

Code for atomic scattering factor of Li

```
open(1,file="fsum5.txt")
a1=0.20
a2=1.60
pi=3.141592
!
do i=0,10000
stol=0.0001*float(i)
f=2.0/(1.0+4.0*(pi*a1*stol)**2)**2+(1.0+4.0*(pi*a2*stol)**2)**(-2)
!
if(i.ne.0) then
fsum=0.0
dr=0.2 ← smaller, better
do j=0,50 ← larger, better
rr=dr*float(j)
fsum1=1.0/(pi*a1**3*stol)*rr*exp(-2.0*rr/a1)*sin(4.0*pi*rr*stol)*dr
fsum2=1.0/(pi*a2**3*stol)*rr*exp(-2.0*rr/a2)*sin(4.0*pi*rr*stol)*dr
fsum=fsum+2.0*fsum1+fsum2
end do
else
fsum=3.0
end if
write(1,*) stol,f,fsum
!
end do
!
close(1)
stop
end
```

