S(p) = K'$. Since M-orbits are transitive under S, we have $Mp = Sp$. Let $P' = Mp$. We can check then that this is a M-equivariant set. Further, since $M \subset N_G(S,K')$, we see that this is an exact K'-partial symmetry breaking set. Hence, it is an ideal M-equivariant K'-partial SBS. Also note that since $M \subset N_G(S,K')$, we have $M = N_M(S,K')$. So by Theorem 4.5, $N_S(K')/K'$ must have a complement in $N_M(K')/K'$.

Conversely, suppose $N_S(K')/K'$ has a complement in $N_M(K')/K'$. Again, we note $M = N_M(S,K')$ so by Theorem 4.5 we have an ideal M-equivariant K'-partial SBS for S. We can lift this to G-equivariance by taking the orbit under $N_G(S,K)$.

To see the order of such a P, we consider the S-orbits. Let T be a transversal of S/K. For each S-orbit, we can pick some p in that orbit so that $\mathrm{Stab}_S(p) \leq K$. We put the elements of Kp in our P_t. Within each S-orbit, any p' can be written as sp for some $s \in S$ and any s is uniquely written as $s = tk$ for some $t \in T$ and $k \in K$. So $p' = tkp$. However, note that any other s' where $p' = s'p = sp$ can be written as $s' = sk'$ for some $k' \in \mathrm{Stab}_S(p)$. Hence, p' is uniquely written as $p' = t(kp)$ since $kk'p = kp$. So each S-orbit contributes $|K/\mathrm{Stab}_S(p)|$ elements to P_t. However, since $\mathrm{Stab}_S(p) \in \mathrm{Cl}_{N_G(S,K)}(K')$, we must have $|K/\mathrm{Stab}_S(p)| = |K/K'|$. Finally, we know each S-orbit is also an M-orbit, since P is transitive under $N_G(S,K)$, there are at most $|N_G(S,K)/M|$ different S-orbits. So

$$\mathrm{Deg}_{S,K}(P) = |P_t| \leq |K/K'| \cdot |N_G(S,K)/M|.$$

□

E.8 Proof of Lemma 5.1

Lemma 5.1. *We have the following formula*

$$N_G(S,K) = S(N_G(S) \cap N_G(K)).$$

Proof. For any $n \in N_G(S,K)$, by definition we must have $nKn^{-1} = sKs^{-1}$ for some $s \in S$. Hence, $s^{-1}nKn^{-1}s = K$ so $s^{-1}n \in N_G(K)$. Further, clearly $s \in N_G(S)$ and $n \in N_G(S)$ so also $s^{-1}n \in N_G(S)$. Therefore, $s^{-1}n \in N_G(S) \cap N_G(K)$. So $n = s(s^{-1}n) \in S(N_G(S) \cap N_G(K))$. Hence

$$N_G(S,K) \subseteq S(N_G(S) \cap N_G(K)).$$

Next, consider any $n' = sn \in S(N_G(S) \cap N_G(K))$ where $s \in S, n \in N_G(S) \cap N_G(K)$. Since $s \in N_G(S), n \in N_G(S)$ clearly $sn \in N_G(S)$. Further, we find

$$snK(sn)^{-1} = s(nKn^{-1})s^{-1} = sKs^{-1} \in \mathrm{Cl}_S(K).$$

Therefore by definition $sn \in N_G(S,K)$. So also

$$S(N_G(S) \cap N_G(K)) \subseteq N_G(S,K).$$

Hence, we find that

$$N_G(S,K) = S(N_G(S) \cap N_G(K)).$$

□

F Classification of full symmetry breaking cases for $O(3)$

Here we tabulate the cases for full symmetry breaking for the finite subgroups of $O(3)$. These are the point groups and the normalizers are tabulated in the International Tables for Crystallography in Hermann–Mauguin notation Koch & Fischer (2006). We have translated these to Schönflies notation in Table 4.

Table 4: Normalizers of the point groups in Schönflies notation. Note we have the equivalences $C_1 = 1$, $S_2 = C_i$, $C_{1h} = C_{1v} = C_s$, $D_1 = C_2$, $D_{1h} = C_{2v}$, $D_{1d} = C_{2h}$.

Normalizer:	Groups:
K_h	1, C_i
$D_{\infty h}$	C_n, S_{2n}, C_{nh} $\forall n \geq 2$; C_s
$D_{(2n)h}$	C_{nv}, D_{nd}, D_{nh} $\forall n \geq 2$; D_n $\forall n \geq 3$
I_h	I, I_h
O_h	D_2, D_{2h}, T, T_d, T_h, O, O_h

In the following subsections we do casework by normalizers. For each, subgroup with a given normalizer, we give a valid complement by name if it exists. In some normalizers, the name of a subgroup is not sufficient to identify it. This is because there are multiple copies of subgroups with that name in the normalizer. In such cases, we must identify which copy of the subgroup we care about. To do so, we give the normalizers in terms of a group presentation found with the help of GAP. Group presentations are essentially a set of generators and relations among the generators. We can then specify any specific subgroups of the normalizer using the generators of the normalizer.

F.1 Normalizer: K_h

All the groups with this normalizer do have complements. Note that in Schönflies notation, K_h is just the entire group $O(3)$. The only subgroups with $O(3)$ as normalizer are the trivial group C_1 and inversion C_i. Clearly for the trivial group the complement is $O(3)$. For inversion, the complement is just $SO(3)$.

Table 5: Groups with normalizer $K_h = O(3)$ and their complements.

