

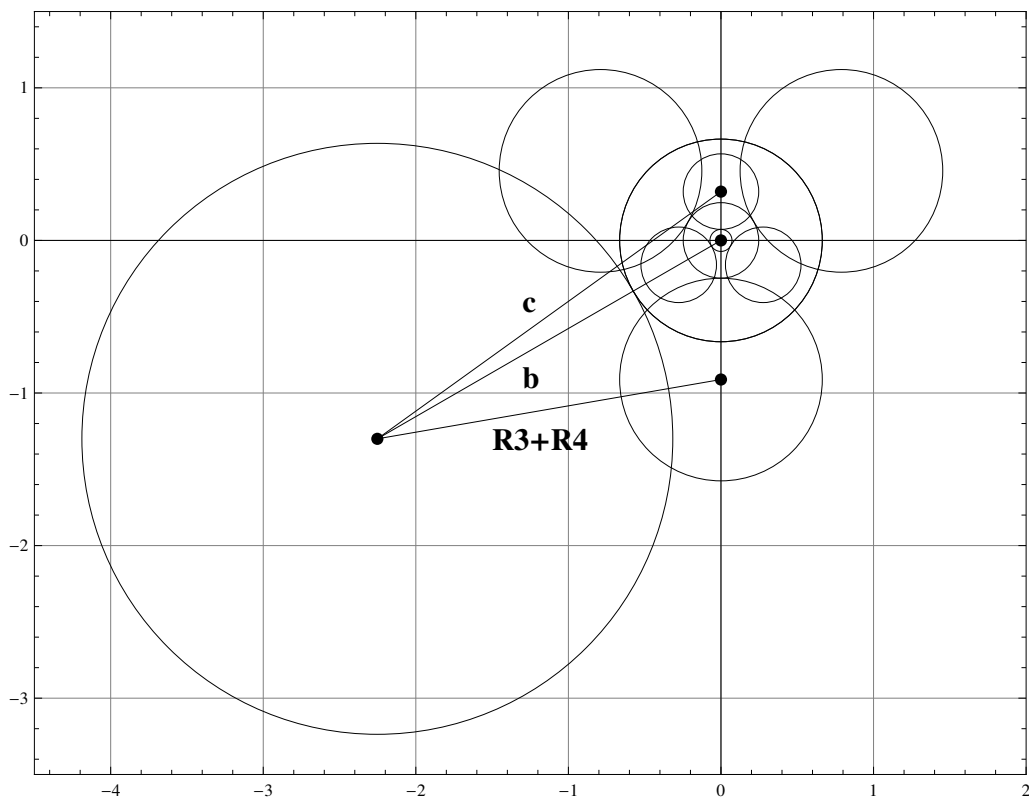
# K atom nach Kimball, Aussen-sp-Kugeln 18.12.2012, W. Heinzelmann, 1963

```
Clear[k1,k2,k3,k4,sig1,sig2,sig3,c,z,R1,R2,R3,R4,a,b,k];
k = {k1 -> 1.0, k2 -> 1.0, k3->1.0, k4->1.0, sig1 -> 0.3, sig2 -> 0.3, sig3 -> 0.3};
z=19.0; si=Sin[π/3];
T = 2.25*k1/R1^2+9.0*k2/R2^2+9.0*k3/R3^2+1.125*k4/R4^2 /. k;
a = (R1+R2)/3+Sqrt[(R2+R3)^2-8*(R1+R2)^2/9];
b = a/3+Sqrt[(R3+R4)^2-8*a*a/9];
c = b+Sqrt[((R1+R2)/3)^2+8*(R1+R2)^2/9];
Vee = 3.0*sig1/R1+4.0*3.0*sig2/R2+4.0*3.0*sig3/R3+16/(R1+R2)+24/((R1+R2)*Sqrt[8/3])+
      16/a+48/(R2+R3)+16/(R1+R2+a)+24*Sqrt[3/8]/a+2/b+6/(R3+R4)+2/(a+b)+2/(b-R1-R2)+6/c /.
Vne = -3.0*z/R1-8*z/(R1+R2)-8*z/a-z/b;
Vir = (Vee+Vne)/T;
func = T+Vee+Vne;
t = FindMinimum[func, {R1,0.0727274}, {R2,0.25108}, {R3,0.689122}, {R4,1.9368},{Method->Newt}
{-598.129, {R1 -> 0.0722919, R2 -> 0.247526, R3 -> 0.664106, R4 -> 1.93648}}]
```

