CHARACTERIZATION AND CATALYTIC PROPERTIES OF MoO$_3$/V$_2$O$_5$/Nb$_2$O$_5$ IN THE REACTION OF DECOMPOSITION OF THE ISOPROPANOL

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Abstract. The influence of molybdenum oxide as a promoter on the V$_2$O$_5$/Nb$_2$O$_5$ system was investigated. A series of MoO$_3$/V$_2$O$_5$/Nb$_2$O$_5$ catalysts with MoO$_3$ loading ranging from 1 to 3 wt% MoO$_3$ and fixed V$_2$O$_5$ content (21 wt%), were prepared by impregnation of support by an aqueous solution of ammonium metavanadate and ammonium molybdate. The catalysts were characterized by chemical analysis (atomic absorption spectroscopy), nitrogen volumetry (BET surface area and pore volume), temperature-programmed reduction (TPR), X-ray diffractometry (XRD) and tested in the isopropanol decomposition reaction. The properties acid-basic of the catalyst was investigated by the selectivity during the isopropanol decomposition reaction. The X-ray diffraction results showed the presence of the β-(Nb,V)$_2$O$_5$ phase since was added the V$_2$O$_5$ on Nb$_2$O$_5$. The results of temperature programmed showed that the reducibility of vanadium was affected with the addition of molybdenum up to a loading of 3 wt% MoO$_3$. The results of catalytic activity for the isopropanol decomposition revealed that the molybdenum oxide, at high loadings, affects the properties acid-base of the V$_2$O$_5$/Nb$_2$O$_5$ catalyst, providing a decrease in the propylene formation (acid sites) and acetone (basic sites).

Keywords: niobium, vanadium, molybdenum, isopropanol.

1. Introduction

Supported vanadium oxide catalysts have been used in a great number of reactions of selective oxidation (Cortez, et. al. 2003). The catalytic properties of the vanadium oxide are influenced strongly by several variables, such as the preparation method, nature of the support and promoter type. Vanadium and molybdenum oxides are important components of catalysts used for selective oxidation of light alkanes (Lopez Nieto, et al. 1995). The molybdenum has been used frequently as a promoter in V$_2$O$_5$-supported (Satsuma et al. 1991). Dejoz et al. (1999) reported the role of the molybdenum in Mo doped V-Mg-O catalysts during oxidative dehydrogenation of n-butane. Lietti et al. (1999) showed that the V$_2$O$_5$-MoO$_3$/TiO$_2$ catalysts could be used in the selective catalytic reduction (SCR) of NO$_X$ In recent years, niobium-based materials have been employed as supports in numerous catalytic applications. The use of Nb$_2$O$_5$ as support in catalysts that contain vanadium can represent an alternative synergic, once the two elements besides belong to the same group of the periodic table, present several similar chemical properties (Tanabe, 2003). The catalytic applications of the niobium oxide as support, promoter or a solid with acid properties, have been reported in the last years (Ziolek, 2003). Isopropanol

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decomposition in the absence of oxygen is used widely as a chemical probe reaction to determine acid-basic properties. In the absence of oxygen the selectivity in the conversion of isopropanol into propylene by dehydration and acetone by dehydrogenation has been employed to determine the balance between surface acidity and basicity (Haffad, et al. 2001). In the presence of oxygen is a measure of the surface redox potential of the catalyst or of its activity as a selective oxidation catalyst (Kulkarni et al., 2002). The reactions oxidation and decomposition reactions of isopropanol are analogous, since the only role of oxygen is to prevent the reduction of the metal oxide surface.

In the present study were prepared and characterized $MoO_3/V_2O_5/Nb_2O_5$ catalysts with MoO_3 contents of 1 and 3 wt.% and with 21 wt.% V_2O_5 loading. The catalytic activity was evaluated in the isopropanol decomposition in the presence of oxygen over the catalysts.

