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!! PES of CO on Rigid Ru(0001) surface
!! Jun Chen, 2022/11/1
!! Dynamics results published in:
!!   Jun Chent, Tan Jint, Tonghao Shen*, Mingjun Yang*, Zhe-Ning Chen*
!!   Toward Accurate and Efficient Dynamic Computational Strategy for Heterogeneous Catalysis: Temperature-Depen-
!!   Chin. Chem. Lett., 2022, 33(11): 4936-4942.

program main
implicit none
real*8 :: c(6,1),v0(1),vnn(1),dv(6,1)

c(1:6,1)=[0.799719d0, 0.231485d0, 6.057808d0, &
           0.619534d0,-0.024350d0, 5.003163d0]
v0(1)=-190.06859437d0
!! corresponding VASP OUTCAR (part) of this point is:
!! POSITION                                     TOTAL-FORCE (eV/Angst)
!! -----
!!    0.79107    2.43599    0.00000    0.001841   -0.000380    0.710451
!!    3.16424    1.06584    0.00000    0.001858   -0.000450    0.710888
!!    0.79107   -0.30431    0.00000    0.002165   -0.000369    0.711189
!!    3.16424   -1.67446    0.00000    0.001949   -0.000395    0.711136
!!    1.58209    1.06584    2.13254   -0.002757   -0.000079   -0.711276
!!    3.95526   -0.30431    2.13254   -0.002906   -0.000029   -0.710960
!!    1.58209    3.80613    2.13254   -0.002788   0.000339   -0.710793
!!    3.95526    2.43599    2.13254   -0.002785   0.000207   -0.711006
!!    0.79107    2.43599    4.26507   0.000885   0.000270    0.001468
!!    3.16424    1.06584    4.26507   0.000800   0.000588    0.001936
!!    0.79107   -0.30431    4.26507   0.000799   0.000224    0.001592
!!    3.16424   -1.67446    4.26507   0.000866   -0.000088    0.001688
!!    1.58176    1.06581    6.41455   0.001133   0.001091    0.001868
!!    3.95493   -0.30434    6.41455   0.000817   0.000921    0.001110
!!    1.58176    3.80611    6.41455   0.001210   0.000909    0.001723
!!    3.95493    2.43596    6.41455   0.000478   0.001315    0.001775
!!    0.79117    2.43599    8.47202   -0.000087   -0.000312   -0.001975
!!    3.16433    1.06584    8.47202   -0.000066   -0.000510   -0.001827
!!    0.79117   -0.30431    8.47202   0.000310   -0.000457    0.001443
!!    3.16433   -1.67446    8.47202   -0.000184   -0.000282   -0.002047
!!    1.59089   -0.07283    14.52983   0.951355   1.352979    5.552712
!!    1.41070   -0.32866    13.47519   -0.954893   -1.355494   -5.561094

call co_ru_pes(c,vnn,1,dv)

write(*,*) " potential energy : VASP vs NN"
write(*,*) v0,vnn
write(*,*) " derivatives"
write(*,*) dv

end program

subroutine co_ru_pes(c,v,idv,dv)
implicit none

real*8,intent(in) :: c(6,1)!! Cartesian of C O on Ru(0001) surface, Angstrom
real*8,intent(out) :: v(1) !! Potential Energy in eV
integer,intent(in) :: idv   !! 0: energy only; 1: energy and force
real*8,intent(out) :: dv(6,1)
real*8 :: ctrans(6,1),dvtrans(6,1),frac(6,1),zmat(6,1),dc,cx(6,1),cy(6,1),vx(1),vy(1),dvt(6,1)
integer :: j

real*8 :: v1,v2,v3,v4,v5

!! calculate potential energy
ctrans=c
call cart2frac(ctrans,frac)
call frac2unit(frac,ctrans,zmat,2,0)
call nnfit_1(6,1,ctrans,v,0,dvtrans)
!
!                               1 analytical derivatives, but directions should be rotated back

!! calculate derivatives numerically
if(idv.eq.1) then
  dv=0.d0
  dc=1.d-3
  do j=1,6
    cx=c; cx(j,1)=cx(j,1)-dc
    cy=c; cy(j,1)=cy(j,1)+dc

    ctrans=cx
    call cart2frac(ctrans,frac)
    call frac2unit(frac,ctrans,zmat,2,0)
    call nnfit_1(6,1,ctrans,vx,0,dvt)
  end do
end if

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ctrans=cy
call cart2frac(ctrans,frac)
call frac2unit(frac,ctrans,zmat,2,0)
call nnfit_1(6,1,ctrans,vy,0,dvt)

dv(j,1)=(vy(1)-vx(1))/2.d0/dc
enddo
endif

return
end subroutine

subroutine nnfit_1(ndim,ntot,r0,vx,idv,dv)
implicit none
integer,intent(in) :: ndim,ntot
real*8,intent(in) :: r0(ndim,ntot)
real*8,intent(out) :: vx(ntot)

integer,parameter :: s0=6,s1=40,s2=40
character*99,save :: wfile="nnfit_3.14.txt"
real*8,save :: w1(s0,s1),b1(s1),w2(s1,s2),b2(s2),w3(s2),rg(2,s0),vg(2)

