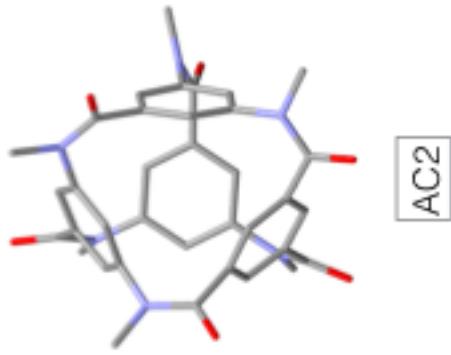
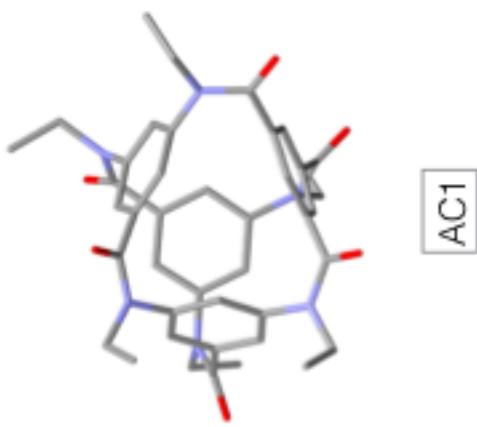


CAGEDATABASE

MARCIN MIKLITZ
JELFS GROUP

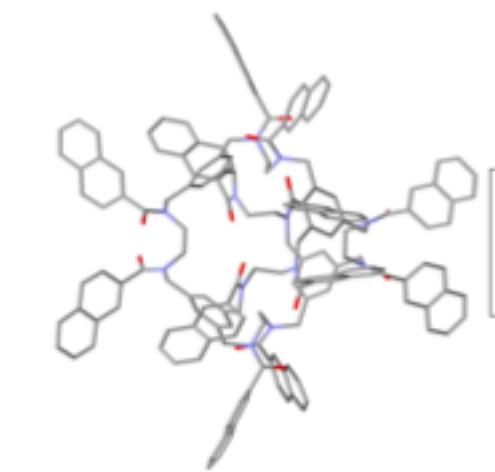


AZUMAYA CAGES

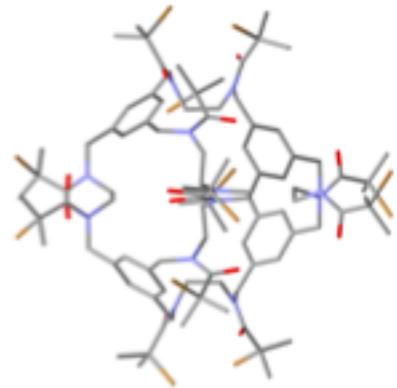


- (1) Masu, H.; Katagiri, K.; Kato, T.; Kagechika, H.; Tominaga, M.; Azumaya, I. *J. Org. Chem.* 2008, 73, 5143.
(2) Masu, H.; Sagara, Y.; Imabeppu, F.; Takayanagi, H.; Katagiri, K.; Kawahata, M.; Tominaga, M.; Kagechika, H.; Yamaguchi, K.; Azumaya, I. *CrystEngComm* 2011, 13, 406.

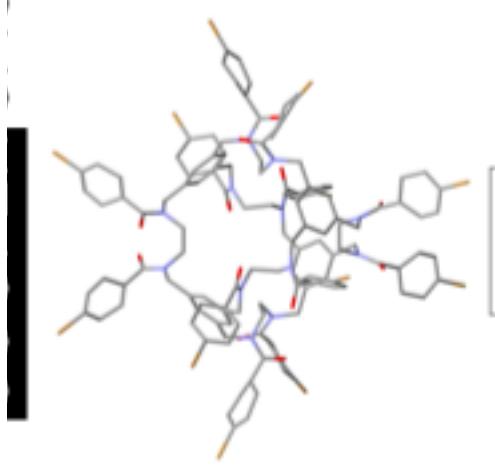
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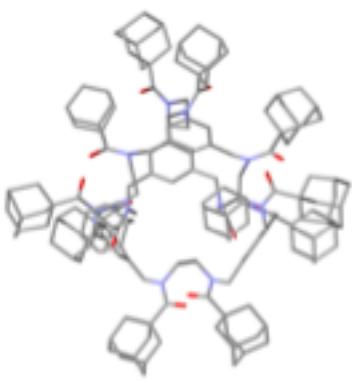
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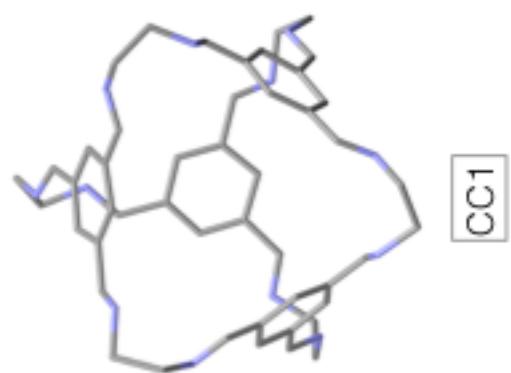
CC1_R4



CC1_R1



CC1_R3



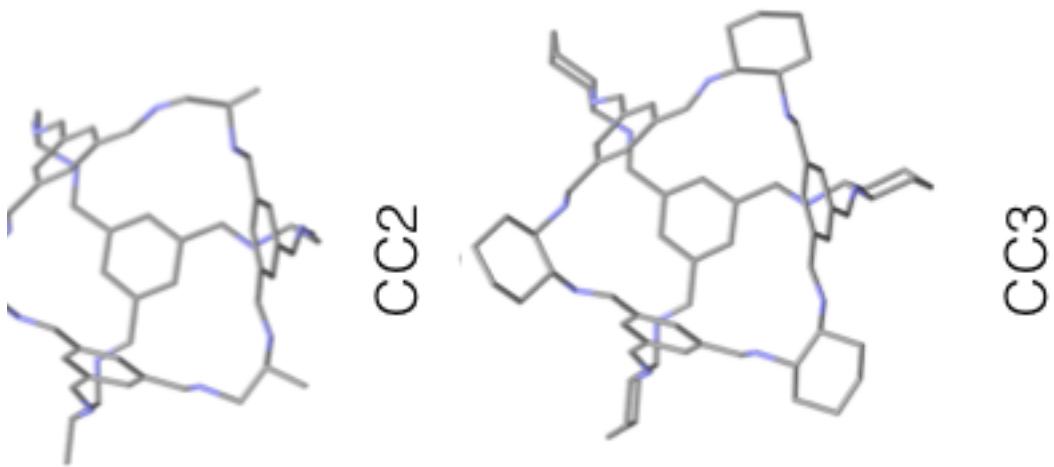
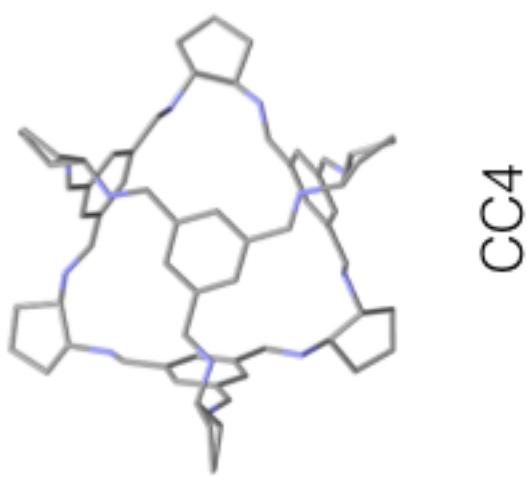
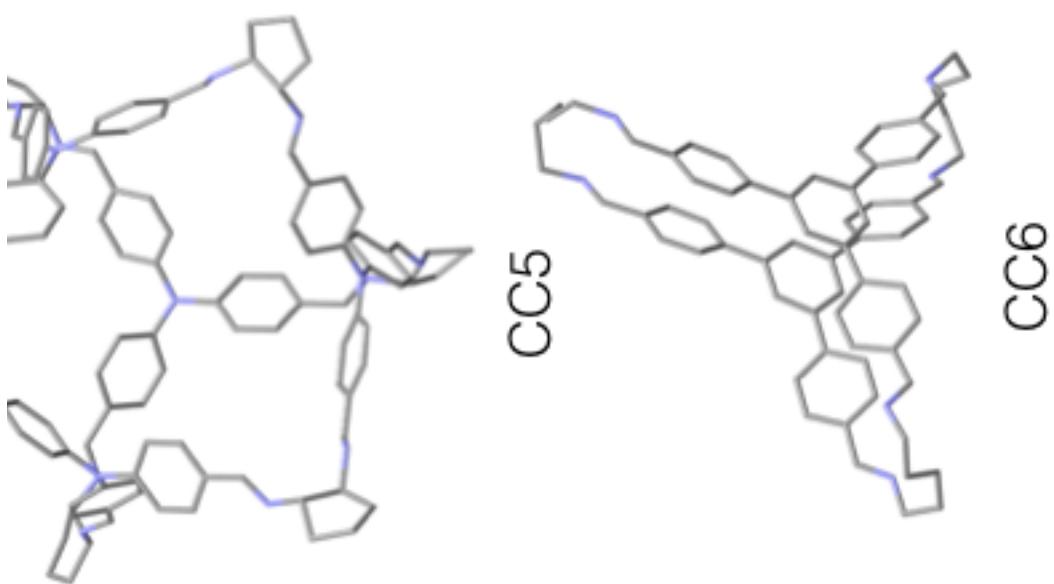
CC1

R1-R4: culshaw, J. L.; Cheng, G.; Schmidtmann, M.; Hasell, T.; Liu, M.; Adams, D. J.; Cooper, A. I. J. Am. Chem. Soc. 2013, 135, 10007.

