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!234567890
!   Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine gen_sg_lat(indexsg,volume,wmat)
implicit none
integer indexsg
real*8 wmat(3,3),volume
real*8 rlat(6),pi
logical llattice,l2d

l2d=.false. ; pi=4.0d0*atan(1.0d0)
do while(.true.)
call genrlat(rlat)
select case(indexsg)
case(1:2)
rlat(4:6)=rlat(4:6)*pi/2.0d0
! 1:2, Triclinic, a /= b /= c and alpha /= beta /= gamma

case(3:4)
rlat(4)=pi/2.0d0 ; rlat(6)=pi/2.0d0 ; rlat(5)=rlat(5)*pi/2.0d0

case(6:7)
rlat(4)=pi/2.0d0 ; rlat(6)=pi/2.0d0 ; rlat(5)=rlat(5)*pi/2.0d0

case(5)
rlat(1)=rlat(2) ; rlat(4)=rlat(5) ; rlat(4:5)=rlat(4:5)*pi ; rlat(6)=rlat
(6)*pi/2.0d0

case(8:9)
rlat(1)=rlat(2) ; rlat(4)=rlat(5) ; rlat(4:5)=rlat(4:5)*pi ; rlat(6)=rlat
(6)*pi/2.0d0

case(10:11)
rlat(4)=pi/2.0d0 ; rlat(6)=pi/2.0d0 ; rlat(5)=rlat(5)*pi/2.0d0

case(12)
rlat(1)=rlat(2) ; rlat(4)=rlat(5) ; rlat(4:5)=rlat(4:5)*pi ; rlat(6)=rlat
(6)*pi/2.0d0

case(13:14)
rlat(4)=pi/2.0d0 ; rlat(6)=pi/2.0d0 ; rlat(5)=rlat(5)*pi/2.0d0

case(15)
rlat(1)=rlat(2) ; rlat(4)=rlat(5) ; rlat(4:5)=rlat(4:5)*pi ; rlat(6)=rlat
(6)*pi/2.0d0
! 3:15, Monoclinic, a /= b /= c and alpha = gamma = 90 deg, beta /= 90 deg

case(16:19)
rlat(4)=0.5d0 ; rlat(5)=0.5d0 ; rlat(6)=0.5d0 ; rlat(4:6)=rlat(4:6)*pi

case(20:21)
rlat(1)=rlat(2) ; rlat(4)=0.5d0*pi ; rlat(5)=0.5d0*pi ; rlat(6)=rlat(6)*p
i/2.0d0

case(22)
rlat(4)=acos((rlat(2)**2+rlat(3)**2-rlat(1)**2)/2.0d0/rlat(2)/rlat(3))
rlat(5)=acos((rlat(1)**2+rlat(3)**2-rlat(2)**2)/2.0d0/rlat(1)/rlat(3))
rlat(6)=acos((rlat(2)**2+rlat(1)**2-rlat(3)**2)/2.0d0/rlat(1)/rlat(2))

case(23:24)
rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=rlat(4:6)*pi/2.0d0
if(cos(rlat(4))+cos(rlat(5)) > 0.0d0)then
rlat(6)=acos(-1.0d0+(cos(rlat(4))+cos(rlat(5))))
else
rlat(6)=acos(-1.0d0-cos(rlat(4))-cos(rlat(5)))
endif

case(25:34)
rlat(4)=0.5d0 ; rlat(5)=0.5d0 ; rlat(6)=0.5d0 ; rlat(4:6)=rlat(4:6)*pi

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case(35:41)
rlat(1)=rlat(2) ; rlat(4)=0.5d0*pi ; rlat(5)=0.5d0*pi ; rlat(6)=rlat(6)*p
i/2.0d0

case(42:43)
rlat(4)=acos((rlat(2)**2+rlat(3)**2-rlat(1)**2)/2.0/rlat(2)/rlat(3))
rlat(5)=acos((rlat(1)**2+rlat(3)**2-rlat(2)**2)/2.0/rlat(1)/rlat(3))
rlat(6)=acos((rlat(2)**2+rlat(1)**2-rlat(3)**2)/2.0/rlat(1)/rlat(2))

case(44:46)
rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=rlat(4:6)*pi/2.0d0
if(cos(rlat(4))+cos(rlat(5)) > 0.0d0)then
rlat(6)=acos(-1.0d0+(cos(rlat(4))+cos(rlat(5))))
else
rlat(6)=acos(-1.0d0-cos(rlat(4))-cos(rlat(5)))
endif

