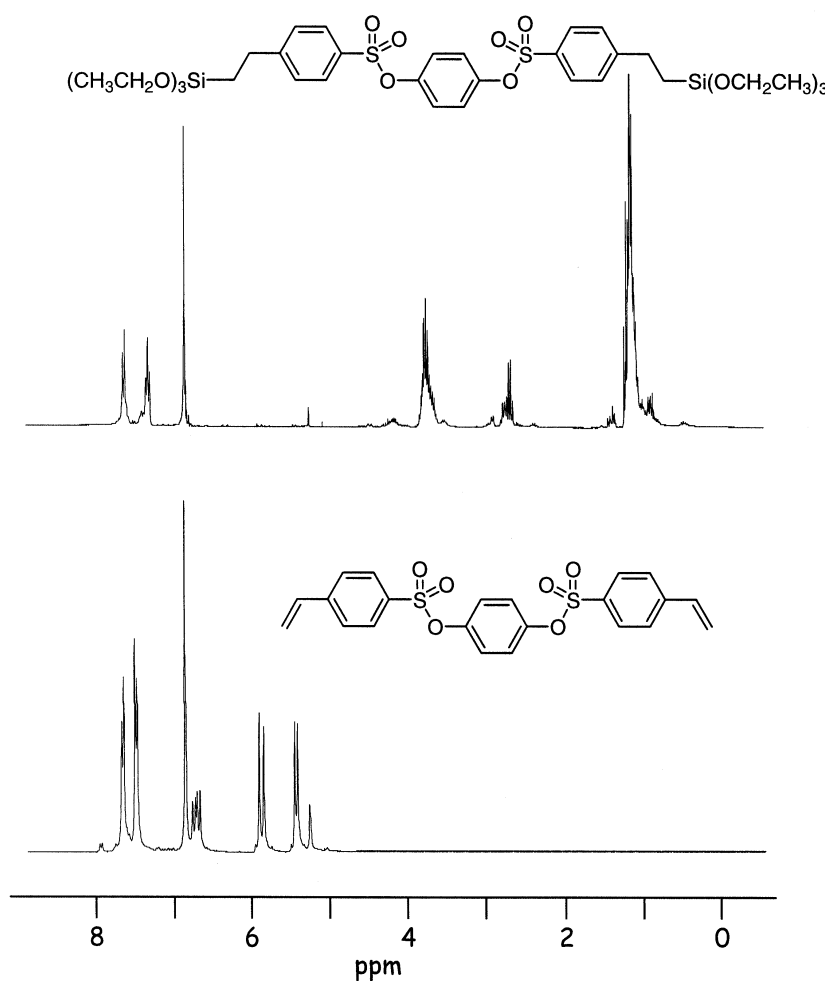


# Design of Heterogeneous Catalysts Via Multiple Active Site Positioning in Organic-Inorganic Hybrid Materials

Véronique Dufaud<sup>‡</sup> and Mark E. Davis<sup>\*</sup>

Contribution from the Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125 USA.

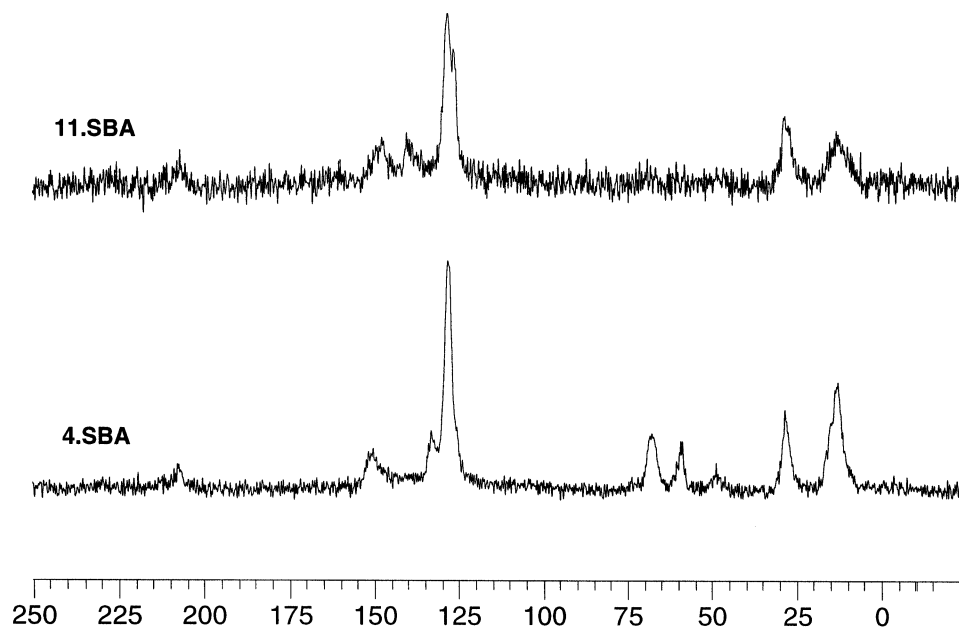
## Supporting Information for the Journal of American Chemical Society



