

Supporting Information

Knowledge Graph Representation of Zeolitic Crystalline Materials

Aleksandar Kondinski^{a,†}, Pavlo Rutkevych^{a,†}, Laura Pascazio^a, Dan N. Tran^a, Feroz Farazi^b, Srishti Ganguly^a, Markus Kraft^{a,b,c,d,e,*}

^aCARES, Cambridge Centre for Advanced Research and Education in Singapore, 1 Create Way, CREATE Tower, #05-05, Singapore, 138602

^bDepartment of Chemical Engineering and Biotechnology, University of Cambridge, Philippa Fawcett Drive, Cambridge, CB3 0AS, UK

^cCMCL Innovations, Sheraton House, Castle Park, Cambridge CB3 0AX, UK

^dSchool of Chemical and Biomedical Engineering, Nanyang Technological University, 62 Nanyang Drive, Singapore, 637459

^eThe Alan Turing Institute, 2QR, John Dodson House, 96 Euston Rd, London NW1 2DB, UK

[†]These authors contributed equally to this work.

*Corresponding author: mk306@cam.ac.uk

SI.1 Ontology Design and Data Details

The measured data in the Crystal Information File (CIF) typically have the uncertainty of measurement, which is not yet supported in the most recent version of the Units Of Measurement Ontology (OM2) [2, 3]. We introduce a `ocr:MeasureWithUncertainty` class Fig. S1.a which is an extension of the `om:Measure` class with additional property `hasUncertaintyValue`. This data property shares the same unit of measurement with the `hasNumericalValue` property.

Also, the CIF format contains a variety of array-like data types, and it is convenient to store such data as components of a single structure. Although not all of these sets are vectors in strict mathematical meaning, we name the new class as `ocr:MeasureVector`, to highlight that this data structure is a set of `om:Measure` values with value, units of measurement. This data structure is flexible in terms of the number of components, labelling of the components, and individual units of measurement for the components, and may contain uncertainties. Depending on the implementation the components can be accessed by the index and/or by the label of the component. The same applies to the components of `ocr:MeasureMatrix`. Large data sets, like spectrum plots, can be represented by two arrays of points for the X and Y axes, measured in their respective units. The data arrays are stored as `MeasureVector`, and may contain uncertainties to represent the plot with error bars.

Data details

CIF files cover the majority of the crystal properties and details on the measurement procedure. The total count of keywords reaches over 3000 in the recent standard [1], plus it allows non-standard keywords defined by software and hardware developers. Within this extensive list, certain keywords emerge as more prevalent than others. We studied the occurrence of the keywords in the CIF files in the COD database [4]. As COD contains CIF files from a variety of sources, we assume that this is a good representation of CIF files in general. Figure S2 shows the cumulative distribution function for the top 350 keywords. Our analysis shows that the top 50 keywords cover over 80% of the information contained in the CIF files. These top keywords include the crystal unit cell data, the atomic structure, and the citation. The OntoCrystal ontology mainly

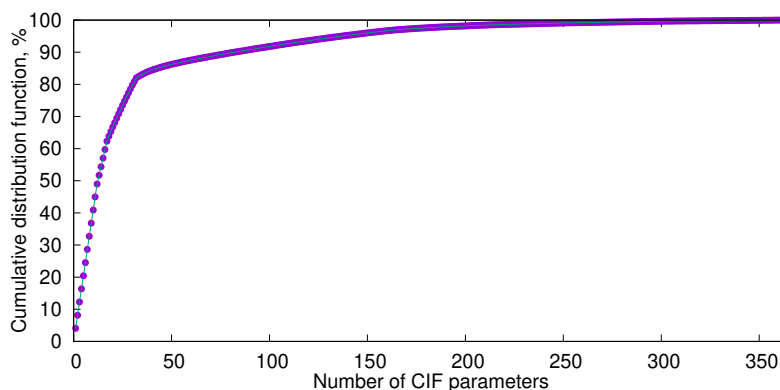


Figure S2: Analysis of Crystallographic Information Files (CIF). The cumulative distribution function for the most common keywords in the COD database. Top 50 keywords cover over 80% of the data contained in the CIF files.

APC, APD, AST, ASV, ATN, ATO, ATS, ATT, ATV, AWO, AWW, BCT, BEC, BIK, BOG, BPH, BRE, CAN, CAS, CDO, CFI, CGF, CGS, CHA, CHI, CLO, CON, CZP, DAC, DDR, DFO, DFT, DOH, DON, EAB, EDI, EMT, EON, EPI, ERI, ESV, ETR, EUO, EZT, FAR, FAU, FER, FRA, GIS, GIU, GME, GON, GOO, HEU, IFR, IHW, IMF, ISV, ITE, ITH, ITW, IWR, IWV, IWW, JBW, KFI, LAU, LEV, LIO, LIT, LOS, LOV, LTA, LTL, LTN, MAR, MAZ, MEI, MEL, MEP, MER, MFI, MFS, MON, MOR, MOZ, MSE, MSO, MTF, MTN, MTT, MTW, MWW, NAB, NAT, NES, NON, NPO, NSI, OBW, OFF, OSI, OSO, OWE, PAR, PAU, PHI, PON, RHO, RON, RRO, RSN, RTE, RTH, RUT, RWR, RWY, SAO, SAS, SAT, SAV, SBE, SBS, SBT, SFE, SFF, SFG, SFH, SFN, SFO, SGT, SIV, SOD, SOS, SSY, STF, STI, STT, SZR, TER, THO, TOL, TON, TSC, TUN, UEL, UFI, UOZ, USI, UTL, VET, VFI, VNI, VSV, WEI, WEN, YUG, ZON.

All codes related to the conversion of files are accessible on The World Avatar Git repository (<https://github.com/cambridge-cares/TheWorldAvatar>). Data files suitable for the regeneration of the knowledge graph are made accessible through the University of Cambridge Data Repository.

SI.2 NLP Workflow, Questions and Responses

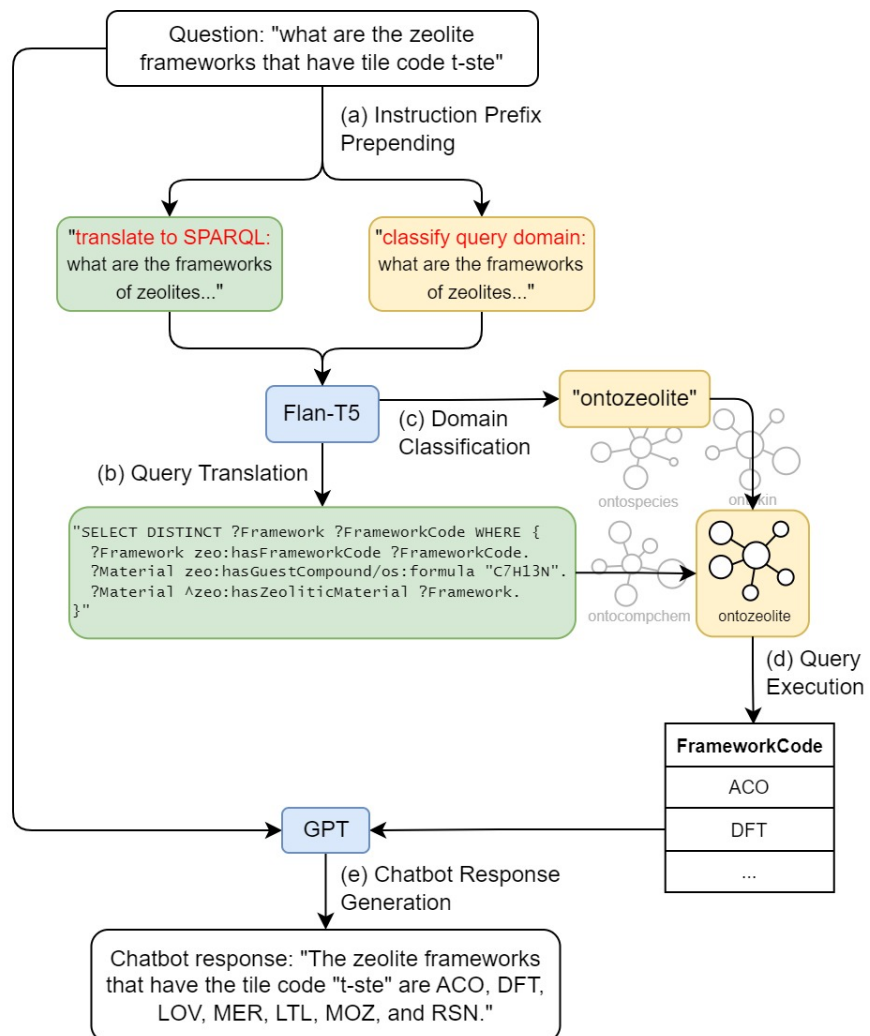


Figure S3: Workflow demonstrating the translation of a natural language question about zeolite frameworks into a SPARQL query, including query execution and chatbot response generation.

Marie Responses

What is the unit cell information of zeolite framework ...

User

User: What is the unit cell information of zeolitic framework ABW?

Bot

Marie's response:

The unit cell information of zeolitic framework ABW includes the following details:

- Lengths:
 - a : 9.873 Å
 - b : 5.254 Å
 - c : 8.77 Å
- Angles:
 - alpha: 90.0°
 - beta: 90.0°
 - gamma: 90.0°
- Volume: 454.9239 cubic Ångstroms
- Lattice system: Orthorhombic
- Space group number (ITCr): 74

Correct Response

This response is correct. For comparison see IZA - Framework Type ABW

User

User: What is the unit cell information of zeolite AHT?

