To have an idea of the order of magnitude of C, we can therefore replace all the energy denominators of (19) by $2E_I$. Using the closure relation and the fact that the diagonal element of W_{dd} is zero (§2-a-β), we then get :

$$C \simeq \frac{e^4}{2E_I} \langle \varphi^A_{1,0,0} ; \varphi^B_{1,0,0} \,|\, (X_A X_B + Y_A Y_B - 2Z_A Z_B)^2 \,|\, \varphi^A_{1,0,0} ; \varphi^B_{1,0,0} \rangle \qquad (20)$$

This expression is simple to calculate: because of the spherical symmetry of the $1s$ state, the mean values of the cross terms of the type $X_A Y_A$, $X_B Y_B$, ..., are zero. Furthermore, and for the same reason, the various quantities:

$$\langle \varphi^A_{1,0,0} \,|\, X_A^2 \,|\, \varphi^A_{1,0,0} \rangle, \langle \varphi^A_{1,0,0} \,|\, Y_A^2 \,|\, \varphi^A_{1,0,0} \rangle \;\; ..., \langle \varphi^B_{1,0,0} \,|\, Z_B^2 \,|\, \varphi^B_{1,0,0} \rangle$$

are all equal to one third of the mean value of $\mathbf{R}_A^2 = X_A^2 + Y_A^2 + Z_A^2$. We finally obtain, therefore, using the expression for the wave function $\varphi_{1,0,0}(\mathbf{r})$:

$$C \simeq \frac{e^4}{2E_I} \times 6 \left| \langle \varphi^A_{1,0,0} \,|\, \frac{\mathbf{R}_A^2}{3} \,|\, \varphi^A_{1,0,0} \rangle \right|^2 = 6\, e^2 a_0^5 \qquad (21)$$

(where a_0 is the Bohr radius) and, consequently:

$$\varepsilon_2 \simeq -\, 6e^2 \frac{a_0^5}{R^6} = -\, 6 \frac{e^2}{R} \left(\frac{a_0}{R} \right)^5 \qquad (22)$$