Group	Complement
1	$K_h = O(3)$
C_i	$K = SO(3)$

F.2 Normalizer: $D_{\infty h}$

Unfortunately, most of the groups in this case have no complements. We provide a proof of this fact here. We begin by showing no nontrivial cyclic group has a complement in C_∞ (which is $SO(2)$ in Schönflies notation).

Table 6: Groups with normalizer $D_{\infty h}$ and their complements.

Group	Complement
C_s	$C_{\infty v}$, D_∞
C_n, S_{2n}, C_{nh} $\forall n \geq 2$	None

Lemma F.1. *Let C_n be a cyclic group of order $n \geq 2$ which is embedded in C_∞. Note that it is a normal subgroup since all groups here are abelian. Then C_n does not have a complement in C_∞.*

Proof. **1** Suppose there was a complement H. By definition, for any $g \in C_\infty$ we have $g = ch$ for unique $h \in H$ and $c \in C_n$.

Next, note that C_∞ is a divisible group. In particular, for any $g \in C_\infty$, there exists some g' such that $g = (g')^n$. Let g' be uniquely written as $h'c'$ for some $h' \in H$ and $c' \in C_n$. Then we have

$$g = (c'h')^n = (c')^n(h')^n = (h')^n$$

where we noted $(c')^n = e$. So g is uniquely written as $g = ch$ for $c = e$ and $h = (h')^n$. But this holds for all g so all elements of C_∞ are just elements of H. This contradicts the fact that $H \cap C_n = \{e\}$. □

Proof. **2** For those familiar with exact sequences, one can consider the following alternative proof. Consider short exact sequence

$$1 \to C_n \to C_\infty \to C_\infty/C_n \to 1.$$

We can check that $C_\infty/C_n \cong C_\infty$. Existence of a complement for C_n implies the above sequence is split, which by the splitting lemma Hatcher (2002) implies $C_\infty \cong C_\infty \oplus C_n$, a contradiction. □

We can now extend the lemma above to there being no complement of any cyclic group in D_∞ (which is $O(2)$ in Schönflies notation).

Lemma F.2. *Let C_n be a cyclic group of order $n \geq 2$ which is embedded in D_∞ such that the rotation axis aligns with the infinite rotation axis in D_∞. Note that it is a normal subgroup since all groups here are abelian. Then C_n does not have a complement in D_∞.*

Proof. Suppose there was a complement H. Consider $H' = H \cap C_\infty$. Clearly, we have $H' \cap C_n = \{e\}$. Next, for any $g \in C_\infty$, there is unique $c \in C_n$ and $h \in H$ such that $g = ch$. But $h = c^{-1}g \in C_\infty$ so $h \in H'$. So H' is a complement of C_n in C_∞. But this contradicts Lemma F.1. □

Finally, we can prove that no subgroups except for C_s in this case have complements. Note here that K_h is just $O(3)$ and K just $SO(3)$ in Schönflies notation.

Theorem F.3. *Consider any point group A which has normalizer $D_{\infty h}$ in K_h. If A has a nontrivial pure rotation, then it has no complement in $D_{\infty h}$.*

Proof. First, note that K_h is the direct product of K and inversion C_i. Suppose A had a complement H.

We can split $A = A_e \sqcup A_i$ where $A_e = A \cap K$ is the subgroup of pure rotations and A_i is a coset consisting of elements with an inversion. Similarly, we can split $H = H_e \sqcup H_i$ and $D_{\infty h} = D_\infty \sqcup D_i$ into subgroups of pure rotations and coset of elements with inversions.

We claim the elements of $G = A_eH_e$ form a group. Consider any $a, a' \in A_e$ and $h, h' \in H_e$. Since A is a normal subgroup of $D_{\infty h} = AH$, we have $hA = Ah$ so $ha' = a''h$ for some $a'' \in A$. But since $h, a' \in K$, we have $a''h \in K$ so $a'' \in K$. Hence $a'' \in A_e$. Therefore,

$$(ah)(a'h') = a(ha')h' = a(a''h)h' = (aa'')(hh') \in A_eH_e.$$

So $G = A_eH_e$ is a group.

Next, since H is a complement of A, clearly $A_e \cap H_e = \{e\}$. Since $G \leq AH = D_{\infty h}$, any $g = ah$ for unique $a \in A$ and $h \in H$ which by construction of G are $a \in A_e$ and $h \in H_e$. So H_e is certainly a complement of A_e in G.

Now, we claim either $G = D_\infty$ or $G = C_\infty$. For any $g \in D_\infty$, since H is a complement, there is a unique $a \in A$ and $h \in H$ such that $g = ah$. In particular, we note we must either have $a \in A_e$ and $h \in H_e$ or $a \in A_i$ and $h \in H_i$ to have the right inversion parity. One possibility is $G = A_eH_e = D_\infty$. For the other possibility, suppose $D_\infty - G$ is nonempty. Fix $g \in D_\infty - G$ and consider any $g' \in D_\infty - G$. Then $g = ah$ and $g' = a'h'$ where $a, a' \in A_i$ and $hh' \in H_i$. Now, note that $a^{-1}a'$ is the combination of 2 elements with odd parity in i so $a^{-1}a' \in A_e$. Next, since A is a normal subgroup, we have $h^{-1}A = Ah^{-1}$ and in particular,

$h^{-1}a^{-1}a' = a''h^{-1}$ for some $a'' \in A$. But since h has odd parity and $a^{-1}a'$ has even parity in inversion, a'' must have even parity in inversion. Hence, we have

$$g^{-1}g' = (ah)^{-1}(a'h') = h^{-1}a^{-1}a'h' = a''(h^{-1}h').$$

Since h, h' both have odd parity, $h'' = h^{-1}h'$ has even parity so in fact $g^{-1}g' = a''h''$ where $a'' \in A_e$ and $h'' \in H_e$. Therefore, $g^{-1}g' \in G$ so $D_\infty - G = gG$ is just a G-coset of D_∞. We can similarly also show that $D_\infty - G = Gg$. Now, we claim $gG \cap C_\infty = \phi$. Suppose not. Then there is some $c \in gG \cap C_\infty$. Since C_∞ is a divisible group, there is some c' where $c = (c')^2$. But we must have $(c')^2 \in G$, a contradiction. Hence $gG \cap C_\infty = \phi$ so $G \cap C_\infty = C_\infty$. To conclude, we must have $g \in D_\infty - C_\infty$ and it is clear gC_∞ would generate the remaining elements in D_∞. So $G = C_\infty$ in this case.