Bot

Marie response:

The unit cell information of zeolite AHT is as follows:

- Lengths: $a = 15.794$ Å, $b = 9.206$ Å, $c = 8.589$ Å
- Angles: $\alpha = 90.0^\circ$, $\beta = 90.0^\circ$, $\gamma = 90.0^\circ$
- Volume: 1248.8369 cubic Å
- Lattice System: Orthorhombic
- Space Group Number (ITCr): 63

Correct Response

This response is correct. For comparison see IZA - Framework Type AHT

User

User: What is the unit cell information of zeolite LAU?

Bot

Marie response:

The unit cell information of zeolite LAU is as follows:

- Lengths: The lengths of the unit cell are $a = 14.587 \text{ \AA}$, $b = 12.877 \text{ \AA}$, $c = 7.613 \text{ \AA}$.
- Angles: The angles of the unit cell are $\alpha = 90.0^\circ$, $\beta = 111.159^\circ$, $\gamma = 90.0^\circ$.
- Volume: The volume of the unit cell is 1333.5942 cubic \AA .
- Lattice System: The zeolite LAU belongs to the monoclinic lattice system.
- Space Group Number: The space group number (according to the International Tables of Crystallography) for zeolite LAU is 12.

Correct Response

This response is correct. For comparison see IZA - Framework Type AHT

Show me zeolite frameworks incorporating ...

User

User: Show me zeolite frameworks incorporating pyridine.

Bot

Marie's response: Zeolite frameworks incorporating pyridine include RFE, FER, and CHA.

Correct Response

This response is correct. For comparison see. Figure S4 documents the IZA response for comparison.

The screenshot shows the IZA-SC website interface. The search criteria are OSDA = C₅H₅N = pyridine. The search results show one material found: RFE (RUB-58, as-made). The table below summarizes the search results.

FTC	Material	Si/Al	Short Fw Formula	Stoichiometry (if available)
RFE	RUB-58, as-made		[Si - O]	[PYr _{1.33} EDA _{0.67}][Si ₄₈ O ₉₆]-RFE, Pyr = C ₅ H ₅ N = pyridine, EDA = C ₂ H ₈ N ₂ = ethylenediamine

Copyright © 2020 Structure Commission of the International Zeolite Association (IZA-SC)

Figure S4: IZA Search for pyridine as guest molecule. Query from 14 April 2024.

Find zeolites with framework element components ...

User

User: Find zeolites with framework element components Ga and Se only.

Bot

Marie's response:

I found two zeolites with framework element components Ga and Se only:

1. Chemical Formula: $[Ga_4Se_8]$
2. Chemical Formula: $[(CID85631)][Ga_4Se_8]$

These zeolites have Ga and Se as their framework element components.

The screenshot shows a search interface with a search bar containing the query "Find zeolites with framework element components Ga and Se only". Below the search bar, there are two buttons: "Click to view the predicted SPARQL query" and "Click to view the post-processed SPARQL query". A "Hide IRIs" button is also present. The search results are displayed in a table with columns for "#", "Material", and "ChemicalFormul".

#	Material	ChemicalFormul
1	http://www.theworldavatar.com/kg/ontozeolite/ZeoliticMaterial_4d09f275-af0e-480b-8f87-04780571bc46	[Ga4Se8]
2	http://www.theworldavatar.com/kg/ontozeolite/ZeoliticMaterial_50294a38-280a-4139-abee-37e14f0bc824	[(CID85631)][Ga4Se8]

Below the table, it says "Showing 1 to 2 of 2 entries" and "Previous 1 Next". To the right of the table, there is a section titled "IRI details" with the following information:

IRI: http://www.theworldavatar.com/kg/ontozeolite/ZeoliticMaterial_4d09f275-af0e-480b-8f87-04780571bc46
doi: 10.1126/science.1078663
Zeolite Framework: RWY
Chemical Formula: [Ga4Se8]

Below the IRI details, there is a 3D ball-and-stick model of a zeolite framework. The model shows a complex, interconnected network of atoms. The atoms are represented by small spheres, with orange spheres likely representing Gallium (Ga) and grey spheres representing Selenium (Se). The model is labeled with "P 1 [P 1] #1" and "a=21.893Å, b=21.893Å, c=21.893Å, α=90.000°, β=90.000°, γ=90.000°".

Figure S5: IZA Search for pyridine as guest molecule. Query from 14 April 2024.

Correct Response

This answer and reference are correct, and they link to an influential work published in DOI: 10.1126/science.1078663.

ChatGPT Responses

What is the unit cell information of zeolite framework ...

User

User: What is the unit cell information of zeolite ABW?

Bot

ChatGPT:

Zeolite ABW, one of the many types of zeolite frameworks, has a unique unit cell structure characterized by specific lattice parameters and symmetry. Here are the details of the zeolite ABW unit cell:

- Crystal System: Hexagonal
- Space Group: P6₃/mmc
- Lattice Parameters:
 - a = about 10.4 Å
 - c = about 6.4 Å

This framework consists of a three-dimensional network of aluminum, silicon, and oxygen that forms channels and cavities. These properties make it useful for various applications including ion exchange, adsorption, and catalysis.

Incorrect Response

The chatbot hallucinates. A shared response can be found on the following link: <https://chat.openai.com/share/64e1673a-ffe-484a-882e-f29939c7f058> For comparison see IZA - Framework Type ABW

User

User: What is the unit cell information of zeolite framework AHT?

Bot

ChatGPT: The zeolite framework type designated as "AHT" refers to a specific structure within the family of zeolite materials. Zeolites are microporous, aluminosilicate minerals commonly used as commercial adsorbents and catalysts. The framework type of a zeolite is determined by its unique three-dimensional arrangement of silica and alumina tetrahedra.

The "AHT" framework type is less commonly discussed compared to more well-known zeolites like Type A (LTA), Type X, and Type Y. To provide accurate unit cell information for the AHT zeolite framework, including its dimensions, symmetry, and typical chemical composition, I'll need to check some detailed resources. Let me do that right now.

The zeolite framework type AHT has specific unit cell information detailed in the databases of the International Zeolite Association. The AHT structure has a monoclinic unit cell with the following dimensions and angles: $a = 9.4860 \text{ \AA}$, $b = 9.9140 \text{ \AA}$, $c = 8.1260 \text{ \AA}$, $\alpha = 90.000^\circ$, $\beta = 90.000^\circ$, $\gamma = 121.490^\circ$. This framework is characterized by its framework density and specific geometric configuration suitable for various applications.

Another specification for the AHT framework is its orthorhombic cell parameters under a different configuration or material composition: $a = 15.7940 \text{ \AA}$, $b = 9.2060 \text{ \AA}$, $c = 8.5890 \text{ \AA}$, with all angles (α, β, γ) at 90.000° , giving a volume approximately 1248.8 \AA^3 . This demonstrates the versatility and structural variations within the AHT type frameworks depending on the specific synthesis and material composition.

These details highlight the complex nature of zeolite framework structures, which are crucial for their function in catalysis and adsorption processes due to the precise arrangement of pores and channels within the material.

For more detailed information and visual representations of the AHT framework, you can visit the IZA Structure Commission's database: Zeolite AHT Framework.

Partially Correct Response

The chatbot originally hallucinates, but the second part of the response provides correct information on the framework parameters. The chatbot provides the correct link to the IZA webpage. A shared response can be found on the following link: <https://chat.openai.com/share/443d6bcb-228e-40e5-b68c-a1b8a9643e36>

User

User: What is the unit cell information of zeolite LAU?

Bot

ChatGPT: Zeolite LAU, also known as Linde Type A or LTA, is a synthetic zeolite with a well-defined structure and specific properties that make it suitable for various industrial applications, especially in adsorption and ion exchange processes. Here's the unit cell information for zeolite LAU (LTA):

- **Chemical Formula:** The chemical formula of zeolite LAU is typically given as $\text{Na}_{12}[\text{Al}_{12}\text{Si}_{12}\text{O}_{48}] \cdot 27\text{H}_2\text{O}$.
- **Crystal System:** Zeolite LAU crystallizes in the cubic crystal system.
- **Unit Cell Dimensions:** The unit cell parameter a is approximately 24.60 Å.
- **Framework Type:** The framework type of zeolite LAU is designated as LTA. It features a three-dimensional network of AlO_4 and SiO_4 tetrahedra linked together to form a characteristic sodalite cage structure. This arrangement creates a system of pores and channels, ideal for molecular sieving.
- **Space Group:** The space group for zeolite LAU is $\bar{3}m$, indicating a highly symmetric structure.
- **Pore Dimensions:** It has uniform pore openings of about 4 Å, making it particularly useful for size-selective adsorption of small molecules.

Zeolite LAU is utilized in processes like water softening and the separation of small molecules due to its ability to selectively adsorb molecules that fit within its pores, which is largely determined by the aforementioned structural characteristics.

Incorrect Response

The chatbot clearly mixes framework-type LAU with framework-type LTA. A shared response can be found on the following link: <https://chat.openai.com/share/25dcedbd-f2ba-40de-a619-83942e29d82e>

Show me zeolite frameworks incorporating ...

User

User: Show me zeolite frameworks incorporating pyridine.

Bot

ChatGPT: Zeolites with incorporated pyridine represent a specialized topic within materials science, focusing on modifying the properties of zeolite frameworks through the introduction of organic molecules like pyridine. Pyridine is a basic, nitrogen-containing heterocycle that can interact with the acidic sites of zeolites, potentially affecting the catalytic and adsorptive properties of the zeolite. Incorporating pyridine into zeolite frameworks can be done in several ways:

Synthesis Modification: Pyridine can be added during the synthesis of the zeolite to direct the assembly of the zeolite framework, acting as a structure-directing agent (SDA). This incorporation can influence the pore size, topology, and framework stability.

