Comparing Data for InChI=1S/N2/c1-2 9 8 8 Entropy (kcal/mol.K) Enthalpy (kcal/mol) 3 3 · Mech 1 Mech 1 2 -2 · - Mech 2 Mech 2 800 1000 1200 800 1200 1400 1400 600 600 1000 0.058 0.058 Gibbs Free Energy (kcal/mol)
0.00
0.00
52
0.00
0.00 0.056 Heat Capacity (kcal/K) 0.054 0.052 Mech 1 Mech 1 0.050 0.050 Mech 2 Mech 2

600

800

1000

Temperature (K)

1200

1400

800

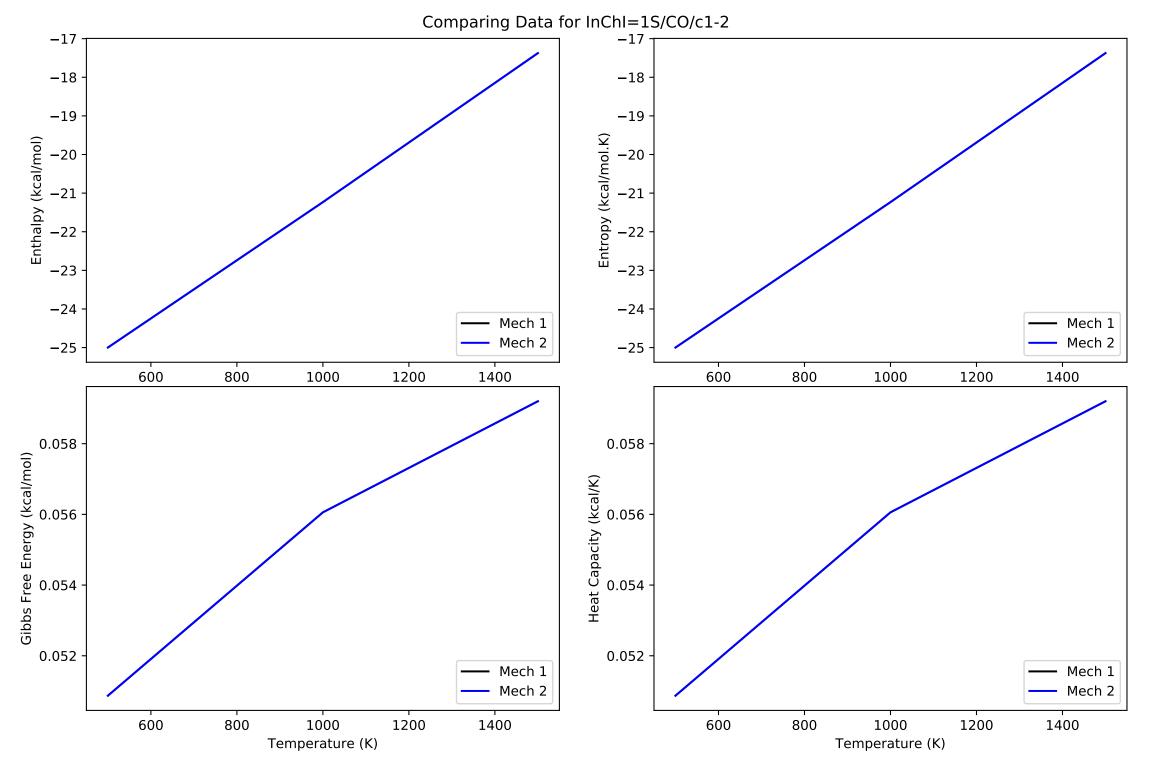
1000

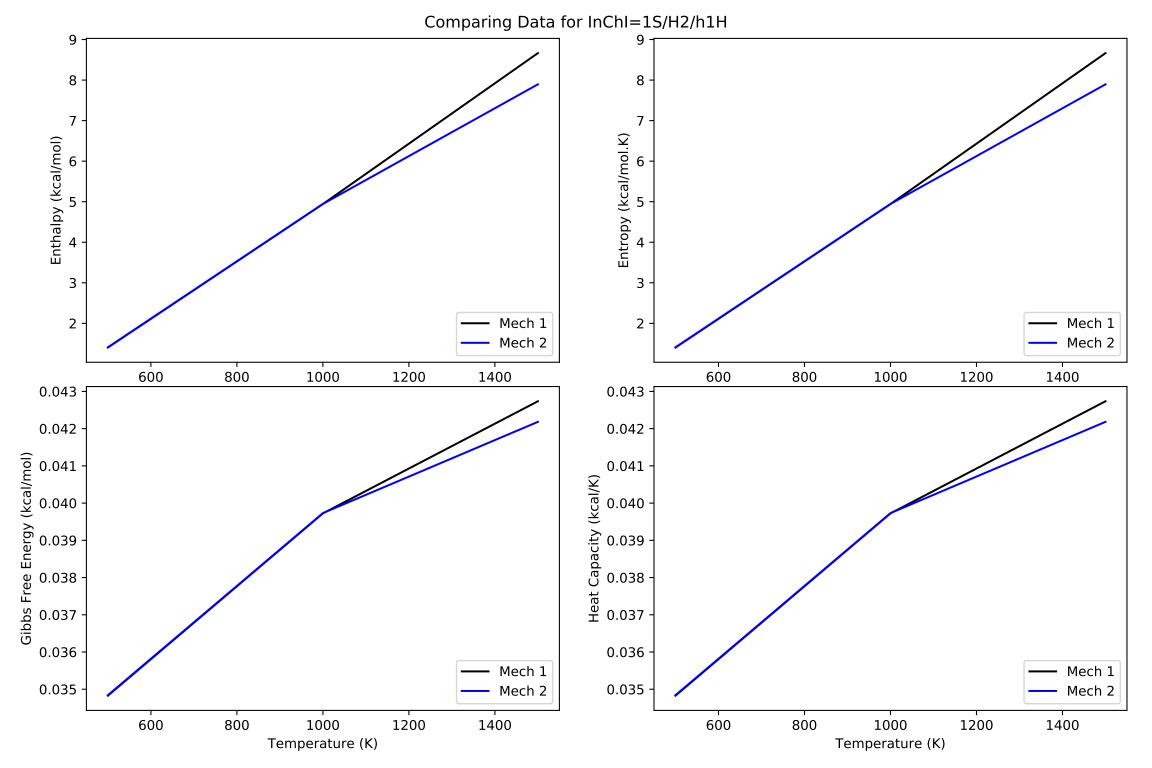
Temperature (K)