COOPER CAGES

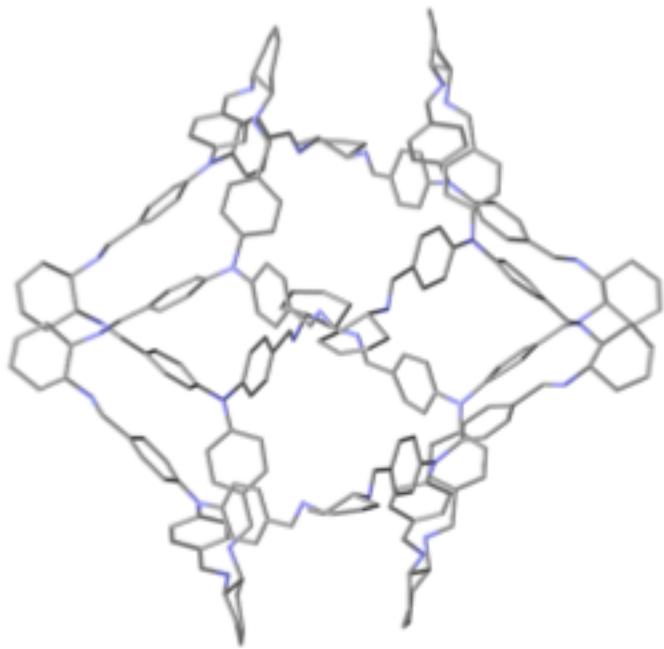


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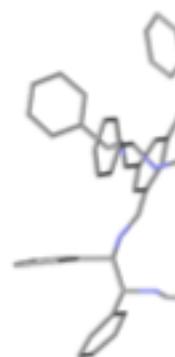
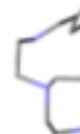
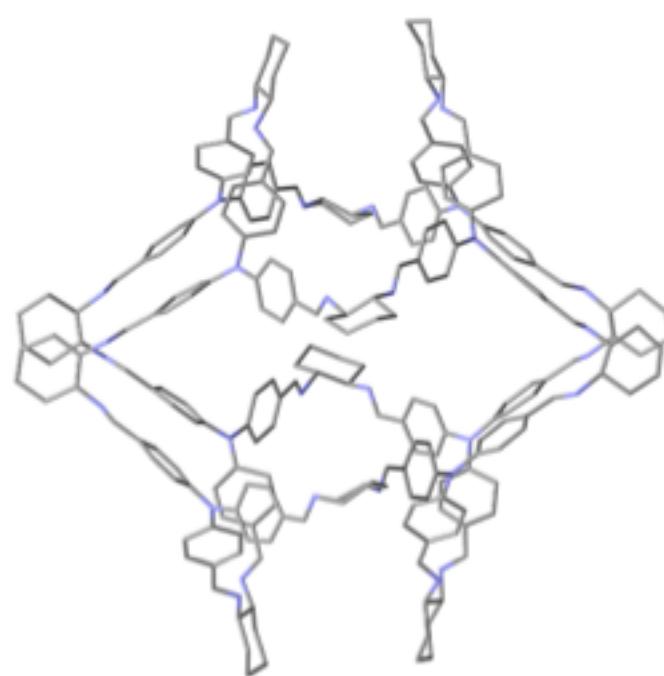


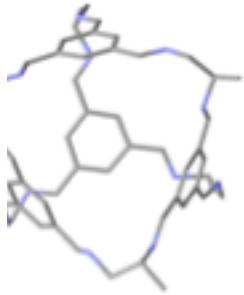
COOPER CAGES

CC8

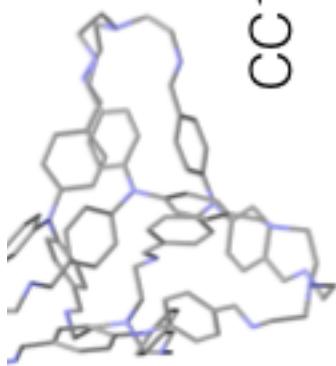


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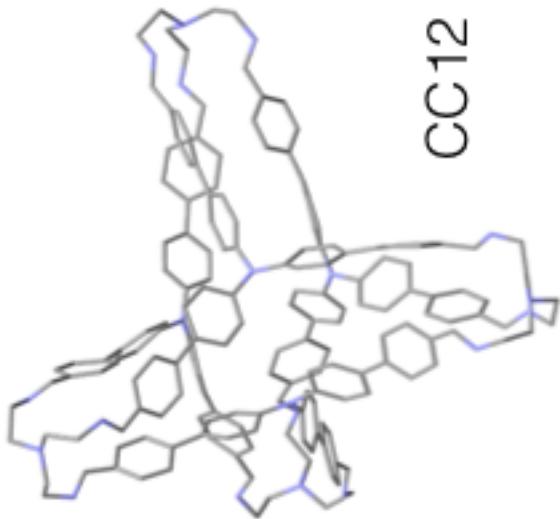




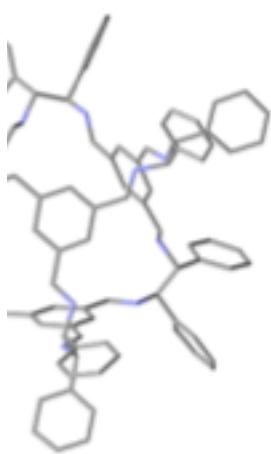
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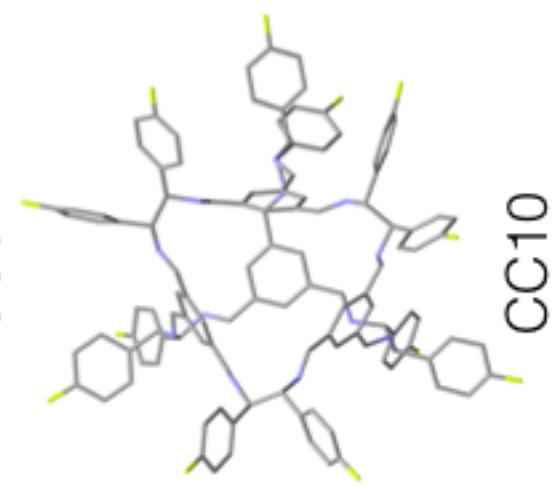
CC11



CC12



CC9



CC10

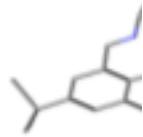
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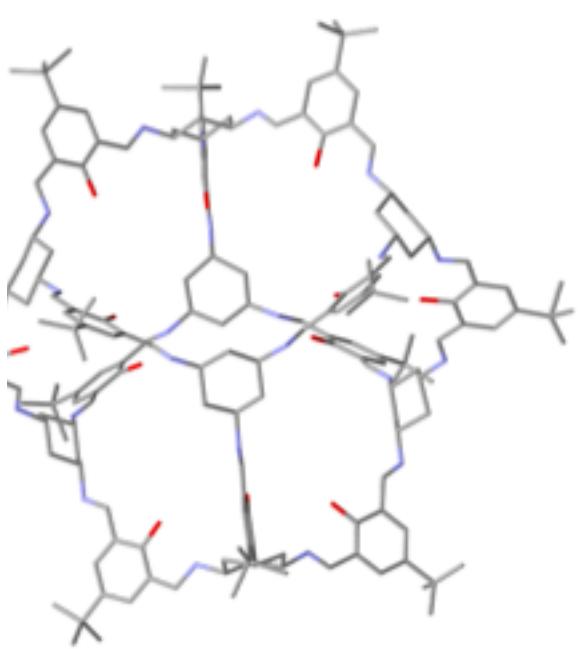


DC1

(1) Avellaneda, A.; Valente, P.; Burgun, A.; Evans, J. D.; Markwell-Heys, A. W.; Rankine, D.; Nielsen, D. J.; Hill, M. R.; Sumbry, C. J.; Doonan, C. J. *Angew. Chem. Int. Ed. Engl.* 2013, 52, 3746.

GAWRONSKI CAGE

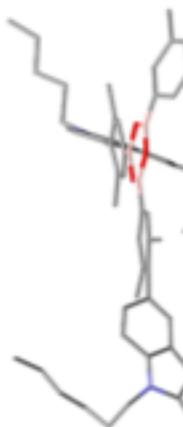


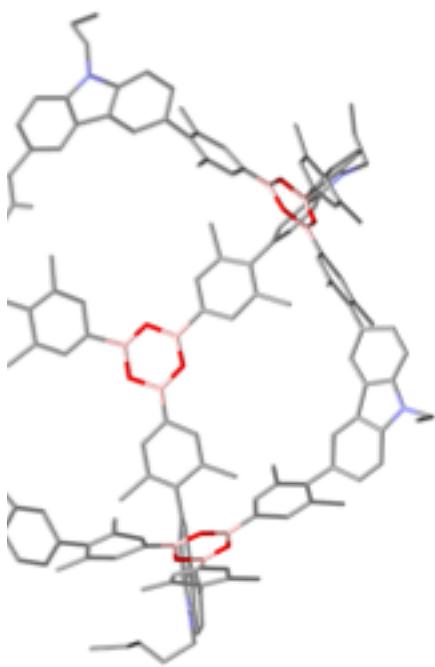


GC1

(1) Skowronek, P.; Waržaitis, B.; Rychlewska, U.; Gawroński, J. Chem. Commun. 2013, 49, 2524.

IWASAWA CAGE

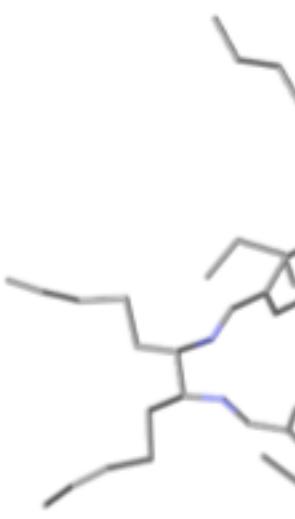


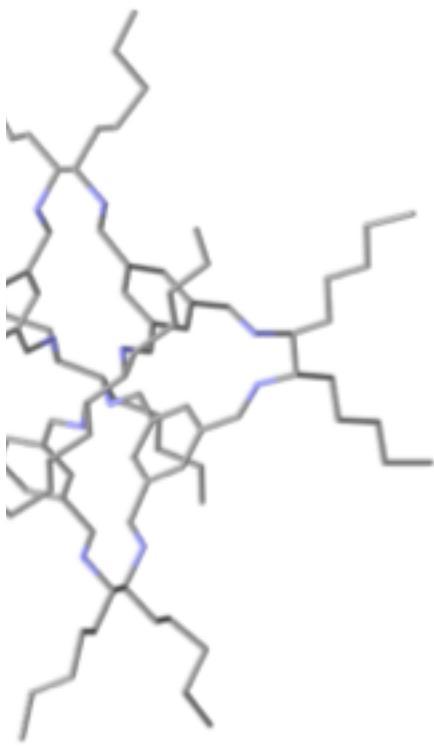


IC1

(1) Ono, K.; Johmoto, K.; Yasuda, N.; Uekusa, H.; Fujii, S.; Kiguchi, M.; Iwasa, N. J. Am. Chem. Soc. 2015, 137, 15006.

