

6.5.6 - CARBON ORBITALS EXPANDED IN STOs with vari

$$\text{NSTO}[l, \zeta] := \frac{(2 \zeta)^{3/2}}{\sqrt{(2l+2)!}} (2 \zeta)^l$$

$$\text{RSTO}[l, \zeta, r] := \text{NSTO}[l, \zeta] r^l \text{Exp}[-\zeta r]$$

$$\text{R1sA}[r] := \text{RSTO}[0, 5.58, r]$$

$$\text{R2sA}[r] := \text{RSTO}[1, 1.57, r]$$

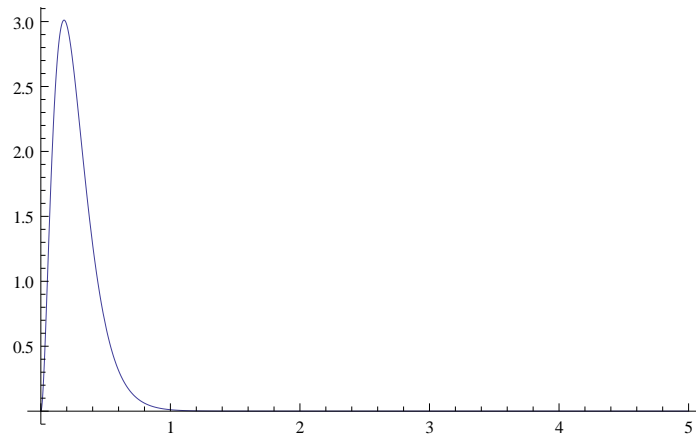
$$\text{R2pA}[r] := \text{RSTO}[1, 1.46, r]$$

$$\phi_{1sA}[r] := 0.998 \text{R1sA}[r] + 0.009 \text{R2sA}[r]$$

$$\phi_{2sA}[r] := -0.231 \text{R1sA}[r] + 1.024 \text{R2sA}[r]$$

$$\phi_{2pA}[r] := \text{R2pA}[r]$$

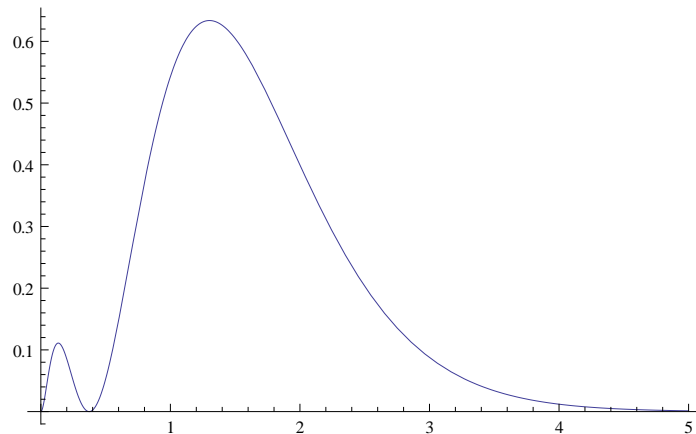
Plot[(r $\phi_{1sA}[r]$)², {r, 0, 5}, PlotRange → All]



Integrate[(r $\phi_{1sA}[r]$)², {r, 0, Infinity}]

0.999962

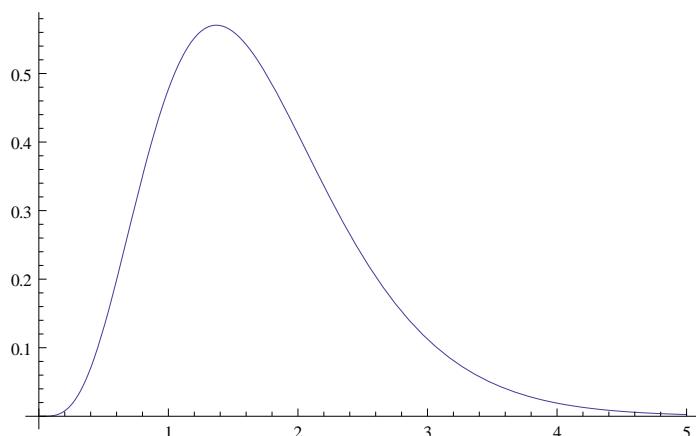
Plot[(r $\phi_{2sA}[r]$)², {r, 0, 5}, PlotRange → All]



Integrate[(r $\phi_{2sA}[r]$)², {r, 0, Infinity}]

0.999827

```
Plot[(r  $\phi_{2pA}[r]$ ) ^ 2, {r, 0, 5}, PlotRange -> All]
```



```
Integrate[(r  $\phi_{2pA}[r]$ ) ^ 2, {r, 0, Infinity}]
```

1.

