



Properties and Applications of Zeolites

Content

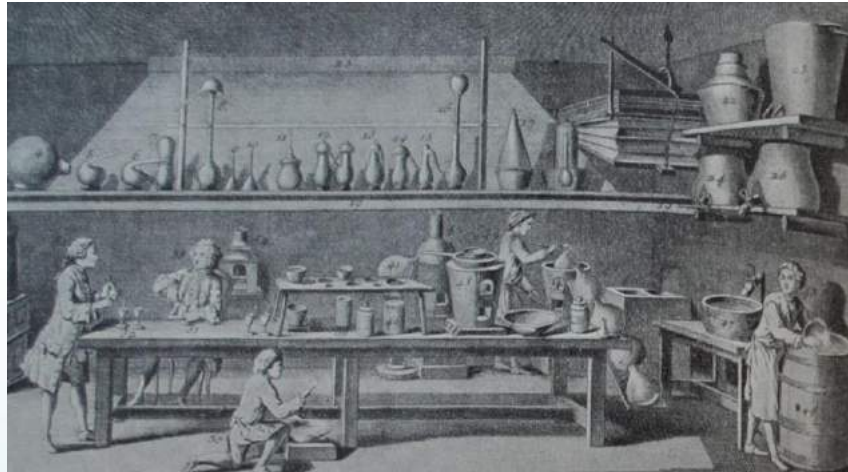
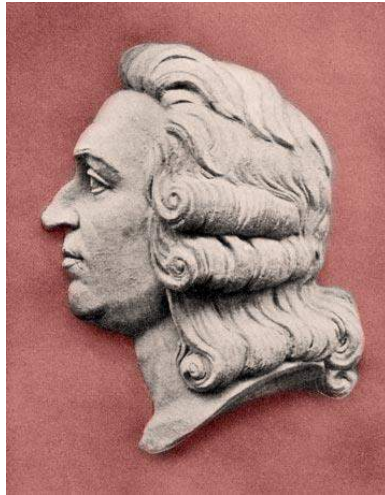
1. Discovery
2. Structure
3. Formation and synthesis
4. Application



Discovery

1756

Axel Fredrick Cronstedt

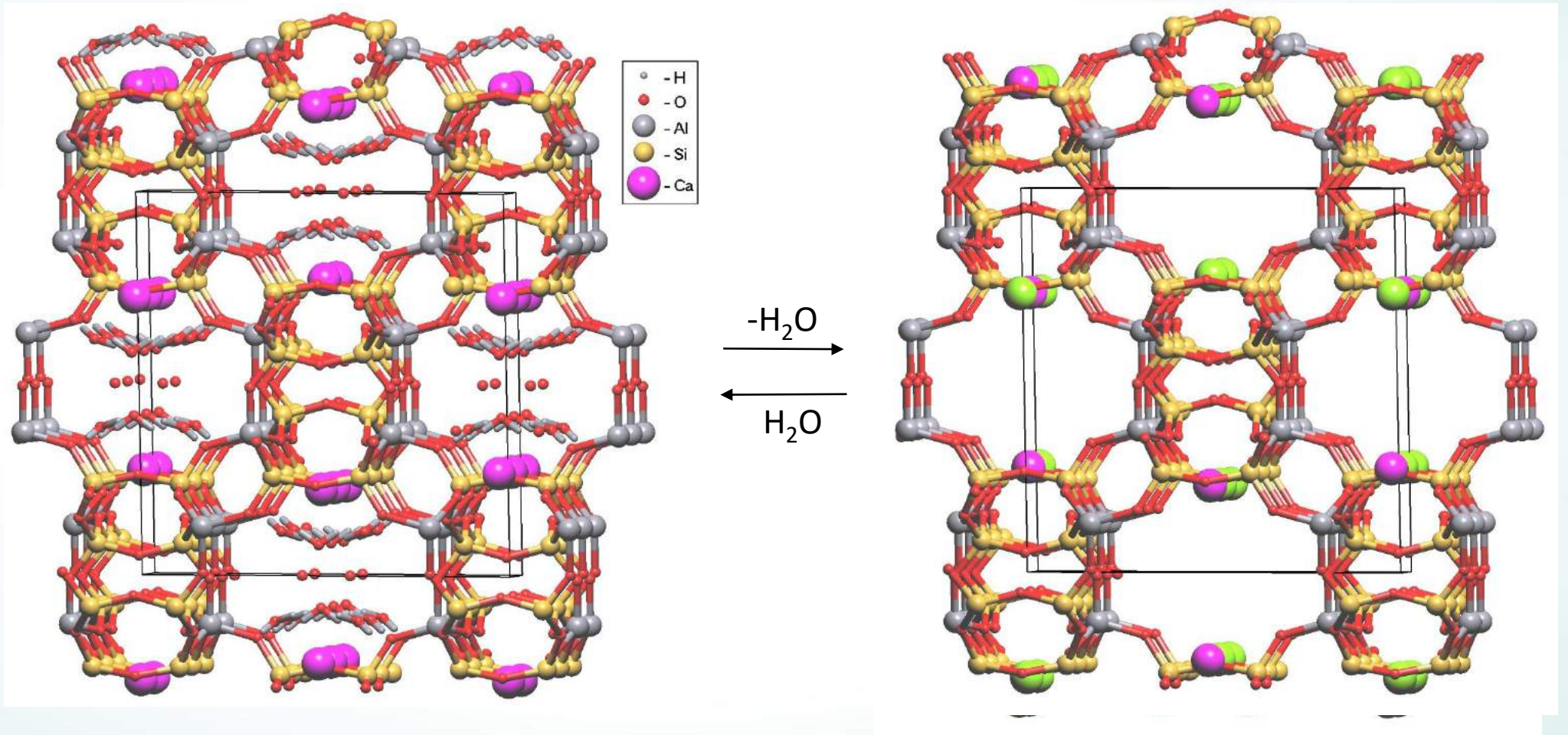


Zein - to boil
Lithos - a stone



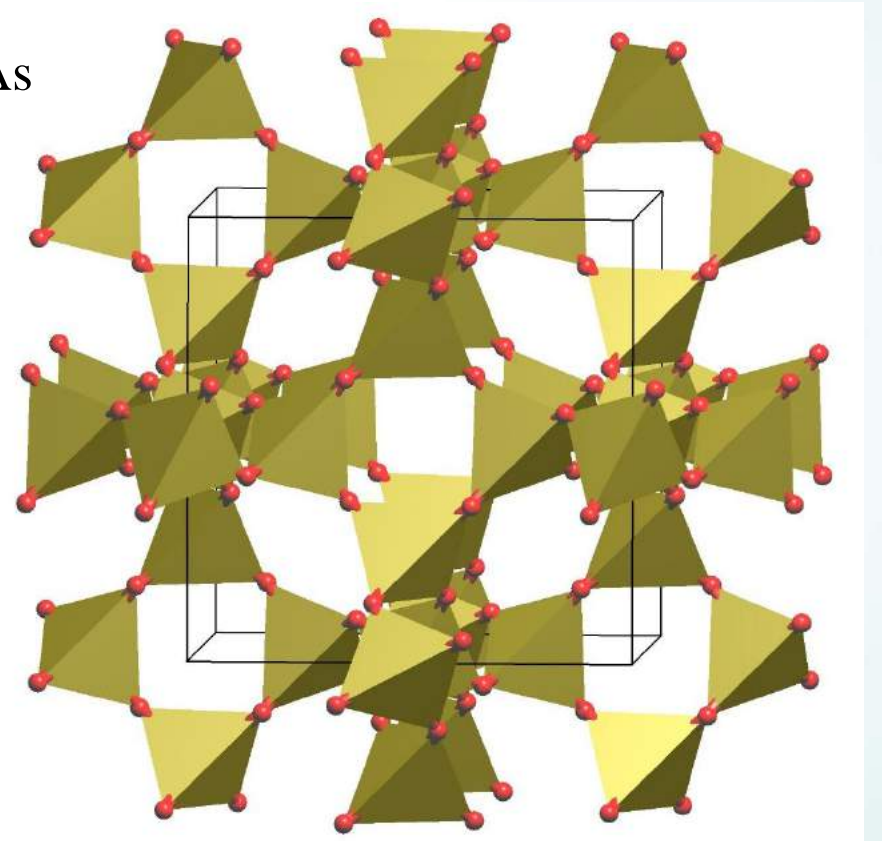
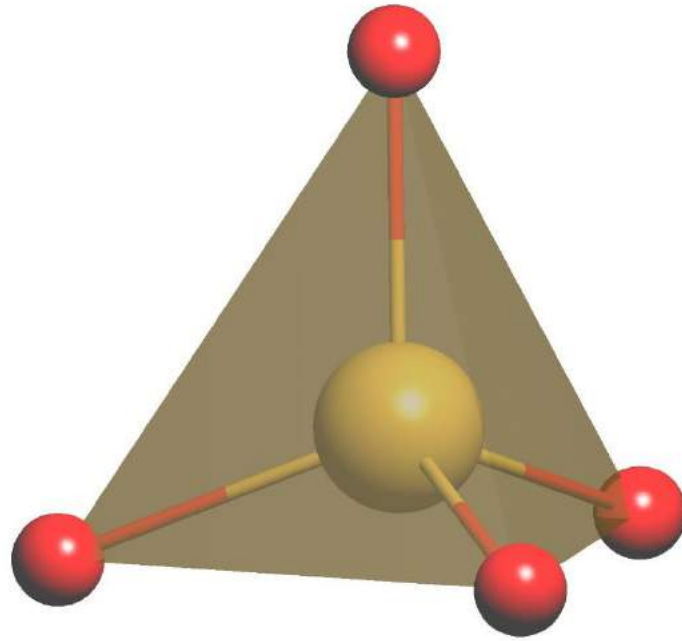
Stilbite

Structure



Structure

Si, Al, Be, Mg, P, Ti, Mn, Fe, Zn, Ga, Ge, Co, B, Li, As




Definition

1. Crystalline substance.
2. Framework consists of linked tetrahedra.
3. Tetrahedron consists of O atoms surrounding the cation.
4. Framework contains open cavities.
5. Cavities are usually occupied by H_2O molecules and extra-framework cations that are usually exchangeable.
6. The channels are large enough to pass the guest species.
7. The framework may be interrupted.



Composition



ToposPro Build - 5. 3. 1. 2 - [C:\Users\20\ICSD\Цеолиты]