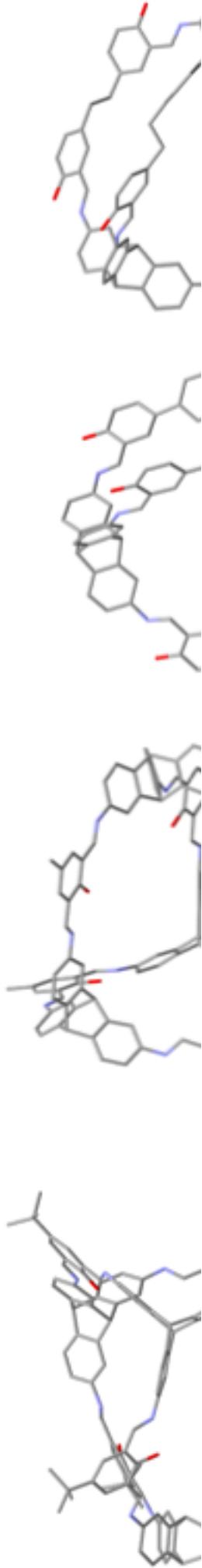
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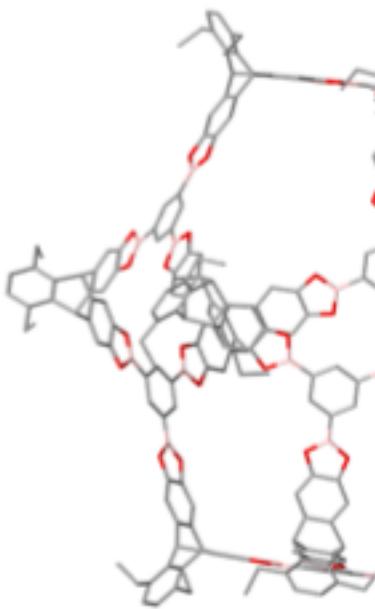
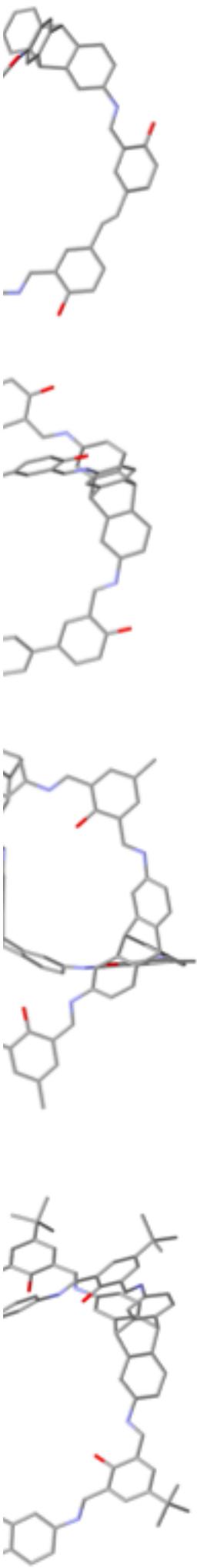


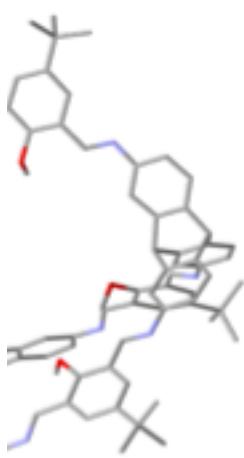
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MASTALERZ CAGES

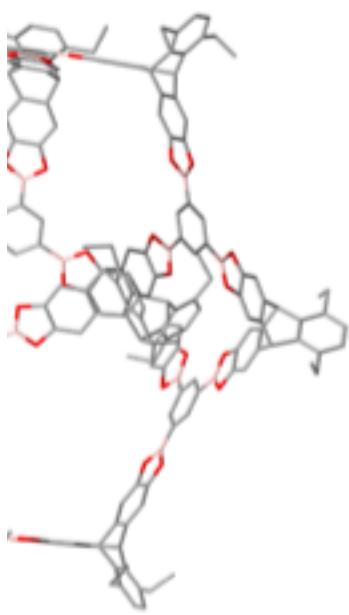


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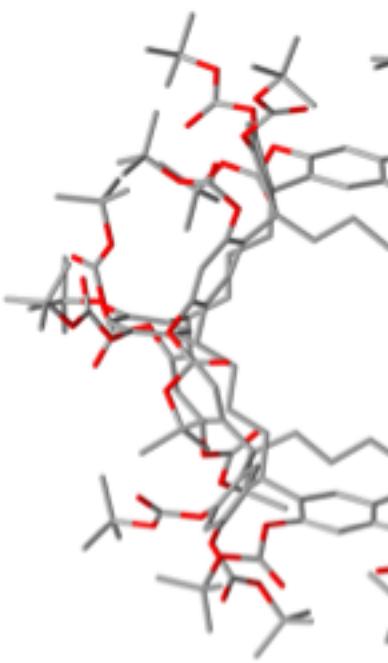
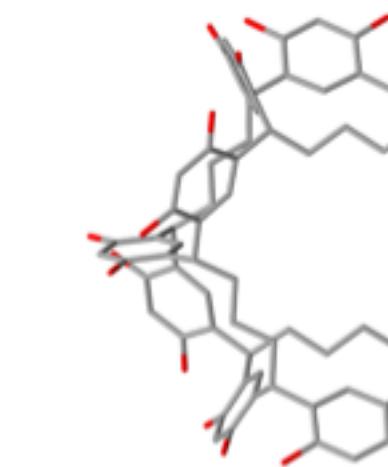


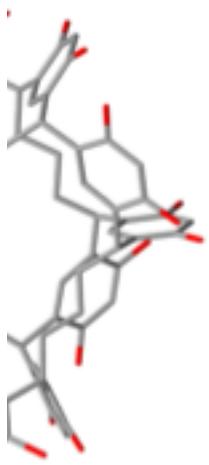
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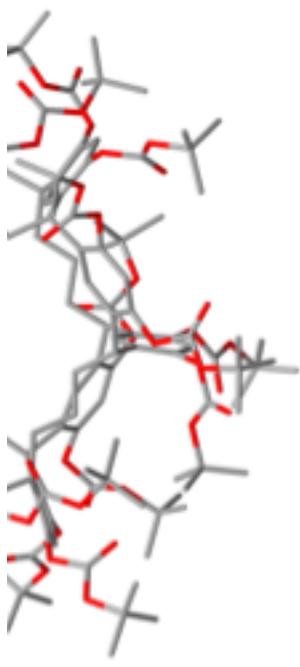
MC6

'NORIA' CAGES





NC1



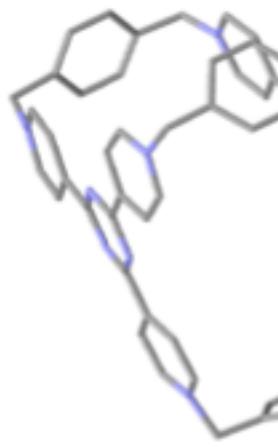
NC2

STODDART CAGES

'ExCage'



'BlueCage'





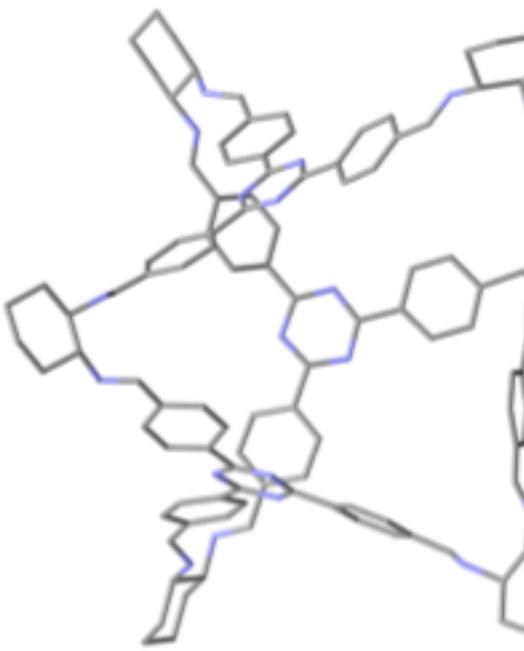
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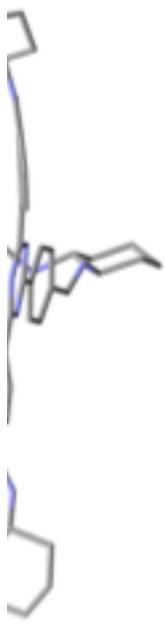
- (1) Dale, E. J.; Vermeulen, N. A.; Thomas, A. A.; Barnes, J. C.; Jur, M.; Blackburn, A. K.; Strutt, N. L.; Sarjeant, A. A.; Stern, C. L.; Denmark, S. E.; Stoddart, J. F. *J. Am. Chem. Soc.* 2014, 136, 10669.
- (2) Hafezi, N.; Holcroft, J. M.; Hartlieb, K. J.; Dale, E. J.; Vermeulen, N. a; Stern, C. L.; Sarjeant, A. a; Stoddart, J. F. *2015*, 456.



SC2

WANG CAGE

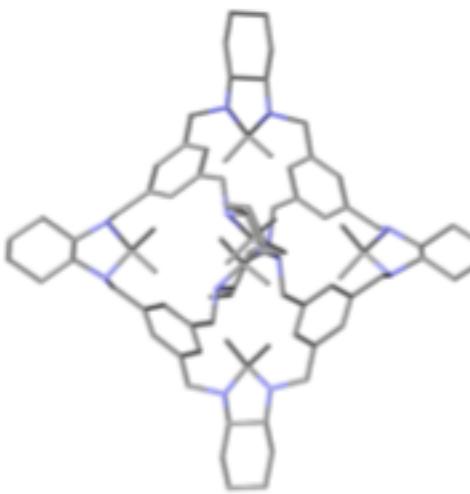




WC1

(1) Ding, H.; Yang, Y.; Li, B.; Pan, F.; Zhu, G.; Zeller, M.; Yuan, D.; Wang, C. Chem. Commun. 2015, 51, 1976.

NEW CAGES (that I would add to the database)



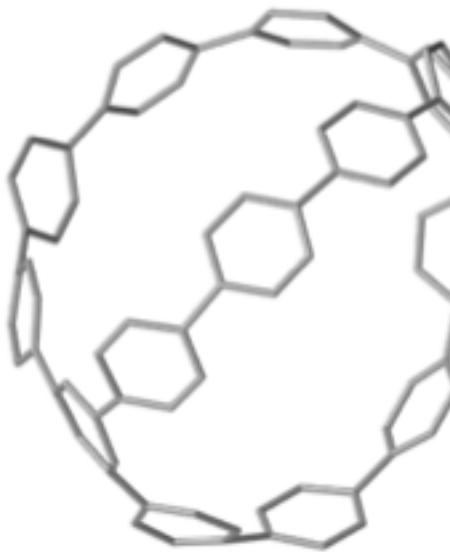
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CC3_R1
VOMPEU

↙

CC3_R2
VOMPAQ

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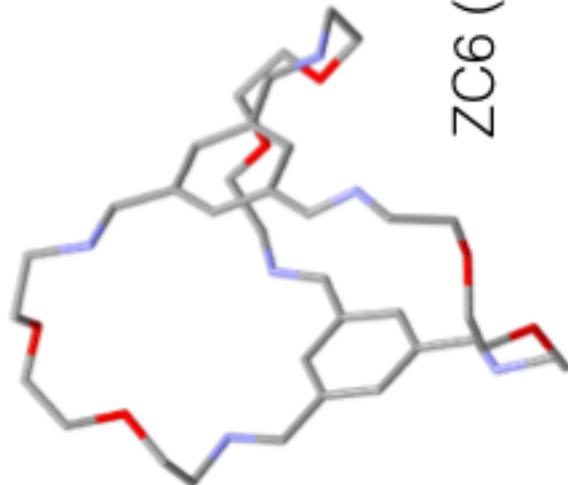




ZC5

(1) Matsui, K.; Segawa, Y.; Itami, K. J. Am. Chem. Soc. 2014, 136, 16452.