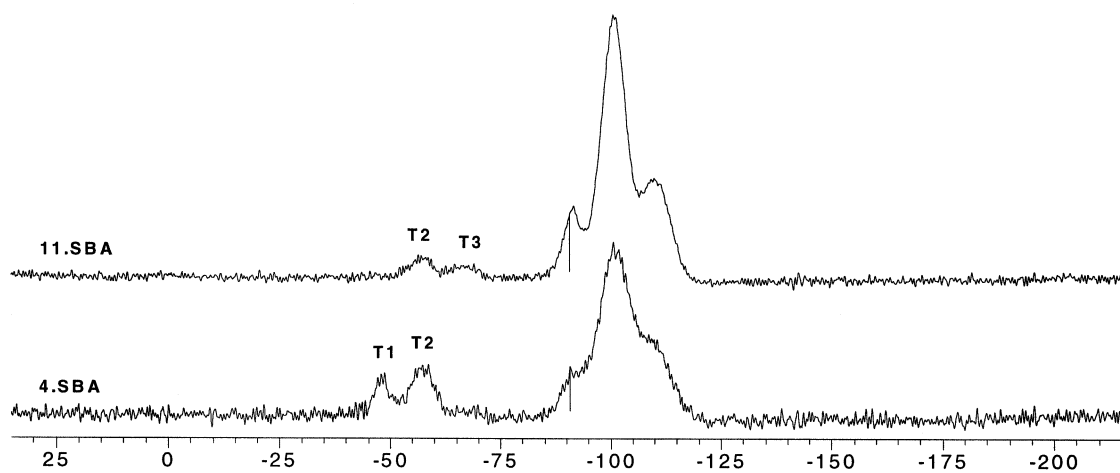
<sup>1</sup>H NMR (CD<sub>2</sub>Cl<sub>2</sub>): Hydrosilylation reaction of **5**

<sup>\*</sup> To whom correspondence should be addressed.

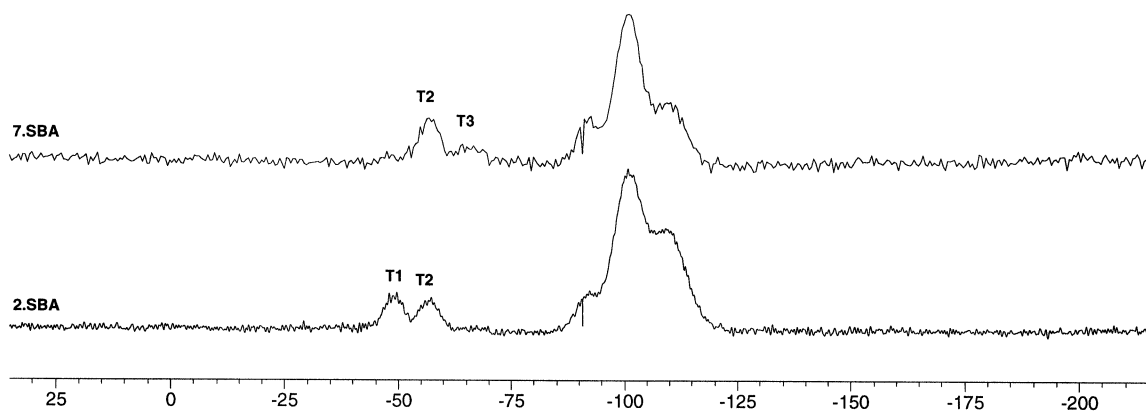
<sup>‡</sup> Present address: Laboratoire de Chimie, Ecole Normale Supérieure de Lyon, 46 allée d'Italie, 69364 Lyon cedex 07, France.

