Response to Reviewer:

1 - In the first version of the article, the proton affinity of vanadyl oxygen of the clusters which model the active center, we calculated on a difference of electronic energies of the neutral and charged clusters received by optimization of their geometry by the DFT method. The expert fairly noticed that these calculations include Born–Oppenheimer approximation which ignores the driving of kernels and can lead to errors in definition of a minimum on a surface of a potential energy. Therefore we carried out the calculations of the frequencies for temperature of the reaction for clusters and complexes of a substratum and an anion with the optimized geometry. The values DPE and DE, certainly, changed, but regularities of influence of the oxide-promoters at these values remained the same.

In accordance with the above proton affinity of vanadyl oxygen (*PA*V=O) of investigated clusters (Table I) was calculated by the formula (1)

*PA*V=O = [(*E*Neutral cluster + *E*therm.Neutral cluster) – (ECharged cluster + *E*therm.Charged cluster)]∙2625.5, (1)

and enthalpy of deprotonation (*DE*) of the methyl group of adsorbed substrate (Table II) by the formula (2)

*DE*=[(*E*anion/clus.+ *E*therm.anion/clus.)–(*E*molecule/clus.+ *E*therm.molecule/clus.)]∙2625.5. (2)

1. - For conclusions about the existence of the linear correlation between *PA* and the experimental results, in classical sense, it is necessary to have kinetic constants of reaction rate. We consider the use of values of experimentally defined conversion for these purposes is incorrect. Therefore we simply note that in the same row of the catalysts the values of PA and conversion change symbatically (in case of DE - antibatically). We will consider this comment in our further research. The figure 2 was deleted according to the remark of the expert.

3. a. Fig.1. and Fig.4. were connected into one figure (corrected Fig.1.). Exp. data was separated from modelling. The text was reshuffled in similar way, first to discuss the exp. data, then computations.

3b. done

 Table I shows *PA*V=O for all systems (V2O5, V2O5-SnO2, V2O5-ZrO2, V2O5-SnO2-TiO2 and V2O5-ZrO2-TiO2) in light of the comment 1.

3c. q = Charge, m = multiplicity

In corrected manuscript we gave the full names of values, rather than abbreviated names.

3d. done

3e. done: TABLE I.

3f. It was non-correct phrase and we don't present it in the corrected manuscript.

3g. done. Fig. 5 (Corrected 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)).

3h. Table II was corrected in light of the comment 1.

Corrected 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.

3i. According to the expert's remark that the cluster with only one vanadium atom is used, we constructed the complexes with plane adsorption of 3-methylpyridine and its carbanion on a cluster with two atoms of vanadium. By their optimization the molecule of a substratum and an anion turned in such a way that they become bonded with the ring nitrogen atom with vanadium cation (vertical adsorption), and results of calculations were the same, as in case of A.

3j. We made the table with the matrixes of the studied clusters and complexes of the substat and its carbanion with the optimized geometry in the Cartesian coordinate system. The table is large, and we are not sure whether it makes sense to place it in the article since its volume will increase. We leave this solution on the discretion of the editorial board and the expert.

3k. Done

 3j. TABLE. XYZ coordinates of the investigated species.