From Table 4, we can see that A_e must in fact be a nontrivial cyclic group. But then the above implies that H_e is a complement of this cyclic group in either $G = D_\infty$ or $G = C_\infty$, which contradict Lemma F.2 and Lemma F.1 respectively. So A cannot have a complement in $D_{\infty h}$. □

F.3 Normalizer: $D_{(2n)h}$

All groups with this normalizer do have complements. We list the subgroup and its complement in Table 7. One presentation of $D_{(2n)h}$ is

$$\langle a, b, m | a^{2n}, b^2, m^2, (ab)^2, (am)^2, (bm)^2 \rangle.$$

Figure 13 depicts an example of a D_{10h} object. The element a correspond to a $2\pi/10$ rotation about the blue vertical axis, b corresponds to a π rotation about the red axis, and m corresponds to a reflection across the mirror plane shown in orange.

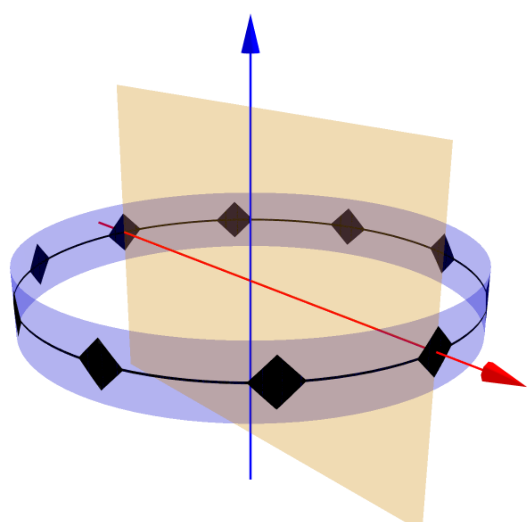


Figure 13: Object with symmetryD_{10h}. We can identify generator a as the 10-fold rotation about the blue axis, generator b as the 2-fold rotation about the red axis, and m as the reflection over the plane shown in orange.

Table 7: Groups with normalizer $D_{(2n)h}$ and their complements.

Group	Generators of group	Complement	Generators of a complement
C_{nv}	a^2, m	C_{2v}	am, bm
D_{nd}	a^2, abm, m	C_s	bm
D_{nh}	a^2, b, m	C_s	am
D_n	a^2, b	C_{2v}	am, bm

F.4 Normalizer: I_h

This case is simple, we either have I or I_h. Clearly we just need to add inversion to get a complement in the former case and in the latter case we can just take the trivial group.

Table 8: Groups with normalizer I_h and their complements.

Group	Complement
I	C_i
I_h	1

F.5 Normalizer: O_h

All subgroups in this case have complements as well. One presentation of O_h is

$$\langle a, b, i | a^4, b^4, i^2, (aba)^2, (ab)^3, iaia^{-1}, ibib^{-1} \rangle.$$

Here, a and b are $\pi/2$ rotations about perpendicular axes and i is just inversion.

Table 9: Groups with normalizer O_h and their complements.

Group	Generators of group	Complement	Generators of a complement
D_2	a^2, b^2	D_{3d}	ab, ba^2, i
D_{2h}	a^2, b^2, i	D_3	ab, ba^2
T	ab, ba	S_4	a^2b, i
T_d	ab, ba, ai	C_2	a^2b
T_h	ab, ba, i	C_2	a^2b
O	a, b	C_i	i
O_h	a, b, i	1	ϕ

G Equivariant full SBS better than exact partial SBS

We provide an outline of the construction of the counterexample. It is easiest to explain this by introducing the concept of a wreath product on groups.

Definition G.1 (Wreath product)**.** Let H be a group with a group action on some set Ω. Let A be another group. We can define a direct product group indexed by Ω as the set of sequences $(a_\omega)_{\omega\in\Omega}$ where $a_\omega \in A$. The action of H on Ω induces a semidirect product by reindexing. In particular, for all $h \in H$ and sequences in A^Ω we define

$$h \cdot (a_\omega)_{\omega\in\Omega} = (a_{h^{-1}\omega})_{\omega\in\Omega}.$$

The resulting group is the unrestricted wreath product and denoted as $A \text{ Wr}_\Omega\ H$.

If rather than a direct product group A^Ω, we restrict ourselves to a direct sum where all but finitely many elements in our sequence is not the identity, then we get the restricted wreath product denoted as $A \text{ wr}_\Omega\ H$.

Note that the direct sum and direct product are the same for finite Ω so the restricted and unrestricted wreath products also coincide in those cases.