6.5.7 - CARBON ORBITALS EXPANDED IN STOs with vari

```
 $\zeta_{1s1}$  = 9.2863;
```

```
 $\zeta_{1s2}$  = 5.4125;
```

```
 $\zeta_{2s1}$  = 4.2595;
```

```
 $\zeta_{2s2}$  = 2.5897;
```

```
 $\zeta_{2s3}$  = 1.5020;
```

```
 $\zeta_{2s4}$  = 1.0311;
```

```
 $C_{1s1s1}$  = 0.07657;
```

```
 $C_{1s1s2}$  = 0.92604;
```

```
 $C_{1s2s1}$  = 0.00210;
```

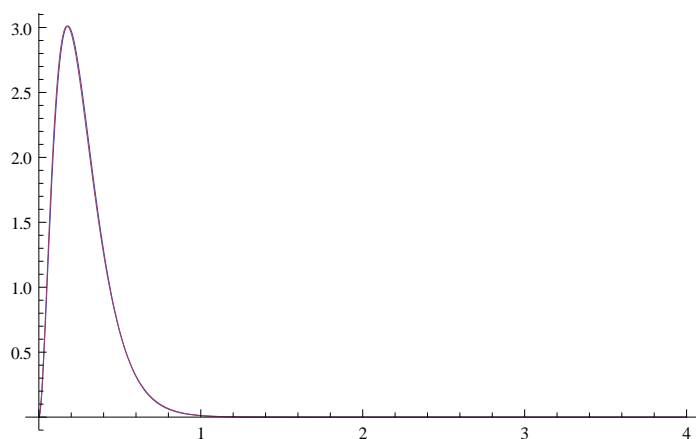
```
 $C_{1s2s2}$  = 0.00638;
```

```
 $C_{1s2s3}$  = 0.00167;
```

```
 $C_{1s2s4}$  = -0.00073;
```

```
 $\phi_{1sB}[r_] := C_{1s1s1}$  RSTO[0,  $\zeta_{1s1}$ , r] +  $C_{1s1s2}$  RSTO[0,  $\zeta_{1s2}$ , r] +  $C_{1s2s1}$  RSTO[1,  $\zeta_{2s1}$ , r] +  
 $C_{1s2s2}$  RSTO[1,  $\zeta_{2s2}$ , r] +  $C_{1s2s3}$  RSTO[1,  $\zeta_{2s3}$ , r] +  $C_{1s2s4}$  RSTO[1,  $\zeta_{2s4}$ , r]
```

```
Plot[{{(r  $\phi_{1sA}[r]$ ) ^ 2, (r  $\phi_{1sB}[r]$ ) ^ 2}, {r, 0, 4}, PlotRange -> All]
```



```
Integrate[(r  $\phi_{1sB}[r]$ ) ^ 2, {r, 0, Infinity}]
```

0.999995

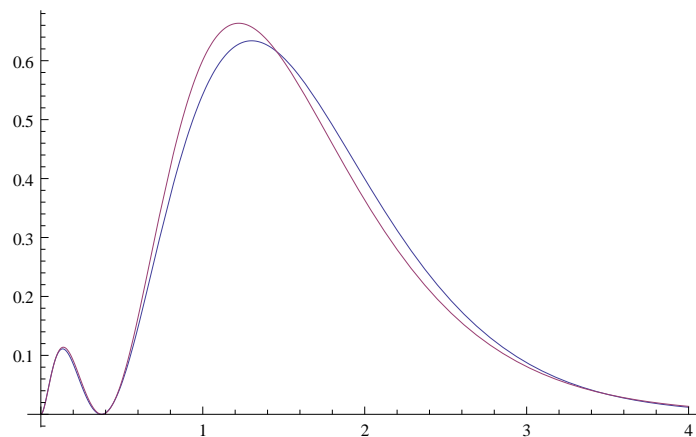
```

C2s1s1 = -0.01196;
C2s1s2 = -0.21041;
C2s2s1 = -0.13209;
C2s2s2 = 0.34624;
C2s2s3 = 0.74108;
C2s2s4 = 0.06495;

φ2sB[r_] := C2s1s1 RSTO[0, ζ1s1, r] + C2s1s2 RSTO[0, ζ1s2, r] + C2s2s1 RSTO[1, ζ2s1, r] +
  C2s2s2 RSTO[1, ζ2s2, r] + C2s2s3 RSTO[1, ζ2s3, r] + C2s2s4 RSTO[1, ζ2s4, r]

Plot[{(r φ2sA[r])^2, (r φ2sB[r])^2}, {r, 0, 4}, PlotRange -> All]

```



```
Integrate[(r φ2sB[r])^2, {r, 0, Infinity}]
```

```
0.999983
```

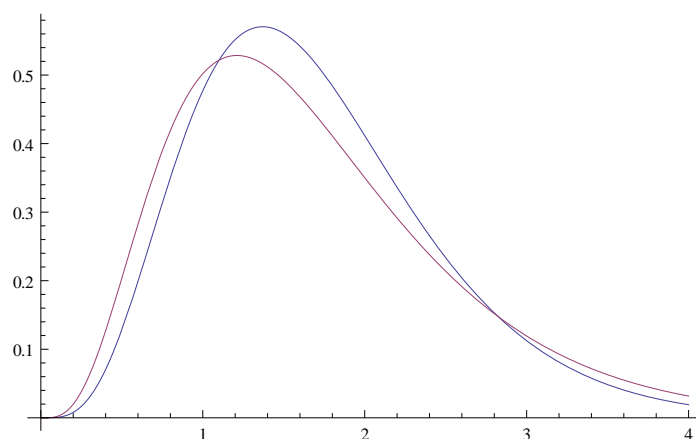
```

ζ2p1 = 6.3438;
ζ2p2 = 2.5873;
ζ2p3 = 1.4209;
ζ2p4 = 0.9554;
C2p2p1 = 0.01090;
C2p2p2 = 0.23563;
C2p2p3 = 0.57774;
C2p2p4 = 0.24756;

φ2pB[r_] := C2p2p1 RSTO[1, ζ2p1, r] +
  C2p2p2 RSTO[1, ζ2p2, r] + C2p2p3 RSTO[1, ζ2p3, r] + C2p2p4 RSTO[1, ζ2p4, r]

Plot[{(r φ2pA[r])^2, (r φ2pB[r])^2}, {r, 0, 4}, PlotRange -> All]