|  |  |  |
| --- | --- | --- |
| Example | Neutral cluster | Charged cluster |
| A | O 0.000000 0.000000 1.997788V 0.000000 1.648939 1.330098V 0.000000 -1.648939 1.330098O 0.000000 0.000000 -1.997788V 0.000000 -1.648939 -1.330098V 0.000000 1.648939 -1.330098O 1.208572 1.806815 0.000000O -1.208572 1.806815 0.000000O 1.208572 -1.806815 0.000000O -1.208572 -1.806815 0.000000O 0.000000 2.816185 2.399776O 0.000000 -2.816185 2.399776O 0.000000 -2.816185 -2.399776O 0.000000 2.816185 -2.399776 | V -0.300140 -0.073570 0.135564O -0.392509 0.065929 1.815150O 1.274519 -0.325202 -0.557675O -0.741514 -1.604267 -0.561585V 0.814439 -1.825689 -1.559019O 1.642534 -3.132342 -1.295614O -1.073740 1.148766 -0.772593O 0.564672 -1.431455 -3.231348V -1.386248 1.639662 -2.527307O -2.216633 2.946301 -2.794900O -1.895150 0.201600 -3.465720O 0.131320 1.489534 -3.466487V -0.266511 -0.123115 -4.178303O -0.213429 -0.207913 -5.745843H -0.446330 0.146396 2.786440 |
| B | V 0.066146 0.043156 0.096367 O 0.098580 0.175060 1.678603O 1.601313 0.141121 -0.859003O -0.122165 -1.582145 -0.679424V 1.037624 -1.146920 -2.000174O 2.060210 -2.227966 -2.554771O -1.053386 1.068192 -0.810632O 0.034838 -0.264900 -3.159122Sn -1.297876 1.110223 -2.752508O -2.390330 2.091825 -3.815921 | V 0.018934 -0.026433 -0.001370O -0.028372 0.028447 1.688805O 1.543437 0.018885 -0.845415O -0.303167 -1.516102 -0.847325V 0.967328 -1.164606 -2.164048O 1.890173 -2.273875 -2.787083O -0.905434 1.086745 -0.916359O 0.095920 -0.114920 -3.241600Sn -1.145362 1.377983 -2.892520O -2.128668 2.563396 -3.838475H -0.053505 0.057309 2.664183 |
| C | V -0.082003 0.030789 0.035769O -0.107046 0.082160 1.623973O 1.525670 -0.023441 -0.800637O -0.402315 -1.521349 -0.843739V 0.890095 -1.160047 -2.062103O 1.847296 -2.311944 -2.593662O -0.958266 1.274316 -0.861165O 0.143464 -0.075319 -3.238791Ti -0.960001 1.345375 -2.729427O -2.456055 1.200977 -3.340700 | V 0.026272 0.017404 -0.022875O -0.051195 0.059673 1.668429O 1.591008 -0.051223 -0.810855O -0.387000 -1.412876 -0.909360V 0.970201 -1.127233 -2.184864O 1.907114 -2.239448 -2.783255O -0.741753 1.266709 -0.902932O 0.274189 0.032797 -3.269134Ti -0.910256 1.432430 -2.816905O -2.389705 0.949569 -3.199349H -0.083817 -0.029564 2.639163 |
| D | V 0.000000 0.000000 0.000000O 0.000000 0.000000 1.590970O 1.598638 0.000000 -0.860579O -0.300222 -1.538247 -0.910841V 1.000203 -1.165453 -2.117500O 1.985095 -2.312954 -2.611878O -0.912711 1.255123 -0.822255O 0.272838 -0.126457 -3.332391Zr -0.932876 1.445814 -2.852002O -2.575256 1.121170 -3.449227 | V 0.009070 -0.044199 0.091115O -0.026106 0.112876 1.779592O 1.553467 -0.015353 -0.733474O -0.269724 -1.583954 -0.662264V 1.044860 -1.303268 -1.973963O 2.076315 -2.395145 -2.446310O -0.919683 1.042500 -0.833192O 0.250331 -0.371864 -3.187186Zr -1.218731 1.043846 -2.914930O -2.717548 0.151603 -3.121962H -0.020434 0.098855 2.753921 |
