TOPOLOGICAL BAND STRUCTURE CLASSIFICATION USING CRYSTALLOGRAPHIC SPACE GROUPS

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ABSTRACT

The interplay between symmetry and topology leads to a rich variety of electronic topological phases, protecting states such as the topological insulators and Dirac semimetals. The algorithm applies to crystals without time-reversal, particle-hole, chiral, or any other anticommuting or anti-unitary symmetries. Using a straight forward counting procedure, we classify all allowed topological phases of spinless particles in crystals in class A. The properties of electrons in magnetically ordered crystals are of interest both from the viewpoint of realizing novel topological phases, such as magnetic Weyl semimetals, and from the application perspective of creating energy-efficient memories. Employing this classification, we study transitions between topological phases within class A that are driven by band inversions at high-symmetry points in the first Brillouin zone. We compute constraints on electron fillings and band connectivity compatible with insulating behavior. In addition, by contrasting with atomic insulators, we identify band topology entailed by the symmetry transformation of bands, as determined. This is achieved by first developing an efficient way to represent band structures in terms of elementary basis states, and then isolating the topological ones by removing the subset of atomic insulators, defined by the existence of localized symmetric Wannier functions.

Keywords: *band structures, symmetry and topology, energy-efficient, electronic topological phases, high-symmetry points, atomic insulators.*

INTRODUCTION

Analyzing phase transitions, domain creation, and diffraction patterns are all examples of crystal structures and phenomena that may be defined and predicted using crystallographic group theory. Important in materials research for establishing relationships between a crystal's symmetry and its optical, photo-elastic, elastic, and other physical properties. On top of that, it helps reduce complicated crystal systems into more understandable mathematical models and has applications in the development of novel materials with desirable features via the knowledge of symmetry constraints on physical processes. Crucially, optical transitions can only take place between levels that have certain characteristics or follow specific laws. Quantum mechanics should provide these guidelines. Atomic spectrum analysis makes use of symmetric and unitary matrix groups. Here we study non-Abelian groups of reflections and rotations. Different types of unitary group representations are also under investigation. A great deal of physics now makes use of group theory. Specifically, basic particle physics makes use of group theory. The unitary groups are the backbone of contemporary particle physics. The groups of spin and isotopic transformations, as well as the groups of weak interaction transformations, are formed by these categories. Topics in nuclear and atomic physics are also addressed by group theory. Determining the energy levels of a system of comparable particles is one of the primary goals of atomic and nuclear physics. The use of perturbation theory approaches is necessary since exact solutions for systems of interacting particles are not feasible. Here, the perturbation will include both the particles' interactions and a portion of each particle's field. Assuming all particles are of the same type, a symmetric interaction operator will hold. Here is another viewpoint. In the n-dimensional space that basis vectors cover, the wave function is seen as a vector.

LITERATURE REVIEW

Konrat, Robert, et al. (2025) Structure-guided optimization often makes use of high-resolution 3D structural information to enhance early hits from screening campaigns to clinical drug candidates, which is essential for drug development. Although it has its drawbacks, X-ray crystallography is usually the go-to technique for medicinal chemists when they're designing new products. In this article, we go over the process of creating protein-ligand ensembles using solution-state NMR spectroscopy, selective side-chain labeling, and sophisticated computational algorithms. For medicinal chemists, this means precise and dependable structural data regarding protein-ligand complexes that may be used for high-throughput experiments.

Caserotto, Hugo et al. (2025) In recent years, serial macromolecular crystallography has emerged as a potent tool for time-resolved investigations and the discovery of room temperature structures of biological macromolecules. Among the 4th generation synchrotrons at the European Synchrotron Radiation Facility (ESRF), ID29 stands out as the world's first synchrotron beamline that can generate high brightness microsecond X-ray pulses at a high repetition rate, making it possible to determine the room temperature structure of biological macromolecules. We collectively refer to this technique as serial microsecond crystallography (SμX) because it enables high-quality full data to be obtained from a very little quantity of crystalline material by combining microsecond exposure lengths with unique beam characteristics and an adaptive sample environment. We used SμX on an integral membrane receptor after we validated the use of different sample delivery methods with different model systems.

