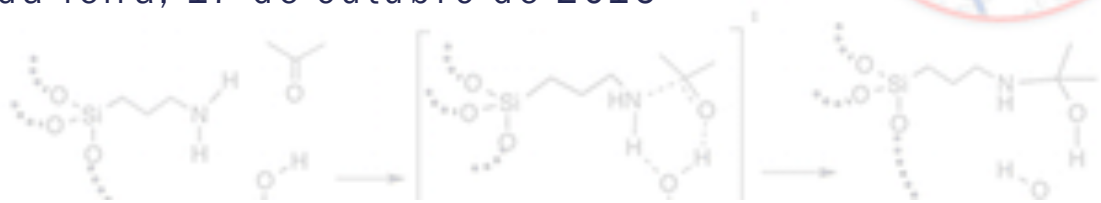


Explorando Reatividade Química Com Cálculos de Estrutura Eletrônica

Ana Paula de Lima Batista

Segunda-feira, 17 de outubro de 2016



Química Computacional

Reatividade
em Química

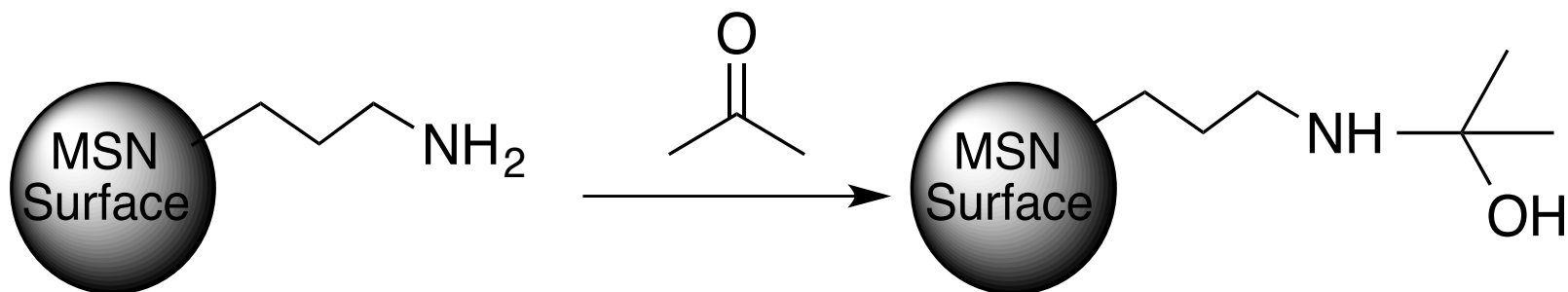
Arranjo molecular das espécies químicas envolvidas