Consider the space $\Omega = \{1, -1\}$ and an action of D_4 on Ω corresponding to the A_2 representation. Intuitively, if we think of D_4 as the rotational symmetries of a square in the xy-plane, this corresponds to how the z coordinate transforms by flipping signs. Define a group G' as $G' = C_2 \text{ wr}_\Omega\ D_4$. This is a group of order 32 and is `SmallGroup(32,28)` in the Small Groups library GAP. One presentation of this group is

$$\langle a, b, c | a^2, b^4, (ab)^4, c^2, bcb^{-1}c, (ac)^4\rangle. \tag{1}$$

In this presentation, we can interpret a, b as generators of D_4 and c as the generator one copy of C_2.

Consider the group $G = G' \times G'$ defined using the direct product. We can write generators of G as $a_1, b_1, c_1, a_2, b_2, c_2$ corresponding to two copies of those in the presentation given in equation 1 where generators with different indices commute. Define S as the subgroup generated by $a_1, b_1^2, c_1, a_2, b_2^2, c_2$ and K as the subgroup generated by c_1c_2.

We can check that $N_G(S) = N_G(S, K) = G$. It is also not hard to check that a_1b_1, a_2b_2 generate a complement for S in G. Hence, by Theorem 3.3, we know that an ideal G-equivariant SBS is possible for S. Hence, we know the size of the equivariant full SBS is $|S| = 256$.

Next, suppose we wanted a G-equivariant exact partial SBS. We can always generate this partial SBS by taking the orbit of some element p under action by $N_G(S, K) = G$ where $\text{Stab}_S(p) = K$. We claim we must also have $\text{Stab}_G(p) = K$. Suppose not, then there must be some $g \in \text{Stab}_G(p)$ such that $g \notin S$. However, we can check through casework or brute force that for all such g, either $gKg^{-1} \neq K$ or $g^2 \in S - K$. But would mean that there are elements not in K which stabilize p so $\text{Stab}_S(p) \neq K$, a contradiction. Hence, no such g can exist so $\text{Stab}_G(p) = K$. Finally, by Orbit-Stabilizer theorem, this means the set must have size $|P| = |\text{Orb}_G(p)| = |G|/|\text{Stab}_G(p)| = (8^2 \cdot 2^4)/2 = 512$. This is larger than the equivariant full SBS.

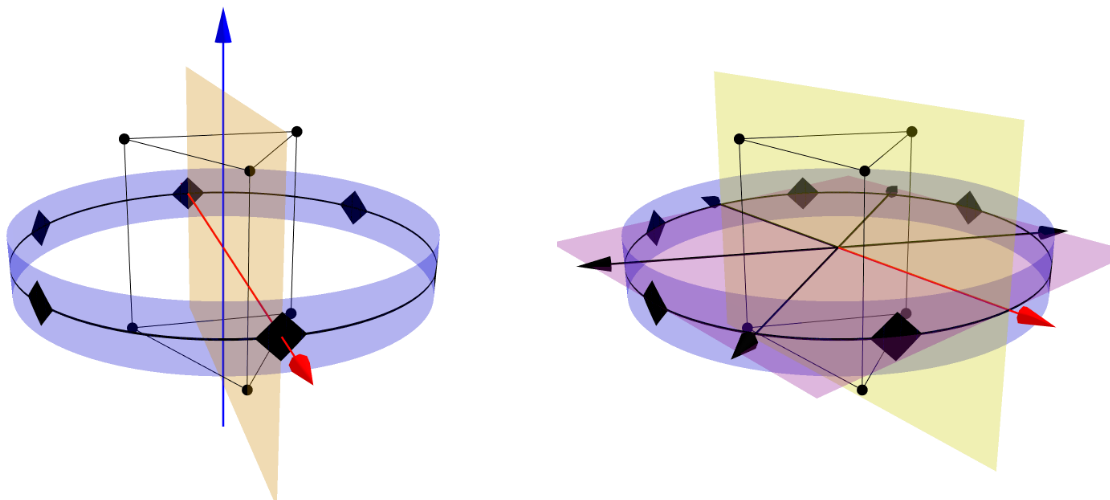
In our supplementary material, we provide a script in GAP which verifies our claims above. In particular it performs a brute force check that $\text{Stab}_S(p) = K$ implies $\text{Stab}_G(p) = K$ for the group G, S, K described above.

H Experiments

We provide some additional details on our experiments here. We also provide our code for running these experiments in the supplementary material.

H.1 Triangular prism

H.1.1 Obtaining an ideal SBS



(a) (b)

