```
(*Ne-Atom and homologues 1s(2)2s(2) 2p(6), all p equal size, with
exchange correction page 40; 25.12.2012*)
```

In[69]:=
```
Clear[z, sig]; sig = 0.24;
T = 9 / (4 * P^2) + 9 * 4 / (4 * Q^2) + 12 / R^2;
Vne = -3 * z / P - 3 * z / Q - 6 * z / R;
Vee = (2 / Q) * (3 - (6 / 10) * (P / Q) ^2) - 6 * sig * P^2 / Q^3 + 3 * sig / P + 3 * sig / Q +
    12 * (1 - (3 / 20) * (P / R) ^2 + (1 / 32) * (P / R) ^3) / R + 4.5 * sig / R + 12 *
     (1 - (3 / 20) * (Q / R) ^2 + (1 / 32) * (Q / R) ^3) / R + 6.582336 / R; (* 8.48528/R *)
func = T + Vne + Vee; Vir = (Vne + Vee) / T;
(* Etot, P, Q *)
t = Table[FindMinimum[func, {P, 0.15}, {Q, 1.6},
    {R, 0.6}, {MaxIterations → 800}, {Method → "Newton"}], {z, 10, 18}]
```

FindMinimum::lstol :

The line search decreased the step size to within the tolerance specified by AccuracyGoal and PrecisionGoal but was unable to find a sufficient decrease in the function. You may need more than MachinePrecision digits of working precision to meet these tolerances. ≫

Out[74]=
```
{{-129.9055, {P → 0.15398422, Q → 1.5885139, R → 0.61773588}},
 {-162.97479, {P → 0.13969193, Q → 1.2913826, R → 0.53277971}},
 {-200.04569, {P → 0.12782468, Q → 1.0244339, R → 0.47243877}},
 {-241.21944, {P → 0.11781805, Q → 0.74977754, R → 0.43602427}},
 {-286.4546, {P → 0.10926171, Q → 0.64663703, R → 0.39616564}},
 {-335.69948, {P → 0.10186175, Q → 0.57726543, R → 0.3614698}},
 {-388.94878, {P → 0.095399027, Q → 0.52353136, R → 0.33197443}},
 {-446.20084, {P → 0.089706291, Q → 0.47979764, R → 0.30677916}},
 {-507.45489, {P → 0.084653803, Q → 0.4432097, R → 0.28506814}}}
```

In[75]:=
```
(* Virial ratio *)
```

In[76]:=
```
Table[N[Vir /. t[[z - 9, 2]], 10], {z, 10, 18}]
Table[N[Vne /. t[[z - 9, 2]], 10], {z, 10, 18}]
Table[N[Vee /. t[[z - 9, 2]], 10], {z, 10, 18}]
```

Out[76]=
```
{-2., -2., -2., -2., -2., -2., -2., -2., -2.}
```

Out[77]=
```
{-310.83963, -385.66672, -469.17781, -561.92343,
 -661.38209, -768.71245, -884.01374, -1007.3035, -1138.5875}
```

Out[78]=
```
{51.028635, 59.717145, 69.086421, 79.484547,
 88.472899, 97.313494, 106.11618, 114.90185, 123.67769}
```

In[79]:=
```
(* Etot in eV *)
```

In[80]:=
```
Table[N[t[[i, 1]] * 27.21138, 10], {i, 1, 9}];
PA = Table[P /. t[[i, 2]], {i, 1, 9}];
QA = Table[Q /. t[[i, 2]], {i, 1, 9}];
RA = Table[R /. t[[i, 2]], {i, 1, 9}];
at = {"Ne", "Na+", "Mg+2", "Al+3", "Si+4", "P+5", "S+6", "Cl+7", "Ar+8"};
```

In[85]:=
```
Table[
 Show[Graphics[{{Thickness[0.01],
   {RGBColor[1, 0, 0],
       Circle[{0, -RA[[i]]}, RA[[i]]], Circle[{0, RA[[i]]}, RA[[i]]]},
   {RGBColor[1, 0, 1], Circle[{-RA[[i]], 0}, RA[[i]]], Circle[{RA[[i]], 0},
   RA[[i]]]}, {RGBColor[0, 1, 1], Circle[{0, 0}, RA[[i]]]}}, {Thickness[0.015],
     {RGBColor[0, 0, 0], Circle[{0, 0}, PA[[i]]], Circle[{0, 0}, QA[[i]]]}}],
   {AspectRatio -> Automatic, PlotLabel → at[[i]],
  Axes -> True, GridLines -> Automatic, ColorOutput → Automatic,
  PlotRange -> {{-1.6, 1.6}, {-1.6, 1.6}}, Frame -> True}], {i, 1, 9}]
```

Out[85]=