Post-synthesis Modification: Pyridine can be introduced into pre-formed zeolites through ion-exchange processes, where pyridine molecules replace other cations in the zeolite's structure. This modification can enhance the selectivity and efficiency of zeolites in various reactions.

Functionalization and Adsorption: Pyridine can also be adsorbed onto the surface of zeolites, modifying the surface characteristics and interacting with reactant molecules in catalytic processes. These modifications aim to enhance the utility of zeolites in applications such as catalysis (e.g., cracking, isomerization, and fine chemical synthesis), gas separation, and pollution control.

For visualization or specific structures of these frameworks, diagrams or modeling software like those used in materials science or chemistry would be helpful to see how pyridine is arranged within the zeolite matrix. If you're looking for more detailed explanations or visual materials, specific research articles or textbooks on zeolite chemistry would be ideal sources.

Incorrect/Partially Correct Response

The chatbot hallucinates and does not answer the question asked. A shared response can be found on the following link: <https://chat.openai.com/share/6f312790-5401-4568-a7c3-b66c2c2f8a6f> Rerunning the prompt links provides to NMR studies linking pyridine to HZSM-5 (DOI: 10.1039/D1CP01515J) <https://chat.openai.com/share/04686096-ee95-440e-ad15-5c3a43b3413d>

User

User: What is the tile information of zeolite framework SOD?

Bot

ChatGPT: The "SOD" in zeolite framework refers to sodalite, a type of zeolite mineral characterized by its cubic framework. The "SOD" topology in zeolites has a three-dimensional structure composed of six-membered rings of SiO₄ and AlO₄ tetrahedra. This forms a distinctive cubic lattice.

The tile information, which describes the types of secondary building units (SBUs) used to construct the framework, includes the following for the SOD framework:

- Primary Building Unit (PBU): The SOD framework is typically built from a primary building unit consisting of β -cages, which are cubic units made up of 24 tetrahedral units (T-atoms).
- Secondary Building Unit (SBU): The SOD framework does not have traditional larger SBUs like some other zeolites but is primarily constructed from the interconnected β -cages.

The sodalite cage itself is a truncated octahedron and is a key characteristic unit in many zeolites, not just those with the SOD framework. These cages are connected in such a way that they form a dense, yet porous structure, ideal for various applications including ion-exchange, gas separation, and catalysis.

Correct/partially Response

The sodalite framework contains only a single tiling unit also called sodalite or β -cage. This cage is well known to be a truncated octahedron. The response is available through the following link: <https://chat.openai.com/share/42d3c2d9-85be-4020-ba42-ef35dc8ccd69>

User

User: What is the tile information of zeolite framework CGF?

Bot

ChatGPT: The zeolite framework type CGF, abbreviated from "Chabazite Germanium Framework," is a hypothetical ordered zeolite framework constructed through simulations by substituting the silicon atoms in the CHA (chabazite) framework type with germanium. In the context of zeolite frameworks, "tiles" often refer to the basic building blocks that make up the framework structure, which could be rings or secondary building units (SBUs) such as polyhedral clusters.

The tile information of the CGF framework can be described as follows:

- Framework Code: CGF
- Topology: This framework is related to the chabazite (CHA) type but with germanium substitution.
- Tile Composition: The tiles in CGF would likely include 4-, 6-, and 8-membered rings, similar to those found in the CHA framework.
- Dimensionality: It is a three-dimensional framework.
- Pore System: The framework contains pores defined by the arrangement and connectivity of its tiles.

These hypothetical zeolites like CGF often explore substitutions of atoms like silicon with other tetrahedral atoms (like germanium) to predict new material properties or understand the structural impacts of such substitutions. The tile-based description is crucial for understanding the pore structure and potential applications in catalysis, gas separation, or ion exchange.

Incorrect/Partially Correct Response

This answer is a hallucination. The abbreviation CGF derives from **C**obalt-**G**allium-**P**hosphate-**F**ive. Consequently information related to tiling is incorrect. The response can be accessed via the link: <https://chat.openai.com/share/87dc6e33-fe50-4341-9b77-5a7f55df1b3e>

Find zeolites with framework element components ...

User

User: Find zeolites with framework element components Ga and Se only.

Bot

ChatGPT: Zeolites are microporous, aluminosilicate minerals commonly used in industrial applications such as catalysis, ion exchange, and gas separation. The structure of a zeolite is characterized by its framework, which consists of tetrahedrally coordinated atoms linked by oxygen atoms.

To find a zeolite that specifically uses gallium (Ga) and selenium (Se) as the framework components is quite unique. Typically, zeolites do not include selenium in their framework because it is not commonly tetrahedrally coordinated in minerals. Selenium usually prefers other types of coordination geometries due to its larger size and different electronic properties compared to silicon or aluminum, which are more commonly found in zeolite frameworks.

Gallium, however, can substitute for aluminum in some zeolite frameworks due to its similar size and charge. It is known to be used in some special synthetic zeolites for specific catalytic or adsorption properties.

Given the unconventional nature of using selenium in a zeolite framework, it is unlikely that such a zeolite with only Ga and Se as framework elements exists based on common knowledge and typical properties of zeolite structures. If such materials were to be synthesized or discovered, they would likely be highly novel and possibly reported in specialized scientific research focused on advanced materials or novel crystallography.

For accurate and current information, searching through scientific literature databases such as SciFinder or Web of Science or reading recent publications in materials science journals would be necessary. These platforms would provide the most up-to-date research on the synthesis and properties of such unique zeolitic materials, if they exist.

Lack of information response

This answer suggests that the chatbot does not have information that such zeolite structural composition exists. The response can be accessed via the link: <https://chat.openai.com/share/33187465-1dc6-4629-91ed-28d628cded70>

Gemini Advanced Responses

What is the unit cell information of zeolitic framework ...

User

User: What is the unit cell information of zeolitic framework ABW?

Bot

Gemini Advanced: Here's the unit cell information of the zeolitic framework ABW:

Framework Type: ABW

Crystal System: Orthorhombic

Space Group: Pna21 (No. 33)

Typical Unit Cell Parameters:

- $a = 10.3 \text{ \AA}$
- $b = 8.2 \text{ \AA}$
- $c = 5.0 \text{ \AA}$

Important Notes:

- **Composition:** The ABW framework is typically formed with aluminosilicate and gallosilicate compositions. The specific unit cell parameters can slightly vary depending on the exact Si/Al or Si/Ga ratio.
- **Structure:** The ABW framework is known for its small pore system, limiting the size of molecules that can enter it. The framework structure features a combination of 4-rings, 6-rings, and 8-rings.

Database References: You can find detailed information about the ABW framework topology, including unit cell data, on the International Zeolite Association (IZA) Structure Commission website: <http://www.iza-structure.org/databases/>

Where to Find More Information:

- **Atlas of Zeolite Framework Types:** This comprehensive resource provides detailed structural descriptions and illustrations of zeolite frameworks, including ABW. (https://books.google.co.uk/books?id=c5_JGBc7VZgC&pg=PA21&lpg=PA21&dq=unit+cell+information+of+zeolitic+framework+ABW&source=bl&ots=xUsyysbLI-&sig=ACfU3U0jG8701C3zbNnVvmYYzsvWnknB0g&hl=en)
- **Research Publications:** Check scientific journals and databases for publications on zeolite synthesis and characterization for more specific experimental unit cell parameters and structural analyses of ABW zeolites.

Let me know if you'd like more information on the ABW framework!

Lack of information response

The chatbot indeed provides link to the IZA database, however, the provided data for ABW are made up and do not correspond to what is being reported there. The response can be accessed via the link: <https://g.co/gemini/share/aa8a2031e241>

User

User: What is the unit cell information of zeolite AHT?

Bot

Gemini Advanced: Here's a breakdown of the unit cell information for zeolite AHT:

Structure and Framework Type

- **Framework Type Code:** AHT (assigned by the International Zeolite Association's Structure Commission)
- **Construction:** AHT is built from unique secondary building units (SBUs) called the 10-ring tube. These tubes connect to each other to form the overall framework.
- **Topology:** The AHT framework has a complex topology with interconnected channels and cages.

Unit Cell Parameters

- **Crystal System:** Tetragonal
- **Space Group:** I4/mmm (No. 139)
- **Lattice Parameters:**
 - $a \approx 18.9 \text{ \AA}$
 - $c \approx 8.4 \text{ \AA}$

- **Unit Cell Volume:** Approximately 3000 \AA^3
- **Zeolite formula per unit cell:** The specific formula depends on the cations present, but a general form is $|M_{12}(H_2O)_{27}][Al_{12}Si_{36}O_{96}]$, where M represents exchangeable cations.

Key Characteristics

- **Pore System:** Zeolites AHT has a pore system formed by interconnected channels with 10-membered ring openings.
- **Channel Dimensions:** The approximate pore size is around $4.4 \times 7.2 \text{ \AA}$.

Important Notes:

- Unit cell parameters can slightly vary based on variations in chemical composition or synthesis conditions. The values provided above are representative.
- Zeolites are complex materials, and detailed structural information is best obtained from crystallographic databases and research papers.

Where to Find More Information

- International Zeolite Association Structure Database: <http://www.iza-structure.org/databases/>
- Research publications: Search for research articles specifically focusing on the structure and properties of zeolite AHT.