case(47:62)
rlat(4)=0.5d0 ; rlat(5)=0.5d0 ; rlat(6)=0.5d0 ; rlat(4:6)=rlat(4:6)*pi

case(63:68)
rlat(1)=rlat(2) ; rlat(4)=0.5d0*pi ; rlat(5)=0.5d0*pi ; rlat(6)=rlat(6)*p
i/2.0d0

case(69:70)
rlat(4)=acos((rlat(2)**2+rlat(3)**2-rlat(1)**2)/2.0/rlat(2)/rlat(3))
rlat(5)=acos((rlat(1)**2+rlat(3)**2-rlat(2)**2)/2.0/rlat(1)/rlat(3))
rlat(6)=acos((rlat(2)**2+rlat(1)**2-rlat(3)**2)/2.0/rlat(1)/rlat(2))

case(71:74)
rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=rlat(4:6)*pi/2.0d0
if(cos(rlat(4))+cos(rlat(5)) > 0.0d0)then
rlat(6)=acos(-1.0d0+(cos(rlat(4))+cos(rlat(5))))
else
rlat(6)=acos(-1.0d0-cos(rlat(4))-cos(rlat(5)))
endif
! 16:74, Orthorhombic, a /= b /= c and alpha = beta = gamma= 90 deg

case(75:78)
rlat(1)=rlat(2) ; rlat(4:6)=0.5d0 ; rlat(4:6)=rlat(4:6)*pi

case(81)
rlat(1)=rlat(2) ; rlat(4:6)=0.5d0 ; rlat(4:6)=rlat(4:6)*pi

case(83:86)
rlat(1)=rlat(2) ; rlat(4:6)=0.5d0 ; rlat(4:6)=rlat(4:6)*pi

case(89:96)
rlat(1)=rlat(2) ; rlat(4:6)=0.5d0 ; rlat(4:6)=rlat(4:6)*pi

case(99:106)
rlat(1)=rlat(2) ; rlat(4:6)=0.5d0 ; rlat(4:6)=rlat(4:6)*pi

case(111:118)
rlat(1)=rlat(2) ; rlat(4:6)=0.5d0 ; rlat(4:6)=rlat(4:6)*pi

case(123:138)
rlat(1)=rlat(2) ; rlat(4:6)=0.5d0 ; rlat(4:6)=rlat(4:6)*pi

case(79:80)
rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4)=rlat(5) ; rlat(4:6)=rlat(4:6)
*pi/2.0d0
if(cos(rlat(4))+cos(rlat(5)) > 0.0d0)then
rlat(6)=acos(-1.0d0+(cos(rlat(4))+cos(rlat(5))))
else
rlat(6)=acos(-1.0d0-cos(rlat(4))-cos(rlat(5)))
endif

case(82)

