

Table SI_XYZ. Total B3LYP/6-311G* energies/enthalpies of different species studied including the xyz file names contained in this SI_XYZ.zip.

	E	H	NAME.xyz
³ [NiL] ²⁻	-3250.503603	-3250.142369	3NiL2_Red.xyz
¹ [NiL] ²⁻	-3250.510626	-3250.118574	1NiL2_Red.xyz
² [NiL] ⁻	-3250.466015	-3250.101912	2NiL1_Red.xyz
¹ [NiL] ⁰	-3250.378540	-3250.011645	1NiL0.xyz
² [NiL] ⁺	-3250.186230	-3249.819337	2NiL1_Ox.xyz
¹ [NiL] ²⁺	-3249.948182	-3249.580637	1NiL2_Ox.xyz
¹ [NiLH] ⁰	-3258.616497	-3258.079627	1NiLH0.xyz
² [NiLH] ⁺	-3258.578456	-3258.036079	2NiLH1.xyz
² [NiLH _{C1}] ⁺	-3258.574194	-3258.031725	2NiLH1_C1.xyz
² [NiLH _{C5}] ⁺	-3258.577090	-3258.034923	2NiLH1_C5.xyz
¹ [NiLH] ²⁺	-3258.432714	-3257.886345	1NiLH2.xyz
¹ [NiLH _{C1}] ²⁺	-3258.428449	-3257.881841	1NiLH2_C1.xyz
¹ [NiLH _{C3}] ²⁺	-3258.430081	-3257.883263	1NiLH2_C3.xyz
¹ [NiLH _{C5}] ²⁺	-3258.430207	-3257.882894	1NiLH2_C5.xyz
¹ [NiLH _{C1C3}] ²⁺	-3258.422065	-3257.875684	1NiLH2_C1_C3.xyz
³ [NiL-CO ₂] ²⁻	-3439.157621	-3438.780621	3NiLCO22_Red.xyz
¹ [NiL-CO ₂] ²⁻	-3439.157234	-3438.778617	1NiLCO22_Red.xyz
² [NiL-CO ₂] ⁻	-3439.111696	-3438.730981	2NiLCO21_Red.xyz
¹ [NiL-CO ₂] ⁰	-3439.023880	-3438.640248	1NiLCO20.xyz
² [NiL-CO ₂] ⁺	-3438.830920	-3438.448238	2NiLCO21_Ox.xyz
¹ [NiL-CO ₂] ²⁺	-3438.592560	-3438.208037	1NiLCO22_Ox.xyz
¹ [NiLH-CO ₂] ⁰	-3447.321361	-3446.765337	1NiLHCO20.xyz
² [NiLH-CO ₂] ⁺	-3447.22514	-3446.665791	2NiLHCO21.xyz
² [NiLH _{C1} -CO ₂] ⁺	-3447.221017	-3446.661914	2NiLHCO21_C1.xyz
² [NiLH _{C5} -CO ₂] ⁺	-3447.224161	-3446.664701	2NiLHCO21_C5.xyz
¹ [NiL _{fr} -CO ₂] ⁰	-3438.976674	-3438.542170	1NiLfrCO20.xyz
CO₂	-188.643673	-188.628479	CO2.xyz