Let me know if you'd like any specific details or have further questions!

Lack of information response

The chatbot indeed provides link to the IZA database, however, the provided data for AHT are made up and do not correspond to what is being reported there. The response can be accessed via the link: <https://g.co/gemini/share/b1f7ff2d5365>

User

User: What is the unit cell information of zeolite LAU?

Bot

Gemini Advanced: Zeolite LAU (Laumontite) has the following unit cell information:

Crystal System: Monoclinic **Lattice Parameters:**

- $a \approx 13.7 \text{ \AA}$
- $b \approx 13.1 \text{ \AA}$
- $c \approx 7.5 \text{ \AA}$
- $\alpha = 90^\circ$
- $\beta \approx 112^\circ$
- $\gamma = 90^\circ$

Space group: C2/m

Important Notes:

- Zeolite structures, including laumontite, can be somewhat flexible. Variations in hydration state or chemical substitutions can slightly alter unit cell dimensions.
- Laumontite is known to transition to a lower symmetry form upon dehydration.

Key Structural Features of the LAU Framework

- **Building Units:** The LAU framework consists of 4-rings of tetrahedra (where each tetrahedron commonly represents a SiO₄ or AlO₄ unit). These combine to form larger structural units such as double 6-rings.
- **Channels:** The LAU framework has a system of one-dimensional channels running parallel to the c-axis.
- **Cages:** The structure contains 'lau' cages that are accessible through the channels.

Where to Find More Information

- International Zeolite Association Structure Database: This is the authoritative source for zeolite framework information (<http://www.iza-structure.org/databases/>)
- Scientific Publications: Research articles on the synthesis, properties, and modification of laumontite often detail its crystallographic information.

Let me know if you'd like more details on the LAU structure or zeolites in general!

Incorrect Data

The chatbot indeed provides link to the IZA database, however, the provided data for LAU are made up and do not correspond to what is being reported there. The response can be accessed via the link: <https://g.co/gemini/share/f49751046133>

Show me zeolite frameworks incorporating ...

User

User: Show me zeolite frameworks incorporating pyridine.

Bot

Gemini Advanced:

Unfortunately, it's difficult to find examples of zeolite frameworks that directly incorporate pyridine within their structure. Here's why and some alternative ways pyridine is used with zeolites:

Challenges of Direct Pyridine Incorporation

- **Size and Shape Mismatch:** Pyridine is a relatively bulky molecule compared to the typical building blocks of zeolite frameworks (silica and alumina tetrahedra). Incorporating it directly would disrupt the zeolite's regular structure.
- **Stability:** The nitrogen atom in pyridine can act as a Lewis base. This basicity could make the zeolite unstable in acidic or reactive environments, as the nitrogen could interact with other molecules.

How Pyridine is Used with Zeolites

- **Templating Agent:** Pyridine-like molecules can be used during zeolite synthesis to direct the formation of specific pore structures. The pyridine-like molecule is later removed, leaving behind a zeolite with a tailored structure.
- **Post-Synthesis Modification:** Pyridine can be attached to existing zeolites through chemical reactions. This creates functionalized zeolites with sites for:
 - **Catalysis:** Pyridine's basic nitrogen can participate in catalytic reactions.
 - **Adsorption:** Pyridine-functionalized zeolites can selectively adsorb molecules that interact with the nitrogen.
- **Guest Molecule:** Pyridine can be trapped within zeolite pores without being chemically bound to the framework. This is useful for:
 - **Catalysis:** Confining pyridine in the zeolite can influence its reactivity in catalytic processes.
 - **Molecular Sensing:** The interaction of pyridine with the zeolite framework can be used for sensing specific molecules.

Note: While it's less common to directly incorporate pyridine into the framework, there are zeolite-like materials called Metal-Organic Frameworks (MOFs) that are much more flexible in terms of the organic molecules they can incorporate. You might find examples of MOFs with integrated pyridine components.

Irrelevant response

The response can be accessed via the link: <https://g.co/gemini/share/52dad5f8579b>

Find zeolites with framework element components ...

User

User: Find zeolites with framework element components Ga and Se only.

Bot

Gemini Advanced:

Unfortunately, it's highly unlikely that zeolites with a framework composed solely of gallium (Ga) and selenium (Se) exist. Here's why:

Zeolites Fundamentals

- **Definition:** Zeolites are crystalline microporous aluminosilicates. This means their framework primarily consists of aluminum (Al), silicon (Si), and oxygen (O).
- **Tetrahedral Building Blocks:** The fundamental building units in zeolites are tetrahedra where a silicon or aluminum atom sits at the center, surrounded by four oxygen atoms. These tetrahedra link together to form the intricate zeolite frameworks.
- **Charge Balancing:** Aluminum has a +3 charge, while silicon has a +4 charge. This charge imbalance necessitates the presence of cations (often sodium, potassium, etc.) within the zeolite structure to maintain neutrality.

Why Ga and Se Are Unlikely

- **Charge Considerations:** Gallium (Ga), like aluminum, has a +3 charge. Selenium (Se) can have varying oxidation states (-2, +4, +6). It's difficult to envision a stable zeolite framework where Ga and Se are the only elements present while maintaining charge neutrality.
- **Coordination Preference:** Gallium tends to favor tetrahedral coordination (like aluminum and silicon). However, selenium often prefers different coordination geometries, making it less compatible with the tetrahedral building blocks of zeolites.

Possible Alternatives

- **Gallosilicates:** These are zeolite-like materials where some silicon atoms are replaced by gallium. However, they typically still contain aluminum in their framework.
- **Chalcogenide Zeolite Analogs:** These materials replace the oxygen in traditional zeolites with heavier chalcogen elements like sulfur (S) or selenium (Se). They can incorporate a wider range of metals into their framework.
- **Metal Selenides:** While not true zeolites, certain metal selenides might display porous or zeolite-like structural characteristics.

Where to Search To find potentially relevant materials, consider searching these resources:

- **Scientific Databases:** Web of Science, SciFinder, Google Scholar, etc.
- **Crystallographic Databases:** The Cambridge Structural Database (CSD), the Inorganic Crystal Structure Database (ICSD).
- **Materials Science Journals:** Focus on publications within materials chemistry, catalysis, and inorganic chemistry.

Let me know if you'd like me to help you refine your search or explore any of these alternative directions!

Lack of information response

The response is of low relevance. The chatbot even argues that structures based on Ga and Se atoms do not exist. The response can be accessed via the link: <https://g.co/gemini/share/9681daaf22f2>

List of Competency Questions

1. What are the channel properties of a specific zeolite formulation?
2. Given a chemical species/counterion, find matching zeolitic frameworks and list their channel properties.
3. Given a chemical species/counterion, find zeolitic frameworks and formulations and filter based on element X, then list characteristic X-ray Diffraction (XRD) signals.
4. Find zeolite materials containing elements X and Y (e.g. Al and P) and list their properties.
5. Given a chemical species/counterion, what is the zeolitic frameworks exhibiting the highest accessible surface area?
6. Plot zeolite frameworks as a function of their occupiable volume and framework density.
7. Show me a crystal structure of a framework that can be described based on natural t-kdq tiling.
8. Show a crystal structure that includes “6-2” secondary building units.
9. Identify a crystal structure that features double zigzag chain structuring.
10. Display the crystallographic structure of a framework containing '6T' secondary building units (SBUs).
11. How many distinct T-atom positions are there in the -LTA structure, and what is their site multiplicity?
12. Which zeolite framework likely shows 2θ peaks at 18, 27, and 29 degrees?
13. Which frameworks contain $4 \times 4 \times 4$ loop configurations, and what are the expected X-ray Diffraction (XRD) peaks for these structures?

SI.3 Structured Queries and Responses

ZeoliteName	GuestIUPACName	GuestFormula	MolecularWeight	BoilingPoint_value	BoilingPoint_unit
FeAPO-LAU	1<I>H</I>-imidazole	C3H4N2	68.08	530.15	K
Laumontite	oxidane	H2O	18.015	373.124	K
Laumontite	deuterated water	H2O	20.028	374.57	K
Laumontite	potassium(1+)	K+	39.0983	1962.15	K
Laumontite	calcium(2+)	Ca+2	40.08		
Laumontite	sodium(1+)	Na+	22.989769		
Leonhardite	oxidane	H2O	18.015	373.124	K
Leonhardite	potassium(1+)	K+	39.0983	1962.15	K
Leonhardite	calcium(2+)	Ca+2	40.08		
Leonhardite	sodium(1+)	Na+	22.989769		
MnAPO-LAU	1<I>H</I>-imidazole	C3H4N2	68.08	530.15	K
Primary leonhardite	oxidane	H2O	18.015	373.124	K
Primary leonhardite	potassium(1+)	K+	39.0983	1962.15	K
Primary leonhardite	iron(3+)	Fe+3	55.84	1535.0	
Primary leonhardite	calcium(2+)	Ca+2	40.08		
Primary leonhardite	sodium(1+)	Na+	22.989769		
Synthetic laumontite	oxidane	H2O	18.015	373.124	K
Synthetic laumontite	calcium(2+)	Ca+2	40.08		
[Co-Ga-P-O]-LAU	oxidane	H2O	18.015	373.124	K
[Co-Ga-P-O]-LAU	1<I>H</I>-imidazole	C3H4N2	68.08	530.15	K
[Co-Ga-P-O]-LAU	ammonium	H4N+	18.039		
[Fe-Ga-P-O]-LAU	1<I>H</I>-imidazole	C3H4N2	68.08	530.15	K
[Mn-Ga-P-O]-LAU	1<I>H</I>-imidazole	C3H4N2	68.08	530.15	K
[Zn-Ga-P-O]-LAU	1,4-diazabicyclo[2.2.2]octane	C6H12N2	112.17	447.15	K

