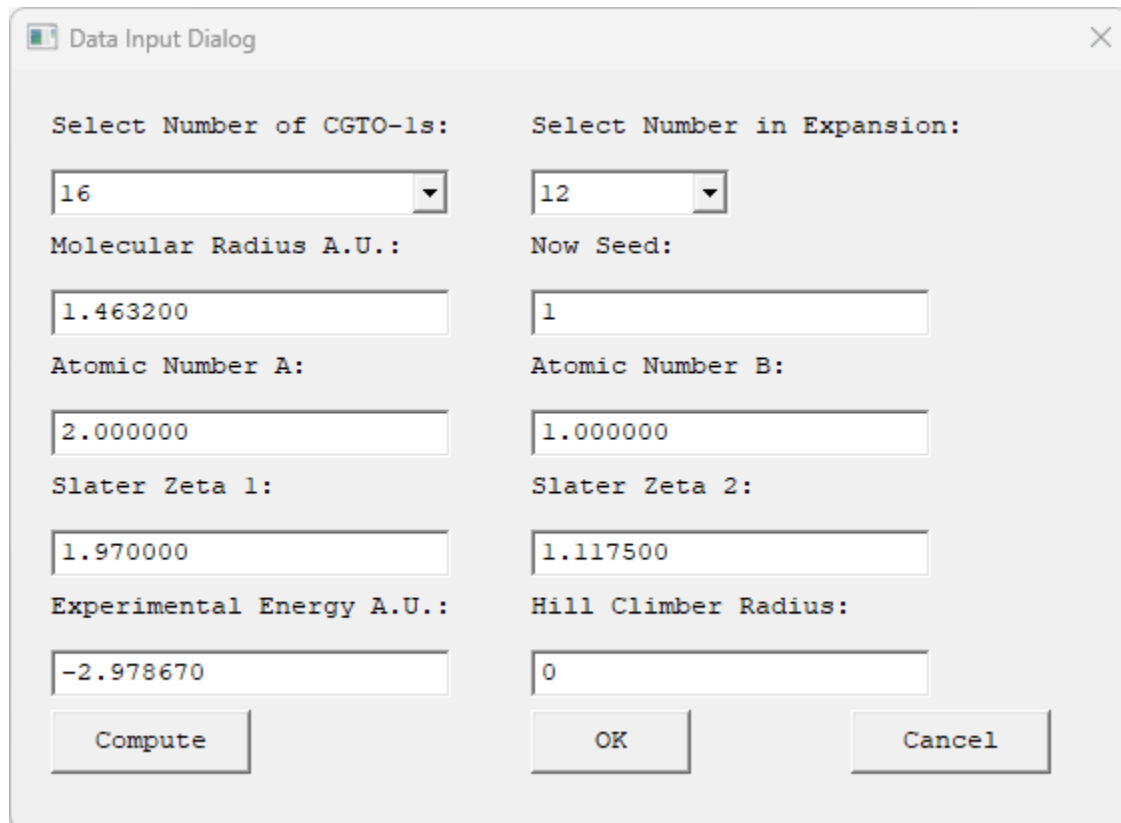


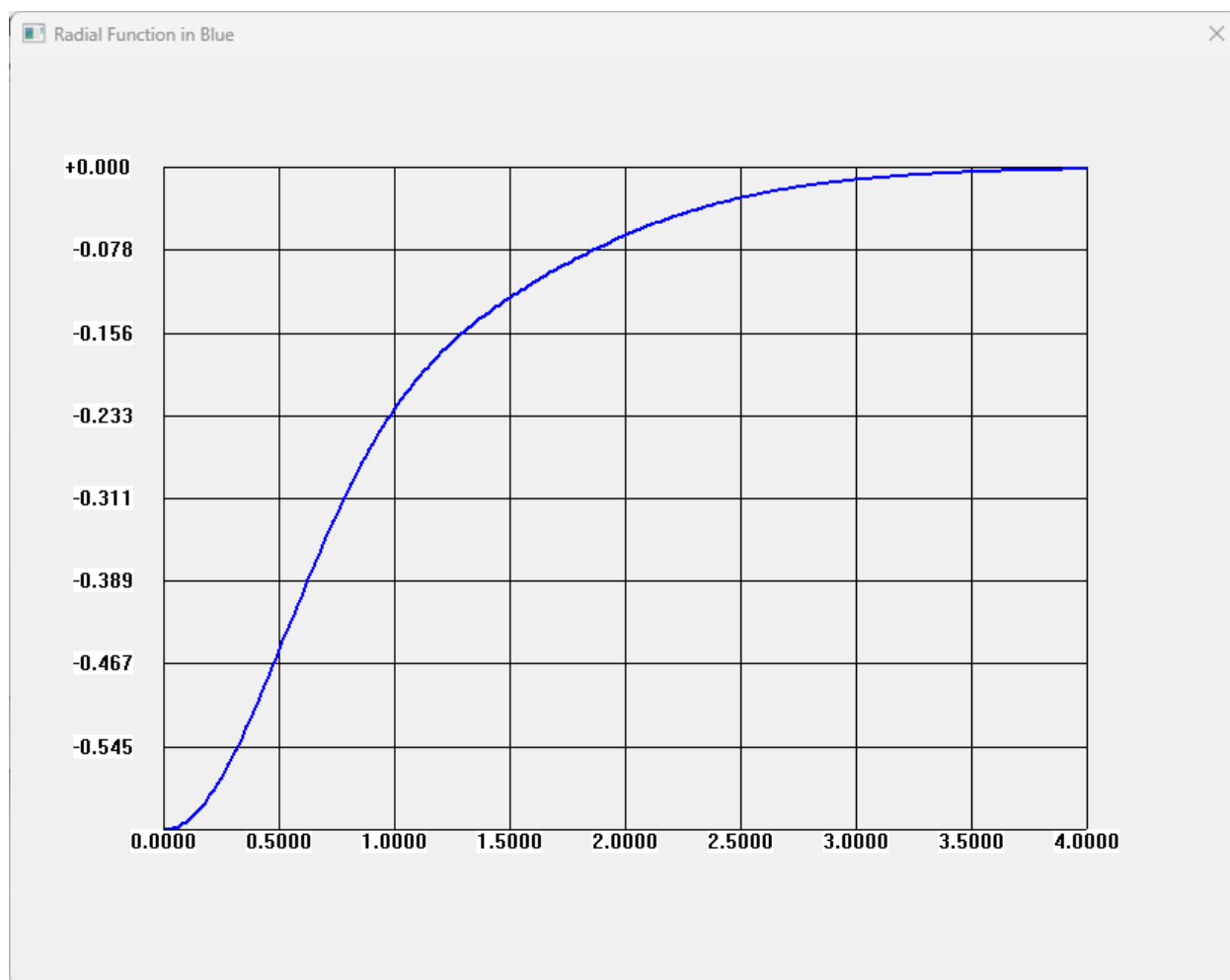
Blog Entry © Sunday, August 24, 2025, by James Pate Williams, Jr. Corrections to New Quantum Chemical Total Molecular Ground-State Energies for the Helium Hydride Cation (a Hetero Nuclear molecule) and the Hydrogen Molecule (a Homo Nuclear Molecule)