System Compound Filter Database Program Results Window Cancel Help

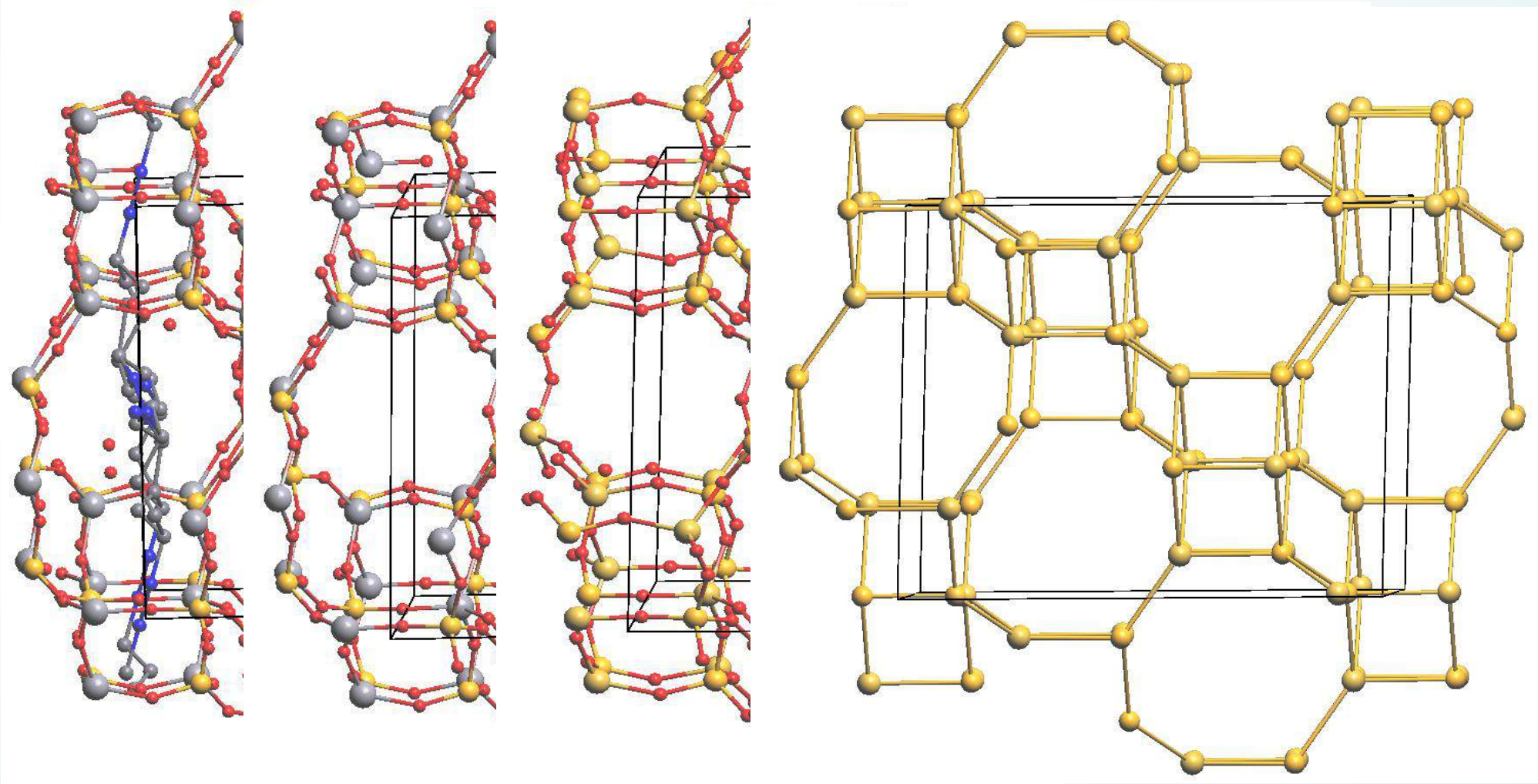
Compounds

K13.5(Si10Al10O40)(OH)3(H2O)13
Ca1.64K2(Si10.67Al5.33O32)(H2O)12
KCa0.92Mg0.82(Si13.52Al4.48O36)(H2O)9.84
K12(Al12Si12O48)(H2O)20
Mn4.5Na3Al12Si12O48(C2H2)4.5
Co.333Na.333(AlSiO4)(H2O)2.92
Ca0.07(AlO.1629SiO.8375O2)
K2.76Mg2Ca0.84(Si36O72)(OH)8.44(H2O)23.94
Mn4.5Na3(Si12Al12O48)
Na5(Al5Si5O20)(H2O)9
Na88(Al88Si104O384)(H2O)172.1
Na(AlSiO4)
Ca28(Al57Si135O384)
Ca43.3Al76.8Si115.2O384
K54.7Al54.7Si137.3O384
Na11Al11Si13O48S16
Na11Al11Si13O48(NH3)32
Ti11Al11Si13O48
Ti11Al11Si13O48(H2O)20
Ca40Al80Si112O384(H2O)116
(Ba13.42(Al30Si66O192))(BaCl2)8.22
(Ba5.12(Al30Si66O192))(BaBr2)7.92
Na17.28Ba8.88(Al30.048Si65.952O192)Cl3.84(H2O)70
Na6(Al6Si10O32)(H2O)12
Na11Fe10(Si15Al4)O384(H2O)164
H11Na29Cu7(Al56Si136O384)(H2O)250
H11Na21Cu12(Al56Si136O384)(H2O)250
H10Al11Cu11Fe(Al56Si136O384)(H2O)250

1678:0:26

3D Framework

4-connected net



Database of Zeolite Structures

IZA-SC

All Codes

Advanced Search ▾

Tools ▾

Other Links ▾

Home > Codes

Help Credits

Zeolite Framework Types

Search for a Framework Type Code

Enter one character to search for a code or
two or more to search for a code or material name

or select one from the tables below:

Fully ordered
Type Materials *

Partially disordered
Type Materials

ABW	ACO	AEI	AEL	AEN	AET	AFG	AFI	AFN	AFO	AFR	AFS	AFT	AFV	AFX
AFY	AHT	ANA	APC	APD	AST	ASV	ATN	ATO	ATS	ATT	ATV	AVL	AWO	AWW
BCT	BEC	BIK	BOF	BOG	BOZ	BPH	BRE	BSV	CAN	CAS	CDO	CFI	CGF	CGS
CHA	-CHI	-CLO	CON	CSV	CZP	DAC	DDR	DFO	DFT	DOH	DON	EAB	EDI	EEI
EMT	EON	EPI	ERI	ESV	ETL	ETR	EUO	EWS	EZT	FAR	FAU	FER	FRA	GIS
GIU	GME	GON	GOO	HEU	IFO	IFR	-JFT	-JFU	IFW	IFY	IHW	IMF	IRN	IRR
-JRY	ISV	ITE	ITG	ITH	ITR	ITT	-ITV	ITW	IWR	IWS	IWV	IWW	JBW	JNT
JOZ	JRY	JSN	JSR	JST	JSW	KFI	LAU	LEV	LIO	-LIT	LOS	LOV	LTA	LTF
LTJ	LTL	LTN	MAR	MAZ	MEI	MEL	MEP	MER	MFI	MFS	MON	MOR	MOZ	MSE
MSO	MTF	MTN	MTT	MTW	MVY	MWF	MWW	NAB	NAT	NES	NON	NPO	NPT	NSI
OBW	OFF	OKO	OSI	OSO	OWE	-PAR	PAU	PCR	PHI	PON	POS	PSI	PUN	RHO
-RON	RRO	RSN	RTE	RTH	RUT	RWR	RWY	SAF	SAO	SAS	SAT	SAV	SBE	SBN
SBS	SBT	SEW	SFE	SFF	SFG	SFH	SFN	SFO	SFS	SFW	SGT	SIV	SOD	SOF
SOR	SOS	SSF	SSY	STF	STI	STT	STW	-SVR	SVV	SWY	SZR	TER	THO	TOL
TON	TSC	TUN	UEI	UFI	UOS	UOV	UOZ	USI	UTL	UWY	VET	VFI	VNI	VSV
WEI	-WEN	YFI	YUG	ZON										

*BEA

*CTH

*-EWT

*-ITN

*MRE

*SFV

*-SSO

*STO

*-SVY

245

50

Building units

Database of Zeolite Structures

IZA-SC All Codes Framework Material 3D Drawing Powder Pattern CIF PDF References

Home Codes Framework Characteristic Units Help Credits

Framework Type FAU

Framework

Cell Parameters: cubic F d -3 m (# 227)
 $a = 24.3450 \text{ \AA}$ $b = 24.3450 \text{ \AA}$ $c = 24.3450 \text{ \AA}$
 $\alpha = 90.000^\circ$ $\beta = 90.000^\circ$ $\gamma = 90.000^\circ$
 Volume = 14428.8 \AA^3
 $R_{\text{pLS}} = 0.0009$

Framework density (FD_{SI}): 13.3 T/1000 A^3
Topological density: TD₁₀ = 579 TD = 0.476190

Ring sizes (# T-atoms): 12 6 4


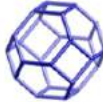
Channel dimensionality: Topological (pore opening > 6-ring): 3-dimensional

Maximum diameter of a sphere:
 that can be included: 11.24 A
 that can diffuse along: a: 7.35 A b: 7.35 A c: 7.35 A

Accessible volume: 27.42 %

Secondary Building Units: 6-6 or 6-2 or 6 or 4-2 or 1-4-1 or 4

Composite Building Units:

Natural Tiling: t-fau t-hpr t-foe

Year code assigned: 1978
 Data last updated: Jul 1, 2007

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FAU $Fd\bar{3}m$

$$2[4^6.6^2] + [4^6.6^8] + [4^{18}.6^4.12^4]$$

1453

TILES

Face symbol:

$[4^6.6^2]$

$[4^6.6^8]$

$[4^{18}.6^4.12^4]$



V, E, F:

(12, 18, 8)

(24, 36, 14)

(48, 72, 26)

Symmetry:

$\bar{3}m$

$\bar{4}3m$

$\bar{4}3m$

Wyckoff:

16c

8a

8b

Label:

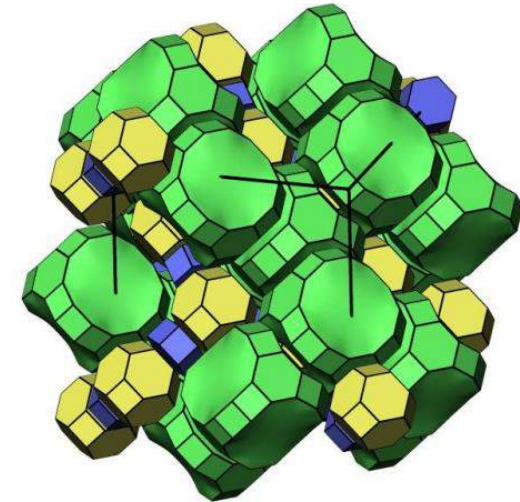
t-hpr

t-toc

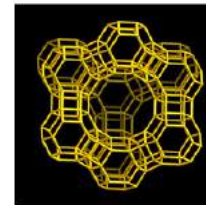
t-fau

Special features: simple

TILING



Framework images
 (click on icon for larger image)



Viewed along [111]



viewed along [110]



Polyhedral model viewed along [110]



an 'artist impression' of a catalytic reaction

Framework Type MFI

ZSM-5

Type Material ¹

Material Name: ZSM-5

Chemical Formula[§]: $[\text{Na}^+_n(\text{H}_2\text{O})_{16}] [\text{Al}_n\text{Si}_{96-n}\text{O}_{192}]\text{-MFI}$, $n < 27$

Unit Cell[§]: orthorhombic $P n m a$ (# 62)

$a' = 20.0700\text{\AA}$	$b' = 19.9200\text{\AA}$	$c' = 13.4200\text{\AA}$
$\alpha' = 90.000^\circ$	$\beta' = 90.000^\circ$	$\gamma' = 90.000^\circ$

Framework density: ³ 17.9 T/1000 \AA^3

Channels: ³ $\{[100] 10 \ 5.1 \times 5.5 \leftrightarrow [010] 10 \ 5.3 \times 5.6\}^{***}$

Dimensionality ³

Sorption (molecular cross section > 3.4 \AA): 3-dimensional
 Topological (pore opening > 6-ring): 3-dimensional

References:

Kokotailo, G.T., Lawton, S.L., Olson, D.H. and Meier, W.M.
 "Structure of synthetic zeolite ZSM-5"
Nature, **272**, 437-438 (1978)

[§] Olson, D.H., Kokotailo, G.T., Lawton, S.L. and Meier, W.M.
 "Crystal Structure and Structure-Related Properties of ZSM-5"
J. Phys. Chem., **85**, 2238-2243 (1981)

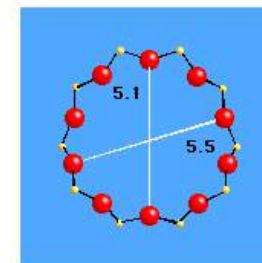
van Koningsveld, H., van Bekkum, H. and Jansen, J.C.
 "On the location and disorder of the tetrapropylammonium (TPA) ion in zeolite ZSM-5 with improved framework accuracy"
Acta Crystallogr., **B43**, 127-132 (1987)

Name and Code derivation:

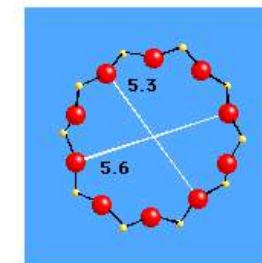
Zeolite Socony Mobil - five
 → ZSM-5 (five)
 → MFI

[§] Chemical Formula and Unit Cell taken from the reference marked with this sign

Limiting Rings



10-ring viewed along [100]



10-ring viewed along [010]

Zeolite Socony Mobil-five

Materials

Database of Zeolite Structures

IZA-SC All Codes Framework Material 3D Drawing Powder Pattern CIF PDF References

Home » Codes » Framework

Characteristic Units Help Credits

MFI Type Material
F MFI Related materials MFI

Framework

Cell Parameters:

orthorhombic	P n m a (# 62)	
a = 20.0900 Å	b = 19.7380 Å	c = 13.1420 Å
α = 90.000°	β = 90.000°	γ = 90.000°
Volume =	5211.3 Å ³	
R _{DL} =	0.0020	

Framework density (FD_{Si}): 18.4 T/1000 Å³

Topological density: TD₁₀ = 960 TD = 0.825819

Ring sizes (# T-atoms): 10 6 5 4

Channel dimensionality: Topological (pore opening > 6-ring): 3-dimensional


Maximum diameter of a sphere:

that can be included	6.36 Å		
that can diffuse along	a: 4.7 Å	b: 4.46 Å	c: 4.46 Å


Accessible volume: 9.81 %

Secondary Building Units: 5-1


Composite Building Units:




mor (t-tes)



cas



mfi (t-pen)

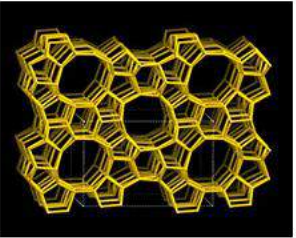


mel

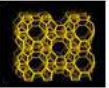
Natural Tiling

t-bog-1	t-kah	t-mel	t-mel-1	t-mel-2	t-mfi-1	t-mfi-2	t-pen
t-pes	t-tes						

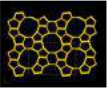
Framework images
(click on icon for larger image)



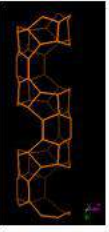
Viewed along [010]




framework, viewed along [100]




projection along [010]



