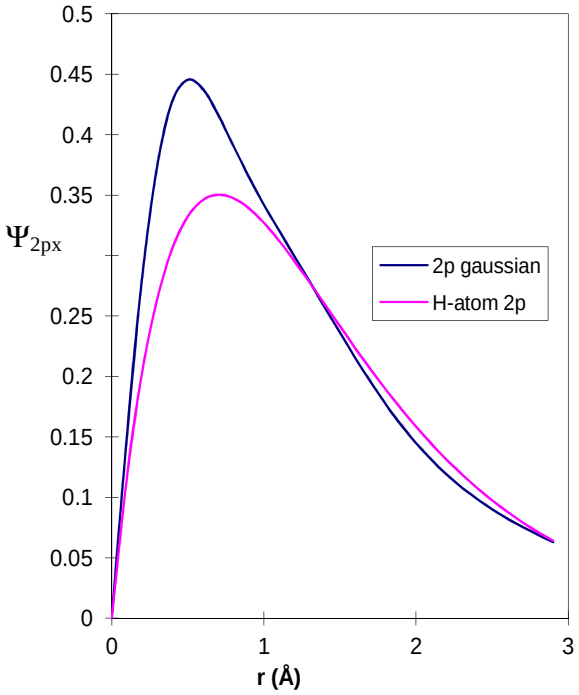
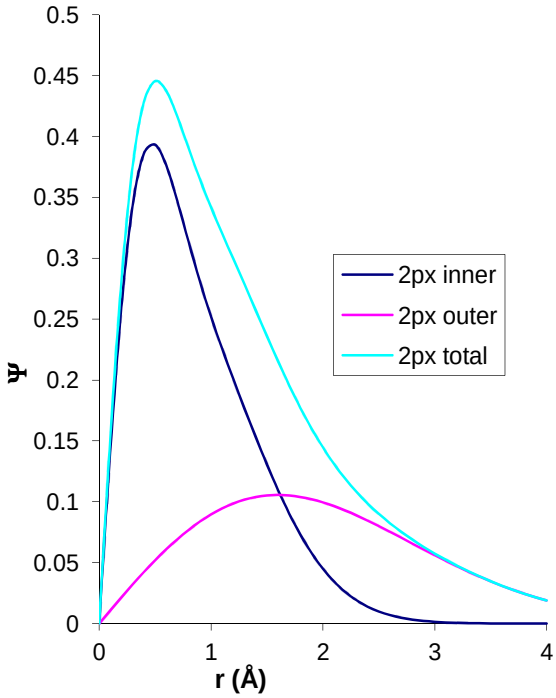
Carbon Atom Gaussian Atomic Orbitals

$2p_X$ orbital with $Z_{eff} = 1.5$ for the Hydrogen-like orbital along the x-axis





Carbon 3-21G basis set as listed in Gaussian94.

	α_i (Å^{-1})	d_{si}	d_{xi}
C			
S	3 1.00		
	0.1722560000D+03	0.6176690000D-01	
	0.2591090000D+02	0.3587940000D+00	
	0.5533350000D+01	0.7007130000D+00	
SP	2 1.00		
	0.3664980000D+01	-0.3958970000D+00	0.2364600000D+00
	0.7705450000D+00	0.1215840000D+01	0.8606190000D+00
SP	1 1.00		
	0.1958570000D+00	0.1000000000D+01	0.1000000000D+01

$\Psi_{2px}(\text{inner}) = 0.2365\ g_X(3.665,r) + 0.8606\ g_X(0.771,r)$

$\Psi_{2px}(\text{outer}) = 1.00\ g_X(0.196,r)$

$\Psi_{2px} = 0.55646\ \Psi_{2px}(\text{inner}) + 0.58708\ \Psi_{2px}(\text{outer})$

Even though we are comparing the Gaussian orbitals with H-atom style orbitals, note that the H-atom orbitals are **not** the correct orbitals for **any** multi-electron atom.