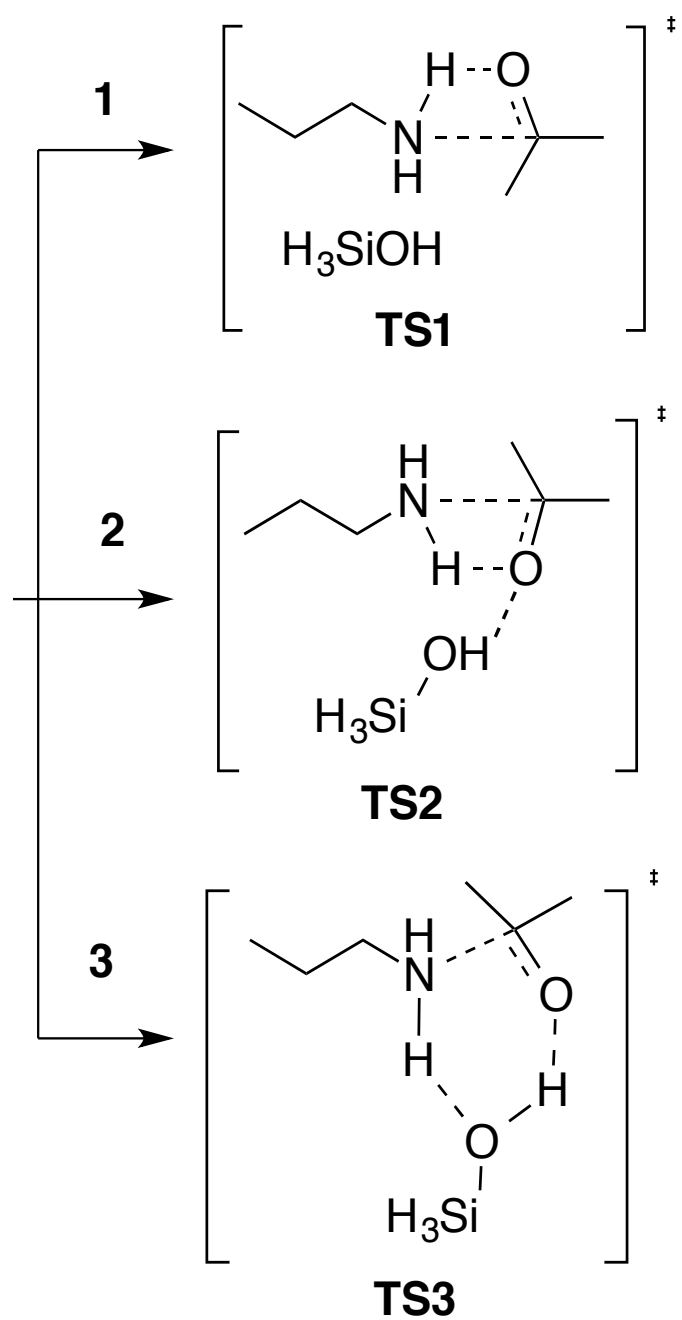
Quebra e formação de ligações químicas

Energia envolvida nestes processos