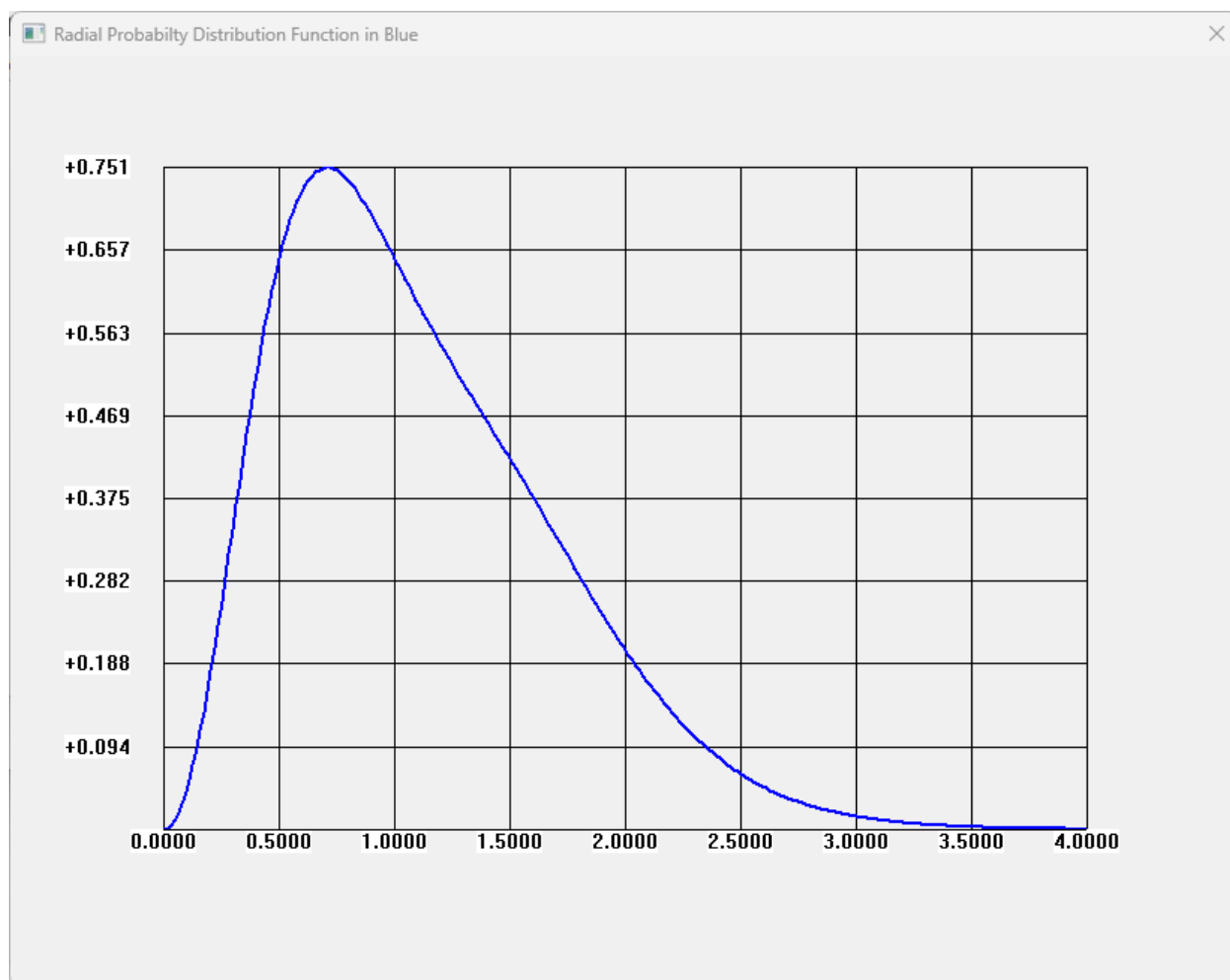
The first four pages are for helium hydride also known as the helium-hydrogen molecular ion (cation) or hydro-helium:



A screenshot of a 'Data Input Dialog' window. The window has a title bar with a green icon and a close button. It contains two columns of input fields. The left column has labels: 'Select Number of CGTO-1s:', 'Molecular Radius A.U.:', 'Atomic Number A:', 'Slater Zeta 1:', and 'Experimental Energy A.U.:'. The right column has labels: 'Select Number in Expansion:', 'Now Seed:', 'Atomic Number B:', 'Slater Zeta 2:', and 'Hill Climber Radius:'. At the bottom, there are three buttons: 'Compute', 'OK', and 'Cancel'.

Parameter	Value
Select Number of CGTO-1s:	16
Molecular Radius A.U.:	1.463200
Atomic Number A:	2.000000
Slater Zeta 1:	1.970000
Experimental Energy A.U.:	-2.978670
Select Number in Expansion:	12
Now Seed:	1
Atomic Number B:	1.000000
Slater Zeta 2:	1.117500
Hill Climber Radius:	0





Tabular Data

Coefficient	Exponent
-0.2973313847	1.5732503608
-0.0886162593	0.4012384272
-0.7498583117	0.7506017658
-0.2195240891	1.7800956781
+0.0323230688	1.5838029656
-0.3720876739	0.2608863793
-0.2670720158	0.4362224893
-0.3612747124	0.9002464775
+0.8029632368	1.2485599268
+0.7357321178	0.9032906615
-0.4287687746	1.6663274257
+0.0112803175	1.2929422434

