List of Captures

Fig.1. The effect of the temperature and composition of the catalyst (1 – V2O5, 2 – V2O5-SnO2, 3 – V2O5-ZrO2, 4 – V2O5-SnO2-TiO2, 5 – V2O5-ZrO2-TiO2) upon the conversion of 3-methylpyridine (A) and yield of nicotinic acid (B).

Fig.2. Clusters modeling active centers of V2O5 (A), V2O5-SnO2 (B), V2O5-ZrO2 (C),

V2O5-SnO2-TiO2 (D) and V2O5-ZrO2-TiO2 (E).

Fig. 3. Deprotonation of the methyl group of 3-methylpyridine connected with the Lewis acidic center (vanadium ion) of V2O5 (A), V2O5-SnO2 (B) and V2O5-TiO2 (C).

TABLE I. Total energy (Еtot.) and thermal energy (*E*therm.) of vanadium containing clusters and their charged forms (Fig.3), proton affinity of oxygen, bonded to vanadium-ion (*PA*V=O). Temperature 573.15 K.

TABLE II. Total energies (*Е*tot.) and thermal energy (*E*therm.) of the 3-methylpyrine and its carbanion, connected with the vanadium pentoxide and binary catalysts and enthalpy deprotonation (*DE*) of substrate. Temperature 573.15 K.