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*pi/2.0d0	<pre> rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4)=rlat(5) ; rlat(4:6)=rlat(4:6) if(cos(rlat(4))+cos(rlat(5)) > 0.0d0)then rlat(6)=acos(-1.0d0+(cos(rlat(4))+cos(rlat(5)))) else rlat(6)=acos(-1.0d0-cos(rlat(4))-cos(rlat(5))) endif </pre>	
	<pre> case(87:88) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4)=rlat(5) ; rlat(4:6)=rlat(4:6) </pre>	
*pi/2.0d0	<pre> if(cos(rlat(4))+cos(rlat(5)) > 0.0d0)then rlat(6)=acos(-1.0d0+(cos(rlat(4))+cos(rlat(5)))) else rlat(6)=acos(-1.0d0-cos(rlat(4))-cos(rlat(5))) endif </pre>	
	<pre> case(97:98) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4)=rlat(5) ; rlat(4:6)=rlat(4:6) </pre>	
*pi/2.0d0	<pre> if(cos(rlat(4))+cos(rlat(5)) > 0.0d0)then rlat(6)=acos(-1.0d0+(cos(rlat(4))+cos(rlat(5)))) else rlat(6)=acos(-1.0d0-cos(rlat(4))-cos(rlat(5))) endif </pre>	
	<pre> case(107:110) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4)=rlat(5) ; rlat(4:6)=rlat(4:6) </pre>	
*pi/2.0d0	<pre> if(cos(rlat(4))+cos(rlat(5)) > 0.0d0)then rlat(6)=acos(-1.0d0+(cos(rlat(4))+cos(rlat(5)))) else rlat(6)=acos(-1.0d0-cos(rlat(4))-cos(rlat(5))) endif </pre>	
	<pre> case(119:122) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4)=rlat(5) ; rlat(4:6)=rlat(4:6) </pre>	
*pi/2.0d0	<pre> if(cos(rlat(4))+cos(rlat(5)) > 0.0d0)then rlat(6)=acos(-1.0d0+(cos(rlat(4))+cos(rlat(5)))) else rlat(6)=acos(-1.0d0-cos(rlat(4))-cos(rlat(5))) endif </pre>	
	<pre> case(139:142) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4)=rlat(5) ; rlat(4:6)=rlat(4:6) </pre>	
*pi/2.0d0	<pre> if(cos(rlat(4))+cos(rlat(5)) > 0.0d0)then rlat(6)=acos(-1.0d0+(cos(rlat(4))+cos(rlat(5)))) else rlat(6)=acos(-1.0d0-cos(rlat(4))-cos(rlat(5))) endif </pre>	
	<pre> ! 75:142, Tetragonal, a = b, a /= c and alpha = beta = gamma= 90 deg </pre>	
66d0 ; rlat(4:6)=rlat(4:6)*pi	<pre> case(143:145) rlat(1)=rlat(2) ; rlat(5)=0.5d0 ; rlat(4)=rlat(5) ; rlat(6)=0.666666666666 </pre>	
	<pre> case(147) rlat(1)=rlat(2) ; rlat(5)=0.5d0 ; rlat(4)=rlat(5) ; rlat(6)=0.666666666666 </pre>	
66d0 ; rlat(4:6)=rlat(4:6)*pi	<pre> case(149:154) rlat(1)=rlat(2) ; rlat(5)=0.5d0 ; rlat(4)=rlat(5) ; rlat(6)=0.666666666666 </pre>	
	<pre> case(156:159) rlat(1)=rlat(2) ; rlat(5)=0.5d0 ; rlat(4)=rlat(5) ; rlat(6)=0.666666666666 </pre>	

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66d0 ; rlat(4:6)=rlat(4:6)*pi	<pre> case(162:165) rlat(1)=rlat(2) ; rlat(5)=0.5d0 ; rlat(4)=rlat(5) ; rlat(6)=0.666666666666 </pre>	
	<pre> case(168:194) rlat(1)=rlat(2) ; rlat(5)=0.5d0 ; rlat(4)=rlat(5) ; rlat(6)=0.666666666666 </pre>	
lat(4:6)=rlat(4:6)*pi/2.0d0	<pre> case(146) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4)=rlat(5) ; rlat(6)=rlat(5) ; r </pre>	
	<pre> case(148) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4)=rlat(5) ; rlat(6)=rlat(5) ; r </pre>	
lat(4:6)=rlat(4:6)*pi/2.0d0	<pre> case(155) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4)=rlat(5) ; rlat(6)=rlat(5) ; r </pre>	
	<pre> case(160:161) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4)=rlat(5) ; rlat(6)=rlat(5) ; r </pre>	
lat(4:6)=rlat(4:6)*pi/2.0d0	<pre> case(166:167) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4)=rlat(5) ; rlat(6)=rlat(5) ; r </pre>	
	<pre> ! 143:167, Trigonal, a = b= c and alpha = beta = gamma /= 90 deg ! 168:194, Hexagonal, a = b /= c and alpha, beta, gamma = 120 deg </pre>	
*pi	<pre> case(195) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=0.5d0 ; rlat(4:6)=rlat(4:6) </pre>	
	<pre> case(198) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=0.5d0 ; rlat(4:6)=rlat(4:6) </pre>	
*pi	<pre> case(200:201) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=0.5d0 ; rlat(4:6)=rlat(4:6) </pre>	
	<pre> case(205) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=0.5d0 ; rlat(4:6)=rlat(4:6) </pre>	
*pi	<pre> case(207:208) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=0.5d0 ; rlat(4:6)=rlat(4:6) </pre>	
	<pre> case(212:213) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=0.5d0 ; rlat(4:6)=rlat(4:6) </pre>	
*pi	<pre> case(215) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=0.5d0 ; rlat(4:6)=rlat(4:6) </pre>	
	<pre> case(218) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=0.5d0 ; rlat(4:6)=rlat(4:6) </pre>	
*pi	<pre> case(221:224) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=0.5d0 ; rlat(4:6)=rlat(4:6) </pre>	
	<pre> case(196) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=1.0d0/3.0d0 ; rlat(4:6)=rla </pre>	