2. Experimental

For this study, the catalyst preparation involves two steps. Prior to impregnation, the Nb_2O_5 was prepared by calcination of hydrated niobium (supplied by CBMM, Brazil HY-340) at 500^oC for 6 h. In the first step, the support was added in the aqueous solution heated up to 70^0C containing the NH_4VO_3 (Merck) salt. The theoretical amount of vanadium on the support was of 21wt.% of V_2O_5. The mixture was maintained under agitation and vacuous in the temperature of 70^0C to remove all the water. Therefore after, the sample was dried at 110^0C for 12 h and subsequently calcined at 450^0C for 4 h. In the second stage, a theoretical amount (1 or 3 wt.% of MoO_3) of $(NH_4)_6Mo_7O_{24}.4H_2O$ (Mallinckrodt) salt was added to the mixed V_2O_5/Nb_2O_5 catalyst with water in excess in the temperature of 70^0C. The mixture was maintained in the same conditions described previously until drying the solid totally. The obtained solid was dried and calcined in the same previous conditions. The final amount of MoO_3 on V_2O_5/Nb_2O_5 was of 1 and 3% wt, respectively. Samples are labeled as xMo/21V/Nb, where x is MoO_3 loading with 1 and 3 wt.%.

The elemental composition of the samples was determined by atomic absorption spectroscopy (AAS). The samples were digested with a mixture acid of HNO_3 and HF. The measurements were carried out by standard addition solution method by using a Perkin-Elmer Analyst equipment.

BET surface areas were measured by using a Quantachrome NOVA 1000 instrument by adsorption of nitrogen at $– 196^0C$ on 150 mg of sample previously degassed at 200^0C under high vacuum atmosphere for 2 h.

XDR diffraction patterns were obtained with a SEISERT Isodebyeflex 1001 diffractometer operated at 40 kV and 30 mA by using Ni-filtered $CuK\alpha$ radiation ($\lambda = 0.15418$ nm). The samples in powder form were analyzed without previous treatment after deposition on a quartz sample holder. The identification of crystalline phases was made by using references from the ASTM files.

Temperature-programmed reduction (TPR) results were obtained in a Quantachrome Chembet-3000 apparatus loaded with 25 mg of catalyst. The samples were first treated in helium at temperature of 150^0C for 1 h. The samples were cooled to room temperature and were subsequently contacted with an H_2/N_2 mixture (H_2/N_2 molar ratio of 0.15 and a total flow of 40 cm^3/min) and heated, at a rate of 10^0C/min, to a final temperature of 900^0C.

The catalytic test of decomposition of isopropanol was realized out in a fixed bed quartz tubular reactor (i.d. 10 mm, length 400 mm) operated at atmospheric pressure and temperature in the range of 170-290^{0}C. The reactor was equipped with a coaxial thermocouple for catalytic bed temperature profiling. The isopropanol (99.7%, Merck) was injected in the piping of feeding of gases flowing of the reactor with aid of a pump Thermo Separation Product Spectra P100, in the flow rate of 0.05 cm^3/min and diluted in a mixture of He and O$_2$ (molar ratio of 3/1) in the flow rate of 74 cm^3/min. Reactants and reaction products were analyzed by on-line gas chromatography (VARIAN 3350), equipped with a thermal conductivity detector (TCD). A Carbowax 20 M on Chromosorb W column was used for separation of products. The catalyst mass was 100 mg, particle size 0.5-0.85 mm and the time contact was 2.4 g.h/mol$_{Isop}$. The conversion was calculated from the reaction product on the basis of the carbon balance: the total molar amount of carbon in the effluent was assumed to be equal to the molar amount of carbon in the isopropanol fed to the reactor.

3. Results and discussion

The results of the chemical composition determined by atomic absorption (AA), BET specific areas and volumes of pores of the samples are presented in Table 1. These results demonstrate that the amounts of V$_2$O$_5$ and MoO$_3$ in the samples are close of the theoretical values. The vanadium presence on the Nb$_2$O$_5$ reduces the specific area and the volume of pores being this more pronounced effect when molybdenum is added on the V$_2$O$_5$/Nb$_2$O$_5$ catalyst. This effect is related to the blockade of the pores of the Nb$_2$O$_5$ for the high loadings of V$_2$O$_5$ (21 wt.%) and also of MoO$_3$ (1 and 3 wt.%).

Table 1. Results of chemical composition of V and Mo obtained by AA, BET specific areas (Sg$_{BET}$) and volumes of pores (Vp) of the samples.