 $^{13}\text{C}$  CP-MAS NMR

Transformation of the sulfonate ester functionalized **4**·SBA to  
the sulfonic acid functionalized **11**·SBA

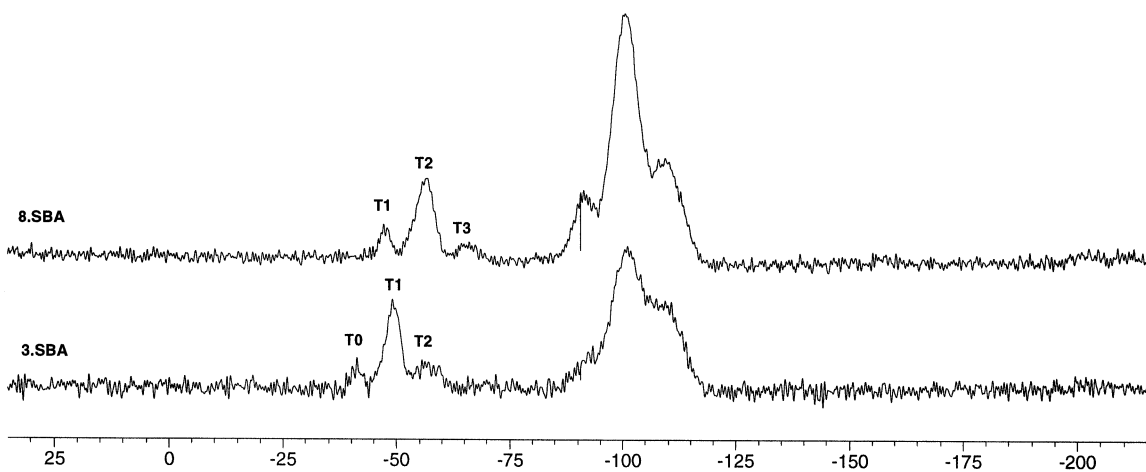
 $^{29}\text{Si}$  CP-MAS NMR

Transformation of the sulfonate ester functionalized **4**·SBA to  
the sulfonic acid functionalized **11**·SBA



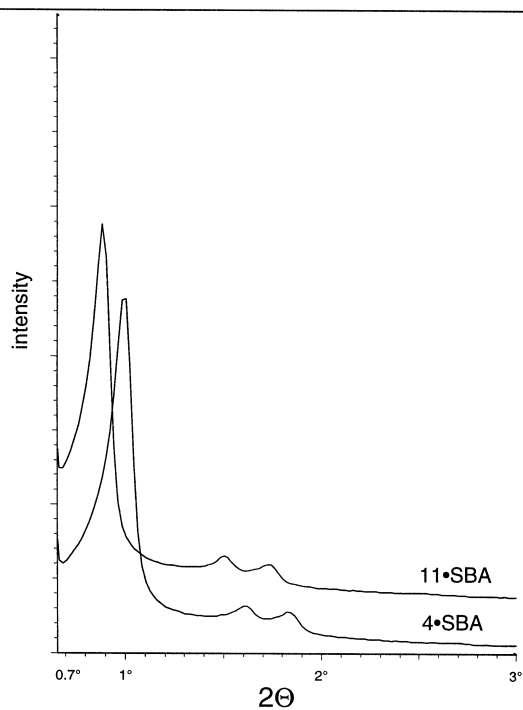
$^{29}\text{Si}$  CP-MAS NMR

Cleavage of the S-S linkage of the disulfide functionalized **2**·SBA to  
the thiol functionalized **7**·SBA