NEW CAGES (that I would add to the database)

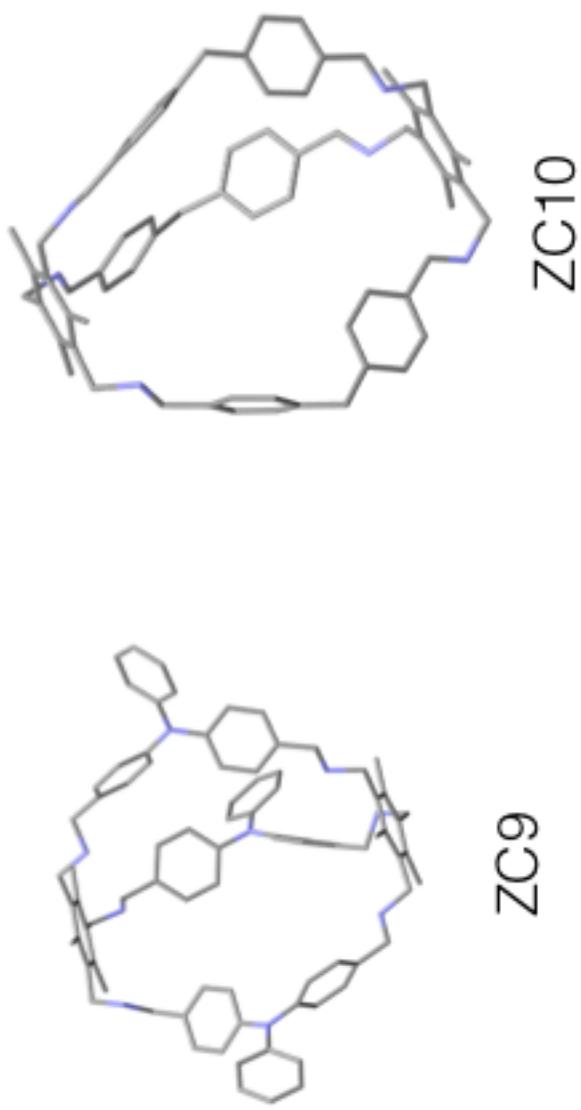


ZC6 (NITYOG)

(1) Pun, A. B.; Gagnon, K. J.; Klivansky, L. M.; Teat, S. J.; Li, Z.-T.; Liu, Y. Org. Chem. Front. 2014, 1, 167.

(2) Pun, A.; Hanifi, D. a; Kiel, G.; O'Brien, E.; Liu, Y. Angew. Chem. Int. Ed. Engl. 2012, 51, 13119.

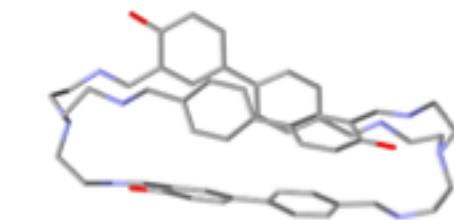
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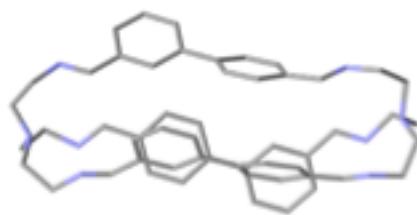
(1) Acharyya, K.; Mukherjee, P. S. Chem. Commun. 2014, 50, 15788.

(2) Acharyya, K.; Mukherjee, S.; Mukherjee, P. S. J. Am. Chem. Soc. 2013, 135, 554.

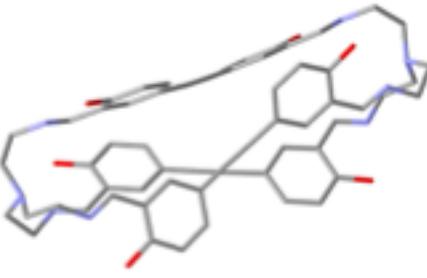
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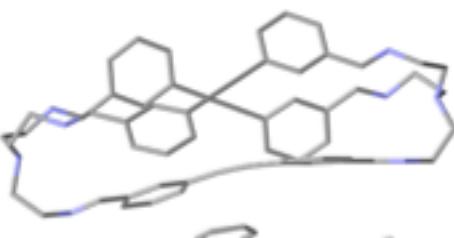
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ZC13



ZC12

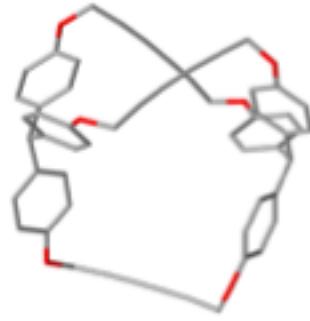


ZC11

(1) Acharyya, K.; Mukherjee, P. S. Chemistry 2014, 20, 1646.

(2) Acharyya, K.; Mukherjee, P. S. Chem. Commun. 2015, 51, 4241.

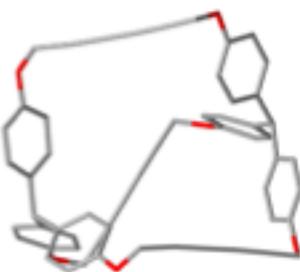
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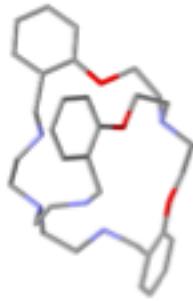
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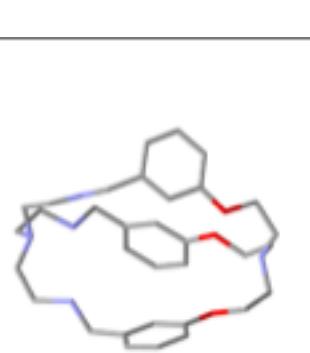
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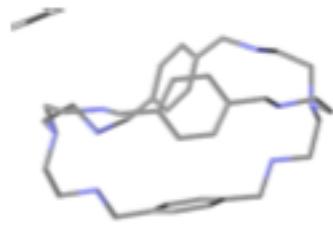


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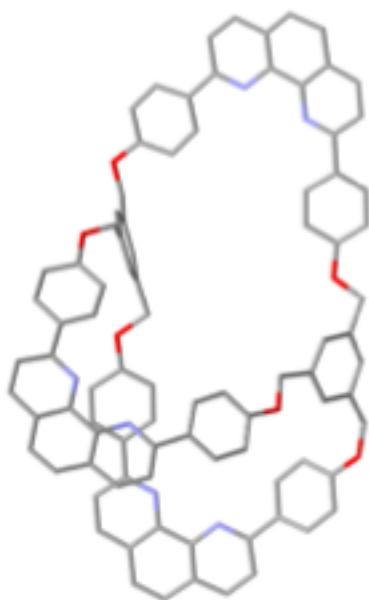


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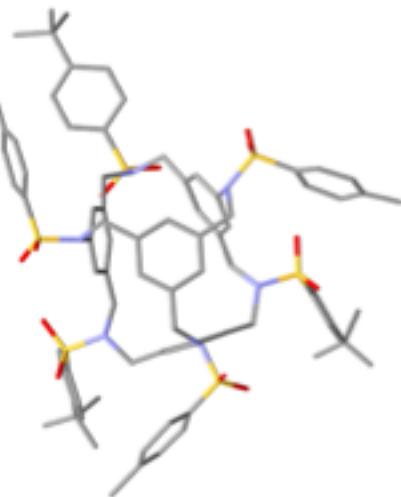
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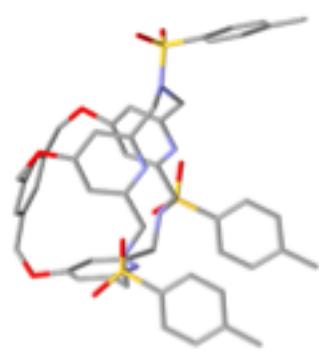


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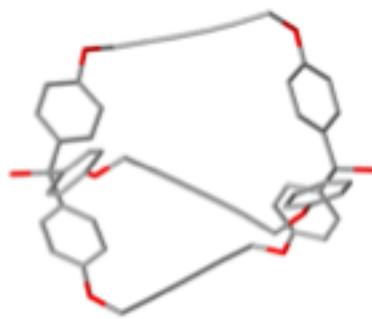


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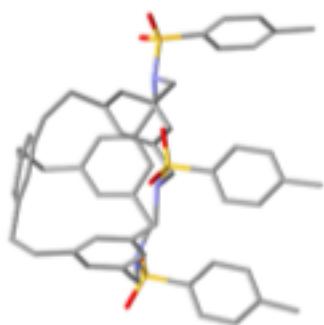
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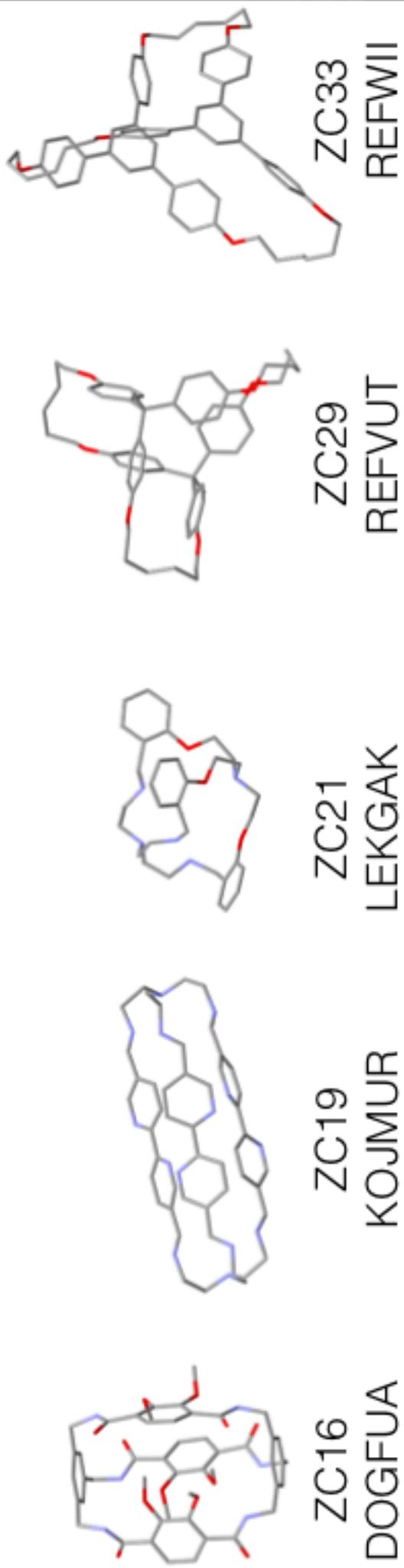


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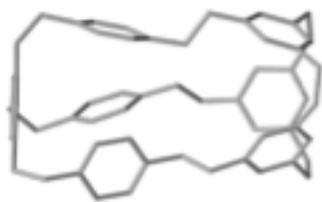
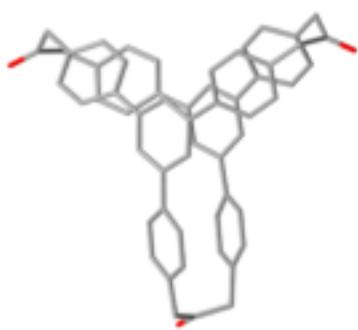


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NEW CAGES (that I *wouldn't* add to the database)