| E | V 2.307295 1.616931 0.314239O 3.452982 2.684578 0.557869O 2.856311 -0.068889 0.512327V 2.305397 -1.646101 -0.113404O 3.449822 -2.741785 -0.153288O 1.759667 1.561751 -1.429264O 1.758099 -1.142879 -1.783727Ti 1.004389 0.320159 -2.447999O -0.667666 0.274636 -2.093218O 0.926127 1.914919 1.307049O 0.923734 -2.188272 0.769291V -0.766881 1.418430 1.790832V -0.768775 -1.831286 1.364937O -1.387647 2.347017 2.918934O -1.390764 -3.018502 2.215752O -0.704233 -0.297036 2.268963O -1.752817 1.362470 0.386331O -1.754443 -1.414170 0.022439Sn -2.417280 0.137813 -1.041466O -3.962589 0.264211 -1.999045 | V 0.320529 0.351081 0.281309O 0.189184 1.330737 1.506772O 1.787969 0.606382 -0.664961V 2.270004 0.267767 -2.362346O 3.416743 1.200584 -2.906451O -0.931396 0.637946 -0.991487O 0.665482 0.567529 -3.171727Ti -1.039584 0.338270 -2.747246O -1.389567 -1.328219 -2.941656O 0.219104 -1.363061 0.764447O 2.652924 -1.424453 -2.519730V 0.212437 -3.064235 0.346933V 2.151211 -3.143034 -2.317693O 0.045875 -4.092081 1.685716O 3.222758 -4.199961 -2.789374O 1.642153 -3.346174 -0.554367O -0.966243 -3.267163 -0.818552O 0.630550 -3.392014 -3.057006Sn -1.348861 -3.351999 -2.864512O -2.659713 -4.369809 -3.604698H -0.137969 -4.794664 2.334382 |
| F | V -2.055999 1.635480 -0.652493 O -2.907662 2.721031 -1.438770O -2.297243 0.000001 -1.330816V -2.055999 -1.635479 -0.652497O -2.907662 -2.721029 -1.438776O -2.639922 1.457067 1.002444O -2.639923 -1.457070 1.002441Ti -3.048241 -0.000003 2.067709O -2.314423 -0.000004 3.517095O -0.322285 1.972677 -0.715928O -0.322285 -1.972676 -0.715932V 1.379183 1.649014 -1.108097V 1.379183 -1.649011 -1.108100O 1.976685 2.722022 -2.116378O 1.976686 -2.722018 -2.116382O 1.445999 0.000002 -1.793508O 2.376565 1.523707 0.327164O 2.376564 -1.523707 0.327162Zr 3.161582 -0.000001 1.395839O 2.536908 -0.000002 3.061863 | V 0.293014 0.319957 0.265275O 0.180709 1.286569 1.503962O 1.769268 0.558142 -0.669489V 2.242915 0.227231 -2.371812O 3.413925 1.138698 -2.902633O -0.954058 0.657033 -1.001019O 0.651994 0.578525 -3.189349Ti -1.072516 0.497015 -2.778074O -1.598472 -1.103332 -3.095986O 0.164291 -1.393847 0.730376O 2.590229 -1.466481 -2.539104V 0.208137 -3.114938 0.384957V 2.165448 -3.210114 -2.321797O 0.145411 -4.083936 1.778461O 3.309815 -4.220597 -2.726206O 1.615696 -3.374904 -0.555749O -1.033092 -3.400196 -0.690140O 0.712814 -3.517837 -3.153365Zr -1.343534 -3.201823 -2.837231O -2.496698 -4.248480 -3.681114H -0.011707 -4.763260 2.457790 |
| Example | Molecule/cluster | Anione/cluster |
| A | V -0.469299 -0.051292 0.090029O -1.163181 -0.008192 1.511772O 1.230427 0.245637 0.155364O -0.891633 -1.482695 -0.752314V -1.487627 -3.182994 -1.117472O -1.997418 -3.941939 0.349190O -0.232842 -4.087311 -1.892895O -2.720011 -3.019908 -2.098152H 2.020825 0.379968 0.711193H -2.734965 -4.361361 0.829390H 0.008691 -4.603579 -2.683945N -1.314884 1.469541 -0.882989C -2.367157 2.178710 -0.361475C -2.976934 3.230485 -1.063481C -2.459650 3.539106 -2.344951C -1.378500 2.811386 -2.874414C -0.819811 1.775961 -2.122028C -4.135905 3.995415 -0.465612H -2.704746 1.885887 0.626529H -2.901858 4.346921 -2.922606H -0.971860 3.039492 -3.853356H 0.017855 1.189955 -2.486546H -4.395920 3.626542 0.531244H -3.896856 5.062482 -0.378180H -5.027650 3.911186 -1.099061 | V 0.734103 -0.319385 -1.273678 O 1.107421 -0.109763 0.255873 O 2.038571 -0.355978 -2.434407 O -0.541277 -1.594054 -1.400108 V -1.696750 -2.821958 -1.122099 O -3.119861 -1.846644 -0.707420 O -1.260907 -3.751493 0.256709 O -1.943440 -3.750492 -2.541516 H 2.981261 -0.404780 -2.668072 H -4.019261 -2.135195 -0.445805 H -0.869854 -3.927093 1.130415 H -1.963211 -4.441170 -3.222169 N -0.481104 1.234792 -1.735910 C -1.778169 1.231955 -1.361453 C -2.537713 2.457175 -1.263266 C -1.850042 3.676770 -1.629274 C -0.528128 3.636786 -2.060180 C 0.145755 2.396979 -2.109485 C -3.872305 2.446309 -0.860540 H -2.237126 0.274291 -1.131829 H -2.379789 4.623717 -1.562022 H -0.001169 4.538827 -2.350536 H 1.175445 2.314130 -2.438031 H -4.362546 1.526651 -0.553542 H -4.466393 3.356295 -0.848415 |