1200

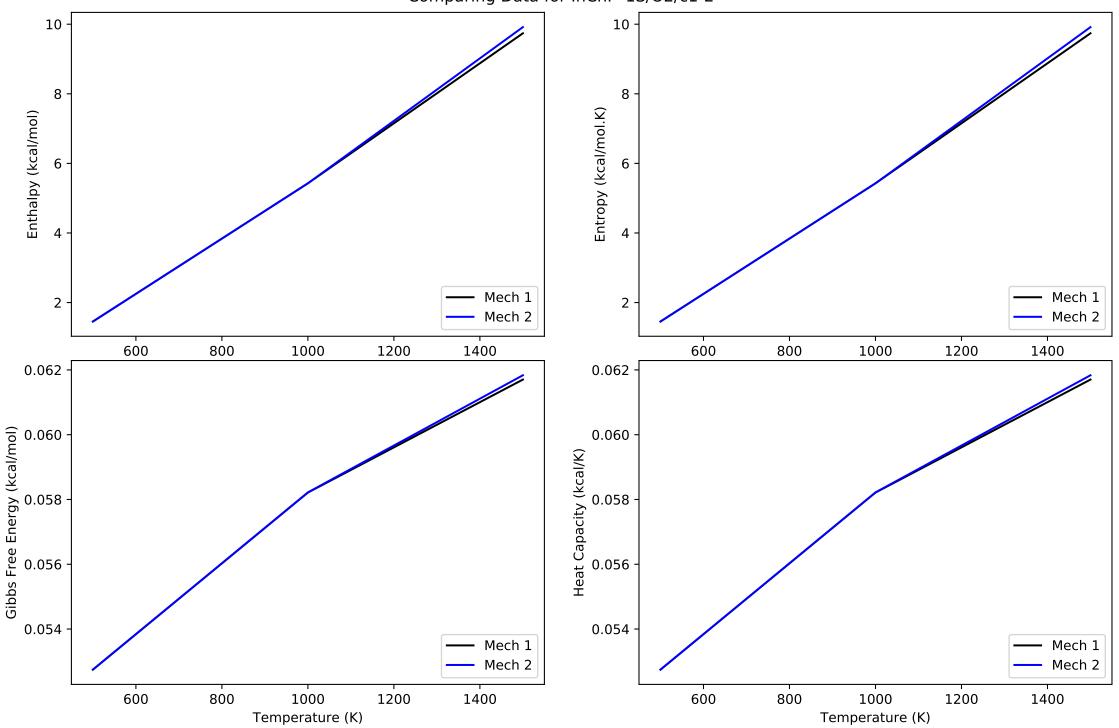
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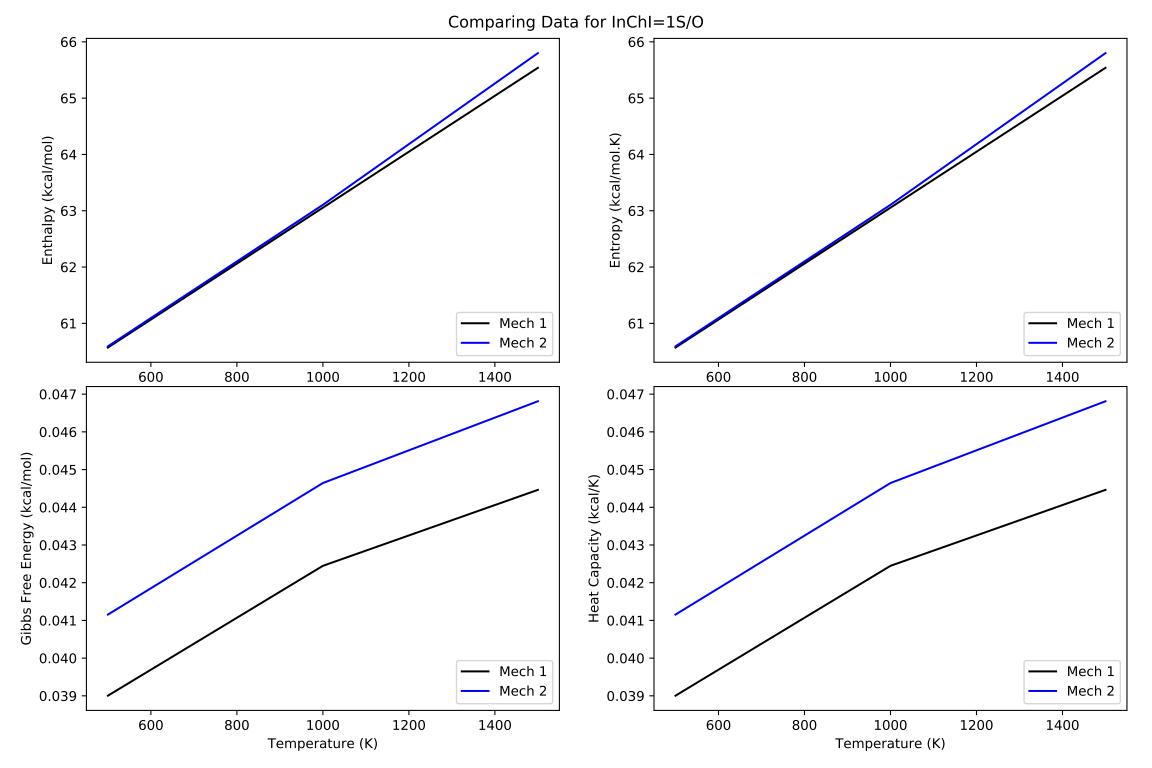




