

Fig. S1. R. Kumashiro et al.,

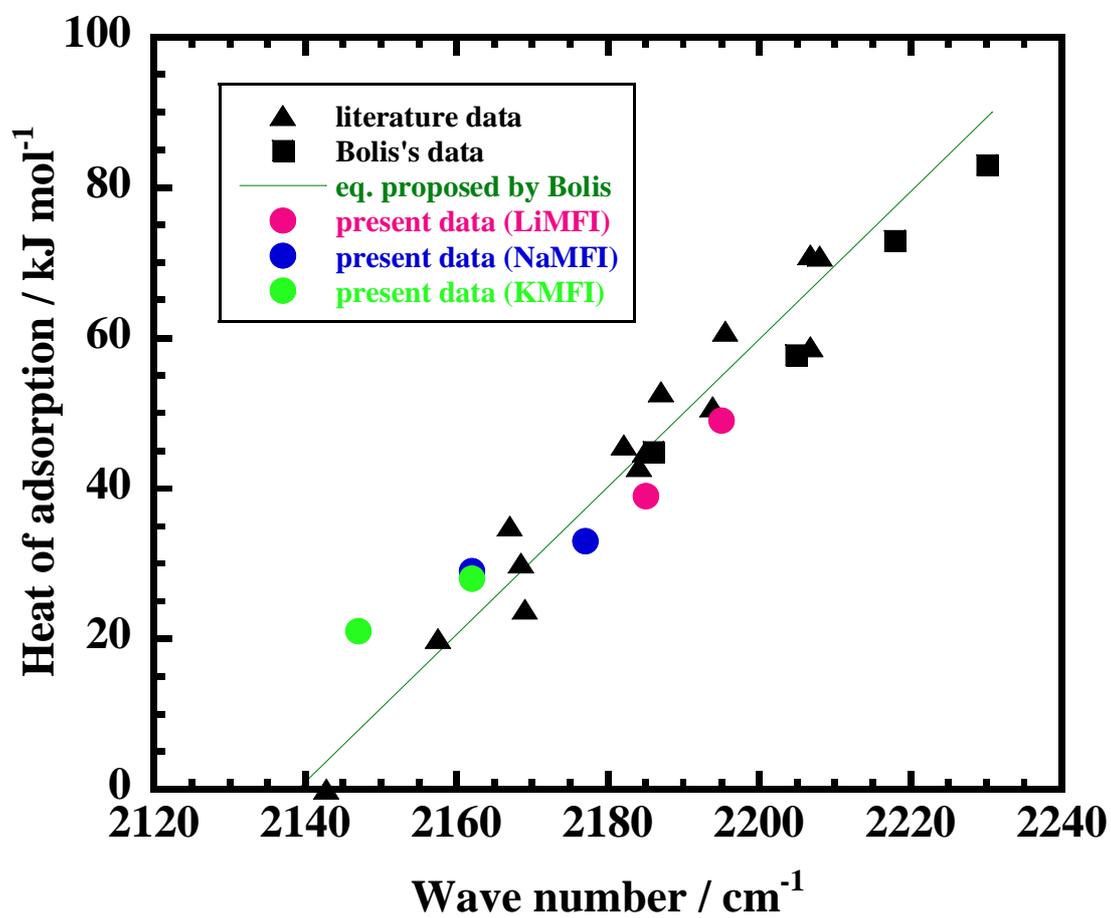


Fig. S2. R. Kumashiro et al.,

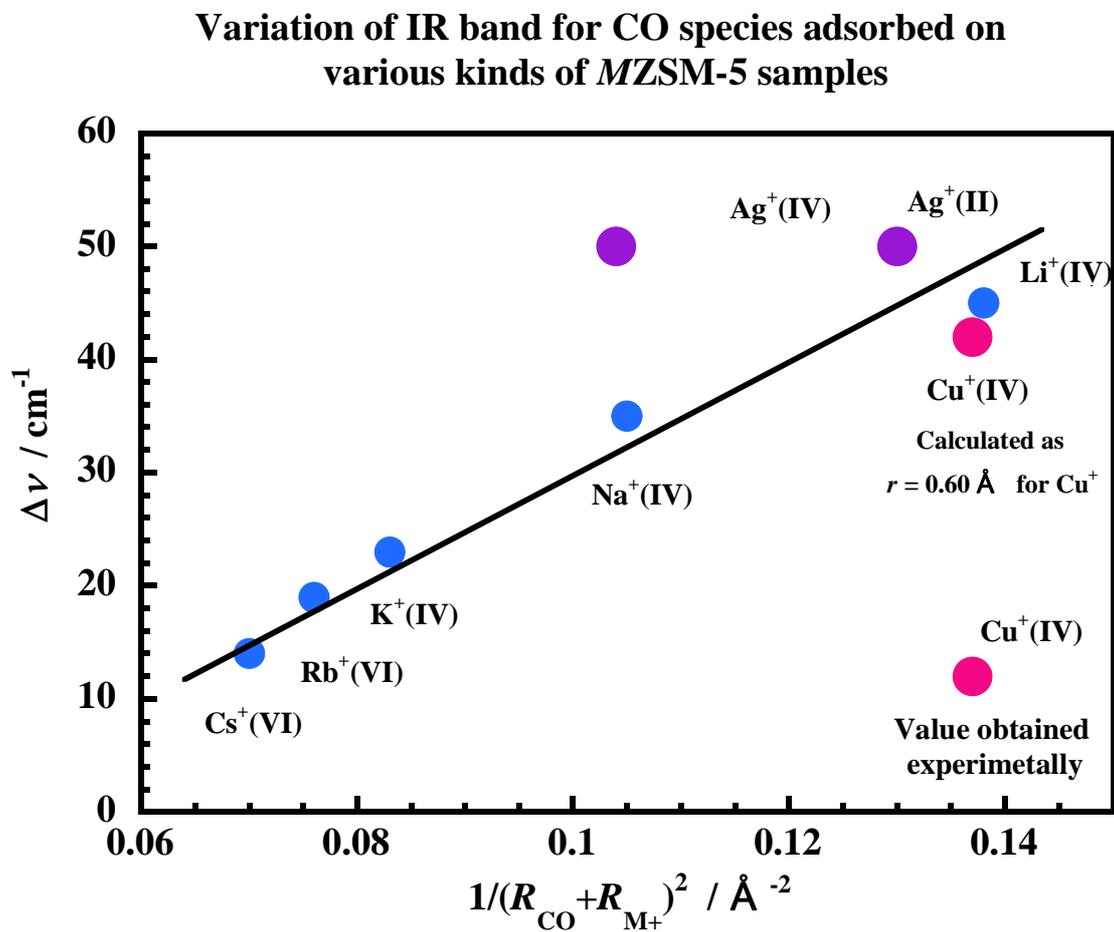


Figure S-3 (a). R. Kumashiro et al.,

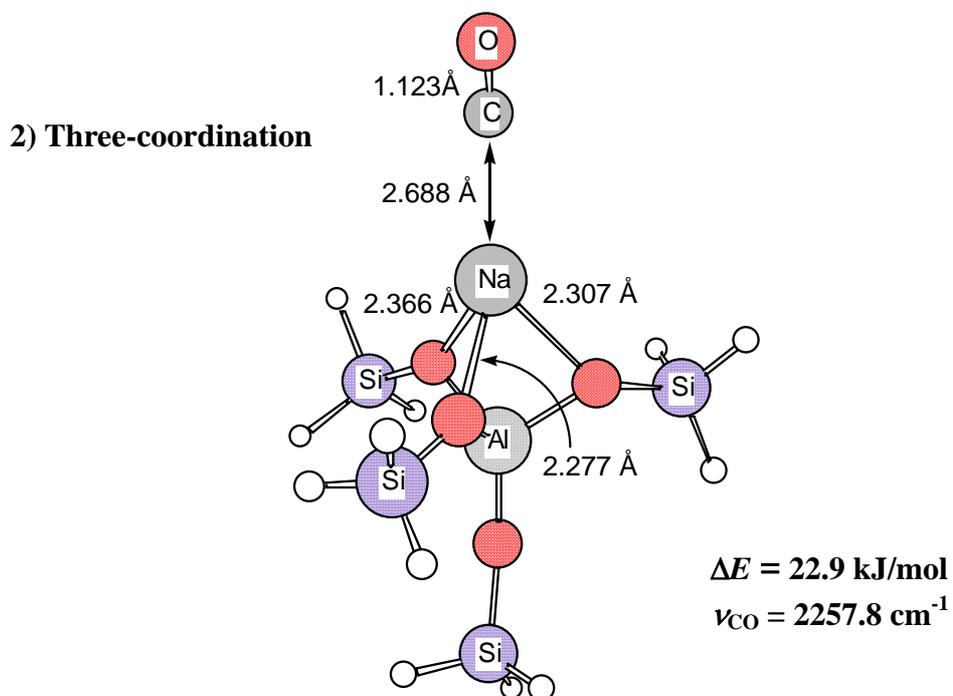
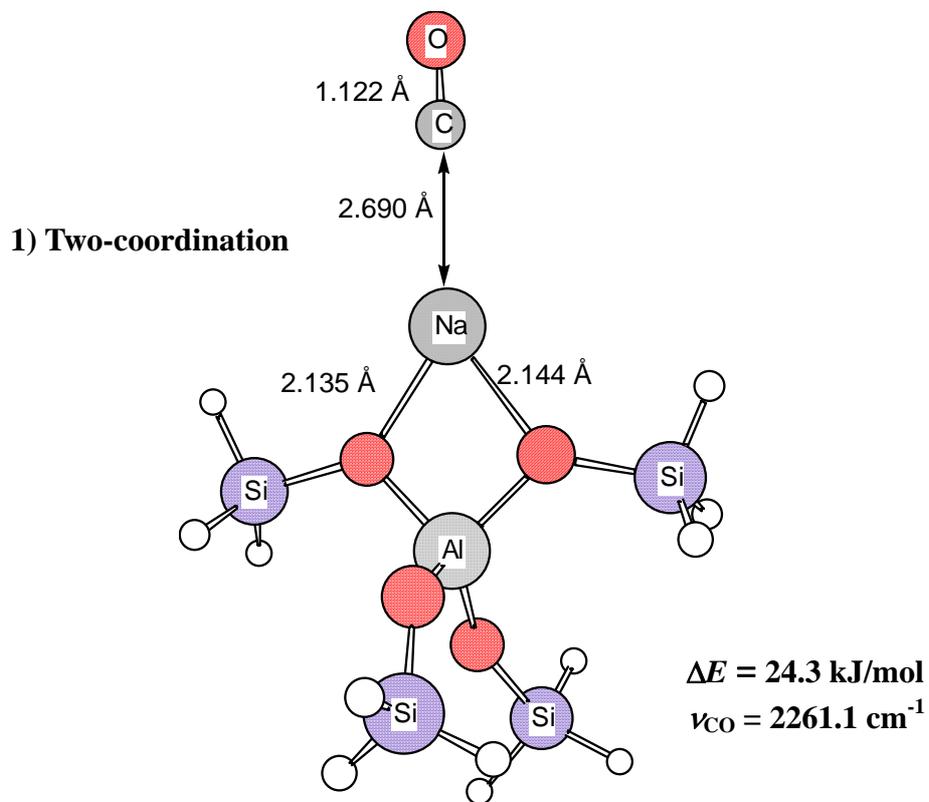