10ring straight channel



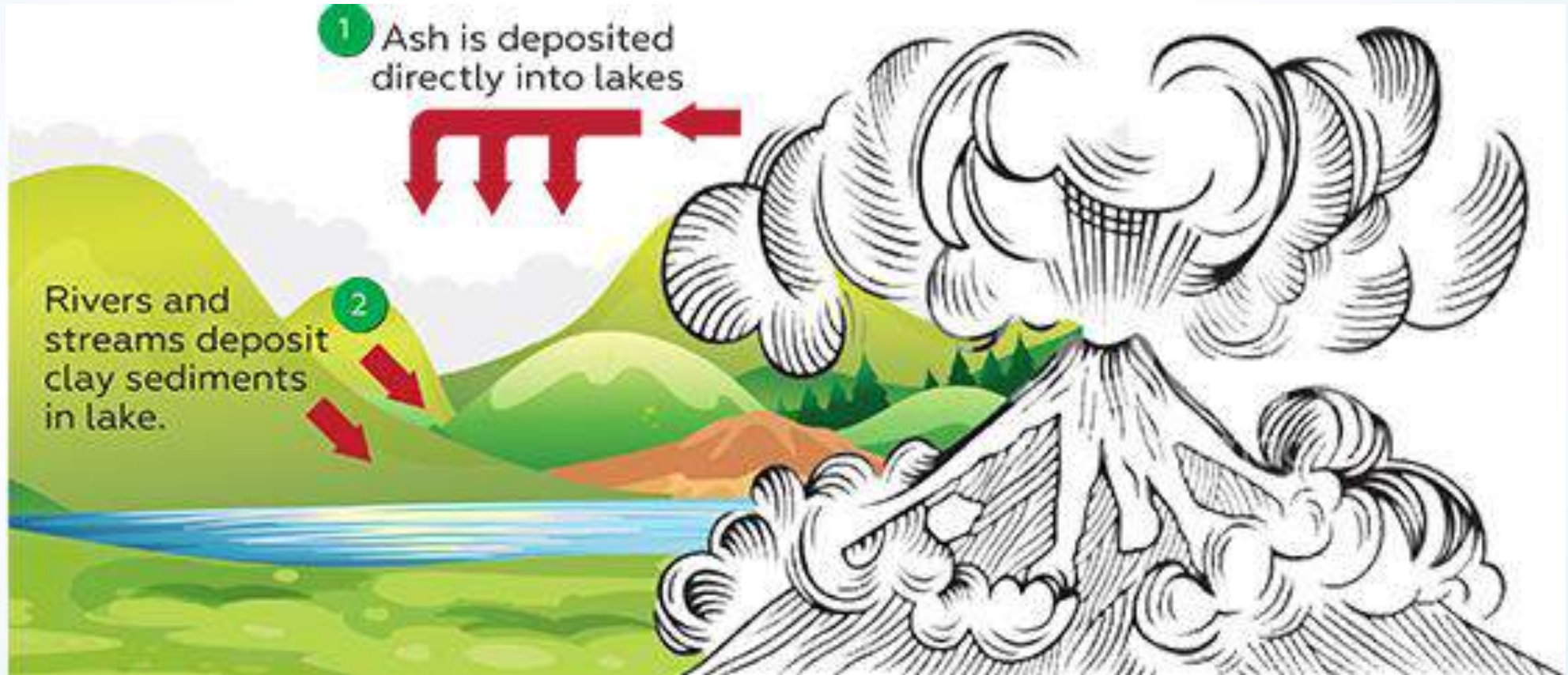
complex of 10rings viewed along [010]



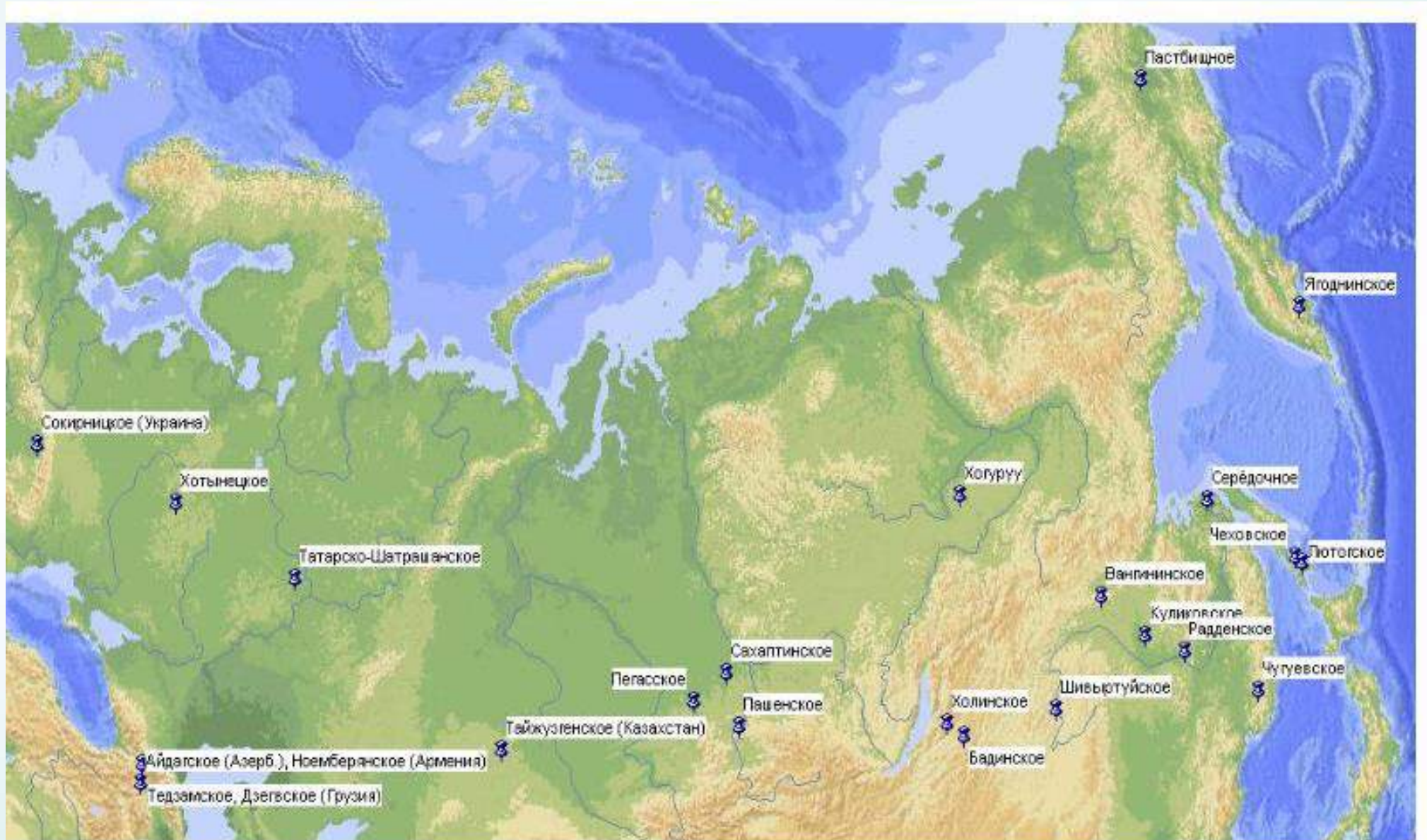
complex of 10rings viewed along [100]

ZSM-5
 FeS-1
 MnS-1
 Mutinaite
 [As-Si-O]-MFI
 [Ga-Si-O]-MFI
 [Fe-Si-O]-MFI
 NU-4
 TSZ-III
 ZBH
 Encilite
 AZ-1
 TSZ
 ZKQ-1B
 TS-1
 USI-108
 ZMQ-TB
 NU-5
 TZ-01
 USC-4
 AMS-1B
 FZ-1
 LZ-105
 Bor-C
 Boralite C
 Silicalite

Formation



Deposits



Natural zeolites



analcime



chabasite



heulandite



clinoptilolite



natrolite



sodalite



stilbite



phillipsite



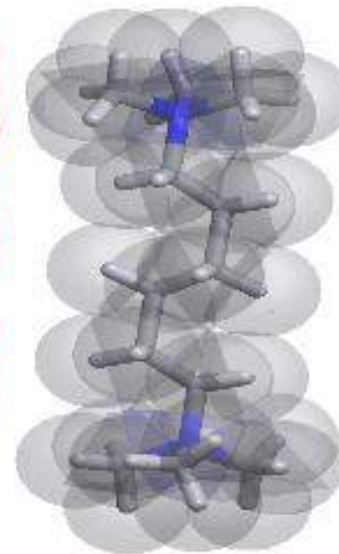
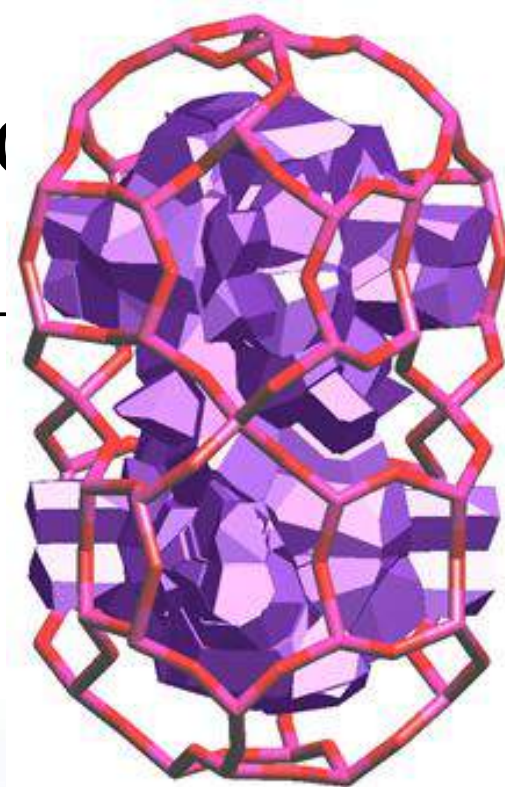
Synthesis

Mixing

$\text{NaAl}(\text{OH})_4 + \text{Na}_2\text{SiO}_3 + \text{NaOH} + \text{template}$, 25⁰C gel formation

$\text{Na}_n(\text{AlO})_m$

F



5-175⁰C

n

Synthesis

Composition

Concentrations and reactant ratio

Order of mixing

Temperature

Ageing time

Crystallization time

pH

Stirring/No stirring

Seeding

Templates



Hypothetical zeolites

1. M. M. J. Treacy, I. Rivin, E. Balkovsky, K. H. Randall, M. D. Foster, Enumeration of Periodic Tetrahedral Frameworks. II. Polynodal Graphs. *Micropor. Mesopor. Mater.* **2004**, 74, 121.
2. R. Pophale, P. A. Cheeseman, M. W. Deem, A database of new zeolite-like materials. *Phys. Chem. Chem. Phys.* **2011**, 13, 12407.
3. Y. Li, J. Yu, R. Xu, Criteria for Zeolite Frameworks Realizable for Target Synthesis. *Angew. Chem. Int. Ed.* **2013**, 52, 1673.



Application

Database of Zeolite Structures

IZA-SC

All Codes

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Home > Codes

Help Credits

Zeolite Framework Types

Search for a Framework Type Code

Enter one character to search for a code or
two or more to search for a code or material name

or select one from the tables below:

Fully ordered
Type Materials *

Partially disordered
Type Materials

ABW	ACO	AEI	AEL	AEN	AET	AFG	AFI	AFN	AFO	AFR	AFS	AFT	AFV	AFX
AFY	AHT	ANA	APC	APD	AST	ASV	ATN	ATO	ATS	ATT	ATV	AVL	AWO	AWW
BCT	BEC	BIK	BOF	BOG	BOZ	BPH	BRE	BSV	CAN	CAS	CDO	CFI	CGF	CGS
CHA	-CHI	-CLO	CON	CSV	CZP	DAC	DDR	DFO	DFT	DOH	DON	EAB	EDI	EEI
EMT	EON	EPI	ERI	ESV	ETL	ETR	EUO	EWS	EZT	FAR	FAU	FER	FRA	GIS
GIU	GME	GON	GOO	HEU	IFO	IFR	-JFT	-JFU	IFW	IFY	IHW	IMF	IRN	IRR
-JRY	ISV	ITE	ITG	ITH	ITR	ITT	-ITV	ITW	IWR	IWS	IWV	IWW	JBW	JNT
JOZ	JRY	JSN	JSR	JST	JSW	KFI	LAU	LEV	LIO	-LIT	LOS	LOV	LTA	LTF
LTJ	LTL	LTN	MAR	MAZ	MEI	MEL	MEP	MER	MFI	MFS	MON	MOR	MOZ	MSE
MSO	MTF	MTN	MTT	MTW	MVY	MWF	MWW	NAB	NAT	NES	NON	NPO	NPT	NSI
OBW	OFF	OKO	OSI	OSO	OWE	-PAR	PAU	PCR	PHI	PON	POS	PSI	PUN	RHO
-RON	RRO	RSN	RTE	RTH	RUT	RWR	RWY	SAF	SAO	SAS	SAT	SAV	SBE	SBN
SBS	SBT	SEW	SFE	SFF	SFG	SFH	SFN	SFO	SFS	SFW	SGT	SIV	SOD	SOF
SOR	SOS	SSF	SSY	STF	STI	STT	STW	-SVR	SVV	SWY	SZR	TER	THO	TOL
TON	TSC	TUN	UEI	UFI	UOS	UOV	UOZ	USI	UTL	UWY	VET	VFI	VNI	VSV
WEI	-WEN	YFI	YUG	ZON										

