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Adsorption and Chemical Reaction of Cu(hfac)(vtms) on Clean and Modified Cu(111) Surface

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We have investigated the adsorption and reaction of Cu(hfac)(vtms) on Cu(111) surface using TPD. The recombinative desorption of Cu(hfac)(vtms) reversibly occurs between 240 and 340K. The remaining Cu(hfac) after the desorption of vtms preferentially undergo the desorption between 330 and 370K as intact Cu(hfac) than the disproportionation reaction. The disproportionation reaction between adsorbed Cu(hfac) was observed to occur between 420 and 520K with an activation energy of 34~37 kcal/mol. The geometries and adsorption sites of Cu(hfac) have been also calculated by means of extended Hückel method. It is found that standing Cu(hfac) is more stable than lying-down Cu(hfac) on the Cu(111) surface and the Cu(hfac) molecule prefers to adsorb on the hollow site over the top or bridge sites. We also have investigated the surface modification effect by preadsorbed I and Na atoms on the reaction of Cu(hfac)(vtms).