Slater Zeta 1 = 1.9700000000

Slater Zeta 2 = 1.1175000000

Electronic Energy = -4.3422295086

Total Energy = -2.9753623681

Exp Energy = -2.9786700000

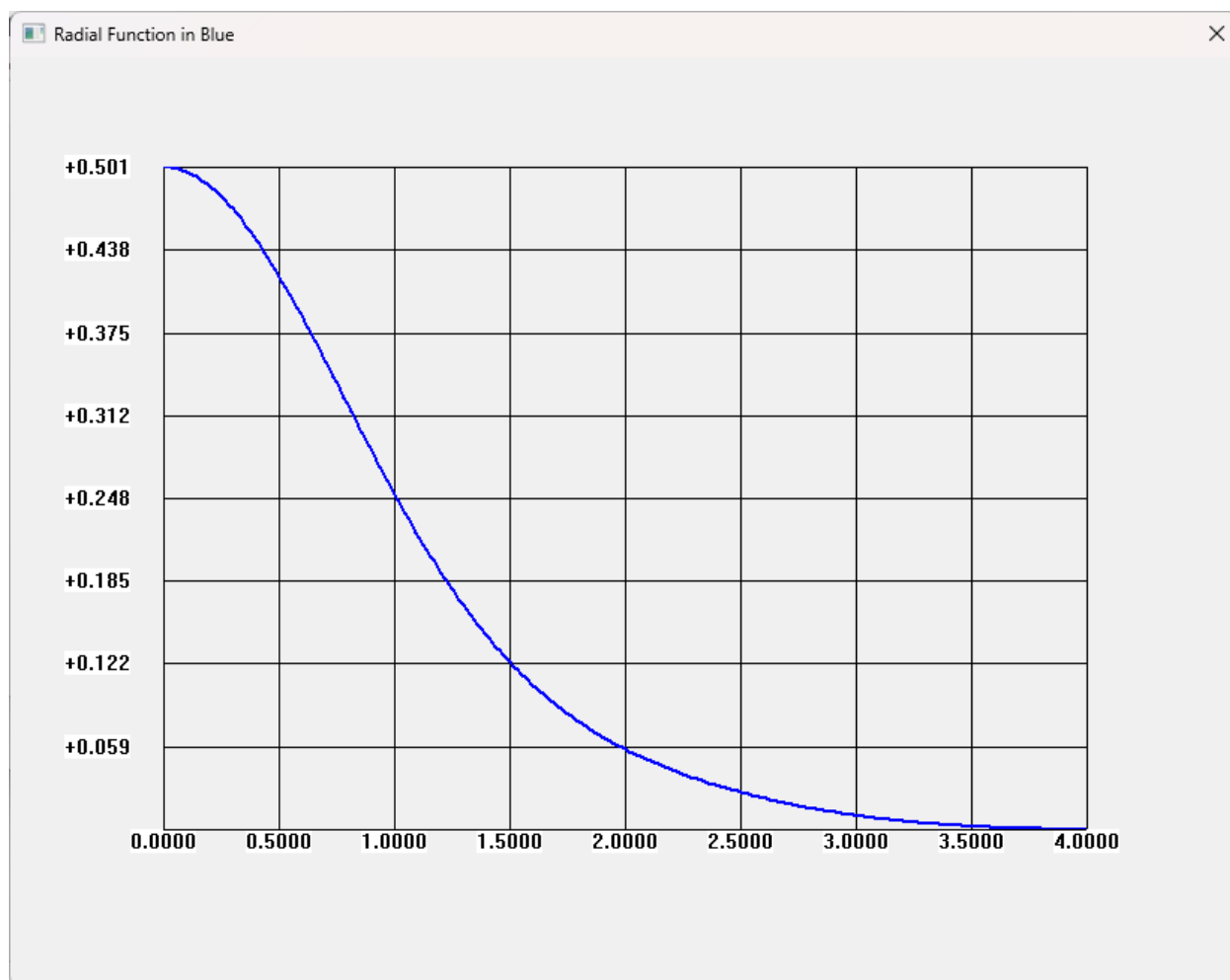
Percent Error = 0.1110439178

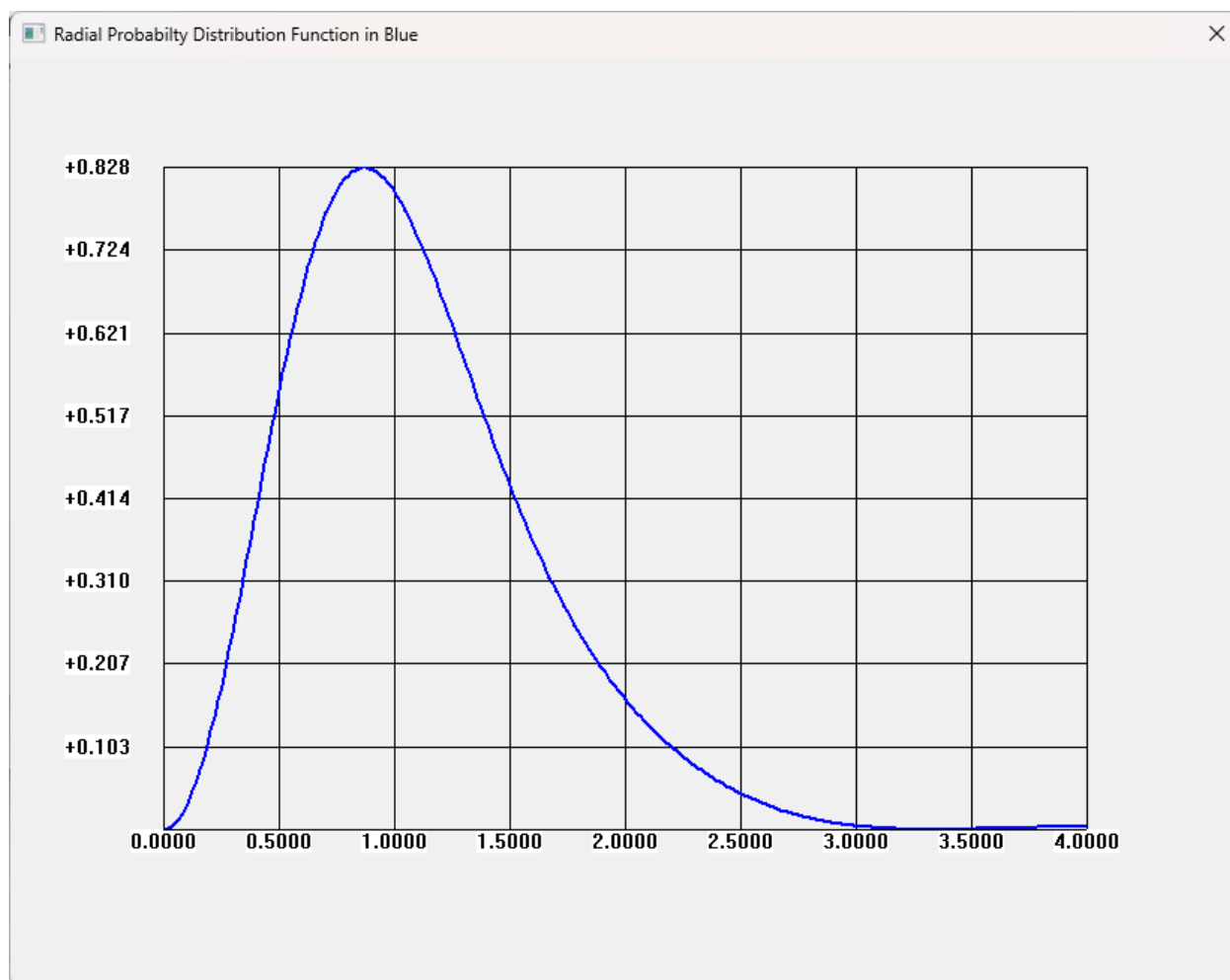
Runtime Millis = 234

The next four pages are for the hydrogen molecule:

Data Input Dialog

Select Number of CGTO-1s:	Select Number in Expansion:
16	12
Molecular Radius A.U.:	Now Seed:
1.401100	1
Atomic Number A:	Atomic Number B:
1.000000	1.000000
Slater Zeta 1:	Slater Zeta 2:
0.887900	0.887900
Experimental Energy A.U.:	Hill Climber Radius:
-1.174476	0
Compute	OK
	Cancel





Tabular Data		X	
Coefficient	Exponent		
-0.6981456844	0.7631405669		
+1.1004293377	0.2371470363		
+0.0116857227	0.2575769983		
+1.0245058221	0.1815604970		
+0.5330934849	0.8136767553		
+0.0743113448	0.8425966925		
+1.0554124393	0.8318454340		
-0.1597587538	0.5690597811		
-0.3929707770	0.2018283134		
-0.1275095561	0.7604624330		
-0.2314129955	0.7248385067		
-1.0990897098	0.1424337116		
Slater Zeta 1 =		0.8879000000	
Slater Zeta 2 =		0.8879000000	
Electronic Energy =		-1.8476700669	
Total Energy =		-1.1339451365	
Exp Energy =		-1.1744760000	
Percent Error =		3.4509741779	
Runtime Millis =		292	