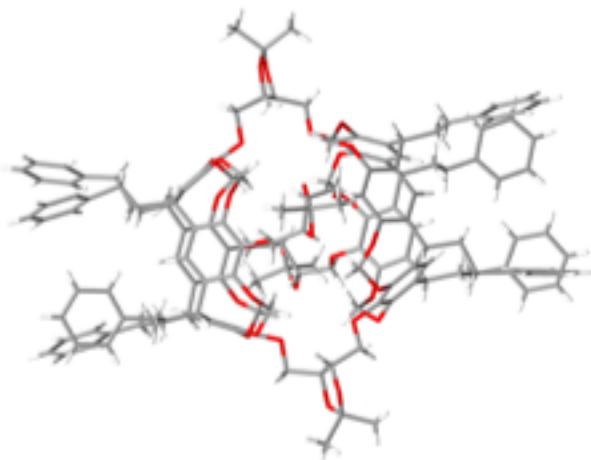
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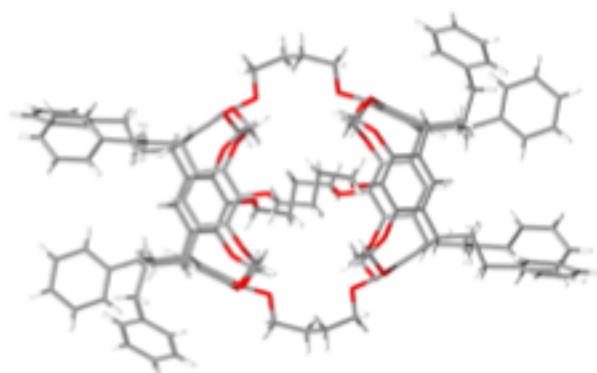
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ZC35
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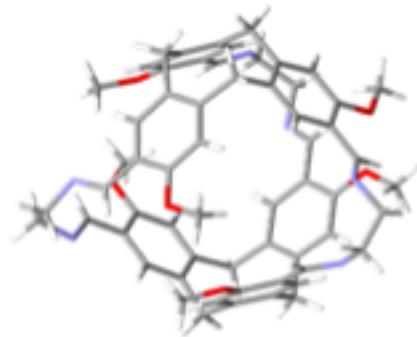
NEW CAGES (that I would add to the database)



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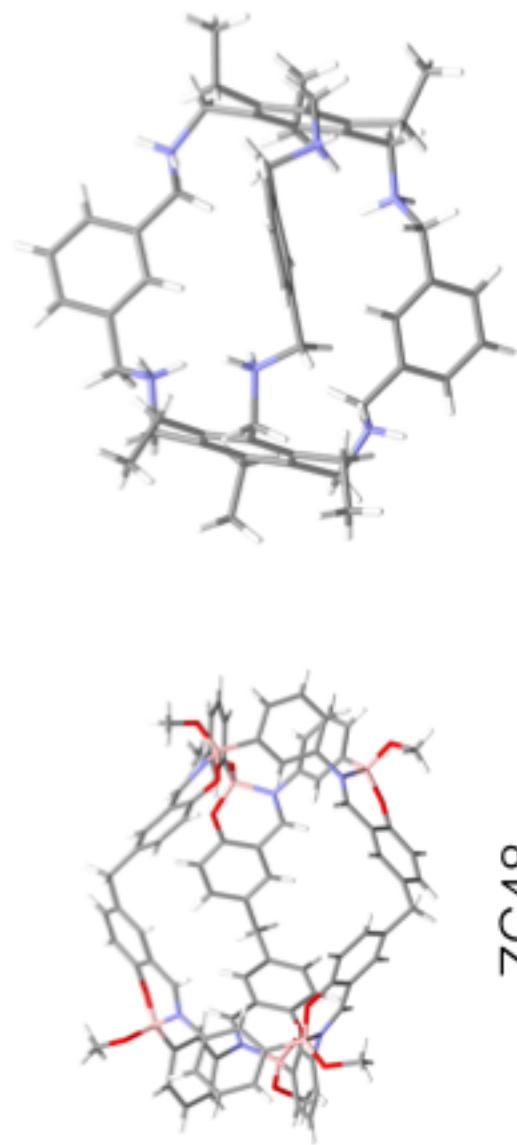
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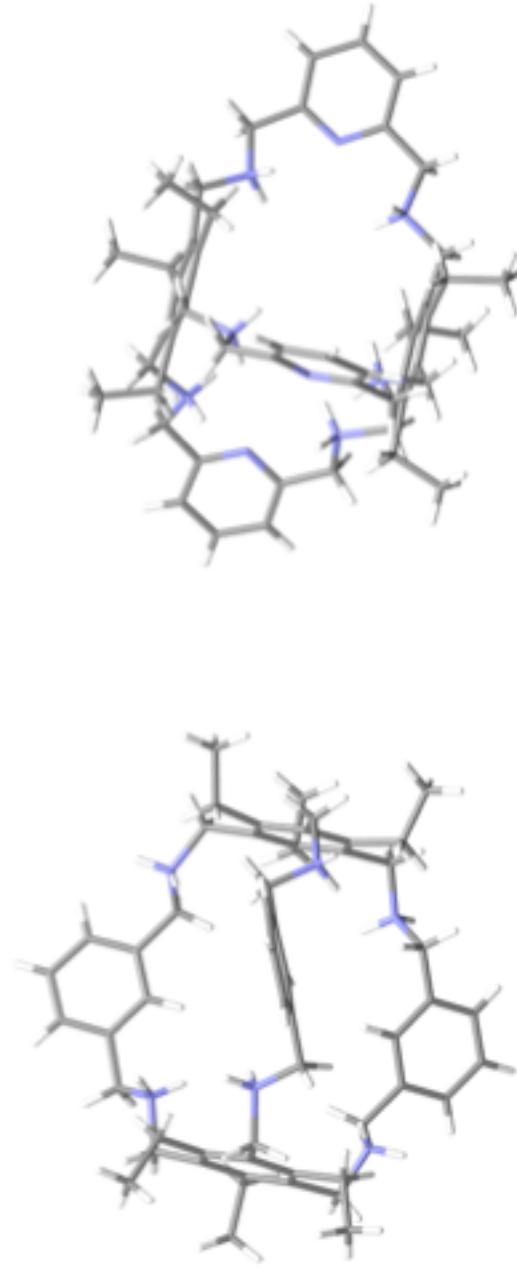
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NEW CAGES (that I would add to the database)

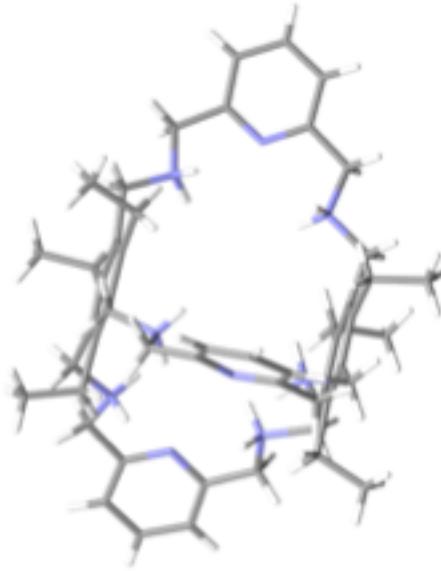
NEW CAGES (that I would add to the database)



ZC48
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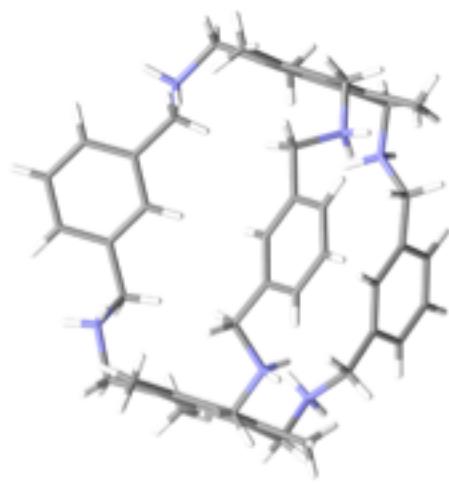
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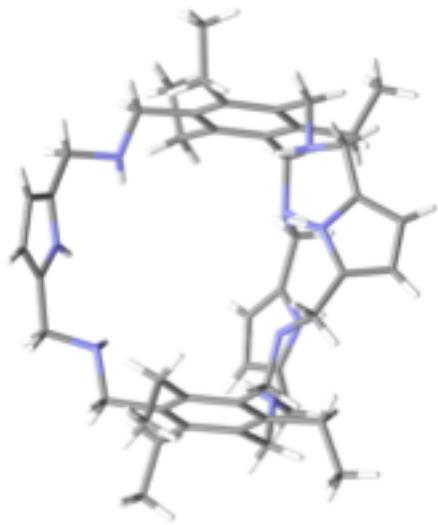
ZC50
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- (1) Barba, V.; Betanzos, I. J. Organomet. Chem. 2007, 692, 4903.
- (2) Mateus, P.; Delgado, R.; Brandão, P.; Carvalho, S.; Félix, V. Org. Biomol. Chem. 2009, 7, 4661.
- (3) Mateus, P.; Delgado, R.; Brandão, P.; Félix, V. J. Org. Chem. 2009, 74, 8638.

NEW CAGES (that I would add to the database)



