ZSE Manuscript Outline

Jerry T. Crum[a], Justin R. Crum[b], Cameron Taylor[a], William F. Schneider[a,c]

[a] Department of Chemical and Biolmolecular Engineering, University of Notre Dame, 250 Nieuwland Science Hall, Notre Dame, IN 46556, USA

[b] Department of Applied Mathematics, University of Arizona, 617 N Santa Rita Ave, Tucson, AZ 85721, USA

[c] Department of Chemistry and Biochmeistry, University of Notre Dame, 251 Nieuwland Science Hall, Notre Dame, IN 46556, USA

1 Abstract

The topology of zeolite frameworks and of associated tetrahedral sites (T-sites) are commonly characterized by their associated rings, typically defined as some set of closed paths or cycles through a framework that cannot be decomposed into shorter cycles. These ring descriptors have been used to identify feasible zeolite topologies, to describe the similarity and differences between zeolites, to identify sites or voids of catalytic relevance, and as machine learning fingerprints. Numerous definitions and algorithms for finding zeolite rings have been proposed and applied throughout the literature. Here we report an analysis of rings and T-sites in a large number of zeolite frameworks using Zeolite Simulation Environment, a Python package that implements an efficient algorithm presented by Goetzke and Klein for finding rings in arbitrary frameworks. We compare the result of a number of common and new ring definitions applied to a large number of common zeolite frameworks. We discover previously unrecognized rings in a number of frameworks. We show that the vertex symbol, a common approach used to characterize T-sites, misses important parts of the stereochemistry around a T-site, and propose an alternative definition. This tool provides an effective platform for characterizing zeolite and T-site structures useful for building models and doing machine learning.

2 Discussion With Bill:

1. Go through table again to make sure we agree
   (a) Will move vertex symbol outside of table
2. Naming the ring conventions:
   (a) Goetzke: ring, primitive ring, fundamental ring[1–3]
   (b) Sastre: Shortest path ring, something else?
   (c) Crum: Unstacked rings, something else?
3. Look at updated highlights
4. Look at intro again

3 Highlights

What is the main point of the paper? What problem is it addressing? What are the main insights?

1. Zeolite framework and nodes commonly classified in terms of rings
2. Various conventions for associating some subsets of rings with either a framework, the T-sites of a framework, or the oxygens of a framework.
3. PROBLEM TO ADDRESS: The convention used will provide different ring counts
4. SOLUTION: We provide a Python package that has the ability to identify and classify these rings based on previously published and new conventions
5. This software tool uses a node-based search procedure that takes advantage of algorithms developed for general nets
6. We compute and compare conventions across all known frameworks
7. Some features treated by convention as rings are not rings in a topological sense but are rather defined by the void space they create.

8. We enumerate all rings, defined as paths with no short-cut, up to 18 T-sites across all known Fws
    (a) Would be very cool to classify Fws according to these rings....
        i. Not sure what approach to use for that, but it is a good idea
    (b) Compare to other classifications, eg cage-window vs channel

4 Introduction

Paragraph 1: background on uses for zeolite rings

- Zeolites are microporous and crystalline, natural to characterize by the sizes of the features present in the crystal. Rings are one common type of feature widely reported and used, both to characterize a zeolite crystal and as descriptors of the individual tetrahedral sites of the zeolite.
- Rings have been used to identify feasible zeolite topologies,[4] to describe the similarity and differences between zeolites,[5] to identify sites or voids of catalytic relevance,[6,7] and as machine learning finger prints [will get citations for this]

Paragraph 2: Explain features of graph representing zeolites

- Zeolites can naturally be represented using graph theory, where atoms are nodes, and bonds are edges. REFS
    - Sometimes in the literature, oxygen atoms are used as bridges instead of nodes, since they only connect to two T-sites
- Table 1 summarizes the various topological features based on connectivity that can be used to describe a framework, T-site, or oxygen atom
- A path is a series of connected nodes from some source node to some target node
- A cycle is a path that starts and ends at the same node, and doesn't repeat any other nodes

Paragraph 3: Explain the various ring counting methodologies we intend to cover

- Rings in zeolites are defined as a cycle traversing the T-site and oxygen atoms (nodes) of the framework, and cannot be decomposed into smaller cycles by a shortcut.[2,3]
- A shortcut is defined as a path connecting two nodes of a cycle that is shorter than both the paths connecting those nodes along the cycle[2,3]
- Shortest path ring is a ring that is the shortest ring for at least one set of O-T-O on the cycle,[8] this ring will be contained in the vertex symbol for at least one of the T-sites within the framework
- See Figure 1 for example of rings
    - The pink highlighted cycle (1-2-3-17-20-14-15-16) is a 8-membered ring (8-MR)
    - The green highlighted cycle (14-20-12-13) is a 4-MR
    - The red outlined cycle following 3-4-18-19-20-17 is not an 6-MR because there is a shortcut connecting nodes 17 and 18.
    - Nodes 5-6-7-8-9 outlined in teal represent a path through the framework.

