

Möbius Basket Molecule: Structure and Properties

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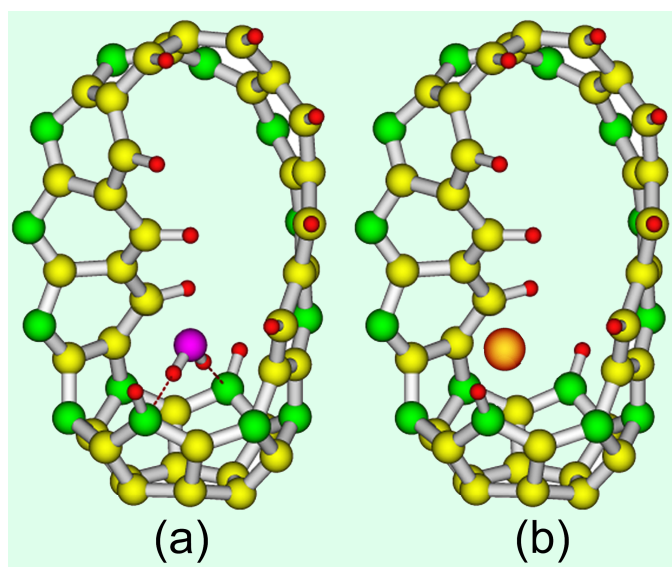


Fig. S1. (a) Complex $\text{H}_2\text{O} \cdots$ Möbius basket, and (b) complex $\text{Fe}^{2+} \cdots$ Möbius basket showing the container characteristic of the Möbius basket.

B3LYP/6-31G(d) level for the optimized Cartesian Coordinates.

Möbius Basket. -2219.9585 au.

C	-4.61431000	2.06414500	-0.83013800
N	-5.22756800	1.12331000	-1.56802500
C	-5.59453900	1.19893400	1.25786900
H	-5.72434000	1.22491800	2.33849100
H	-3.95298400	2.96376700	2.44959800
C	-3.86127400	2.89896000	1.36656700
C	-4.81541600	2.17685500	0.62080200
N	-3.60363100	2.70057000	-1.46264800
C	1.98289500	2.57706500	-0.65550000
C	2.10277400	2.60868300	0.80867000
C	1.00314600	2.90765200	1.54304800
C	-0.25506200	3.00621300	-0.63376800
C	-0.23262100	3.10794700	0.83358100
H	1.02332500	2.96154500	2.62822900
N	0.90967200	2.76849900	-1.34713200
C	-4.80425000	-2.19031500	0.61889300
C	-4.60328400	-2.07504100	-0.83189100
C	-5.76458200	-0.00911900	0.55693500
C	-0.21640700	-3.10318500	0.83147900
C	-0.23969700	-3.00182000	-0.63661400
C	2.11882400	-2.59931300	0.80942000
C	1.99613400	-2.56505900	-0.66020600
C	-5.50891000	-0.00777700	-0.89084200
C	-5.58828200	-1.21774900	1.25671900
C	-3.84650800	-2.90955200	1.36408400
C	1.01835900	-2.90178700	1.54227700
N	-5.22143600	-1.13608300	-1.56900100
N	-3.59012900	-2.70587300	-1.46488500
N	0.92259100	-2.76137400	-1.35064400
H	-5.71826100	-1.24548600	2.33727300
H	-3.93832400	-2.97614800	2.44699100
H	1.03825900	-2.96015500	2.62707800
N	3.26764800	-2.28039400	-1.17607100
C	3.74211500	-1.14315800	-1.95885000
C	4.14578200	-2.31420000	-0.07419400
N	2.95781500	-0.00283000	-2.27585500
C	4.93853900	-0.70770500	-1.39107400
N	3.45009700	-2.30697400	1.15058100
C	5.19894800	-1.45045200	-0.15287400
C	3.69420000	1.11803400	-1.87420800
H	2.14922500	0.00724300	-2.88767300

