Electron repulsion integrals

```
prefac = 1
```

1

```
f0 = Subscript[F, 0]
f1 = Subscript[F, 1]
f2 = Subscript[F, 2]
f3 = Subscript[F, 3]
f4 = Subscript[F, 4]
```

```
ssss0 = prefac * f0
```

F_0

```
ssss1 = prefac * f1
```

F_1

```
ssss2 = prefac * f2
```

F_2

```
ssss3 = prefac * f3
```

F_3

```
ssss4 = prefac * f4
```

F_4

```
pai = Subscript[PA, i]
paj = Subscript[PA, j]
pbj = Subscript[PB, j]
pci = Subscript[PC, i]
pcj = Subscript[PC, j]
wpi = Subscript[WP, i]
wpj = Subscript[WP, j]
qck = Subscript[QC, k]
qdl = Subscript[QD, l]
wqk = Subscript[WQ, k]
wql = Subscript[WQ, l]
dij = Subscript[δ, ij]
djk = Subscript[δ, jk]
dik = Subscript[δ, ik]
dil = Subscript[δ, il]
djl = Subscript[δ, jl]
dkl = Subscript[δ, kl]
```

```
psss0 = Collect[Expand[pai * ssss0 + wpi * ssss1],
  {f0, f1, f2, f3, f4, dij, dkl, djk, dil}]
```

$F_0\, PA_i + F_1\, WP_i$

```
psss1 = Collect[Expand[pai * ssss1 + wpi * ssss2],
  {f0, f1, f2, f3, f4, dij, dkl, djk, dil}]
```

$F_1\, PA_i + F_2\, WP_i$

```
psss2 = Collect[Expand[pai * ssss2 + wpi * ssss3],
  {f0, f1, f2, f3, f4, dij, dkl, djk, dil}]
```

$$F_2\ PA_i + F_3\ WP_i$$

```
psss3 = Collect[Expand[pai * ssss3 + wpi * ssss4],
  {f0, f1, f2, f3, f4, dij, dkl, djk, dil}]
```

$$F_3\ PA_i + F_4\ WP_i$$

```
spss0 = Collect[Expand[pbj * ssss0 + wpj * ssss1],
  {f0, f1, f2, f3, f4, dij, dkl, djk, dil}]
```

$$F_0\ PB_j + F_1\ WP_j$$

```
spss1 = Collect[Expand[pbj * ssss1 + wpj * ssss2],
  {f0, f1, f2, f3, f4, dij, dkl, djk, dil}]
```

$$F_1\ PB_j + F_2\ WP_j$$

```
spss2 = Collect[Expand[pbj * ssss2 + wpj * ssss3],
  {f0, f1, f2, f3, f4, dij, dkl, djk, dil}]
```

$$F_2\ PB_j + F_3\ WP_j$$

```
spss3 = Collect[Expand[pbj * ssss3 + wpj * ssss4],
  {f0, f1, f2, f3, f4, dij, dkl, djk, dil}]
```

$$F_3\ PB_j + F_4\ WP_j$$

```
psps0 =
 Collect[Expand[qck * psss0 + wqk * psss1 + (dik / (2 * (ζ + η))) * ssss1],
  {f0, f1, f2, f3, f4, dij, dkl, djk, dil}]
```

$$F_0\ PA_i\ QC_k + F_2\ WP_i\ WQ_k + F_1\left(QC_k\ WP_i + PA_i\ WQ_k + \frac{\delta_{ik}}{2\ (\zeta + \eta)}\right)$$

```
psps1 =
 Collect[Expand[qck * psss1 + wqk * psss2 + (dik / (2 * (ζ + η))) * ssss2],
  {f0, f1, f2, f3, f4, dij, dkl, djk, dil}]
```

$$F_1\ PA_i\ QC_k + F_3\ WP_i\ WQ_k + F_2\left(QC_k\ WP_i + PA_i\ WQ_k + \frac{\delta_{ik}}{2\ (\zeta + \eta)}\right)$$

```
spps0 =
 Collect[Expand[qck * spss0 + wqk * spss1 + (djk / (2 * (ζ + η))) * ssss1],
  {f0, f1, f2, f3, f4, dij, dkl, djk, dil}]
```

$$F_0\ PB_j\ QC_k + F_2\ WP_j\ WQ_k + F_1\left(QC_k\ WP_j + PB_j\ WQ_k + \frac{\delta_{jk}}{2\ (\zeta + \eta)}\right)$$

```
spps1 =
 Collect[Expand[qck * spss1 + wqk * spss2 + (djk / (2 * (ζ + η))) * ssss2],
  {f0, f1, f2, f3, f4, dij, dkl, djk, dil}]
```