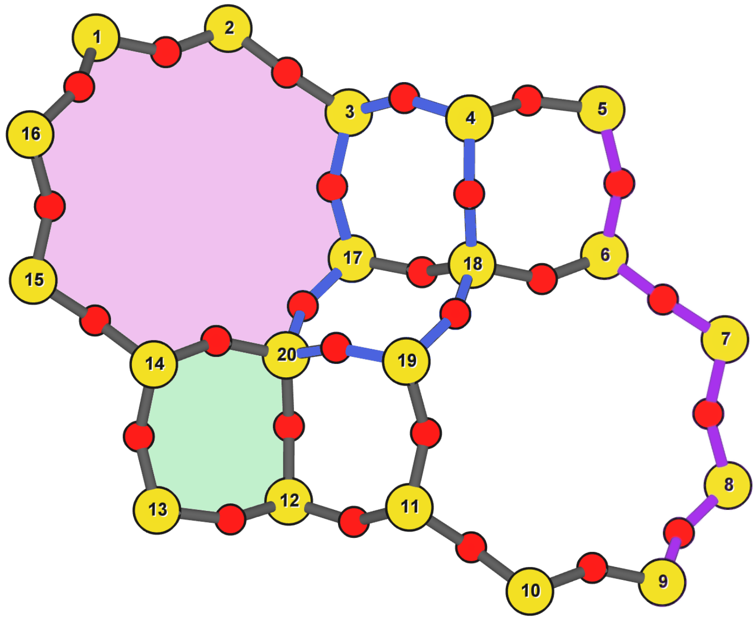

Figure 1: Cutout of the Chabazite framework showing a path (5-6-7-8-9) highlighted with purple bonds, a cycle (3-4-18-19-20-17) highlighted with blue bonds, an 8-MR filled in with pink, and a 4-MR filled in with green. Yellow atoms are Si (T-sites), and red atoms are oxygen.

Table 1: Matrix showing relationship between frameworks, nodes, paths, cycles, and various ring types. Vertex symbol doesn't belong in the first column. It isn't a topological feature.

	Description	Framework	Node (T-Sites)	Node (Oxygen)
Nodes	T-sites and oxygen atoms	Contains some set of symmetry distinct T-sites and oxygen atoms		
Paths	Collection of connected nodes from source to target	Periodic cell contains an infinite number of paths		
Cycles	Path that starts and ends at the same node	Periodic cell contains an infinite number of cycles		
Rings	Cycle that contains no shortcuts	Contains a finite number of unique rings	All rings that pass through particular T-site	All rings that pass through particular oxygen atom
Unstacked Rings	Ring that does not traverse two stacked rings	A subset of the Rings above	All unstacked rings that pass through T-site	All unstacked rings that pass through oxygen atom
Shortest Path Rings	Ring that is the shortest ring for at least one set of O-T-O on the cycle	A smaller subset of the rings above	All shortest path rings starting from a T-site (Vertex)	All shortest path rings that pass through oxygen atom
Vertex Symbol	Way to classify the rings around a T-site, shortest ring (and its multiplicity) for each O-O pair around a T-site	Collection of vertex symbols for all symmetry distinct T-sites in framework	Vertex symbol for particular T-site	
Geometric rings	A cycle that may contain a shortcut, but has similar geometric/chemical properties to a ring without a shortcut	Contains a finite number of geometric rings	Can be described by the geometric rings that pass through	Can be described by the geometric rings that pass through

Paragraph 4: Problem to address

- Different conventions exist that can reduce the set of rings to more strictly defined properties

- These methods return different sets of rings
- We can use rings to characterize oxygen atoms, T-sites, and entire frameworks
- T-sites:
  - Vertex symbols are the set of shortest paths connecting the 6 oxygen-oxygen pairs around a T-site[9]
  - Shortest path rings count all the vertex symbol rings that pass through a T-site or an oxygen atom[8]
  - Or we can count all the rings that do not have a short cut[3]
- Oxygen atoms:
  - Shortest path rings
  - All rings with out a shortcut
- Framework
  - Vertex symbol rings
  - Shortest path rings
  - All rings with out a shortcut
- Differences in ring counts leads to differences in how we describe the topology of zeolites. Therefore, when discussing the rings in a zeolite it is important to also state which method of ring counting is used.

Paragraph 5: Our solution to the problem

- Here we present Zeolite Simulation Environment (ZSE), a Python package that implements the ring finding algorithm presented by Goetzke and Klein[3] to find rings up to a user defined cutoff size, and can implement the previously published ring set reduction conventions.
- We use ZSE to provide an analysis of rings using each of these conventions on the entire set of IZA zeolite frameworks to compare how they result in different characterizations

Using ZSE we show the differences in framework, T-site, and oxygen ring descriptors when using the various ring counting conventions. We highlight rings that are found by these conventions but not typically discussed for a number of frameworks. We also show that the vertex symbol, a common approach used to characterize T-sites misses important parts of the stereochemistry around a T-site.