Comparing Data for InChI=1S/O2/c1-2



Comparing Data for InChI=1S/H 58 58 57 57 Enthalpy (kcal/mol) Entropy (kcal/mol.K) 56 55 54 54 Mech 1 Mech 1 Mech 2 Mech 2 53 -53 1200 800 1000 1200 1400 800 1400 600 600 1000 0.035 0.035 (kcal/mol) (kcal/mol) (cal/mol) (cal/mol) (cal/mol) (cal/mol) 0.034 Heat Capacity (kcal/K) 0.033 0.032 0.031 Mech 1 Mech 1 Mech 2 Mech 2 0.030 0.030 800 800 600 1000 1200 600 1000 1200 1400 1400 Temperature (K) Temperature (K)



Comparing Data for InChI=1S/HO/h1H 18 -18 17 17 16 16 Enthalpy (kcal/mol) 11 12 13 13 -12 · 12 11 11 -Mech 1 Mech 1 - Mech 2 Mech 2 10 -10 -800 1000 1200 1200 1400 1400 800 600 600 1000 0.056 -0.056 -0.055 0.055 Gipps Lee Energy (Kcal/mol)
0.053
0.052
0.051
0.050
0.049 0.054 Heat Capacity (Kcal/K) 0.053 0.051 0.055 0.050 0.049 0.049 Mech 1 Mech 1 0.048 0.048 Mech 2 Mech 2

600

800

1000

Temperature (K)

1200

1400

600

800

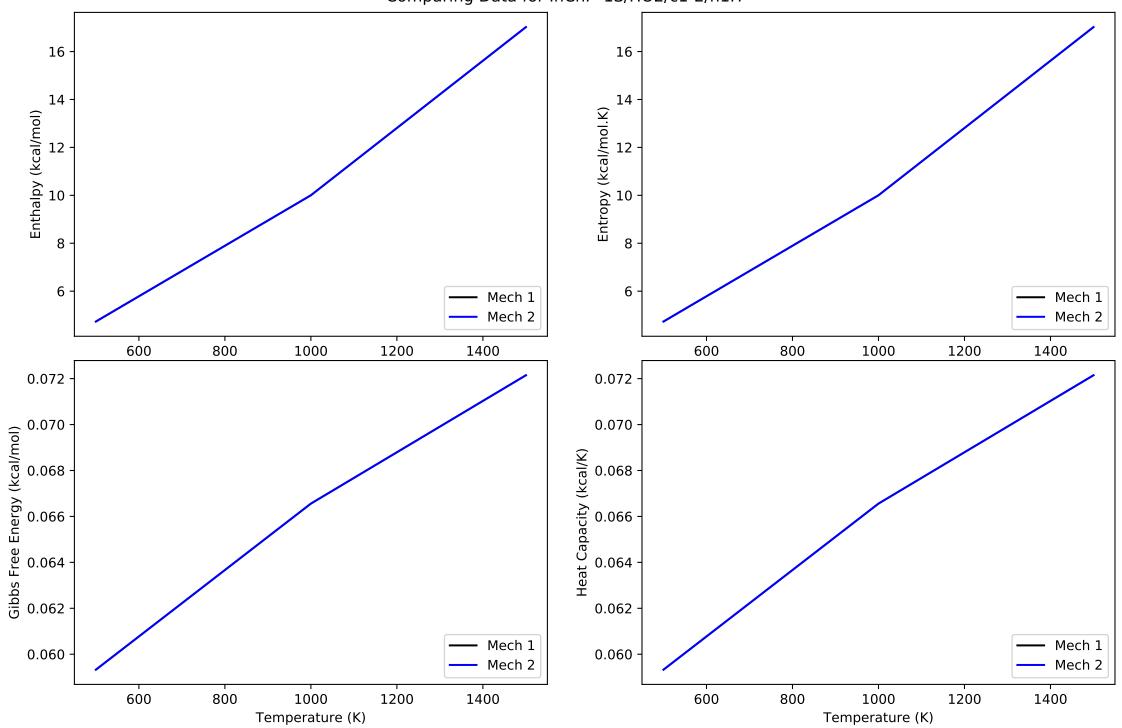
1000

Temperature (K)

