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In[23]:= (* Al atom Kimball, Ne-tbp core 15.09.2012 *)
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In[24]:= Clear[k1,k2,k3,k4, sig1,sig2,c,z,R1,R2,R3,R4,a,b,f,g,d];
c = {k1 -> 1.0, k2 -> 1.0, k3 -> 1.0, k4 -> 1.0, sig1 -> 0.28, sig2 -> 0.3,
sig3 -> 0.3};
z=13.0;
ad = Sqrt[3]/2;
T = 2.25*k1/R1^2+6.75*k2/R2^2+3.375*k3/R3^2+2.25*k4/R4^2 /. c;
b = (R1+R2)/2+Sqrt[(R2+R3)^2-3*(R1+R2)^2/4];
a = (R1+R2)*Sqrt[3];d = b*Sqrt[3];
f =
Sqrt[(R1+R4)^2+(R1+R2)^2];g=Sqrt[b^2+(R1+R4)^2];Vee=3.0*sig1/R1+3.0*3.0*sig2/R2
/. c;
Vee = Vee +
12/(R1+R2)+6/b+12/a+4/(R1+R4)+12/f+3/d+12/(R2+R3)+6/(b+R1+R2)+6/g+0.5/(R1+R4);
Vne=-3.0*z/R1-6*z/(R1+R2)-2*z/(R1+R4)-3*z/b;

func = T + Vee + Vne /. c;

t = FindMinimum[func, {R1,0.109}, {R2,0.4198},
{R3,1.668},{R4,0.416},{MaxIterations -> 500},{Method-> "Newton"}]
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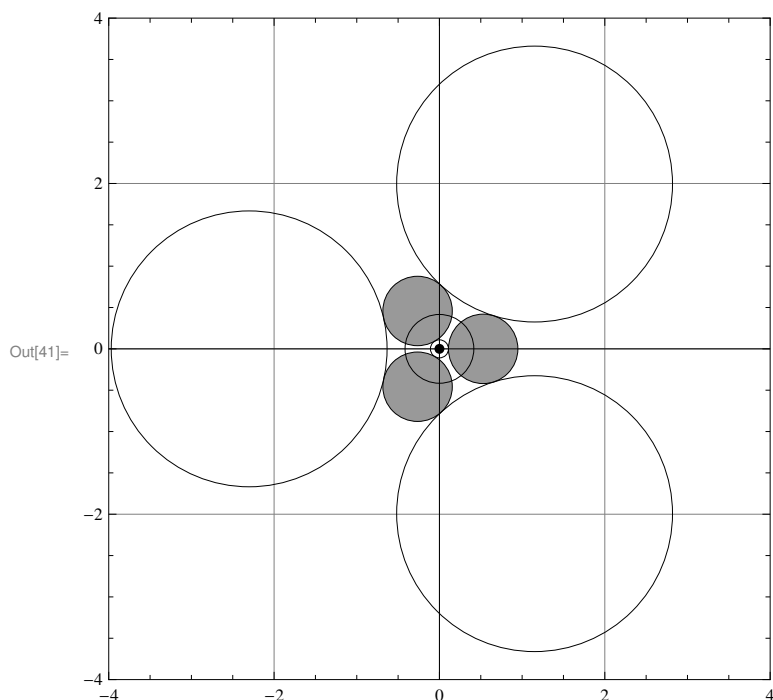
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Out[37]= {-241.501, {R1 -> 0.109113, R2 -> 0.419818, R3 -> 1.66817, R4 -> 0.415972}}
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In[38]:= -(Vne+Vee)/T /. t[[2]]
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Out[38]= 2.
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In[39]:= plot1=Graphics[{{GrayLevel[0.6],Disk[{R1+R2,0},R2],Disk[{-
(R1+R2)/2,ad*(R1+R2)},R2],Disk[{-(R1+R2)/2,-
ad*(R1+R2)},R2]},Circle[{R1+R2,0},R2],Circle[{-(
R1+R2)/2,ad*(R1+R2)},R2],Circle[{-(R1+R2)/2,-
ad*(R1+R2)},R2],Circle[{0,0},R1],Disk[{0,0},0.06],Circle[{0,0},R4],Circle[{
-b,0},R3],Circle[{b/2,ad*b},R3], Circle[{b/2,-ad*b},R3]}} /. t[[2]];

Show[plot1,{AspectRatio -> Automatic, Axes -> True, GridLines -> Automatic,
PlotRange -> {{-4,4},{-4,4}}, Frame -> True}]
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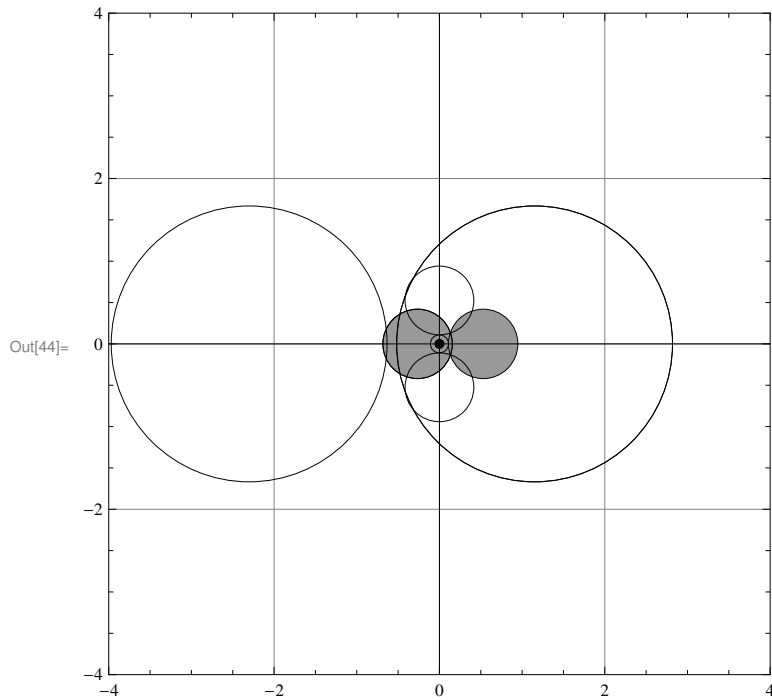
plot2=Graphics[{{GrayLevel[0.6],Disk[{R1+R2,0},R2],Disk[{-(R1+R2)/2,0},R2],Disk[{-(R1+R2)/2,0},R2]},Circle[{R1+R2,0},R2],Circle[{-(R1+R2)/2,0},R2],Circle[{-(R1+R2)/2,0},R2],Circle[{0,0},R1],Disk[{0,0},0.06],Circle[{0,R1+R4},R4],Circle[{0,-(R1+R4)},R4],Circle[{-b,0},R3],Circle[{b/2,0},R3],Circle[{b/2,0},R3]}} /.
t[[2]];

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Show[plot2,{AspectRatio -> Automatic, Axes -> True, GridLines -> Automatic,
PlotRange -> {{-4,4},{-4,4}}, Frame -> True}]

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- Graphics -