Answer to the Letter by Bredikhin and Lokhov

Dear Sir,

Bredikhin and Lokhov present a couple of very high quality spectra and, by that, substantially broaden the existing literature. The authors think that their data are at variance with the conclusions in our paper (Ref. 1) but actually the data confirm our results and conclusions.

Figure 1 in the paper by Bredikhin and Lokhov shows the following:

(i) According to the segment A, the highest frequency peak at 2097 cm⁻¹ shifts with decreasing θ by about 25 cm⁻¹ in good agreement with our data (see Ref. (*I*, Fig. 1)); we have found $\Delta \nu = 21-25$ cm⁻¹ for the peak of approx the same position. Thus, there is no problem with this peak.

(ii) The shape of the broadened peak between 2000 and 1800 cm⁻¹ as shown in sequent A indicates that there are at least two distinct states of adsorbed CO being monitored here. Actually, the segment B suggests that under better resolution (no island formation upon desorption) there are probably three states to be identified. Each of the peaks shifts by about 20 cm^{-1} by variations in $\theta(CO)$. This is again the same finding as made by us in Ref. (1). Our Figs. 1 and 2 show the presence of two states, each of them shifting with $\theta(CO)$ by 28 and 33 cm⁻¹, respectively. There is a small difference in the lowest value of $\nu(\theta \rightarrow 0)$: while our extrapolations (see Ref. (1, Fig. 1)) do not reach lower than $1910-1915 \text{ cm}^{-1}$, Bredikhin and Lokhov's lowest value is about 1895 cm⁻¹. However, the authors themselves say that they observed variations in the singletone value of 10-15 cm⁻¹

for different supports and Pd particle sizes (our experience is similar, see Ref. (1, Fig. 1)), so that the data can be considered as being in agreement, within the possible variations between the various sets of results.

(iii) We were unable to detect a separate peak at 1805 cm⁻¹ as the authors do in segment B of their Fig. 1. Our detection system was probably less sensitive. Comparison of the segments A and B of the authors Fig. 1 reveals that the identification of the absorption at 1805 cm^{-1} is not easy. Either it was absent with our catalysts or we have missed it. However, it is incorrect (in our opinion) to ascribe the whole $\Delta \nu$ value 1805–1965 (or even 1805–1910) cm^{-1} to a shift of one single state and then to say that $\Delta \nu$ is the same on powders and single crystal planes. "Singletone value" does not mean "the lowest possible value," as Bredikhin and Lokhov understand it, but it's the lowest possible value of ν for a given state, and there are clearly two or three states discernible in the spectra by Bredikhin and Lokhov in the region 1800- 2000 cm^{-1} .

REFERENCE

1. Hendrickx, H. A. C. M., Bouvrie, C. des, and Ponec, V., J. Catal. 109, 120 (1988).

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