

(\* [Fe(CN)6]--- computation;  
coordinates and radii from FeCN6m06.exe, 05.02.2012 \*)

```
t = {{0.00000, 0.00000, 0.00000, 1.28759},  
     {2.63524, 0.00000, 0.00000, 1.34765}, {4.22692, 0.00000, 0.00000, 0.24403},  
     {5.18906, 0.00000, 0.00000, 0.71812}, {5.35906, 1.94986, 0.00000, 1.77986},  
     {5.35906, 0.00000, 1.94986, 1.77986}, {5.35906, -1.94986, 0.00000, 1.77986},  
     {5.35906, 0.00000, -1.94986, 1.77986}, {6.12140, 0.00000, 0.00000, 0.21422},  
     {7.41822, 0.00000, 0.00000, 1.08261}, {0.00000, 2.63524, 0.00000, 1.34765},  
     {0.00000, 4.22692, 0.00000, 0.24403}, {0.00000, 5.18906, 0.00000, 0.71812},  
     {1.94986, 5.35906, 0.00000, 1.77986}, {0.00000, 5.35906, 1.94986, 1.77986},  
     {-1.94986, 5.35906, 0.00000, 1.77986}, {0.00000, 5.35906, -1.94986, 1.77986},  
     {0.00000, 6.12140, 0.00000, 0.21422}, {0.00000, 7.41822, 0.00000, 1.08261},  
     {-2.63524, 0.00000, 0.00000, 1.34765}, {-4.22692, 0.00000, 0.00000, 0.24403},  
     {-5.18906, 0.00000, 0.00000, 0.71812}, {-5.35906, -1.94986, 0.00000, 1.77986},  
     {-5.35906, 0.00000, -1.94986, 1.77986},  
     {-5.35906, 1.94986, 0.00000, 1.77986}, {-5.35906, 0.00000, 1.94986, 1.77986},  
     {-6.12140, 0.00000, 0.00000, 0.21422}, {-7.41822, 0.00000, 0.00000, 1.08261}};
```

```
x = Table[t[[i, 1]], {i, 1, 28}];  
y = Table[t[[i, 2]], {i, 1, 28}];  
z = Table[t[[i, 3]], {i, 1, 28}];  
r = Table[t[[i, 4]], {i, 1, 28}];
```

(\* one of the three sigma planes \*)

```
plot2 = Graphics[{Circle[{x[[1]], y[[1]]}, r[[1]]],  
                 Circle[{x[[2]], y[[2]]}, r[[2]]],  
                 Circle[{x[[9]], y[[9]]}, r[[9]]], Circle[{x[[3]], y[[3]]}, r[[3]]],  
                 Circle[{x[[10]], y[[10]]}, r[[10]]], Circle[{x[[4]], y[[4]]}, r[[4]]],  
                 Circle[{x[[11]], y[[11]]}, r[[11]]], Circle[{x[[5]], y[[5]]}, r[[5]]],  
                 Circle[{x[[12]], y[[12]]}, r[[12]]], Circle[{x[[6]], y[[6]]}, r[[6]]],  
                 Circle[{x[[13]], y[[13]]}, r[[13]]], Circle[{x[[7]], y[[7]]}, r[[7]]],  
                 Circle[{x[[14]], y[[14]]}, r[[14]]], Circle[{x[[8]], y[[8]]}, r[[8]]],  
                 Circle[{x[[15]], y[[15]]}, r[[15]]], Circle[{x[[16]], y[[16]]}, r[[16]]],  
                 Circle[{x[[17]], y[[17]]}, r[[17]]], Circle[{x[[18]], y[[18]]}, r[[18]]],  
                 Circle[{x[[19]], y[[19]]}, r[[19]]], Circle[{x[[20]], y[[20]]}, r[[20]]],  
                 Circle[{x[[21]], y[[21]]}, r[[21]]], Circle[{x[[22]], y[[22]]}, r[[22]]],  
                 Circle[{x[[23]], y[[23]]}, r[[23]]], Circle[{x[[24]], y[[24]]}, r[[24]]],  
                 Circle[{x[[25]], y[[25]]}, r[[25]]], Circle[{x[[26]], y[[26]]}, r[[26]]],  
                 Circle[{x[[27]], y[[27]]}, r[[27]]], Circle[{x[[28]], y[[28]]}, r[[28]]],  
                 Circle[{x[[11]], -y[[11]]}, r[[11]]], Circle[{x[[12]], -y[[12]]}, r[[12]]],  
                 Circle[{x[[13]], -y[[13]]}, r[[13]]], Circle[{x[[14]], -y[[14]]}, r[[14]]],  
                 Circle[{x[[15]], -y[[15]]}, r[[15]]], Circle[{x[[16]], -y[[16]]}, r[[16]]],  
                 Circle[{x[[17]], -y[[17]]}, r[[17]]], Circle[{x[[18]], -y[[18]]}, r[[18]]],  
                 Circle[{x[[19]], -y[[19]]}, r[[19]]],  
                 Circle[{x[[1]], y[[1]]}, 0.05], Circle[{x[[1]], y[[1]]}, 0.25],  
                 Circle[{x[[1]], y[[1]]}, 0.636],  
                 Disk[{x[[3]], y[[3]]}, 0.1], Disk[{x[[9]], y[[9]]}, 0.1],  
                 Disk[{x[[12]], y[[12]]}, 0.1], Disk[{x[[12]], -y[[12]]}, 0.1],  
                 Disk[{x[[18]], y[[18]]}, 0.1], Disk[{x[[18]], -y[[18]]}, 0.1],  
                 Disk[{x[[21]], y[[21]]}, 0.1], Disk[{x[[27]], y[[27]]}, 0.1],  
                 Disk[{0, 0}, 0.16] ] ]
```