integer :: idv
real*8 :: dv(ndim,ntot)
integer :: i,j,k,l
integer,save :: init=0
integer :: fid
if(ndim.ne.s0) stop "ndim .ne. s0"
if (init.eq.0) then
    init=1
!fid=123456
!open(fid,file=trim(wfile),status='old',action='read')
!read(fid,*) w1,b1,w2,b2,w3,rg,vg
!close(fid)
!do j=1,s1
!do i=1,s0
!    write(fid+1,'(4x,a,i4,a,i4,a,es24.16)') "w1(",i,"",j,"")=",w1(i,j)
!enddo
!enddo
!do j=1,s1
!    write(fid+1,'(4x,a,i4,a,es24.16)') "b1(",j,"")=",b1(j)
!enddo
!do k=1,s2
!do j=1,s1
!    write(fid+1,'(4x,a,i4,a,i4,a,es24.16)') "w2(",j,"",k,"")=",w2(j,k)
!enddo
!enddo
!do k=1,s2
!    write(fid+1,'(4x,a,i4,a,es24.16)') "b2(",k,"")=",b2(k)
!enddo
!do k=1,s2
!    write(fid+1,'(4x,a,i4,a,es24.16)') "w3(",k,"")=",w3(k)
!enddo
!write(fid+1,'(4x,a,es24.16)') "b3=",b3
!do j=1,s0
!do i=1,2
!    write(fid+1,'(4x,a,i4,a,i4,a,es24.16)') "rg(",i,"",j,"")=",rg(i,j)
!enddo
!enddo
!do i=1,2
!    write(fid+1,'(4x,a,i4,a,es24.16)') "vg(",i,"")=",vg(i)
!enddo

w1( 1, 1)= -2.0506595834700500E-01
w1( 2, 1)= -1.3955749911561499E-01
w1( 3, 1)=  8.6309827904072201E-01
w1( 4, 1)= -1.7261056142074299E-01
w1( 5, 1)= -1.1723721059029900E-01
w1( 6, 1)=  7.7359541804345247E-02
w1( 1, 2)= -2.5615690256426898E-01
w1( 2, 2)= -2.0457378657918199E-01
w1( 3, 2)=  1.9928697148143499E+00
w1( 4, 2)=  2.6451781389495299E-01
w1( 5, 2)=  2.1018562165276200E-01
w1( 6, 2)= -1.9541897708176199E+00
w1( 1, 3)= -4.0722228734867499E-01
w1( 2, 3)=  7.2081664290937697E-01
w1( 3, 3)= -4.6886703029766302E-01
w1( 4, 3)=  1.4430835173131501E-01
w1( 5, 3)= -2.8190381405838599E-01
w1( 6, 3)=  5.1121310071646697E-01
w1( 1, 4)=  1.2455494201877799E-01
w1( 2, 4)=  7.6612887978460220E-02

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w1( 3,  4)= 7.4371838561955095E-01
w1( 4,  4)= 1.5948250551583501E-01
w1( 5,  4)= 1.3802632807870299E-01
w1( 6,  4)= 1.9009339222552499E+00
w1( 1,  5)= -3.2338881598980401E-01
w1( 2,  5)= -2.3116774064105799E-01
w1( 3,  5)= -1.9441995235932599E-01
w1( 4,  5)= 7.9250959889926598E-01
w1( 5,  5)= 6.2348823677816800E-01
w1( 6,  5)= -6.8762852082289827E-02
w1( 1,  6)= 1.0904393178197900E+00
w1( 2,  6)= 4.3904050132490802E-01
w1( 3,  6)= 1.2321806617366200E+00
w1( 4,  6)= -1.2567015562342601E+00
w1( 5,  6)= -4.3117381416732298E-01
w1( 6,  6)= 1.2621570154931701E+00
w1( 1,  7)= 2.5575933212724900E-01
w1( 2,  7)= 9.4332210490800497E-02
w1( 3,  7)= -1.5844548027150900E+00
w1( 4,  7)= -3.6069987661340902E-01
w1( 5,  7)= -2.2591182893066400E-01
w1( 6,  7)= 2.1000440917857699E-01
w1( 1,  8)= -6.0137538440460103E-01
w1( 2,  8)= 1.3476600977953099E-01
w1( 3,  8)= -1.5675079699009000E+00
w1( 4,  8)= 6.3020958575156705E-01
w1( 5,  8)= -1.4102809282401599E-01
w1( 6,  8)= 1.5346030485728701E+00
w1( 1,  9)= 5.7582085579562503E-01
w1( 2,  9)= -3.2610185566580802E-01
w1( 3,  9)= 1.1721700721749100E+00
w1( 4,  9)= -2.3803169429074500E-01
w1( 5,  9)= 1.2136411279102600E-01
w1( 6,  9)= -3.6806039454088801E-01
w1( 1, 10)= 1.1450634303475200E-01
w1( 2, 10)= -6.9150116537808304E-01
w1( 3, 10)= 5.8963878118905699E-01
w1( 4, 10)= -1.2137300038178900E-01
w1( 5, 10)= 7.1411831099627998E-01
w1( 6, 10)= -5.8087586750221099E-01
w1( 1, 11)= 1.8005203706546499E-01
w1( 2, 11)= -6.4024853312810803E-01
w1( 3, 11)= -1.1682384521966700E+00
w1( 4, 11)= 7.1547843021494542E-02
w1( 5, 11)= -3.1756230205852469E-03
w1( 6, 11)= 5.1862158884580500E-01
w1( 1, 12)= 1.1009537298506800E-01
w1( 2, 12)= 2.0246633603900299E-01
w1( 3, 12)= 1.0228085277366801E+00
w1( 4, 12)= -1.1133945101579500E-01
w1( 5, 12)= -2.0914112006816599E-01
w1( 6, 12)= -1.0041051104675600E+00
w1( 1, 13)= -2.8022007819788403E-01
w1( 2, 13)= -1.9497213006956901E-01
w1( 3, 13)= 1.8559122748986900E+00
w1( 4, 13)= 2.9082178712334900E-01
w1( 5, 13)= 1.9959409997275199E-01
w1( 6, 13)= -1.8174077279362599E+00
w1( 1, 14)= 3.0277885285360401E-01
w1( 2, 14)= -5.7552348411102627E-02
w1( 3, 14)= 1.6326609318252101E+00
w1( 4, 14)= -6.2330661870471904E-01
w1( 5, 14)= 2.9650633350379102E-01
w1( 6, 14)= -7.8028757886962097E-01
w1( 1, 15)= -1.6508844768869699E-01
w1( 2, 15)= -1.3567503346399901E-01
w1( 3, 15)= 1.7485164054718999E-01
w1( 4, 15)= -4.1137895081659298E-01
w1( 5, 15)= -2.4836760603006200E-01
w1( 6, 15)= 1.8069218176735400E+00
w1( 1, 16)= 1.0727792733253100E-01
w1( 2, 16)= 1.5180081331467889E-02
w1( 3, 16)= 1.0178187990453900E+00
w1( 4, 16)= 2.6751683333082998E-01
w1( 5, 16)= -5.7714644556529004E-01
w1( 6, 16)= -8.7553547926185904E-01
w1( 1, 17)= 2.0076887155581959E-02
w1( 2, 17)= 8.0462179444227300E-01
w1( 3, 17)= 2.1055895523831598E+00
w1( 4, 17)= -7.8761485806632774E-03
w1( 5, 17)= -8.4508522840833200E-01
w1( 6, 17)= -2.0476425003128700E+00