$$F_1\ PB_j\ QC_k + F_3\ WP_j\ WQ_k + F_2\left(QC_k\ WP_j + PB_j\ WQ_k + \frac{\delta_{jk}}{2\ (\zeta + \eta)}\right)$$

```
ppss0 = Collect[Expand[
    pbj * psss0 + wpj * psss1 + (dij / (2 * ζ)) * (ssss0 - (ρ / ζ) * ssss1)],
  {f0, f1, f2, f3, f4, dij, dkl, djk, dil}]
```

$$F_2\, WP_i\, WP_j + F_0 \left(PA_i\, PB_j + \frac{\delta_{ij}}{2\,\zeta}\right) + F_1 \left(PB_j\, WP_i + PA_i\, WP_j - \frac{\rho\,\delta_{ij}}{2\,\zeta^2}\right)$$

```
ppss1 = Collect[Expand[
    pbj * psss1 + wpj * psss2 + (dij / (2 * ζ)) * (ssss1 - (ρ / ζ) * ssss2)],
  {f0, f1, f2, f3, f4, dij, dkl, djk, dil}]
```

$$F_3\, WP_i\, WP_j + F_1 \left(PA_i\, PB_j + \frac{\delta_{ij}}{2\,\zeta}\right) + F_2 \left(PB_j\, WP_i + PA_i\, WP_j - \frac{\rho\,\delta_{ij}}{2\,\zeta^2}\right)$$

```
ppss2 = Collect[Expand[
    pbj * psss2 + wpj * psss3 + (dij / (2 * ζ)) * (ssss2 - (ρ / ζ) * ssss3)],
  {f0, f1, f2, f3, f4, dij, dkl, djk, dil}]
```

$$F_4\, WP_i\, WP_j + F_2 \left(PA_i\, PB_j + \frac{\delta_{ij}}{2\,\zeta}\right) + F_3 \left(PB_j\, WP_i + PA_i\, WP_j - \frac{\rho\,\delta_{ij}}{2\,\zeta^2}\right)$$

```
ppps0 = Collect[Expand[qck * ppss0 + wqk * ppss1 +
     (1 / (2 * (ζ + η))) * (dik * spss1 + djk * psss1)],
  {f0, f1, f2, f3, f4, dij, dkl, djk, dil}]
```

$$\begin{aligned}
&F_3\, WP_i\, WP_j\, WQ_k + F_0 \left(PA_i\, PB_j\, QC_k + \frac{QC_k\, \delta_{ij}}{2\,\zeta}\right) + \\
&\quad F_1 \left(PB_j\, QC_k\, WP_i + PA_i\, QC_k\, WP_j + PA_i\, PB_j\, WQ_k + \right. \\
&\qquad \left. \left(-\frac{\rho\, QC_k}{2\,\zeta^2} + \frac{WQ_k}{2\,\zeta}\right) \delta_{ij} + \frac{PB_j\, \delta_{ik}}{2\,(\zeta+\eta)} + \frac{PA_i\, \delta_{jk}}{2\,(\zeta+\eta)}\right) + \\
&\quad F_2 \left(QC_k\, WP_i\, WP_j + PB_j\, WP_i\, WQ_k + PA_i\, WP_j\, WQ_k - \right. \\
&\qquad \left. \frac{\rho\, WQ_k\, \delta_{ij}}{2\,\zeta^2} + \frac{WP_j\, \delta_{ik}}{2\,(\zeta+\eta)} + \frac{WP_i\, \delta_{jk}}{2\,(\zeta+\eta)}\right)
\end{aligned}$$

```
ppps1 = Collect[Expand[qck * ppss1 + wqk * ppss2 +
     (1 / (2 * (ζ + η))) * (dik * spss2 + djk * psss2)],
  {f0, f1, f2, f3, f4, dij, dkl, djk, dil}]
```

$$F_4\, WP_i\, WP_j\, WQ_k + F_1 \left(PA_i\, PB_j\, QC_k + \frac{QC_k\, \delta_{ij}}{2\, \zeta} \right) +$$

$$F_2 \left(PB_j\, QC_k\, WP_i + PA_i\, QC_k\, WP_j + PA_i\, PB_j\, WQ_k + \right.$$

$$\left. \left(-\frac{\rho\, QC_k}{2\, \zeta^2} + \frac{WQ_k}{2\, \zeta} \right) \delta_{ij} + \frac{PB_j\, \delta_{ik}}{2\, (\zeta + \eta)} + \frac{PA_i\, \delta_{jk}}{2\, (\zeta + \eta)} \right) +$$

