

Supplementary Information

Table S1

complex	energy [Hartree]	zero point + thermal correction [Hartree]	entropy [cal/mol K]	G [kcal/mol]	ΔG [kcal/mol] ^a
II	-2783.56267866	0.386552	201.913	-1746530.03	0
III	-2782.32973149	0.369409	210.249	-1745769.61	19.33
TS^{III-IV}	-2782.31214093	0.368908	201.017	-1745756.11	32.83
IV	-2782.46608897	0.370219	212.536	-1745855.35	-66.41
V	-3112.56942207	0.423163	226.433	-1952969.27	-80.40
H ₂	-1.17957102	0.013459	31.136	-741.09	-
MeSiH ₃	-331.253258	0.066753	61.137	-207841.02	-

^a ΔG relative to **II** taking into account consumed MeSiH₃ and produced H₂ molecules.