Gupta, Satya P., et al. (2024) Targeted treatments, such as those for cancer and viruses, rely heavily on protein-ligand interactions. Therefore, a number of theoretical and experimental approaches have been devised to investigate the mechanism of enzyme activities, rapid binding, and selectivity in the last few years. There is a growing importance of AI techniques, big data, and neural networks, with combinatorial and graph theoretical approaches serving as major subfields within these techniques. Surface plasmon resonance and isothermal titration calorimetry are two common experimental approaches for measuring binding affinity. Electrostatic calculations, molecular dynamics simulation, hybrid dynamics approaches, etc. are some of the computational tools used to study protein-ligand interactions; these tools provide insight into structural stability, binding, protein activities, and more.

Armin Wagner et al. (2021) elements like sulfur, phosphorus, potassium, chlorine, or calcium are often found naturally in macromolecules, and the anomalous scattering characteristics of these elements may be used in long-wavelength macromolecular crystallography (MX). Proteins and nucleic acids may now be directly solved for their structures via experimental phasing, all without the requirement for further labeling. These investigations are conducted in a vacuum to avoid the substantial air absorption of X-rays in this range of wavelengths. Beamline I23, located at Diamond Light Source in the United Kingdom, is the first synchrotron device of its kind. It was specifically designed and fine-tuned for MX research in the extended wavelength range approaching 5 Å. This is accomplished by enclosing all endstation components of the sample environment in a huge vacuum vessel. Use of thermally conductive sample holders is necessary to keep samples at cryogenic temperatures throughout storage and data collecting in vacuum. This allows for effective heat removal, guaranteeing that the sample will cool to about 50 K. Beamline I23 sample preparation and vacuum transfer processes are detailed in the current protocol.

Ziqiang Zhou et.al (2018) In this study I examine the mathematical and physical descriptions of micro-images of material systems through symbolic logic, set theory, and topology. I prove the existence of a naturally morphological equation, which is a law of the qualitative structure of matter systems and the law of the unity of two types of morphological structures (Jordan and hidden structure). This equation can be employed to describe not only the shared properties of various correlated matter, but also to accurately categorize micro-images into different groups for the purpose of studying the morphology groups in algebraic geometry and materials science. In addition to its many uses in microscopy and other areas of applied mathematics, the morphology equation has the potential to shed new light on some fundamental ideas in algebraic geometry.

The science of crystal analysis

The study of the structure and characteristics of molecules and crystalline materials is known as crystallography. The Ancient Greek words κρύσταλλος (krústallos), meaning "clear ice, rock-crystal," and ιράφειν (gráphein), meaning "to write," are the origins of the English term crystallography. The UN declared 2014 the International Year of Crystallography in July 2012 to honor the field's significance.

Many of crystallography's subfields, including X-ray crystallography, are significant in their own right as scientific disciplines. From non-periodic or quasicrystal crystals to the mathematics of crystal geometry, crystallography covers it all. Utilizing X-ray diffraction, which generates experimental data usable by X-ray crystallography, may provide precise atomic locations and, on occasion, electron density on an atomic scale. In order to study the relative orientations at the grain boundary in materials at greater scales, it incorporates experimental procedures such orientational imaging. The study of crystals is essential to many branches of science, including physics, chemistry, and biology, and to many recent advances in these domains. Crystallography relied on goniometer observations of crystal geometry prior to the twentieth century.

System of crystals

The point groups and the space groups they belong to are arranged in a lattice structure in a crystal system. If the majority of the 32-point groups in three dimensions are associated with a single lattice system, then the names of the crystal system and the lattice system are interchangeable. As a result of their shared threefold rotational symmetry, two lattice systems—the rhombohedral and the hexagonal—are designated with five-point groups. The trigonal crystal system is given these point groups.