Figure S6: Molecular weights and boiling points of guest species for materials with framework LAU obtained as results of the federated query

Example queries

QUERY 1: Extract crystal lattice parameters with uncertainties (when available)

```
PREFIX zeo: <http://www.theworldavatar.com/kg/ontozeolite/>
PREFIX ocr: <http://www.theworldavatar.com/kg/ontocrystal/>
PREFIX om: <http://www.ontology-of-units-of-measure.org/resource/om-2/>

SELECT ?zeoname ?a ?d_a ?b ?d_b ?c ?d_c ?alpha ?d_alpha ?beta ?d_beta ?gamma ?d_gamma ?volume ?d_vol ?lattice ?symmNum
↔ ?unit_length ?unit_angle

WHERE {
  ?zeo zeo:hasFrameworkCode ?zeoname .
  ?zeo ocr:hasCrystalInformation/ocr:hasUnitCell ?unitcell .

  ?unitcell ocr:hasUnitCellLengths/ocr:hasVectorComponent ?abc_a, ?abc_b, ?abc_c .
  ?abc om:hasUnit/rdfs:label ?unit_length .
  ?abc_a ocr:hasComponentLabel "a"; ocr:hasComponentValue ?a .
  ?abc_b ocr:hasComponentLabel "b"; ocr:hasComponentValue ?b .
  ?abc_c ocr:hasComponentLabel "c"; ocr:hasComponentValue ?c .
  ?unitcell ocr:hasUnitCellAngles/ocr:hasVectorComponent ?abg_a, ?abg_b, ?abg_g .
  ?abg om:hasUnit/rdfs:label ?unit_angle .
  ?abg_a ocr:hasComponentLabel "alpha"; ocr:hasComponentValue ?alpha .
  ?abg_b ocr:hasComponentLabel "beta"; ocr:hasComponentValue ?beta .
  ?abg_g ocr:hasComponentLabel "gamma"; ocr:hasComponentValue ?gamma .

  OPTIONAL { ?unitcell ocr:hasUnitCellVolume/om:hasNumericalValue ?volume . }
  OPTIONAL { ?abc_a ocr:hasComponentUncertainty ?d_a . }
  OPTIONAL { ?abc_b ocr:hasComponentUncertainty ?d_b . }
  OPTIONAL { ?abc_c ocr:hasComponentUncertainty ?d_c . }
  OPTIONAL { ?abg_a ocr:hasComponentUncertainty ?d_alpha . }
  OPTIONAL { ?abg_b ocr:hasComponentUncertainty ?d_beta . }
  OPTIONAL { ?abg_g ocr:hasComponentUncertainty ?d_gamma . }
  OPTIONAL { ?Volume ocr:hasUncertaintyValue ?d_vol . }
  OPTIONAL { ?unitcell ocr:hasLatticeSystem ?lattice . }
  OPTIONAL { ?unitcell ocr:hasSymmetryNumber ?symmNum . }
}
```

QUERY 2: Extract the coordinate transformation matrix and shift

```
# Fractional to cartesian transformation:
PREFIX zeo: <http://www.theworldavatar.com/kg/ontozeolite/>
PREFIX ocr: <http://www.theworldavatar.com/kg/ontocrystal/>
PREFIX om: <http://www.ontology-of-units-of-measure.org/resource/om-2/>

SELECT ?zeo ?mc_xx ?mc_xy ?mc_xz ?mc_yx ?mc_yy ?mc_yz ?mc_zx ?mc_zy ?mc_zz ?vc_x ?vc_y ?vc_z ?mc_unit ?vc_unit
WHERE {
  ?zeo zeo:hasFrameworkCode ?zeo .
  ?zeo ocr:hasCrystalInformation/ocr:hasCoordinateTransformation ?trans .
  ?trans ocr:hasTransformationMatrixToCartesian ?mCart ;
         ocr:hasTransformationVectorToCartesian ?vCart .

  ?mCart ocr:hasMatrixComponent ?mc_11, ?mc_12, ?mc_13, ?mc_21, ?mc_22, ?mc_23, ?mc_31, ?mc_32, ?mc_33 ;
  ↪ om:hasUnit/rdfs:label ?mc_unit .
  ?mc_11 ocr:hasComponentValue ?mc_xx ; ocr:hasComponentLabel "xx" .
  ?mc_12 ocr:hasComponentValue ?mc_xy ; ocr:hasComponentLabel "xy" .
  ?mc_13 ocr:hasComponentValue ?mc_xz ; ocr:hasComponentLabel "xz" .
  ?mc_21 ocr:hasComponentValue ?mc_yx ; ocr:hasComponentLabel "yx" .
  ?mc_22 ocr:hasComponentValue ?mc_yy ; ocr:hasComponentLabel "yy" .
  ?mc_23 ocr:hasComponentValue ?mc_yz ; ocr:hasComponentLabel "yz" .
  ?mc_31 ocr:hasComponentValue ?mc_zx ; ocr:hasComponentLabel "zx" .
  ?mc_32 ocr:hasComponentValue ?mc_zy ; ocr:hasComponentLabel "zy" .
  ?mc_33 ocr:hasComponentValue ?mc_zz ; ocr:hasComponentLabel "zz" .
  ?vCart ocr:hasVectorComponent ?vc_1, ?vc_2, ?vc_3 ; om:hasUnit/rdfs:label ?mc_unit .
  ?vc_1 ocr:hasComponentValue ?vc_x ; ocr:hasComponentLabel "x" .
  ?vc_2 ocr:hasComponentValue ?vc_y ; ocr:hasComponentLabel "y" .
  ?vc_3 ocr:hasComponentValue ?vc_z ; ocr:hasComponentLabel "z" .
}

# Cartesian to fractional transformation:
PREFIX zeo: <http://www.theworldavatar.com/kg/ontozeolite/>
PREFIX ocr: <http://www.theworldavatar.com/kg/ontocrystal/>
PREFIX om: <http://www.ontology-of-units-of-measure.org/resource/om-2/>

SELECT ?zeo ?mf_xx ?mf_xy ?mf_xz ?mf_yx ?mf_yy ?mf_yz ?mf_zx ?mf_zy ?mf_zz ?vf_x ?vf_y ?vf_z ?mf_unit ?vf_unit
WHERE {
  ?zeo zeo:hasFrameworkCode ?zeo .
  ?zeo ocr:hasCrystalInformation/ocr:hasCoordinateTransformation ?trans .
  ?trans ocr:hasTransformationMatrixToCartesian ?mFrac ;
         ocr:hasTransformationVectorToCartesian ?vFrac .

  ?mFrac ocr:hasMatrixComponent ?mf_11, ?mf_12, ?mf_13, ?mf_21, ?mf_22, ?mf_23, ?mf_31, ?mf_32, ?mf_33 ;
  ?mf_11 ocr:hasComponentValue ?mf_xx ; ocr:hasComponentLabel "xx" .
  ?mf_12 ocr:hasComponentValue ?mf_xy ; ocr:hasComponentLabel "xy" .
  ?mf_13 ocr:hasComponentValue ?mf_xz ; ocr:hasComponentLabel "xz" .
  ?mf_21 ocr:hasComponentValue ?mf_yx ; ocr:hasComponentLabel "yx" .
  ?mf_22 ocr:hasComponentValue ?mf_yy ; ocr:hasComponentLabel "yy" .
  ?mf_23 ocr:hasComponentValue ?mf_yz ; ocr:hasComponentLabel "yz" .
  ?mf_31 ocr:hasComponentValue ?mf_zx ; ocr:hasComponentLabel "zx" .
  ?mf_32 ocr:hasComponentValue ?mf_zy ; ocr:hasComponentLabel "zy" .
  ?mf_33 ocr:hasComponentValue ?mf_zz ; ocr:hasComponentLabel "zz" .
  ?vFrac ocr:hasVectorComponent ?vf_1, ?vf_2, ?vf_3 ; om:hasUnit/rdfs:label ?mf_unit .
  ?vf_1 ocr:hasComponentValue ?vf_x ; ocr:hasComponentLabel "x" .
  ?vf_2 ocr:hasComponentValue ?vf_y ; ocr:hasComponentLabel "y" .
  ?vf_3 ocr:hasComponentValue ?vf_z ; ocr:hasComponentLabel "z" .
}
```

QUERY 3: Extract the atomic coordinates (fractional or Cartesian)

```
PREFIX zeo: <http://www.theworldavatar.com/kg/ontozeolite/>
PREFIX ocr: <http://www.theworldavatar.com/kg/ontocrystal/>
PREFIX om: <http://www.ontology-of-units-of-measure.org/resource/om-2/>

SELECT ?zeoname ?afx ?afy ?afz ?acx ?acy ?acz ?af_unit ?ac_unit ?aoccup ?alabel

WHERE {
  ?zeo zeo:hasFrameworkCode ?zeoname .
  ?zeo ocr:hasCrystalInformation/ocr:hasAtomicStructure/ocr:hasAtomSite ?atom .
  ?atom ocr:hasFractionalPosition ?aF_xyz ; ocr:hasCartesianPosition ?aC_xyz .

  ?aF_xyz ocr:hasVectorComponent ?aF_x, ?aF_y, ?aF_z ; om:hasUnit/rdfs:label ?af_unit .
  ?aF_x ocr:hasComponentValue ?afx ; ocr:hasComponentLabel "x" .
  ?aF_y ocr:hasComponentValue ?afy ; ocr:hasComponentLabel "y" .
  ?aF_z ocr:hasComponentValue ?afz ; ocr:hasComponentLabel "z" .

  ?aC_xyz ocr:hasVectorComponent ?aC_x, ?aC_y, ?aC_z ; om:hasUnit/rdfs:label ?ac_unit .
  ?aC_x ocr:hasComponentValue ?acx ; ocr:hasComponentLabel "x" .
  ?aC_y ocr:hasComponentValue ?acy ; ocr:hasComponentLabel "y" .
  ?aC_z ocr:hasComponentValue ?acz ; ocr:hasComponentLabel "z" .

  OPTIONAL { ?atom ocr:hasAtomSiteLabel ?alabel . }
  OPTIONAL { ?atom ocr:hasOccupancy ?aoccup . }
}
```