5 Software Description

Paragraph 1: Basics of ZSE tootls

- All of the frameworks listed on the IZA Database of zeolite structures[10] are included in a database with ZSE
- These structures are Atomic Simulation Environment Atoms objects,[11] and can be used with any of the functions in ZSE
- ZSE also includes CIF tools to read structure files for frameworks not listed in the IZA website, such as hypothetical zeolites, and return an Atoms object that can be used with ZSE

Paragraph 2: Implementation of ring counting methodologies

- ZSE has 3 previously published rules for ring finding implemented
  - All cycles without a shortcut[3]
  - All shortest path cycles[8]
  - Cycles that compose the vertex symbol for a T-site[9]
- We have also implemented a new rule that finds all rings with out a shortcut, but excludes rings that are made by traversing a stacked set of rings. Have to define stacked ring.
  - Figure showing example of 8-MR in the d6r of CHA and 14-MR in AFI
- Each of the rules: shortest path, vertex symbols, and our new rule are a subset of the no shortcuts rule

Paragraph 3: Process to find rings

Process to find rings:

1. To find rings in a zeolite, ZSE makes a custom connectivity matrix for the Si and O atoms in the framework
2. We use NetworkX[12] to build a shortest path matrix for every atom pair in the zeolite framework
3. We then find all the rings up to some cutoff size base on the algorithm presented by Goetzke and Klein[3]
4. Depending on the rule chosen by the user, ZSE then removes rings from this list that don't meet the qualifications of the rule
5. ZSE returns a list of the rings found, a list of the atom indicies that compose each ring, Atoms objects for each ring that can be further analyzed or visualized by the user

6 Results

Paragraph 1: Differences in frameworks

- Ring counts frequency plots
  - Plot showing how many frameworks on the IZA contain each size ring found using the various ring counting methods
  - This highlights the differences in the ring rules, and shows that results will vary depending on rule.

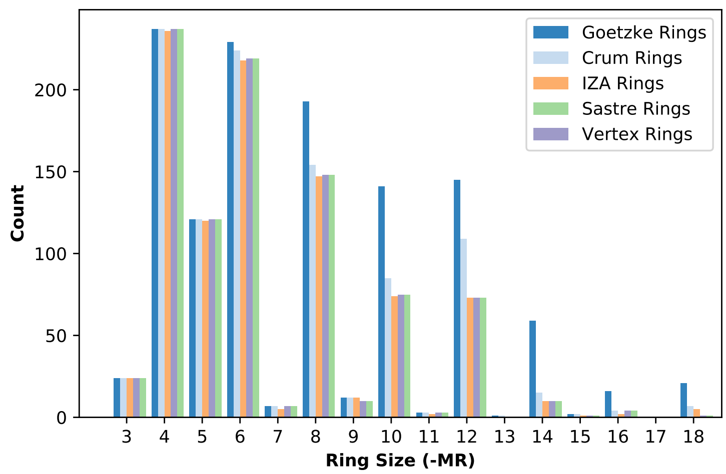

Figure 2: Number of IZA frameworks containing each size ring, using the various ring counting rules. [This will be updated with the Sastre method, vertex method, and the rings listed on the IZA website. Currently the IZA does not show any ring data for the SVY framework, providing one less framework to count.

Paragraph 2: Differences in T-sites

- Number of unique T-sites
  - There are 1460 T-sites through all the frameworks listed on the IZA website.
  - We can characterize those T-sites by the rings that pass through them
  - Sastre did this, and called the list of rings, the ring index
  - If we do this using different rules for ring finding how do the results change?
    - See Figure 3
  - Most common T-site ring index using Goetzke method is: $5_6 \bullet 10_4$ showing up 23 times through the IZA frameworks.
  - Most common T-site ring index using Crum method is: $4_3 \bullet 8_4$ showing up 31 times through the IZA frameworks.
    - Next most common T-site with Crum method is $5_6 \bullet 10_4$ showing up 25 times
  - This raises the question, if you want to use machine learning to correlate T-site rings to chemical properties, which ring method should you use?

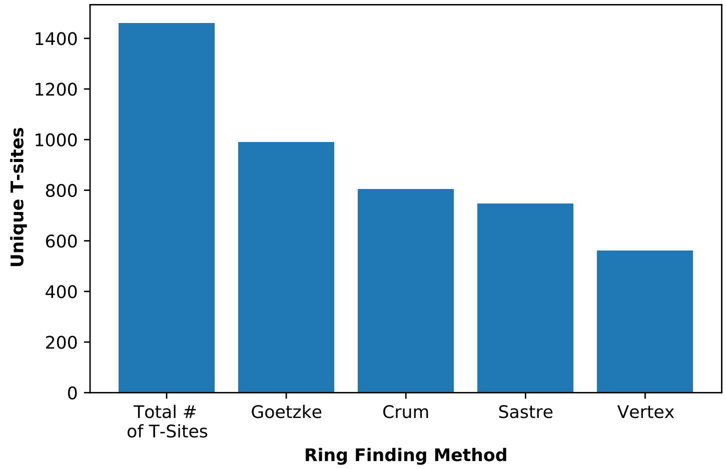

Figure 3: Number of unique T-sites when classified by the rings passing through them using varrious ring finding rules.

