

Supplementary Materials

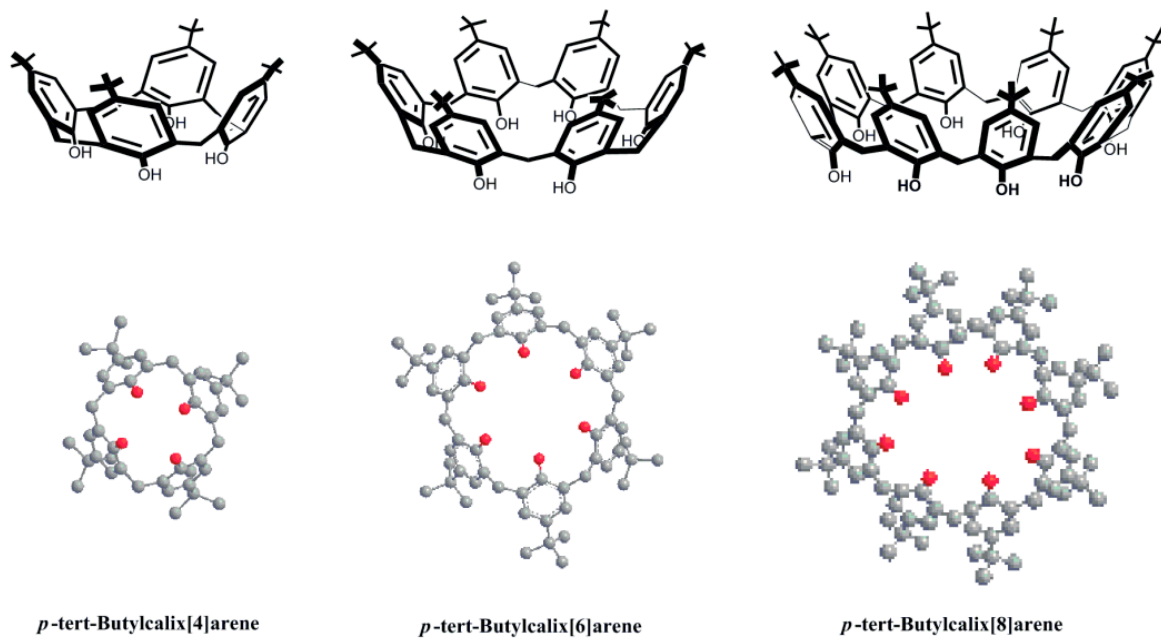


Figure S1. Structures of *p*-tert-butylcalix[n]arenes [24].

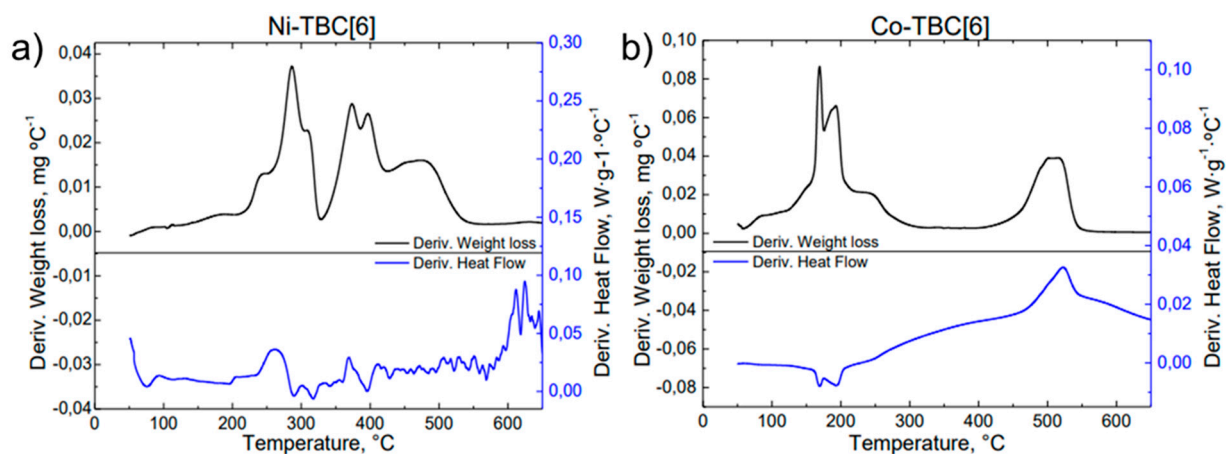


Figure S2. Differential thermogravimetric (DTG) and Differential heat flow profiles of a) Ni-TBC[6] and b) Co-TBC[6].

