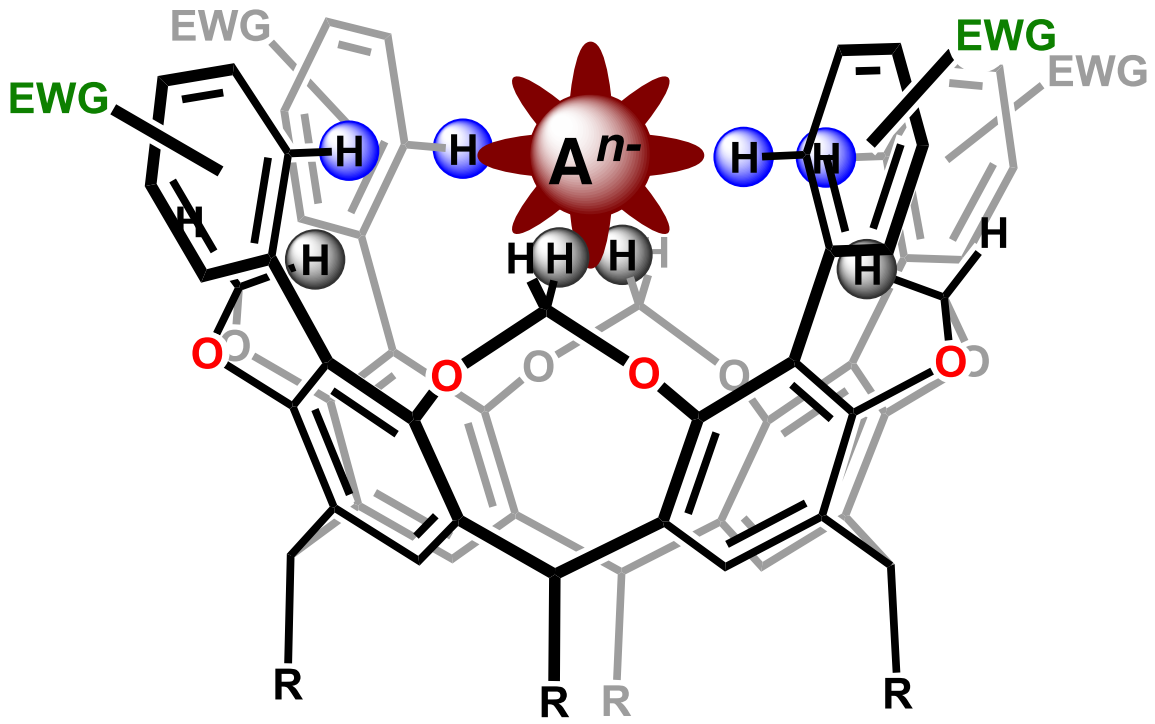
University of Pittsburgh



