# Computational Chemistry Example

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## Example Table

Table 1: Basis set sizes

| Basis Set | Basis Functions Count |
|---|---|
| 6-31G* | 19 |
| cc-pVTZ | 58 |

## Using Latex Equations and Python

$$N! = \int_0^\infty e^{Ng(x)} dx = \int_0^\infty e^{N\ln(N) - 1 - \frac{(x-N)^2}{2N^2}} dx$$

The exponential terms that do not contain an x can be separated out and pulled out to the front.

$$N! = e^{N(\ln(N)-1)} \int_0^\infty e^{\frac{(x-N)^2}{2N^2}} dx$$

```python
import sympy as sp

x = sp.Symbol("x")
N = sp.Symbol("N", positive=True)
# N = sp.Symbol("N")
gx = sp.exp(-(x-N)**2/(2*N))
out = sp.integrate(gx, (x, 0, sp.oo))
print(sp.latex(out))

N = sp.oo
erfc_eval = (2 - sp.erfc(sp.sqrt(2)*sp.sqrt(N)/2))/2
print(erfc_eval)
```

```
\frac{\sqrt{2} \sqrt{\pi} \sqrt{N} \left(2 - \operatorname{erfc}{\left(\frac{\sqrt{2} \sqrt{N}}{2} \right)}\right)}{2}
1
```

This ultimately yields...

$$N! = e^{N\ln(N)-N} \frac{\sqrt{2\pi N}\left(2 - \operatorname{erfc}\left(\frac{\sqrt{2}\sqrt{N}}{2}\right)\right)}{2}$$

Since N is very large, the erfc portion of the equation effectively becomes 1, allowing us to remove the portion through an approximation.

$$N! \approx e^{N \ln(N) - N} \sqrt{2\pi N}$$

Taking the natural log of this produces...

$$\ln N! = ln(e^{N \ln(N) - N} \sqrt{2\pi N}) = ln(e^{N \ln(N) - N}) + \ln \sqrt{2\pi N} = N \ln(N) - N + \ln \sqrt{2\pi N}$$

# Images

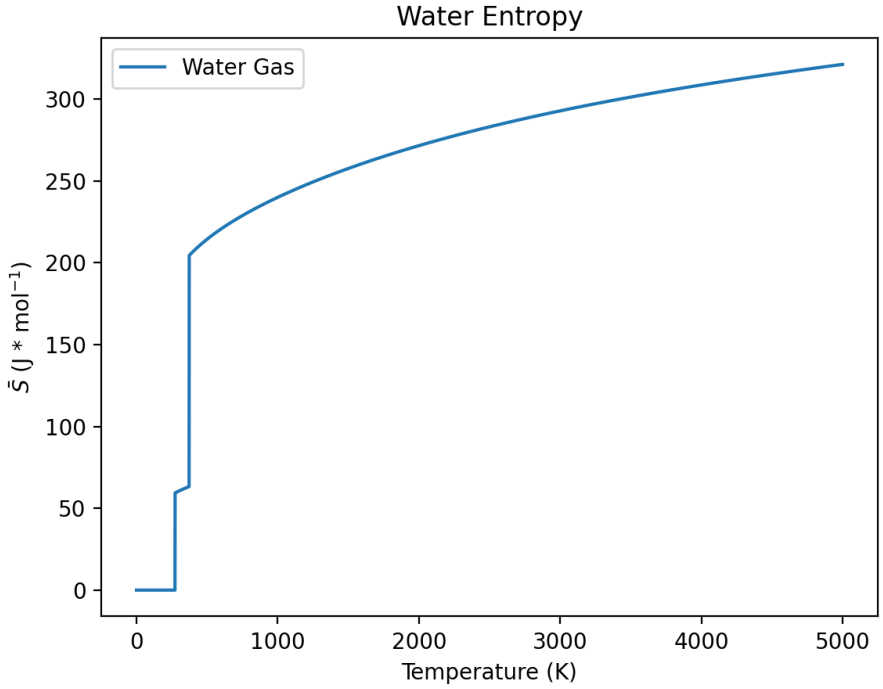
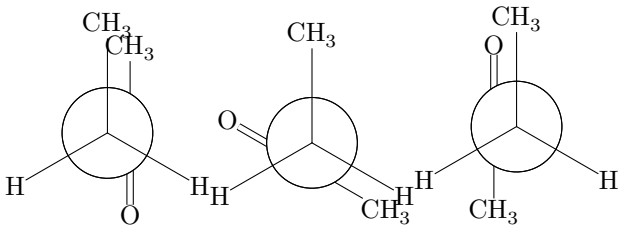



Figure 1: The water entropy vs. temperature plot shows large jumps in entropy between the major phase transitions of solid to liquid and liquid to gas.

# Latex Sections




# Citations

Table 2: Water rotational constants[1]

| Rotational Constants | Frequency ($cm^{-1}$) |
|---|---|
| A | 27.8761 |
| B | 14.5074 |
| C | 9.2877 |

# References

(1) Hall, R. T.; Dowling, J. M. Pure Rotational Spectrum of Water Vapor. *The Journal of Chemical Physics* **1967**, *47* (7), 2454–2461.