

```

In[678]:= (* [ H3SiCH3 computation;
           coordinates and radii from SiH3CH31.exe, 07.02.2012 *)

t = {{-1.95516, 0.00000, 0.00000, 0.59369}, {1.62462, 0.00000, 0.00000, 0.26315},
     {-2.68291, 2.05840, 0.00000, 1.58958}, {-2.68291, -1.02920, 1.78263, 1.58958},
     {-2.68291, -1.02920, -1.78263, 1.58958},
     {0.00000, 0.00000, 0.00000, 1.36147}, {2.12872, -1.42580, 0.00000, 1.24913},
     {2.12872, 0.71290, 1.23478, 1.24913}, {2.12872, 0.71290, -1.23478, 1.24913}};
u = {{-1.95516, 0.00000, 0.00000}, {1.62462, 0.00000, 0.00000},
     {-2.88858, 2.64013, 0.00000}, {-2.88858, -1.32007, 2.28642},
     {-2.88858, -1.32007, -2.28642}, {2.30993, -1.93836, 0.00000},
     {2.30993, 0.96918, 1.67867}, {2.30993, 0.96918, -1.67867}};

In[680]:= 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;*)

In[685]:= 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],
                 Text[StyleForm["Si", FontSize -> 16, FontWeight -> "Bold"],
                    {-2.05, -0.9}, {-1, 0}],
                 Text[StyleForm["C", FontSize -> 16, FontWeight -> "Bold"],
                    {1.55, -0.9}, {-1, 0}]]];

Show[plot2, {AspectRatio -> Automatic, Axes -> True,
           GridLines -> Automatic, PlotRange -> {{-5, 4}, {-3, 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,
}

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```
PlotRange -> {{-4.5, 4.5}, {-4.5, 4.5}}, Frame -> True}}
```

```
(* xz plane *)
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```
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],
  Text[StyleForm["Si", FontSize -> 16, FontWeight -> "Bold"],
    {-2.05, -0.9}, {-1, 0}],
  Text[StyleForm["C", FontSize -> 16, FontWeight -> "Bold"],
    {1.55, -0.9}, {-1, 0}]]];
```

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