Samples	V$_2$O$_5$ (wt.%)	MoO$_3$ (wt.%)	Sg$_{BET}$ (m^2.g^{-1})	Vp (cm^3.g^{-1})
Nb$_2$O$_5$	0	0	112	0,08
21V/Nb	24,2	0	39	0,04
1Mo/21V/Nb	21,0	1,2	17	0,02
3Mo/21V/Nb	19,2	2,9	6	nd

nd: not determined

Figure 1 presents the XRD patterns of V$_2$O$_5$ bulk, Nb$_2$O$_5$ support and of the catalysts xMo/21V/Nb calcined at 500^{0}C. The profile of XRD of V$_2$O$_5$ bulk is represented in Figure 1-a, where the most intense peaks correspond to 2θ at 20.3^o (100%), 26.1^o (90%) and 30.95^o (85%). The Figure 1-b presents the profile of XRD of Nb$_2$O$_5$ with a most intense peak at 2θ = 23,14^0 corresponding the TT-phase or T-phase of Nb$_2$O$_5$. The X-ray diffractograms of the sample calcined, after the addition of V$_2$O$_5$ on Nb$_2$O$_5$ (Figure 1-c), show the presence of a β-(Nb,V)$_2$O$_5$ phase as evidenced by the peaks to 2θ at 23.67^0, 24.97^0 and 26.19^0. A more intense peak to 2θ = 22.33^0 and other less intense, are characteristic of V$_2$O$_5$ dispersed on Nb$_2$O$_5$. The absence of peaks of the crystalline phase of MoO$_3$ for samples containing 1 and 3 wt.% MoO$_3$ supported on V$_2$O$_5$/Nb$_2$O$_5$, represented respectively by the Figure 1-d and

1-e, indicates that the molybdenum oxide is present in a state amorphous or highly dispersed on V_2O_5/Nb_2O_5. In previous studies, Ko and Weissman (1990) reported that the forms of the TT and T-phases of Nb_2O_5, when calcined at 500°C, present a profile of X-ray diffraction similar. Other authors (Chary et al. 2002) identified the TT-phase and T-phase of crystalline Nb_2O_5 with different spacing intensities at d = 3,94Å ($2\theta = 22.6^0$) and d = 3.14Å ($2\theta = 28.42^0$). The intensity of β-$(Nb,V)_2O_5$ phase, identified in $2\theta = 23.6^0$ and 25^0, increases with the addition of molybdena (1 wt.% of MoO_3) to the V_2O_5/Nb_2O_5 catalysts and decreases with the increase in molybdenum loading from 2 to 4 wt.%. In this study, this behavior was confirmed in all the samples. In more recent works, Chary et al. (2002) identified the β-$(Nb,V)_2O_5$ phase to 2θ at 22.5^0 (100%) and 28.5^0 (90%) for samples containing 10 to 12 wt.% V_2O_5 supported on Nb_2O_5. Watling et al. (1996) also observed the presence of β-$(Nb,V)_2O_5$ phase for concentration of vanadium around 7 mol-% in vanadia-niobia catalysts.
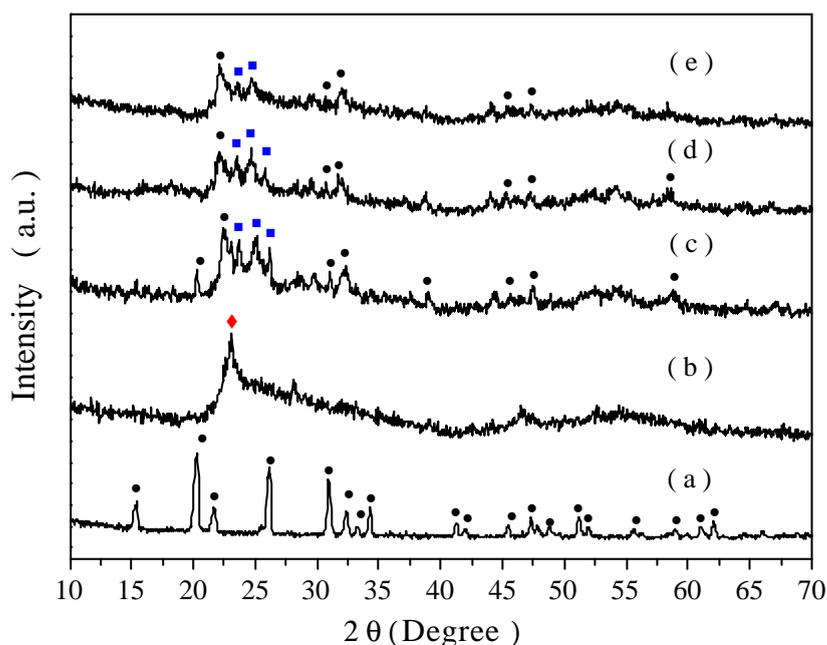
Fig. 1. XDR patterns of (a) V_2O_5 bulk; (b) N_2O_5; (c) 21V/Nb; (d) 1Mo/21V/Nb and (e) 3Mo/21V/Nb. Peaks due to ( ) V_2O_5 phase; ($\blacklozenge$) TT-phase or T-phase of Nb_2O_5 and ( ) β-$(Nb,V)_2O_5$ phase.