Groups of points

The mathematical set of symmetry operations that preserve the appearance of a crystal structure while leaving at least one point untouched is called the crystal class or crystallographic point group.

Some examples of symmetry operations include Using a reflection plane, which mirrors the building, Changing the structure's orientation such that it spins around a predetermined axis When a coordinate system is inverted, the sign of the coordinates relative to a symmetry or inversion point changes. Performing a rotation around an axis and then inverting it is an example of improper rotation. Symmetry elements include reflection planes, centers of symmetry, rotation axes (both proper and improper), and centers of inversion. Each crystal may belong to one of 32 distinct types. There are seven distinct crystal systems that each of them fits into.

Crystallography using X-rays and the invention of new drugs

In order to determine the structures of organic molecules, X-ray structural analysis has lately emerged as the most effective approach. The rational foundation for the design and development of new drugs with the necessary properties can be provided by using structural information alone or in conjunction with methods of theoretical conformational analysis to begin the analysis of the relationship between structure and biological activity. It is critical to restrict the prescription of antibiotics to their most suitable applications once they have been recognized, as there is no such thing as a perfect antibiotic. As a result, agents that are defined as "boys" should be derived from boys. It should now be feasible to have early warning of potential resistance mechanisms to new or old antibiotics, and so prepare for difficulties in the clinic in a proactive way, given the expanding understanding of environmental reservoirs of resistance. We must resume a coordinated attack that makes full use of new knowledge and technology. Our offspring will have to endure life before antibiotics if we do not. Studying the composition and characteristics of solids in their crystalline form is known as crystallography.

Applications of crystallography in medicine

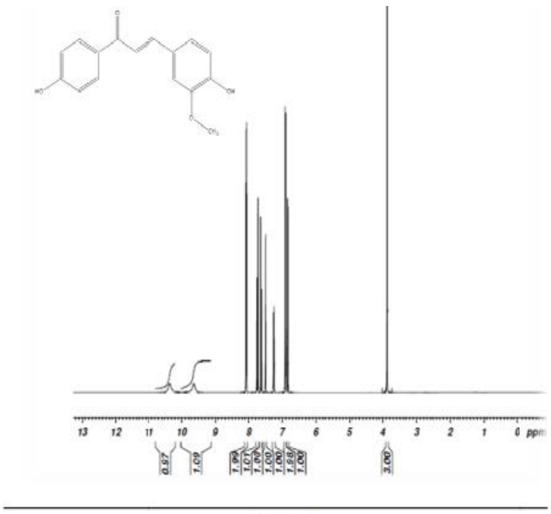
When it comes to X-ray crystallography, substance synthesis is where it really shines. The spontaneous production of substantial quantities of many of the therapeutic compounds found by science is very challenging. This calls for the development of synthetic methods for producing the compounds in question. A chemist needs an atomic structure map of a material before they can make it synthetic. Only by using X-ray crystallography is it possible to create this map. Dorothy Hydykin, a British chemist, was one of the few scientists to achieve this level of accomplishment (1910). Hadykin and her colleagues discovered penicillin's molecular structure during WWII (1939–1945). Producing this medicine on a large scale during the war required its synthesis. Pernicious anemia is a chronic blood condition that causes weakness and pallor; the hodykims team is now working on mapping this vitamin. Insulin mapping was another area of focus for the team. Treatment of diabetes and other blood disorders involves the use of insulin. The compounds were all created in our lab using materials sourced from their natural environments, with the exception of one crystal. An X-ray crystal structure may be obtained in four stages. An X-ray grade crystal is often grown as the first step by the experimental chemist. In order to solve a crystal structure, a crystallographer must first gather relevant data, then build an initial structure.

