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Supporting Information

Covalent Triazine Framework C_6N_6 as an Electrochemical Sensor for Hydrogen-Containing Industrial Pollutants. A DFT Study

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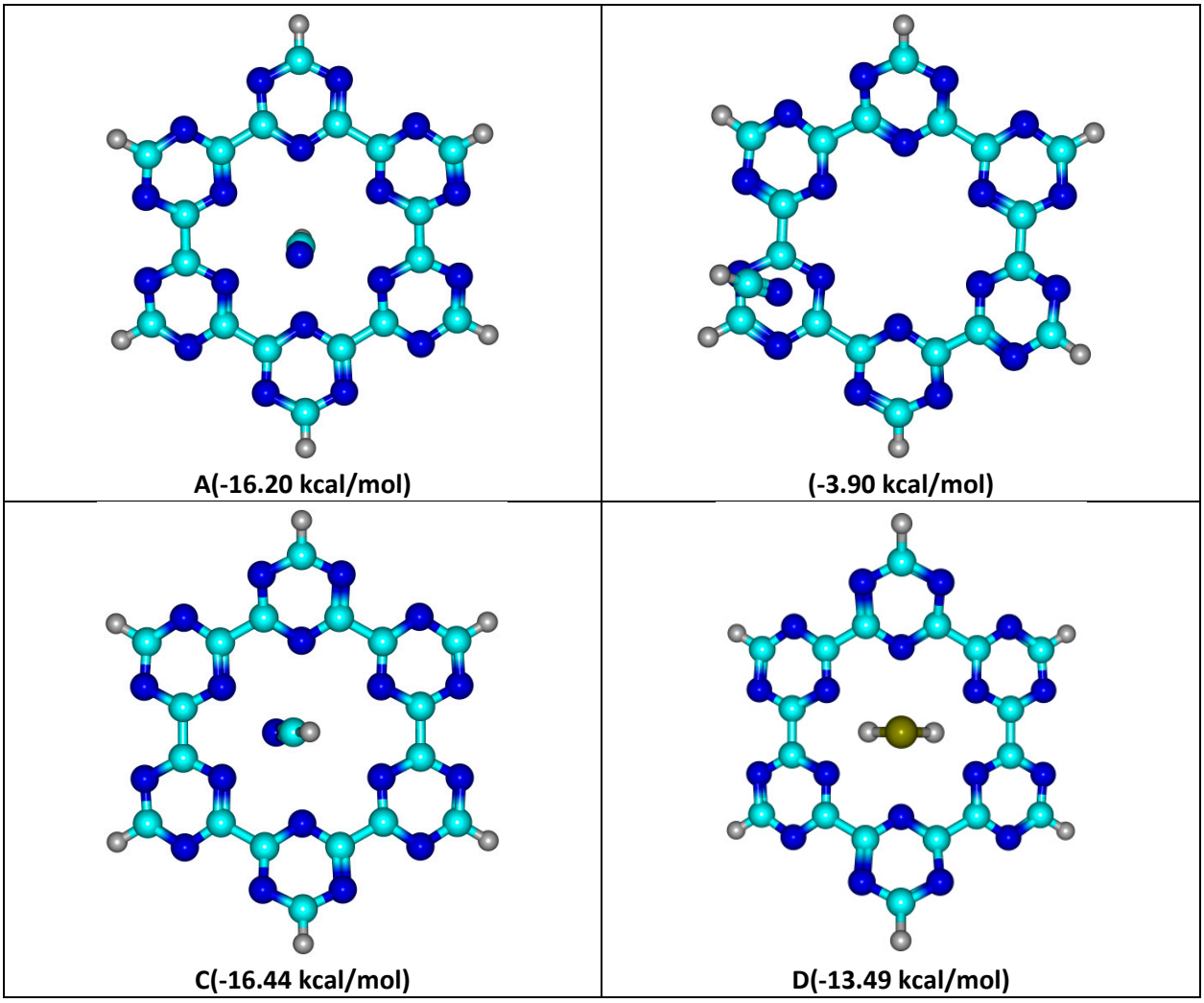