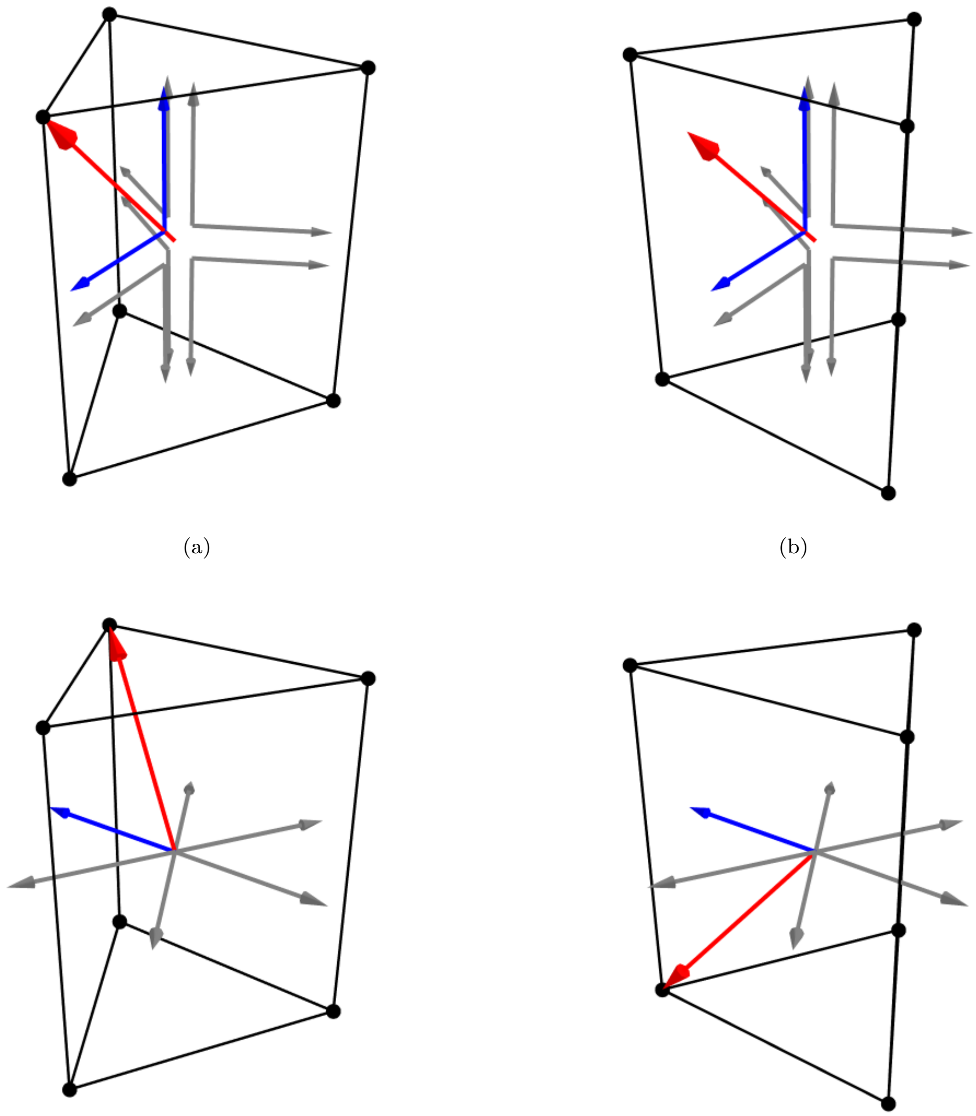
Figure 14: (a) Triangular prism with D_3 symmetry and patterned cylinder with D_{6h} symmetry. The generators are a, b, m where a is a $2\pi/6$ rotation about the blue axis, b is a π rotation about the red axis, and m is a reflection across the orange plane. (b) An ideal symmetry breaking set for the triangular prism. A complement of D_3 in D_{6h} is generated by the mirror planes shown here in yellow and purple. The vector in red is a symmetry breaking object with this complement as stabilizer. The orbit of this vector under the normalizer generates the other vectors shown in black.

Table 7 tells us D_3 is generated by a^2, b and that a complement H is generated by am, bm. By Theorem 3.3, we know that if we can pick some object v with stabilizer $\mathrm{Stab}_{D_{6h}}(v) = H$, then the orbit of v under D_3 gives an ideal equivariant SBS. In this case, one such v that works is a vector parallel to the triangular faces of the prism and one of the sides of the prism. This is shown in Figure 14b. Note reflection across the yellow plane corresponds to am and across the purple plane corresponds to bm. It is clear the arrow in red is stabilized by this complement. One can further check it shares no symmetries with the triangular prism. The other 5 arrows in black are the other symmetry breaking objects we obtain by taking the orbit of the red arrow under action by D_{6h}.

H.1.2 Nonequivariant SBS

In addition to using an equivariant SBS as presented in the main paper, we also tried training with the non-equivariant SBS described in Section 3.2. Recall that the symmetry breaking objects here are a vector pointing to one of the vertices of the triangle projected in the xy plane and a vector pointing up or down corresponding to which triangle we pick from. We fix one pair of vectors as our symmetry breaking object and train our equivariant model to match it with a vertex.

As shown in Figure 15a, our model is able to complete this. However, rotating the prism by 180° and feeding this rotated prism along with our symmetry breaking object, we find that our model outputs a vector which does not point to any vertex. This is shown in Figure 15b. Contrast this with the equivariant case in Figures 15c and 15d where our model still produces a vector which points to a vertex of the prism.

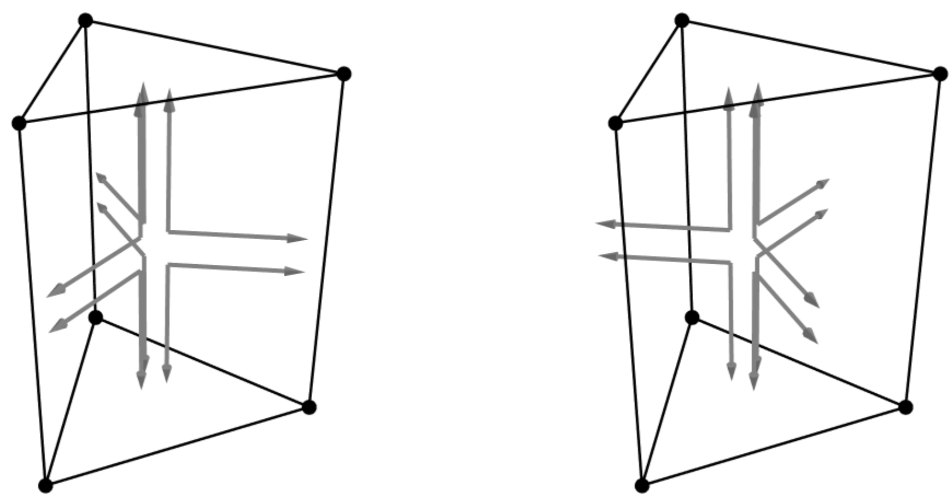


(a) (b) (c) (d)

Figure 15: (a) Output (red) generated by our model and symmetry breaking object (blue) given that is chosen from a non-equivariant SBS (b) Output (red) generated by our model and symmetry breaking object (blue) given when our prism is rotated by 180° (c) Output (red) generated by our model and symmetry breaking object (blue) given that is chosen from an equivariant SBS (d) Output (red) generated by our model and symmetry breaking object (blue) given when our prism is rotated by 180°

H.1.3 Nonideal SBS

We can modify the nonequivariant SBS into an equivariant one by adding the additional objects needed for closure under the normalizer. Doing so we see there are 2 S-orbits in this nonideal equivariant SBS shown in Figure 16. This corresponds to a degeneracy of 2 as defined in Section H.1.3.

