Pyridine adsorption on the polar ZnO(0001) surface: Zn termination versus O termination

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The interaction of pyridine (C_5H_5N) with the two differently terminated ZnO(0001) surfaces has been investigated using thermal desorption spectroscopy (TDS), x-ray photoelectron spectroscopy (XPS), and x-ray absorption spectroscopy (NEXAFS). The binding energy of pyridine on the O-terminated ZnO(000-1) surface amounts to 57 kJ/mol and the spectroscopic data reveal only small modifications of the pyridine electronic structure, indicating the presence of a physisorbed species. On the Zn-terminated ZnO(0001) surface, the binding energy is substantially higher, 112 kJ/mol, and the N1*s* NEXAFS data for the pyridine π^* resonance shows a shift of 0.6 eV toward higher binding energies. This observation indicates a substantial interaction between the nitrogen lone pair and Zn, as is confirmed by precise *ab initio* calculations of the core-level excitation. [S0021-9606(00)71106-8]