```



```
Integrate[(r φ2pB[r])^2, {r, 0, Infinity}]
```

```
1.
```

6.6.5 - CARBON ORBITALS EXPANDED IN SPHERICAL-T

$$\text{RGTO}[\alpha n l, l, r] := \frac{2 (2 \alpha n l)^{3/4}}{\pi^{1/4}} \sqrt{\frac{2^l}{(2 l + 1)!!}} (\sqrt{2 \alpha n l} r)^l \text{Exp}[-\alpha n l r^2]$$

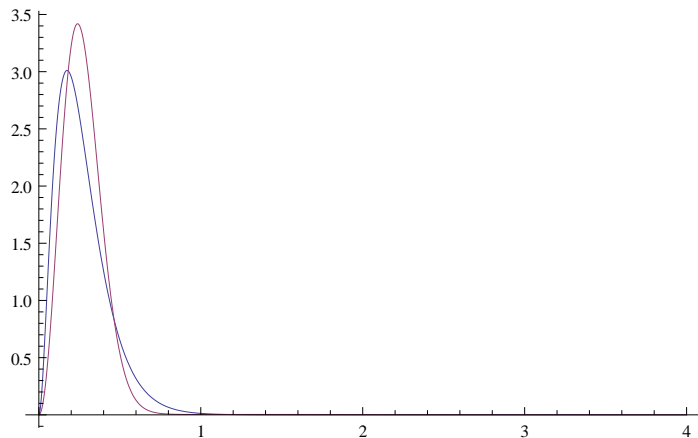
RGTO1s[r_] := RGTO[8.80, 0, r]

RGTO2s[r_] := RGTO[0.252, 0, r]

RGTO2p[r_] := RGTO[0.385, 1, r]

$\phi_{\text{GTO1s}}[r] := 0.982 \text{RGTO1s}[r] + 0.077 \text{RGTO2s}[r]$

Plot[{{($\phi_{1sB}[r] r$)², ($\phi_{\text{GTO1s}}[r] r$)²}, {r, 0, 4}, PlotRange -> All]

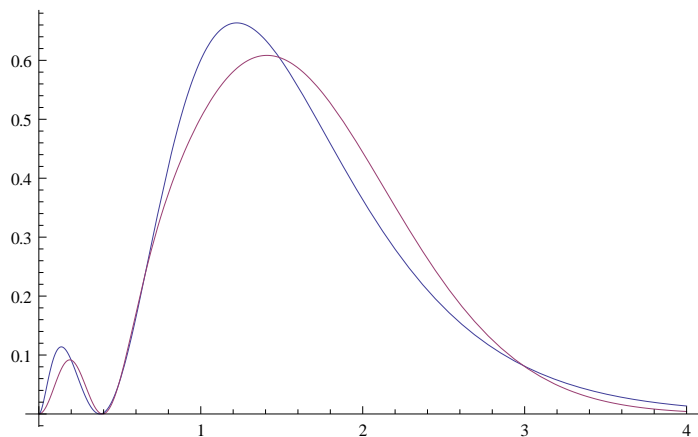


Integrate[($\phi_{\text{GTO1s}}[r] r$)², {r, 0, Infinity}]

0.998794

$\phi_{\text{GTO2s}}[r] := -0.266 \text{RGTO1s}[r] + 1.016 \text{RGTO2s}[r]$

Plot[{{($\phi_{2sB}[r] r$)², ($\phi_{\text{GTO2s}}[r] r$)²}, {r, 0, 4}, PlotRange -> All]

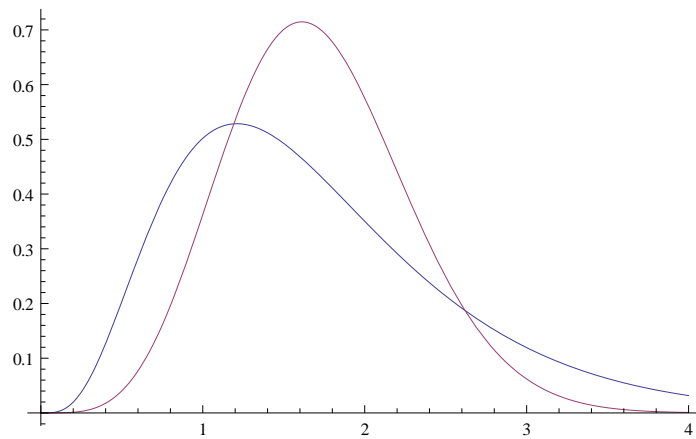


Integrate[($\phi_{\text{GTO2s}}[r] r$)², {r, 0, Infinity}]

1.001

$\phi_{\text{GTO2p}}[r] := \text{RGTO2p}[r]$

```
Plot[{(ϕ2pB[r] r)2, (ϕGTO2p[r] r)2}, {r, 0, 4}, PlotRange → All]
```



```
Integrate[(ϕGTO2p[r] r)2, {r, 0, Infinity}]
```

1.

