

```
1 using System;
2
3 namespace InteractionEnergies
4 {
5     public class RadialWaveFunction
6     {
7         // SI Units from NIST website
8
9         public double alpha = 1.0 / 137.0;
10        public double c = 299792458;
11        public double h = 6.62607015e-34;
12        public double hbar = 1.054571817e-34;
13        public double me = 9.1093837015e-31;
14        public double mn = 1.67492749804e-27;
15        public double mp = 1.67262192369e-27;
16        public double e = 1.602176634e-19;
17        public double e0 = 8.8541878128e-12;
18
19        // constants are updated from Schiff's
20        // cgs system numbers found in the
21        // first page of his "Quantum Mechanics"
22
23        public double e_schiff = 4.806529902e-10;
24        public double hbar_schiff = 1.054571817e-27;
25        public double me_schiff = 0.91093837015e-27;
26        public double mn_schiff = 1.674927498045e-24;
27        public double mp_schiff = 1.67262192369e-24;
28
29        public double a_mu_schiff_unscaled(double mu)
30        {
31            return hbar_schiff * hbar_schiff / (mu * e_schiff * e_schiff);
32        }
33
34        public double a_mu_schiff_scaled(double mu)
35        {
36            return 1.0e8 * a_mu_schiff_unscaled(mu);
37        }
38
39        public double En_schiff_unscaled(double amu, int Z, int n)
40        {
41            return -Z * Z * e_schiff * e_schiff
42                / (2.0 * amu * n * n);
43        }
44
45        public double En_schiff_scaled(double amu, int Z, int n)
46        {
47            return 6.24150907446076e11 * En_schiff_unscaled(amu, Z, n);
48        }
49
50        public double a_mu_SI_Units_unscaled(double mu, int Z)
51        {
52            return 4.0 * Math.PI * e0 * hbar * hbar / (mu * Z * e * e);
```

```
53     }
54
55     public double a_mu_SI_Units_scaled(double mu, int Z)
56     {
57         return 1e-10 * a_mu_SI_Units_unscaled(mu, Z);
58     }
59
60     public double En_SI_Units_unscaled(double amu, double mu, int Z, int n)
61     {
62         return -Z * Z * mu * e * e * e * e /
63             (8.0 * n * n * h * h * e0 * e0);
64     }
65
66     public double En_SI_Units_scaled(double amu, double mu, int Z, int n)
67     {
68         return 6.24150907446076e18 * En_SI_Units_unscaled(amu, mu, Z, n);
69     }
70
71     public double Mu(double m, double M)
72     {
73         return (m * M) / (m + M);
74     }
75
76     public double Factorial(int n)
77     {
78         double nfact = 1.0;
79
80         for (int i = 2; i <= n; i++)
81             nfact *= i;
82
83         return nfact;
84     }
85
86     // Associated Laguerre Functions
87     // https://mathworld.wolfram.com/AssociatedLaguerrePolynomial.html
88
89     public double Laguerre(double rho, int n, int l)
90     {
91         double sum = 0.0;
92
93         for (int k = 0; k <= n - l - 1; k++)
94         {
95             double factor1 = Math.Pow(-1, k + 2 * l + 1);
96             double factor2 = Factorial(n + l);
97             double factor3 = Math.Pow(rho, k);
98             double numer = factor1 * factor2 * factor2 * factor3;
99             double factor4 = Factorial(n - l - 1 - k);
100             double factor5 = Factorial(2 * l + 1 + k);
101             double factor6 = Factorial(k);
102             double denom = factor4 * factor5 * factor6;
103
104             sum += numer / denom;
```

```
105     }
106
107     return sum;
108 }
109
110 public double Rnl(double amu, double r, int n, int l, int Z)
111 {
112     double factor1 = 2.0 * Z / (n * amu);
113     double rho = factor1 * r;
114     double factor2 = Math.Pow(factor1, 3.0);
115     double numer = Factorial(n - l - 1);
116     double denom = 2.0 * n * Math.Pow(Factorial(n + l), 3.0);
117     double factor3 = Math.Sqrt(factor2 * numer / denom);
118     double factor4 = Math.Exp(-0.5 * rho) * Math.Pow(rho, l);
119     double factor5 = Laguerre(rho, n, l);
120
121     factor5 = -factor3 * factor4 * factor5;
122
123     return factor5;
124 }
125 }
126 }
```