QUERY 4: Extract tile information

```
PREFIX zeo: <http://www.theworldavatar.com/kg/ontozeolite/>
PREFIX ocr: <http://www.theworldavatar.com/kg/ontocrystal/>

SELECT ?zeoname ?nOfTiles ?nOfEdges ?faceNumber ?tileCode ?nFace ?nEdge ?nVert ?tP ?tQ ?tR ?tS ?signature

WHERE {
  ?zeo zeo:hasFrameworkCode ?zeoname .
  ?zeo ocr:hasCrystalInformation/ocr:hasTiledStructure ?structure .

  ?structure ocr:hasTileNumber ?tileNumber ; ocr:hasTileSignature ?signature ; ocr:hasTransitivity ?trans .

  ?tileNumber ocr:hasValue ?nOfTiles .
  ?tileNumber ocr:isNumberOfTiles ?tile .
  ?tile ocr:hasTileFaceNumber ?tfn .
  ?tile ocr:hasTileCode ?tileCode .
  ?tile ocr:hasNumberOfFaces ?nFace .
  ?tile ocr:hasNumberOfEdges ?nEdge .
  ?tile ocr:hasNumberOfVertices ?nVert .

  ?tfn ocr:isNumberOfTileFaces/ocr:hasNumberOfEdges ?nOfEdges .
  ?tfn ocr:hasValue ?faceNumber .

  ?trans ocr:hasVectorComponent ?transP, ?transQ, ?transR, ?transS .
  ?transP ocr:hasComponentLabel "p" ; ocr:hasComponentValue ?tP .
  ?transQ ocr:hasComponentLabel "q" ; ocr:hasComponentValue ?tQ .
  ?transR ocr:hasComponentLabel "r" ; ocr:hasComponentValue ?tR .
  ?transS ocr:hasComponentLabel "s" ; ocr:hasComponentValue ?tS .
}
```


QUERY 5: Extract peaks info of an XRD spectrum

```
PREFIX zeo: <http://www.theworldavatar.com/kg/ontozeolite/>
PREFIX ocr: <http://www.theworldavatar.com/kg/ontocrystal/>
PREFIX om: <http://www.ontology-of-units-of-measure.org/resource/om-2/>

SELECT ?zeoname ?2theta ?i ?h ?k ?l ?simulated

WHERE {
  ?zeo zeo:hasFrameworkCode ?zeoname .
  ?zeo ocr:hasCrystalInformation/ocr:hasXRDspectrum/ocr:hasCharacteristicPeak ?peak .
  ?peak ocr:hasTwoThetaPosition ?2theta ; ocr:hasRelativeIntensity ?i .

  ?peak ocr:hasMillerIndices/ocr:hasVectorComponent ?hkl_h, ?hkl_k, ?hkl_l ;
    ocr:isSimulated ?simulated .

  ?hkl_h ocr:hasComponentLabel "h" ; ocr:hasComponentValue ?h .
  ?hkl_k ocr:hasComponentLabel "k" ; ocr:hasComponentValue ?k .
  ?hkl_l ocr:hasComponentLabel "l" ; ocr:hasComponentValue ?l .
}
```

SI.4 Description Logic

TBox for OntoZeolite

The OntoZeolite ontology defines 26 classes, 26 Object Properties, and 28 Data Properties:

AccessibleAreaPerCell \sqsubseteq Measure
AccessibleAreaPerGram \sqsubseteq Measure
AccessibleVolume \sqsubseteq Measure
AccessibleVolumePerCell \sqsubseteq Measure
CompositeBU \sqsubseteq MeasureVector
CoordinationSequence \sqsubseteq MeasureVector
FrameworkDensity \sqsubseteq Measure
OccupiableAreaPerCell \sqsubseteq Measure
OccupiableAreaPerGram \sqsubseteq Measure
OccupiableVolume \sqsubseteq Measure
OccupiableVolumePerCell \sqsubseteq Measure
Precursor \sqsubseteq Species
RingSizes \sqsubseteq MeasureVector
SecondaryBU \sqsubseteq MeasureVector
SpecificAccessibleArea \sqsubseteq Measure
SpecificOccupiableArea \sqsubseteq Measure
SphereDiameter \sqsubseteq MeasureVector
TAtom \sqsubseteq Measure
VertexSymbol \sqsubseteq MeasureVector
 \exists hasAccessibleAreaPerCell. \top \sqsubseteq FrameAccessibleArea
 \exists hasAccessibleAreaPerCell. \top \sqsubseteq FrameworkTopology
 \top \sqsubseteq \forall hasAccessibleAreaPerCell.AccessibleAreaPerCell
 \exists hasAccessibleAreaPerGram. \top \sqsubseteq FrameworkTopology
 \top \sqsubseteq \forall hasAccessibleAreaPerGram.AccessibleAreaPerGram
 \exists hasAccessibleVolume. \top \sqsubseteq FrameworkTopology
 \top \sqsubseteq \forall hasAccessibleVolume.AccessibleVolume
 \exists hasAccessibleVolumePerCell. \top \sqsubseteq FrameworkTopology
 \top \sqsubseteq \forall hasAccessibleVolumePerCell.AccessibleVolumePerCell
 \exists hasChemicalComposition. \top \sqsubseteq ZeoliticMaterial
 \top \sqsubseteq \forall hasChemicalComposition.ChemicalComponent
 \exists hasCitation. \top \sqsubseteq Recipe
 \top \sqsubseteq \forall hasCitation.Document
 \exists hasCompositeBU. \top \sqsubseteq FrameworkTopology
 \top \sqsubseteq \forall hasCompositeBU.CompositeBU
 \exists hasCoordinationSequence. \top \sqsubseteq TAtom
 \top \sqsubseteq \forall hasCoordinationSequence.CoordinationSequence
 \exists hasDensity. \top \sqsubseteq ZeoliticMaterial
 \top \sqsubseteq \forall hasDensity.Density
 \exists hasFrameworkDensity. \top \sqsubseteq FrameworkTopology
 \top \sqsubseteq \forall hasFrameworkDensity.FrameworkDensity
 \exists hasFrameworkTopology. \top \sqsubseteq ZeoliticMaterial
 \top \sqsubseteq \forall hasFrameworkTopology.FrameworkTopology
 \exists hasOccupiableAreaPerCell. \top \sqsubseteq FrameworkTopology
 \top \sqsubseteq \forall hasOccupiableAreaPerCell.OccupiableAreaPerCell
 \exists hasOccupiableAreaPerGram. \top \sqsubseteq FrameworkTopology
 \top \sqsubseteq \forall hasOccupiableAreaPerGram.OccupiableAreaPerGram
 \exists hasOccupiableVolume. \top \sqsubseteq FrameworkTopology
 \top \sqsubseteq \forall hasOccupiableVolume.OccupiableVolume
 \exists hasOccupiableVolumePerCell. \top \sqsubseteq FrameworkTopology
 \top \sqsubseteq \forall hasOccupiableVolumePerCell.OccupiableVolumePerCell

\exists hasPrecursor. $\top \sqsubseteq$ Recipe
 $\top \sqsubseteq \forall$ hasPrecursor.Precursor
 \exists hasRecipe. $\top \sqsubseteq$ ZeoliticMaterial
 $\top \sqsubseteq \forall$ hasRecipe.Recipe
 \exists hasRingSizes. $\top \sqsubseteq$ FrameworkTopology
 $\top \sqsubseteq \forall$ hasRingSizes.RingSizes
 \exists hasSecondaryBU. $\top \sqsubseteq$ FrameworkTopology
 $\top \sqsubseteq \forall$ hasSecondaryBU.SecondaryBU
 \exists hasSpecificAccessibleArea. $\top \sqsubseteq$ FrameworkTopology
 $\top \sqsubseteq \forall$ hasSpecificAccessibleArea.SpecificAccessibleArea
 \exists hasSpecificOccupiableArea. $\top \sqsubseteq$ FrameworkTopology
 $\top \sqsubseteq \forall$ hasSpecificOccupiableArea.SpecificOccupiableArea
 \exists hasSphereDiameter. $\top \sqsubseteq$ FrameworkTopology
 $\top \sqsubseteq \forall$ hasSphereDiameter.SphereDiameter
 \exists hasTAtom. $\top \sqsubseteq$ FrameworkTopology
 $\top \sqsubseteq \forall$ hasTAtom.TAtom
 \exists hasTopologicalDensity. $\top \sqsubseteq$ FrameworkTopology
 $\top \sqsubseteq \forall$ hasTopologicalDensity.TopologicalDensity
 \exists hasVertexSymbol. $\top \sqsubseteq$ TAtom
 $\top \sqsubseteq \forall$ hasVertexSymbol.VertexSymbol
 \exists hasZeoliticMaterial. $\top \sqsubseteq$ ZeoliteFramework
 $\top \sqsubseteq \forall$ hasZeoliticMaterial.ZeoliticMaterial $\top \sqsubseteq \forall$ hasAmount.Datatype string
 $\top \sqsubseteq \forall$ hasBatchComposition.Datatype string
 $\top \sqsubseteq \forall$ hasBatchPreparation.Datatype string
 $\top \sqsubseteq \forall$ hasCage.Datatype string
 $\top \sqsubseteq \forall$ hasChannelDimension.Datatype string
 $\top \sqsubseteq \forall$ hasCharacterization.Datatype string
 $\top \sqsubseteq \forall$ hasComposition.Datatype string
 $\top \sqsubseteq \forall$ hasCrystallization.Datatype string
 $\top \sqsubseteq \forall$ hasDOI.Datatype string
 $\top \sqsubseteq \forall$ hasFrameworkCode.Datatype string
 $\top \sqsubseteq \forall$ hasNotes.Datatype string
 $\top \sqsubseteq \forall$ hasProductRecovery.Datatype string
 $\top \sqsubseteq \forall$ hasRCSRLink.Datatype string
 $\top \sqsubseteq \forall$ hasRingCount.Datatype integer
 $\top \sqsubseteq \forall$ hasRingSize.Datatype integer