$$F_3 \left(QC_k\, WP_i\, WP_j + PB_j\, WP_i\, WQ_k + PA_i\, WP_j\, WQ_k - \frac{\rho\, WQ_k\, \delta_{ij}}{2\, \zeta^2} + \frac{WP_j\, \delta_{ik}}{2\, (\zeta + \eta)} + \frac{WP_i\, \delta_{jk}}{2\, (\zeta + \eta)} \right)$$

```
pppp0 = Collect[Expand[qdl * ppps0 +
     wql * ppps1 + (1 / (2 * (ζ + η))) * (dil * spps1 + djl * psps1) +
     (dkl / (2 * η)) * (ppss0 - (ρ / η) * ppss1)],
  {f0, f1, f2, f3, f4, dij, dkl, djk, dil}]
```

$$
\begin{aligned}
&F_4\, WP_i\, WP_j\, WQ_k\, WQ_l + \\
&F_3 \left(QD_l\, WP_i\, WP_j\, WQ_k + QC_k\, WP_i\, WP_j\, WQ_l + PB_j\, WP_i\, WQ_k\, WQ_l + PA_i\, WP_j\, WQ_k\, WQ_l - \right. \\
&\quad \frac{\rho\, WQ_k\, WQ_l\, \delta_{ij}}{2\,\zeta^2} + \frac{WP_j\, WQ_l\, \delta_{ik}}{2\,(\zeta+\eta)} + \frac{WP_j\, WQ_k\, \delta_{il}}{2\,(\zeta+\eta)} + \\
&\quad \left. \frac{WP_i\, WQ_l\, \delta_{jk}}{2\,(\zeta+\eta)} + \frac{WP_i\, WQ_k\, \delta_{jl}}{2\,(\zeta+\eta)} - \frac{\rho\, WP_i\, WP_j\, \delta_{kl}}{2\,\eta^2} \right) + \\
&F_0 \left(PA_i\, PB_j\, QC_k\, QD_l + \frac{PA_i\, PB_j\, \delta_{kl}}{2\,\eta} + \delta_{ij} \left(\frac{QC_k\, QD_l}{2\,\zeta} + \frac{\delta_{kl}}{4\,\zeta\,\eta} \right) \right) + \\
&F_2 \left(QC_k\, QD_l\, WP_i\, WP_j + PB_j\, QD_l\, WP_i\, WQ_k + PA_i\, QD_l\, WP_j\, WQ_k + \right. \\
&\quad PB_j\, QC_k\, WP_i\, WQ_l + PA_i\, QC_k\, WP_j\, WQ_l + PA_i\, PB_j\, WQ_k\, WQ_l + \\
&\quad \frac{QD_l\, WP_j\, \delta_{ik}}{2\,(\zeta+\eta)} + \frac{PB_j\, WQ_l\, \delta_{ik}}{2\,(\zeta+\eta)} + \left(\frac{QC_k\, WP_j}{2\,(\zeta+\eta)} + \frac{PB_j\, WQ_k}{2\,(\zeta+\eta)} \right) \delta_{il} + \\
&\quad \left(\frac{QD_l\, WP_i}{2\,(\zeta+\eta)} + \frac{PA_i\, WQ_l}{2\,(\zeta+\eta)} + \frac{\delta_{il}}{4\,(\zeta+\eta)^2} \right) \delta_{jk} + \frac{QC_k\, WP_i\, \delta_{jl}}{2\,(\zeta+\eta)} + \\
&\quad \frac{PA_i\, WQ_k\, \delta_{jl}}{2\,(\zeta+\eta)} + \frac{\delta_{ik}\, \delta_{jl}}{4\,(\zeta+\eta)^2} + \left(-\frac{\rho\, PB_j\, WP_i}{2\,\eta^2} - \frac{\rho\, PA_i\, WP_j}{2\,\eta^2} + \frac{WP_i\, WP_j}{2\,\eta} \right) \delta_{kl} + \\
&\quad \left. \delta_{ij} \left(-\frac{\rho\, QD_l\, WQ_k}{2\,\zeta^2} - \frac{\rho\, QC_k\, WQ_l}{2\,\zeta^2} + \frac{WQ_k\, WQ_l}{2\,\zeta} + \frac{\rho^2\, \delta_{kl}}{4\,\zeta^2\,\eta^2} \right) \right) + \\
&F_1 \left(PB_j\, QC_k\, QD_l\, WP_i + PA_i\, QC_k\, QD_l\, WP_j + PA_i\, PB_j\, QD_l\, WQ_k + \right. \\
&\quad PA_i\, PB_j\, QC_k\, WQ_l + \frac{PB_j\, QD_l\, \delta_{ik}}{2\,(\zeta+\eta)} + \frac{PB_j\, QC_k\, \delta_{il}}{2\,(\zeta+\eta)} + \frac{PA_i\, QD_l\, \delta_{jk}}{2\,(\zeta+\eta)} + \\
&\quad \frac{PA_i\, QC_k\, \delta_{jl}}{2\,(\zeta+\eta)} + \left(-\frac{\rho\, PA_i\, PB_j}{2\,\eta^2} + \frac{PB_j\, WP_i}{2\,\eta} + \frac{PA_i\, WP_j}{2\,\eta} \right) \delta_{kl} + \\
&\quad \left. \delta_{ij} \left(-\frac{\rho\, QC_k\, QD_l}{2\,\zeta^2} + \frac{QD_l\, WQ_k}{2\,\zeta} + \frac{QC_k\, WQ_l}{2\,\zeta} + \left(-\frac{\rho}{4\,\zeta\,\eta^2} - \frac{\rho}{4\,\zeta^2\,\eta} \right) \delta_{kl} \right) \right)
\end{aligned}
$$