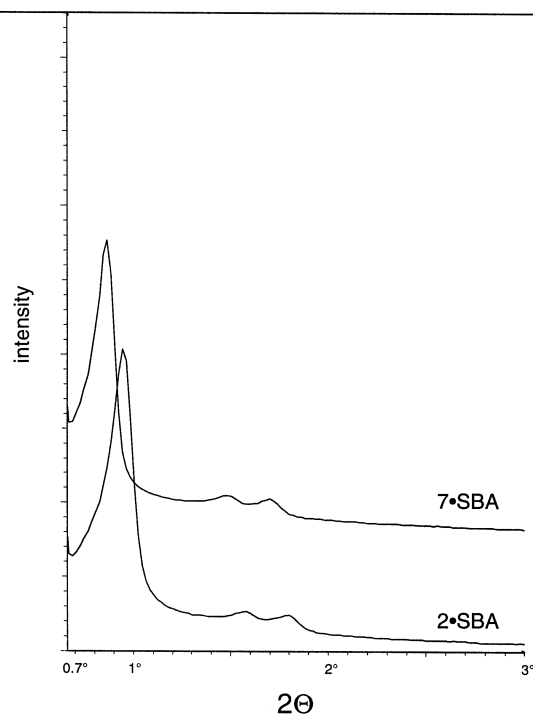


$^{29}\text{Si}$  CP-MAS NMR

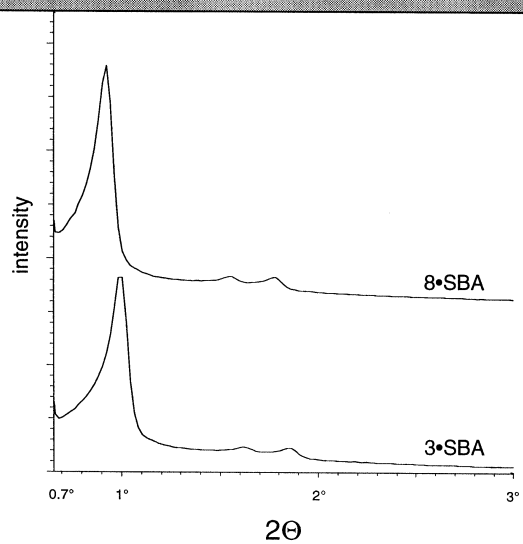
Cleavage of the S-S linkage of the disulfide functionalized **3**·SBA to  
the thiol functionalized **8**·SBA

**Powder X-ray diffraction patterns**

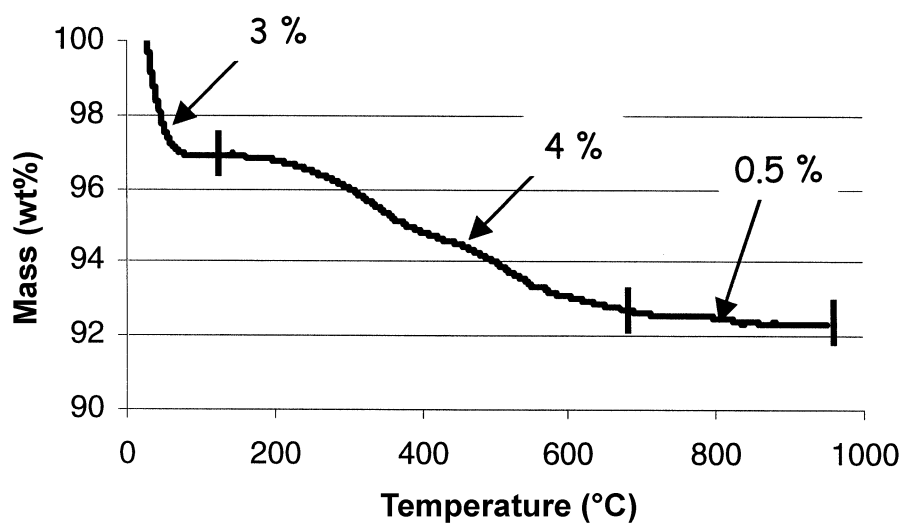
Transformation of ethyl sulfonate **4•SBA** into sulfonic acid **11•SBA**