TBox for OntoCrystal

The OntoCrystal ontology defines 18 classes, 43 Object Properties, and 25 Data properties:

AbscissaData \sqsubseteq MeasureVector
AtomCartesianPosition \sqsubseteq MeasureVector
AtomFractionalPosition \sqsubseteq MeasureVector
AtomSite $\sqsubseteq \forall$ hasCartesianPosition.PositionVector
AtomSite $\sqsubseteq \forall$ hasElement.OntoSpecies:Species
AtomSite $\sqsubseteq \forall$ hasFractionalPosition.PositionVector
AtomicStructure $\sqsubseteq \forall$ hasAtomSite.AtomSite
CoordinateTransformation $\sqsubseteq \forall$ hasTransformationMatrixToCartesian.TransformationMatrix
CoordinateTransformation $\sqsubseteq \forall$ hasTransformationMatrixToFractional.TransformationMatrix
CoordinateTransformation $\sqsubseteq \forall$ hasTransformationVectorToCartesian.TransformationVector
CoordinateTransformation $\sqsubseteq \forall$ hasTransformationVectorToFractional.TransformationVector
CrystalInformation $\sqsubseteq \forall$ hasAtomicStructure.AtomicStructure
CrystalInformation $\sqsubseteq \forall$ hasCoordinateTransformation.CoordinateTransformation
CrystalInformation $\sqsubseteq \forall$ hasUnitCell.UnitCell
MatrixComponent $\sqsubseteq \forall$ hasUnit.om:Unit
MatrixWithUncertainty \sqsubseteq MeasureMatrix
MeasureMatrix $\sqsubseteq \forall$ hasMatrixComponent.MatrixComponent
MeasureMatrix $\sqsubseteq \forall$ hasUnit.om:Unit
MeasureVector $\sqsubseteq \forall$ hasUnit.om:Unit
MeasureVector $\sqsubseteq \forall$ hasVectorComponent.VectorComponent
MeasureWithUncertainty \sqsubseteq om:Measure
MeasureWithUncertainty $\sqsubseteq \forall$ hasUnit.om:Unit
MillerIndices \sqsubseteq MeasureVector
OrdinateData \sqsubseteq MeasureVector
PositionVector \sqsubseteq MeasureVector
TransformationMatrix \sqsubseteq MatrixWithUncertainty
TransformationVector \sqsubseteq VectorWithUncertainty
Transitivity \sqsubseteq MeasureVector
UnitCell $\sqsubseteq \forall$ hasReciprocalUnitCellAngles.UnitCellAngles
UnitCell $\sqsubseteq \forall$ hasReciprocalUnitCellLengths.UnitCellLengths
UnitCell $\sqsubseteq \forall$ hasReciprocalUnitCellVectorSet.UnitCellVectorSet
UnitCell $\sqsubseteq \forall$ hasUnitCellAngles.UnitCellAngles
UnitCell $\sqsubseteq \forall$ hasUnitCellLengths.UnitCellLengths
UnitCell $\sqsubseteq \forall$ hasUnitCellVectorSet.UnitCellVectorSet
UnitCell $\sqsubseteq \forall$ hasUnitCellVolume.UnitCellVolume
UnitCellAngles \sqsubseteq MeasureVector
UnitCellLatticeVector \sqsubseteq MeasureVector
UnitCellLengths \sqsubseteq MeasureVector
UnitCellVectorSet $\sqsubseteq \forall$ hasUnitCellVector.UnitCellLatticeVector
UnitCellVolume \sqsubseteq MeasureWithUncertainty
VectorComponent $\sqsubseteq \forall$ hasUnit.om:Unit
VectorWithUncertainty \sqsubseteq MeasureVector
 \exists hasAbscissaData. \top \sqsubseteq PlotXY
 \exists hasAtomSite. \top \sqsubseteq AtomicStructure
 \exists hasAtomicStructure. \top \sqsubseteq CrystalInformation
 \exists hasAuthor. \top \sqsubseteq Citation
 \exists hasAuthorIndex. \top \sqsubseteq Citation
 \exists hasCartesianPosition. \top \sqsubseteq AtomSite
 \exists hasCharacteristicPeak. \top \sqsubseteq XRDSpectrum
 \exists hasCoordinateTransformation. \top \sqsubseteq CrystalInformation
 \exists hasElement. \top \sqsubseteq AtomSite

\exists hasFractionalPosition. $\top \sqsubseteq$ AtomSite
 \exists hasMatrixComponent. $\top \sqsubseteq$ MeasureMatrix
 \exists hasMillerIndices. $\top \sqsubseteq$ CharacteristicPeak
 \exists hasOrdinateData. $\top \sqsubseteq$ PlotXY
 \exists hasPlotData. $\top \sqsubseteq$ XRDSpectrum
 \exists hasPosition. $\top \sqsubseteq$ TileVertex
 \exists hasReciprocalUnitCellAngles. $\top \sqsubseteq$ UnitCell
 \exists hasReciprocalUnitCellLengths. $\top \sqsubseteq$ UnitCell
 \exists hasReciprocalUnitCellVectorSet. $\top \sqsubseteq$ UnitCell
 \exists hasTile. $\top \sqsubseteq$ TiledStructure
 \exists hasTileFace. $\top \sqsubseteq$ Tile
 \exists hasTileFaceNumber. $\top \sqsubseteq$ Tile
 \exists hasTileNumber. $\top \sqsubseteq$ TiledStructure
 \exists hasTileVertex. $\top \sqsubseteq$ Tile
 \exists hasTiledStructure. $\top \sqsubseteq$ CrystalInformation
 \exists hasTransformationMatrixToCartesian. $\top \sqsubseteq$ CoordinateTransformation
 \exists hasTransformationMatrixToFractional. $\top \sqsubseteq$ CoordinateTransformation
 \exists hasTransformationVectorToCartesian. $\top \sqsubseteq$ CoordinateTransformation
 \exists hasTransformationVectorToFractional. $\top \sqsubseteq$ CoordinateTransformation
 \exists hasTransitivity. $\top \sqsubseteq$ TiledStructure
 \exists hasUnit. $\top \sqsubseteq$ (MatrixComponent \sqcup MeasureMatrix \sqcup MeasureVector \sqcup MeasureWithUncertainty \sqcup VectorComponent)
 \exists hasUnitCell. $\top \sqsubseteq$ CrystalInformation
 \exists hasUnitCellAngles. $\top \sqsubseteq$ UnitCell
 \exists hasUnitCellLengths. $\top \sqsubseteq$ UnitCell
 \exists hasUnitCellVector. $\top \sqsubseteq$ UnitCellVectorSet
 \exists hasUnitCellVectorSet. $\top \sqsubseteq$ UnitCell
 \exists hasUnitCellVolume. $\top \sqsubseteq$ UnitCell
 \exists hasVectorComponent. $\top \sqsubseteq$ MeasureVector
 \exists hasXRDSpectrum. $\top \sqsubseteq$ CrystalInformation
 \exists isAbscissaOf. $\top \sqsubseteq$ OrdinateData
 \exists isAuthorIndexOf. $\top \sqsubseteq$ AuthorIndex
 \exists isNumberOfTileFaces. $\top \sqsubseteq$ TileFaceNumber
 \exists isNumberOfTiles. $\top \sqsubseteq$ TileNumber
 $\top \sqsubseteq \forall$ hasAbscissaData. AbscissaData
 $\top \sqsubseteq \forall$ hasAtomSite. AtomSite
 $\top \sqsubseteq \forall$ hasAtomicStructure. AtomicStructure
 $\top \sqsubseteq \forall$ hasAuthor. Author
 $\top \sqsubseteq \forall$ hasAuthorIndex. AuthorIndex
 $\top \sqsubseteq \forall$ hasCartesianPosition. PositionVector
 $\top \sqsubseteq \forall$ hasCharacteristicPeak. CharacteristicPeak
 $\top \sqsubseteq \forall$ hasCoordinateTransformation. CoordinateTransformation
 $\top \sqsubseteq \forall$ hasCrystalInformation. CrystalInformation
 $\top \sqsubseteq \forall$ hasElement. OntoSpecies:Species
 $\top \sqsubseteq \forall$ hasFractionalPosition. PositionVector
 $\top \sqsubseteq \forall$ hasMatrixComponent. MatrixComponent
 $\top \sqsubseteq \forall$ hasMillerIndices. MillerIndices
 $\top \sqsubseteq \forall$ hasOrdinateData. OrdinateData
 $\top \sqsubseteq \forall$ hasPlotData. PlotXY
 $\top \sqsubseteq \forall$ hasPosition. MeasureVector
 $\top \sqsubseteq \forall$ hasReciprocalUnitCellAngles. UnitCellAngles
 $\top \sqsubseteq \forall$ hasReciprocalUnitCellLengths. UnitCellLengths
 $\top \sqsubseteq \forall$ hasReciprocalUnitCellVectorSet. UnitCellVectorSet
 $\top \sqsubseteq \forall$ hasTile. Tile