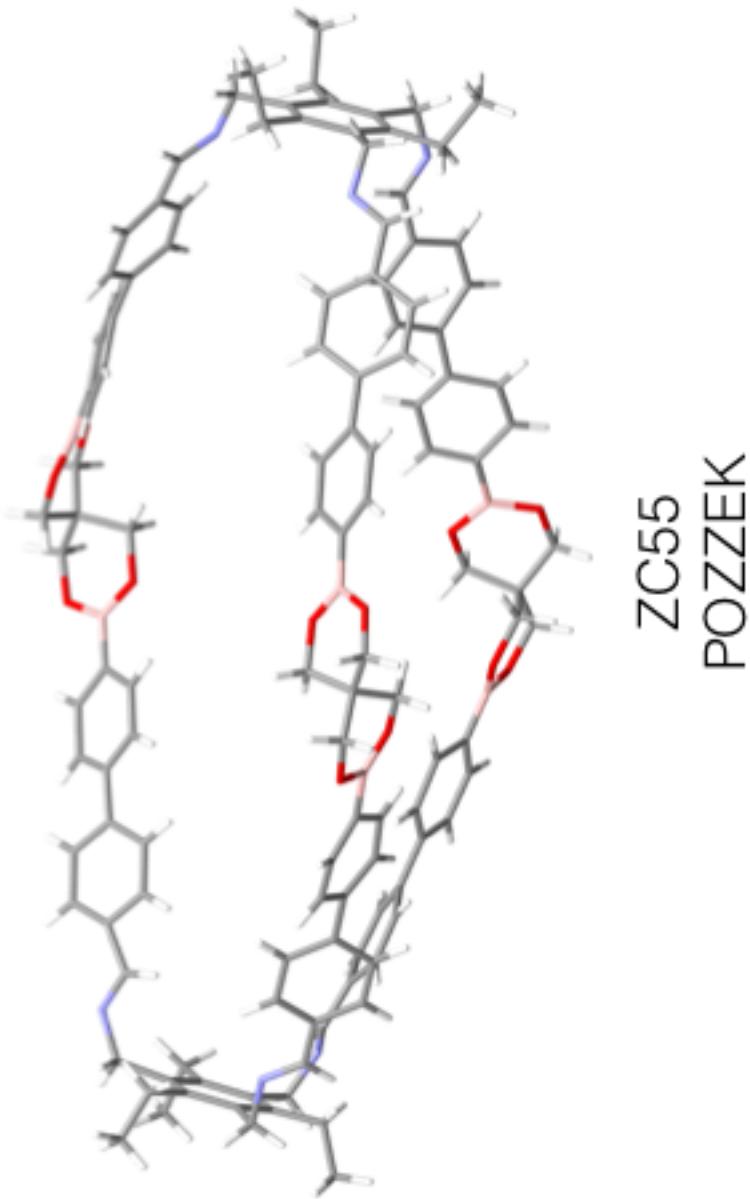
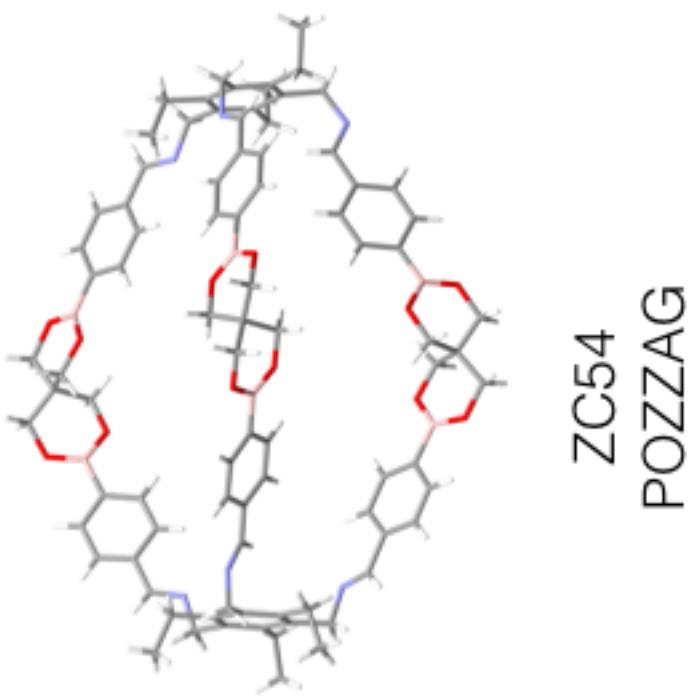
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ZC53
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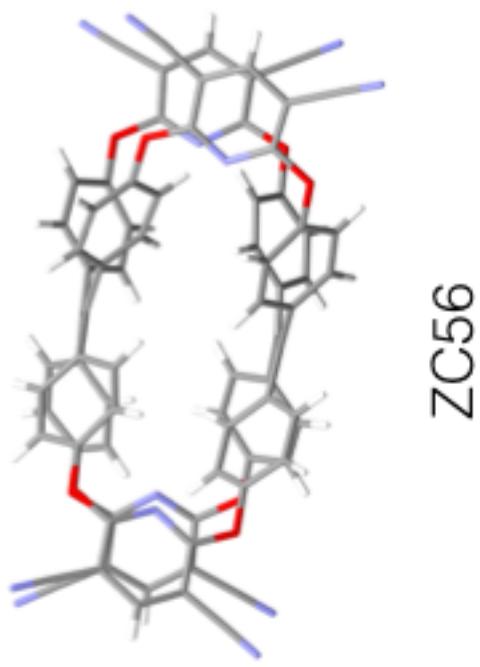
- (1) Arunachalam, M.; Ravikumar, I.; Ghosh, P. 2008, 9144.
(2) Francesconi, O.; Ienco, A.; Moneti, G.; Nativi, C.; Roelens, S. Angew. Chemie - Int. Ed. 2006, 45, 6693.

NEW CAGES (that I would add to the database)



(1) Igli, B.; Christinat, N.; Tönnemann, J.; Schüttler, C.; Scopelliti, R.; Severin, K. *J. Am. Chem. Soc.* 2009, 131, 3154.

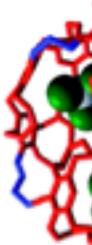
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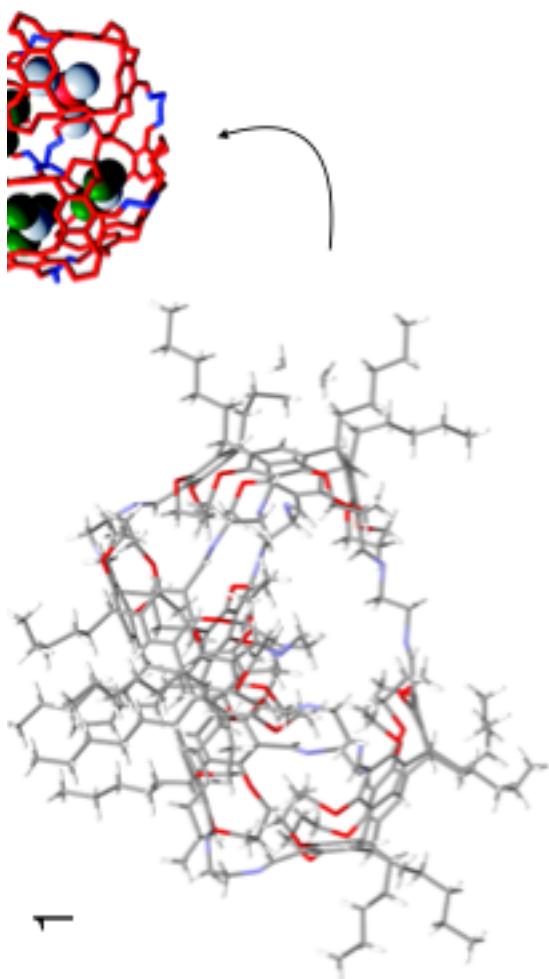


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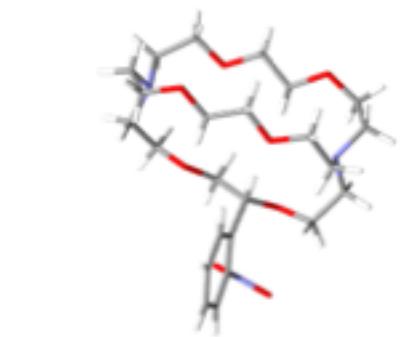
(1) Zhang, C.; Wang, Z.; Tan, L.; Zhai, T.-L.; Wang, S.; Tan, B.; Zheng, Y.-S.; Yang, X.-L.; Xu, H.-B. Angew. Chemie Int. Ed. 2015, n/a.

NEW CAGES (that I *wouldn't* add to the database)





ZC37
AVAFIN

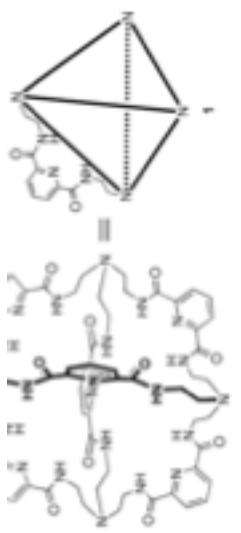
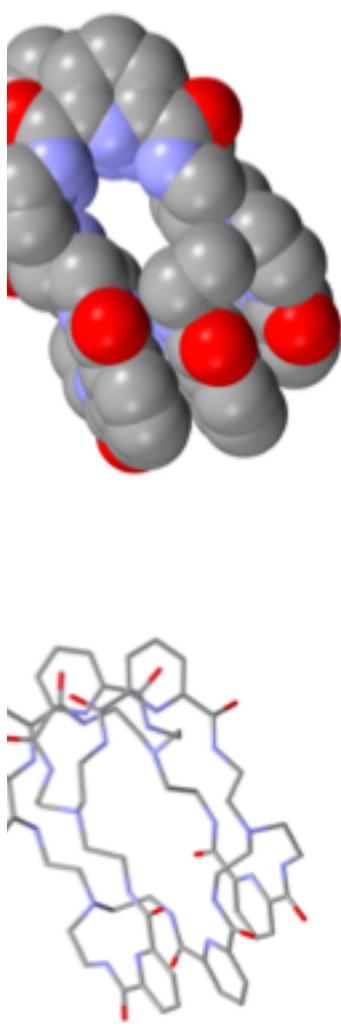


ZC39
KIZLAG

(1) Sun, J.; Bennett, J. L.; Emge, T. J.; Warmuth, R. J. Am. Chem. Soc. 2011, 133, 3268.

NEW CAGES (that I *wouldn't* add to the database)



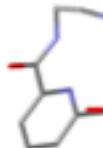
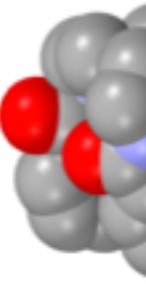


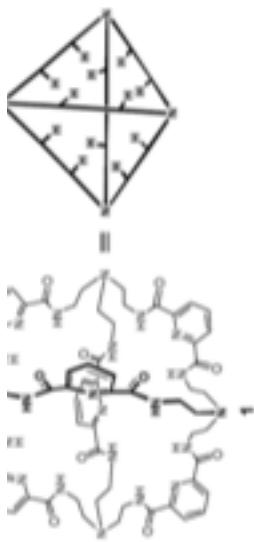
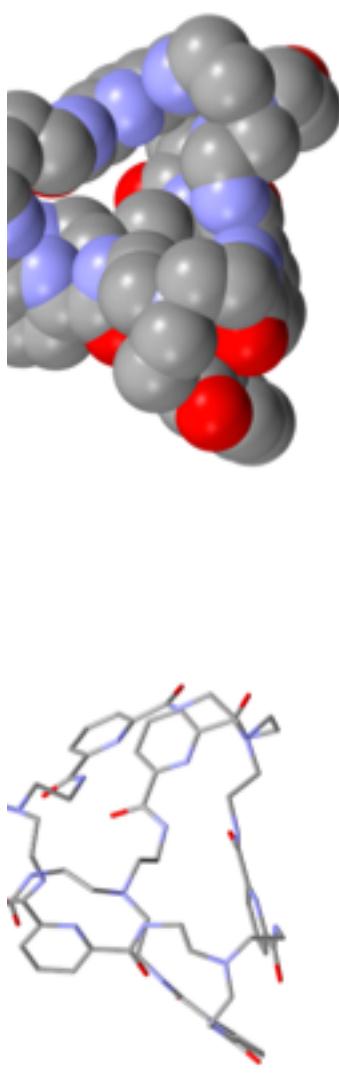
Scheme 1. Synthesis of the covalent organic tetrahedral cage 1.

ZC2 (LAXRUZ)

(1) Wang, Q.-Q.; Day, V. W.; Bowman-James, K. *Angew. Chem. Int. Ed. Engl.* 2012, 51, 2119.