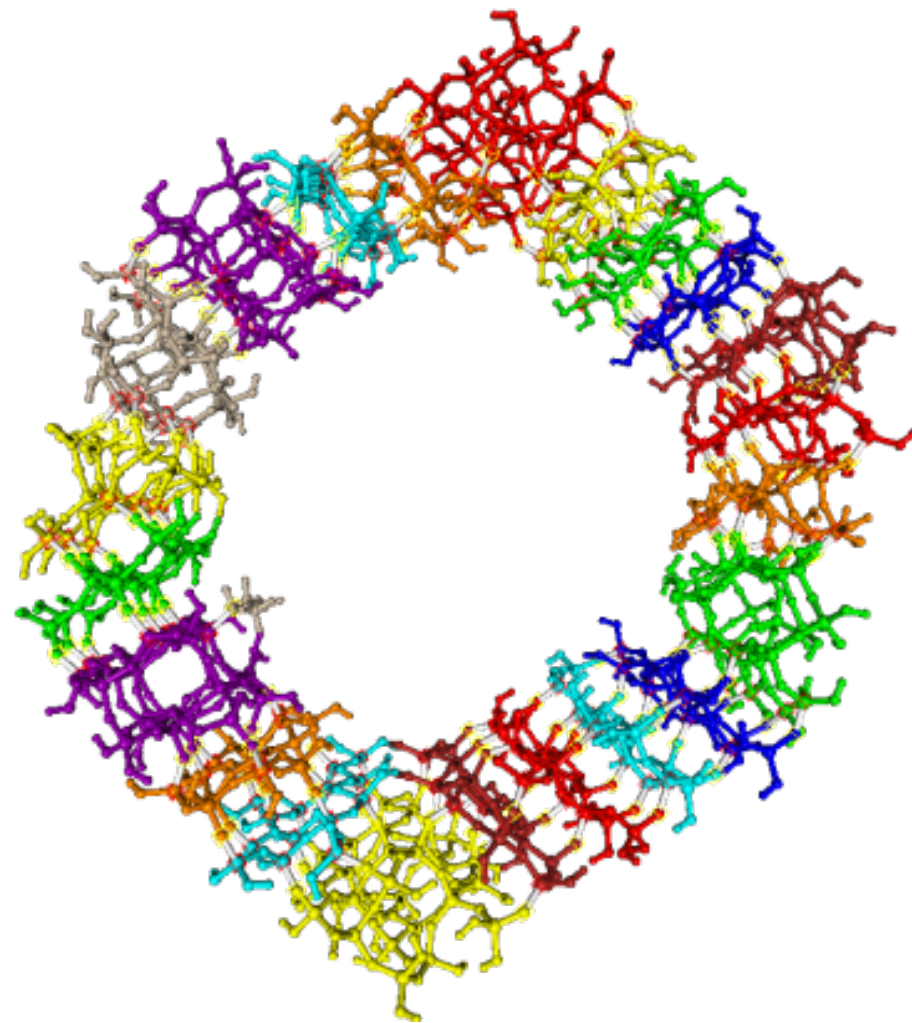
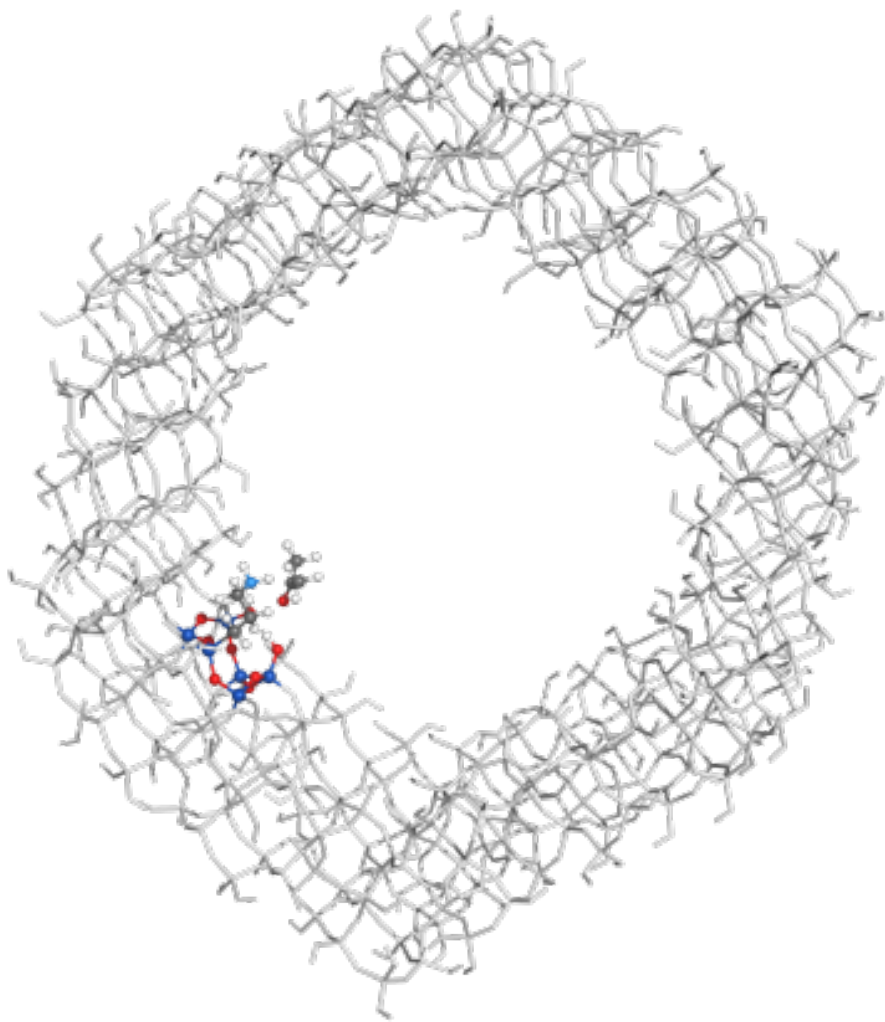
Catálise Heterogênea