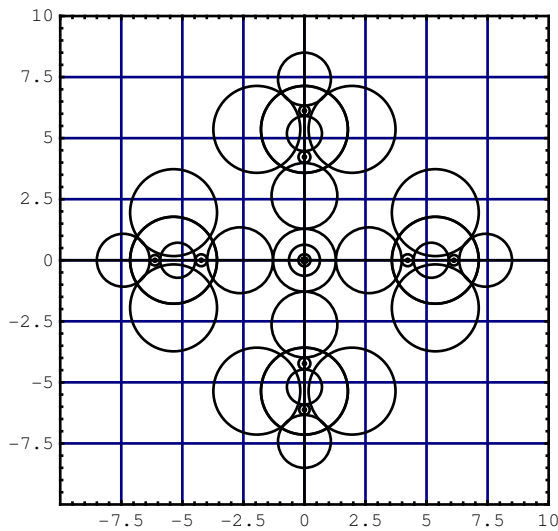
```
Show[plot2, {AspectRatio -> Automatic, Axes -> True,
  GridLines -> Automatic, PlotRange -> {{-10, 10}, {-10, 10}}, Frame -> True}]
```

```
(* xz plane *)
```

```
(* plot3=Graphics[{Circle[{x[[1]],z[[1]]},r[[1]]},
  Circle[{sq*x[[2]],z[[2]]},r[[2]]},Circle[{sq*x[[3]],z[[3]]},r[[3]]},
  Circle[{sq*x[[4]],z[[4]]},r[[4]]},Circle[{sq*x[[5]],z[[5]]},r[[5]]},
  Circle[{sq*x[[6]],z[[6]]},r[[6]]},Circle[{sq*x[[7]],z[[7]]},r[[7]]},
  Circle[{sq*x[[8]],z[[8]]},r[[8]]},Circle[{sq*x[[9]],z[[9]]},r[[9]]},
  Circle[{sq*x[[10]],z[[10]]},r[[10]]},Circle[{sq*x[[11]],z[[11]]},r[[11]]},
  Circle[{sq*x[[12]],z[[12]]},r[[12]]},Circle[{sq*x[[13]],z[[13]]},r[[13]]},
  Circle[{sq*x[[14]],z[[14]]},r[[14]]},Circle[{sq*x[[15]],z[[15]]},r[[15]]},
  Circle[{sq*x[[16]],z[[16]]},r[[16]]},Circle[{sq*x[[17]],z[[17]]},r[[17]]},
  Circle[{sq*x[[18]],z[[18]]},r[[18]]},Circle[{sq*x[[19]],z[[19]]},r[[19]]},
  Circle[{sq*x[[20]],z[[20]]},r[[20]]},Circle[{sq*x[[21]],z[[21]]},r[[21]]},
  Circle[{x[[22]],z[[22]]},r[[22]]},Circle[{x[[23]],z[[23]]},r[[23]]},
  Circle[{x[[24]],z[[24]]},r[[24]]},Circle[{x[[25]],z[[25]]},r[[25]]},
  Circle[{x[[26]],z[[26]]},r[[26]]},Circle[{x[[27]],z[[27]]},r[[27]]},
  Circle[{x[[28]],z[[28]]},r[[28]]},Disk[{sq*x[[3]],z[[3]]},0.1],
  Disk[{sq*x[[9]],z[[9]]},0.1], Disk[{sq*x[[21]],z[[21]]},0.1],
  Disk[{sq*x[[27]],z[[27]]},0.1], Disk[{0,0},0.16}]]
```

```
Show[plot3,{AspectRatio -> Automatic,Axes -> True,GridLines -> Automatic,
  PlotRange -> {{-10,10},{-5,5}}, Frame -> True}] *)
```

```
- Graphics -
```



```
- Graphics -
```