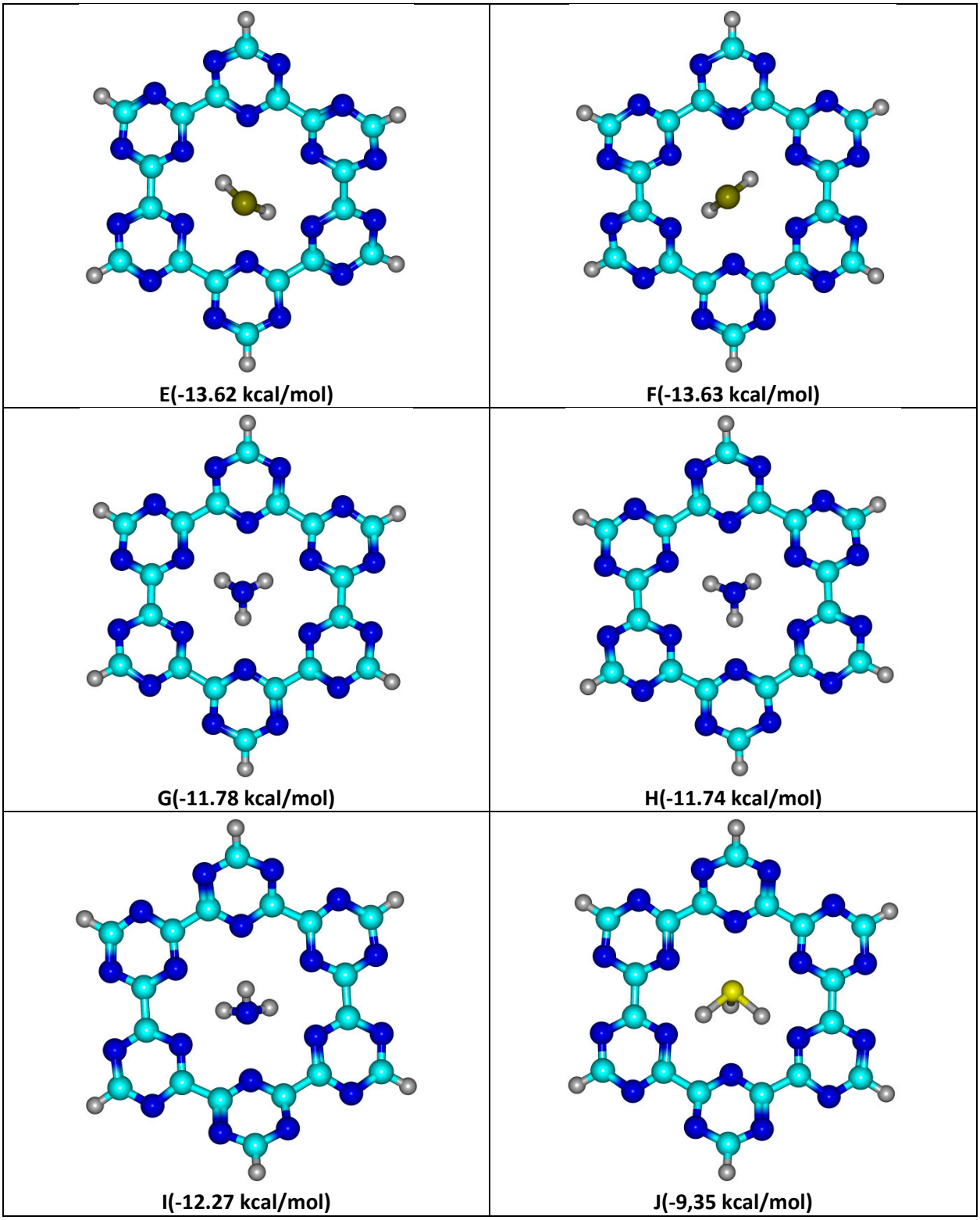

Figure S1. Optimized geometries of least stable complexes of each analyte over C_6N_6 at ωb97XD/6-31G (d,p) level of theory.(HCN/C_6N_6 complexes (A-C), H_2S/C_6N_6 complexes (D-F), NH_3/C_6N_6 complexes (G-I), PH_3/C_6N_6 complexes (J),.