The temperature programmed reduction (TPR) profiles of V_2O_5 bulk, Nb_2O_5 and catalysts are presented in Figure 2. The TPR profile of pure V_2O_5 shown in Figure 2-a, presents three peaks of reduction at 663^0C, 696^0C and 836^0C. Komandur et al. (2003) obtained the same profile, whose peaks were attributed to the following sequence of reduction of the vanadium oxide: 675^0C ($V_2O_5 \rightarrow V_6O_{13}$), 705^0C ($V_6O_{13} \rightarrow V_2O_4$) and 780^0C ($V_2O_4 \rightarrow V_2O_3$). In the three reduction stages, the vanadium (V^{+5}) is reduced to the species $V^{+4,33}$, V^{+4} and V^{+3}, the measure that the reduction temperature increases.

The profile of reduction of Nb_2O_5, presented in Figure 2-b, shows a peak of reduction around 781°C. The reducibility of Nb_2O_5 is more difficult than of vanadium oxide. The complete reduction of pure niobium with hydrogen is initiated at 800^0C. However, the reduction of bulk Nb_2O_5 to Nb_2O_4 happens around 1300°C (20). The

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21V/Nb catalyst, presented in Figure 2-c, exhibits four peaks of reduction: a little defined one around 595°C and other three located at 640°C, 680°C and 830°C, being the first three corresponding to the reduction of the vanadium species and the last correspondent the reduction of Nb_2O_5. The profile of reduction of 1Mo/21V/Nb catalyst, presented in Figure 2-d, shows four regions of reduction at 608°C, 644°C, 692°C and 850°C. The presence of MoO_3 in low concentrations (1 wt.%) on V_2O_5/Nb_2O_5 modifies the reducibility of V^5 species on Nb_2O_5, promoting a significant change in the reduction temperatures for higher values. The profile of reduction of 3Mo/21V/Nb catalyst (Figure 1-e) presents maximum temperatures of reduction at 630°C and 858°C.
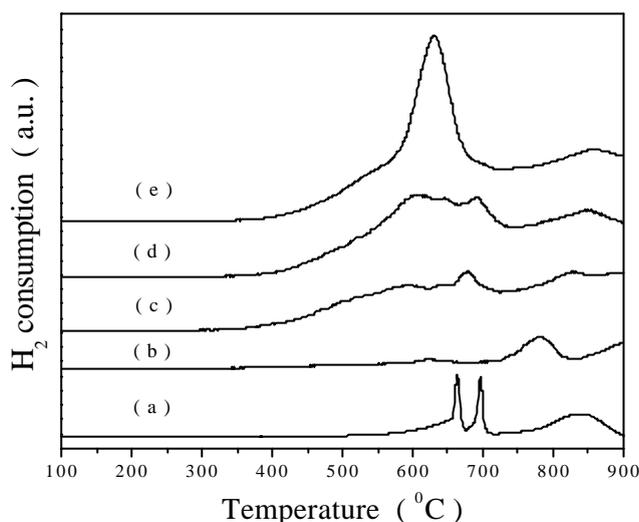

Fig. 2. TPR profiles of (a) V_2O_5 (bulk); (b) Nb_2O_5; (c) 21V/Nb; (d) 1Mo/21V/Nb and (e) 3Mo/21V/Nb.

The modification in the reducibility of V^{+5} species with the support can be attributed to the addition of molybdenum oxide through the formation of β-$(Nb,V)_2O_5$ phase, which promote an increase of the maximum temperature of reduction. Other authors (Chary et al. 2002) found that the addition of molybdenum oxide over V_2O_5/Nb_2O_5 catalysts favors the formation of β-$(Nb,V)_2O_5$ phase up to 3 wt.% MoO_3 loading and increases the reducibility of the catalysts. The reduction of MoO_3 was studied for Grunert et al. (1992). They identified reduced species of Mo^{+6}, Mo^{+5}, Mo^{+4} and Mo^{+2}, and a located region around of 630°C was attributed to the formation of metallic Mo. In more recent works, Bhaskar et al. (2001) identified two peaks of pure MoO_3 at 767 and 997^{0}C and one minor reduction peak at 797^{0}C. The sharp peak at 767^{0}C corresponds to reduction of MoO_3 ($MoO_3 \rightarrow MoO_2$) and the peak at 997^{0}C is associated with the reduction of de MoO_2 ($MoO_2 \rightarrow Mo$). A minor peak at 797^{0}C can correspond at Mo_4O_{11} formed by reduction of MoO_3. In the present work, a reduction peak at 630°C (Figure 2-e) can be attributed to the metallic Mo reduced on V_2O_5/Nb_2O_5.