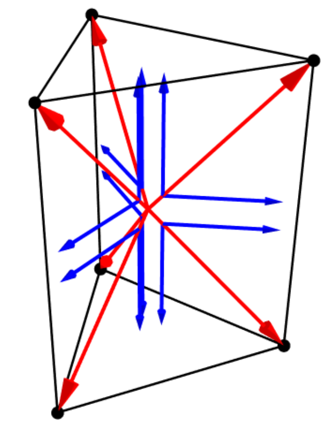
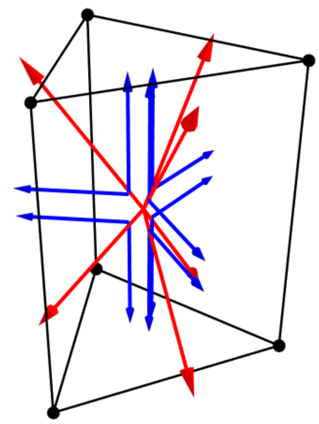
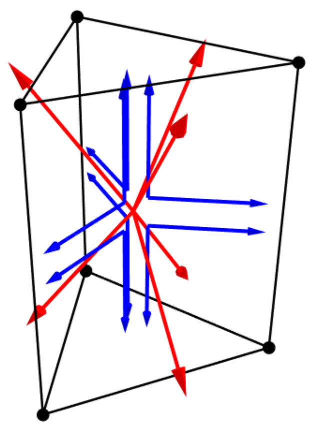
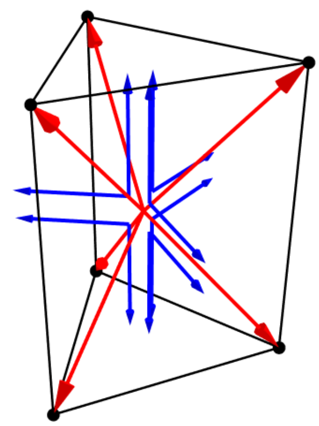
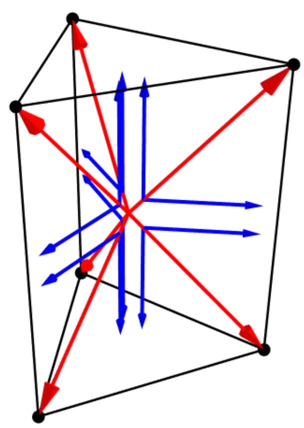
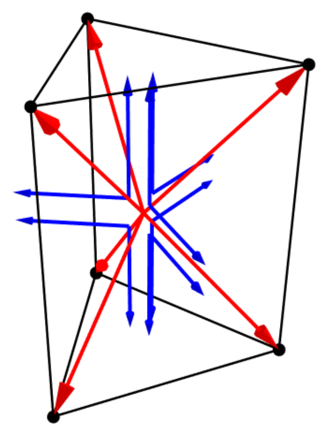


(a) S-orbit 1 (b) S-orbit 2

Figure 16: (a) S-orbit corresponding to the original nonequivariant SBS (b) Additional S-orbit needed which makes the set closed under the normalizer.

From the discussion in Section 3.4, we expect this SBS to be less efficient than an ideal one. We first train using only a symmetry breaking object from one of the S-orbits. We see that when given objects from that orbit, the network correctly outputs vectors pointing to vertices of the prism but fails when given objects from the other S-orbit. However, if we use objects from both orbits in training, the output vectors point to vertices when given objects from either S-orbit. Hence, we need to use at minimum 2 symmetry breaking objects during training to guarantee correct behavior for all objects in the SBS compared to only needing one example to train for an ideal SBS.

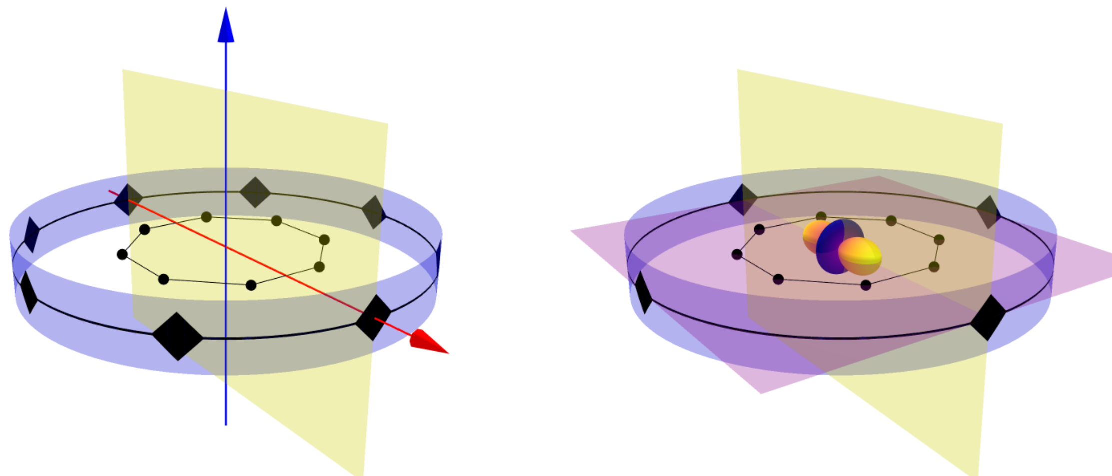
Table 10: Results of training using a nonideal equivariant SBS. If we only see one of the S-orbits in training, the network fails on the unseen orbits. If we see both S-orbits then the network behaves correctly.

