Symmetry-break-induced variation of energy-level degeneracy observed on individual molecules by low temperature STM/STS

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In order to experimentally analyze the influence of a small symmetry break on the degeneracy of discrete energy levels we have carried out comparative STM/STS investigations on benzene [C6H6] and triphenylphosphine [P(C6H5)3] molecules adsorbed to Au(111) surfaces. Due to the high symmetry of benzene, most of its energy levels are degenerated. The phenyl rings [C6H5] of P(C6H5)3 are structurally identical with benzene except the substituted H-atom, which is replaced by a P-atom. Therefore P(C6H5)3 should exhibit an additional splitting of certain energy levels due to the slightly reduced symmetry. A similar behavior has already been observed in UPS spectra of bromobenzene [C6H5Br]. The measurements were performed with a variable-temperature UHV-STM system. By using a continuous flow cryostat the microscope can be operated between 6.5 K and room temperature. From the experimentally obtained I-V-data the energy level distribution is derived for both molecules. In this way a symmetry-reduction-induced decrease of the level degeneracy can be observed in detail and compared with theoretical results.