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Chemical Zeolites	Unit-distan	ice Rea	alizations of Comb	inatorial Zeolites
Combinatorial				
Realization		E	Brigitte Servatius — WPI	
2d Zeolites				
Finite Zeolites				
The Layer				
Holes in Zeolites	14			
Motions	ITA TO			
A geometric	T_T			
Open Problems		6	MINISTRSTVO ZA IZOBRAZEVANJE, ZNANOST IN ŠPORT	INALOZDA O VASO PHINOANOSE OPERACIJO DELNO FINANCIRA EVROPSKA UNIJA Evropski socialni skad
Home Page	UNIVERSIT			
Title Page	OWIVER			
 ↔ 				
Page 1 of 41				
Go Back				
Full Screen				
Close				
Quit				



- Chemical Zeolites
- Realization
- 2d Zeolites
- Finite Zeolites
- The Layer...
- Holes in Zeolites
- Motions
- A geometric . . .
- Open Problems

Home	Page
Title	Page
44	••
•	• •
Page 2	2 of 41



Close

Quit

1. Chemical Zeolites

- crystalline solid
- units: Si + 4O





 \bullet two covalent bonds per oxygen



Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites The Layer... Holes in Zeolites Motions

A geometric... Open Problems

Home Page
Title Page

• •

Page <mark>3</mark> of <mark>41</mark>

Go Back

Full Screen

Close

Quit



- naturally occurring
- synthesized
- theoretical

Used as microfilters.



Chemical Zeolites
Combinatorial
Realization
2d Zeolites
Finite Zeolites
The Layer
Holes in Zeolites

44

A geometric . . .

- -	Open	Problems
------------	------	----------

Home Page	
Title Page	

••

2. Combinatorial Zeolites

Combinatorial d-Dimensional Zeolite

- \bullet A connected complex of corner sharing d-dimensional simplices
- At each corner there are exactly two distinct simplices
- Two corner sharing simplices intersect in exactly one vertex.

There is a one-to-one correspondence between combinatorial

d-dimensional zeolites and d-regular body-pin graphs.

body-pin graph

Vertices: simplices (silicon)

Edges: bonds (oxygen)

Page 4 of 41 Go Back

Full Screen

Close



Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites The Layer... Holes in Zeolites Motions A geometric... Open Problems











Close

Quit

Graph of a Combinatorial Zeolite

is obtained by replacing each d-dimensional simplex with K_{d+1} .

The graph of the zeolite is the line graph of the Body-Pin graph.

Whitney

(1932) proved that connected graphs X on at least 5 vertices are strongly reconstructible from their line graphs L(X). Moreover, $Aut(X) \cong Aut(L(X))$.



Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites The Layer... Holes in Zeolites Motions A geometric...

Open Problems

Home Page
Title Page

Page <mark>6</mark> of <mark>41</mark>

Go Back Full Screen

Close

Quit

3. Realization

A realization of a *d*-dimensional zeolite

An placement (embedding) of vertices of the the *d*-dimensional complex in \mathbb{R}^d . Equivalently a placement (embedding) of the vertices of the line graph of the body-pin graph.

unit-distance realization

A realization where all edges join vertices distance 1 apart in \mathbb{R}^d .

non-interpenetrating realization

A realization where simplices are disjoint except at joined vertices.



Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites The Layer... Holes in Zeolites Motions

A geometric . . .

Open Problems



Full Screen

Close

Quit

The typical situation: Not unit distance realizable.





Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites The Layer... Holes in Zeolites Motions A geometric... Open Problems





Full Screen

Close

Quit

2d Zeolites

4.

Smallest 2d zeolite is the line graph of K_4 : The graph of the octahedron with four (edge disjoint) faces. For body-pin graphs on more than 4 vertices, the zeolite can be

recovered uniquely from the line-graph.





Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites Finite Zeolites The Layer... Holes in Zeolites Motions A geometric... Open Problems

Home Page

Title Page

Page 9 of 41

Go Back

Full Screen

Close

Quit

44

••

It is just as easy to construct infinite symmetric examples:





Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites Finite Zeolites The Layer... Holes in Zeolites Motions A geometric... Open Problems

Home Page

Title Page

Page 10 of 41

Go Back

Full Screen

Close

Quit

••

••

▶

Showing a different symmetry

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XXXXX



- Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites The Layer... Holes in Zeolites Motions
- A geometric . . .
- Open Problems

Home Page
Title Page
•• ••
•
Page 11 of 41
Go Back
Full Screen

Close





●First ●Prev ●Next ●Last ●Go Back ●Full Screen ●Close ●Quit



Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites The Layer... Holes in Zeolites Motions A geometric... Open Problems



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	Ca	Pack	

Full Screen

Close

Quit

5. Finite Zeolites

Body pin graph: $K_{3,3}$. Since the body pin graph is not planar, the resulting zeolite cannot be planar. Its underlying graph is generically globally rigid. However, it has a unit distance realization in the plane which is a mechanism.





Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites Finite Zeolites The Layer... Holes in Zeolites Motions A geometric... Open Problems

Home Page

Title Page

Page 13 of 41

Go Back

Full Screen

Close

••

••

Harborth's Example





Chemical Zeolites

Combinatorial . . .

Realization

2d Zeolites

Finite Zeolites

The Layer...

Holes in Zeolites

Motions

A geometric . . .

Open Problems

Home Page

Title Page



Page 14 of 41

Go Back

Full Screen

Close

Quit



●First ●Prev ●Next ●Last ●Go Back ●Full Screen ●Close ●Qu



Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites

The Layer...

Holes in Zeolites

Motions

A geometric . . .

Open Problems

Home Page

Title Page



Page 15 of 41



Close







Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites The Layer...

Holes in Zeolites Motions

A geometric . . .

Open Problems



Page **17** of **41**



Close

Quit

6. The Layer Construction

Z=(T,C) is a combinatorial zeolite realizable in dimension d. $\mathbb{R}^d\subseteq \mathbb{R}^{d+1}$

Label each $t \in T$ arbitrarily with ± 1 .

For +1, erect a d + 1 dimensional simplex in the upper half space,

For -1, erect a d + 1 dimensional simplex in the lower half space,

Call the Complex Z_a and its mirror image Z_b .



Alternately staking Z_a and Z_b gives a *layered Zeolite* in \mathbb{R}^{d+1} .

●First ●Prev ●Next ●Last ●Go Back ●Full Screen ●Close ●Quit



Chemical Zeolites Combinatorial... Realization

2d Zeolites Finite Zeolites

T mile Zeome.

The Layer...

Holes in Zeolites

Motions

A geometric . . .

Open Problems



Page **18** of **41**

Go Back

Full Screen

Close

Quit

Labels all +1 A two layered zeolite.





Chemical Zeolites
Combinatorial
Realization
2d Zeolites
Finite Zeolites
The Layer
Holes in Zeolites
Motions
A geometric
Open Problems
Home Page
Title Page





Go Back	
Full Screen	

Close

Quit

The general case starting from a finite zeolite.



Theorem: There are uncountably many isomorphism classes of unit distance realizable zeolites in \mathbb{R}^3 . (actually in any dimension d > 1.)



Chemical Zeolites
Combinatorial
Realization
2d Zeolites
Finite Zeolites
The Layer
Holes in Zeolites
Motions
A geometric
Open Problems
Home Page
Title Page
44 >>



Go Back

Full Screen

Close





Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites Finite Zeolites Holes in Zeolites Motions A geometric...

Open Problems





Full Screen

Close







•• ••









Close

Quit

Proof:



●First ●Prev ●Next ●Last ●Go Back ●Full Screen ●Close ●Quit



- Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites Finite Zeolites The Layer... Holes in Zeolites Motions A geometric...
- Open Problems



Full Screen

Close

Quit

7. Holes in Zeolites





Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites The Layer... Holes in Zeolites Motions A geometric...

Open Problems

Home Page
Title Page

Title Vage

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Full Screen

Close

Quit



Degree of Freedom

Each simplex $d\mbox{-dimensional}$ simplex has d(d+1)/2 degrees of freedom

Each contact of the d + 1 contacts removes d degrees.

By a naïve count, a zeolite is rigid - (overbraced by d(d+1)/2.)





Chemical Zeolites

- Combinatorial . . .
- Realization
- 2d Zeolites
- Finite Zeolites
- The Layer . . .
- Holes in Zeolites
- Motions
- A geometric . . .
- **Open Problems**



Title Page



Page 25 of 41

Go Back

Full Screen

Close



Generically globally rigid in the plane.





- Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites
- The Layer...
- Holes in Zeolites
- Motions
- A geometric . . .
- **Open Problems**



Go Back

Full Screen

Close

Quit

Generically globally rigid in the plane.

A 4-regular vertex transitive graph is globally rigid unless it has a 3-factor consisting of s disjoint copies of K_4 with $s \ge 3$. [Jackson, S, S - 2004]





Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites The Layer... Holes in Zeolites Motions

A geometric . . .

Open Problems

Home Page		
Title Page		
44	••	
•		
Page 27 of 41		

Go Back	
Full Screen	

Close





Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites The Layer... Holes in Zeolites Motions

A geometric . . .

Open Problems

Home	Page
Title	Page
44	••
•	>
Page <mark>2</mark>	8 of 41

Go Back	
Full Screen	

Close





Quit

Chemical Zeolites Combinatorial . . . Realization 2d Zeolites Finite Zeolites The Layer... Holes in Zeolites Motions A geometric . . . **Open Problems** Home Page Title Page •• 44 Page **29** of **41** Go Back Full Screen Close

Are there finite generically flexible 2D Zeolites? Yes, line graphs of 3-regular graphs with edge connectivity less than 3.





