```
> restart;
  with(geom3d):
```

PROBLEM 200-3

Si atoms around Si atoms #C- SiC Zink Blende a=4.3596 A

```
> with(Spread):
```

```
> point(origo,0,0,0):
  cellnum:=0:atnum:=0:thelist:='thelist':
  NumSiAtPrCell:=4: #NB for Si around Si
  for ix from -3 to 2 do
   for iy from -3 to 2 do
    for iz from -3 to 2 do
      cellnum:=cellnum+1;
      for j from 1 to NumSiAtPrCell do # NB only 4 Si atoms needed
  here
        atnum:=NumSiAtPrCell*(cellnum-1)+j;# NB
        if   j=1 then point(coords,[ix,iy,iz])
        elif j=2 then point(coords,[ix+0.5,iy+0.5,iz])
        elif j=3 then point(coords,[ix,iy+0.5,iz+0.5])
        elif j=4 then point(coords,[ix+0.5,iy,iz+0.5])
        #elif j=5 then point(coords,[ix+0.25,iy+0.25,iz+0.25])
        #elif j=6 then point(coords,[ix+0.75,iy+0.75,iz+0.25])
        #elif j=7 then point(coords,[ix+0.25,iy+0.75,iz+0.75])
        #elif j=8 then point(coords,[ix+0.75,iy+0.25,iz+0.75])
        end if;
        d:=distance(coords,origo);
        thelist[atnum]:=evalf(d);
        #print(atnum);
       od;#j
     od;#iz
     od;#iy
    od;#ix
   maxatnum:=atnum;
```

$$maxatnum := 864 \qquad (1)$$

```
> sortedlist:=sort([seq(thelist[j],j=1..maxatnum)]):
```

```
> ssisi := CreateSpreadsheet(Si_Si_Shells): SetCellFormula(ssisi,
  1, 1, 'ShellNum'):SetCellFormula(ssisi, 1, 2, 'NumInShell'):
  for j from 3 to 5 do SetCellFormula(ssisi, 1, j,
  'ShellDistance');od:
  shnum:=0:d:=0:cntr:=0:
  #print(shellnum,numinshell, shelldistance,shelldistance,
  shelldistance);
  for j from 1 to maxatnum do
  if ((sortedlist[j]-d)>=0.01)
   then if shnum<8
          then x:=sqrt(convert(d^2,rational));
               #print(shnum,cntr,x*a,d*a,  d*0.43596*nm);
               if shnum>0 then SetCellFormula(ssisi, shnum+1,3 , x*
  a);
                               SetCellFormula(ssisi, shnum+1,2 ,
  cntr);
```

```
                                    SetCellFormula(ssisi, shnum+1,1 ,
shnum);
                                    SetCellFormula(ssisi, shnum+1,4 , d*
a);
                                    SetCellFormula(ssisi, shnum+1,5 , d*
0.43596*nm);
                               end if;
          end if;
shnum:=shnum+1;d:=sortedlist[j];
cntr:=0:
end if:
cntr:=cntr+1:
od:
```

Si_Si_Shells

	A	B	C	D	E	F
1	*ShellNum*	*NumInShell*	*ShellDistance*	*ShellDistance*	*ShellDistance*	
2	1	12	$\frac{1}{2}\sqrt{2}\,a$	$0.7071067812\,a$	$0.3082702723\ nm$	
3	2	6	a	$1.\,a$	$0.43596\ nm$	
4	3	24	$\frac{1}{2}\sqrt{6}\,a$	$1.224744871\,a$	$0.5339397740\ nm$	
5	4	12	$\sqrt{2}\,a$	$1.414213562\,a$	$0.6165405445\ nm$	
6	5	24	$\frac{1}{2}\sqrt{10}\,a$	$1.581138830\,a$	$0.6893132843\ nm$	
7	6	8	$\sqrt{3}\,a$	$1.732050808\,a$	$0.7551048703\ nm$	
8	7	48	$\frac{1}{2}\sqrt{14}\,a$	$1.870828693\,a$	$0.8156064770\ nm$	