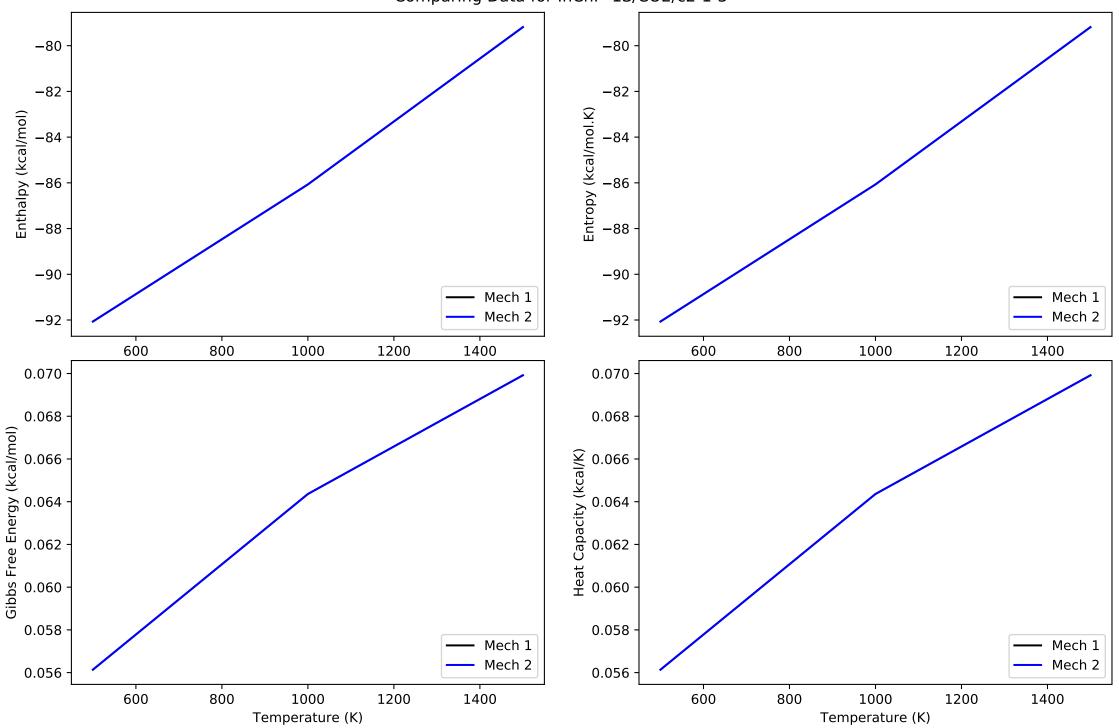
1200

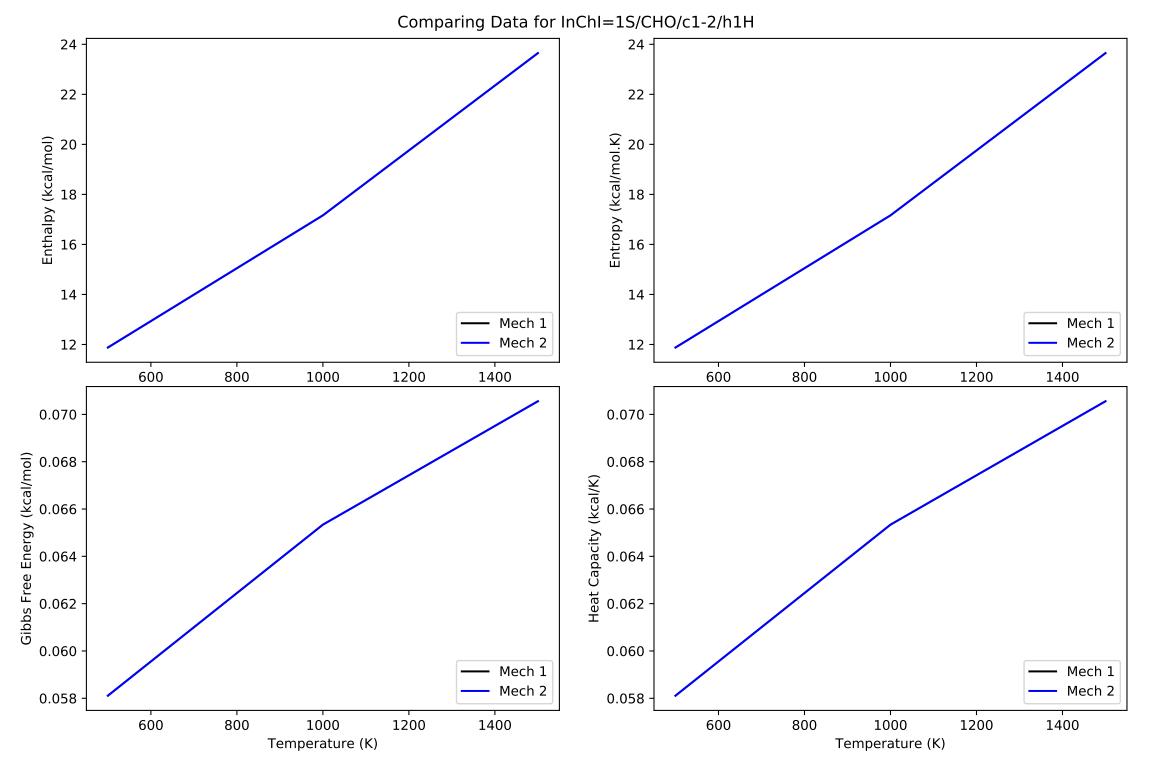
