Supporting Information

Activation of Si-Si and Si-H bonds at Pt: A catalytic hydrogenolysis of silicon-silicon bonds

Jan Voigt, Maren A. Chilleck and Thomas Braun*

DFT calculations

For calculating the Gibbs free energy of reaction, the molecular geometries of $Me_3SiSiMe_3$, H_2, and $HSiMe_3$ were optimized at the B3LYP/cc-pVTZ level of theory using Gaussian09. Vibrational analysis confirmed the calculated structures to be local minima.

$Me_3SiSiMe_3$

SCF energy: -818.6993224 H

Sum of electronic and thermal Free Energies: -818.520008 H

Cartesian coordinates (in Å) of the optimized geometry:

atom	x	y	z
Si	1.18856	0.00026	0.00003
C	1.84996	-1.08846	1.40857
C	1.85224	-0.67475	-1.64652
C	1.84921	1.76471	0.23959
Si	-1.18851	-0.00028	-0.00049
H	2.94480	-0.66913	-1.65328
H	1.51368	-0.07326	-2.49199
H	1.52578	-1.70194	-1.81837
H	2.94247	-1.09993	1.40729
H	1.50863	-2.12052	1.31099
H	1.52417	-0.72209	2.38370
H	2.94172	1.77016	0.24918
H	1.50825	2.19493	1.18299
H	1.52214	2.42672	-0.56419
C	-1.84922	-1.76263	-0.25417
C	-1.85078	1.10064	-1.39890
C	-1.85143	0.66046	1.65194
H	-1.52376	0.04358	2.49059
H	-2.94401	0.66755	1.65396
H	-1.51391	1.68135	1.83934
H	-1.51084	0.75408	-2.37645
H	-1.52383	2.13534	-1.28186
H	-2.94330	1.09786	-1.40825
H	-1.51928	-2.18041	-1.20701
H	-2.94177	-1.76971	-0.25028
H	-1.51148	-2.43421	0.53716

H_2

SCF energy: -1.1799988 H

Sum of electronic and thermal Free Energies: -1.181416 H

Cartesian coordinates (in Å) of the optimized geometry:

atom	x	y	z
H	0.00000	0.00000	0.37143
H	0.00000	0.00000	-0.37143

$HSiMe_3$

SCF energy: -409.949159 H

Sum of electronic and thermal Free Energies: -409.861000 H

Cartesian coordinates (in Å) of the optimized geometry:

atom	x	y	z
Si	-0.00004	-0.00044	0.37494
C	0.09052	1.78846	-0.22186
C	1.50425	-0.97240	-0.22209
C	-1.59470	-0.81567	-0.22209
H	0.00004	-0.00026	1.86756
H	1.54260	-1.00645	-1.31278
H	1.47873	-2.00091	0.14204
H	2.43188	-0.51805	0.13000
H	0.10654	1.83984	-1.31257
H	0.99174	2.28102	0.14728
H	-0.76886	2.36418	0.12590
H	-1.64544	-0.82934	-1.31279
H	-2.47149	-0.27931	0.14483
H	-1.66561	-1.84696	0.12766