Note that in Figure 4 a bar for IZA rings is not present. This is because the IZA does not list rings that pass through specific T-sites.

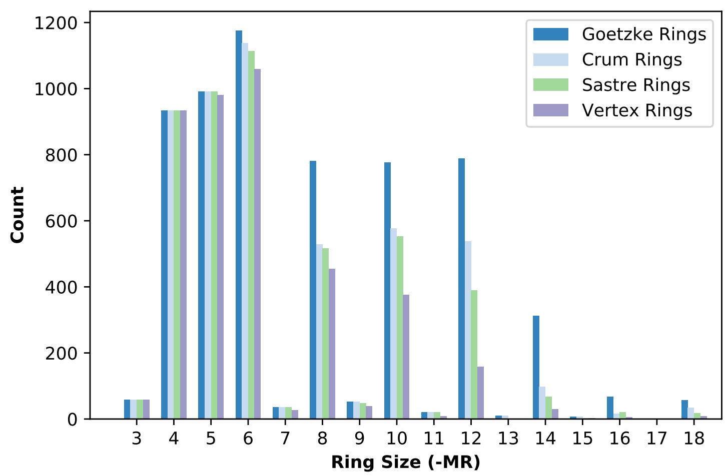

Figure 4: Frequency of T-sites across all IZA frameworks containing ring sizes between 3- and 18-MR.

- Include a heat map based on Cameron's results showing the coefficient of similarity that he defined

Paragraph 3: Differences in O-sites

- Number of unique oxygen sites
  - We can repeat this method for the oxygen atoms in all the frameworks
  - Counting the symmetry distinct oxygen atoms in each framework on the IZA database leads to a total count of 3219
  - We can classify those oxygen atoms based on the rings that pass through them, using the various ring counting rules
  - Figure 5 shows counts based on ring finding rules
  - The percentage of unique oxygen sites is much lower than the percentage of unique T-sites for every ring finding method

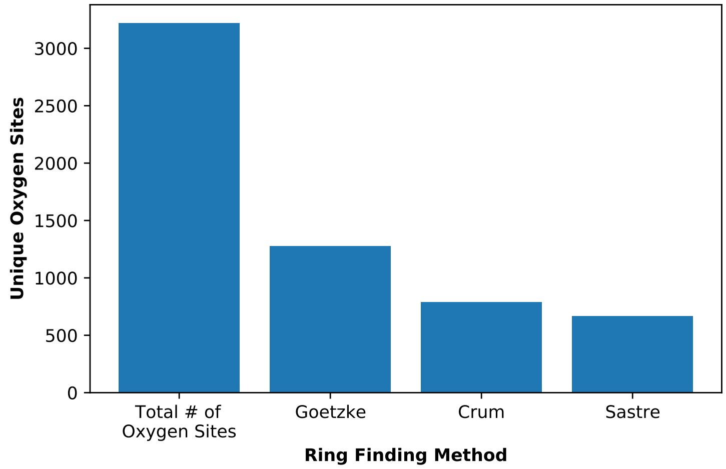

Figure 5: Number of unique oxygen sites when classified by the rings passing through them using varrious ring finding rules. Vertex method not included, since that is a way to classify T-sites only.

Note that in Figure 6 a bar for Vertex rings is not present. This is because the Vertex symbol only defines rings that pass through a specific T-site.

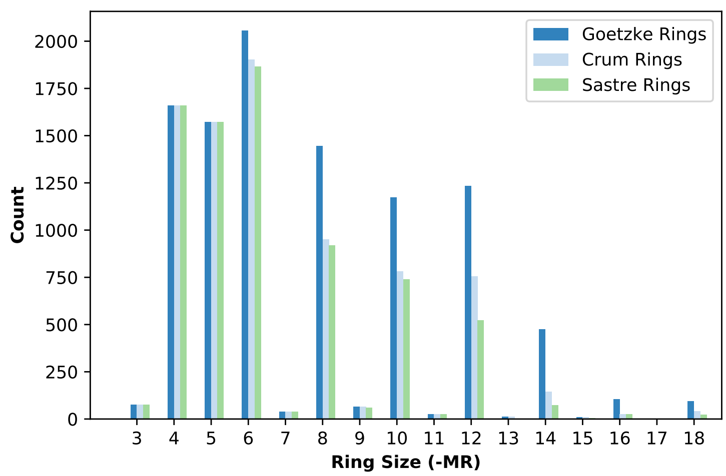

Figure 6: Frequency of O-sites across all IZA frameworks containing ring sizes between 3- and 18-MR.