1400

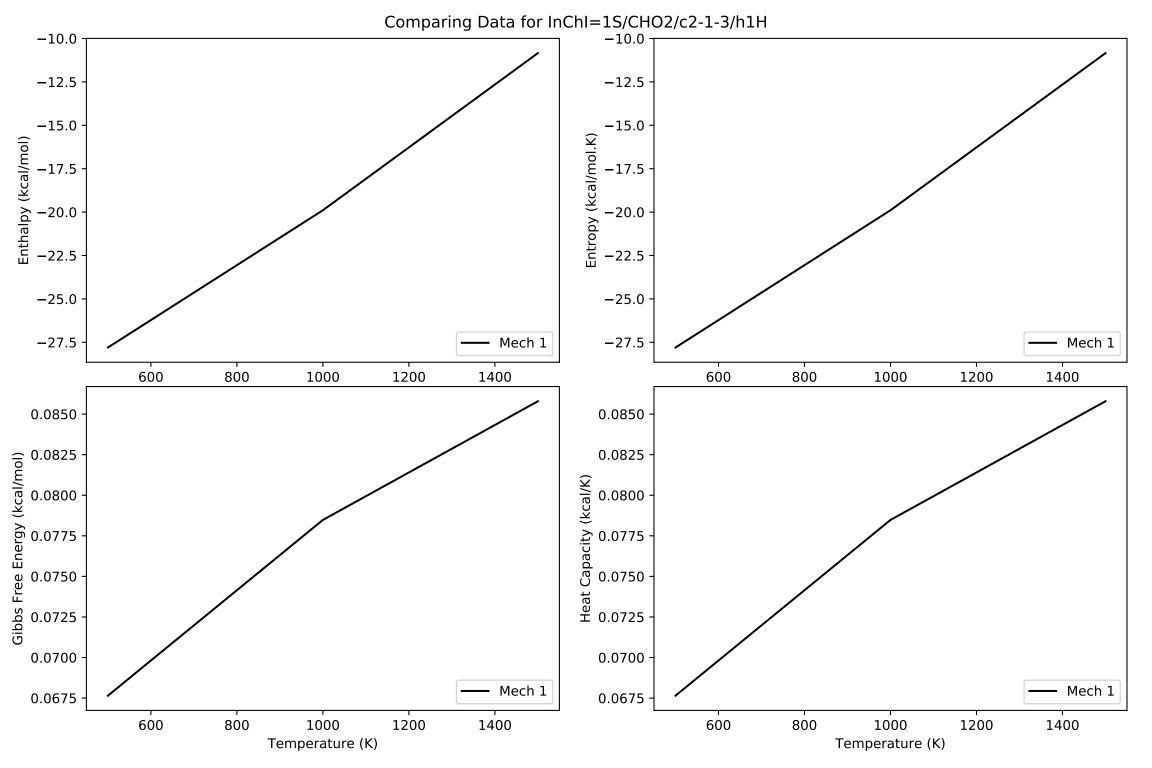
Comparing Data for InChI=1S/HO2/c1-2/h1H