8.2.2 - CARBON ORBITALS EXPANDED IN (9s5p) GTOs I

```
α11 = 4232.61;
```

```
α12 = 634.882;
```

```
α13 = 146.097;
```

```
α14 = 42.4974;
```

```
α15 = 14.1892;
```

```
α16 = 5.1477;
```

```
α17 = 1.9666;
```

```
α18 = 0.4962;
```

```
α19 = 0.1533;
```

```
C1s1 = 0.00122;
```

```
C1s2 = 0.00934;
```

```
C1s3 = 0.04534;
```

```
C1s4 = 0.15459;
```

```
C1s5 = 0.35867;
```

```
C1s6 = 0.43809;
```

```
C1s7 = 0.14581;
```

```
C1s8 = 0.00199;
```

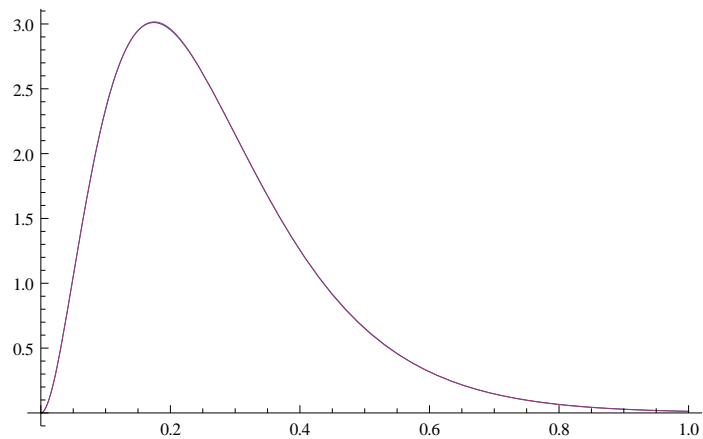
```
C1s9 = 0.00041;
```

```
ϕGTO1s9s5p[r_] := C1s1 RGTO[α11, 0, r] + C1s2 RGTO[α12, 0, r] +
```

```
  C1s3 RGTO[α13, 0, r] + C1s4 RGTO[α14, 0, r] + C1s5 RGTO[α15, 0, r] +
```

```
  C1s6 RGTO[α16, 0, r] + C1s7 RGTO[α17, 0, r] + C1s8 RGTO[α18, 0, r] + C1s9 RGTO[α19, 0, r]
```

```
Plot[{(\phi1sB[r] r)^2, (\phiGTO1s9s5p[r] r)^2}, {r, 0, 1}, PlotRange -> All]
```



```
Integrate[(\phiGTO1s9s5p[r] r)^2, {r, 0, Infinity}]
```

```
0.999924
```

```
C2s1 = -0.00026;
```

```
C2s2 = -0.00202;
```

```
C2s3 = -0.00974;
```

```
C2s4 = -0.03606;
```

```
C2s5 = -0.08938;
```

```
C2s6 = -0.17699;
```

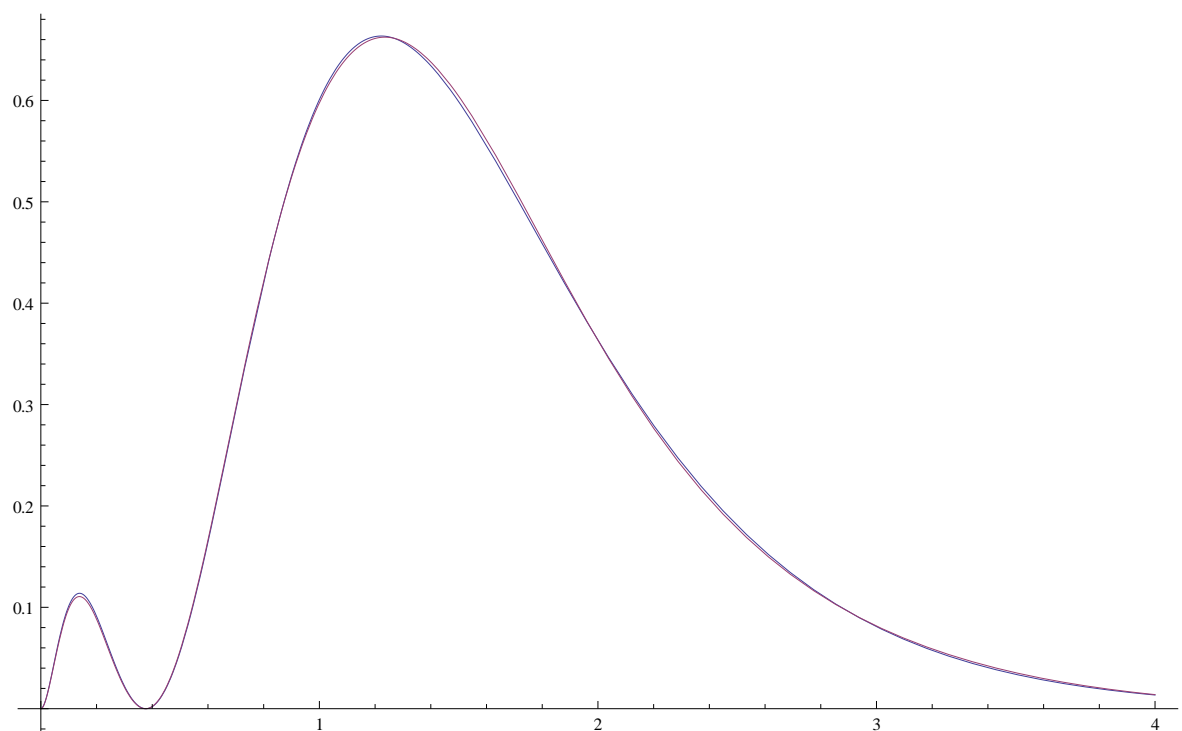
```
C2s7 = -0.05267;
```

```
C2s8 = 0.57408;
```

```
C2s9 = 0.54768;
```

```
\phiGTO2s9s5p[r_] := C2s1 RGTO[\alpha11, 0, r] + C2s2 RGTO[\alpha12, 0, r] +
  C2s3 RGTO[\alpha13, 0, r] + C2s4 RGTO[\alpha14, 0, r] + C2s5 RGTO[\alpha15, 0, r] +
  C2s6 RGTO[\alpha16, 0, r] + C2s7 RGTO[\alpha17, 0, r] + C2s8 RGTO[\alpha18, 0, r] + C2s9 RGTO[\alpha19, 0, r]
```

```
Plot[{(\phi2sB[r] r)^2, (\phiGTO2s9s5p[r] r)^2}, {r, 0, 4}, PlotRange -> All]
```



```
Integrate[( $\phi_{\text{GTO2s9s5p}}[r] r$ )2, {r, 0, Infinity}]
```

```
1.00001
```

```
 $\alpha_{21}$  = 18.1557;
```

```
 $\alpha_{22}$  = 3.9864;
```

```
 $\alpha_{23}$  = 1.1429;
```

```
 $\alpha_{24}$  = 0.3594;
```

```
 $\alpha_{25}$  = 0.1146;
```

```
C2p1 = 0.01469;
```

```
C2p2 = 0.09150;
```

```
C2p3 = 0.30611;
```

