

### H3SiSiH3 computation; coordinates and radii from Si2H6001.exe 07.02.2012

```
t = {{-2.19608, 0.00000, 0.00000, 0.59375}, {2.19608, 0.00000, 0.00000, 0.59375},  
     {-2.89687, 1.98215, 0.00000, 1.50863}, {-2.89687, -0.99107, 1.71659, 1.50863},  
     {-2.89687, -0.99107, -1.71659, 1.50863},  
     {0.00000, 0.00000, 0.00000, 1.60233}, {2.89687, -1.98215, 0.00000, 1.50863},  
     {2.89687, 0.99107, 1.71659, 1.50863}, {2.89687, 0.99107, -1.71659, 1.50863}};  
u = {{-2.19608, 0.00000, 0.00000}, {2.19608, 0.00000, 0.00000},  
     {-3.09274, 2.53615, 0.00000}, {-3.09274, -1.26807, 2.19637},  
     {-3.09274, -1.26807, -2.19637}, {3.09274, -2.53615, 0.00000},  
     {3.09274, 1.26807, 2.19637}, {3.09274, 1.26807, -2.19637}};  
  
x = Table[t[[i, 1]], {i, 1, 9}];  
y = Table[t[[i, 2]], {i, 1, 9}];  
z = Table[t[[i, 3]], {i, 1, 9}];  
r = Table[t[[i, 4]], {i, 1, 9}];  
sq = 1.0 (*Sqrt[2]/2;*)  
  
h = Table[u[[i, 1]], {i, 1, 8}];  
k = Table[u[[i, 2]], {i, 1, 8}];  
l = Table[u[[i, 3]], {i, 1, 8}];  
  
(* xy plane *)  
  
plot2 = Graphics[{Circle[{x[[1]], y[[1]]}, r[[1]]],  
                  Circle[{x[[2]], y[[2]]}, r[[2]]], Circle[{x[[3]], y[[3]]}, r[[3]]],  
                  Circle[{x[[4]], y[[4]]}, r[[4]]], Circle[{x[[5]], y[[5]]}, r[[5]]],  
                  Circle[{x[[6]], y[[6]]}, r[[6]]], Circle[{x[[7]], y[[7]]}, r[[7]]],  
                  Circle[{x[[8]], y[[8]]}, r[[8]]], Circle[{x[[9]], y[[9]]}, r[[9]]],  
                  Disk[{h[[1]], k[[1]]}, 0.08], Disk[{h[[2]], k[[2]]}, 0.08],  
                  Disk[{h[[3]], k[[3]]}, 0.08], Disk[{h[[4]], k[[4]]}, 0.08],  
                  Disk[{h[[5]], k[[5]]}, 0.08], Disk[{h[[6]], k[[6]]}, 0.08],  
                  Disk[{h[[7]], k[[7]]}, 0.08], Disk[{h[[8]], k[[8]]}, 0.08]}];  
  
Show[plot2, {AspectRatio -> Automatic, Axes -> True,  
           GridLines -> Automatic, PlotRange -> {{-4.5, 4.5}, {-4, 4}}, Frame -> True}]  
  
(* yz plane *)  
plot3 = Graphics[{Circle[{y[[1]], z[[1]]}, r[[1]]],  
                  Circle[{sq*y[[2]], z[[2]]}, r[[2]]], Circle[{sq*y[[3]], z[[3]]}, r[[3]]],  
                  Circle[{sq*y[[4]], z[[4]]}, r[[4]]], Circle[{sq*y[[5]], z[[5]]}, r[[5]]],  
                  Circle[{sq*y[[6]], z[[6]]}, r[[6]]], Circle[{sq*y[[7]], z[[7]]}, r[[7]]],  
                  Circle[{sq*y[[8]], z[[8]]}, r[[8]]], Circle[{sq*y[[9]], z[[9]]}, r[[9]]],  
                  Disk[{k[[1]], l[[1]]}, 0.08], Disk[{k[[2]], l[[2]]}, 0.08],  
                  Disk[{k[[3]], l[[3]]}, 0.08], Disk[{k[[4]], l[[4]]}, 0.08],  
                  Disk[{k[[5]], l[[5]]}, 0.08], Disk[{k[[6]], l[[6]]}, 0.08],  
                  Disk[{k[[7]], l[[7]]}, 0.08], Disk[{k[[8]], l[[8]]}, 0.08]}];  
  
Show[plot3, {AspectRatio -> Automatic, Axes -> True, GridLines -> Automatic,  
           PlotRange -> {{-4.5, 4.5}, {-4.5, 4.5}}, Frame -> True}]
```

```
(* xz plane *)
plot1 = 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]]],
  Disk[{h[[1]], l[[1]]}, 0.08], Disk[{h[[2]], l[[2]]}, 0.08],
  Disk[{h[[3]], l[[3]]}, 0.08], Disk[{h[[4]], l[[4]]}, 0.08],
  Disk[{h[[5]], l[[5]]}, 0.08], Disk[{h[[6]], l[[6]]}, 0.08],
  Disk[{h[[7]], l[[7]]}, 0.08], Disk[{h[[8]], l[[8]]}, 0.08]}];

Show[plot1, {AspectRatio -> Automatic, Axes -> True, GridLines -> Automatic,
  PlotRange -> {{-4.5, 4.5}, {-4.5, 4.5}}, Frame -> True}]
```