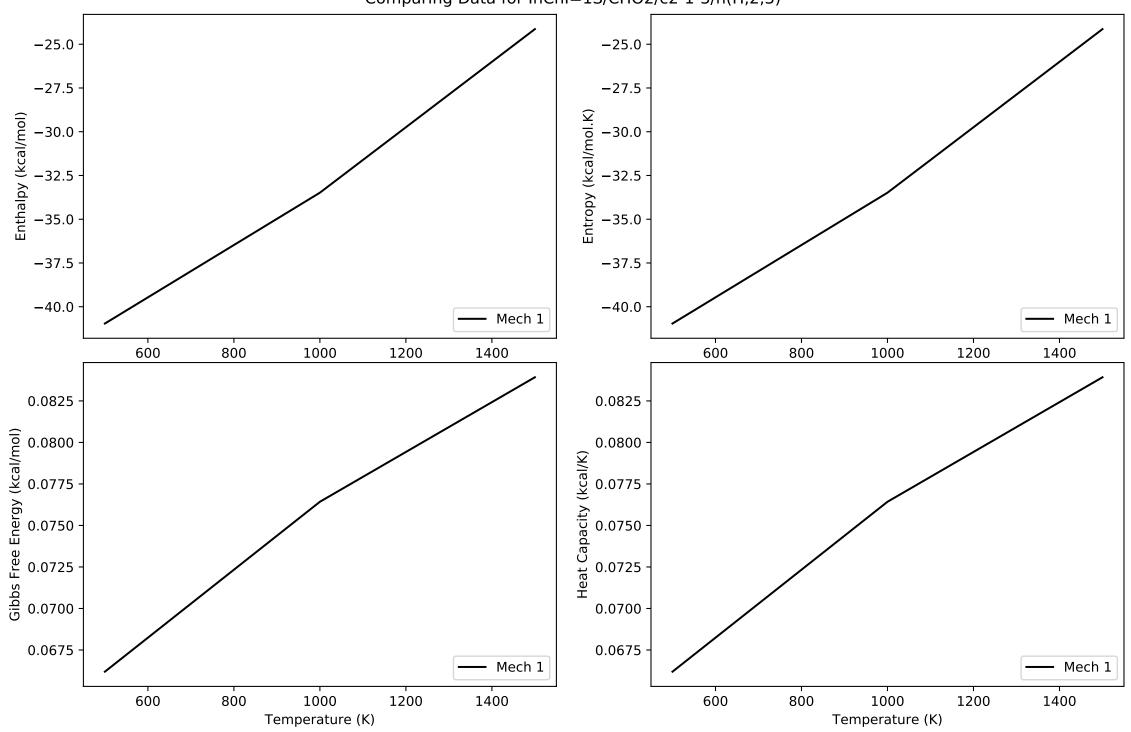
Comparing Data for InChI=1S/CO2/c2-1-3

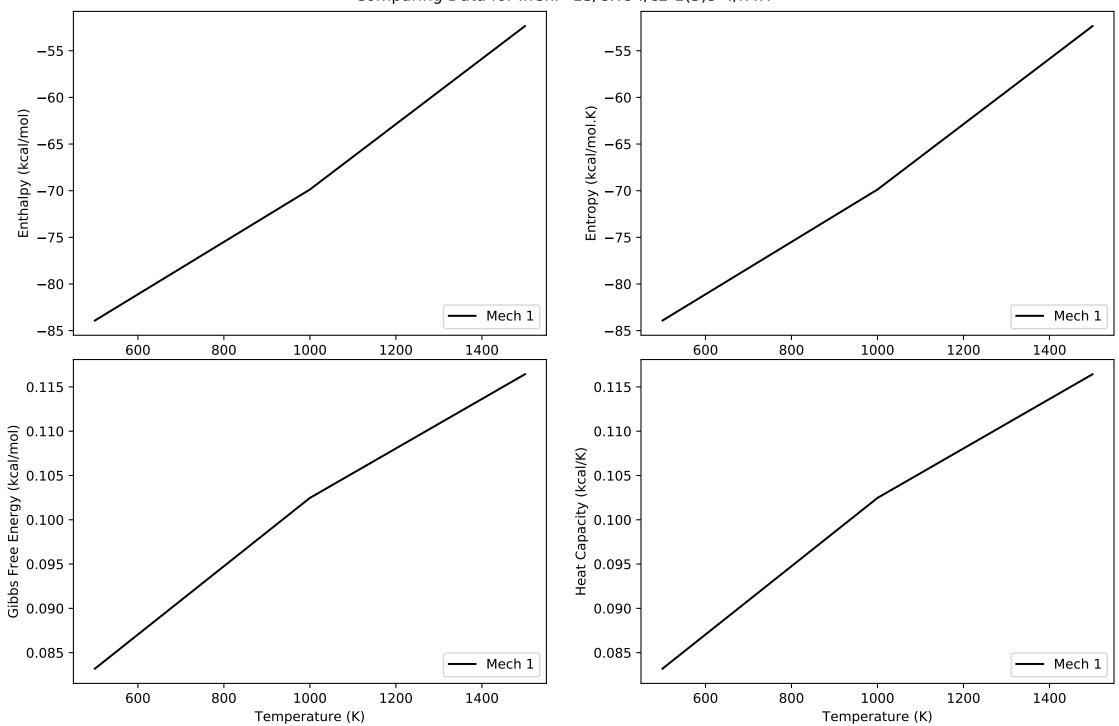


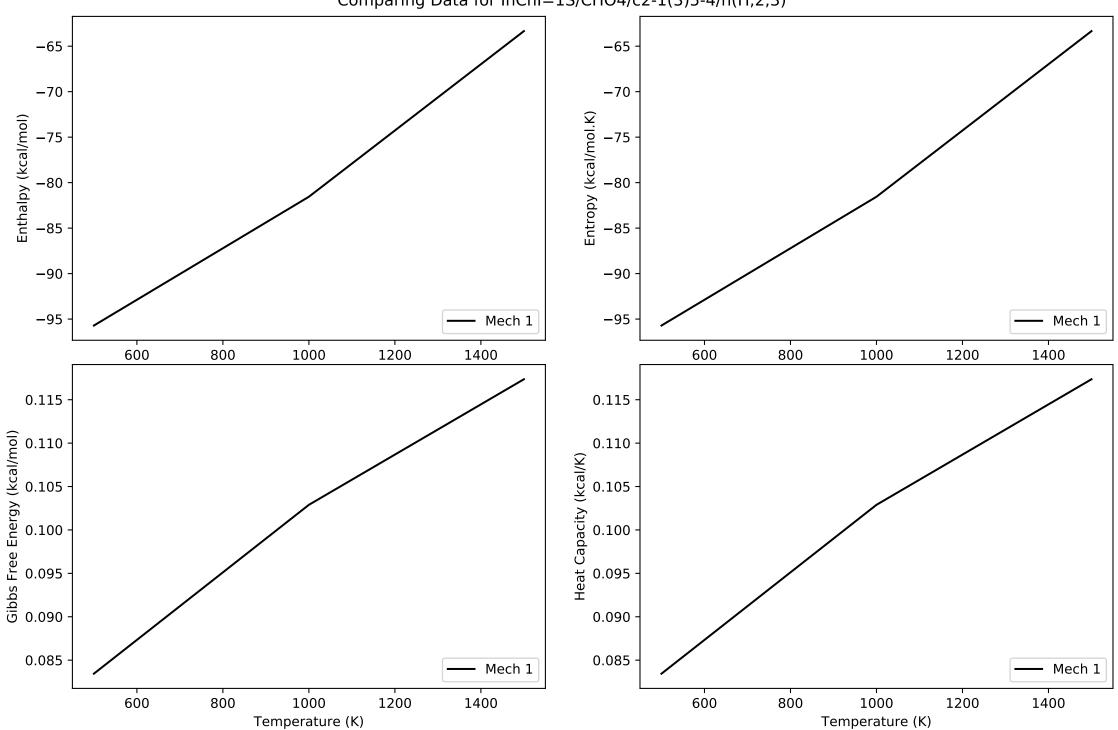




Comparing Data for InChI=1S/CHO2/c2-1-3/h(H,2,3)