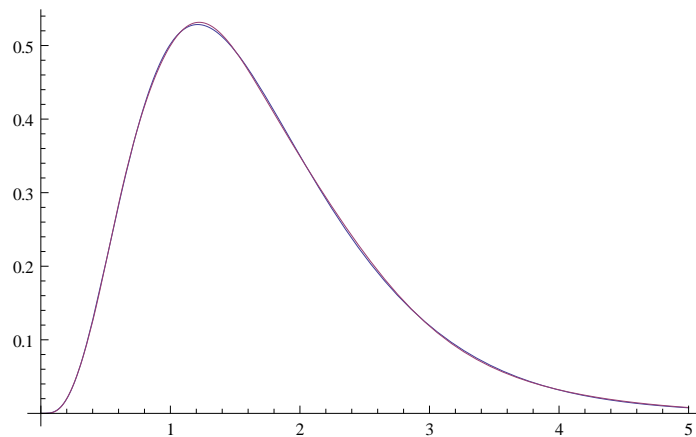
```
C2p4 = 0.50734;
```

```
C2p5 = 0.31735;
```

```
 $\phi_{\text{GTO2p9s5p}}[r_] :=$  C2p1 RGTO[ $\alpha_{21}$ , 1, r] + C2p2 RGTO[ $\alpha_{22}$ , 1, r] +
```

```
  C2p3 RGTO[ $\alpha_{23}$ , 1, r] + C2p4 RGTO[ $\alpha_{24}$ , 1, r] + C2p5 RGTO[ $\alpha_{25}$ , 1, r]
```

```
Plot[{( $\phi_{2pB}[r] r$ )2, ( $\phi_{\text{GTO2p9s5p}}[r] r$ )2}, {r, 0, 5}, PlotRange -> All]
```



```
Integrate[( $\phi_{\text{GTO2p9s5p}}[r] r$ )2, {r, 0, Infinity}]
```

```
0.999989
```

8.2.5 - CARBON ORBITALS EXPANDED IN (9s5p) GTOs I

```
 $\alpha_{31}$  = 4232.61;
```

```
 $\alpha_{32}$  = 634.882;
```

```
 $\alpha_{33}$  = 146.097;
```

```
 $\alpha_{34}$  = 42.4974;
```

```
 $\alpha_{35}$  = 14.1892;
```

```
 $\alpha_{36}$  = 1.9666;
```

```
 $\alpha_{37}$  = 5.1477;
```

```
 $\alpha_{38}$  = 0.4962;
```

```
 $\alpha_{39}$  = 0.1533;
```

```
C3s1 = 0.002029;
```

```
C3s2 = 0.015535;
```

```
C3s3 = 0.075411;
```

```
C3s4 = 0.257121;
```

```
C3s5 = 0.596555;
```

```
C3s6 = 0.242517;
```

```
C3s7 = 1.000000;
```