$\top \sqsubseteq \forall \text{ hasTileFace. TileFace}$
 $\top \sqsubseteq \forall \text{ hasTileFaceNumber. TileFaceNumber}$
 $\top \sqsubseteq \forall \text{ hasTileNumber. TileNumber}$
 $\top \sqsubseteq \forall \text{ hasTileVertex. TileVertex}$
 $\top \sqsubseteq \forall \text{ hasTiledStructure. TiledStructure}$
 $\top \sqsubseteq \forall \text{ hasTransformationMatrixToCartesian. TransformationMatrix}$
 $\top \sqsubseteq \forall \text{ hasTransformationMatrixToFractional. TransformationMatrix}$
 $\top \sqsubseteq \forall \text{ hasTransformationVectorToCartesian. TransformationVector}$
 $\top \sqsubseteq \forall \text{ hasTransformationVectorToFractional. TransformationVector}$
 $\top \sqsubseteq \forall \text{ hasTransitivity. Transitivity}$
 $\top \sqsubseteq \forall \text{ hasUnit.om:Unit}$
 $\top \sqsubseteq \forall \text{ hasUnitCell. UnitCell}$
 $\top \sqsubseteq \forall \text{ hasUnitCellAngles. UnitCellAngles}$
 $\top \sqsubseteq \forall \text{ hasUnitCellLengths. UnitCellLengths}$
 $\top \sqsubseteq \forall \text{ hasUnitCellVector. UnitCellLatticeVector}$
 $\top \sqsubseteq \forall \text{ hasUnitCellVectorSet. UnitCellVectorSet}$
 $\top \sqsubseteq \forall \text{ hasUnitCellVolume. UnitCellVolume}$
 $\top \sqsubseteq \forall \text{ hasVectorComponent. VectorComponent}$
 $\top \sqsubseteq \forall \text{ hasXRDSpectrum. XRDSpectrum}$
 $\top \sqsubseteq \forall \text{ isAbscissaOf. AbscissaData}$
 $\top \sqsubseteq \forall \text{ isAuthorIndexOf. Author}$
 $\top \sqsubseteq \forall \text{ isNumberOfTileFaces. TileFace}$
 $\top \sqsubseteq \forall \text{ isNumberOfTiles. Tile}$
 $\exists \text{ http://purl.org/ontology/bibo/doi. } \top \sqsubseteq \text{ Citation}$
 $\exists \text{ hasAtomSiteLabel. } \top \sqsubseteq \text{ AtomSite}$
 $\exists \text{ hasColumnIndex. } \top \sqsubseteq \text{ MatrixComponent}$
 $\exists \text{ hasComponentIndex. } \top \sqsubseteq \text{ VectorComponent}$
 $\exists \text{ hasComponentLabel. } \top \sqsubseteq (\text{MatrixComponent} \sqcup \text{VectorComponent})$
 $\exists \text{ hasComponentUncertainty. } \top \sqsubseteq (\text{MatrixComponent} \sqcup \text{VectorComponent})$
 $\exists \text{ hasComponentValue. } \top \sqsubseteq (\text{MatrixComponent} \sqcup \text{VectorComponent})$
 $\exists \text{ hasFaceCode. } \top \sqsubseteq \text{ TileFace}$
 $\exists \text{ hasLatticeSystem. } \top \sqsubseteq \text{ UnitCell}$
 $\exists \text{ hasNumberOfEdges. } \top \sqsubseteq (\text{Tile} \sqcup \text{TileFace})$
 $\exists \text{ hasNumberOfFaces. } \top \sqsubseteq \text{ Tile}$
 $\exists \text{ hasNumberOfVertices. } \top \sqsubseteq \text{ Tile}$
 $\exists \text{ hasOccupancy. } \top \sqsubseteq \text{ AtomSite}$
 $\exists \text{ hasPeakWidth. } \top \sqsubseteq \text{ CharacteristicPeak}$
 $\exists \text{ hasRelativeIntensity. } \top \sqsubseteq \text{ CharacteristicPeak}$
 $\exists \text{ hasRowIndex. } \top \sqsubseteq \text{ MatrixComponent}$
 $\exists \text{ hasSpaceGroupHM. } \top \sqsubseteq \text{ UnitCell}$
 $\exists \text{ hasSpaceGroupSymbol. } \top \sqsubseteq \text{ UnitCell}$
 $\exists \text{ hasSymmetryNumber. } \top \sqsubseteq \text{ UnitCell}$
 $\exists \text{ hasTileCode. } \top \sqsubseteq \text{ Tile}$
 $\exists \text{ hasTileSignature. } \top \sqsubseteq (\text{Tile} \sqcup \text{TiledStructure})$
 $\exists \text{ hasTwoThetaPosition. } \top \sqsubseteq \text{ CharacteristicPeak}$
 $\exists \text{ hasUncertaintyValue. } \top \sqsubseteq \text{ MeasureWithUncertainty}$
 $\exists \text{ hasValue. } \top \sqsubseteq (\text{TileFaceNumber} \sqcup \text{TileNumber})$
 $\exists \text{ hasVectorLabel. } \top \sqsubseteq \text{ UnitCellLatticeVector}$
 $\exists \text{ isSimulated. } \top \sqsubseteq \text{ CharacteristicPeak}$
 $\exists \text{ rdfs:label. } \top \sqsubseteq \text{ om:Unit}$
 $\exists \text{ http://xmlns.com/foaf/0.1/family_name. } \top \sqsubseteq \text{ Author}$
 $\exists \text{ http://xmlns.com/foaf/0.1/firstName. } \top \sqsubseteq \text{ Author}$
 $\top \sqsubseteq \forall \text{ http://purl.org/ontology/bibo/doi.xsd:string}$
 $\top \sqsubseteq \forall \text{ hasAtomSiteLabel.xsd:string}$

T \sqsubseteq \forall hasColumnIndex.xsd:integer
T \sqsubseteq \forall hasComponentIndex.xsd:integer
T \sqsubseteq \forall hasComponentLabel.xsd:string
T \sqsubseteq \forall hasComponentUncertainty.rdfs:Literal
T \sqsubseteq \forall hasComponentValue.rdfs:Literal
T \sqsubseteq \forall hasFaceCode.xsd:string
T \sqsubseteq \forall hasLatticeSystem.xsd:string
T \sqsubseteq \forall hasNumberOfEdges.xsd:integer
T \sqsubseteq \forall hasNumberOfFaces.xsd:integer
T \sqsubseteq \forall hasNumberOfVertices.xsd:integer
T \sqsubseteq \forall hasOccupancy.xsd:decimal
T \sqsubseteq \forall hasPeakWidth.xsd:decimal
T \sqsubseteq \forall hasRelativeIntensity.xsd:decimal
T \sqsubseteq \forall hasRowIndex.xsd:integer
T \sqsubseteq \forall hasSpaceGroupHM.xsd:string
T \sqsubseteq \forall hasSpaceGroupSymbol.xsd:string
T \sqsubseteq \forall hasSymmetryNumber.xsd:integer
T \sqsubseteq \forall hasTileCode.xsd:string
T \sqsubseteq \forall hasTileSignature.xsd:string
T \sqsubseteq \forall hasTwoThetaPosition.xsd:decimal
T \sqsubseteq \forall hasUncertaintyValue.xsd:string
T \sqsubseteq \forall hasValue.xsd:integer
T \sqsubseteq \forall hasVectorLabel.xsd:string
T \sqsubseteq \forall isSimulated.xsd:boolean
T \sqsubseteq \forall rdfs:label.xsd:string
T \sqsubseteq \forall http://xmlns.com/foaf/0.1/family_name.xsd:string
T \sqsubseteq \forall http://xmlns.com/foaf/0.1/firstName.xsd:string

References

- [1] Herbert J. Bernstein, John C. Bollinger, I. David Brown, Saulius Gražulis, James R. Hester, Brian McMahon, Nick Spadaccini, John D. Westbrook, and Simon P. Westrip. Specification of the Crystallographic Information File format, version 2.0. *J. Appl. Crystallogr.*, 49(1):277–284, Feb 2016.
- [2] Hajo Rijgersberg. OM - ontology of units of measure, 2023. 2023.
- [3] HajoF Rijgersberg, Mark van Assem, and Jan Top. Ontology of units of measure and related concepts. *Semant. Web.*, 4:3–13, 2013.
- [4] G. Saulius, A. Daškevič, A. Merkys, D. Chateigner, L. Lutterotti, M. Quirós, N.R. Serebryanaya, P. Moeck, R.T. Downs, and A.L. Bail. Crystallography open database—an open-access collection of crystal structures. *J. Appl. Crystallogr.*, 42(4):726–729, 2009.
- [5] M.M.J. Treacy and J.B. Higgins, editors. *Collection of Simulated XRD Powder Patterns for Zeolites (Fifth Edition)*. Elsevier Science B.V., Amsterdam, fifth edition edition, 2007.