

Iron Assisted Formation of CO₂ over Condensed CO and Its Relevance to Interstellar Chemistry

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Supporting Information

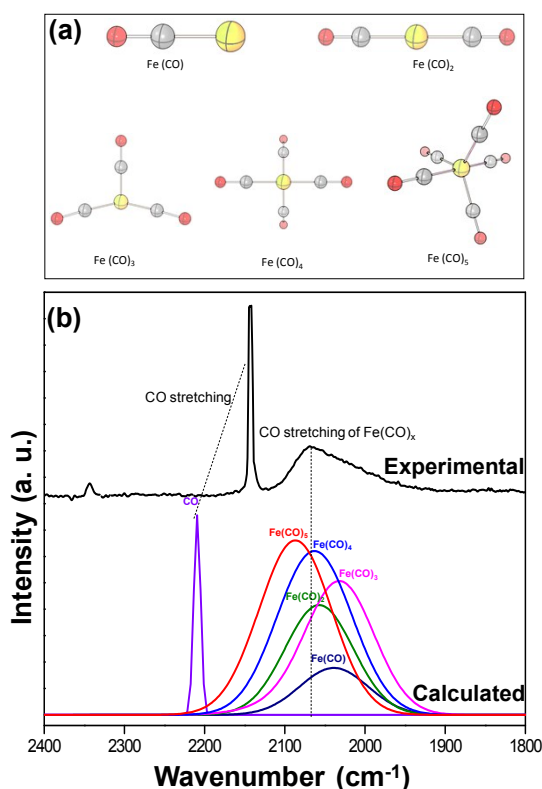


Fig S1. (a) Optimized geometry of Fe(CO)_x (x=1-5) at the B3LYP/LANL2DZ: (Fe)/6-31G* (C and O) level. Colour code: C: grey; O: red; Fe: yellow (b) Calculated vibration frequencies for CO and Fe(CO)_x (x=1-5) complexes compared with the experimental spectrum.

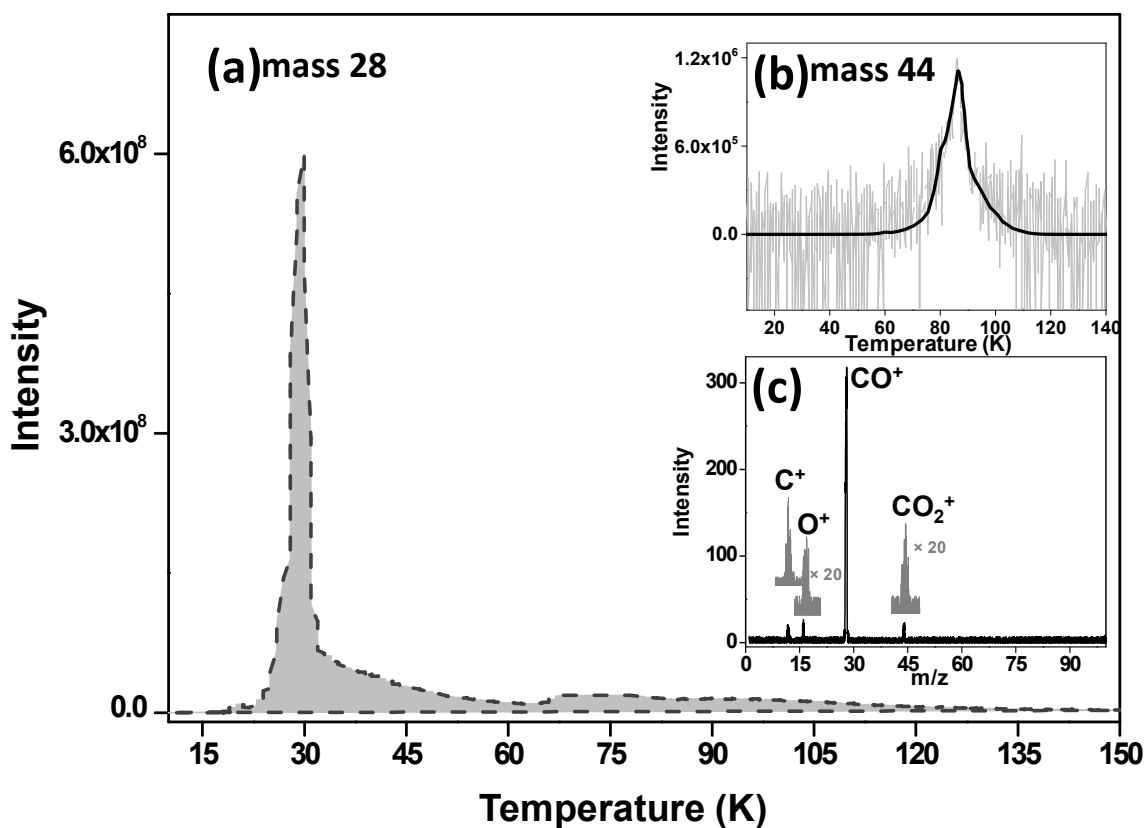


Fig S2. (a) Temperature programmed desorption profile of Fe + CO deposited at 10 K at a heating rate of 30 K/min for mass 28 (for CO). (b) The TPD of mass 44 (for CO₂) and (c) the mass spectrum obtained at 85 K from the TPD profile showing the CO and CO₂ concentration ratio (inset, the peaks are enlarged by multiplying by a factor of 20). CO in spectrum (c) is due to the dissociation of Fe(CO)_x.