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TI Structure determination of PF3 adsorption on Cu(100) using X-ray standing waves

AU Kariapper, MS Fisher, CJ Woodruff, DP Chan, ASY Jones, RG

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AB The local structure of the Cu(1 0 0)c(4 x 2)-PF3 adsorption phase has been investigated through the use of normal-incidence X-ray standing waves (NIXSW), monitored by P 1s and F 1s photoemission, together with P K-edge near-edge X-ray absorption fine structure (NEXAFS). NEXAFS shows the molecule to be oriented with its C-3v symmetry axis essentially perpendicular to the surface, while the P NIXSW data show the molecule to be adsorbed in atop sites 2.37 +/- 0.04 angstrom above the surface, this distance corresponding to the Cu-P nearest-neighbour distance in the absence of any surface relaxation. F NIXSW indicates a surprisingly small height difference of the P and F atoms above the surface 0.44 +/- 0.06 angstrom, compared with the value expected for an undistorted gas-phase geometry of 0.77 angstrom, implying significant increases in the F-P-F bond angles. In addition, however, the F NIXSW data indicate that the molecules have a well-defined azimuthal orientation with a molecular mirror plane aligned in a < 0 1 1 > substrate mirror plane, and with a small (5-10 degrees) tilt of the molecule in this plane such that the two symmetrically-equivalent F atoms in each molecule are tilted down towards the surface.

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