Overlap, Potential and Kinetic Integrals

```
ss =.
integrals Overlap
```

```
ps = pai * ss
```

$$\text{ss}\ \text{PA}_i$$

```
pp = Simplify[pbj * ps + (dij / 2 ζ) ss]
```

$$\text{ss}\ \text{PA}_i\ \text{PB}_j + \frac{1}{2}\ \text{ss}\ \zeta\ \delta_{ij}$$

```
sks = Simplify[ξ (3 - 2 ξ * R^2) ss]
```

$$\text{ss}\ \xi\ \left(3 - 2\ \text{R}^2\ \xi\right)$$

```
pks = Simplify[pai * sks + 2 ξ * ps]
```

$$\text{ss}\ \xi\ \left(5 - 2\ \text{R}^2\ \xi\right)\ \text{PA}_i$$

```
pkp = Simplify[pbj * pks + (dij / 2 ζ) * sks + 2 ξ * pp]
```

$$-\frac{1}{2}\ \text{ss}\ \xi\ \left(2\ \left(-7 + 2\ \text{R}^2\ \xi\right)\ \text{PA}_i\ \text{PB}_j + \zeta\ \left(-5 + 2\ \text{R}^2\ \xi\right)\ \delta_{ij}\right)$$

```
scs0 = Simplify[2 Sqrt[ζ / π] * ss * f0]
```

$$\frac{2\ \text{ss}\ \sqrt{\zeta}\ \text{F}_0}{\sqrt{\pi}}$$

```
scs1 = Simplify[2 Sqrt[ζ / π] * ss * f1]
```

$$\frac{2\ \text{ss}\ \sqrt{\zeta}\ \text{F}_1}{\sqrt{\pi}}$$

```
scs2 = Simplify[2 Sqrt[ζ / π] * ss * f2]
```

$$\frac{2\ \text{ss}\ \sqrt{\zeta}\ \text{F}_2}{\sqrt{\pi}}$$

```
pcs0 = Simplify[pai * scs0 - pci * scs1]
```

$$\frac{2\ \text{ss}\ \sqrt{\zeta}\ \left(\text{F}_0\ \text{PA}_i - \text{F}_1\ \text{PC}_i\right)}{\sqrt{\pi}}$$

```
pcs1 = Simplify[pai * scs1 - pci * scs2]
```

$$\frac{2\ \text{ss}\ \sqrt{\zeta}\ \left(\text{F}_1\ \text{PA}_i - \text{F}_2\ \text{PC}_i\right)}{\sqrt{\pi}}$$

```
pcp0 = Simplify[pbj * pcs0 - pcj * pcs1 + (dij / 2 ζ) (scs0 - scs1)]
```

$$\frac{\text{ss}\ \sqrt{\zeta}\ \left(2\ \text{F}_2\ \text{PC}_i\ \text{PC}_j + \text{F}_0\ \left(2\ \text{PA}_i\ \text{PB}_j + \zeta\ \delta_{ij}\right) - \text{F}_1\ \left(2\ \text{PB}_j\ \text{PC}_i + 2\ \text{PA}_i\ \text{PC}_j + \zeta\ \delta_{ij}\right)\right)}{\sqrt{\pi}}$$