Adsorption forms of NO on Rh_5Ir cationic clusters investigated by the infrared multiple photon dissociation spectroscopy

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Rhodium is known to be a commonly used element for three-way catalysts. Previous researches revealed that the adsorption form of NO on the rhodium cluster can be changed from the molecular attachment to the dissociative attachment after one Rh atom substituted by a Ta atom.[1] This result indicates that the substitution of Rh atom by other transition metal atom can alter the ability of NO dissociation. Rhodium's same group element, Iridium, was proved to have the ability of NO dissociation in the previous research. The combination of these two elements can change their catalytical ability.

In the present research, the Rh_5IrNO cationic clusters were prepared by laser ablation method with NO gas. Then those Rh_5IrNO cationic clusters were investigated by the infrared multiple photon dissociation (IRMPD) after tagged with argon. Figure 1 shows the infrared vibrational spectra of different isomers (b-e) obtained by DFT calculation and experimental IRMPD spectrum (a). Vibrational bands which exist at 1800 cm^{-1}, 900 cm^{-1} in Figure 1 (a) suggest that both molecular and dissociative NO attachments on Rh_5Ir^+ coexist. In addition, vibrational bands locating at 600 cm^{-1}, 550 cm^{-1} and 480 cm^{-1} suggest that Rh_5IrNO^+ should have several isomers after compared with calculated spectra of the most stable structures. The ratio between dissociative and molecular NO attachment on Rh_5IrNO^+ will be discussed. Therefore, the efficiency of NO dissociation on Rh_5Ir^+ cluster will be compared with Rh_6^+ and other clusters and the effect of Ir atom will be discussed.

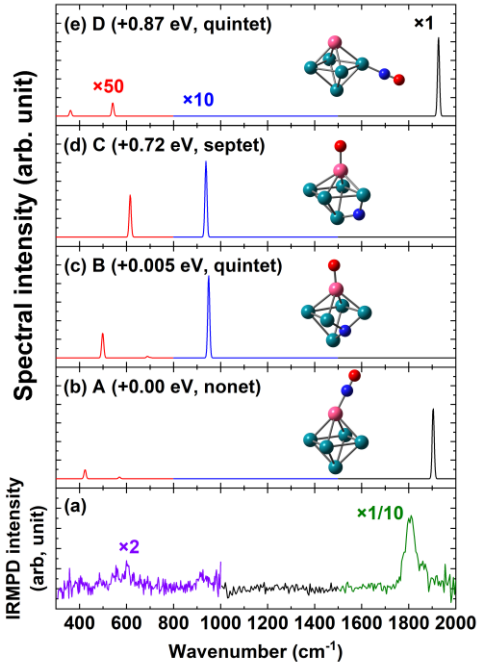

Figure 1 (a) Experimental IRMPD spectrum and (b, c, d, e) vibrational spectra of possible isomers of Rh_5IrNO^+ with molecular and dissociative NO adsorption.

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