Surface Chemistry of 1H-1,2,3-Triazole on Cu(100) and Oxygen-Precovered Cu(100)

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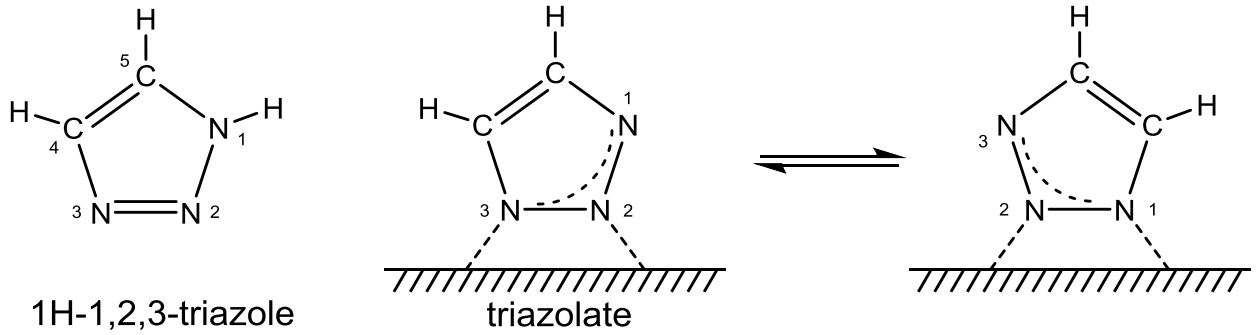
1,2,3-Benzotriazole has been considered as an effective corrosion inhibitor of metals, especially for copper [1]. The active part playing a key role in surface bonding and stability is the triazole ring. We have employed combinative surface analytical techniques (X-ray photoelectron spectroscopy, temperature-programmed reaction/desorption, reflection-absorption infrared spectroscopy, and near-edge X-ray absorption fine structure), with the aid of theoretical calculation to investigate the bonding and chemistry of 1H-1,2,3-triazole on Cu(100). In general, the copper surfaces under protection with corrosion inhibitors are partially or locally oxidized, therefore the effect of oxygen is also studied in the present research. On Cu(100), adsorbed 1H-1,2,3-triazole molecules are predominant at 120 K, with N_{1s} binding energies at 401.5 and 402.5 eV for the imine (-N=) and amine (-NH-) groups, respectively. At this temperature, a small amount of the 1H-1,2,3-triazole has dissociated by N-H bond scission, forming triazolate surface intermediate with N_{1s} binding energy shifted to 400.3 eV for all the nitrogen atoms. The surface triazolate has three characteristic infrared bands at 975, 1164 and 1442 cm^{-1}, indicating that it is perpendicularly adsorbed on the surface and is consistent with the results of the calculation and NEXAFS studies. The reaction of 1H-1,2,3-triazole on Cu(100) begins with N-H cleavage to form H_2 below 320 K. The triazolate is stable up to ~500 K and decomposes into H_2, N_2, HCN and CH_3CN at a higher temperature (~550 K). On O/Cu(100), the adsorbed oxygen atoms abstract the H from the amine group of 1H-1,2,3-triazole to form adsorbed OH and triazolate. Recombination of the OH groups generates H_2O at 210 K. In the presence of oxygen on Cu(100), triazolate is less stable and decomposes at 465 K mainly to form H_2O, N_2, CO and CO_2.



Reference:
[1] M. Finšgar, I. Milošev, Corros. Sci. **52**, 2737 (2010).