Reação Aldol





GAMESS

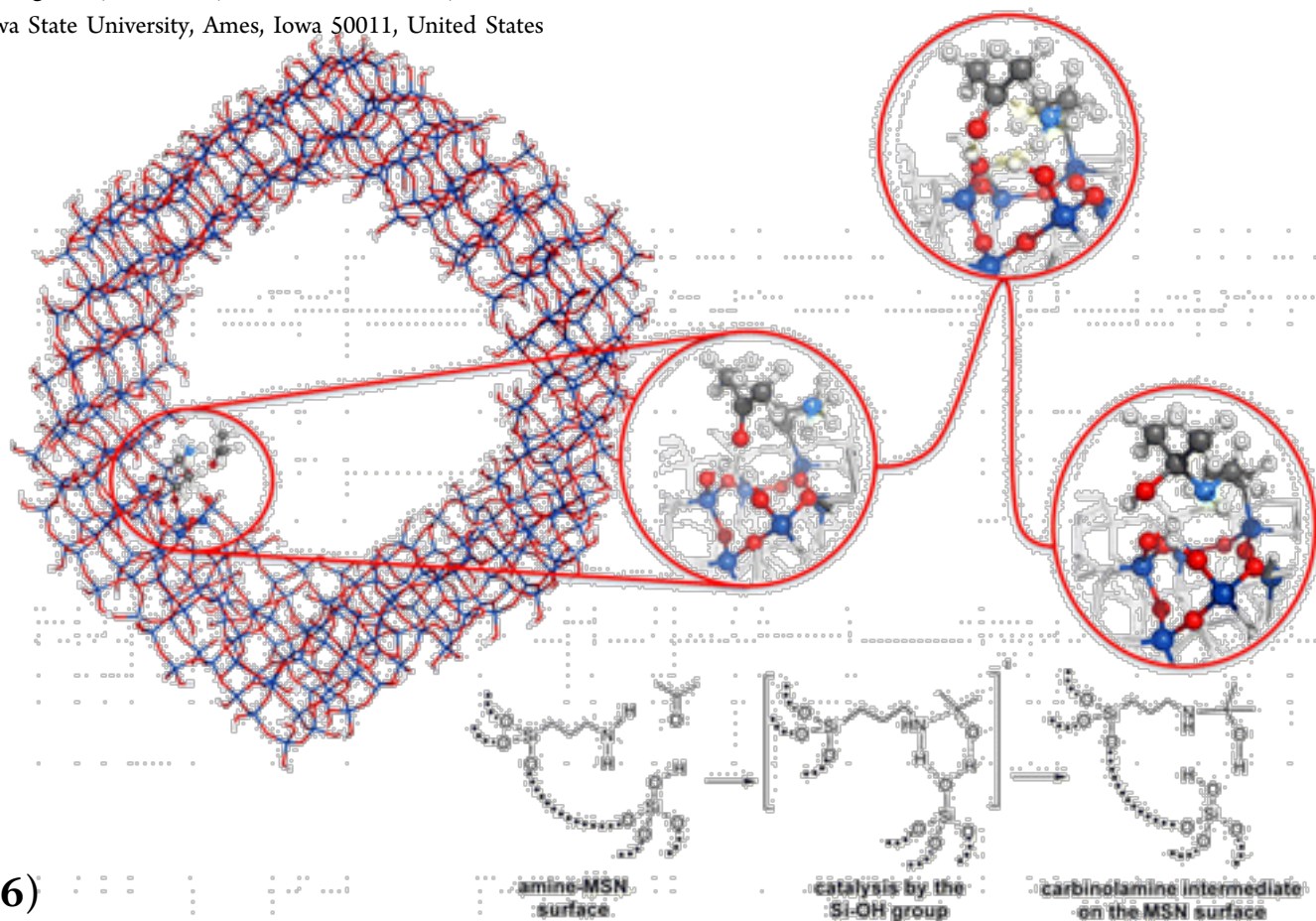


Silanol-Assisted Carbinolamine Formation in an Amine-Functionalized Mesoporous Silica Surface: Theoretical Investigation by Fragmentation Methods

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Outros Resultados

1- **DE LIMA BATISTA, ANA P.; BRAGA, ATAUALPA A. C.** Mor-Dalphos-Pd (II) oxidative addition complexes and related NH₃ adducts: Insights into bonding and nonbonding interactions. *J. Mol. Struct.*, v. 1120, p. 245-249, 2016

2- **GUEST, DANIEL; MENEZES DA SILVA, VITOR H.; DE LIMA BATISTA, ANA P.; ROE, S. MARK; BRAGA, ATAUALPA A. C.; NAVARRO, OSCAR.** (N-Heterocyclic Carbene)-Palladate Complexes in Anionic Mizoroki-Heck Coupling Cycles: A Combined Experimental and Computational Study. *Organometallics*, v. 34, p. 2463-2470, 2015.