Blog Entry Friday, March 7, 2025, by James Pate Williams, Jr.

Hydrogen Molecule Results
(Parameters of the Gaussians from file >):

(Number of Gaussians >): 3
Gaussian # 0 1.0e-7
Gaussian # 1 2.0e-7
Gaussian # 2 3.0e-7
(H2 distance(a.u.) : Min >>): 1.398397231548386
(H2 distance(a.u.) : Max >>): 1.998397231548386
(H2 distance(a.u.) : Step >>): 0.1
(d electron, nuclear, total (Hartree) and binding (eV) energy):

1.398397	0.456743	0.715104	1.171847	29.549715
1.498397	0.456743	0.667380	1.124122	28.900383
1.598397	0.456743	0.625627	1.082369	28.332299
1.698397	0.456742	0.588790	1.045533	27.831112
1.798397	0.456742	0.556051	1.012793	27.385661
1.898397	0.456742	0.526760	0.983503	26.987140
1.998397	0.456742	0.500401	0.957143	26.628502

C:\Users\James\source\repos\H2_HF_Gauss\x64\Debug\H2_HF_Gauss.exe (process 4320) exited with code 0 (0x0).
Press any key to close this window . . .

Hydrogen Molecular Ion Results
(Parameters of the Gaussians from file >):

(Number of Gaussians >): 3
Gaussian # 0 1.27
Gaussian # 1 2.27
Gaussian # 2 3.27
(H2 distance(a.u.) : Min >>): 1.9971934
(H2 distance(a.u.) : Max >>): 1.9991934
(H2 distance(a.u.) : Step >>): 0.001
(d electron, nuclear, total (Hartree) and binding (eV) energy):

1.997193	0.101806	0.500703	0.602509	15.000513
1.998193	0.102453	0.500452	0.602905	15.005909
1.999193	0.103099	0.500202	0.603301	15.011293

C:\Users\James\source\repos\H2_HF_Gauss\x64\Debug\H2_HF_Gauss.exe (process 31184) exited with code 0 (0x0).
Press any key to close this window . . .

These numbers compare well with the research paper:

1509.00477

From the paper hydrogen molecule -1.73427 and hydrogen molecular ion -0.602501700.