Paragraph 4: Comparison to previously published results by Sastre

- Reproduce the results from Sastre paper, show ring counts with the other rules, Table 2
  - Ring index was presented by Sastre and Corma as a way to list the rings that pass through a node in a zeolite[8]
  - List rings from smallest to largest, and any multiplicities are shown by a subscript
  - This is a convenient way to characterize the atoms of a zeolite by the rings they are associated with
  - Results in the Sastre column were found using ZSE but agree directly with the results shown by Sastre and Corma[8]
  - This provides an in depth look at some of the frameworks and the differences in rings found by each rule.

- Leads into the next section discussing the specific rings of CHA and pentasil that do or don't get counted by each rule.

Table 2: Comparison of Ring Indices for the T-sites in Various Uninodal Zeolite Frameworks

Framework	Goetzke	Crum	Sastre[8]
ABW	$4_2 \bullet 6_3 \bullet 8_4$	$4_2 \bullet 6_3 \bullet 8_4$	$4_2 \bullet 6_3 \bullet 8_4$
ACO	$4_3 \bullet 6_3 \bullet 8_6 \bullet 10_{15}$	$4_3 \bullet 8_6$	$4_3 \bullet 8_6$
AFI	$4_1 \bullet 6_{13} \bullet 12_1 \bullet 14_7$	$4_1 \bullet 6_{13} \bullet 12_1$	$4_1 \bullet 6_{13}$
ANA	$4_2 \bullet 6_2 \bullet 8_{16}$	$4_2 \bullet 6_2 \bullet 8_{16}$	$4_2 \bullet 6_2 \bullet 8_{16}$
ATO	$4_1 \bullet 6_9 \bullet 8_8 \bullet 12_{20}$	$4_1 \bullet 6_9 \bullet 12_{20}$	$4_1 \bullet 6_9$
BCT	$4_1 \bullet 6_6 \bullet 8_{20}$	$4_1 \bullet 6_6 \bullet 8_{12}$	$4_1 \bullet 6_6$
CHA	$4_3 \bullet 6_1 \bullet 8_6 \bullet 12_1$	$4_3 \bullet 6_1 \bullet 8_2 \bullet 12_1$	$4_3 \bullet 6_1 \bullet 8_2$
DFT	$4_2 \bullet 6_6 \bullet 8_{10} \bullet 10_{10}$	$4_2 \bullet 6_6 \bullet 8_{10}$	$4_2 \bullet 6_6 \bullet 8_{10}$
GIS	$4_3 \bullet 8_4$	$4_3 \bullet 8_4$	$4_3 \bullet 8_4$
GME	$4_3 \bullet 6_1 \bullet 8_6 \bullet 12_7$	$4_3 \bullet 6_1 \bullet 8_2 \bullet 12_1$	$4_3 \bullet 6_1 \bullet 8_2$
MER	$4_3 \bullet 8_4 \bullet 10_{10} \bullet 14_{14}$	$4_3 \bullet 8_4$	$4_3 \bullet 8_4$
MON	$4_1 \bullet 5_5 \bullet 8_6$	$4_1 \bullet 5_5 \bullet 8_6$	$4_1 \bullet 5_5 \bullet 8_6$
NPO	$3_1 \bullet 6_6 \bullet 12_{40}$	$3_1 \bullet 6_6 \bullet 12_{40}$	$3_1 \bullet 6_6$

Paragraph 5: Rings that are found using Goetzke method, but not discussed in most literature

- These ring finding rules often find rings that are not commonly discussed in literature, and are not listed by the IZA
- These are classified as untabulated rings by Curtis and Deem[5]
- However it is possible that these rings are relevant for describing chemical, catalytic, or topological properties of zeolites
- Here we show an example of untabulated rings in the Chabazite framework
- Show the cage belts results for CHA, AFT, etc... and discuss how those rings don't show up in previous literature, Figure 7
  - Looking at results for CHA in Table 2 we see the Goetzke method finds $4_3 \bullet 6_1 \bullet 8_6 \bullet 12_1$
  - This is different from the results in the Sastre paper,[8] in that they only show 2 8-MRs and no 12-MRs
  - The extra 8-MRs result from cycles traversing nodes in both 6-MRs of the d6r
    * Crum rule removes these 8-MRs while still finding the 12-MR
    * Sastre rule does not find the 8-MRs in the d6r or the 12-MR
  - The 12-MR is a cycle that circumferences the CHA cage

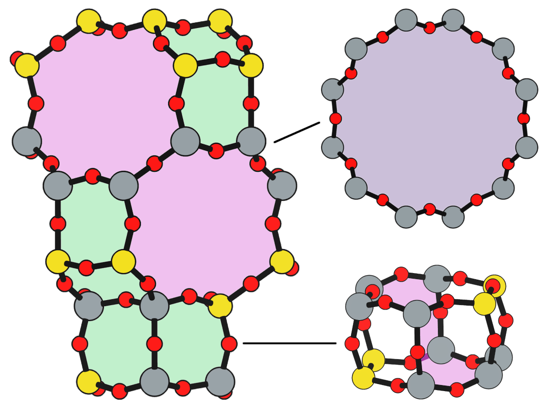

Figure 7: Chabazite cage and d6r with highlighted rings: 4-MR in green, 8-MR in pink, and 12-MR in purple. The 8-MR in the d6r and the 12-MR are rings not typically discussed in literature, Si atoms have been replaced with Al atoms to help identify those rings in the overall cage structure..