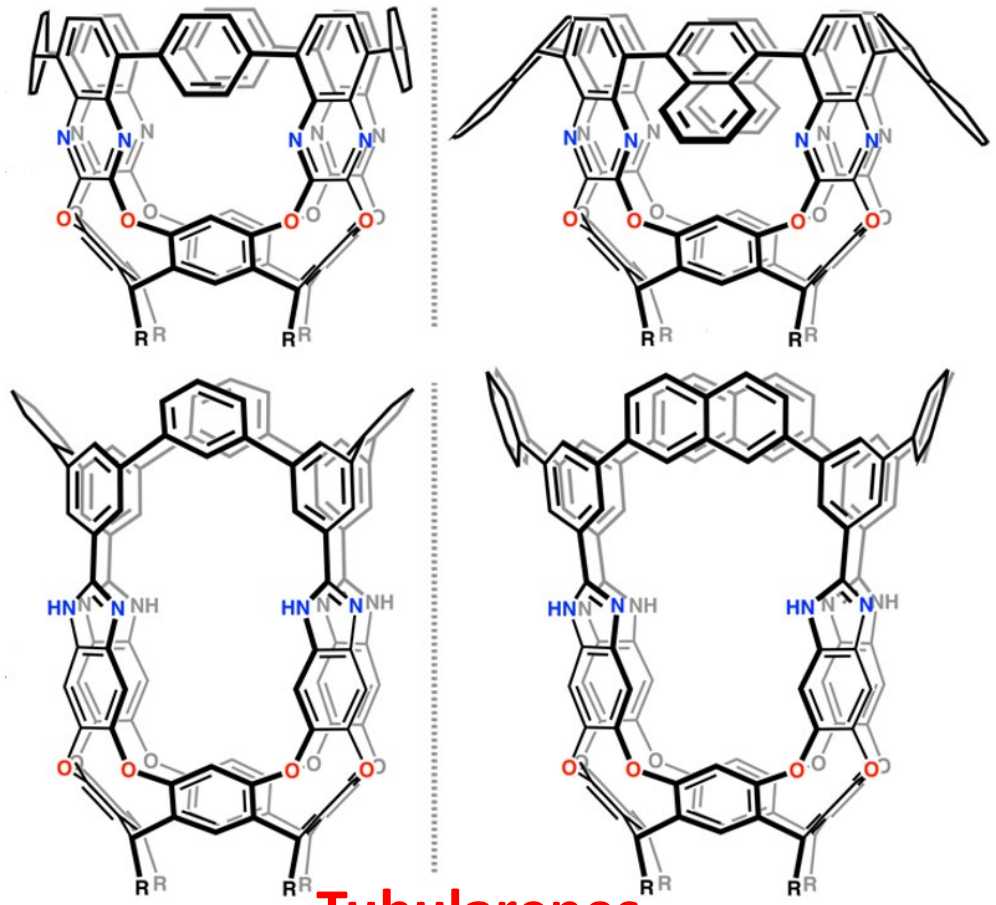
Fluorocages: C–H hydrogen bonding for the recognition of anions

