

STO-1G for Atomic Numbers 1 and 1

R = Rab = 1.401100e+00

Zeta 1 = 1.240000e+00 Zeta 2 = 1.240000e+00

Overlap integral = 4.221463e-01

Kinetic energy integrals:

t11 = +6.249191e-01 t12 = +3.019920e-01

t21 = +3.019920e-01 t22 = +6.249191e-01

Potential energy integrals on center A:

v11-A = -1.029998e+00 v12-A = -6.014846e-01

v21-A = -6.014846e-01 v22-A = -6.634196e-01

Potential energy integrals on center B:

v11-B = -6.634196e-01 v12-B = -6.014846e-01

v21-B = -6.014846e-01 v22-B = -1.029998e+00

Direct and exchange integrals:

v[1, 1, 1, 1] = 7.283185e-01 v[2, 1, 1, 1] = 4.528791e-01

v[2, 1, 2, 1] = 3.214666e-01 v[2, 2, 1, 1] = 5.703512e-01

v[2, 2, 2, 1] = 4.528791e-01 v[2, 2, 2, 2] = 7.283185e-01

Overlap integral = 4.221463e-01

Kinetic energy integrals:

T11 = +6.249191e-01 T12 = +3.019920e-01

T21 = +3.019920e-01 T22 = +6.249191e-01

Potential energy integrals on center A:

V11-A = -1.029998e+00 V12-A = -6.014324e-01

V21-A = -6.014324e-01 V22-A = -6.634085e-01

Potential energy integrals on center B:

V11-B = -6.634085e-01 V12-B = -6.014324e-01

V21-B = -6.014324e-01 V22-B = -1.029998e+00

Direct and exchange integrals:

V[1, 1, 1, 1] = 7.283185e-01 V[2, 1, 1, 1] = 4.528205e-01

V[2, 1, 2, 1] = 3.214666e-01 V[2, 2, 1, 1] = 5.703248e-01
V[2, 2, 2, 1] = 4.528205e-01 V[2, 2, 2, 2] = 7.283185e-01

Comparison of Two Error Functions

ERF from Abramowitz and Stegun

erf from C Translation of NUMAL by H. T. Lau

Difference below is the percent difference

x	ERF	erf	Difference
0.000000	0.000000	0.000000	0.000000
0.100000	0.112492	0.112463	0.025545
0.200000	0.222750	0.222703	0.021135
0.300000	0.328684	0.328627	0.017486
0.400000	0.428454	0.428392	0.014386
0.500000	0.520561	0.520500	0.011733
0.600000	0.603913	0.603856	0.009473
0.700000	0.677853	0.677801	0.007569
0.800000	0.742145	0.742101	0.005985
0.900000	0.796946	0.796908	0.004684
1.000000	0.842731	0.842701	0.003628