

Structural and Energetic Properties of Pyridine–SiCl₄ Complexes

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We are interested in the structural and energetic properties of pyridine–SiCl₄ complexes and how these change in different chemical environments (e.g., gas phase, solvents, etc.) Using the M06 method along with 6-311+G (2df,2pd), we computed equilibrium geometries, binding energies, and vibrational frequencies for the pyridine–SiCl₄ and 3,5 pyridine–SiCl₄ complexes. In addition, we mapped the N–Si potentials from 1.7 Å to 5.0 Å. For pyridine–SiCl₄ the equilibrium structure has an N–Si distance of 3.351 Å and the binding energy is 4.6 kcal/mol. Also, 3,5-difluoropyridine–SiCl₄ has an N–Si distance of 3.389 Å and the binding energy is 4.3 kcal/mol. Furthermore, the N–Si potentials are relatively similar; they are flat and anharmonic with a long minimum and a flat shelf-like region along the inner wall. We also performed bulk reactivity experiments and found that, in spite of the weak interactions predicted by the computations, combining SiCl₄ and these pyridine compounds immediately produces a stable reaction product.

