Written by Alexander Sauter. Small correction by Ladislav

1. Calculating the Integral

Radial Part $R_{1,0}(r)$:

$$R_{1,0}(r) = 2 \cdot \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \cdot e^{-\frac{Z \cdot r}{a_0}} = R^*_{1,0}(r)$$

Integral:

$$\int_0^\infty \int_0^\infty r_1^2 \cdot r_2^2 \cdot R_{1,0}(r_1)^2 \cdot R_{1,0}(r_2)^2 \frac{e^2}{r_>} dr_1 dr_2$$
$$= \int_0^\infty \int_0^\infty 2^4 \left(\frac{Z}{a_0}\right)^6 e^{-\frac{2Z}{a_0}(r_1+r_2)} r_1^2 \cdot r_2^2 \frac{e^2}{r_>} dr_1 dr_2$$
$$= 2^4 \left(\frac{Z}{a_0}\right)^6 \cdot e^2 \int_0^\infty \int_0^\infty e^{-\frac{2Z}{a_0}(r_1+r_2)} r_1^2 \cdot r_2^2 \frac{1}{r_>} dr_1 dr_2$$

With substitution:

$$= \frac{1}{2}\frac{Ze^2}{a_0}\underbrace{\int_0^\infty \int_0^\infty r_1^2 r_2^2 e^{-r_1} e^{-r_2} \frac{1}{r_>} dr_1 dr_2}_{intA}$$

Attend that $\frac{e^2}{a_0} = a.u. = E_0$
To calculate the rest-integral, we split it into two integrals. For each r_1 are we taking the integral over r_2 and than can we take the integrale over r_1:

$$\begin{aligned} intA &= \int_0^\infty \left(\int_0^{r_1} e^{-r_1-r_2} r_1 r_2^2 dr_2 \right) dr_1 + \int_0^\infty \left(\int_{r_1}^\infty e^{-r_1-r_2} r_1^2 r_2 dr_2 \right) dr_1 \\ &= \int_0^\infty r_1 e^{-r_1} \underbrace{\int_0^{r_1} r_2^2 e^{-r_2} dr_2}_{intB} dr_1 + \int_0^\infty r_1^2 e^{-r_1} \underbrace{\int_{r_1}^\infty e^{-r_2} r_2 dr_2}_{intC} dr_1 \end{aligned}$$

With partial integration one get:

$$intB = 2 - e^{-r_1}(r_1^2 + 2r_1 + 2)$$

$$intC = e^{-r_1}(r_1 + 1)$$

And with this you get by again merging the two split integrals:

$$intA = \int_0^\infty 2r_1 e^{-r_1} - e^{-2r_1}(r_1^2 + 2r_1)dr_1$$

With substitution and the knowledge that:

$$\int_0^\infty x^n e^{-x} dx = n!$$

Added expression for Substitutions (Ladislav): if the exponent contains α, we make substitution

$$x = \frac{1}{\alpha} y \qquad dx = \frac{1}{\alpha}\ dy$$

so that

$$\int_0^\infty \ x^n \ dx\ e^{-\alpha x} \ = \ \frac{1}{\alpha^{n+1}} \int_0^\infty \ y^n \ dy\ e^{-y}$$

Alexander gets:

$$intA = 2 - \frac{1}{8} - \frac{1}{2} = \frac{5}{4}$$

This however does not give the right result, so we do it step by step (added Ladislav) We re-write $intA$ as

$$intA = \int_0^\infty 2r_1 e^{-r_1} dr_1 - \int_0^\infty e^{-2r_1} r_1^2 dr_1 - \int_0^\infty e^{-2r_1} 2r_1 dr_1$$

We see that the first integral has $n = 1$ and no constant in the exponential; thus we get 2. Second term contains $n = 2$ and $\alpha = 2$. It thus gives

$$-\frac{1}{2^3} 2! = \frac{1}{4}$$

The third term has $n = 1$ and $\alpha = 2$. It gives

$$-2\frac{1}{2^2} 1! = \frac{1}{2}$$

The correct expression is thus

$$intA = 2 - \frac{1}{4} - \frac{1}{2} = \frac{5}{4}$$

Now Alexander continues:

And with this we get for the whole integral from the begining

$$\int_0^\infty \int_0^\infty \ldots = \frac{5}{8} \frac{Ze^2}{a_0}$$

2. Formula for the values of the table

"$2E_{10}$": (just two electrons)

$$E = 2 \cdot (-\frac{1}{2} E_0 Z^2)$$

"$2E_{10} + \frac{5}{8}Z$": (two electrons and their interaction)

$$E = 2 \cdot (-\frac{1}{2} E_0 Z^2) + \frac{5}{8} Z E_0$$

"Variational": ($z = Z - \frac{5}{16}$)

$$E(z, Z) = E_0 \cdot (z^2 - 2zZ + \frac{5}{8} z)$$

The value for the "2. Ion.pot." do one get with the formula:

$$\frac{1}{2} E_0 Z^2$$

And the Value from the "Ion.pot." by subtracting the 2. ionization potential from the experimental binding energy.