RESEARCH METHODOLOGY

Diseases pose the greatest danger to humans, and medical professionals are still battling to develop effective treatments. Modern medicine is the product of constant, resolute endeavor by human society. A plethora of new synthetic compounds with action potential were unlocked with the dawn of the synthetic drug era. The synthesis of chalcones, which are donor-acceptor conjugated dienes, relies heavily on the Claisen-Schmidt reaction. The medicinal properties of natural goods are attracting more and more attention. An essential class of naturally occurring substances is chalcones. Their chemical composition is that of open chain flavanoids, whereby a three-carbon α, β unsaturated carbonyl system connects the two aromatic rings. Research has shown that chalcones' antibacterial action is caused by the presence of a reactive α, β unsaturated keto function. The incorporation of biocidal moieties into the main or side chains of polymers makes macromolecular compounds biologically active. The biological effects of chalcones and related compounds are well-documented. According to the literature review, several chalcones and their derivatives have a wide range of pharmacological effects, including anti-inflammatory, anti-fungal, anti-oxidant, anti-malarial, anti-TB, analgesic, and anti-human immune syndrome. Several coordination compounds based on chalcones have been studied for their potential biocidal effects. The antibacterial activity of several newly synthesized 3-(aryl)-1-(4-(quinolin-8-ylamino)phenyl)prop-2-en-1-ones was reported after they were characterized using standard procedures.

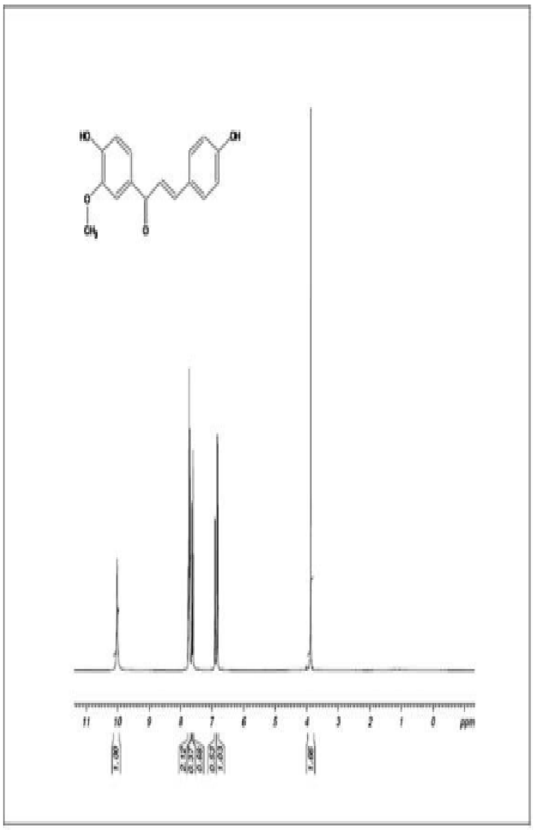
RESULTS AND DISCUSSIONS

Using Q-switched Nd: YAG with an input wavelength of 1064 nm and an input power of 0.68 J, the efficiency of the sample's second harmonic generation was determined. The sample's SHG efficiency was measured by measuring the amplitude of the green signal it produced, which was detected using a photomultiplier tube at 532 nm.



