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Methanol Formation from Carbon Monoxide and Hydrogen on Neutral Nb_8 Clusters in the Gas Phase YAN XIE, SHENG-GUI HE, ELLIOT BERNSTEIN, Department of Chemistry, Colorado State University, Fort Collins, CO, 80523-1872 — Reactions of neutral V_n, Nb_n, and Ta_n metal clusters ($n \leq 11$) with (CO + H_2)/He mixed gases and CH_3OH/He in a flow tube reactor (P $\sim$ 14 Torr) are studied by time of flight mass spectroscopy. Metal clusters are generated by 532 nm laser ablation and reactants and products are ionized by low fluence ($\sim$200 μJ/cm^2) 193 nm excimer laser light. Nb_n clusters exhibit strong size dependent reactivity in reactions both with CO + H_2 and CH_3OH compared with V_n and Ta_n clusters. A remarkably strong mass peak Nb_8COH_4 is observed in the reaction of Nb_n clusters with the mixed gases CO + H_2 at various concentration of H_2. This suggests a stable, low energy CH_3OH structure may form on an Nb_8 cluster. Methanol formation is not found on other Nb_n ($n \neq 8$), V_n, and Ta_n clusters. In reactions of CH_3OH with metal clusters M_n(M= V, Nb, Ta, n = 3-11), molecularly adsorbed products (M_nCH_3OH) are only observed on Nb_8 and Nb_{10}, whereas dehydrogenated products (M_nCO) are observed for all other clusters. This observation supports the suggestion that CH_3OH can be formed on Nb_8 in the reaction of Nb_n with CO + H_2. Reaction mechanisms are discussed based on the experimental results in this work and those in the literature. Theoretical calculations are carried out to confirm our experimental results and suggested reaction mechanisms.

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