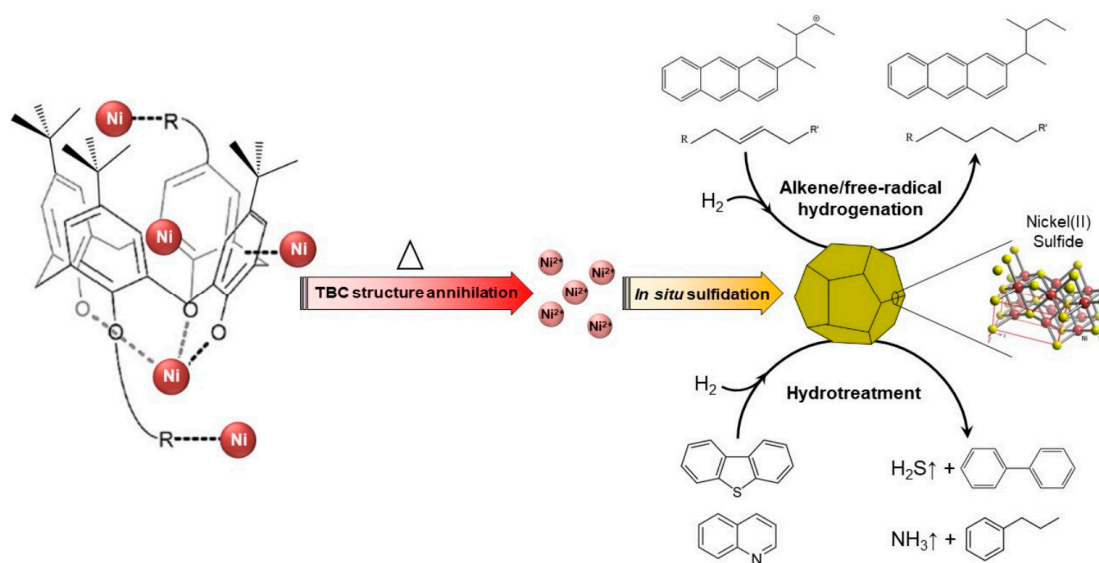


Figure S3. Mechanism of in situ sulfidation to form the active metal sulfide from metal-based calixarenes.

Table S1. Features and Advantages Offered by Calixarene [11].

Features	Subsequent advantages
Inexpensive and easily synthesized	Milligram quantities
Ability to be functionalized	Solubility control (including water)
Ability to incorporate chirality	Enantio-discrimination
Presence of cavity	Multiple-substrate recognition
Multiple binding sites	Cooperative effects
Ability to be fixed on solid supports	Heterogeneous catalysis

Table S2. Physical and chemical properties of the vacuum gas oil (VGO).

Properties	Value
Appearance	soft but solid at room temperature
Color	greenish dark brown
Density (g/cm ³ at 15°C)	0.892
Molecular weight	442.7
Initial boiling point, IBP (°C)	343
Final boiling point, FBP (°C)	641
Elemental analysis (wt.%)	
Carbon	85.10
Hydrogen	11.95
Sulfur	2.667
Nitrogen	0.215
HPLC analysis (wt.%)	
Saturates	13.3
Aromatics	68.1
Polars	18.6

Table S3. Temperature of peaks in DTG.

Catalyst	1 st Step (°C)	2 nd Step (°C)	3 rd Step (°C)
Ni-TBC[6]	285	373	474
Co-TBC[6]	167	236	504

Table S4. Characteristic peaks in DSC.

Peak (°C)	Ni-TBC[6]	Co-TBC[6]
1	75 ^a	-
2	-	168 ^b
3	-	194 ^b
4	262 ^d	209 ^d
5	318 ^b	-
6	370 ^c	523 ^c
7	395 ^b	-

^aglass transition^bendothermic^cexothermic^dre-crystallization**Table S5.** Properties of the Commercial Hydrocracking Catalyst (KC-2710).

Property	Unit	Value
BET specific surface area	m ² /g	346
Specific pore volume	mL/g	0.37
Average pore diameter	nm	4.3
Specific total acidity	μmol/g	844
Chemical composition:		
SiO ₂	wt. %	33
Al ₂ O ₃	wt. %	38
WO ₃	wt. %	23
NiO	wt. %	6
Support phase	amorphous SiO ₂ -Al ₂ O ₃ and Y zeolite (45 wt. %)	