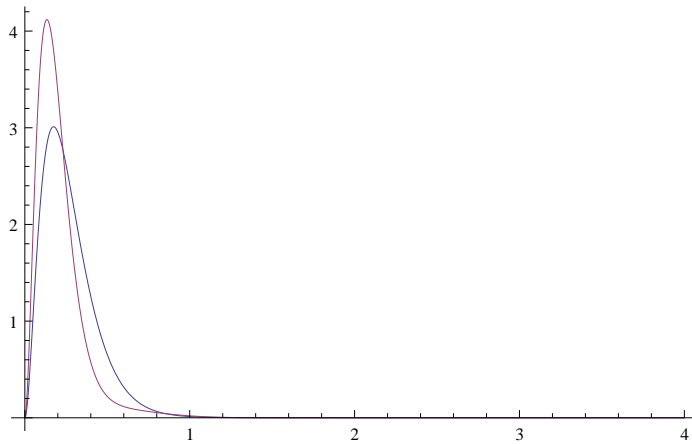
```
C3s8 = 0.542048;
```

```
C3s9 = 0.517121;
```

```

χGTO1s9s5p[r_] := C3s1 RGTO[α31, 0, r] + C3s2 RGTO[α32, 0, r] +
  C3s3 RGTO[α33, 0, r] + C3s4 RGTO[α34, 0, r] + C3s5 RGTO[α35, 0, r] + C3s6 RGTO[α36, 0, r]
Plot[{{(φ1sB[r] r)^2, (χGTO1s9s5p[r] r)^2}, {r, 0, 4}, PlotRange -> All]

```



```
Integrate[(χGTO1s9s5p[r] r)^2, {r, 0, Infinity}]
```

1.

```

C4s1 = 0.002029;
C4s2 = 0.015535;
C4s3 = 0.075411;
C4s4 = 0.257121;
C4s5 = 0.596555;
C4s6 = 0.242517;
C4s7 = 1.000000;
C4s8 = 1.000000;
C4s9 = 1.000000;

```

```
χGTO2s9s5p[r_] := RGTO[α37, 0, r]
```

```
Integrate[(χGTO2s9s5p[r] r)^2, {r, 0, Infinity}]
```

1.

```

C5s1 = 0.006228;
C5s2 = 0.047676;
C5s3 = 0.231439;
C5s4 = 0.789108;
C5s5 = 0.791751;
C5s6 = 0.321870;
C5s7 = 1.000000;
C5s8 = 1.000000;
C5s9 = 1.000000;

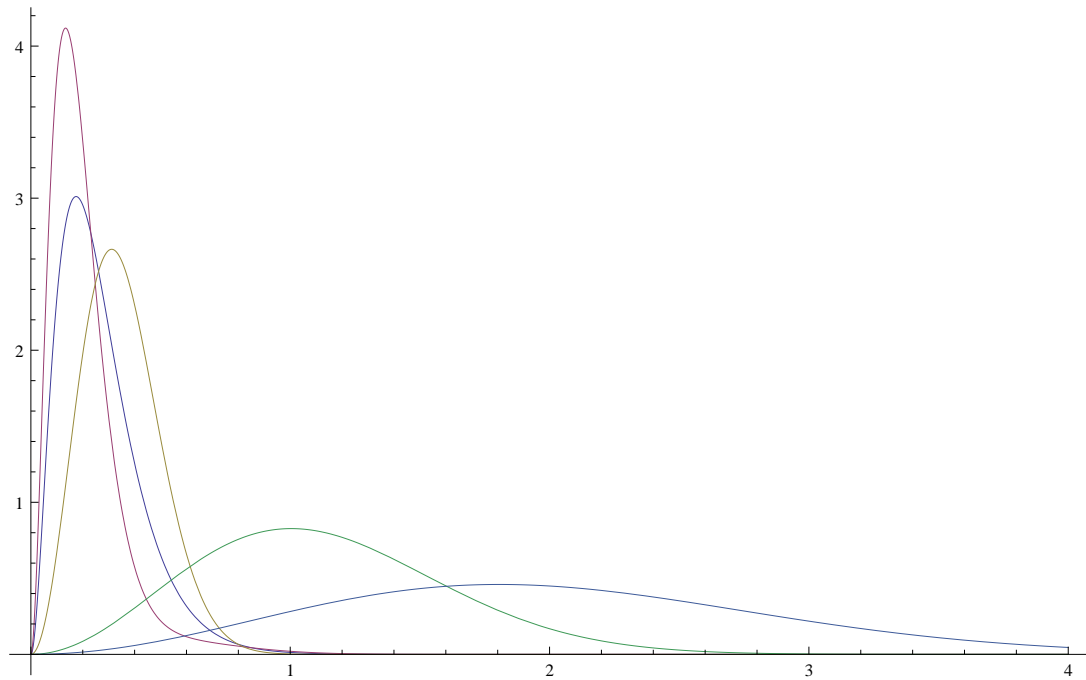
```

```
χGTO3s9s5p[r_] := RGTO[α38, 0, r]
```

```
χGTO4s9s5p[r_] := RGTO[α39, 0, r]
```



```
Plot[{{(phi1sB[r] r)^2, (chiGT01s9s5p[r] r)^2, (chiGT02s9s5p[r] r)^2,
      (chiGT03s9s5p[r] r)^2, (chiGT04s9s5p[r] r)^2}, {r, 0, 4}, PlotRange -> All]
```



