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Di- σ and dative binding of benzene and pyridine on a Si(5 5 12)-2x1 at 80K

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We investigated the adsorption of benzene and pyridine on Si(5 5 12)-(2x1) by using variable-low temperature scanning tunneling microscopy (STM) and density functional theory (DFT) calculations. The benzene molecule most strongly binds to two adatoms on the *D3* and *D2* units in a tilted butterfly configuration, which consists of di- σ bonds between C atoms and Si adatoms and two C=C double bonds in the benzene molecule. Pyridine molecules interact with adatom(s) on the *D2* and *D3* units through both Si-N dative bonding and di- σ bonds. The dative bonding through the lone pair electrons of N atom produces a vertical configuration (pyridine-like), which is more stable than di- σ bonds. Di- σ bonds can be formed either through Si-N^1 and Si-C^4 or Si-C^2 and Si-C^5.