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Formation, stability, and reactivity studies of neutral iron sulfide clusters SHI YIN, ZHECHEN WANG, ELLIOT BERNSTEIN, Chemistry Department, Colorado State University — Different methods are used to generate neutral iron sulfide clusters to study their formation, stability, and reactivity, employing a time of flight mass spectrometer (TOFMS) with VUV (118 nm) radiation single photon ionization (SPI). Neutral Fe_mS_n (m = 1-4, n =1-6), and hydrogen containing $Fe_mS_nH_x$ (x >0,n >m) clusters are generated by the reaction of seeded H_2S in a helium carrier gas with laser ablated iron metal within a supersonic nozzle. The observed strong signal of association products $Fe_2S_2(SH)_{0,1}M$ (M = CO, C_2H_4, C_3H_6) suggest that the $Fe_2S_2(SH)_{0,1}$ clusters have the high activity for interactions with these small molecules. In order to avoid the effect for reactivity from hydrogen containing clusters, pure Fe_mS_nclusters are generated through laser ablation of a mixed iron/sulfur target in the presence of a pure helium carrier gas. $(FeS)_m$ (m = 1-4) is observed to be the most stable series. Reaction of CO and H_2 on neutral $(FeS)_{1,2}$clusters is farther investigated both experimentally and theoretically. A size dependent reactivity of iron sulfide clusters toward CO is characterized. The reaction FeS + CO → Fe + OCS is found for the FeS cluster. Products $Fe_2S_2^{13}COH_2$ and $Fe_2S_2^{13}COH_4$ are identified for reactions of ^{13}CO and H_2 on Fe_2S_2 clusters: this suggests that the Fe_2S_2 cluster has a high catalytic activity for hydrogenation reactions of CO to form formaldehyde and methanol. DFT calculations are performed to explore the potential energy surfaces for the two reactions: Fe_2S_2 + CO + $2H_2$ → Fe_2S_2 + CH_3OH; and Fe_2S_2 + CO + H_2 → Fe_2S_2 + CH_2O.

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