- *BEA
- *CTH
- *EWT
- *ITN
- *MRE
- *SFV
- *SSO
- *STO
- *SVY

Database of Zeolite Structures

IZA-SC All Codes Framework Material 3D Drawing Powder Pattern CIF PDF References

Home » Codes » Framework

Characteristic Units Help Credits

Framework Type LTA

Framework ¹

Cell Parameters: cubic P m -3 m (# 221)
a = 11.9190 Å b = 11.9190 Å c = 11.9190 Å
α = 90.000° β = 90.000° γ = 90.000°
Volume = 1693.2 Å³
R_{DLS} = 0.0026

Framework density (FD_{SI}): ¹ 14.2 T/1000 Å³
Topological density: ¹ TD₁₀ = 641 TD = 0.533333

Ring sizes (# T-atoms): 8 6 4

Channel dimensionality: ¹ Topological (pore opening > 6-ring): 3-dimensional

Maximum diameter of a sphere: ¹

that can be included 11.05 Å
that can diffuse along a: 4.21 Å b: 4.21 Å c: 4.21 Å

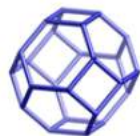
Accessible volume: 21.43 %

Secondary Building Units: ¹ 8 or 4-4 or 6-2 or 6 or 1-4-1 or 4

Composite Building Units: ¹



d4r (t-cub)



sod (t-toc)

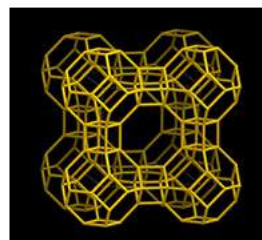


lta (t-grc)

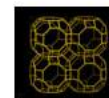
Natural Tiling ¹

t-cub t-grc t-toc

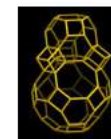
Framework images
(click on icon for larger image)



Viewed along [100]



framework, showing the alpha cages



alpha-cage, sodalite cage and 4MR



projection along [100]

Zeolite A

Year code assigned 1978
Data last updated Jul 1, 2007

Database of Zeolite Structures

IZA-SC All Codes Framework Material 3D Drawing Powder Pattern CIF PDF References

Home » Codes » Framework

Characteristic Units Help Credits

Framework Type FAU

Framework

Cell Parameters:
cubic F d -3 m (# 227)
a = 24.3450 Å b = 24.3450 Å c = 24.3450 Å
 $\alpha = 90.000^\circ$ $\beta = 90.000^\circ$ $\gamma = 90.000^\circ$
Volume = 14428.8 Å³
R_{DLS} = 0.0009

Framework density (FD_{Si}): 13.3 T/1000 Å³

Topological density: TD₁₀ = 579 TD = 0.476190

Ring sizes (# T-atoms): 12 6 4

Channel dimensionality: Topological (pore opening > 6-ring): 3-dimensional

Maximum diameter of a sphere:

that can be included 11.24 Å

that can diffuse along a: 7.35 Å b: 7.35 Å c: 7.35 Å

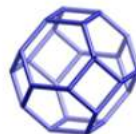
Accessible volume: 27.42 %

Secondary Building Units: 6-6 or 6-2 or 6 or 4-2 or 1-4-1 or 4

Composite Building Units:



d6r (t-hpr)

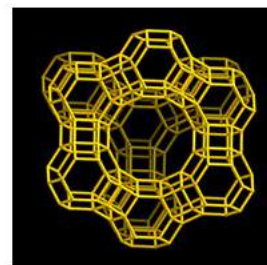


sod (t-toc)

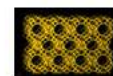
Natural Tiling

t-fau t-hpr t-toc

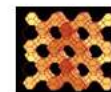
Framework images
(click on icon for larger image)



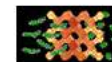
Viewed along [111]



viewed along [110]



Polyhedral model viewed along [110]



an 'artist impression' of a catalytic reaction

Year code assigned 1978
Data last updated Jul 1, 2007

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Zeolite X Si/Al 1.25

Zeolite Y Si/Al 2.3

USY (Ultra-Stable-Y) Si/Al 5.6

Database of Zeolite Structures

IZA-SC All Codes Framework Material 3D Drawing Powder Pattern CIF PDF References

Home » Codes » Type Material

Characteristic Units Help Credits

Framework Type MFI

Type Material ?

Material Name: ZSM-5

Chemical Formula[§]: $[\text{Na}^+_n (\text{H}_2\text{O})_{16}] [\text{Al}_n \text{Si}_{96-n} \text{O}_{192}] \text{-MFI}$, $n < 27$

Unit Cell[§]: orthorhombic $P n m a$ (# 62)
 $a' = 20.0700 \text{ \AA}$ $b' = 19.9200 \text{ \AA}$ $c' = 13.4200 \text{ \AA}$
 $\alpha' = 90.000^\circ$ $\beta' = 90.000^\circ$ $\gamma' = 90.000^\circ$

Framework density: ? 17.9 T/1000 \AA^3

Channels: ? $\{[100] 10 \ 5.1 \times 5.5 \leftrightarrow [010] 10 \ 5.3 \times 5.6\}^{***}$
Dimensionality ?
Sorption (molecular cross section > 3.4 \AA): 3-dimensional
Topological (pore opening > 6-ring): 3-dimensional

References:

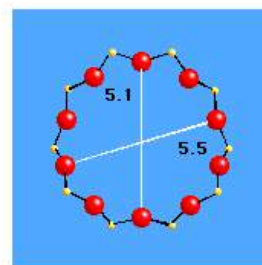
- Kokotailo, G.T., Lawton, S.L., Olson, D.H. and Meier, W.M.
"Structure of synthetic zeolite ZSM-5"
Nature, **272**, 437-438 (1978)
- [§] Olson, D.H., Kokotailo, G.T., Lawton, S.L. and Meier, W.M.
"Crystal Structure and Structure-Related Properties of ZSM-5"
J. Phys. Chem., **85**, 2238-2243 (1981)
- van Koningsveld, H., van Bekkum, H. and Jansen, J.C.
"On the location and disorder of the tetrapropylammonium (TPA) ion in zeolite ZSM-5 with improved framework accuracy"
Acta Crystallogr., **B43**, 127-132 (1987)

Name and Code derivation:

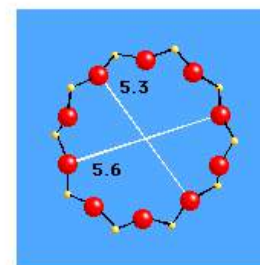
- Zeolite **S**ocony **M**obil - five
→ ZSM-5 (five)
→ MFI

[§] Chemical Formula and Unit Cell taken from the reference marked with this sign

Limiting Rings



10-ring viewed along [100]



10-ring viewed along [010]

H-ZSM-5

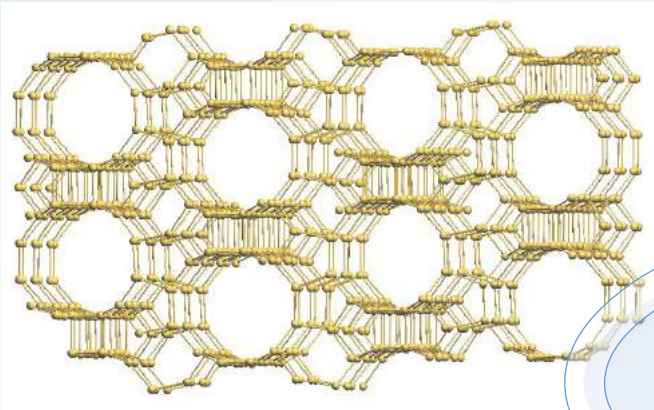
Application: building



4 000 000 t



Si, Al, Be, Mg, P, Ti, Mn, Fe,
Zn, Ga, Ge, Co, B, Li, As

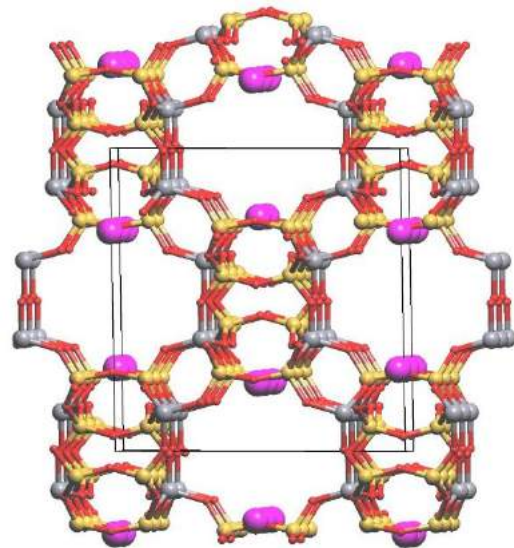
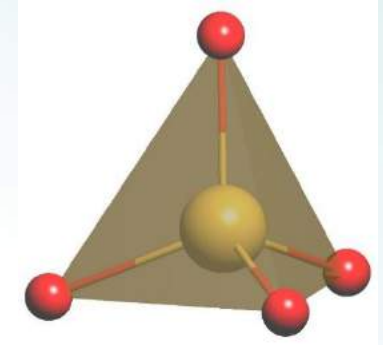


