Fig.1. The effect of the temperature and composition of the catalyst on the conversion of 3-methylpyridine (A) and yield of nicotinic acid (B).

Fig.2. Conversion of 3-methylpyridine and proton affinity of the binary and three-component catalysts (I – V2O5, II – V2O5-SnO2, III - V2O5-ZrO2, IV - V2O5-SnO2-TiO2, V - V2O5-ZrO2-TiO2) to V2O5 vanadyl oxygen.

Fig.3. Clusters modeling active centers of V2O5, the binary and three-component catalysts.

Fig.4. The effect of temperature and composition of the catalyst on the conversion of 3-methylpyridine (A) and yield of nicotinic acid (B).

Fig. 5. Deprotonation of the methyl group of 3-methylpyridine connected with the Lewis acidic center (vanadium ion) of various catalysts.

TABLE. Total energies of 3-methylpyrine and its carbanion, connected with the vanadium pentoxide and binary catalysts (*Е*tot.) and enthalpy deprotonation of the substrate (*DE*). (*DE* = (*E*anion/cat. − *E*molecule/cat.)×2625.5)