

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

```
In[97]:= 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}]
```

```
Out[102]= {{-129.905, {P -> 0.153984, Q -> 1.58851, R -> 0.617736}},
{-162.975, {P -> 0.139692, Q -> 1.29138, R -> 0.53278}},
{-200.046, {P -> 0.127825, Q -> 1.02443, R -> 0.472439}},
{-241.219, {P -> 0.117818, Q -> 0.749778, R -> 0.436024}},
{-286.455, {P -> 0.109262, Q -> 0.646637, R -> 0.396166}},
{-335.699, {P -> 0.101862, Q -> 0.577265, R -> 0.36147}},
{-388.949, {P -> 0.095399, Q -> 0.523531, R -> 0.331974}},
{-446.201, {P -> 0.0897063, Q -> 0.479798, R -> 0.306779}},
{-507.455, {P -> 0.0846538, Q -> 0.44321, R -> 0.285068}}}
```

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In[103]:= (* Virial ratio *)
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```
In[104]:= 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[104]= {-2., -2., -2., -2., -2., -2., -2., -2., -2.}
```

```
Out[105]= {-310.84, -385.667, -469.178, -561.923,
-661.382, -768.712, -884.014, -1007.3, -1138.59}
```

```
Out[106]= {51.0286, 59.7171, 69.0864, 79.4845, 88.4729, 97.3135, 106.116, 114.902, 123.678}
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In[107]:= (* Etot in eV *)
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```
In[108]:= 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}];
```

```

In[112]:= 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,
  Axes -> True, GridLines -> Automatic, ColorOutput -> Automatic,
  PlotRange -> {{-1.6, 1.6}, {-1.6, 1.6}}, Frame -> True}], {i, 1, 9}]

```

