

$$\begin{aligned}
G &= \int \eta_1(\vec{A}, \alpha_1, \ell_1, m_1, n_1)(\vec{r}_{A1}) \eta_2(\vec{B}, \alpha_2, \ell_2, m_2, n_2)(\vec{r}_{B1}) \\
&\times \frac{1}{r_{12}} \eta_3(\vec{C}, \alpha_3, \ell_3, m_3, n_3)(\vec{r}_{C2}) \eta_4(\vec{D}, \alpha_4, \ell_4, m_4, n_4)(\vec{r}_{D2}) dV_1 dV_2 \\
&= \Omega \sum_{\ell=0}^{\ell_1+\ell_2} \sum_{r=0}^{[\ell/2]} \sum_{\ell'=0}^{\ell_3+\ell_4} \sum_{r'=0}^{[\ell'/2]} \sum_{i=0}^{[(\ell+\ell'-2r-2r')/2]} \\
&\quad B_{\ell,\ell',r,r',i}(\ell_1, \ell_2, \vec{A}_x, \vec{B}_x, \vec{P}_x, \gamma_1; \ell_3, \ell_4, \vec{C}_x, \vec{D}_x, \vec{Q}_x, \gamma_2) \\
&\times \sum_{m=0}^{m_1+m_2} \sum_{s=0}^{[m/2]} \sum_{m'=0}^{m_3+m_4} \sum_{s'=0}^{[m'/2]} \sum_{j=0}^{[(m+m'-2s-2s')/2]} \\
&\quad B_{m,m',s,s',j}(m_1, m_2, \vec{A}_y, \vec{B}_y, \vec{P}_y, \gamma_1; m_3, m_4, \vec{C}_y, \vec{D}_y, \vec{Q}_y, \gamma_2) \\
&\times \sum_{n=0}^{n_1+n_2} \sum_{t=0}^{[n/2]} \sum_{n'=0}^{n_3+n_4} \sum_{t'=0}^{[n'/2]} \sum_{k=0}^{[(n+n'-2t-2t')/2]} \\
&\quad B_{n,n',t,t',k}(n_1, n_2, \vec{A}_z, \vec{B}_z, \vec{P}_z, \gamma_1; n_3, n_4, \vec{C}_z, \vec{D}_z, \vec{Q}_z, \gamma_2) \\
&\times F_\nu(\vec{p}^2/4\delta) \tag{1}
\end{aligned}$$

where

$$\begin{aligned}
\nu &= \ell + \ell' + m + m' + n + n' - 2(r + r' + s + s' + t + t') - (i + j + k) \\
\delta &= \frac{1}{4\gamma_1} + \frac{1}{4\gamma_2}
\end{aligned}$$

and the ‘‘Gaussian product factor’’ Ω , involving the original factors K_1 and K_2 , is given by

$$\Omega = \frac{2\pi^2}{\gamma_1\gamma_2} \left(\frac{\pi}{\gamma_1 + \gamma_2} \right)^{1/2} \exp \left(-\frac{\alpha_1\alpha_2\vec{A}\vec{B}^2}{\gamma_1} - \frac{\alpha_3\alpha_4\vec{C}\vec{D}^2}{\gamma_2} \right)$$

One thing is clear from this rather awesome formula; the electron-repulsion integral is simply a weighted sum of the integrals $F_\nu(x)$. The coefficients which multiply the $F_\nu(x)$ involve

1. The powers of x , y , and z in the Cartesian factors of each of the GTFs.
2. The exponents of each of the GTFs.

3. The components of the position vectors of each GTF.

The B terms can be simplified by the definition of

$$\theta(\ell, \ell_1, \ell_2, a, b, r, \gamma) = f_\ell(\ell_1, \ell_2, a, b) \frac{\ell! \gamma^{r-\ell}}{r!(\ell - 2r)!}$$

Then the B involving the “ x -components” is

$$\begin{aligned} & B_{\ell, \ell', r_1, r_2, i}(\ell_1, \ell_2, \vec{A}_x, \vec{B}_x, \vec{P}_x, \gamma_1; \ell_3, \ell_4, \vec{C}_x, \vec{D}_x, \vec{Q}_x, \gamma_2) \\ = & (-1)^\ell \theta(\ell, \ell_1, \ell_2, \vec{P}\vec{A}_x, \vec{P}\vec{B}_x, r, \gamma_1) \theta(\ell', \ell_3, \ell_4, \vec{Q}\vec{C}_x, \vec{Q}\vec{D}_x, r', \gamma_2) \\ \times & \frac{(-1)^i (2\delta)^{2(r+r')} (\ell + \ell' - 2r - 2r')! \delta^i \vec{p}_x^{\ell+\ell'-2(r+r'+i)}}{(4\delta)^{\ell+\ell'} i! [\ell + \ell' - 2(r + r' + i)]!} \end{aligned}$$

With completely analogous expressions for the other two B factors.