The acid-base properties of catalysts were compared using the isopropanol test reaction. The results of catalytic activity for the oxidative decomposition of isopropanol as a function of reaction temperature are shown in Table 2. The catalytic activity was evaluated being taken as base the rate of formation of the products (mol g_{cat}^- ^{1}min^{-1}). The results show that the Nb_2O_5 is only selective to propylene in the temperature of 230°C. The vanadium

addition over niobium produces propylene and acetone in the three temperature intervals, being growing with the increase of this parameter. The addition of 1 wt.% of MoO_3 over 21V/Nb increase the propylene production and reduces the production of acetone, when compared with the catalyst 21V/Nb. Already in the catalysts containing 3 wt.% of MoO_3 on 21V/Nb, the propylene production and of acetone decrease. The results of catalytic activity versus reaction temperature for the isopropanol oxidation of 1Mo/21V/Nb catalyst are shown in Figure 3. The conversion of the isopropanol increases with the rise of temperature and reaches a maximum in the temperature of 260^{0}C. The propylene formation is favored starting from the temperature of 210^{0}C, however, the formation of acetone is disfavored starting from this temperature. In works mentioned previously (Wang et al. 1999), the increase of the temperature favors the propylene formation through the dehydration of the isopropanol.

Table 2. Results of catalytic activity of Nb_2O_5 and xMo/21V/Nb at different temperatures, in the isopropanol oxidation reaction.

Catalyst	RFP - Rate of formation of the products (mol.g$_{cat}$$^{-1}$min^{-1})					
	Propylene			Acetone		
	210℃	220℃	230℃	210℃	220℃	230℃
Nb_2O_5	0	0	8,1	0	0	0
21V/Nb	38,8	46,6	51,5	14,3	13,0	11,1
1Mo/21V/Nb	33,4	46,9	55,1	4,8	4,7	4,5
3Mo/21V/Nb	5,5	35,8	43,1	4,0	3,0	2,8
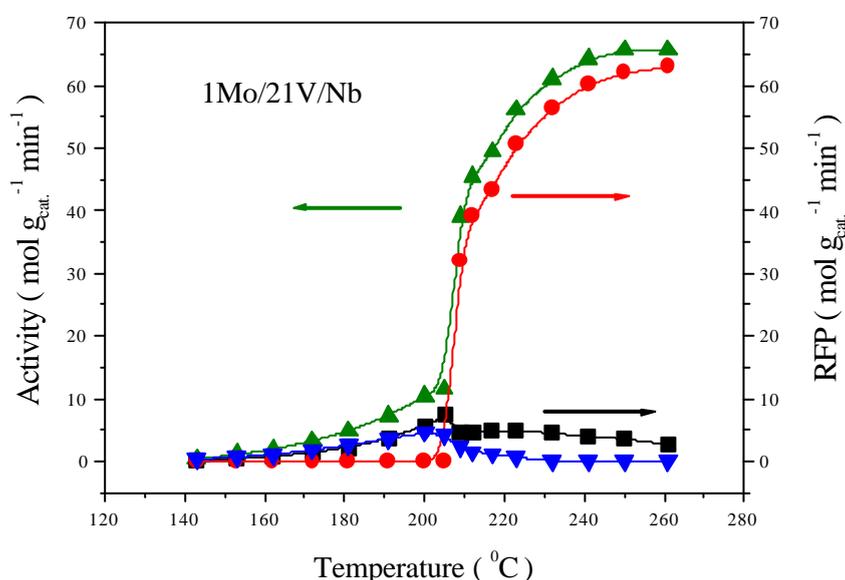
Fig. 3. Catalytic results for the isopropanol oxidation of 1Mo/21V/Nb catalyst versus reaction temperature. ( ) Isopropanol; (●) propylene; (■) acetone and ( ) di-isopropylether.