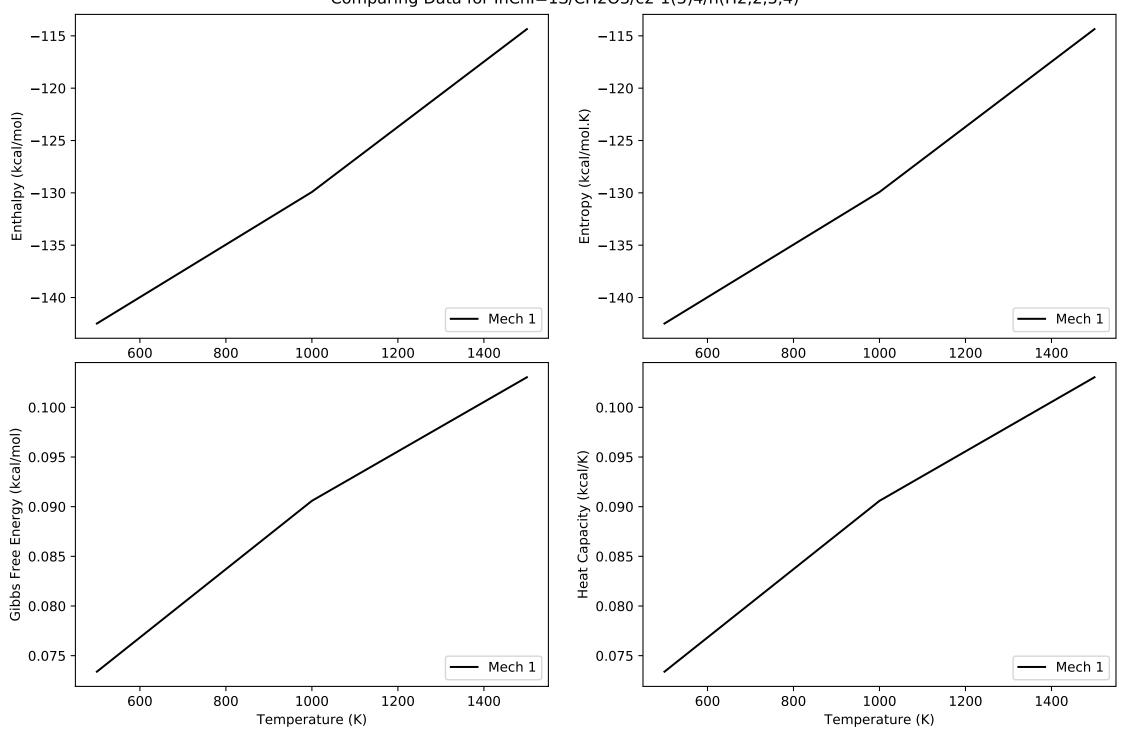


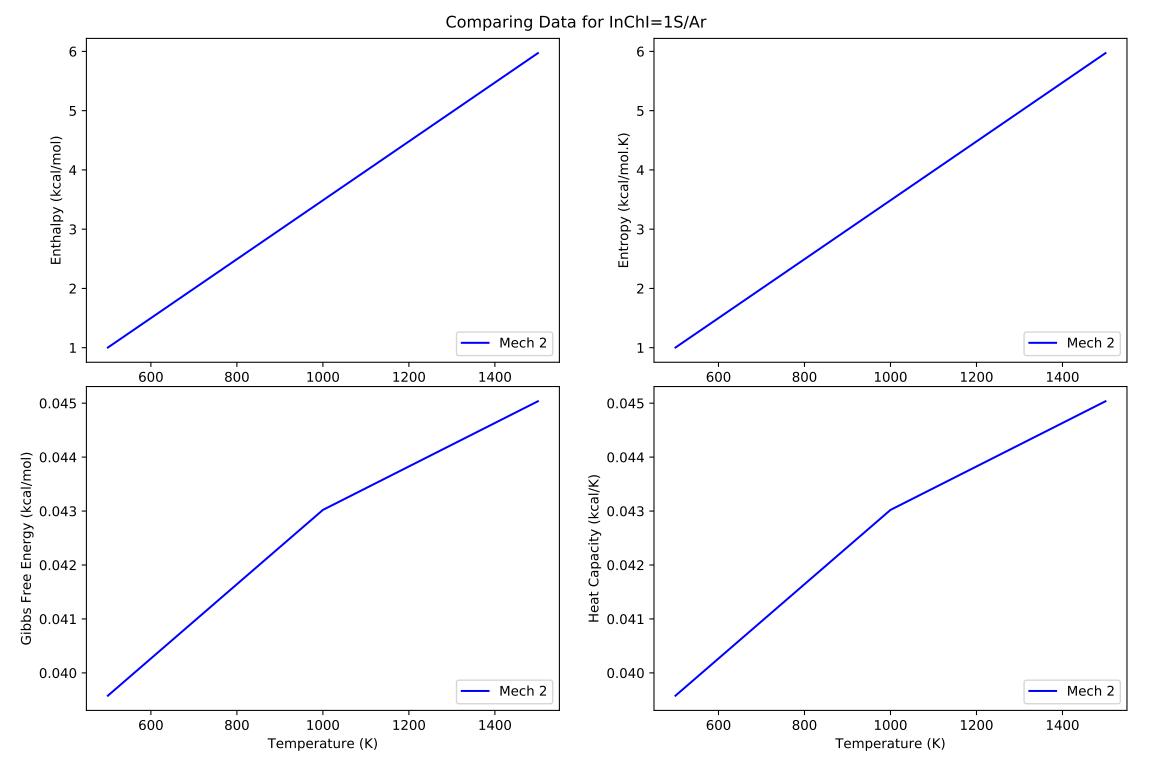


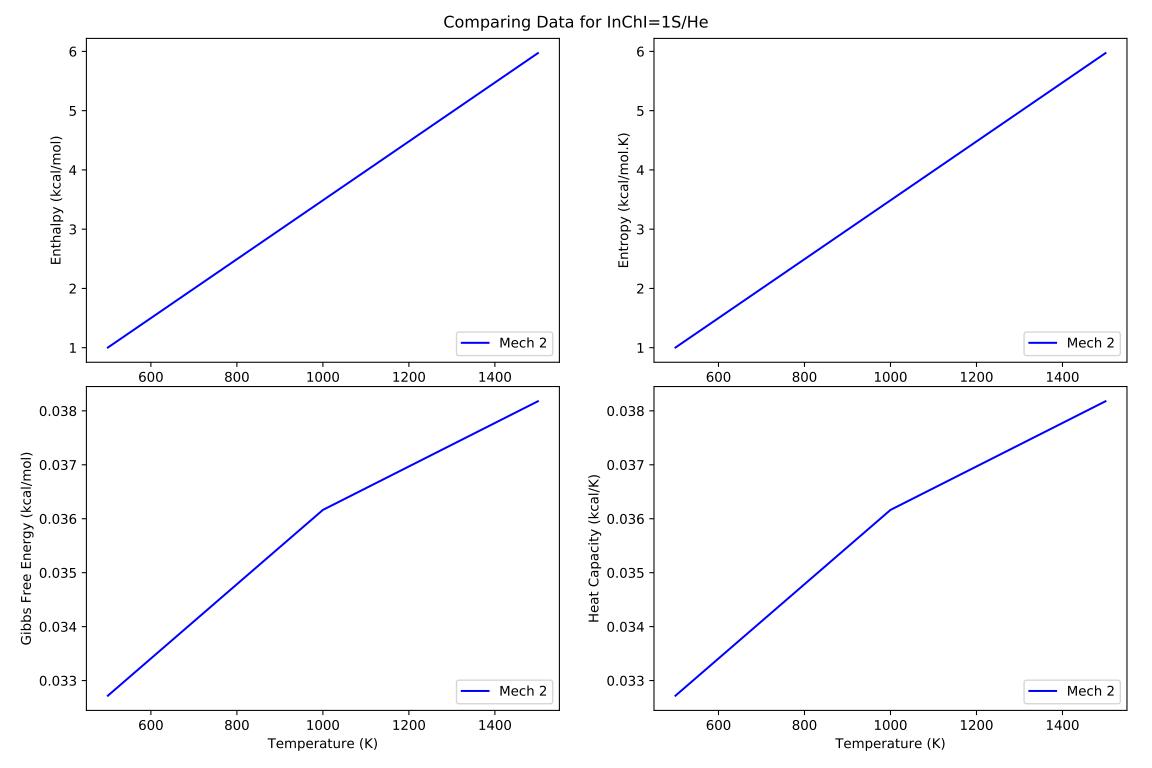
Temperature (K)

Temperature (K)

Comparing Data for InChI=1S/CH2O3/c2-1(3)4/h(H2,2,3,4)







Temperature (K)

Temperature (K)