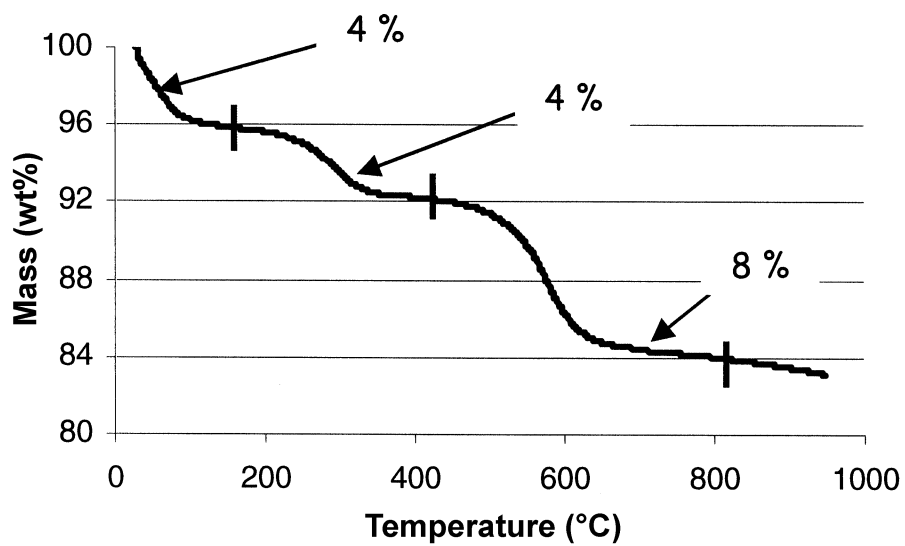
Cleavage of the unsymmetrical disulfide bond in **2•SBA** to produce surface thiol species **7•SBA**



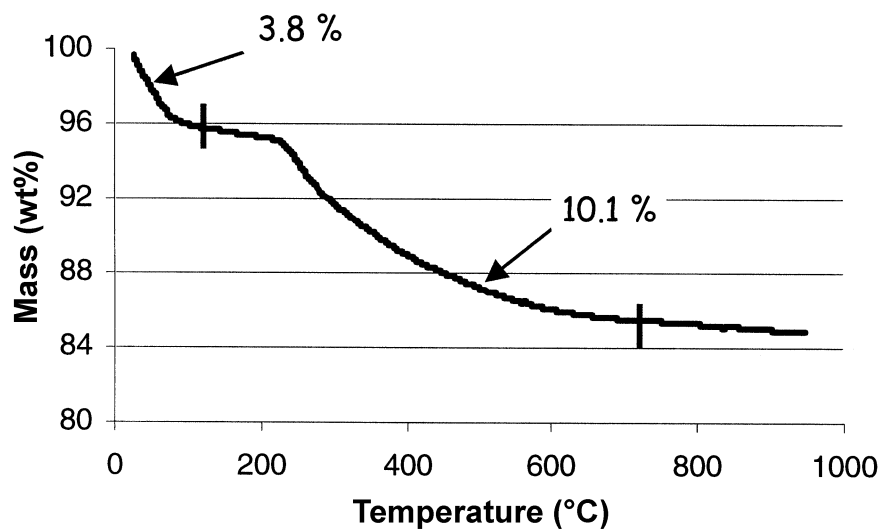
Cleavage of the symmetrical disulfide bond in **3•SBA** to produce proximal surface thiol species **8•SBA**



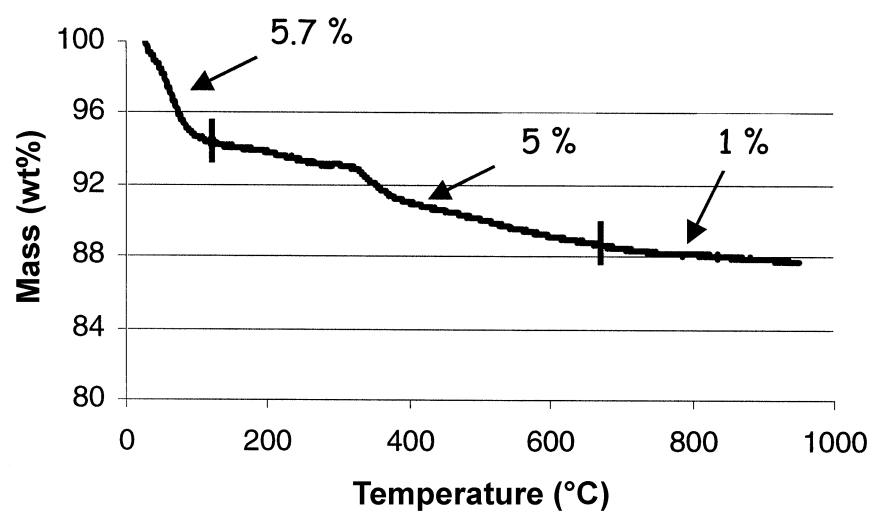
TGA measurement of 1•SBA



TGA measurement of 4•SBA



TGA measurement of 2•SBA



TGA measurement of 3•SBA