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w1( 1, 18)= -4.3544002229486067E-02
w1( 2, 18)=  3.0644680949102970E-02
w1( 3, 18)= -1.3681075156592699E+00
w1( 4, 18)=  6.7144368733846146E-02
w1( 5, 18)= -1.0788683128676700E-01
w1( 6, 18)=  3.0432392809287161E-02
w1( 1, 19)=  1.1206031857744001E+00
w1( 2, 19)=  6.8943857327431102E-01
w1( 3, 19)=  4.9465051340335302E+00
w1( 4, 19)= -4.7726895088037502E-01
w1( 5, 19)= -3.2261449713906998E-01
w1( 6, 19)= -1.6832979658505600E+00
w1( 1, 20)= -5.2589469657469801E-01
w1( 2, 20)=  2.3703483502709499E-01
w1( 3, 20)=  4.8234018493273501E-01
w1( 4, 20)=  5.4663383261737097E-01
w1( 5, 20)= -2.4409260076454900E-01
w1( 6, 20)= -4.7130148599702099E-01
w1( 1, 21)= -7.2175317550550200E-01
w1( 2, 21)=  3.2029862551720001E-01
w1( 3, 21)=  6.2993565833426501E-01
w1( 4, 21)=  7.4964808381232395E-01
w1( 5, 21)= -3.2868338458750301E-01
w1( 6, 21)= -6.1983450993436395E-01
w1( 1, 22)=  9.7106784157472303E-01
w1( 2, 22)=  5.5163655187215899E-01
w1( 3, 22)=  2.3135828748459599E+00
w1( 4, 22)= -4.1722216573561499E-01
w1( 5, 22)= -4.3922845647000502E-01
w1( 6, 22)= -1.8287675499255800E+00
w1( 1, 23)= -6.8719896991660101E-01
w1( 2, 23)= -5.2544923881451899E-01
w1( 3, 23)=  7.9623935517755193E-02
w1( 4, 23)=  7.1283297225211895E-01
w1( 5, 23)=  5.3711642322871100E-01
w1( 6, 23)= -7.5706278485819650E-02
w1( 1, 24)=  6.6137372164290706E-02
w1( 2, 24)= -3.1087165870201100E-01
w1( 3, 24)= -1.0334798987574101E+00
w1( 4, 24)= -3.2627464362428020E-02
w1( 5, 24)=  2.6984085105684402E-01
w1( 6, 24)=  1.0606346412338099E+00
w1( 1, 25)=  1.7949283644847120E-02
w1( 2, 25)= -8.3759927018974334E-02
w1( 3, 25)=  9.0438692982000102E-01
w1( 4, 25)= -9.6559623896292787E-02
w1( 5, 25)= -4.9852640919902991E-02
w1( 6, 25)=  5.3588554921857101E-01
w1( 1, 26)= -4.2311129938409398E-01
w1( 2, 26)=  8.4982845018524586E-02
w1( 3, 26)= -1.1603247851511800E+00
w1( 4, 26)=  4.3426613107203799E-01
w1( 5, 26)= -8.4342076962622886E-02
w1( 6, 26)=  1.1386011135681600E+00
w1( 1, 27)= -6.1483196682869008E-02
w1( 2, 27)=  7.8942752269793123E-02
w1( 3, 27)= -1.0324524724760400E+00
w1( 4, 27)=  6.2237476678483020E-02
w1( 5, 27)=  3.2802107279979580E-05
w1( 6, 27)= -4.5404511513603502E-01
w1( 1, 28)=  4.9197675273609770E-02
w1( 2, 28)=  4.0304183060807838E-02
w1( 3, 28)= -1.5065070910109100E+00
w1( 4, 28)=  5.4316748846674250E-02
w1( 5, 28)=  1.4089953316283399E-01
w1( 6, 28)= -1.9203232182274399E+00
w1( 1, 29)= -1.0460717233233401E-01
w1( 2, 29)= -8.9520564440339498E-02
w1( 3, 29)= -2.7689435538249301E+00
w1( 4, 29)=  1.9311579847037100E-01
w1( 5, 29)=  1.4555299502497801E-01
w1( 6, 29)=  1.2512693347568700E+00
w1( 1, 30)= -5.8590915760900997E-01
w1( 2, 30)=  6.7919513348222804E-01
w1( 3, 30)= -1.4719751762944500E+00
w1( 4, 30)=  5.4813656782739295E-01
w1( 5, 30)= -5.3832350041709098E-01
w1( 6, 30)=  1.2571164121671401E+00
w1( 1, 31)= -2.6652282335664002E-01
w1( 2, 31)=  2.4808928993303800E-01
w1( 3, 31)=  3.9188209354786029E-02
w1( 4, 31)=  4.9388505686232521E-02