N[-Vir /. t[[2]], 10]

2.

```
Show[Graphics[{Circle[{0,0},R1],Circle[{0,0},R2],Circle[{0,0},R3],Circle[{0,R1+R2},R2],
Circle[{-si*(R1+R2),-(R1+R2)/2},R2],Circle[{si*(R1+R2),-(R1+R2)/2},R2],
Circle[{-si*(R2+R3),(R2+R3)/2},R3],Circle[{si*(R2+R3),(R2+R3)/2},R3],
Circle[{0,-(R2+R3)},R3],Circle[{0,0},R3],Circle[{-si*(R3+R4),-(R3+R4)/2},R4],
Disk[{0,0},0.04],Disk[{-si*(R3+R4),-(R3+R4)/2},0.04],Disk[{0,R1+R2},0.04],
Disk[{0,-(R2+R3)},0.04],Line[{{0,0},{-si*(R3+R4),-(R3+R4)/2}},
Line[{{0,R1+R2},{-si*(R3+R4),-(R3+R4)/2}},Line[{{0,-(R2+R3)},{-si*(R3+R4),-(R3+R4)},
Text[StyleForm["R3+R4",FontSize->16,FontWeight->"Bold"],{-1.5,-1.3},{-1,0}],
Text[StyleForm["b",FontSize->16,FontWeight->"Bold"],{-1.3,-0.9},{-1,0}],
Text[StyleForm["c",FontSize->16,FontWeight->"Bold"],{-1.3,-0.4},{-1,0}]] /. t[[2]
Axes -> True,GridLines -> Automatic,PlotRange -> {{-4.5,2.0},{-3.5,1.5}},Frame -> True
```



```
Show[Graphics[
  {Circle[{0, 0}, R1], Circle[{(R1 + R2) / 2, 0}, R2], Circle[{(R1 + R2) / 2, si * (R1 + R2)}, R2],
    Circle[{-(R1 + R2), 0}, R2], Circle[{(R1 + R2) / 2, -si * (R1 + R2)}, R2],
    Circle[{-(R2 + R3) / 2, si * (R2 + R3)}, R3], Circle[{R2 + R3, 0}, R3],
    Circle[{-(R2 + R3) / 2, -si * (R2 + R3)}, R3], Circle[{-(R2 + R3) / 2, 0}, R3],
    Circle[{-b, 0}, R4], Disk[{0, 0}, 0.04], Disk[{-b, 0}, 0.04],
    Disk[{(R1 + R2) / 2, si * (R1 + R2)}, 0.04], Disk[{-(R2 + R3) / 2, -si * (R2 + R3)}, 0.04],
    Line[{0, 0}, {-b, 0}], Line[{-b, 0}, {(R1 + R2) / 2, si * (R1 + R2)}],
    Line[{-(R2 + R3) / 2, -si * (R2 + R3)}, {-b, 0}],
    Text[StyleForm["R3+R4", FontSize -> 16, FontWeight -> "Bold"], {-2.2, -0.5}, {-1, 0}],
    Text[StyleForm["b", FontSize -> 16, FontWeight -> "Bold"], {-2, -0.15}, {-1, 0}],
    Text[StyleForm["c", FontSize -> 16, FontWeight -> "Bold"], {-2, 0.2}, {-1, 0}]] /. t[[2]],
  {AspectRatio -> Automatic, PlotRange -> {{-4.8, 1.8}, {-2, 2}}, Frame -> True}]
```