NEW CAGES (that I **wouldn't add to the database)**

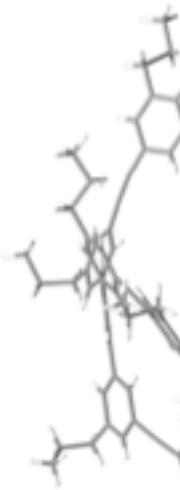


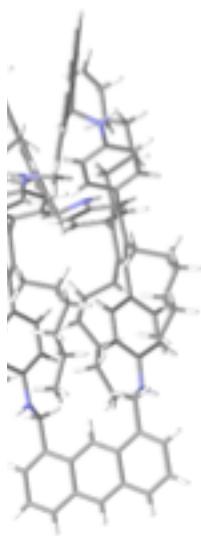


ZC4 (SETNEM)

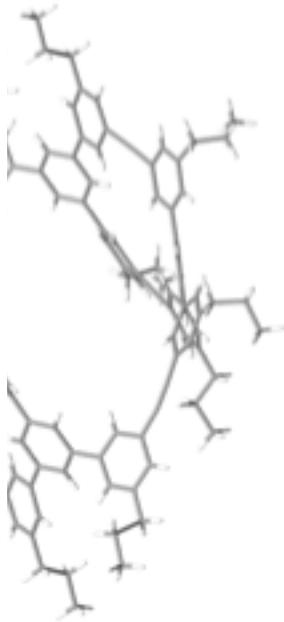
(1) Wang, Q.; Day, V. W.; Bowman-james, K. J. Am. Chem. Soc. 2013, 135, 392.

NEW CAGES (that I **wouldn't** add to the database)



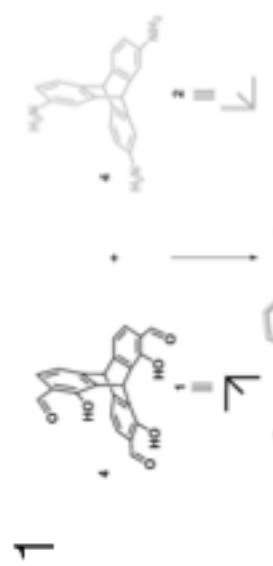
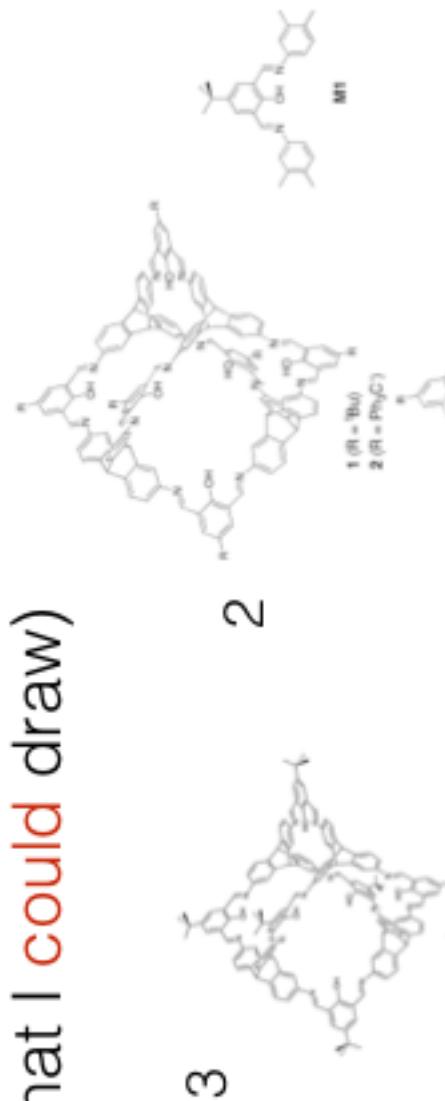


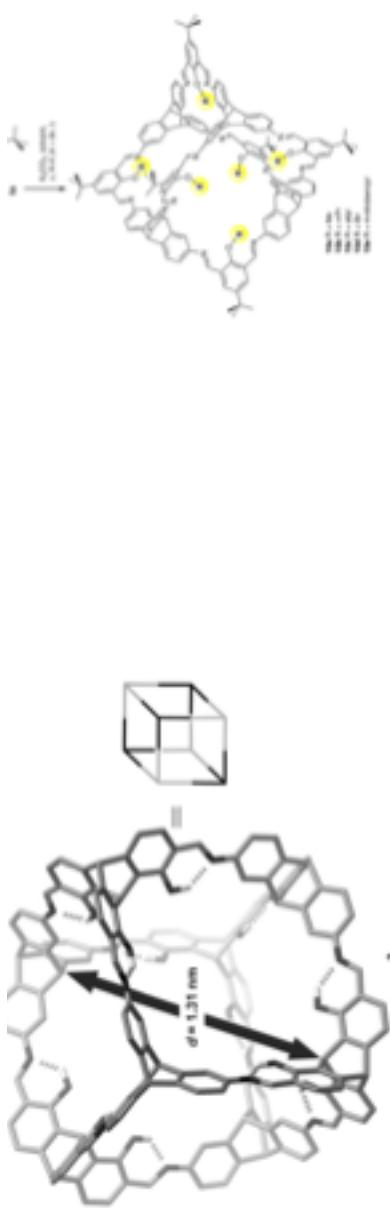
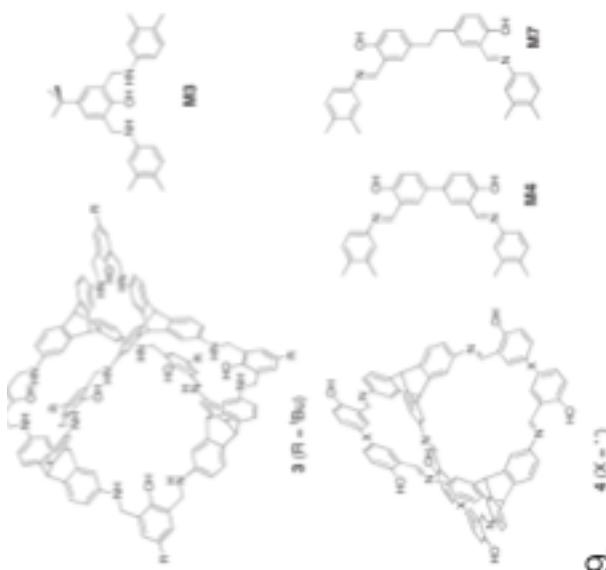
ZC45
PUTREC



ZC46
YOHXOK

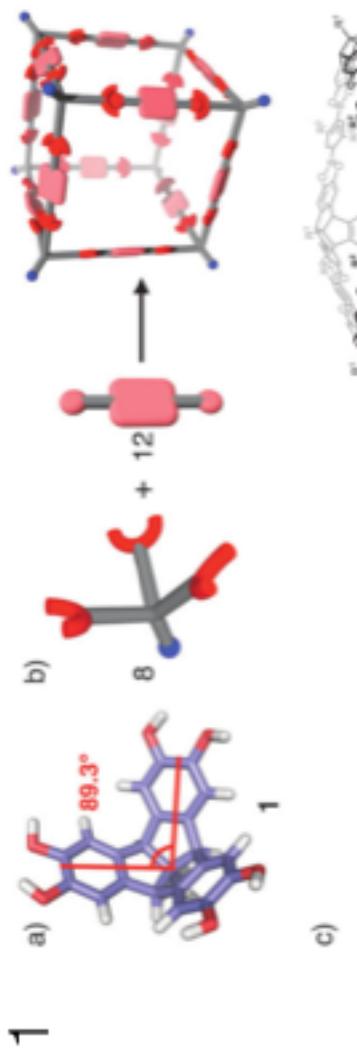
NEW CAGES (that I could draw)

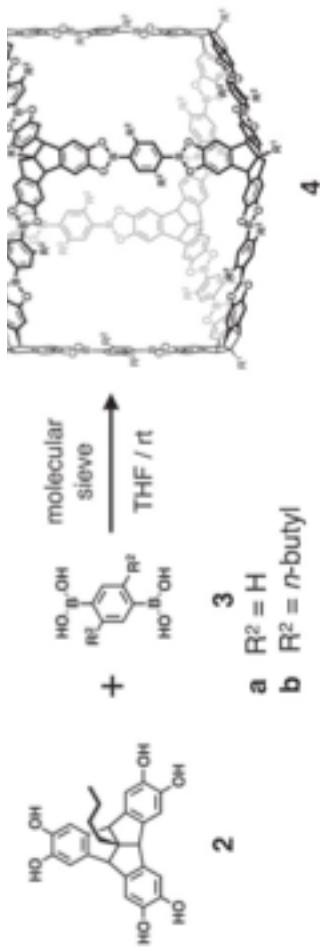




- (1) Elbert, S. M.; Rominger, F.; Mastalerz, M. Chem. - A Eur. J. 2014, 20, 1.
- (2) Brutschy, M.; Schneider, M. W.; Mastalerz, M.; Waldvogel, S. R. Adv. Mater. 2012, 24, 6049.
- (3) Mastalerz, M. Synlett 2013, 24, 781.

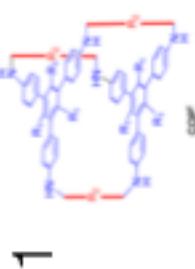
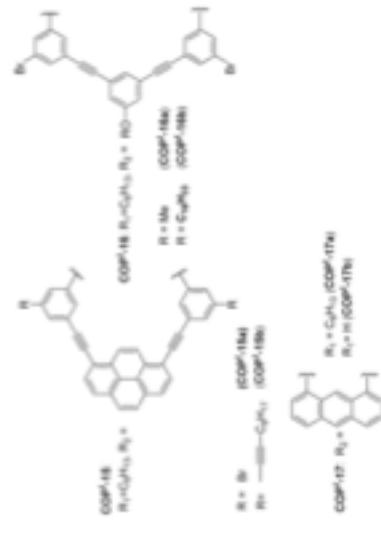
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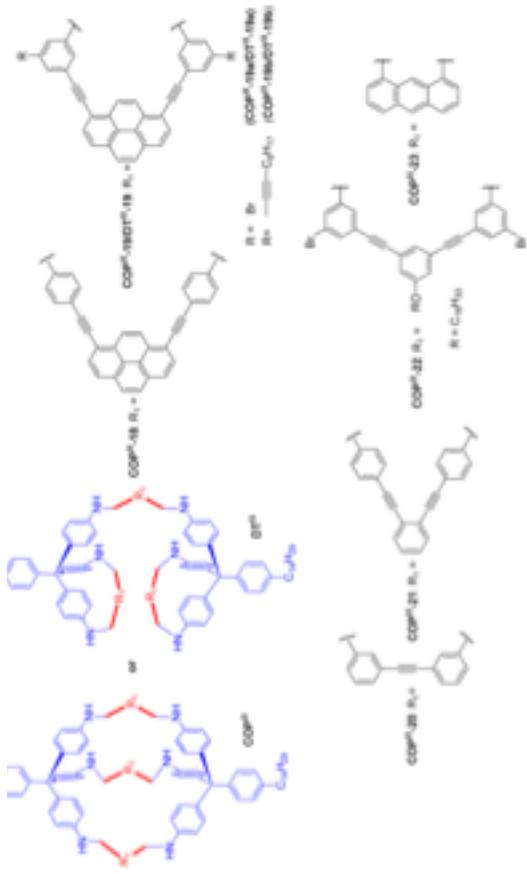


(1) Klotzbach, S.; Scherpf, T.; Beuerle, F. Chem. Commun. (Camb). 2014, 50, 12454.