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w1( 5, 31)= 8.7113643111328326E-02
w1( 6, 31)= 5.6352463183064405E-01
w1( 1, 32)= -1.2821362242034600E+00
w1( 2, 32)= -7.2093087509691700E-01
w1( 3, 32)= 3.1984917820874798E-01
w1( 4, 32)= 2.7930501433516441E-02
w1( 5, 32)= 1.2387722524101729E-02
w1( 6, 32)= 1.9760810552779001E-01
w1( 1, 33)= -5.4620800742438702E-01
w1( 2, 33)= -3.8899434244686598E-01
w1( 3, 33)= 3.5549859579241033E-02
w1( 4, 33)= 5.6625504287642303E-01
w1( 5, 33)= 3.9916443742481300E-01
w1( 6, 33)= -3.7730287059362787E-02
w1( 1, 34)= -1.2678104696595399E-01
w1( 2, 34)= 6.3717477171090897E-01
w1( 3, 34)= -5.4298194494470498E-01
w1( 4, 34)= 1.2980125222934399E-01
w1( 5, 34)= -6.5059240510162997E-01
w1( 6, 34)= 5.3254456647593396E-01
w1( 1, 35)= -6.5722456884999303E-01
w1( 2, 35)= 1.2497169790723800E-01
w1( 3, 35)= -1.4953963031470701E+00
w1( 4, 35)= 6.7281552683799595E-01
w1( 5, 35)= -1.2310588114354901E-01
w1( 6, 35)= 1.4668063682513199E+00
w1( 1, 36)= -6.4307632429818490E-02
w1( 2, 36)= -2.1801914003036901E-01
w1( 3, 36)= 1.7610100663285899E-01
w1( 4, 36)= -5.4708493301694805E-01
w1( 5, 36)= 4.4369418778333097E-01
w1( 6, 36)= 2.6600688213995798E+00
w1( 1, 37)= 3.1749339285973999E-01
w1( 2, 37)= -6.6816750201970199E-01
w1( 3, 37)= -1.9760105050544499E-01
w1( 4, 37)= 5.5356361856973131E-02
w1( 5, 37)= -2.0715946835717148E-03
w1( 6, 37)= 5.7935673386292692E-02
w1( 1, 38)= -5.2213044296158195E-01
w1( 2, 38)= -2.8418335534522299E-01
w1( 3, 38)= -1.3011565585655800E+00
w1( 4, 38)= 5.4185654312408305E-01
w1( 5, 38)= 2.4127456219597801E-01
w1( 6, 38)= 1.2177062790712900E+00
w1( 1, 39)= 1.3799176693895750E-02
w1( 2, 39)= 4.1680150926787102E-01
w1( 3, 39)= 1.0473531918456900E+00
w1( 4, 39)= -1.6323076335620579E-02
w1( 5, 39)= -4.2682354584687199E-01
w1( 6, 39)= -1.0273613424432000E+00
w1( 1, 40)= -4.1636517010758001E-01
w1( 2, 40)= 5.3297406838705796E-01
w1( 3, 40)= -1.4716075162164399E+00
w1( 4, 40)= 3.8065625544342702E-01
w1( 5, 40)= -5.8737189338448104E-01
w1( 6, 40)= 7.3070810894074900E-01
b1( 1)= 1.2356602763579101E+00
b1( 2)= -8.9708599007291201E-01
b1( 3)= 9.9544427325269402E-01
b1( 4)= 2.9037099063111298E+00
b1( 5)= -7.8139642381587104E-01
b1( 6)= 3.8209721611296699E+00
b1( 7)= -6.5692508621978496E-01
b1( 8)= 8.0908598540285104E-01
b1( 9)= 7.5454844543538702E-01
b1( 10)= 8.4737062457397605E-01
b1( 11)= -7.6508974623279602E-01
b1( 12)= -7.5687338141411498E-01
b1( 13)= 7.7800865503612504E-01
b1( 14)= -3.5228176970670300E-01
b1( 15)= 2.3062270140224701E+00
b1( 16)= -1.0558844336900199E+00
b1( 17)= -3.3460288642320002E+00
b1( 18)= -7.0419810601585198E-01
b1( 19)= 5.0425696728970699E+00
b1( 20)= -7.8083344444584202E-01
b1( 21)= 7.5925446564087296E-01
b1( 22)= 1.4666167778421599E+00
b1( 23)= -8.5500369351851102E-01
b1( 24)= 2.8833055071777602E-01
b1( 25)= 3.4272984245590399E+00
b1( 26)= -8.1086602562689503E-01