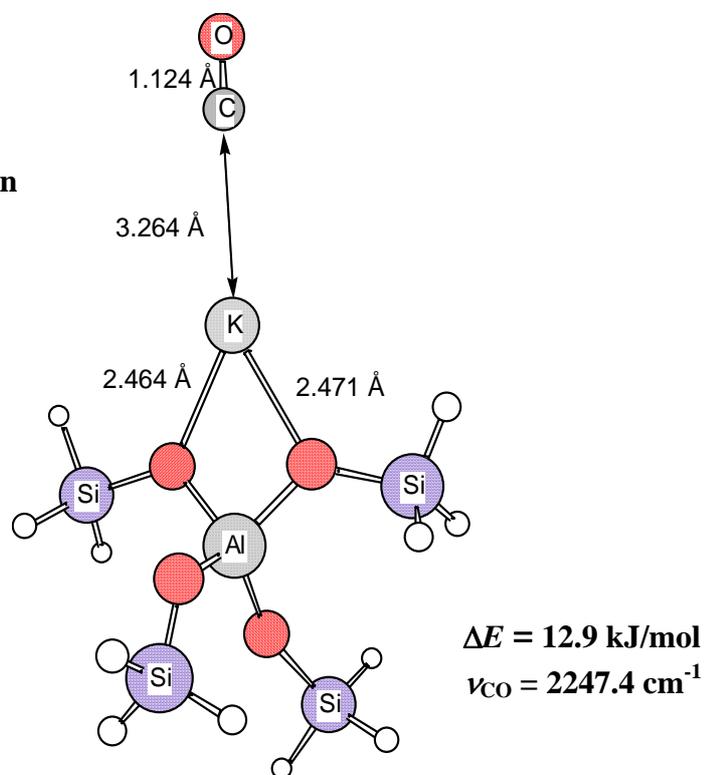
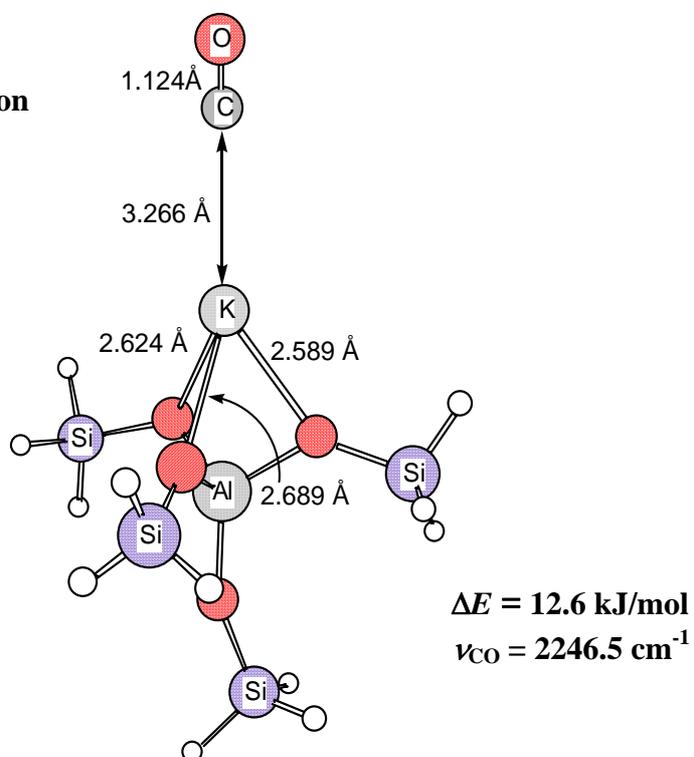


Figure S-3 (b). R. Kumashiro et al.,

1) Two-coordination



2) Three-coordination



### Supplemental information

Figure S-1. The plots for the present *MZSM-5*—CO systems were well expressed by the equation proposed by Bolis et al.<sup>55</sup> in which both our results and the data cited from Bolis's work were also plotted.

Figure S-2. The relation of CO frequency-shifts vs.  $1/(R_M + R_{CO})^2$  for the different alkali-metal-ion exchanged *ZSM-5* samples, as well as copper- and silver-ion-exchanged *ZSM-5* samples for the respective sites having different coordination environments.

Figure S-3. Results of DF calculation for the CO species adsorbed on two types of (a) sodium- and (b) potassium-ion-exchanged sites with the different coordination environments.