In silico search for planar hexacoordinate Silicon atom: A kinetically viable species

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Abstract

In silico search for planar hexacoordinate silicon center has been initiated by global minimum screening with density functional theory and energy refinement using coupled cluster theory. The search resulted in a local minimum of SiAl3Mg3H2+ structure which contains a planar hexacoordinate silicon center (phSi). The phSi structure is 5.8 kcal/mol higher in energy than the global minimum. However, kinetic studies reveal that the local minimum structure has enough stability to be detected experimentally. Born-Oppenheimer molecular dynamics (BOMD) simulations reveal that the phSi structure can be maintained up to 400 K. The formation of multiple bonds between the central silicon atom and framework aluminium atom is the key stabilizing factor for the planar structure.

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