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b1( 27)= -1.5007736765806301E+00
b1( 28)= -3.3908843143634502E+00
b1( 29)= -9.8848285324881302E-01
b1( 30)= 1.2725212450573600E+00
b1( 31)= 3.1376491529846601E-01
b1( 32)= 3.9793315198063500E-01
b1( 33)= 7.8422832960510802E-01
b1( 34)= 7.8818614167985301E-01
b1( 35)= -2.7829070424535400E+00
b1( 36)= 3.0833412728763800E+00
b1( 37)= -7.5636815058865603E-01
b1( 38)= 1.7058353859852300E+00
b1( 39)= 5.5171230238427604E-01
b1( 40)= -6.3164394820663705E-01
w2(  1,  1)= 1.0376435215163700E-01
w2(  2,  1)= 2.6778213695132602E+00
w2(  3,  1)= 1.9466541257131100E+00
w2(  4,  1)= 9.2835247571934698E-01
w2(  5,  1)= -1.1516050348191400E+00
w2(  6,  1)= 1.7507717298408201E+00
w2(  7,  1)= -4.6293369472211197E+00
w2(  8,  1)= 1.4928869866453401E-01
w2(  9,  1)= -2.8828473756242101E-01
w2( 10,  1)= 2.0467168460661700E-01
w2( 11,  1)= -8.3182172990636905E-01
w2( 12,  1)= -2.0789617633392901E+00
w2( 13,  1)= 2.9891481845559498E-01
w2( 14,  1)= -2.5123660132827301E+00
w2( 15,  1)= -2.3037533765822098E+00
w2( 16,  1)= -2.4511508126995500E+00
w2( 17,  1)= -3.2365961951085298E+00
w2( 18,  1)= -3.6957698626283098E-01
w2( 19,  1)= -4.8678139209858502E+00
w2( 20,  1)= 3.1668125189458900E+00
w2( 21,  1)= 1.9049769006024200E+00
w2( 22,  1)= -1.7700685813216399E-01
w2( 23,  1)= -4.3898888724075800E+00
w2( 24,  1)= -1.5184458649654500E+00
w2( 25,  1)= 2.2674119974636802E+00
w2( 26,  1)= 4.5555190225233000E-01
w2( 27,  1)= 1.2634817809506900E+00
w2( 28,  1)= -5.4508348680410801E-01
w2( 29,  1)= 8.5298916285512105E-01
w2( 30,  1)= -6.5110726815358100E-01
w2( 31,  1)= 5.7909903044099398E+00
w2( 32,  1)= 5.5671058344409496E-01
w2( 33,  1)= -4.1394820191708401E+00
w2( 34,  1)= -7.9181520502338815E-02
w2( 35,  1)= 4.4424634619329001E-01
w2( 36,  1)= -4.8072923215404201E-01
w2( 37,  1)= 6.5298299466806498E+00
w2( 38,  1)= -6.0330709872389698E-01
w2( 39,  1)= 1.1460355628023999E-01
w2( 40,  1)= -3.4647232420248799E+00
w2(  1,  2)= 3.9695762004078601E+00
w2(  2,  2)= -1.3199672388415100E+00
w2(  3,  2)= 2.6104169267587398E+00
w2(  4,  2)= -5.8256996993114796E-01
w2(  5,  2)= 2.5326235988714201E+00
w2(  6,  2)= 1.5376790022617301E-01
w2(  7,  2)= 3.9550150710578400E+00
w2(  8,  2)= -7.9139595678401398E-01
w2(  9,  2)= 5.2382498818130996E-01
w2( 10,  2)= 1.6107471827185400E+00
w2( 11,  2)= 3.2144950513982001E-01
w2( 12,  2)= -2.5166379256826479E-02
w2( 13,  2)= 1.2013032649147000E+00
w2( 14,  2)= 1.5262596677301199E+00
w2( 15,  2)= -3.7439920127279600E+00
w2( 16,  2)= 2.5308205614325701E+00
w2( 17,  2)= 6.3203404831094003E+00
w2( 18,  2)= -3.916455761050998E-01
w2( 19,  2)= -3.8274376002593802E+00
w2( 20,  2)= -6.5509824192374400E-01
w2( 21,  2)= 9.5419350016708904E-01
w2( 22,  2)= 1.7031386707611600E+00
w2( 23,  2)= -1.0665392906363500E+00
w2( 24,  2)= 2.7577126691932601E+00
w2( 25,  2)= -2.0149172874781902E+00
w2( 26,  2)= -1.9910473052738900E+00
w2( 27,  2)= -8.1650853332941598E+00
w2( 28,  2)= -3.0230471578916198E+00

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w2( 29, 2)= 4.6421291661330404E+00
w2( 30, 2)= 3.8548086105348198E+00
w2( 31, 2)= -5.7425956603214701E+00
w2( 32, 2)= 1.4040821232119600E+00
w2( 33, 2)= 4.3229286675594096E+00
w2( 34, 2)= -7.5441659160793995E-01
w2( 35, 2)= 1.7750669169347399E+00
w2( 36, 2)= -1.0655988390101601E-01
w2( 37, 2)= -5.2277676743602397E+00
w2( 38, 2)= -2.8754751541913701E+00
w2( 39, 2)= 1.0759618420711401E+00
w2( 40, 2)= 1.3413771591800601E+00
w2( 1, 3)= -3.9540998565021899E+00
w2( 2, 3)= 2.7304548080642701E+00
w2( 3, 3)= 1.2575337344832599E-01
w2( 4, 3)= -1.9243339583405601E+00
w2( 5, 3)= -3.0107103537542201E+00
w2( 6, 3)= 2.3778064939056600E+00
w2( 7, 3)= 1.6890438493648701E+00
w2( 8, 3)= 3.052853590303098E+00
w2( 9, 3)= -1.8909277300684899E+00
w2( 10, 3)= 3.9857588562389301E-01
w2( 11, 3)= 2.5977295803147199E-01
w2( 12, 3)= -6.7098724135980099E+00
w2( 13, 3)= 1.7497116045333501E+00
w2( 14, 3)= -3.5075774127294880E-02
w2( 15, 3)= -3.3810685460392400E+00
w2( 16, 3)= 1.8887767508545501E+00
w2( 17, 3)= -3.5459504033920699E+00
w2( 18, 3)= -4.8115649453235898E+00
w2( 19, 3)= 2.8861853398338502E+00
w2( 20, 3)= 3.5325837100708402E+00
w2( 21, 3)= 4.6673897361327824E-03
w2( 22, 3)= -1.0224830780439100E+00
w2( 23, 3)= 2.8008379960548400E+00
w2( 24, 3)= 6.1545693836533100E-01
w2( 25, 3)= 8.5109570932357204E-01
w2( 26, 3)= 4.9167552820493499E-01
w2( 27, 3)= -1.2054014633730199E+00
w2( 28, 3)= -1.8403097750816300E+00
w2( 29, 3)= -1.9064573479321201E+00
w2( 30, 3)= -2.7440362096635500E+00
w2( 31, 3)= 1.6479314358699599E+00
w2( 32, 3)= 6.9845820771176667E-02
w2( 33, 3)= -5.6359159140160200E+00
w2( 34, 3)= 8.3449794356943097E-01
w2( 35, 3)= -1.8503555046142901E+00
w2( 36, 3)= 4.0704857199103500E-01
w2( 37, 3)= -7.5471482735632800E-01
w2( 38, 3)= 1.7931760985927201E+00
w2( 39, 3)= -1.7998428004805200E+00
w2( 40, 3)= -4.0753897877910400E-01
w2( 1, 4)= 2.9022973057960502E+00
w2( 2, 4)= -1.0724399317685600E-01
w2( 3, 4)= -3.7166701350682598E+00
w2( 4, 4)= 2.1058668027603802E+00
w2( 5, 4)= 8.6274395791287595E-01
w2( 6, 4)= 8.0934202328511695E-01
w2( 7, 4)= -3.5164595843937798E+00
w2( 8, 4)= -6.2375936001914201E-01
w2( 9, 4)= 2.3275685824037602E+00
w2( 10, 4)= -1.1019493131761000E+00
w2( 11, 4)= -4.1835847914464903E+00
w2( 12, 4)= -2.2262694775459901E+00
w2( 13, 4)= 1.5319879219484001E-01
w2( 14, 4)= 1.5979390092976700E+00
w2( 15, 4)= 3.0386869102559402E+00
w2( 16, 4)= -3.2532698589389701E+00
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w2( 18, 4)= 2.4603790266829502E+00
w2( 19, 4)= -6.3265616236019495E-01
w2( 20, 4)= 9.2202895361334702E-01
w2( 21, 4)= -8.0548845966353100E-01
w2( 22, 4)= -8.5653072987795198E-01
w2( 23, 4)= -9.7901913185563105E-01
w2( 24, 4)= -8.4869618771046396E-01
w2( 25, 4)= -3.0230713076583302E+00
w2( 26, 4)= -4.2370885949170900E-01
w2( 27, 4)= 9.0922484519974296E-01
w2( 28, 4)= 1.2953454299169600E+00
w2( 29, 4)= 1.1699520476200700E+00
w2( 30, 4)= 3.3991871382345300E+00