C	4.93014400	0.71988900	-1.37927600
C	4.02944100	-1.15937800	1.85648300
C	5.11468900	-0.71533600	1.10656900
N	3.25492800	2.29551000	-1.17745100
C	5.17833000	1.47112300	-0.15236600
N	3.27469900	-0.01134700	2.27387300
C	5.10274600	0.71713100	1.09204400
C	4.17172300	2.39450400	-0.07420600
C	3.95722000	1.11422900	1.75856600
H	2.75410400	0.01508900	3.14552000
N	3.43468100	2.31389100	1.16140900
C	-1.43913800	3.30059600	1.47925400
H	-1.47347300	3.37844900	2.56469300
C	-1.42232400	-3.30114900	1.47650500
H	-1.45648100	-3.38033500	2.56184400
C	-2.54404500	-3.05192200	-0.71047000
C	-2.63096900	-3.19689500	0.74483800
C	-2.64680800	3.19313200	0.74728200
C	-2.55933900	3.04968500	-0.70800100
N	-1.35988900	3.08824000	-1.34990600
N	-1.34526500	-3.08686900	-1.35231700

Normal Basket. -2220.0836 au.

C	-4.61431000	2.06414500	-0.83013800
N	-5.22756800	1.12331000	-1.56802500
C	-5.59453900	1.19893400	1.25786900
H	-5.72434000	1.22491800	2.33849100
H	-3.95298400	2.96376700	2.44959800
C	-3.86127400	2.89896000	1.36656700
C	-4.81541600	2.17685500	0.62080200
N	-3.60363100	2.70057000	-1.46264800
C	1.98289500	2.57706500	-0.65550000
C	2.10277400	2.60868300	0.80867000
C	1.00314600	2.90765200	1.54304800
C	-0.25506200	3.00621300	-0.63376800
C	-0.23262100	3.10794700	0.83358100
H	1.02332500	2.96154500	2.62822900
N	0.90967200	2.76849900	-1.34713200
C	-4.80425000	-2.19031500	0.61889300
C	-4.60328400	-2.07504100	-0.83189100
C	-5.76458200	-0.00911900	0.55693500
C	-0.21640700	-3.10318500	0.83147900
C	-0.23969700	-3.00182000	-0.63661400
C	2.11882400	-2.59931300	0.80942000

C	1.99613400	-2.56505900	-0.66020600
C	-5.50891000	-0.00777700	-0.89084200
C	-5.58828200	-1.21774900	1.25671900
C	-3.84650800	-2.90955200	1.36408400
C	1.01835900	-2.90178700	1.54227700
N	-5.22143600	-1.13608300	-1.56900100
N	-3.59012900	-2.70587300	-1.46488500
N	0.92259100	-2.76137400	-1.35064400
H	-5.71826100	-1.24548600	2.33727300
H	-3.93832400	-2.97614800	2.44699100
H	1.03825900	-2.96015500	2.62707800
N	3.26764800	-2.28039400	-1.17607100
C	3.74211500	-1.14315800	-1.95885000
C	4.14578200	-2.31420000	-0.07419400
N	2.95781500	-0.00283000	-2.27585500
C	4.93853900	-0.70770500	-1.39107400
N	3.45009700	-2.30697400	1.15058100
C	5.19894800	-1.45045200	-0.15287400
C	3.69420000	1.11803400	-1.87420800
H	2.14922500	0.00724300	-2.88767300
C	4.93014400	0.71988900	-1.37927600
C	4.02944100	-1.15937800	1.85648300
C	5.11468900	-0.71533600	1.10656900
N	3.25492800	2.29551000	-1.17745100
C	5.17833000	1.47112300	-0.15236600
N	3.27469900	-0.01134700	2.27387300
C	5.10274600	0.71713100	1.09204400
C	4.17172300	2.39450400	-0.07420600
C	3.95722000	1.11422900	1.75856600
H	2.75410400	0.01508900	3.14552000
N	3.43468100	2.31389100	1.16140900
C	-1.43913800	3.30059600	1.47925400
H	-1.47347300	3.37844900	2.56469300
C	-1.42232400	-3.30114900	1.47650500
H	-1.45648100	-3.38033500	2.56184400
C	-2.54404500	-3.05192200	-0.71047000
C	-2.63096900	-3.19689500	0.74483800
C	-2.64680800	3.19313200	0.74728200
C	-2.55933900	3.04968500	-0.70800100
N	-1.35988900	3.08824000	-1.34990600
N	-1.34526500	-3.08686900	-1.35231700