Channels
&
cavities

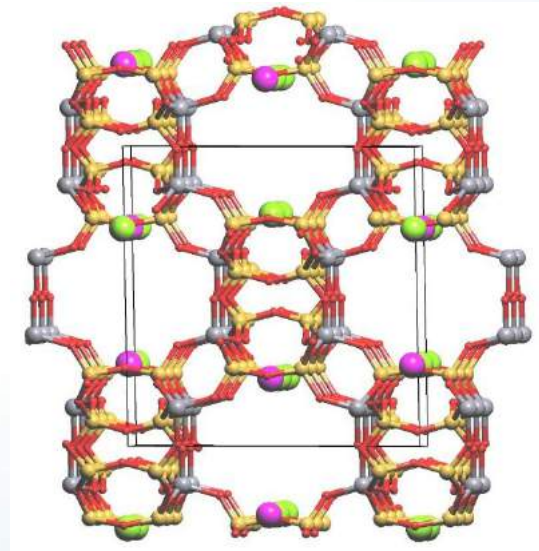
Various
T-atoms

Many
active
centers

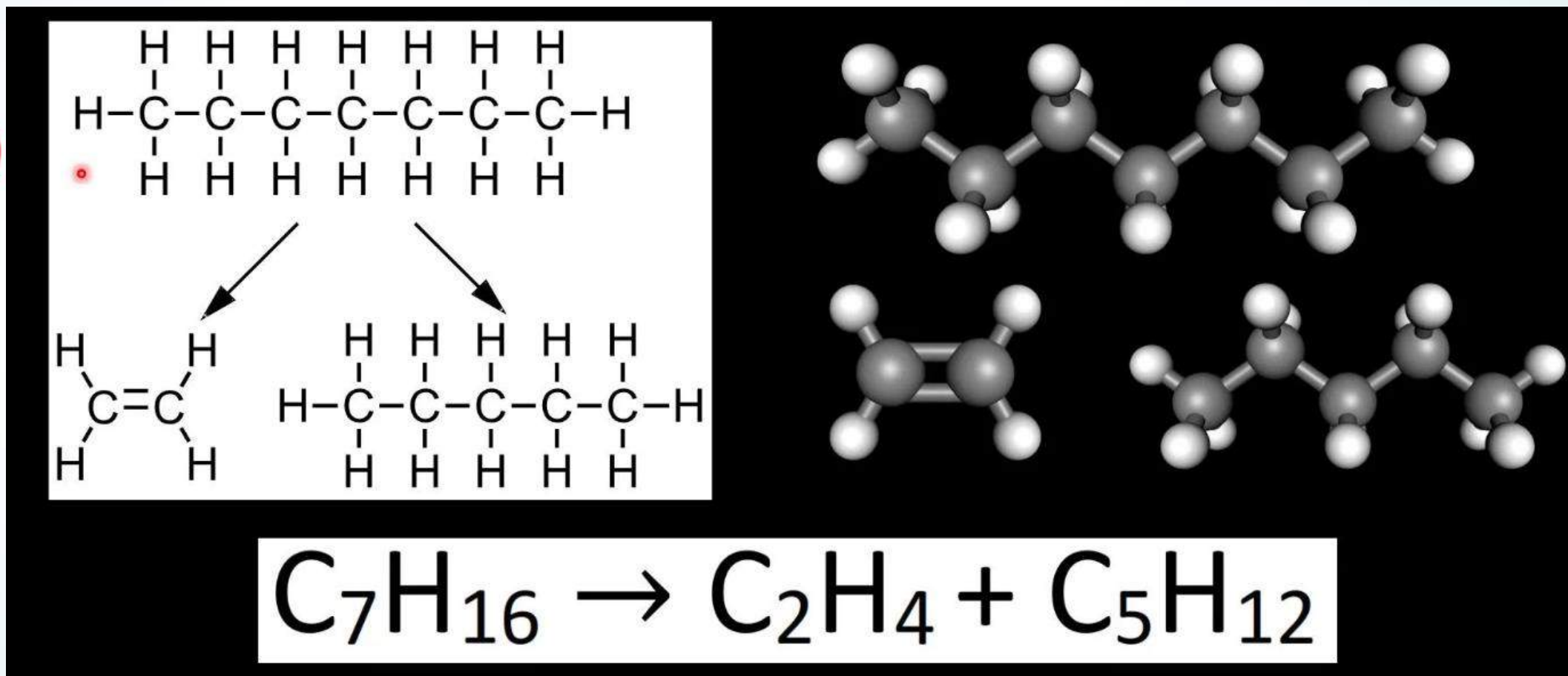
Kt-
exchange



Adsorbents
Molecular sieves
Catalysis
Kt-exchange

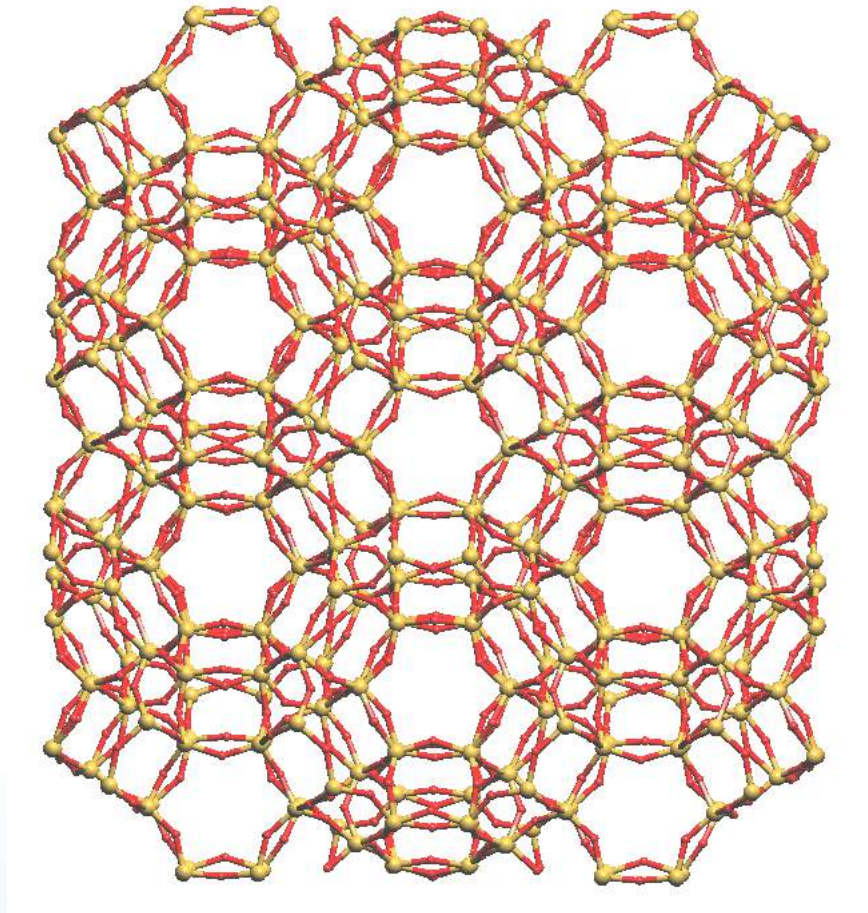


Applications: catalysis



Applications: catalysis

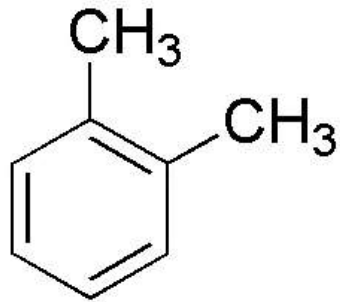
Zeolite Y (FAU) 300 000 t



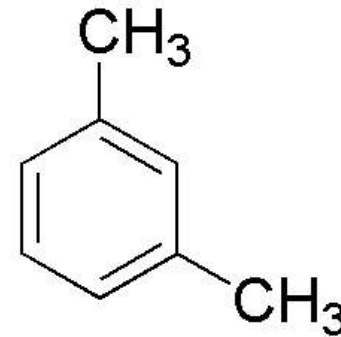
Applications: catalysis

H-ZSM-5 (MFI)

“Polyester” industry



ortho-xylene
(1,2-dimethylbenzene)



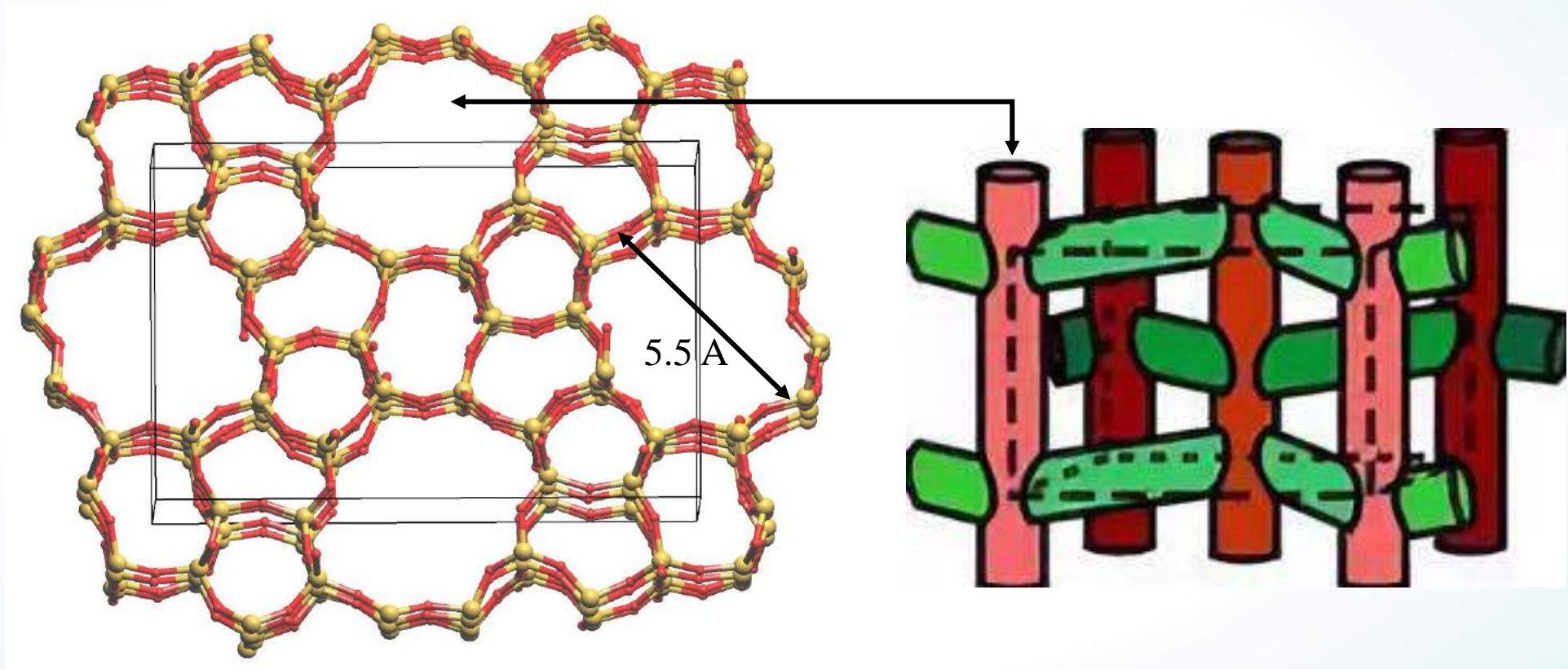
meta-xylene
(1,3-dimethylbenzene)



para-xylene
(1,4-dimethylbenzene)

Applications: catalysis

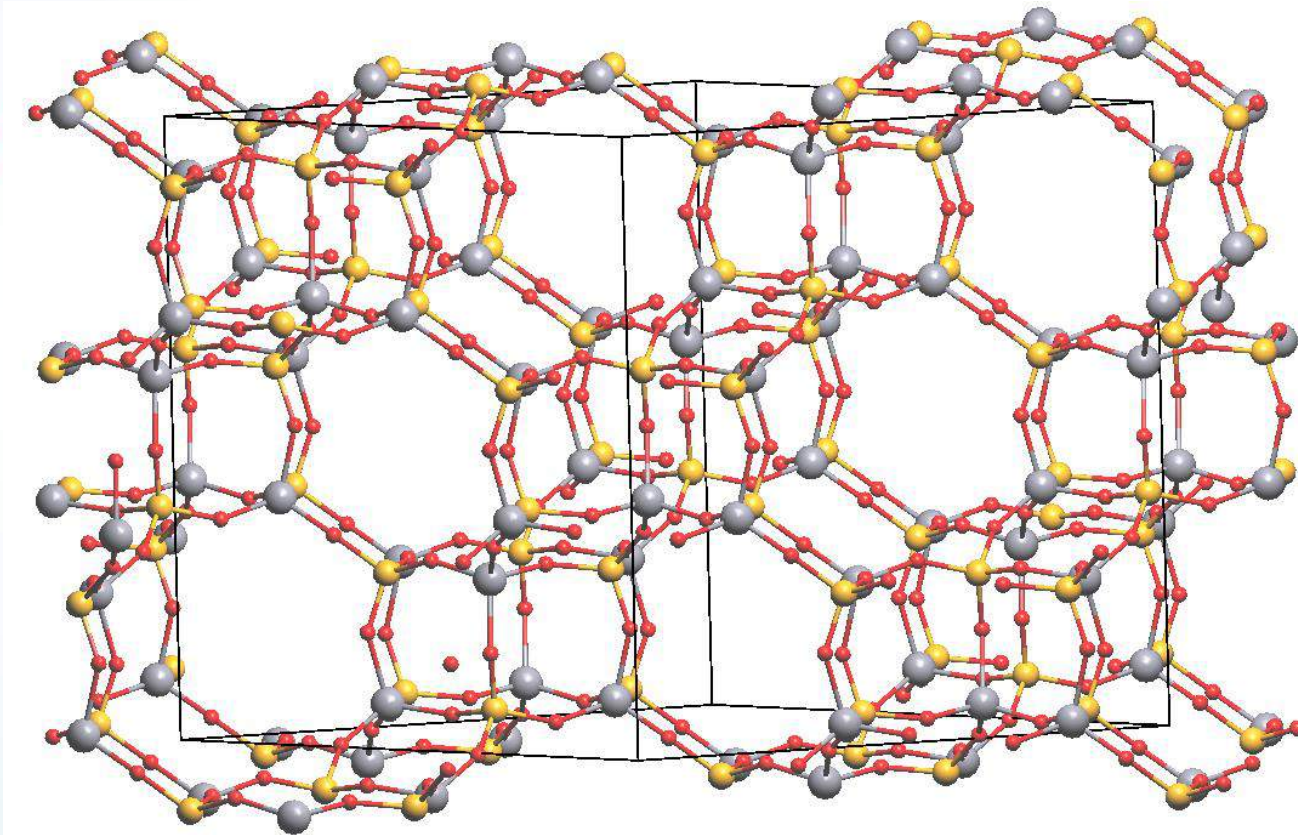
Methanol to Gasoline (MTG) Process



H-ZSM-5 (MFI)

Applications: catalysis

Methanol to Olefins (MTO) Process

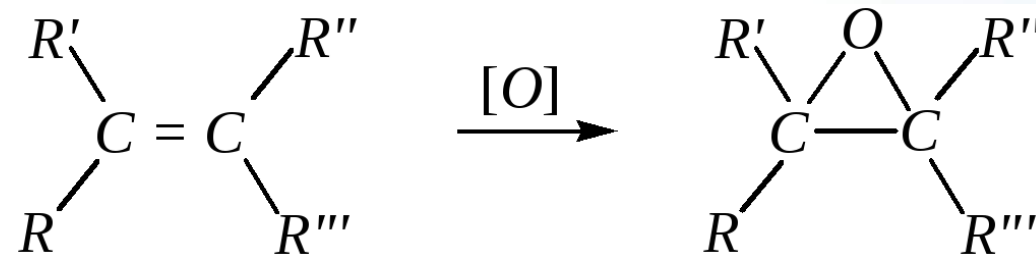
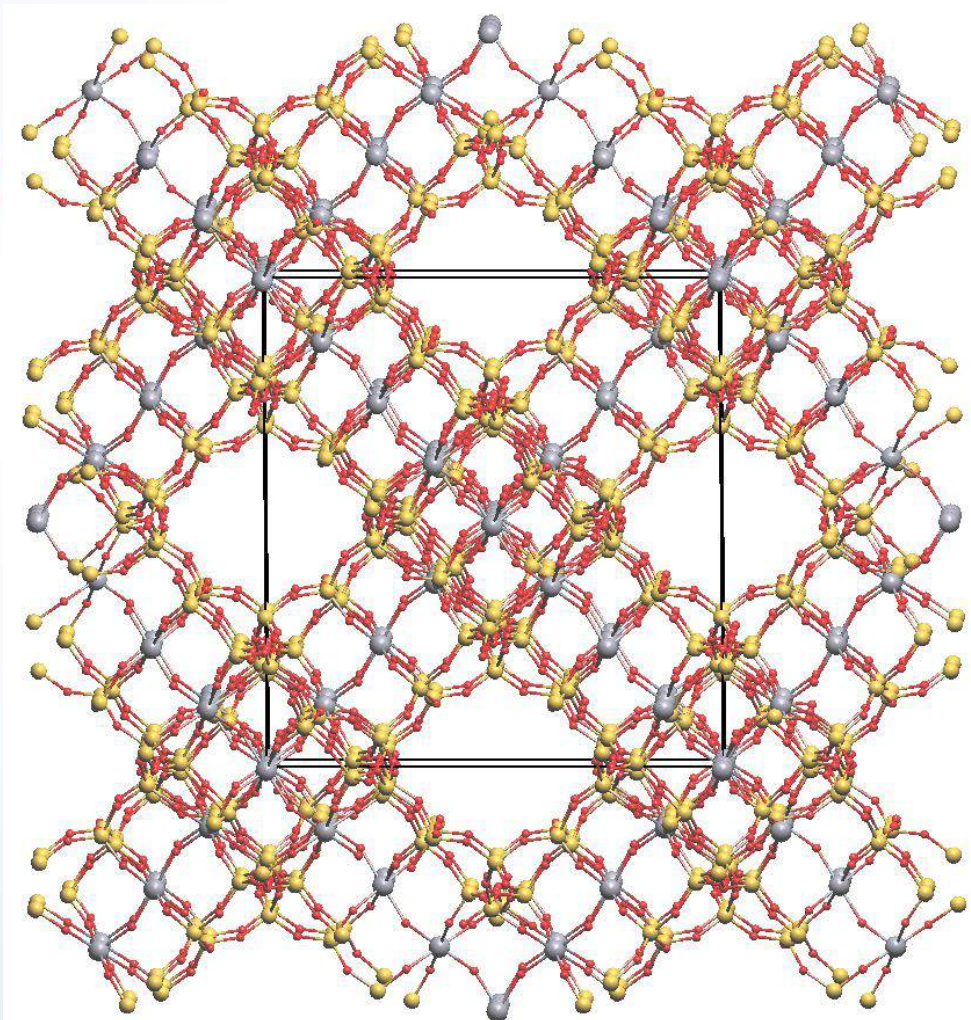