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w2( 31, 4)= -3.2501046958000102E-01
w2( 32, 4)= -1.4339966086213399E-01
w2( 33, 4)= -1.1731413953946599E+00
w2( 34, 4)= 4.1435134216436997E-01
w2( 35, 4)= -1.7710043979898600E+00
w2( 36, 4)= -9.11803865558520599E-01
w2( 37, 4)= 3.2590829072371599E+00
w2( 38, 4)= -2.5800517560425101E-01
w2( 39, 4)= 5.0887134721097205E-01
w2( 40, 4)= 1.5191708588144599E+00
w2( 1, 5)= -1.1958407638395900E+00
w2( 2, 5)= 1.2585325241941700E-01
w2( 3, 5)= 2.1383741132159999E+00
w2( 4, 5)= -5.3229523396983702E-01
w2( 5, 5)= -6.6464762409411404E-01
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w2( 8, 5)= 2.2688395058821600E+00
w2( 9, 5)= -2.6551693187248899E+00
w2( 10, 5)= -5.6100063868374594E-01
w2( 11, 5)= -1.5108211880130500E+00
w2( 12, 5)= 3.2500701898238199E-01
w2( 13, 5)= 1.7463880553151001E+00
w2( 14, 5)= -8.8291714605077398E-01
w2( 15, 5)= 6.6933508094259020E-02
w2( 16, 5)= 3.9223930087354999E+00
w2( 17, 5)= -3.5469944364023700E+00
w2( 18, 5)= -2.9839775183618298E+00
w2( 19, 5)= -5.1042546660232502E-01
w2( 20, 5)= 3.9714491385891599E+00
w2( 21, 5)= -1.6893113238283599E+00
w2( 22, 5)= -1.2279998632714899E+00
w2( 23, 5)= 6.7017890340664099E-01
w2( 24, 5)= 3.5818886831670599E-01
w2( 25, 5)= 3.1467389801807899E+00
w2( 26, 5)= 1.6155578680770399E+00
w2( 27, 5)= -1.8964354897253599E-01
w2( 28, 5)= 9.4449944653557005E-01
w2( 29, 5)= 1.2161946599276701E+00
w2( 30, 5)= -4.7980212847687804E+00
w2( 31, 5)= -1.6231128943271000E+00
w2( 32, 5)= 4.1354461315912799E-01
w2( 33, 5)= -3.3417003895180999E+00
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w2( 35, 5)= -4.9209237379169997E+00
w2( 36, 5)= 5.6848507642046697E-01
w2( 37, 5)= 3.0044651810263001E-01
w2( 38, 5)= -3.9806590893528199E-01
w2( 39, 5)= -7.7607382818127602E-01
w2( 40, 5)= -1.3623855708566901E+00
w2( 1, 6)= 8.7969434938097901E+00
w2( 2, 6)= -2.3321680680691599E+00
w2( 3, 6)= 3.9419666884708653E-02
w2( 4, 6)= 2.8339625349056701E+00
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w2( 8, 6)= 1.8637702983385400E+00
w2( 9, 6)= 1.0562359691594201E+00
w2( 10, 6)= 1.5266982640187099E+00
w2( 11, 6)= 1.1543544402141499E+00
w2( 12, 6)= -1.3742323062579400E+00
w2( 13, 6)= -5.2634308550521403E-01
w2( 14, 6)= 1.6515140629046299E-01
w2( 15, 6)= -3.4846865873175731E-02
w2( 16, 6)= 8.9375583496997901E-01
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w2( 18, 6)= -8.9360328383701504E-01
w2( 19, 6)= 2.1347567299382701E+00
w2( 20, 6)= -1.8249154208448000E+00
w2( 21, 6)= 4.7817376885489579E-02
w2( 22, 6)= 1.0819899575056900E-01
w2( 23, 6)= -1.6541125500195799E+00
w2( 24, 6)= -5.4746513222618498E+00
w2( 25, 6)= 1.3085743833591199E+00
w2( 26, 6)= 3.1238012166439999E+00
w2( 27, 6)= 8.7682891848109392E+00
w2( 28, 6)= 1.3302682980884599E+00
w2( 29, 6)= -3.2067308209926799E+00
w2( 30, 6)= -1.6393363840166799E+00
w2( 31, 6)= 1.0228148470088900E+01
w2( 32, 6)= -2.1047860890648300E+00