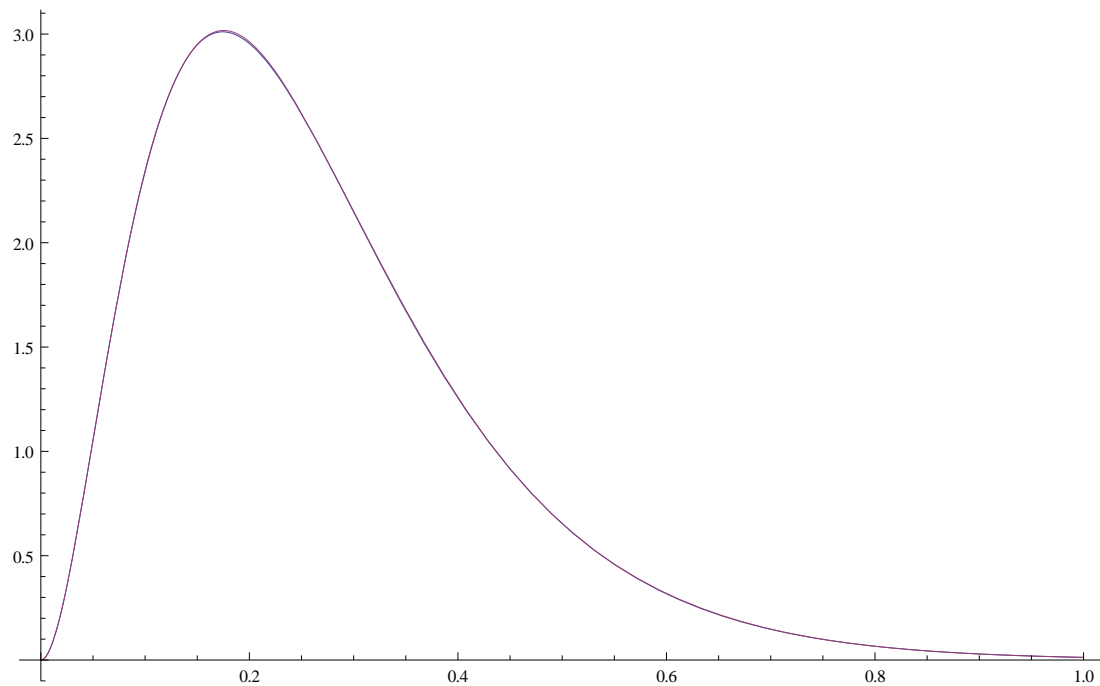
```
Integrate[(chiGT03s9s5p[r] r)^2, {r, 0, Infinity}]
```

1.

```
phiCGT01s4s2p[r_] :=
```

```
0.601 chiGT01s9s5p[r] + 0.438 chiGT02s9s5p[r] + 0.005 chiGT03s9s5p[r] + 0.001 chiGT04s9s5p[r]
```

```
Plot[{{(phi1sB[r] r)^2, (phiCGT01s4s2p[r] r)^2}, {r, 0, 1}, PlotRange -> All]
```



```

α21 = 18.1557;
α22 = 3.9864;
α23 = 1.1429;
α24 = 0.3594;
α25 = 0.1146;
C22p1 = 0.018534;
C22p2 = 0.115442;
C22p3 = 0.386206;
C22p4 = 0.640089;
C22p5 = 1.0;

C3p1 = 0.039196;
C3p2 = 0.244144;
C3p3 = 0.816775;
C3p4 = 1.0;
C3p5 = 1.0;

```

```

χGT01p4s2p[r_] :=
  C22p1 RGTO[α21, 1, r] + C22p2 RGTO[α22, 1, r] + C22p3 RGTO[α23, 1, r] + C22p4 RGTO[α24, 1, r]

```

```

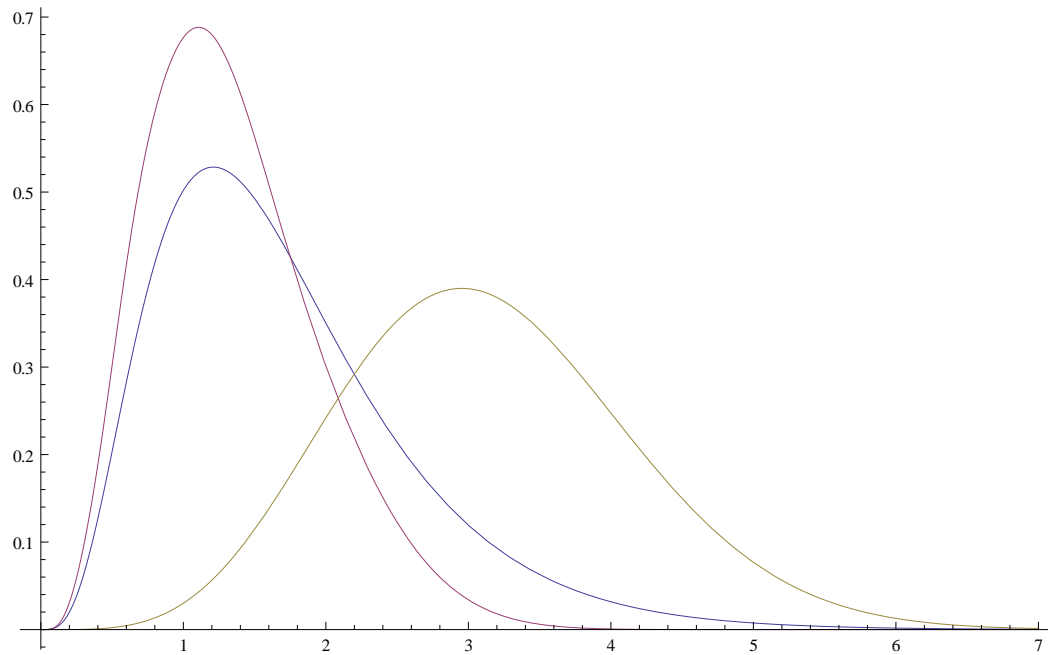
χGT02p4s2p[r_] := C22p5 RGTO[α25, 1, r]

