Fig. 1. The effect of temperature and composition of the catalyst on the conversion of 3,4-dimethylpyridine (A), yield of 3-methyl-4-cyanopyridine (B) and imide of pyridine-3,4-dicarboxylic acid (C): 1 – V2O5, 2 – V2O5·4SnO2, 3 – V2O5·4ZrO2.

Fig. 2. The effect of NH3/3,4-dimethylpyridine mole ratio on the conversion (1) of 3,4-dimethylpyridine , yield (2) and selectivity (3) of 3-methyl-4-cyanopyridine.

Fig.3. Heterolytic cleavage of C−H bond without carry of a proton on vanadyl oxygen (A) and with it (B).

TABLE I. Total energies of molecules of 3,4-dimethylpyridine, о-xylene, mononitriles and corresponding anions (*E*tot.), enthalpy of proton detachment from the methyl groups in the gaseous phase (*DE*), energies of the [highest occupied molecular orbital](https://en.wikipedia.org/wiki/Highest_occupied_molecular_orbital)s of anions (*Е*HOMO), calculated by the *ab initio* method (HF/6-311+G\*\*).

TABLE II. Total energies of the connected with the Lewis acidic center molecule of 3,4-dimethylpyridine and carbanions (*Е*tot.), energy of heterolytic cleavage of С−Н bond of the methyl groups of the adsorbed substrate (*E*C-H), deprotonation enthalpy (*DE*) of the methyl groups, calculated by the DFT method (B3LYP/LanL2DZ)

TABLE III. Total energies (*Е*tot.), zero-point energy (*ZPE*) of the 3,4-dimethylpyridine and carbanions in gaseous phase and enthalpy deprotonation of substitutions, calculated by *ab initio* method (HF/6-311+G\*\* Freq Test).

TABLE IV. Total energies (*Е*tot.) and thermal energy (*E*therm) of the 3,4-dimethylpyridine and carbanions on cluster, enthalpy deprotonation of substitutions (*DE*), calculated by DFT method (B3LYP/Lanl2DZ).

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TABLE V. The total energies of the vanadium-containing clusters and their protonated forms (*E*tot.), proton affinity of oxygen bound to the vanadium ion (*PA*), calculated by the DFT method (B3LYP / LanL2DZ).

Scheme 1 – Formation of imide of pyridine-3,4-dicarboxylic acid from 3,4-dimethylpyridine