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<pre> t(4:6)*pi case(202:203) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=1.0d0/3.0d0 ; rlat(4:6)=rla t(4:6)*pi case(209:210) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=1.0d0/3.0d0 ; rlat(4:6)=rla t(4:6)*pi case(216) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=1.0d0/3.0d0 ; rlat(4:6)=rla t(4:6)*pi case(219) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=1.0d0/3.0d0 ; rlat(4:6)=rla t(4:6)*pi case(225:228) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=1.0d0/3.0d0 ; rlat(4:6)=rla t(4:6)*pi case(197) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=109.471220634491d0/180.d0 ; rlat(4:6)=rlat(4:6)*pi case(199) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=109.471220634491d0/180.d0 ; rlat(4:6)=rlat(4:6)*pi case(204) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=109.471220634491d0/180.d0 ; rlat(4:6)=rlat(4:6)*pi case(206) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=109.471220634491d0/180.d0 ; rlat(4:6)=rlat(4:6)*pi case(211) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=109.471220634491d0/180.d0 ; rlat(4:6)=rlat(4:6)*pi case(214) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=109.471220634491d0/180.d0 ; rlat(4:6)=rlat(4:6)*pi case(217) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=109.471220634491d0/180.d0 ; rlat(4:6)=rlat(4:6)*pi case(220) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=109.471220634491d0/180.d0 ; rlat(4:6)=rlat(4:6)*pi case(229) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=109.471220634491d0/180.d0 ; rlat(4:6)=rlat(4:6)*pi case(230) rlat(1)=rlat(2) ; rlat(3)=rlat(2) ; rlat(4:6)=109.471220634491d0/180.d0 ; rlat(4:6)=rlat(4:6)*pi ! 195:230, Cubic end select call latmatvol(rlat,wmat,volume) call llcheck(llattice,l2d,wmat) if(llattice) return enddo end !234567890 </pre>		

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<pre> ! Written by In-Ho Lee, KRISS, September 11, 2013. subroutine latmatvol(rlat,wmat,volume) implicit none real*8 rlat(6),wmat(3,3),volume real*8 ylat(6),slat(6),zmat(3,3),tmq,tmp slat=rlat call latmat(slat,zmat,1) tmp=(zmat(1,2)*zmat(2,3)-zmat(1,3)*zmat(2,2))*zmat(3,1) & +(zmat(1,3)*zmat(2,1)-zmat(1,1)*zmat(2,3))*zmat(3,2) & +(zmat(1,1)*zmat(2,2)-zmat(1,2)*zmat(2,1))*zmat(3,3) tmq=volume/tmp ; tmq=tmq**(1.0d0/3.0d0) ylat(1)=rlat(1)*tmq ; ylat(2)=rlat(2)*tmq ; ylat(3)=rlat(3)*tmq ylat(4)=rlat(4) ; ylat(5)=rlat(5) ; ylat(6)=rlat(6) call latmat(ylat,wmat,1) return end !234567890 ! Written by In-Ho Lee, KRISS, September 11, 2013. subroutine latmat(rlat,wmat,ksign) implicit none integer ksign real*8 rlat(6),wmat(3,3) real*8 ra,rb,rc,cosinea,cosineb,cosinec real*8 epslat,tmr integer i,j epslat=1.0d-6 if(ksign == 1)then wmat=0.0d0 wmat(1,1)=rlat(1) wmat(2,1)=rlat(2)*cos(rlat(6)) wmat(2,2)=rlat(2)*sin(rlat(6)) wmat(3,1)=rlat(3)*cos(rlat(5)) wmat(3,2)=rlat(3)*cos(rlat(4))*sin(rlat(6)) & -((rlat(3)*cos(rlat(5))-rlat(3)*cos(rlat(4))*cos(rlat(6)))/tan(rlat(6))) tmr=rlat(3)**2-wmat(3,1)**2-wmat(3,2)**2 ; if(tmr <= 1.0d-12) tmr=0.0d0 wmat(3,3)=sqrt(tmr) do i=1,3 do j=1,3 if(abs(wmat(i,j)) < epslat) wmat(i,j)=0.0d0 enddo enddo else rlat=0.0d0 ra=sqrt(wmat(1,1)**2+wmat(1,2)**2+wmat(1,3)**2) rb=sqrt(wmat(2,1)**2+wmat(2,2)**2+wmat(2,3)**2) rc=sqrt(wmat(3,1)**2+wmat(3,2)**2+wmat(3,3)**2) cosinea=(wmat(2,1)*wmat(3,1)+wmat(2,2)*wmat(3,2)+wmat(2,3)*wmat(3,3))/rb/ rc cosineb=(wmat(1,1)*wmat(3,1)+wmat(1,2)*wmat(3,2)+wmat(1,3)*wmat(3,3))/rc/ ra cosinec=(wmat(1,1)*wmat(2,1)+wmat(1,2)*wmat(2,2)+wmat(1,3)*wmat(2,3))/ra/ rb rlat(1)=ra ; rlat(2)=rb ; rlat(3)=rc rlat(4)=acos(cosinea) ; rlat(5)=acos(cosineb) ; rlat(6)=acos(cosinec) endif return end !234567890 ! Written by In-Ho Lee, KRISS, September 11, 2013. subroutine genrlat(rlat) implicit none real*8 rlat(6) real*8 tmp,tmq integer k real ranmar tmp=0.10d0 ; tmq=1.0d0/tmp </pre>		