(2)

C atoms around Si atoms #C- SiC Zink Blende a=4.3596 A

```
> point(origo,0,0,0):
cellnum:=0:atnum:=0:thelist:='thelist':
NumCAtPrCell:=4: #NB for C around Si
for ix from -3 to 2 do
 for iy from -3 to 2 do
  for iz from -3 to 2 do
    cellnum:=cellnum+1;
    for j from 1 to NumCAtPrCell do # NB only 4 C atoms needed
here
      atnum:=NumCAtPrCell*(cellnum-1)+j;# NB
      #if   j=1 then point(coords,[ix,iy,iz])
      #elif j=2 then point(coords,[ix+0.5,iy+0.5,iz])
      #elif j=3 then point(coords,[ix,iy+0.5,iz+0.5])
      #elif j=4 then point(coords,[ix+0.5,iy,iz+0.5])
```

```
        if j=1 then point(coords,[ix+0.25,iy+0.25,iz+0.25])
        elif j=2 then point(coords,[ix+0.75,iy+0.75,iz+0.25])
        elif j=3 then point(coords,[ix+0.25,iy+0.75,iz+0.75])
        elif j=5 then point(coords,[ix+0.75,iy+0.25,iz+0.75])
        end if;
        d:=distance(coords,origo);
        thelist[atnum]:=evalf(d);
        #print(atnum);
      od;#j
    od;#iz
    od;#iy
   od;#ix
 maxatnum:=atnum;
```

$$maxatnum := 864 \tag{3}$$

```
> sortedlist:=sort([seq(thelist[j],j=1..maxatnum)]):
```

```
> ssic := CreateSpreadsheet(Si_C_Shells):
SetCellFormula(ssic, 1, 1, 'ShellNum'):SetCellFormula(ssic, 1, 2,
'NumInShell'):
for j from 3 to 5 do SetCellFormula(ssic, 1, j, 'ShellDistance');
od:

shnum:=0:d:=0:cntr:=0:
#print(shellnum,numinshell, shelldistance,shelldistance,
shelldistance);
for j from 1 to maxatnum do
if ((sortedlist[j]-d)>=0.01)
 then if shnum<8
        then x:=sqrt(convert(d^2,rational));
             #print(shnum,cntr, x*a,d*a,  d*0.43596*nm);
             if shnum>0 then SetCellFormula(ssic, shnum+1,3 , x*
a);
                             SetCellFormula(ssic, shnum+1,2 ,
cntr);
                             SetCellFormula(ssic, shnum+1,1 ,
shnum);
                             SetCellFormula(ssic, shnum+1,4 , d*
a);
                             SetCellFormula(ssic, shnum+1,5 , d*
0.43596*nm);
             end if;
        end if;
shnum:=shnum+1;d:=sortedlist[j];
cntr:=0:
end if:
cntr:=cntr+1:
od:
```

Si_C_Shells						
	A	B	C	D	E	F
1	*ShellNum*	*NumInShell*	*ShellDistance*	*ShellDistance*	*ShellDistance*	
2	1	4	$\frac{1}{4}\sqrt{3}\ a$	$0.4330127019\ a$	$0.1887762175\ nm$	
3	2	12	$\frac{1}{4}\sqrt{11}\ a$	$0.8291561976\ a$	$0.3614789359\ nm$	
4	3	12	$\frac{1}{4}\sqrt{19}\ a$	$1.089724736\ a$	$0.4750763959\ nm$	
5	4	16	$\frac{3}{4}\sqrt{3}\ a$	$1.299038106\ a$	$0.5663286527\ nm$	
6	5	24	$\frac{1}{4}\sqrt{35}\ a$	$1.479019946\ a$	$0.6447935357\ nm$	
7	6	12	$\frac{1}{4}\sqrt{43}\ a$	$1.639359631\ a$	$0.7146952247\ nm$	
8	7	24	$\frac{1}{4}\sqrt{51}\ a$	$1.785357107\ a$	$0.7783442844\ nm$	

(4)