H-SAPO-34 (CHA)



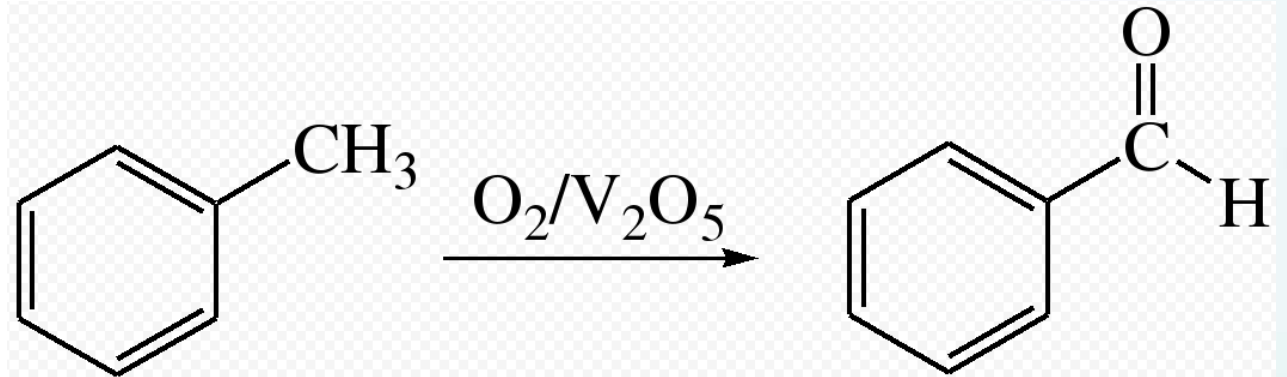
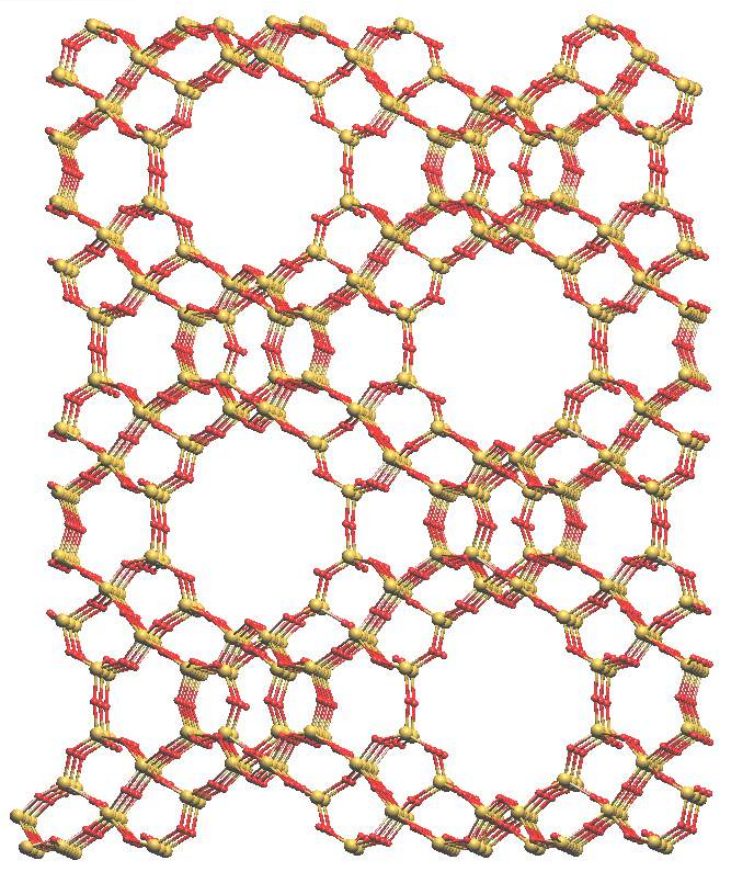
Applications: Chemical oxidation

TS-1 (MFI)



Applications: Photo-oxidation

Zeolite Y (FAU)



Application: “Ship in a bottle” complex



Applications: “Ship in a bottle” complex

Zeolite Y (FAU)

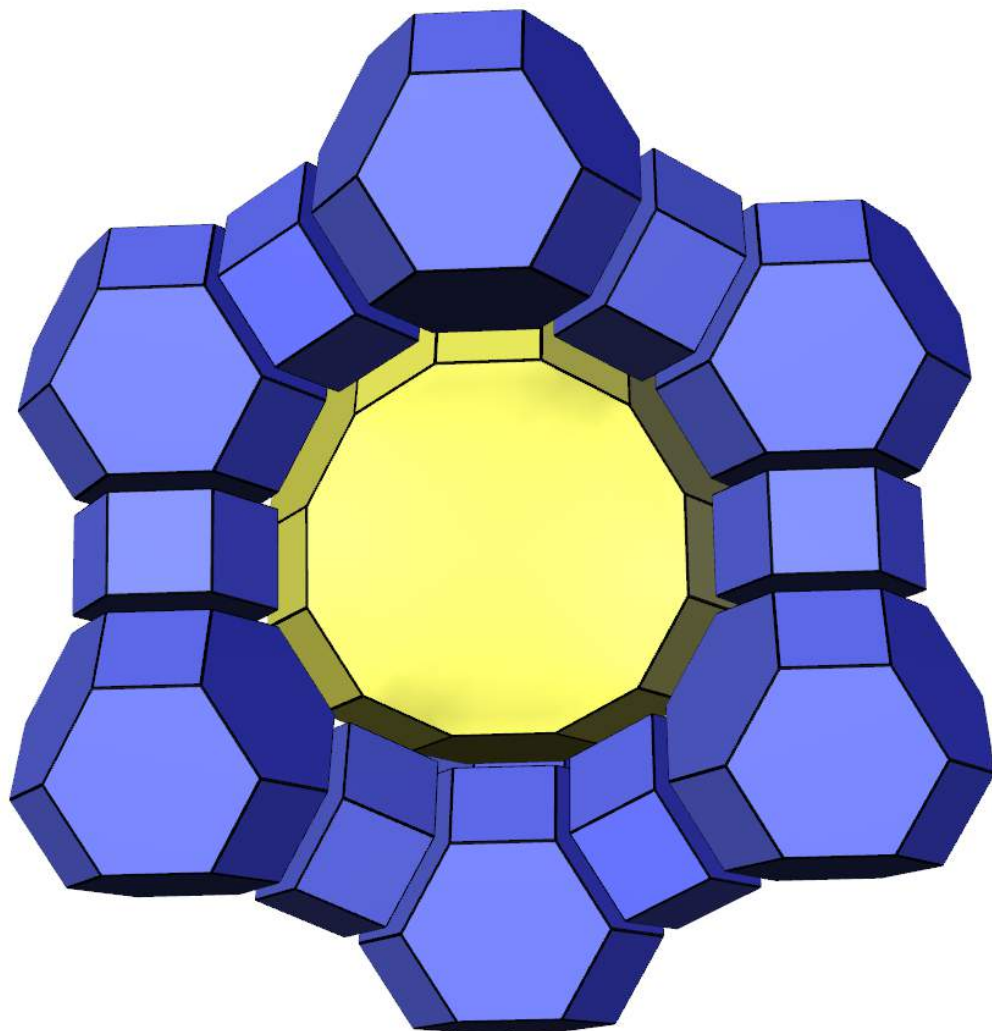
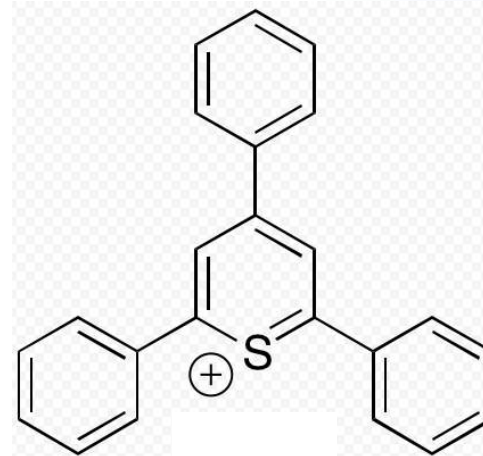
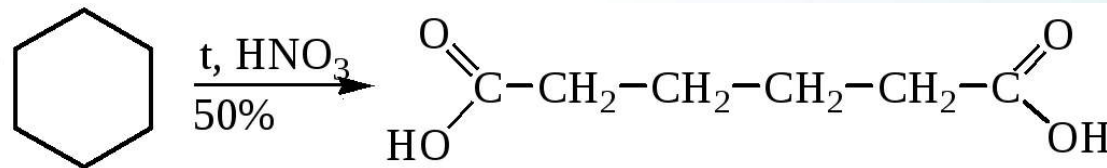


Photo-catalysts



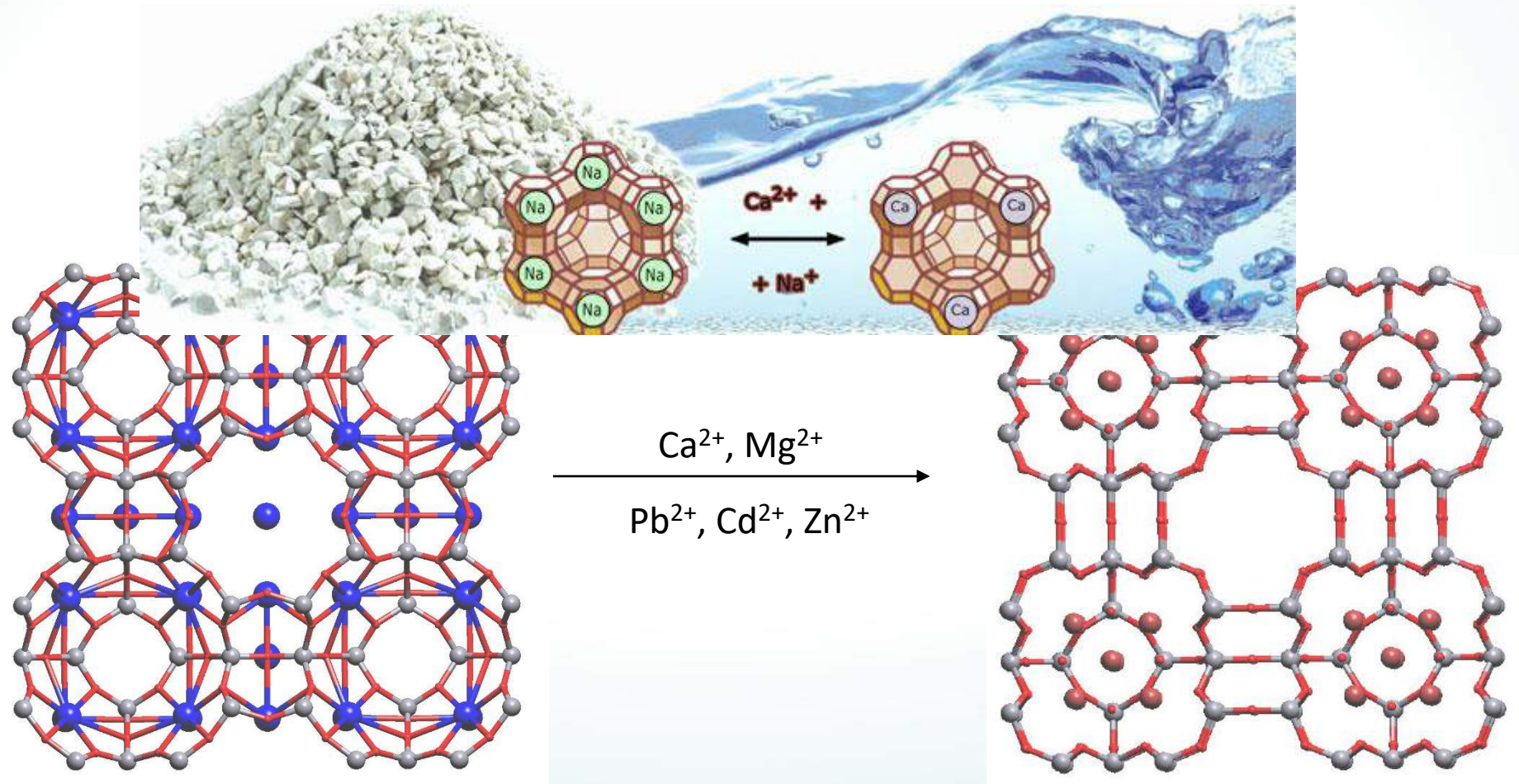
2,4,6-triphenylthiapyrylium cation



Applications: Kt-exchange

Zeolite A (LTA)