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do while(.true.)
do k=1,6
rlat(k)=ranmar()
enddo
if((abs(rlat(1)/rlat(2)) > tmp .or. abs(rlat(1)/rlat(2)) < tmp) .and. &
(abs(rlat(1)/rlat(3)) > tmp .or. abs(rlat(1)/rlat(3)) < tmp) .and. &
(abs(rlat(2)/rlat(3)) > tmp .or. abs(rlat(2)/rlat(3)) < tmp)) exit
enddo
return
end
!234567890
!      Written by In-Ho Lee, KRISS, September 11, 2013.
subroutine l1check(llattice,l2d,zmat)
implicit none
logical llattice,l2d
real*8 zmat(3,3)
real*8 altm(3,3),ra,rb,rc,alpha,beta,gama,pi,tmp
integer i,j

altm=zmat
pi=4.0d0*atan(1.0d0)

!---{
!
do i=1,3
do j=1,3
if(isnan(altm(i,j)))then
llattice=.false.
return
endif
enddo
enddo

!
!---}
ra=sqrt(altm(1,1)**2+altm(1,2)**2+altm(1,3)**2)
rb=sqrt(altm(2,1)**2+altm(2,2)**2+altm(2,3)**2)
rc=sqrt(altm(3,1)**2+altm(3,2)**2+altm(3,3)**2)
alpha=(altm(2,1)*altm(3,1)+altm(2,2)*altm(3,2)+altm(2,3)*altm(3,3))/rb/rc
beta=(altm(1,1)*altm(3,1)+altm(1,2)*altm(3,2)+altm(1,3)*altm(3,3))/rc/ra
gama=(altm(1,1)*altm(2,1)+altm(1,2)*altm(2,2)+altm(1,3)*altm(2,3))/ra/rb

tmp=180.0d0/pi
alpha=tmp*acos(alpha) ; beta=tmp*acos(beta) ; gama=tmp*acos(gama)
llattice=.true.
if(.not. l2d)then
if(ra < 1.20d0 .or. rb < 1.20d0 .or. rc < 1.20d0) llattice=.false.
if(alpha < 20.0d0 .or. alpha > 160.0d0) llattice=.false.
if(beta < 20.0d0 .or. beta > 160.0d0) llattice=.false.
if(gama < 20.0d0 .or. gama > 160.0d0) llattice=.false.
if(ra/rb > 6.0d0 .or. ra/rb < 0.3d0) llattice=.false.
if(ra/rc > 6.0d0 .or. ra/rc < 0.3d0) llattice=.false.
if(rb/rc > 6.0d0 .or. rb/rc < 0.3d0) llattice=.false.
else
if(ra < 1.20d0 .or. rb < 1.20d0) llattice=.false.
if(alpha < 20.0d0 .or. alpha > 160.0d0) llattice=.false.
if(beta < 20.0d0 .or. beta > 160.0d0) llattice=.false.
if(gama < 20.0d0 .or. gama > 160.0d0) llattice=.false.
if(ra/rb > 6.0d0 .or. ra/rb < 0.3d0) llattice=.false.
endif
return
end subroutine l1check
!234567890

```