Seen in training		Outputs	
S-orbit 1	S-orbit 2	S-orbit 1	S-orbit 2
Yes	No		
No	Yes		
Yes	Yes		

H.2 Octagon to rectangle

H.2.1 Obtaining an ideal partial SBS

In this scenario, we want G-equivariance for $G = O(3)$ and we have $S = D_8$ and partial symmetry $K = D_2$.



(a) (b)

Figure 17: (a) Octagon with D_8 symmetry we input and patterned cylinder with $N_G(S, K) = D_{8h}$ symmetry. The generators are a^2, b, m where a^2 is a $2\pi/8$ rotation about the blue axis, b is a π rotation about the red axis, and m is a reflection across the orange plane. (b) A symmetry breaking object which generates an ideal partial SBS. Note that in addition to the D_2 symmetry, this object is also symmetric under reflections across the purple and yellow planes.

The octagon has D_8 symmetry and we know from Table 4 that its normalizer is D_{16h}. We also know from Appendix F.3 that a presentation of this normalizer is

$$\langle a, b, m | a^{16}, b^2, m^2, (ab)^2, (am)^2, (bm)^2 \rangle.$$

Note the symmetry of the octagon S is generated by a^2, b and that of a rectangle K by a^8, b. Next, we can check by brute force that $N_G(S, K)$ is generated by a^2, b, m.

We then need to compute $N_S(K)$ and $N_{N_G(S,K)}(K)$. We note from Table 4 that $N_G(K) = D_{4h}$ and in particular, it is not hard to see the specific copy of D_{4h} is generated by a^4, b, m. We now just have $N_S(K) = S \cap N_G(K)$. Looking at the generators, we can check that m is not present in S so $N_S(K) = D_4$ and is generated by a^4, b. For $N_{N_G(S,K)}$, from the generators of $N_G(S, K)$ we can see that $N_G(K)$ is a subgroup so $N_{N_G(S,K)}(K) = N_G(K) = D_{4h}$ and is generated by a^4, b, m.

Finally, from Theorem 4.5, we need to look at the quotient groups $N_S(K)/K$ and $N_{N_G(S,K)}(K)/K$. For the latter, we can set the cosets

$$X = \{a^4, a^{12}, a^4 b, a^{12} b\} \qquad Y = \{m, a^8 m, bm, a^8 bm\}$$

which we can check generate the quotient group. In particular we have relations $X^2 = Y^2 = (XY)^2 = 1$ so a presentation is given by just

$$\langle X, Y | X^2, Y^2, (XY)^2 \rangle.$$

For $N_S(K)/K$ which is a subgroup of this, we can see that it is just generated by X. But it is easy to see that the quotient group generated by Y forms a complement.

Following the argument in Theorem 4.5, we see that we need a symmetry breaking object with stabilizer generated by group elements in the cosets of the complement of $N_S(K)/K$. Since here the complement is generated by coset Y, we need the stabilizer to be generated by m, a^8m, bm, a^8bm. It is not hard to check we can simplify the list of generators to a^8, b, m. We note that an $l = 2$ irrep with even parity works in this case.

H.3 $BaTiO_3$ experiment

H.3.1 Atom matching algorithm

We would like to predict atom distortions. However, our data consists of atom coordinates in the initial and target structures not necessarily in the same order. Hence, we need an algorithm to match similar atoms together so we know how much they are distorted. This process is complicated by the fact that we have periodic boundary conditions with periodicity determined by lattice vectors and that our atoms may be translated within the lattice. We assume our structures are given in the same rotational orientation.

For our algorithm, we use the insight that the distorted atom should still have similar vectors to neighboring atoms. Hence, we can compute a signature for an atom a by taking the difference of the positions of that atom and all other atoms in the lattice. We call the set of position differences for atom a from all other atoms the signature σ_a of a. Note in our implementation, we also separate out the atom types in addition to the position differences.

Next, we need a way to compare signatures. Suppose we had atom a from the initial structure and atom a' from the target structure. Certainly, if they are different atom types, we assign a cost of ∞ to this pairing. Otherwise, we look at their signatures. However, we actually need to optimally pair the other atoms to do so. For a pair of atoms b and b' from the initial and target structures, we can give a cost of ∞ if they are different atoms and $\sigma_a[b] - \sigma_{a'}[b']$ otherwise. If the atoms are similar, this should be small, but it may also be shifted by lattice parameters from the smallest it could be. So we just look at all small lattice shifts L and set the smallest $||\sigma_a[b] - \sigma_{a'}[b'] + L||^2$ as the cost of pairing b, b'. This gives a cost matrix $M_{b,b'}$. With all the costs, we can run the matching algorithm in Crouse (2016) to match the atoms. The cost of the assignment is the difference in the signatures of a, a'.

Finally, we can match the atoms using the comparison of signatures. We create a cost matrix where $C_{a,a'}$ is the difference in signatures of a, a' from the initial and target structures. We then run another iteration of the algorithm from Crouse (2016) to find our matching.