Chemical Zeolites Combinatorial... Realization 2d Zeolites

Finite Zeolites

The Layer...

Holes in Zeolites

Motions

A geometric . . .

Open Problems



Full Screen

Close

Quit

Are there finite generically rigid but not globally rigid 2D Zeolites?

Yes, line graphs of 3-regular graphs with edge connectivity less than 3.





Chemical Zeolites Combinatorial... Realization 2d Zeolites

Finite Zeolites

The Layer . . .

Holes in Zeolites

Motions

A geometric . . .

Open Problems



Go Back

Full Screen

Close

Quit

Are there finite generically rigid but not globally rigid 2D Zeolites?

Yes, line graphs of 3-regular graphs with edge connectivity less than 3.





Chemical Zeolites	9
Combinatorial	Ŭ
Realization	
2d Zeolites	
Finite Zeolites	
The Layer	
Holes in Zeolites	
Motions	
A geometric	
Open Problems	
Home Page	
I itle Page	
•• ••	
• •	
Page 32 of 41	
Go Back	
Full Screen	
Close	
Quit	

A geometric approach



●First ●Prev ●Next ●Last ●Go Back ●Full Screen ●Close ●Quit



Chemical Zeolites Combinatorial . . . Realization 2d Zeolites Finite Zeolites The Layer . . . Holes in Zeolites Motions A geometric . . . **Open Problems** Home Page Title Page •• 44 Page 33 of 41 Go Back Full Screen Close

Quit

Combinatorial version of the gain graph





Chemical Zeolites	
Combinatorial	
Realization	G
2d Zeolites	
Finite Zeolites	
The Layer	
Holes in Zeolites	
Motions	
A geometric	
Open Problems	
Home Page	
I Itle Page	
44	
• •	
Page 34 of 41	
Go Back	
Full Screen	
Close	
Quit	

Geometric version of the gain graph



●First ●Prev ●Next ●Last ●Go Back ●Full Screen ●Close ●Qui



Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites The Layer... Holes in Zeolites Motions A geometric...

Open Problems



Close

Quit

It's a geometric line graph!







Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites The Layer... Holes in Zeolites Motions A geometric... Open Problems

Home Page	
Title Page	
44 >>	
▲ ▶	
Page <mark>36</mark> of 41	
Go Back	

Full Screen

Close

Quit

10. Open Problems

- 1. Does there exist a finite 2D zeolite with a planar unit distance realization and having no non-simplex triangle?
- 2. Find f(n) so that, given a Unit Distance realization of an *n*-dimensional zeolite, its line graph has a unit distance realization in dimension f(n)

[If f(n) = 2n - 1, then the line graph corresponds to an 2n - 1 dimensional zeolite.]

- 3. In particular, find f(2).
- 4. Do there exist finite non-interpenetrating zeolites with unit distance plane realization which is non-rigid?



Chemical Zeolites Combinatorial... Realization 2d Zeolites Finite Zeolites The Layer... Holes in Zeolites Motions A geometric... Open Problems

Home	e Page
Title	Page
44	••
•	►

Page **37** of **41**

Go	Back	

Full Screen

Close

Quit



Harborth's Construction



Chemical Zeolites

Combinatorial . . .

Realization

2d Zeolites

Finite Zeolites

The Layer...

Holes in Zeolites

Motions

A geometric . . .

Open Problems

Home Page

Title Page



Page <mark>38</mark> of <mark>41</mark>



Full Screen

Close





- Chemical Zeolites
- Combinatorial . . .
- Realization
- 2d Zeolites
- Finite Zeolites
- The Layer...
- Holes in Zeolites
- Motions
- A geometric . . .
- Open Problems
 - Home Page
 - Title Page





Page <mark>39</mark> of <mark>41</mark>

Go Back

Full Screen

Close





- Chemical Zeolites Combinatorial... Realization
- 2d Zeolites
- Finite Zeolites
- The Layer...
- Holes in Zeolites
- Motions
- A geometric . . .
- Open Problems
 - Home Page
 - Title Page
- 44
 >>

 4
 >>
- Page 40 of 41
- Go Back
- Full Screen
 - Close
 - Quit





Chemical Zeolites

Combinatorial . . .

Realization

2d Zeolites

Finite Zeolites

The Layer...

Holes in Zeolites

Motions

A geometric . . .

Open Problems

Home Page

Title Page



Page **41** of **41**

Go Back

Full Screen

Close

Quit



●First ●Prev ●Next ●Last ●Go Back ●Full Screen ●Close ●Quit