Saber Mirzaei

April 6, 2021

Rational design of anion hosts to solve a problem

What we do in our lab:



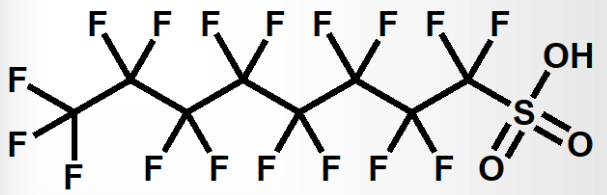
Tubularenes

Chem. Sci., **2020**,11, 8089-8094.
Org. Lett. **2021**, 23, 1, 87–92.

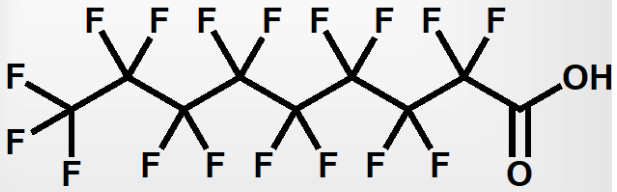
Best current technologies for PFAS removal:

1) Burn contaminated system
   *Activated carbon
2) Bury contaminated system
3) Other traditional systems to clean water not designed for PFAS

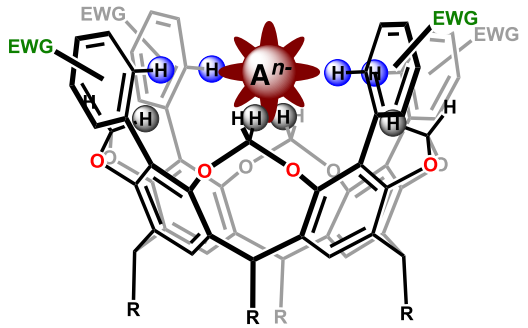
PFAS
>3000 different PFAS

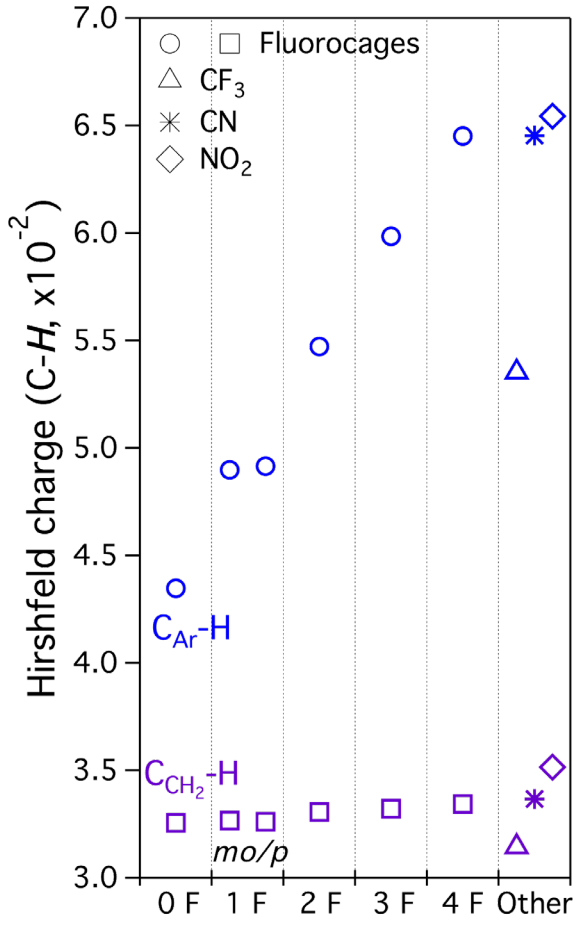


Perfluorooctanesulfonic acid (PFOS)

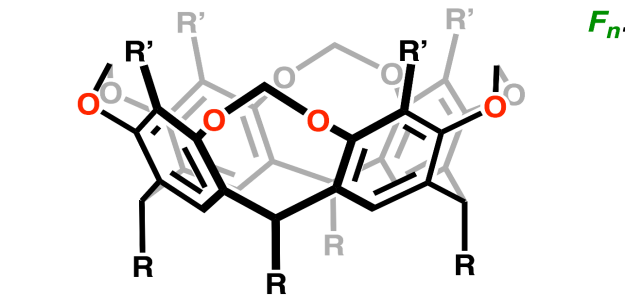


Perfluorooctanoic acid (PFAS)



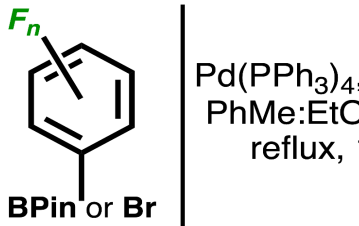


Synthesis & Characterization



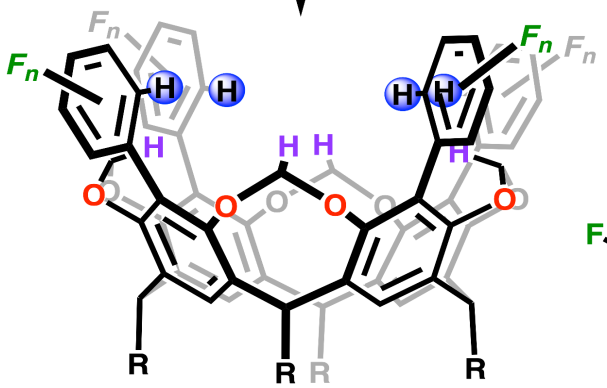
S1 (R' = Br) or **S2** (R' = BPin)