Paragraph 6: Geometric rings

- On the other end of the spectrum, there are cycles that would not be classified as a rings by the connectivity rules previously outlined that display properties similar to rings
- These shortcut containing cycles can display chemical and/or geometric properties consistent with rings, and are of interest to catalysis researchers even though they are not considered rings by connectivity rules
- One example is the 6-membered cycle referred to as the α-6-MR in literature (Figure 8) and is present in a number of frameworks including but not limited to MOR, FER, MFI, and BEA,[13,14] which is a potential location for Co^{2+} uptake when two Al atoms are 3rd nearest neighbor in the cycle. Similar to Co^{2+} uptake in 3NN Al atoms in 6-MRs in other frameworks such as CHA and AEI.
- This 6-membered cycle would not be considered a ring by any of the connectivity rules outlined here due to the shortcut splitting the cycle into two 5-MRs

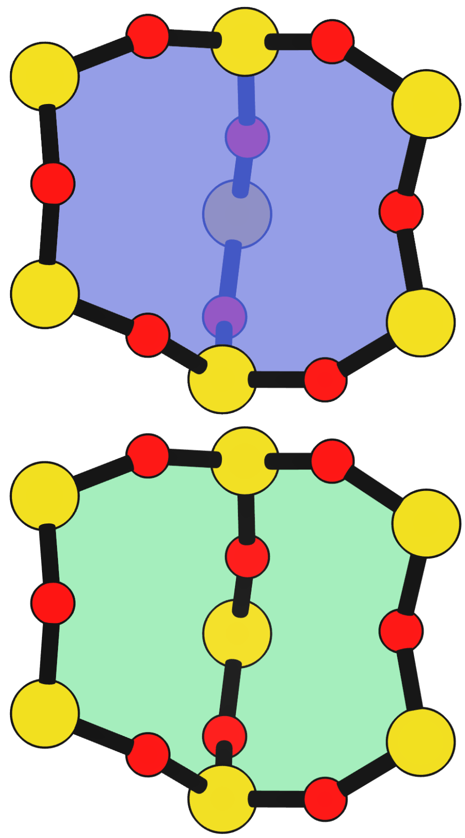

Figure 8: Cutout of MFI framework showing the structure referred to as an α-6-MR in blue, and the two 5-MRs that compose it in green. The 6-membered cycle would not be found as a ring by any of the connectivity ring rules (Goetzke, Crum, Sastre, or vertex symbol).

Paragraph 7: Stereochemistry concerns when using Ring Index

- The ring index for a T-site or O-site only list the size and counts of rings, but does not include any useful information about the orientation of those rings in space
- Because of this, multiple T-sites could have the same ring index, but with very different stereochemisty of those rings
- Stereochemistry could influence the chemical properties we care about, such as deprotonation energy, T-site substitution energy, or catalytic properties
- This would indicate that a ring index is not a complete descriptor, and there is room to define a new descriptor that takes into consideration ring orientation.
- **Here we insert a figure of two T-sites with the same ring index, but very different orientations**

Not sure if this is relevant to include or not, but it provides some context for us too discuss

- Here we show the most common ring indices for T-sites in the IZA database using each of the ring finding rules
- Table 3 shows the five most common ring indices for T-sites using the Goetzke rule

Table 3: Most Common Ring Indices Using the Goetzke Rule

Ring Index	Count	Frameworks Containing Index
$5_6 \bullet 10_4$	23	IMF(2), MEL(1), MFI(2), PRO(1), SVR(2), TUN(2), SFV(13)
$4_1 \bullet 5_3 \bullet 6_2 \bullet 10_3 \bullet 12_4$	14	MEL(1), SFV(13)
$4_1 \bullet 5_3 \bullet 6_2 \bullet 8_5 \bullet 10_1$	14	MEL(1), SFV(13)
$5_5 \bullet 6_3 \bullet 10_1 \bullet 12_1$	14	MEL(1), SFV(13)
$5_4 \bullet 6_3 \bullet 8_2 \bullet 10_3$	14	MEL(1), SFV(13)

- Table 4 shows the five most common ring indices for T-sites using the Crum rule