It is known that the decomposition of isopropanol can happen through different mechanisms, which depend of the acid and basic properties of the catalyst (Gervasini et al., 1997). The identification of the acid and basic properties of the catalyst can determine the mechanism more probable in this reaction (Diez et al. 2003). On the

other hand, the reaction of decomposition of isopropanol doesn't supply information to distinguish among of Lewis and of Brönsted acids sites. The presence of redox species in the catalysts can contribute in the dehydration activity and dehydrogenation in the decomposition of isopropanol. Deo et al. (1994) identified the superficial species of vanadium oxide on different metallic oxides. The VO_4 species on γ-Al_2O_3 are detected to low concentrations of vanadium oxide, and still species poliméricas of the type V-O-V happen with the increase of the concentration of vanadium oxide (Cortez et al. 2002). In higher concentrations, the formation of three-dimensional crystals of V_2O_5 is observed in coordination octahedra (Arena et al. 1999). In this work high vanadium concentration was used on Nb_2O_5, and for DRX was possible to identify only the crystalline phase V_2O_5.

The properties acids of Nb_2O_5, V_2O_5 and MoO_3 have been reported in the literature. Jehng et al. (1990) studied the molecular structure-reactivity relationships for supported niobium oxide catalysts by combining Raman spectroscopy structural studies with chemical probes (pyridine) that measured the acidity and reactivity of the surface niobium oxide sites. The results of Raman spectra showed that the highly distorted NbO_6 octahedral possess Nb-O bonds and are associated with Lewis acid sites, presenting located bands between 850cm^{-1} and 1000cm^{-1}. The slightly distorted NbO_6 octahedral as well as NbO_7 and NbO_8 groups only possess Nb-O bonds and are associated with Brönsted acid sites. Busca et al. (1989) found acidity of Lewis and Brönsted on V_2O_5. The formation of the surface vanadia species on the oxide supports is accompanied by a decrease in the number of surface Lewis acid sites and increase in the number of surface Brönsted acid sites (Blasco, et al. 1997). The decrease of Lewis acidity can be associated with the coordination of VO_X species on support, and the increase of Brönsted acidity to the groups V-OH of the species VOH_4^{-2} and $V_2O_7H_2^{-2}$ on support (Ferreira et al., 1999). Some authors (Abello et al., 2001), in studies with TPD of NH_3 adsorption on Mo/γ-Al_2O_3, observed that the addition of Mo on γ-Al_2O_3 increases the number of acid sites that interact with NH_3. This way, the acid force presents an important decrease with the increase of the molybdenum oxide loading, and new acid sites with weak and moderate forces are formation. In previous works, Aramendia et al. (1996) concluded that the activity of dehydration in the reaction of decomposition of isopropanol on MgO is related with the acidity of Brönsted. Similar results were found by Martin et al. (1996) in the catalysts MoO_3/TiO_2.

The results of the present paper confirm that the propeno formation on xMo/21V/Nb catalysts was due the presence of acid sites with weak and moderate forces (Brönsted acid sites), generated in the surface of the catalyst by the presence of V_2O_5 and MoO_3. The formation of acetone was due the presence of basic sites related to the superficial oxygen of VO_X and MO_X species on niobium oxide.

4. Conclusion

The vanadium addition to the Nb_2O_5 support and of molybdenum on the V/Nb system decreases, significantly, the specific area and the volume of pores of niobium oxide, being this more pronounced effect when the content of MoO_3 assumes values of the order of 3 wt.%. In the results of diffraction of ray-X, was verified that the addition of the vanadium on Nb_2O_5 promotes the formation of β-$(Nb,V)_2O_5$ phase, and the addition of molybdenum on the V/Nb system, alters the intensities of the peaks of this crystalline phase. The addition of

molybdenum, to low concentrations, modifies the reducibility of the vanadium on Nb_2O_5, increasing the maximum temperature of reduction. The presence of 3 wt.% of MoO_3 on the V/Nb system affected the reducibility of VO_X species in the catalyst.

The results of catalytic activity showed, in the catalyst with low MoO_3 content, a larger selectivity to propylene, fact this related to the presence of Brönsted acid sites in the catalyst with low concentration of MoO_3. This effect is due to the decrease of strong acid sites (Lewis) and the increase of weak and moderate acid sites (Brönsted) for the addition of MoO_3.

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