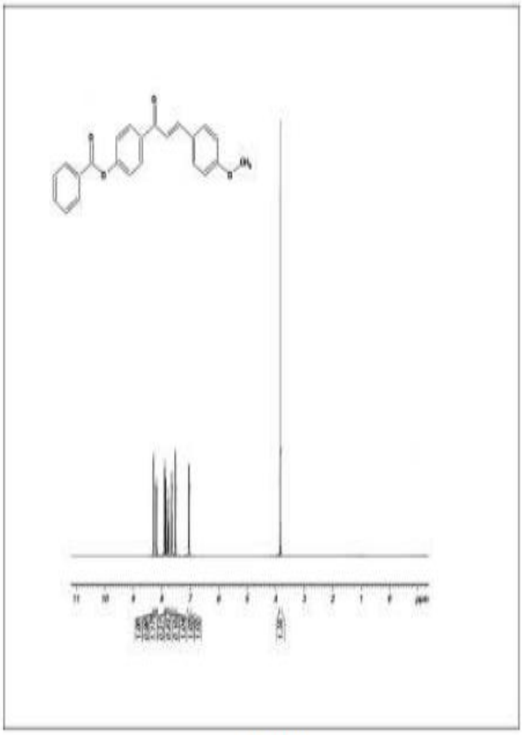
HMHP-I

The presence of green light indicates that the crystals are in the second harmonic generation. Using a reference KDP of the same size as the sample, we discovered that the measured SHG efficiency for HMHP-I was 0.26, for HMHP-II it was 0.96, and for MPEPB it was 0.23 times the size of KDP. Due to its centrosymmetric structure, crystal MPMC does not exhibit SHG efficiency. There has been talk recently that if crystalline perfection is improved, SHG efficiency might go up.

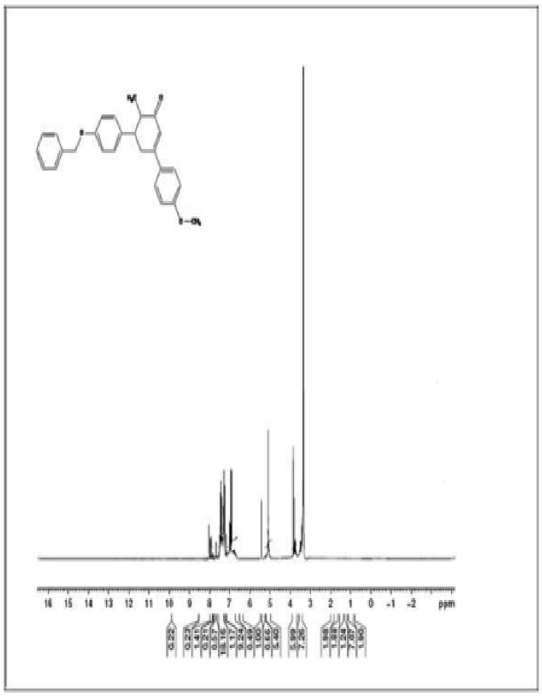


HMHP-II

Graph 1: NMR SPECTRA



MPEPB



MPMC

Graph 2: NMR SPECTRA

Each of the four novel chalcone derivatives—HMHP-I, HMHP-II, MPEPB—and one non-NLO (MPMC) crystal—were created using the slow evaporation solution growth approach and produced at room temperature.

Table 1: The observed values for HMHP-I

S. No	Load (P) X 10^{-3} Kg	Diagonal Length X10^{-3} m			Hardness value of Hv Kg/ mm^2
		d1	d2	D	
1	25	36.85	38.88	37.87	32.3
2	50	43.12	45.62	44.37	47.0
3	100	51.99	54.43	53.21	65.4

CONCLUSIONS

The structural characteristics and basic symmetries of crystalline materials may be better understood with the help of crystallographic group theory. The use of symmetry operations, such as rotations, reflections, inversions, and translations, enables researchers to systematically classify crystal formations. Group theory provides a rigorous mathematical framework that allows crystals to be classified into 230 space groups. These groups are the basis for understanding and forecasting the chemical and physical behavior of crystalline solids. The analysis of crystal structures is a hard process, but this systematic categorization makes it easier by exposing underlying structural patterns that aren't always obvious from experimental observation alone. The importance of crystallographic group theory in predicting material qualities from symmetry considerations is one of the main takeaways from the field's research. The optical behavior, electrical conductivity, magnetism, and flexibility of a crystal are heavily impacted by symmetry limits that arise from its space group. For example, piezoelectricity may be easily described by group theory because it is only seen in non-centrosymmetric crystals. Similarly, the symmetry restrictions on crystal phonon vibrations play a crucial role in elucidating lattice dynamics and thermal conductivity.

In addition to shedding light on current materials, these predictions pave the way for the logical development of new functional materials for applications in areas like electronics, photonics, and catalysis.

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