NEW CAGES (that I could draw)

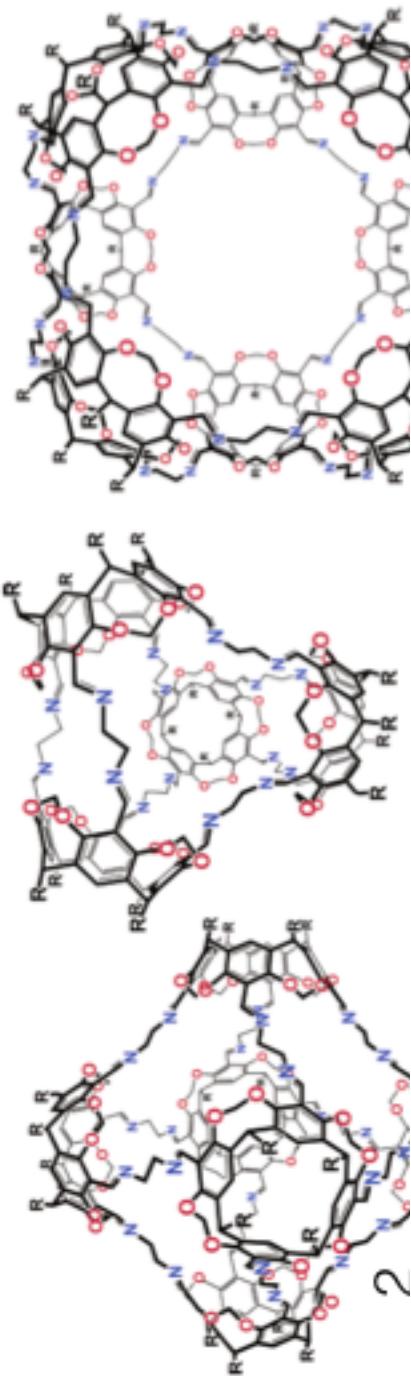


1
2
3

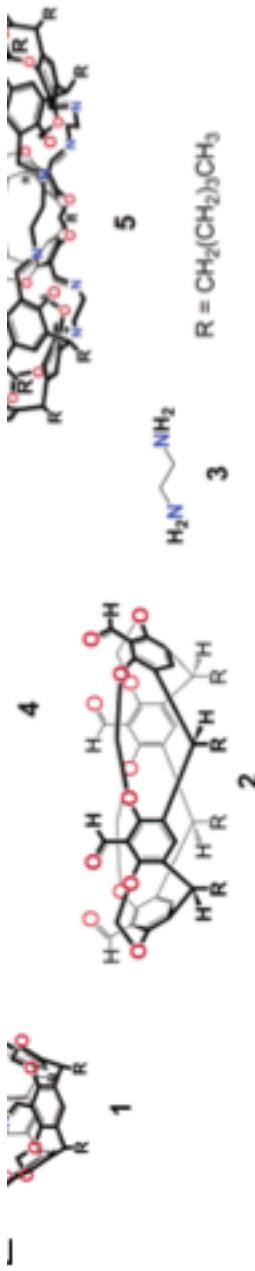


(1) Jin, Y.; Jin, A.; McCaffrey, R.; Long, H.; Zhang, W. J. Org. Chem. 2012, 77, 7392.

NEW CAGES (that I could draw)



2

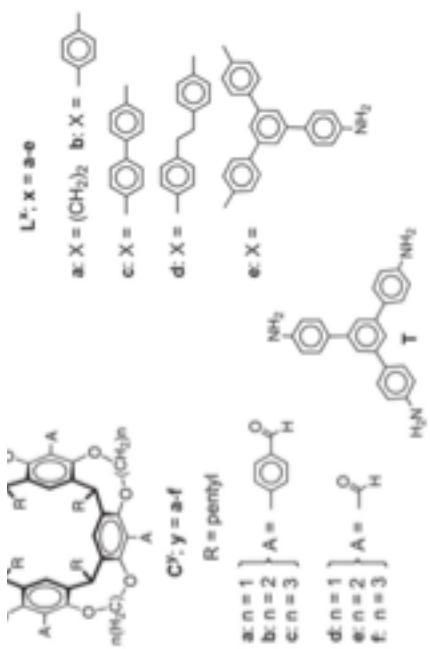


- (1) Liu, X.; Warmuth, R. J. Am. Chem. Soc. 2006, 128, 14120.
- (2) Liu, X.; Liu, Y.; Li, G.; Warmuth, R. Angew. Chem. Int. Ed. Engl. 2006, 45, 901.

NEW CAGES (that I could draw)

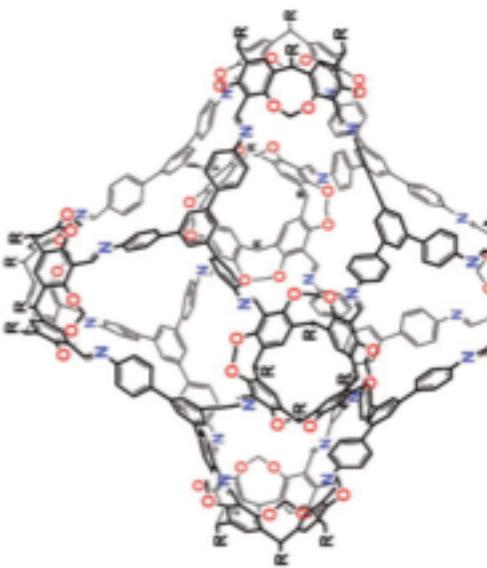
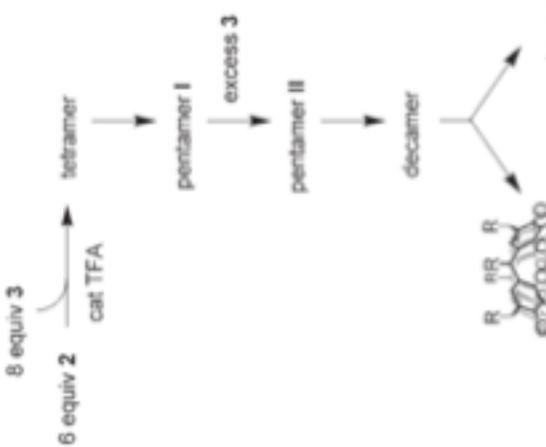


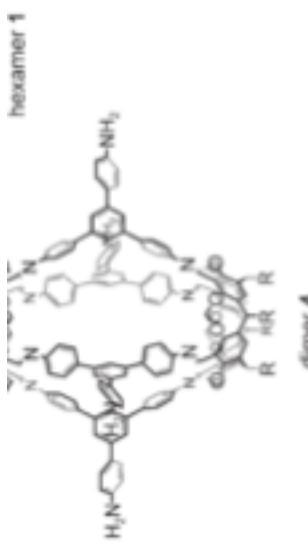
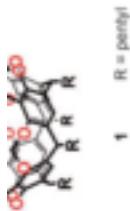
Fig. 1 (A) Edge-directed synthesis of octahedron $\mathbf{C}^8\mathbf{L}^{12}$ from 6 cavitands \mathbf{C}^8 and 12 benzidines \mathbf{L}^{12} . (B) Space-filling model of $\mathbf{C}^8\mathbf{L}^{12}$ (Amber[®], pentyl groups are omitted).



(1) Sun, J.; Warmuth, R. Chem. Commun. (Camb). 2011, 47, 9351.

NEW CAGES (that I could draw)

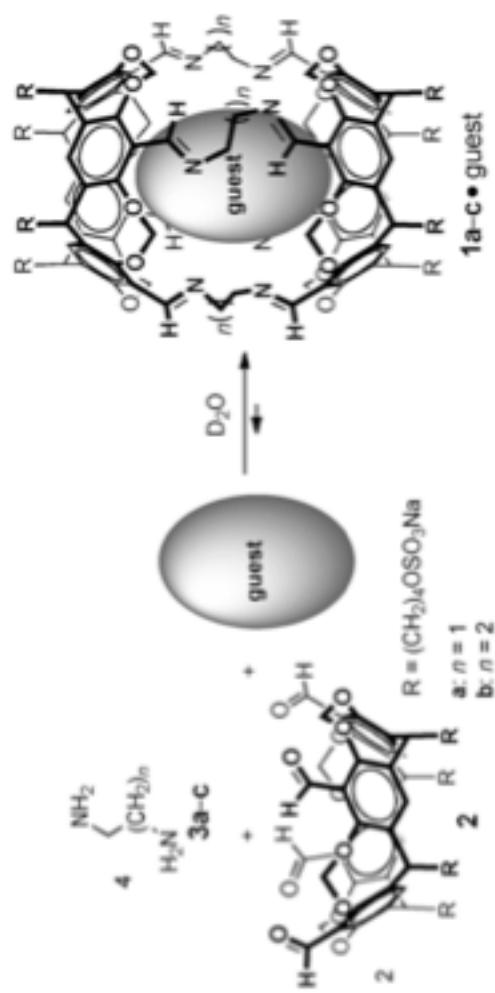




(1) Liu, Y.; Liu, X.; Warmuth, R. Chem. - A Eur. J. 2007, 13, 8953.

SC 2. Proposed association-disproportionation mechanism for the condensation of **1** in the TFA-catalyzed condensation of **2** with **3**.

NEW CAGES (that I could draw)

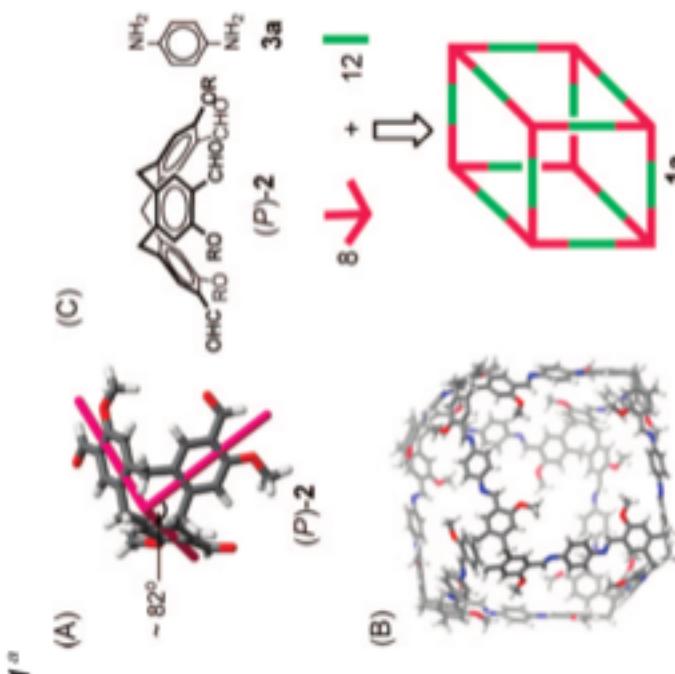


ϵ : $n = 3$

Scheme 1. Assembly of hemicarcerplexes **Ia–e**–guest.

(1) Lin, Z.; Sun, J.; Efremovska, B.; Warmuth, R. *Chemistry* 2012, 18, 12864.

NEW CAGES (that I could draw)



^a Amber*-energy minimized structures of (*P*)-**2** (A) and (*all-P*)-**1a** (B) (hexadecyl groups are replaced with CH₃). (C) Design of nanocube **1a** from 8 tritopic 90° corners **2** (R = hexadecyl) and 12 ditopic 180° spacers **3a**.

