Gamma Term &

From lab slides:

$$Y_{AB} = \sum_{k=1}^{3}\sum_{k'=1}^{3}\sum_{l=1}^{3}\sum_{l'=1}^{3} d'_{k s_A} d'_{k' s_A} d'_{l s_B} d'_{l' s_B} [0]^{(0)}$$

$$[0]^{(0)} = U_A U_B \sqrt{\frac{1}{(R_a - R_B)^2}} \operatorname{erf}(\sqrt{T})$$

This is the term that we need to differentiate wrt $\underline{R_a}$

$$\frac{\partial}{\partial R_A} \frac{1}{\sqrt{(R_a - R_B)^2}} = \text{break into } xyz \text{ components just like overlap term!}$$

lab slide / wolfram

$$= -\frac{R_A - R_B}{|R_a - R_B|^3} = \frac{\partial}{\partial R_a} \text{ term}$$

$$\cancel{\frac{1}{(R_a - R_B)^2}} \quad \cancel{\left((R_a - R_B)^2\right)^{-\frac{1}{2}}} \quad \cancel{-\frac{1}{2}}$$

$$\frac{\partial}{\partial R_a} \operatorname{erf}(\sqrt{T}) =$$

substitute $T = v^2 (R_a - R_B)^2$

$$\frac{\partial \frac{2}{\sqrt{\pi}} \int_0^{\sqrt{T}} \exp(-v^2)\, dv}{\partial R_A} =$$

$$\frac{\partial \frac{2}{\sqrt{\pi}} \int_0^{v\sqrt{(R_a - R_B)^2}} \exp(-v)^2\, dv \cdot \partial\left[v\sqrt{(R_A - R_B)^2}\right]}{\partial R_A \; \partial\left[v\sqrt{(R_A - R_B)^2}\right]}$$

taking derivative wrt same thing as integral!

$= \frac{\partial U}{}$

$$= \frac{2}{\sqrt{\pi}} \exp\left(-V^2 (R_a - R_B)^2\right) \frac{V(R_a - R_B)}{|R_a - R_B|}$$

individual dimensional component

distance

$$= \frac{2V}{\sqrt{\pi}} e^{-T} \cdot \frac{R_A - R_B}{\text{dist}}$$

RECAP

$$[0]^{(0)} = U_A U_B \underbrace{\sqrt{\frac{1}{(R_a - R_B)^2}}}\ \underbrace{\operatorname{erf}(\sqrt{T})}$$

$$\frac{\partial}{\partial R_a} \sqrt{\frac{1}{(R_a - R_B)^2}} \quad \text{This term} = \frac{-(R_a - R_B)}{|R_a - R_B|^3}$$

$$\frac{\partial}{\partial R_A} \operatorname{erf}(\sqrt{T}) \quad \text{this term} = \frac{2V}{\sqrt{\pi}} e^{-T} \frac{R_a - R_B}{|R_a - R_B|}$$

Combine!

$$\frac{\partial}{\partial R_A} [0]^{(0)} = U_A U_B \left[\frac{-R_a - R_B}{|R_a - R_B|^3} \operatorname{erf}(\sqrt{T}) + \sqrt{\frac{1}{(R_a - R_B)^2}} \left(\frac{2U}{\sqrt{\pi}} e^{-T} \frac{R_a - R_B}{|R_a - R_B|} \right) \right]$$

$$\frac{\partial}{\partial R_A \frac{\partial}{B}}[0]^{(0)} = U_A U_B\left[-\frac{R_a-R_B}{|R_a-R_B|^3}\,\mathrm{erf}(\sqrt{T}) + \sqrt{\frac{1}{(R_a-R_B)^2}}\cdot\frac{2V}{\sqrt{\pi}}e^{-T}\cdot\frac{R_a-R_B}{|R_a-R_B|}\right]$$

time to simplify...

erf

$$2\quad -\frac{U_A U_B (R_a-R_B)}{|R_a-R_B|^3}\,\mathrm{erf}(\sqrt{T}) + \frac{U_A U_B\; 2V\; e^{-T}}{|R_a-R_B|\sqrt{\pi}}$$

pull out

$$\frac{+U_A U_B (R_a-R_B)}{|R_a-R_B|^2}$$

from each term

$$\frac{U_A U_B}{\sqrt{(R_a-R_B)^2}}\cdot\frac{2V}{\sqrt{\pi}}e^{-T}\,\frac{R_a-R_B}{|R_a-R_B|}$$

$$\downarrow$$

$$\frac{U_A U_B}{|R_a-R_B|}\,\frac{2V}{\sqrt{\pi}}\,\frac{R_a-R_B}{|R_a-R_B|}e^{-T}$$

$$\frac{(R_a-R_B)U_A U_B}{|R_a-R_B|^2}\,\frac{2V}{\sqrt{\pi}}e^{-T}$$

?

$$\frac{+U_A U_B (R_a-R_B)}{|R_a-R_B|^2}\left(-\frac{\mathrm{erf}\sqrt{T}}{|R_a-R_B|} + \frac{2V}{\sqrt{\pi}}e^{-T}\right)$$

matches slide! Yay!

more clearly $$\frac{\partial}{\partial R_A}[0]^{(0)} = \frac{U_A U_B (R_A-R_B)}{|R_a-R_B|^2}\left(\frac{-\mathrm{erf}(\sqrt{T})}{|R_a-R_B|} + \frac{2V}{\sqrt{\pi}}e^{-T}\right)$$

multiply by all the primatives NORMALIZED coeff!