Table 4: Five Most Common Ring Indices Using the Crum Rule

Ring Index	Count	Frameworks Containing Index
$4_3 \bullet 8_4$	31	APC(1), GIS(1), MER(1), MWF(13), PAU(6), PHI(2), PWN(2), SIV(4)
$5_6 \bullet 10_4$	25	IMF(3), MEL(1), MFI(2), RRO(1), SVR(2), TUN(3), SFV(13)
$4_2 \bullet 6_4$	17	FAR(1), FRA(6), GIU(1), LIO(1), LOS(2), LTN(2), MAR(1), SOD(1), TOL(2)
$5_5 \bullet 6_3 \bullet 10_1$	17	IMF(1), MEL(1), MFI(1), TUN(1), SFV(13)
$4_3 \bullet 6_1 \bullet 8_2 \bullet 12_1$	16	AFS(1), AFT(3), AFV(1), AFX(2), AVL(2), BPH(1), CHA(1), GME(1), SBE(1), SFW(3)

- Table 5 shows the five most common ring indices for T-sites using the Sastre rule
- Table 6 shows the five most common ring indices for T-sites using vertex symbols

Table 5: Five Most Common Ring Indices Using the Sastre Rule

Ring Index	Count	Frameworks Containing Index
$4_2 \bullet 6_4$	39	AFG(3), CAN(1), FAR(4), FRA(6), GIU(5), LIO(4), LOS(2), LTN(2) MAR(4), SOD(1), TOL(7)
$5_6 \bullet 10_4$	33	IMF(3), MEL(2), MFI(2), RRO(1), SVR(2), TUN(2), SFV(21)
$4_3 \bullet 8_4$	30	GIS(1), MER(1), MWF(14), PAU(6), PHI(2), PWN(2), SIV(4)
$4_3 \bullet 6_1 \bullet 8_2$	28	AEI(3), AFT(3), AFV(1), AFX(2), AVL(2), CHA(1), GME(1), KFI(1), LTF(1), MWF(2), PAU(2), PWN(1), RHO(1), SAV(3), SFW(3), TSC(1)
$4_3 \bullet 6_2 \bullet 8_1$	24	AFV(1), AVE(2), AVL(1), CLO(2), EAB(1), ERI(1), IFY(1), IRN(1), LEV(1), LTA(1), LTN(1), MOZ(1), OFF(1), SAT(1), SWY(2), TSC(1), UFI(1), PTT(1), SYT(3)

Table 6: Five Most Common Ring Indices Using Vertex Symbolscite:bernauer-proton-2016

Vertex Symbol	Count	Frameworks Containing Index
$4 \bullet 4 \bullet 6 \bullet 6 \bullet 6 \bullet 6$	40	AFG(3), CAN(1), FAR(4), FRA(6), GIU(5), LIO(4), LOS(2), LTN(2), MAR(4), RON(1), SOD(1), TOL(7)
$4 \bullet 4 \bullet 4 \bullet 6 \bullet 8 \bullet 8$	32	AEI(3), AFT(3), AFV(1), AFX(2), ATT(1), AVL(2), CHA(1), ETV(1), GME(1), KFI(1), LTF(1), MRT(2), MWF(2), PAU(2), PWN(1), RHO(1), SAV(3), SFW(3), TSC(1)
$4 \bullet 4 \bullet 4 \bullet 6 \bullet 6 \bullet 8$	30	AFV(1), AVE(2), AVL(1), CGS(1), CLO(2), EAB(1), ERI(1), ETR(1), IFY(1), IRN(1), JSW(1), LEV(1), LTA(1), LTL(1), LTN(1), MOZ(3), OFF(1), PTT(1), SAT(1), SWY(2), SYT(3), TSC(1), UFI(1)
$4 \bullet 4 \bullet 4 \bullet 8 \bullet 8 \bullet 8_2$	30	GIS(1), MER(1), MWF(14), PAU(6), PHI(2), PWN(2), SIV(4)
$5 \bullet 5 \bullet 5 \bullet 5 \bullet 5 \bullet 6$	26	DDR(1), DOH(2), IHW(1), IMF(1), MEL(1), MEP(1), MFI(1), MTN(1), SFS(1), SFV(15), TUN(1)

7 Conclusions

- Rings of graph are well defined; here identify all rings up to XXX in YYY frameworks. Find that commonly reported (IZA) ring sizes miss certain rings.
- The method used to find rings in a zeolite will provide different ring counts unclear
- When discussing rings in a zeolite it is import to disclose by which method those rings were found
- Using ZSE we can find rings based on various methods
- This provides a foundation for using ring fingerprints in machine learning models to correlate chemical properties and topology

References

[1] Marians, C. S. and Hobbs, L. W. Network properties of crystalline polymorphs of silica. *Journal of Non-Crystalline Solids*, 124(2-3):242–253, October 1990. ISSN 00223093. doi: 10.1016/0022-3093(90)90269-R. URL https://linkinghub.elsevier.com/retrieve/pii/002230939090269R.

[2] Guttman, L. Ring structure of the crystalline and amorphous forms of silicon dioxide. *Journal of Non-Crystalline Solids*, 116(2-3):145–147, February 1990. ISSN 00223093. doi: 10.1016/0022-3093(90)90686-G. URL https://linkinghub.elsevier.com/retrieve/pii/002230939090686G.