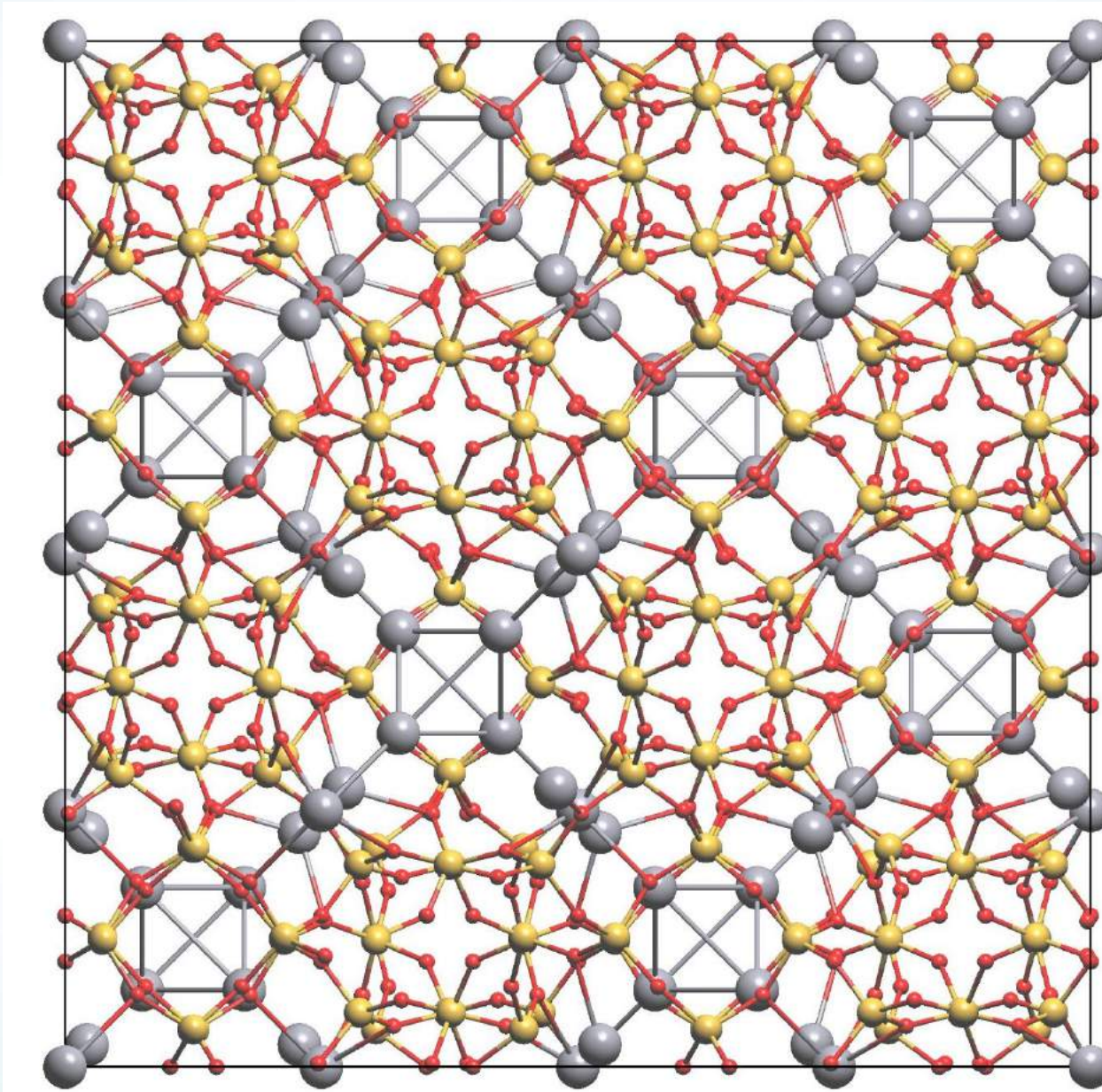
1,400 000 t



Applications: Kt-exchange



Applications: Medicine

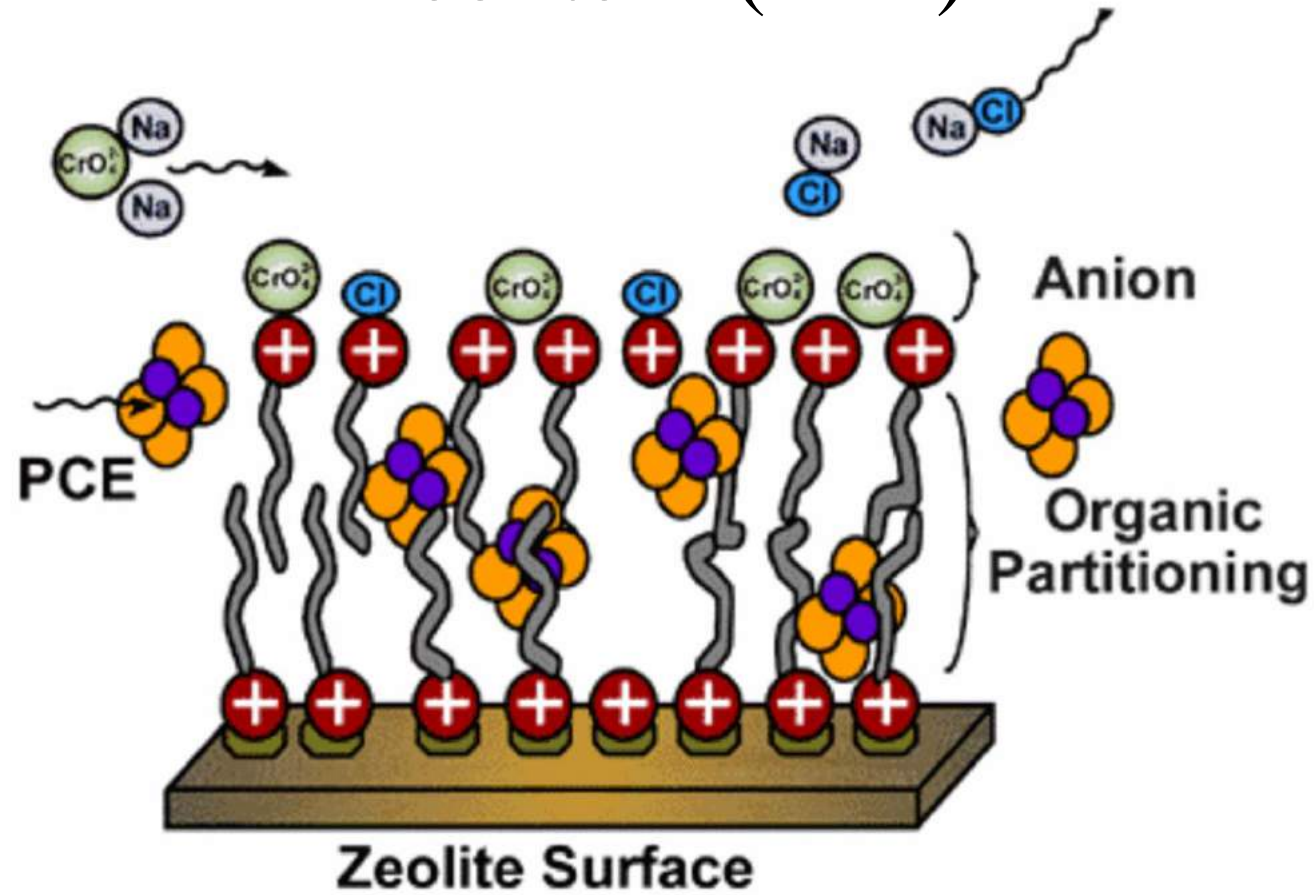


Applications: Agriculture

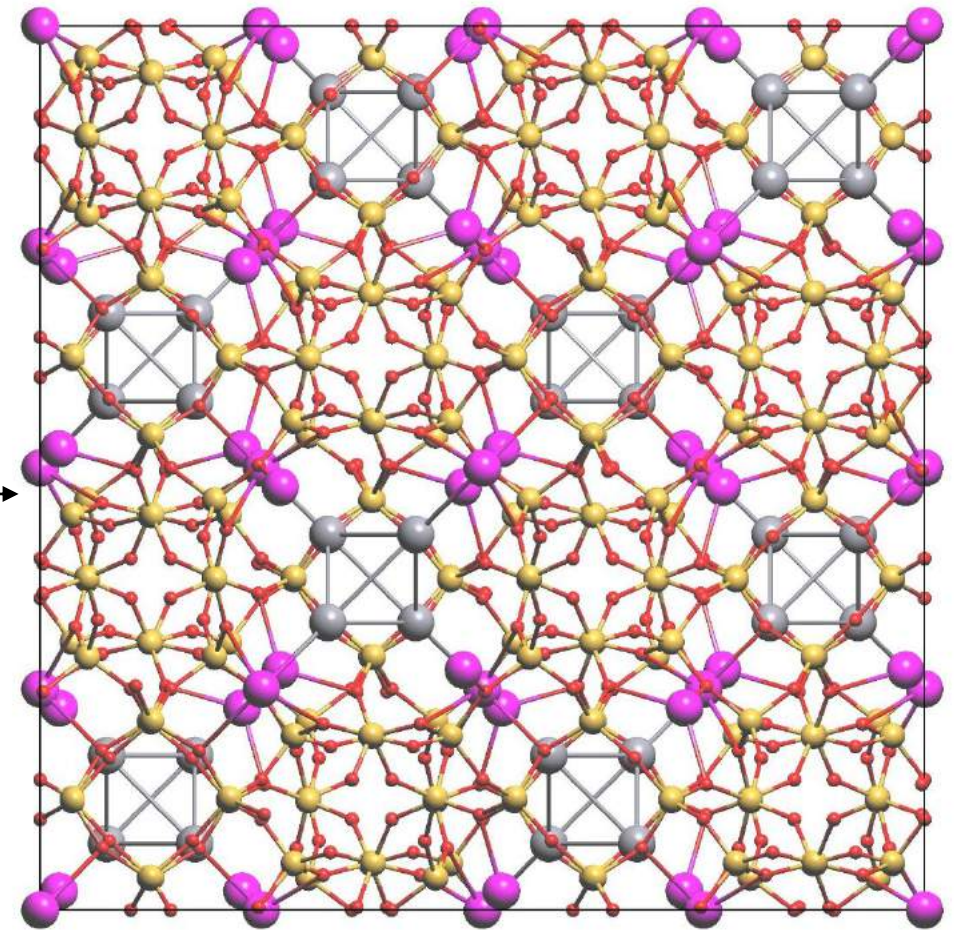
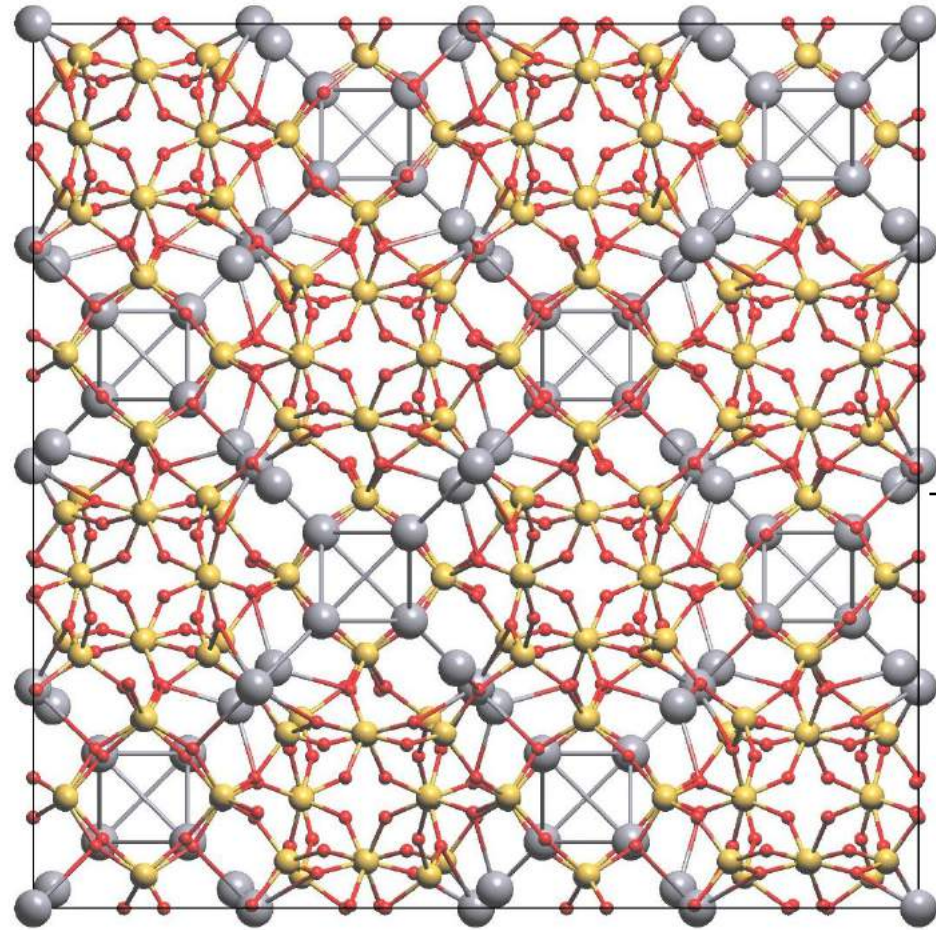
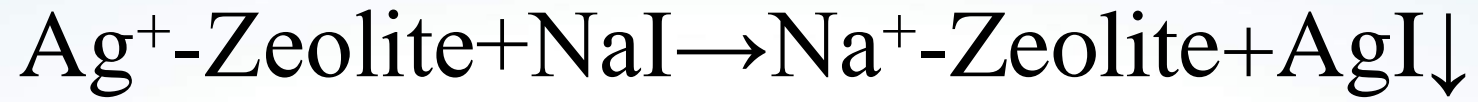


