

```
do i = 1, num_atoms
  do j = 1, i
    zij = z(j) - z(i)
    zijsq = zij * zij
    pot_ij = volfactor * (sqrpialpha * exp(-zijsq*alphasq) &
      + pi * zij * erf(zij*alpha))
    V(j) = V(j) - q_elec(i) * pot_ij
    V(i) = V(i) - q_elec(j) * pot_ij
  end do
end do
```