| B | V -0.474770 0.193002 0.424385O -1.220883 0.303852 1.817342O 1.242635 0.131035 0.614555V 2.700833 1.230360 0.435381O 3.714424 0.534153 -0.559425O 3.455945 1.643155 1.930296O -0.698570 1.635583 -0.509754O 1.899798 2.584526 -0.350722Sn 0.249548 3.275582 -1.039667O -0.329484 4.757334 -1.906611H 4.289236 1.629408 2.439220N -1.213061 -1.449590 -0.419067C -2.358225 -2.037913 0.061300C -2.916891 -3.178627 -0.535768C -2.245879 -3.713164 -1.662892C -1.069694 -3.112801 -2.148287C -0.569944 -1.977263 -1.508616C -4.177777 -3.805837 0.013203H -2.809157 -1.577830 0.933698H -2.642185 -4.598422 -2.153954H -0.544340 -3.517638 -3.006157H 0.341277 -1.489826 -1.840635H -4.967576 -3.825156 -0.747926H -3.995558 -4.842796 0.321358H -4.560059 -3.259622 0.880796 | V -0.027777 -0.167546 0.516798O -0.291078 -0.571715 2.030342O 1.734532 0.143866 0.181753V 2.794957 1.478588 -0.114358O 3.397605 1.406092 -1.718215O 3.984572 1.561605 1.101302O -0.800107 1.334995 -0.039823O 1.648692 2.786901 -0.017037Sn -0.272977 3.196595 -0.083206O -1.176728 4.744924 -0.363645H 4.671987 1.648524 1.780266N -0.683815 -1.725998 -0.575378C -2.024069 -1.800981 -0.732834C -2.693768 -3.058910 -0.958261C -1.845697 -4.235873 -1.010242C -0.468600 -4.115750 -0.883837C 0.107890 -2.837479 -0.680976C -4.075250 -3.110237 -1.129888H -2.584056 -0.871269 -0.676507H -2.304778 -5.210938 -1.149590H 0.178175 -4.984834 -0.932538H 1.177850 -2.690661 -0.584980H -4.691143 -2.216969 -1.064898H -4.582969 -4.047261 -1.342906H 3.755722 1.283343 -2.611191 |
| C | V 0.025978 -0.308673 1.161039O -0.001902 -0.968584 2.599665O 1.606015 0.240878 0.693297V 2.339546 1.765150 -0.009457O 2.778746 1.434287 -1.492599O 3.664498 2.398726 0.894417O -1.030700 1.055847 0.999577O 0.928194 2.837693 -0.008456Ti -0.894594 2.688998 0.070003O -1.488529 2.390909 -1.411411H 4.612768 2.628672 0.854332N -0.586366 -1.744841 -0.069145C -0.613445 -3.058193 0.332397C -0.996215 -4.093752 -0.533255C -1.363786 -3.731842 -1.852543C -1.343061 -2.385107 -2.257651C -0.948930 -1.403060 -1.346398C -1.016339 -5.531224 -0.065581H -0.327354 -3.256285 1.359643H -1.668471 -4.502967 -2.555712H -1.627828 -2.094070 -3.262578H -0.932068 -0.351593 -1.617500H -0.710575 -5.622801 0.981064H -2.021745 -5.959439 -0.161531H -0.339265 -6.147883 -0.669627 | V -0.513085 0.039487 0.672310O -1.171390 -0.474455 2.021085O 1.319705 0.136943 0.755386V 2.591508 1.254539 0.432839O 3.494038 0.785452 -0.950725O 3.540760 1.478660 1.838480O -0.995129 1.650584 0.099513O 1.662710 2.657167 0.033270Ti -0.087953 3.154619 -0.448771O -0.215780 3.312789 -2.059679H 4.222702 1.474230 2.528384N -0.819644 -1.405478 -0.699953C -0.128177 -2.558873 -0.594780C -0.637049 -3.801028 -1.130396C -1.914657 -3.726442 -1.811487C -2.578575 -2.512032 -1.942352C -2.009037 -1.346584 -1.380088C 0.076788 -4.991023 -1.014185H 0.825218 -2.520869 -0.076828H -2.347505 -4.636533 -2.219221H -3.528832 -2.441638 -2.459781H -2.485645 -0.374959 -1.455868H 1.021953 -5.038201 -0.479862H -0.285855 -5.912386 -1.461884H 3.873797 0.592861 -1.821814 |