Applications: Adsorption

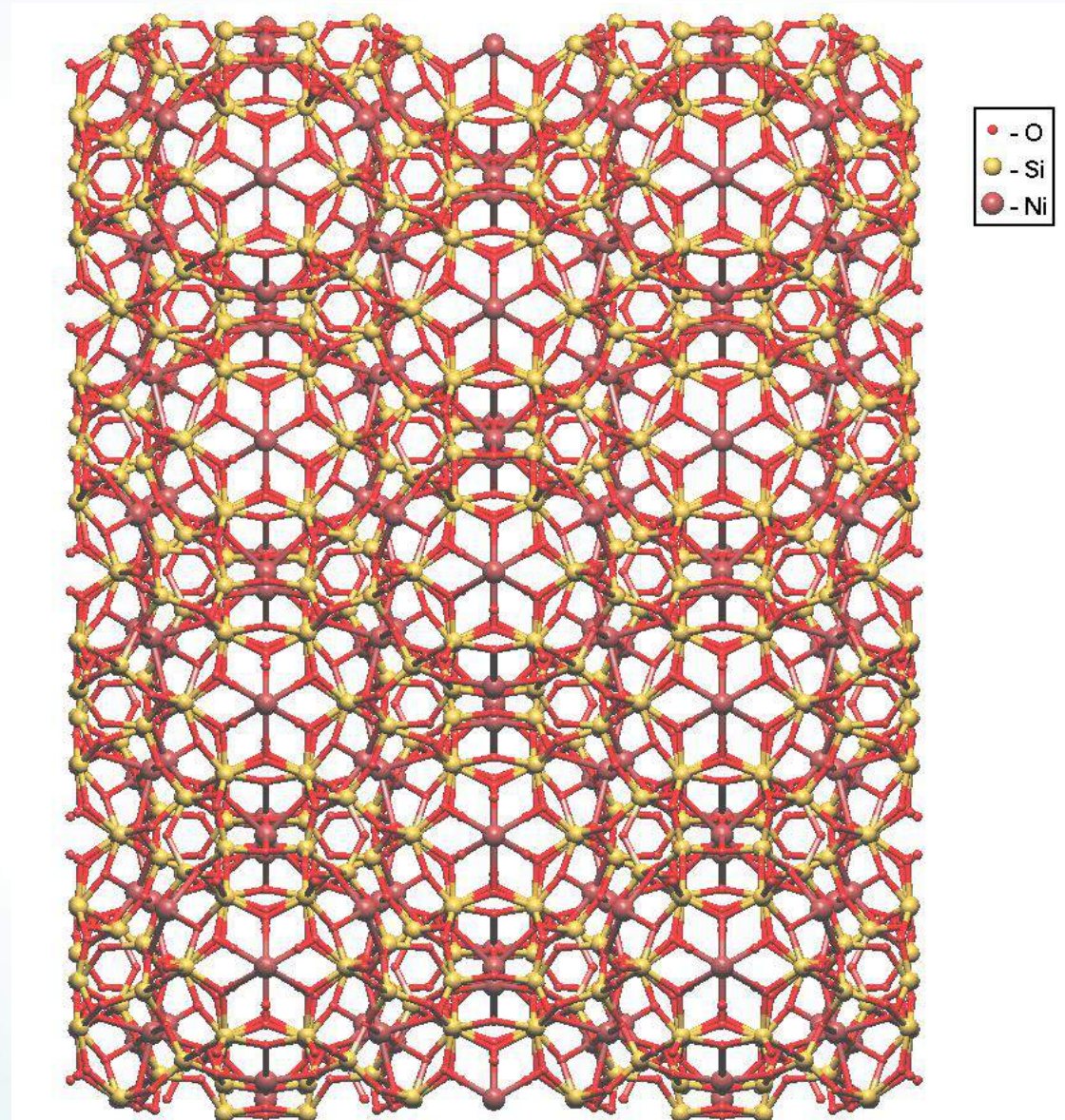
Clinoptilolite (HEU) Zeolite A (LTA)



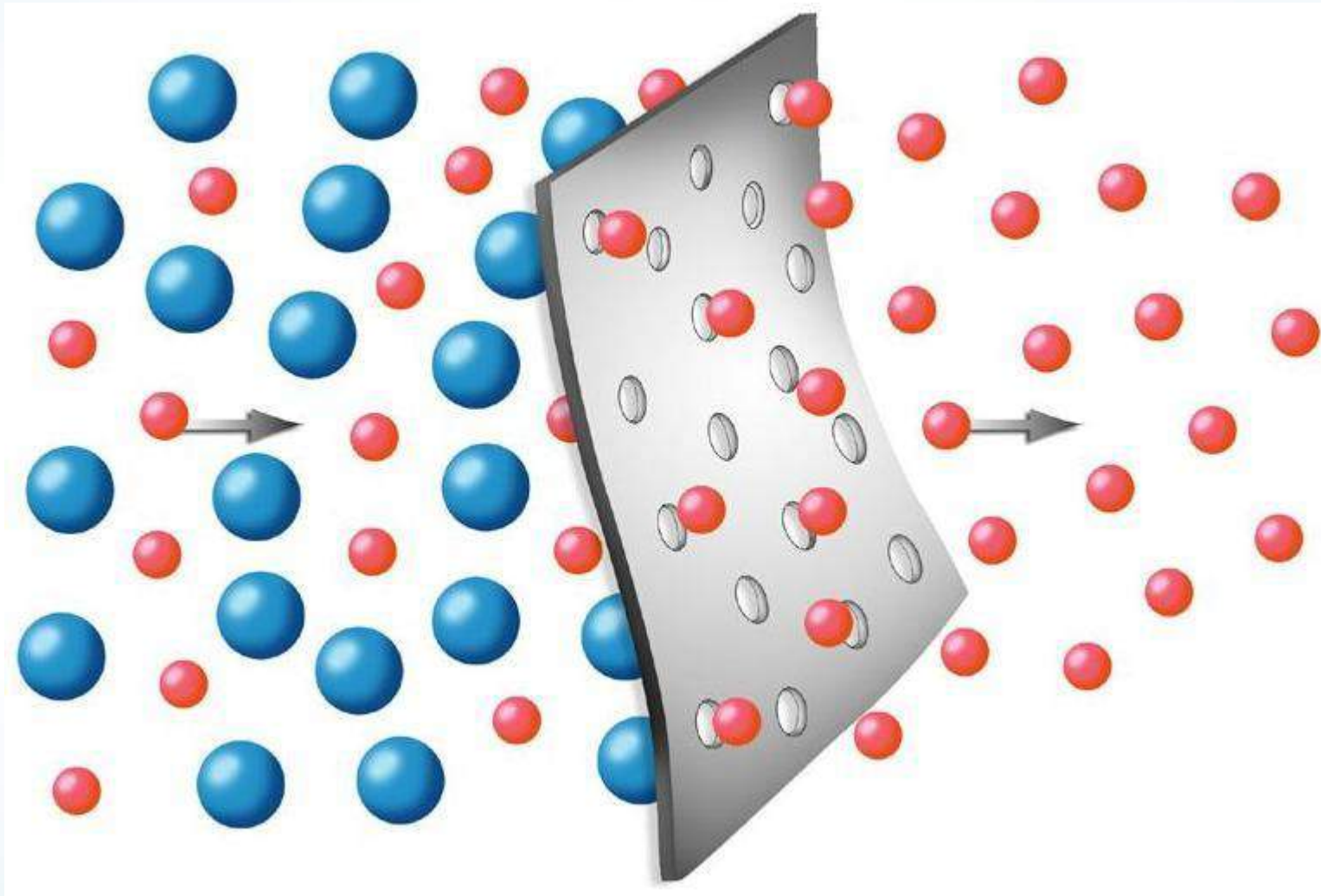
Applications: Anion adsorption



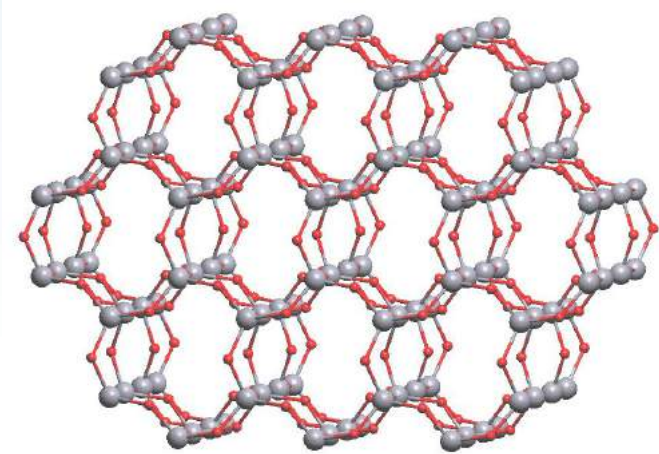
Applications: Adsorption



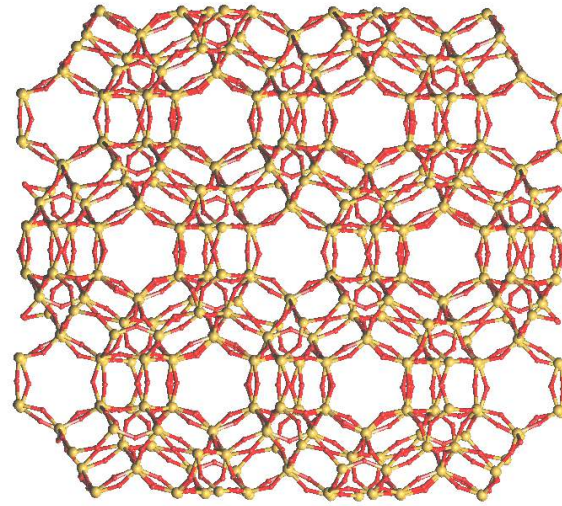
Applications: Molecular sieves



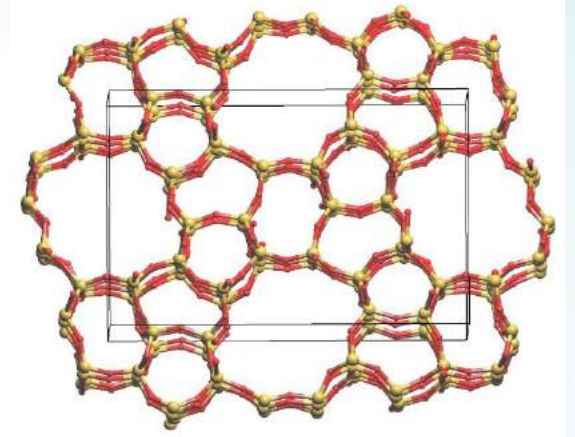
Applications: Molecular sieves



Zeolite A (LTA)



Zeolite Y (FAY)



H-ZSM-5 (MFI)

Drying agent

Hydrocarbon sieving

Separation of gases



References

1. <http://iza-structure.org>
2. Fischer R. X., Baur W. H. Materials with Zeolite-Type Structures. Landolt-Börnstein Numerical Data and Functional Relationships in Science and Technology. Group IV: Physical Chemistry Volume 14.
3. Christopher J. Rhodes Properties and applications of zeolites Science Progress (2010), 93(3), 1–63
4. Haw, J.F. (2002) Phys. Chem. Chem. Phys., 4, 5431.
5. Corma, A. and Garcia, H. (2004) Eur. J. Chem., 1143

Thank you for your attention