[3] Goetzke, K. and Klein, H.-J. Properties and efficient algorithmic determination of different classes of rings in finite and infinite polyhedral networks. *Journal of Non-Crystalline Solids*, 127(2):215–220, February 1991. ISSN 00223093. doi: 10.1016/0022-3093(91)90145-V. URL https://linkinghub.elsevier.com/retrieve/pii/002230939190145V.

[4] Li, X. and Deem, M. W. Why Zeolites Have So Few Seven-Membered Rings. *The Journal of Physical Chemistry C*, 118(29):15835–15839, July 2014. ISSN 1932-7447, 1932-7455. doi: 10.1021/jp504143r. URL https://pubs.acs.org/doi/10.1021/jp504143r.

[5] Curtis, R. A. and Deem, M. W. A Statistical Mechanics Study of Ring Size, Ring Shape, and the Relation to Pores Found in Zeolites. *Journal of Physical Chemistry B*, 107:8612–8620, 2003.

[6] Li, S., Li, H., Gounder, R., Debellis, A., Müller, I. B., Prasad, S., Moini, A., and Schneider, W. F. First-Principles Comparison of Proton and Divalent Copper Cation Exchange Energy Landscapes in SSZ-13 Zeolite. *The Journal of Physical Chemistry C*, 122(41):23564–23573, October 2018. ISSN 1932-7447, 1932-7455. doi: 10.1021/acs.jpcc.8b07213. URL https://pubs.acs.org/doi/10.1021/acs.jpcc.8b07213.

[7] Kester, P. M., Crum, J. T., Li, S., Schneider, W. F., and Gounder, R. Effects of Brønsted acid site proximity in chabazite zeolites on OH infrared spectra and protolytic propane cracking kinetics. *Journal of Catalysis*, 395:210–226, March 2021. ISSN 00219517. doi: 10.1016/j.jcat.2020.12.038. URL https://linkinghub.elsevier.com/retrieve/pii/S0021951721000191.

[8] Sastre, G. and Corma, A. Topological Descriptor for Oxygens in Zeolites. Analysis of Ring Counting in Tetracoordinated Nets. *The Journal of Physical Chemistry C*, 113(16):6398–6405, April 2009. ISSN 1932-7447, 1932-7455. doi: 10.1021/jp8100128. URL https://pubs.acs.org/doi/10.1021/jp8100128.

[9] O'Keeffe, M. and Hyde, S. Vertex symbols for zeolite nets. *Zeolites*, 19(5-6):370–374, November 1997. ISSN 01442449. doi: 10.1016/S0144-2449(97)00133-4. URL https://linkinghub.elsevier.com/retrieve/pii/S0144244997001334.

[10] Baerlocher, C. and McCusker, L. Database of Zeolite Structures. URL http://www.iza-structure.org/databases/.

[11] Larsen, A. H., Castelli, I. E., Christensen, R., Du, M., Groves, M. N., Jennings, P. C., Jensen, P. B., Kermode, J., Kitchin, J. R., Kolsbjerg, E. L., Kubal, J., Kaasbjerg, K., Lysgaard, S., Maxson, T., Olsen, T., Pastewka, L., Peterson, A., Rostgaard, C., Schi, J., Thygesen, K. S., Vegge, T., Vilhelmsen, L., Walter, M., Zeng, Z., and Jacobsen, K. W. The atomic simulation environment—a Python library for working with atoms. *J. Phys.*, page 31, 2017.

[12] Hagberg, A. A., Schult, D. A., and Swart, P. J. Exploring network structure, dynamics, and function using NetworkX. In *Proceedings of the 7th Python in Science Conference*, pages 11–15, Pasadena, CA USA, August 2008.

[13] Dědeček, J., Sobalík, Z., and Wichterlová, B. Siting and Distribution of Framework Aluminium Atoms in Silicon-Rich Zeolites and Impact on Catalysis. *Catalysis Reviews*, 54(2):135–223, April 2012. ISSN 0161-4940, 1520-5703. doi: 10.1080/01614940.2012.632662. URL http://www.tandfonline.com/doi/abs/10.1080/01614940.2012.632662.

[14] Bernauer, M., Tabor, E., Pashkova, V., Kaucký, D., Sobalík, Z., Wichterlová, B., and Dedecek, J. Proton proximity – New key parameter controlling adsorption, desorption and activity in propene oligomerization over H-ZSM-5 zeolites. *Journal of Catalysis*, 344:157–172, December 2016. ISSN 00219517. doi: 10.1016/j.jcat.2016.09.025. URL https://linkinghub.elsevier.com/retrieve/pii/S002195171630197X.

8 Acknowledgments

- Funding
  - CISTAR
  - Schmitt Fellowship
- Discussions
  - Christian Baerlocher
- Software:
  - German Sastre: zeoTsites
- Compute Resources
  - CRC