R =



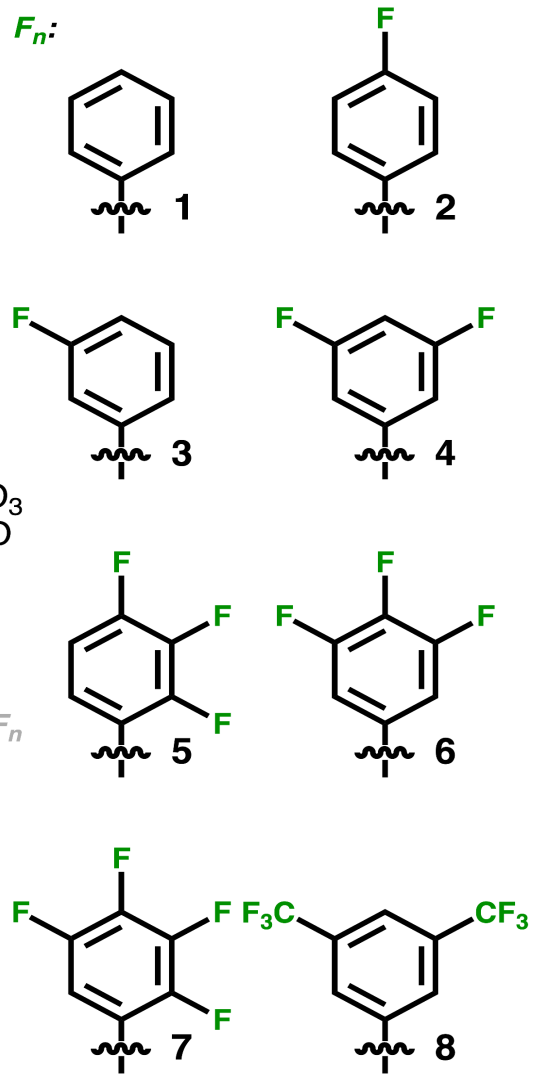
BPin or **Br**

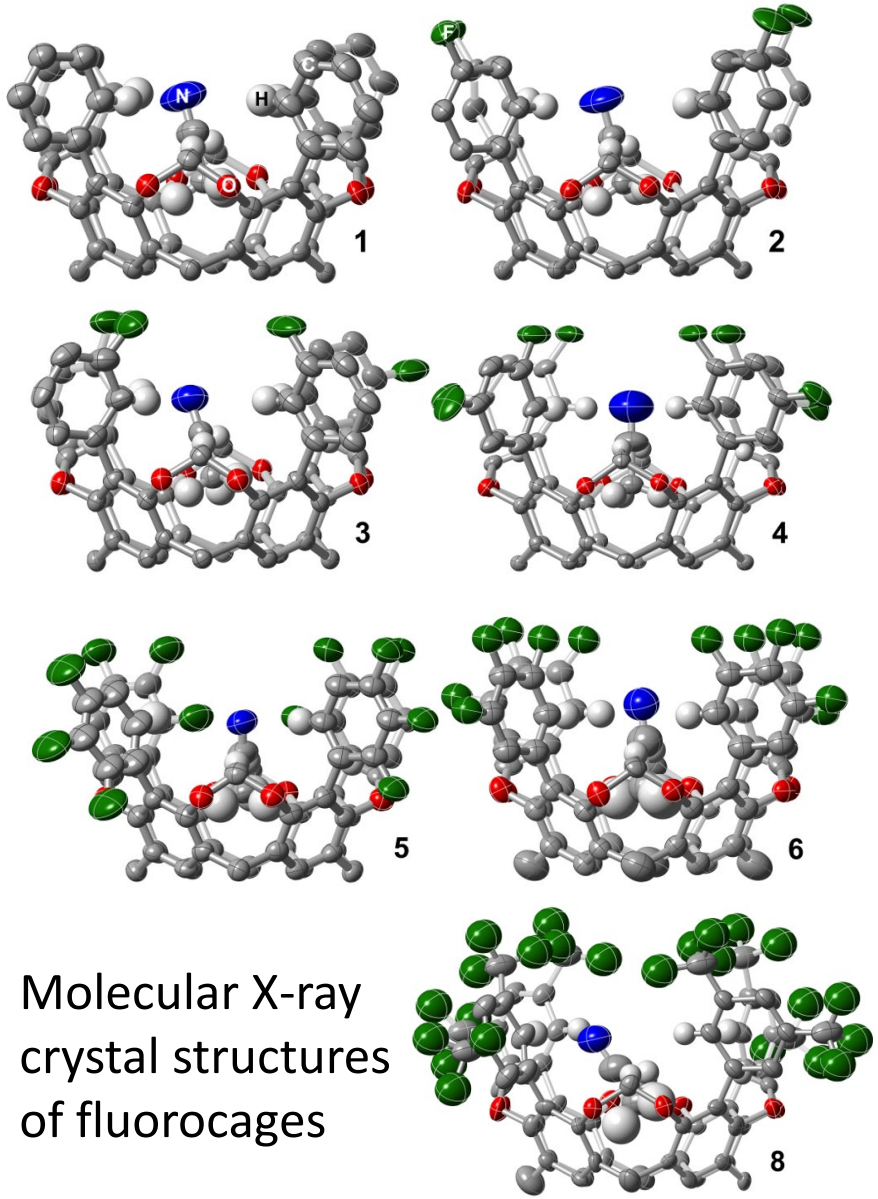
$Pd(PPh_3)_4$, K_2CO_3
PhMe:EtOH:H_2O
reflux, 12 h



Fluorocage

F_n:





Molecular X-ray crystal structures of fluorocages

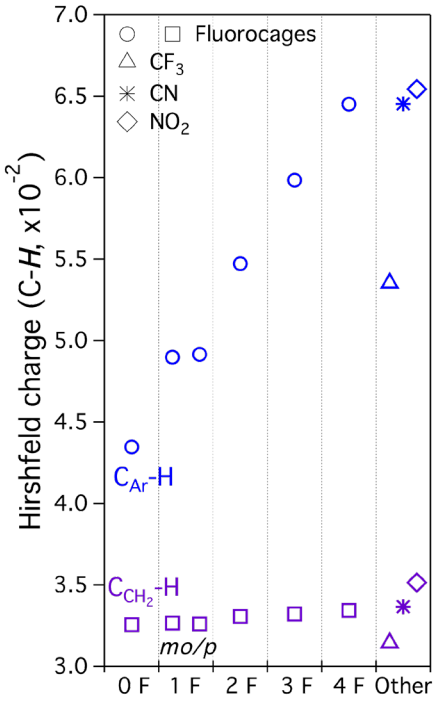
Do they work?

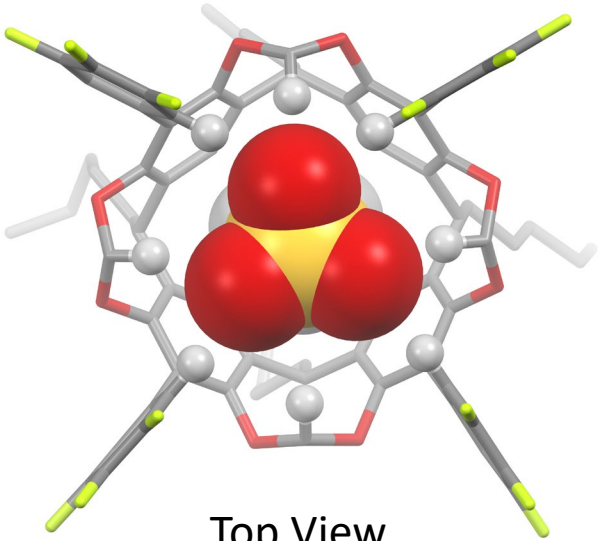
Anion association constants (K_a) of $[PF_6]^-$ and $[MeSO_3]^-$ in fluorocages 1–8.

Salt	Solvent	K_a 1	2	3	4	5	6	7	8
[*n*-Bu_4N] [PF_6]	$CDCl_3$	0.0	0.0	0.0	84±12	ND	15105± 328	ND	279±15
[*n*-Bu_4N] [$MeSO_3$]	$CDCl_3$	0.0	22±4	667±38	TBD	ND	TBD	ND	TBD

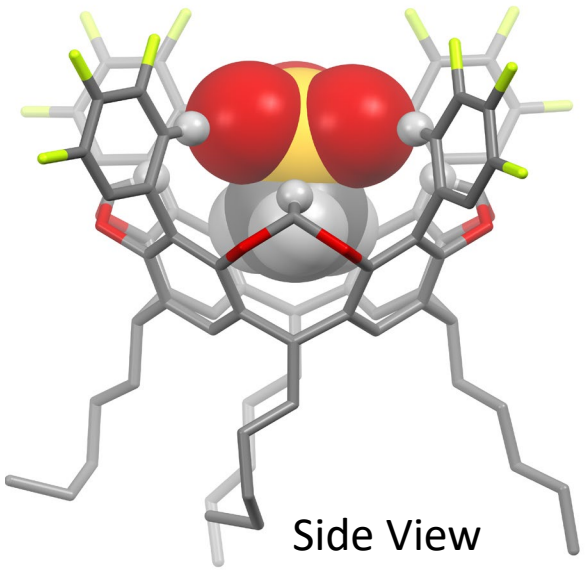
ND = Not determined, TBD = To be determined

Boss: Raúl Hernández Sánchez



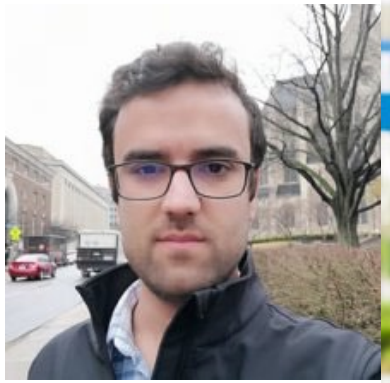


Top View



Side View

Single-crystal structure of $MeSO_3 \subset$ 6 cage



Students: Saber and Victor

Pitt Research
Center for Research Computing

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Arts & Sciences Graduate Fellowship