

special topic

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As deuterium has a lower zero-point energy than hydrogen, it should be possible to calculate the chemical potential energy of reactions that use hydrogen and compare them to their deuterated counterparts to show that deuterium should be the favored species when forming new chemicals. As the paper by TJ Millar (2005) notes a significant enhancement (10^{11}) of deuterated ammonia, the reaction I'll do the calculation for is of the amino radical NH_2 with H to form ammonia, NH_3 .

So, we will be comparing the Gibbs free energies of:

Hydrogenated Reaction	Deuterated Analog
$NH_2 + H \rightarrow NH_3$	$ND_2 + D \rightarrow ND_3$

In order to complete this calculation, it will be necessary to gather the enthalpies of formation, H_f° , and the standard Entropies of each species to then use the formula for Gibbs free energy:

$$\Delta G = \Delta H - T\Delta S$$

This can be done using the NIST Chemistry WebBook, which provides the gas phase thermochemistry data for each of these species. The results are as follows:

			Deuterated			
Species	Quantity	Value	Units	Species	Quantity	Value Units
NH_2	$\Delta_f H_{gas}^\circ$	190.37	kJ/mol	ND_2	$\Delta_f H_{gas}^\circ$	185.35 kJ/mol
NH_2	$S_{gas,1bar}^\circ$	194.71	J/mol*K	ND_2	$S_{gas,1bar}^\circ$	204.30 J/mol*K
H	$\Delta_f H_{gas}^\circ$	218.00	kJ/mol	D	$\Delta_f H_{gas}^\circ$	221.72 kJ/mol
H	$S_{gas,1bar}^\circ$	114.72	J/mol*K	D	$S_{gas,1bar}^\circ$	123.35 J/mol*K
NH_3	$\Delta_f H_{gas}^\circ$	-	kJ/mol	ND_3	$\Delta_f H_{gas}^\circ$	- kJ/mol
		45.90				58.58
NH_3	$S_{gas,1bar}^\circ$	192.77	J/mol*K	ND_3	$S_{gas,1bar}^\circ$	203.93 J/mol*K

Now, we simply have to compute ΔH and ΔS as:

$$\Delta H = H_f^\circ(\text{products}) - H_f^\circ(\text{reactants})$$

$$\Delta S = S^\circ(\text{products}) - S^\circ(\text{reactants})$$

Before setting the temperature of the reaction as 10 K to give $T\Delta S$.

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[17]: T = 10

enthalpy_NH2 = 190.37
enthalpy_H   = 218
enthalpy_NH3 = -45.9

# Converting from J/mol * K to kJ/mol*K
entropy_NH2 = 194.71 / 1000
entropy_H   = 114.72 / 1000
entropy_NH3 = 192.77 / 1000

hydrogen_dH = enthalpy_NH3 - (enthalpy_NH2 + enthalpy_H)
hydrogen_dS = entropy_NH3 - (entropy_NH2 + entropy_H)
hydrogen_dG = hydrogen_dH - (T * hydrogen_dS)
print(f'Change in enthalpy (Hydrogen): {hydrogen_dH:.2f}')
print(f'Change in entropy (Hydrogen): {hydrogen_dS:.2f}')
print(f'Change in Gibbs (Hydrogen): {hydrogen_dG:.2f}\n')

enthalpy_ND2 = 185.35
enthalpy_D   = 221.72
enthalpy_ND3 = -58.58

# Converting from J/mol * K to kJ/mol*K
entropy_ND2 = 204.30 / 1000
entropy_D   = 123.35 / 1000
entropy_ND3 = 203.93 / 1000

deuterium_dH = enthalpy_ND3 - (enthalpy_ND2 + enthalpy_D)
deuterium_dS = entropy_ND3 - (entropy_ND2 + entropy_D)
deuterium_dG = deuterium_dH - (T * deuterium_dS)
print(f'Change in enthalpy (Deuterium): {deuterium_dH:.2f}')
print(f'Change in entropy (Deuterium): {deuterium_dS:.2f}')
print(f'Change in Gibbs (Deuterium): {deuterium_dG:.2f}')

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Change in enthalpy (Hydrogen): -454.27
Change in entropy (Hydrogen): -0.12
Change in Gibbs (Hydrogen): -453.10

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Change in enthalpy (Deuterium): -465.65
Change in entropy (Deuterium): -0.12
Change in Gibbs (Deuterium): -464.41

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The reaction with the more negative ΔG is the more thermodynamically favored. In this reaction, the species which have deuterium instead of hydrogen results in a slightly more favored chemical potential difference, showing that deuterium is likely to be favored in reactions when present.

1 References

1. Millar, T. J. (2005). Deuterium in interstellar clouds. *Astronomy & Geophysics : The Journal of the Royal Astronomical Society*, 46(2), 2.29-2.32. <https://doi.org/10.1111/j.1468-4004.2005.46229.x>