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w2( 33, 6)= -1.4133192089591999E+00
w2( 34, 6)= -6.9308121773483400E-01
w2( 35, 6)= 1.3080636424687000E+00
w2( 36, 6)= 2.1321885227132001E-01
w2( 37, 6)= 6.1077072318607302E+00
w2( 38, 6)= 4.0909006306260798E+00
w2( 39, 6)= 1.1882172357069301E+00
w2( 40, 6)= -1.2169726556403000E+00
w2( 1, 7)= 3.1860807532772899E+00
w2( 2, 7)= -9.3059850913051001E-01
w2( 3, 7)= 4.8044366535644398E+00
w2( 4, 7)= -1.1362310847928601E+00
w2( 5, 7)= 4.0616830609841897E-01
w2( 6, 7)= 1.9287212711950599E-01
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w2( 8, 7)= 7.2363613766164903E-01
w2( 9, 7)= -1.3372294241714999E+00
w2( 10, 7)= -2.1990712104391799E-01
w2( 11, 7)= -1.0151537066284599E+00
w2( 12, 7)= -9.0986824345044504E-01
w2( 13, 7)= 1.1394425001233000E+00
w2( 14, 7)= 6.1780641337719960E-02
w2( 15, 7)= -1.2698789848990699E+00
w2( 16, 7)= -4.4899621678593299E-01
w2( 17, 7)= -3.0775491060179898E+00
w2( 18, 7)= -3.3086460822070900E+00
w2( 19, 7)= 1.7872283875674599E+00
w2( 20, 7)= 1.1578316838229099E+00
w2( 21, 7)= -1.0402509853623999E-01
w2( 22, 7)= -4.9468043234803299E-01
w2( 23, 7)= 1.0804271562733700E+00
w2( 24, 7)= 1.0245780334565799E+00
w2( 25, 7)= 2.6764682102013598E-01
w2( 26, 7)= -1.7871958788001301E+00
w2( 27, 7)= -2.5130824753736700E+00
w2( 28, 7)= 2.3815478266562802E+00
w2( 29, 7)= 1.8368248367196800E+00
w2( 30, 7)= -9.3933008017713304E-01
w2( 31, 7)= -1.6937932579362101E+00
w2( 32, 7)= -8.7304342856360670E-02
w2( 33, 7)= -9.9624220977662403E-01
w2( 34, 7)= -1.7015627293155200E+00
w2( 35, 7)= -1.0653531109262900E-01
w2( 36, 7)= 7.8114554924433839E-03
w2( 37, 7)= 3.0770546585490499E+00
w2( 38, 7)= -1.6077142599407401E-01
w2( 39, 7)= -3.0419502419918301E+00
w2( 40, 7)= 6.5346074978766322E-02
w2( 1, 8)= 2.6203117832546101E+00
w2( 2, 8)= 8.6714427938611505E-01
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w2( 4, 8)= 2.3181005761947202E+00
w2( 5, 8)= -2.2210937901561101E-01
w2( 6, 8)= 9.9669645009806858E-03
w2( 7, 8)= -8.4996836008723797E-01
w2( 8, 8)= -1.9449442009881599E+00
w2( 9, 8)= -2.0399232507996901E-01
w2( 10, 8)= -1.8002951694310600E+00
w2( 11, 8)= 3.6473226940186199E-01
w2( 12, 8)= 3.2787556324828602E+00
w2( 13, 8)= 7.1499421243101102E-01
w2( 14, 8)= 1.0817838964082500E+00
w2( 15, 8)= -7.2816686001955200E-01
w2( 16, 8)= 3.8296648143060602E-01
w2( 17, 8)= -5.6146867650724996E-01
w2( 18, 8)= -1.6957841400794400E+00
w2( 19, 8)= -7.8341155704281795E-01
w2( 20, 8)= -2.5877992984404501E+00
w2( 21, 8)= -2.1792729414367900E+00
w2( 22, 8)= 8.3380337009140174E-02
w2( 23, 8)= 1.4854531567385800E+00
w2( 24, 8)= 1.3119344545847700E+00
w2( 25, 8)= -1.7718999424303801E+00
w2( 26, 8)= -7.0179430948524787E-02
w2( 27, 8)= -2.3572386831066399E+00
w2( 28, 8)= 1.9534802262954101E+00
w2( 29, 8)= 4.4243294037613301E-01
w2( 30, 8)= 5.2934693695242299E+00
w2( 31, 8)= -2.5930440755980699E-01
w2( 32, 8)= -3.0783948471270400E-01
w2( 33, 8)= 2.3602062698668900E+00
w2( 34, 8)= 6.9284860083009003E-01