Because we only ever use differences of atoms, this matching algorithm is independent of translations.

H.3.2 Translation invariant loss

In the previous experiments, we could simply use a MSE loss of the vector differences. However, for crystals we wanted to have a loss which is invariant under translation. We realize that our matching algorithm in fact produces such a loss. By storing the matching information, we can effectively compute the same loss without having to run the matching algorithm every time. This is what we use to evaluate our model.

H.3.3 Symmetrically related outputs

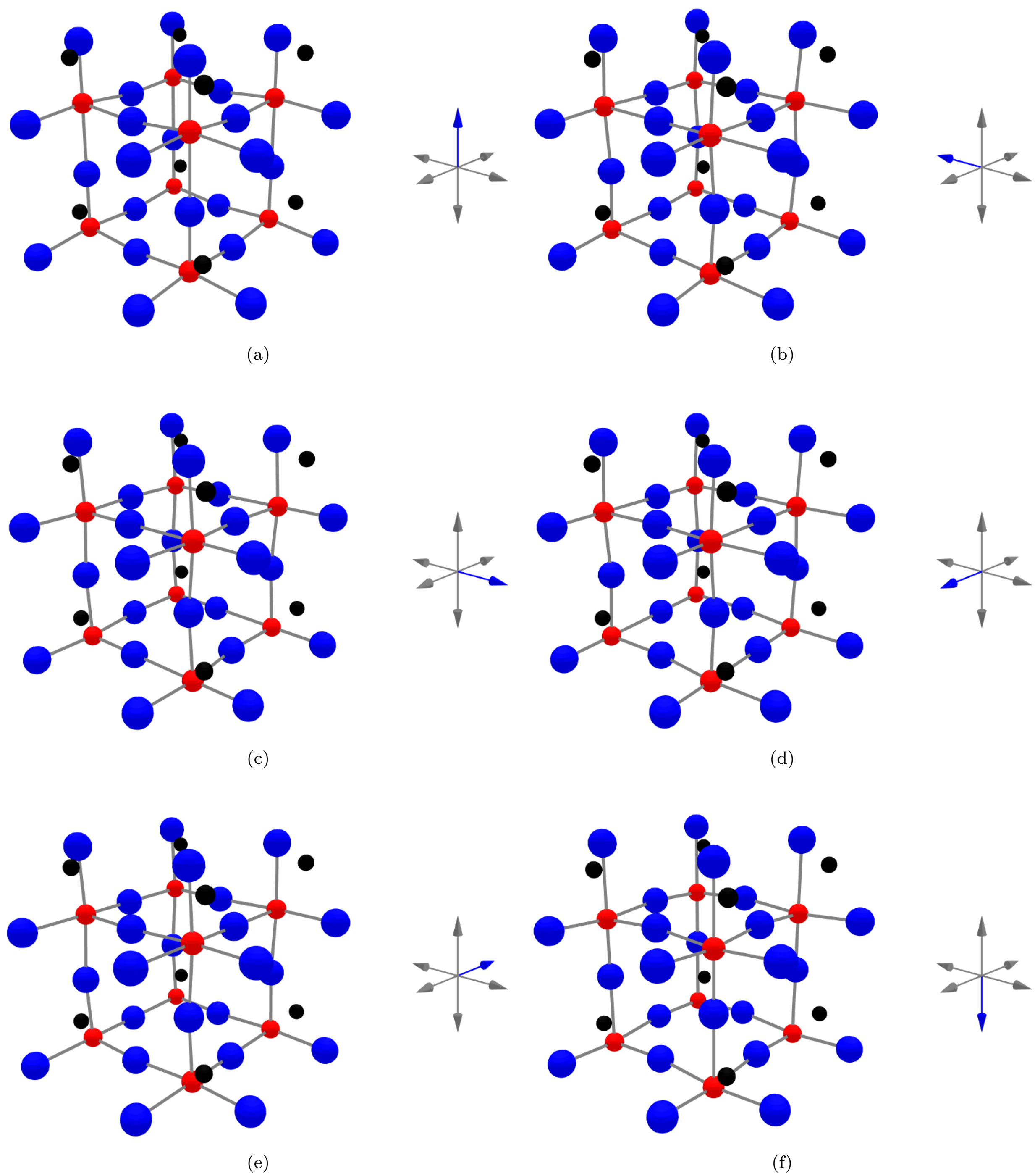


Figure 18: Distortions of a highly symmetric crystal structure of $BaTiO_3$ when provided with each of the possible symmetry breaking objects in our ideal equivariant partial SBS.

Table 11: Values of various quantities which help distinguish the high symmetry and low symmetry structures. Our models here try to distort the high symmetry structure to the low symmetry one.

Structure	SB object	Bond length average	Bond length variance	Ti-O1-Ti	Ti-O2-Ti	Ti-O3-Ti
High symmetry		2	0	180°	180°	180°
Low symmetry		2.003417	0.01392	180°	171.80°	171.80°
Model	None	2	0	180°	180°	180°
Model	$(1, 0, 0)$	2.003417	0.01392	180°	171.80°	171.80°
Model	$(-1, 0, 0)$	2.003417	0.01392	180°	171.80°	171.80°
Model	$(0, 1, 0)$	2.003417	0.01392	171.80°	180°	171.80°
Model	$(0, -1, 0)$	2.003417	0.01392	171.80°	180°	171.80°
Model	$(0, 0, 1)$	2.003417	0.01392	171.80°	171.80°	180°
Model	$(0, 0, -1)$	2.003417	0.01392	171.80°	171.80°	180°