

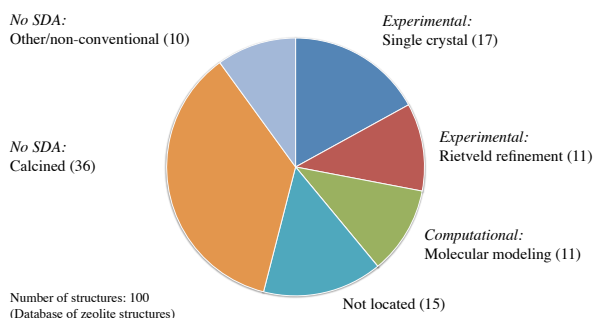
# HOW DO THE POSITIONS OF SDAs DETERMINED FROM XRPD DATA COMPARE WITH THOSE OBTAINED FROM MOLECULAR MODELING?

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## Introduction

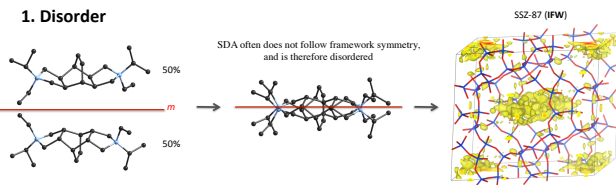
Determining the location of the organic structure-directing agent (SDA) inside the channel system of a zeolite is a long-standing problem in zeolite structural science. We have developed a method that can be used to determine the location of the SDA in most cases.

## Location of organic SDA in zeolite structures 1998-2015

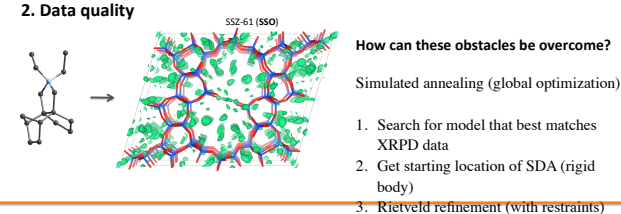


## Obstacles in locating the SDA

### 1. Disorder



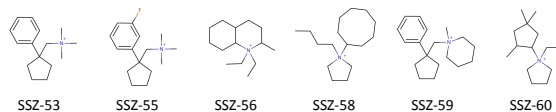
### 2. Data quality



## Can simulated annealing be applied routinely to locate the SDA?

- Six known borosilicate zeolites studied
- Known frameworks
  - Different, flexible SDAs
  - SDA located with molecular modeling<sup>1</sup>
1. Locate SDA with simulated annealing
  2. Verify/refine location via Rietveld refinement
  3. Compare with modeling results

	ftc	a	b	c	$\alpha$	$\beta$	$\gamma$	Spgr.
SSZ-53 <sup>2</sup>	SFH	5.02	33.74	21.17			90.5	C2/c
SSZ-55 <sup>3</sup>	ATS	12.95	21.85	5.08				Cmc2 <sub>1</sub>
SSZ-56 <sup>4</sup>	SFS	13.95	19.90	12.36			106.7	P2 <sub>1</sub> /m
SSZ-58 <sup>5</sup>	SFG	25.11	12.50	12.86				Pmma
SSZ-59 <sup>6</sup>	SFN	5.02	12.74	14.72	103.4		90.5	P-1
SSZ-60 <sup>6</sup>	SSY	21.95	13.70	5.01				P2 <sub>1</sub>

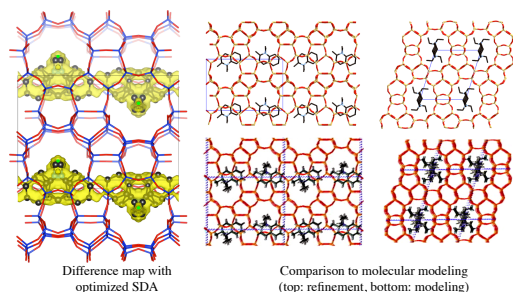


## Conclusions

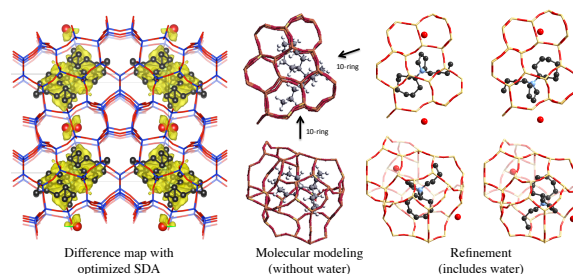
1. Can simulated be applied routinely to locate the SDA? – Yes, in most cases...
2. Flexibility of simulated annealing is ideal for structure completion
3. Difference maps roughly show the location of the SDA
4. Results may differ when simulations are performed using an incomplete model (no B, sorbed H<sub>2</sub>O)
5. The final structure should make chemical sense

## Sometimes the procedure is straightforward

### SSZ-56



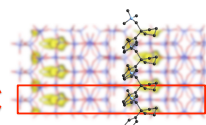
### SSZ-58



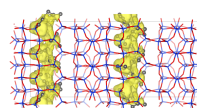
## Sometimes it takes a bit of thinking

1D channel system impedes procedure as SDAs do not fit the unit cell

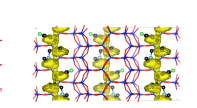
1. Expand unit cell (x3) to allow full ordering of the SDA
2. Locate SDA
3. Reduce unit cell to original (keep location of the SDA)
4. Rietveld refinement



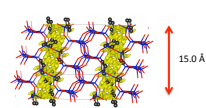
### SSZ-53



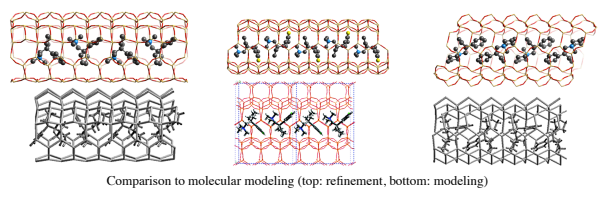
### SSZ-55



### SSZ-59

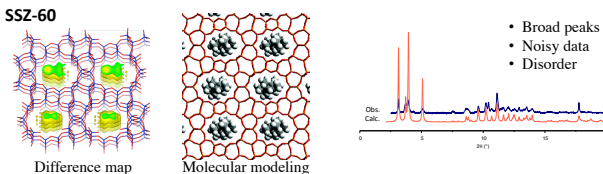


Difference map with optimized SDA



## Sometimes the data are just not good enough

### SSZ-60



## References

- <sup>1</sup> A. Burton, et al., *Micropor. Mesopor. Mat.* **90**(1-3), 129, 2006
- <sup>2</sup> A. Burton, et al., *Chem.-Eur. J.* **9**(23), 5737, 2003
- <sup>3</sup> A. Burton, et al., *J. Phys. Chem. B* **110**(11), 5273, 2006
- <sup>4</sup> S. Elomari, et al., *Micropor. Mesopor. Mat.* **118**(1-3), 325, 2009
- <sup>5</sup> A. Burton, et al., *J. Am. Chem. Soc.* **125**(6), 1633, 2003
- <sup>6</sup> A. Burton, S. Elomari, *Chem. Commun.*, 2618, 2004