```

```

Plot[{(φ2pB[r] r)^2, (χGT01p4s2p[r] r)^2, (χGT02p4s2p[r] r)^2}, {r, 0, 7}, PlotRange -> All]

```

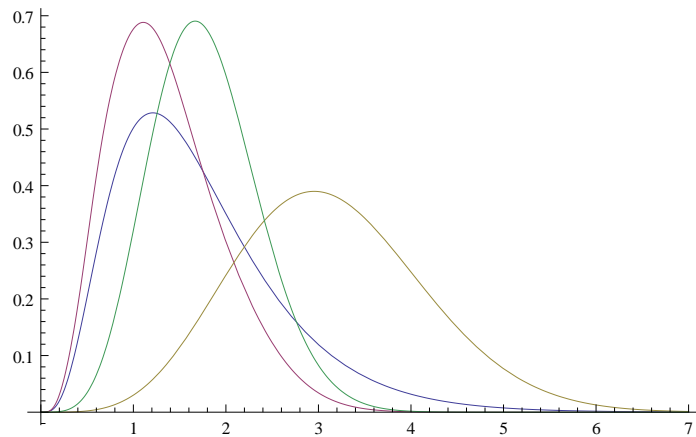


```

χGT02p4s2ptest[r_] := 1.0 RGTO[α24, 1, r]

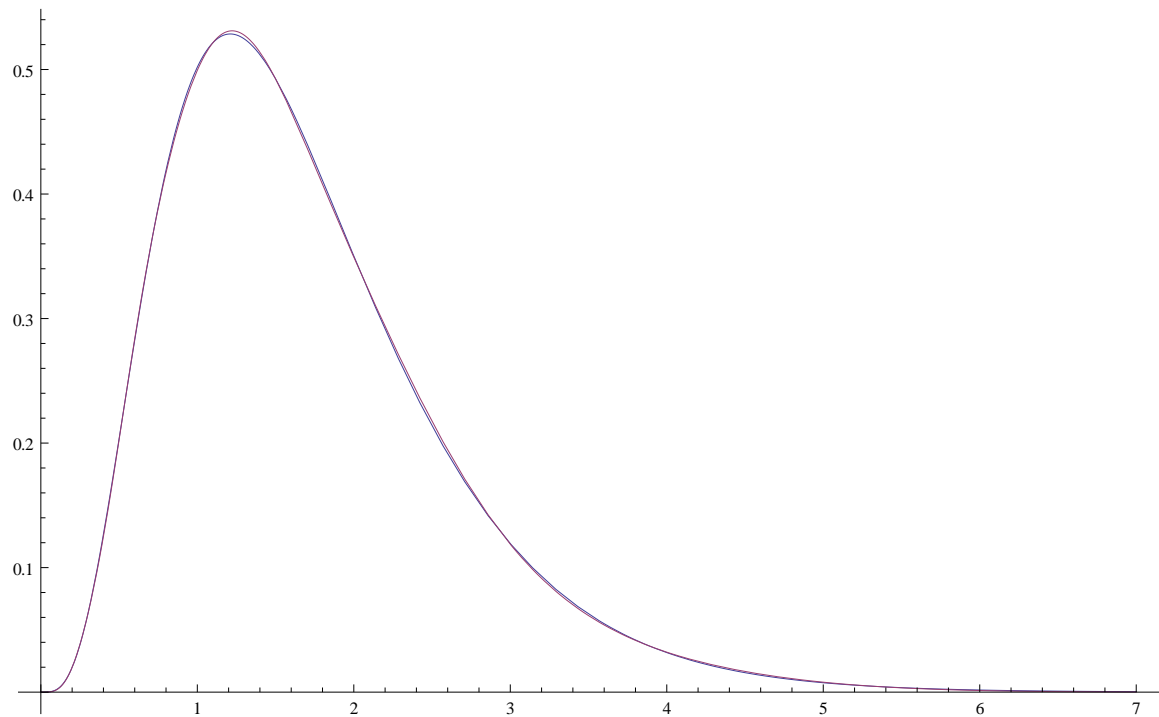
```

```
Plot[{(\phi_{2pB}[r] r)^2, (\chi_{GTO1p4s2p}[r] r)^2, (\chi_{GTO2p4s2p}[r] r)^2, (\chi_{GTO2p4s2ptest}[r] r)^2},
{r, 0, 7}, PlotRange -> All]
```



```
\phi_{CGTO2p4s2p}[r_] := 0.792 \chi_{GTO1p4s2p}[r] + 0.318 \chi_{GTO2p4s2p}[r]
```

```
Plot[{(\phi_{2pB}[r] r)^2, (\phi_{CGTO2p4s2p}[r] r)^2}, {r, 0, 7}, PlotRange -> All]
```



```
\phi_{CGTO2s4s2p}[r_] :=
```

```
-0.142 \chi_{GTO1s9s5p}[r] - 0.195 \chi_{GTO2s9s5p}[r] + 0.562 \chi_{GTO3s9s5p}[r] + 0.553 \chi_{GTO4s9s5p}[r]
```

```
Plot[{(\phi_{2sB}[r] r)^2, (\phi_{CGTO2s4s2p}[r] r)^2}, {r, 0, 7}, PlotRange -> All]
```