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w2( 35,  8)= -3.5930504838080701E-01
w2( 36,  8)=  3.4041030082052698E-01
w2( 37,  8)= -2.0283832064209899E+00
w2( 38,  8)=  1.1102080498526501E+00
w2( 39,  8)=  5.7820701817949804E-01
w2( 40,  8)=  1.8011632388871901E+00
w2(  1,  9)= -3.2764949482257399E-01
w2(  2,  9)=  2.7378633375762219E-02
w2(  3,  9)= -1.4275540419797601E+00
w2(  4,  9)=  3.8634328050454703E-01
w2(  5,  9)=  1.0353631662383260E-02
w2(  6,  9)= -1.3080338381571801E+00
w2(  7,  9)= -4.6382012216148699E-01
w2(  8,  9)= -1.1049194521482399E+00
w2(  9,  9)= -5.5399339329421904E-01
w2( 10,  9)=  8.4519174991167428E-02
w2( 11,  9)=  5.7313435297456905E-01
w2( 12,  9)=  2.5384450107860399E+00
w2( 13,  9)=  2.4394750587296599E-01
w2( 14,  9)=  1.0815931186292510E-02
w2( 15,  9)=  4.2298667142856899E-01
w2( 16,  9)=  9.9029318806769628E-02
w2( 17,  9)= -6.9119088334659096E-01
w2( 18,  9)=  4.8709651227796003E-01
w2( 19,  9)=  7.5239240747818303E-01
w2( 20,  9)= -9.4216933743032805E-01
w2( 21,  9)=  4.6346807930633199E-01
w2( 22,  9)=  2.6381840899411702E-01
w2( 23,  9)= -7.6658688565194100E-01
w2( 24,  9)=  2.9667512842512198E+00
w2( 25,  9)=  1.0173076984710100E-01
w2( 26,  9)= -6.5580013674022597E-01
w2( 27,  9)=  3.4660768737520300E+00
w2( 28,  9)=  4.3365287889028298E-01
w2( 29,  9)= -1.3934729060919601E-01
w2( 30,  9)=  2.2827563718245898E+00
w2( 31,  9)=  7.0200371148756202E-01
w2( 32,  9)=  1.7247742733018521E-02
w2( 33,  9)=  3.0771034282288900E-01
w2( 34,  9)= -6.3933154328670705E-01
w2( 35,  9)=  3.3485775736928098E+00
w2( 36,  9)= -6.8029506301810305E-01
w2( 37,  9)= -8.3364099009752701E-01
w2( 38,  9)=  4.1920237620458201E+00
w2( 39,  9)=  1.9307825577116100E+00
w2( 40,  9)= -1.6247302762615101E-01
w2(  1, 10)= -1.5533721676127501E+00
w2(  2, 10)= -2.1786736048004198E+00
w2(  3, 10)= -1.2965572438053601E+00
w2(  4, 10)=  5.5016899021689367E-02
w2(  5, 10)=  8.6817006158732302E-01
w2(  6, 10)= -2.0118313632820799E+00
w2(  7, 10)= -5.9497558899261505E-01
w2(  8, 10)=  2.9434633591827000E+00
w2(  9, 10)= -9.7687869032958397E-01
w2( 10, 10)=  1.9395666508597400E+00
w2( 11, 10)=  3.1774003591802300E+00
w2( 12, 10)= -7.3712433527147603E+00
w2( 13, 10)= -2.0214574470172599E+00
w2( 14, 10)=  2.2615917970872399E+00
w2( 15, 10)= -1.2893028066455900E+00
w2( 16, 10)=  3.4541724527483701E+00
w2( 17, 10)=  2.7585954592162998E+00
w2( 18, 10)= -1.2269761026470600E+00
w2( 19, 10)=  4.4195823346517900E+00
w2( 20, 10)=  2.9456839672015001E+00
w2( 21, 10)=  3.3719593879305600E+00
w2( 22, 10)=  5.0807843781285200E-01
w2( 23, 10)= -3.0273656741990602E+00
w2( 24, 10)= -1.1622719051018000E+00
w2( 25, 10)= -4.9135258397284798E-01
w2( 26, 10)=  2.2645565687019200E+00
w2( 27, 10)= -1.4805606613846001E+00
w2( 28, 10)=  1.3819543715825100E+00
w2( 29, 10)= -2.3698940739235499E+00
w2( 30, 10)= -1.7898065427733600E+00
w2( 31, 10)= -7.61707771679198401E-01
w2( 32, 10)= -7.4219508989772184E-02
w2( 33, 10)= -4.2206652854774500E+00
w2( 34, 10)=  4.1819810815604003E-01
w2( 35, 10)= -1.5927815635010401E+00
w2( 36, 10)=  1.9999896101370300E+00

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w2( 37, 10)= -4.2228073838260203E+00
w2( 38, 10)= 1.4544114551120499E+00
w2( 39, 10)= -1.8144599758454600E+00
w2( 40, 10)= -2.2765546817745901E+00
w2( 1, 11)= 9.0368093473069538E-02
w2( 2, 11)= 4.8213936080505801E+00
w2( 3, 11)= 1.1166604332560399E-01
w2( 4, 11)= 5.6090375051798103E-01
w2( 5, 11)= 9.7800069485247332E-02
w2( 6, 11)= 1.0860459436948899E+00
w2( 7, 11)= 3.2351476704942201E+00
w2( 8, 11)= 3.8909298087740102E-01
w2( 9, 11)= -1.8533650450482200E-01
w2( 10, 11)= -1.4924729089570701E+00
w2( 11, 11)= -1.0921335482977399E+00
w2( 12, 11)= 6.6013131967700200E+00
w2( 13, 11)= 2.9856717763714302E-01
w2( 14, 11)= 1.0077801009947630E-02
w2( 15, 11)= 2.1214196769704499E-01
w2( 16, 11)= -1.2406726695439001E+00
w2( 17, 11)= -9.1587061799216080E-02
w2( 18, 11)= 1.4826329049307900E+00
w2( 19, 11)= -5.1349598492744297E+00
w2( 20, 11)= -3.0117140630381201E+00
w2( 21, 11)= 4.9951613995619898E-01
w2( 22, 11)= 1.6217639371011501E+00
w2( 23, 11)= 8.2932056819686895E-01
w2( 24, 11)= 5.4603318881300000E-01
w2( 25, 11)= 5.0118589483242804E-01
w2( 26, 11)= 1.2166922350633300E+00
w2( 27, 11)= -5.2003218308697396E-01
w2( 28, 11)= -1.3738881084165799E+00
w2( 29, 11)= 4.1922519467662802E+00
w2( 30, 11)= -1.7394991831243201E+00
w2( 31, 11)= -2.3936374501922102E+00
w2( 32, 11)= 2.8858247990399299E-01
w2( 33, 11)= 3.7817582692995599E+00
w2( 34, 11)= 6.4024943900742102E+00
w2( 35, 11)= 2.4696379997848399E+00
w2( 36, 11)= -3.6821400874179999E-01
w2( 37, 11)= -9.6897262453364597E-01
w2( 38, 11)= -2.6910872904357901E+00
w2( 39, 11)= -1.8912181629958300E+00
w2( 40, 11)= -2.7337005831560002E+00
w2( 1, 12)= 3.6614930872565301E+00
w2( 2, 12)= 2.3062228487228000E+00
w2( 3, 12)= -6.4387019886077002E-01
w2( 4, 12)= -1.0398180301605999E+00
w2( 5, 12)= -1.4740495142989300E-02
w2( 6, 12)= -5.8751521147545915E-04
w2( 7, 12)= 4.0602580879245496E+00
w2( 8, 12)= -1.7458946524112100E+00
w2( 9, 12)= -2.8301912637434001E+00
w2( 10, 12)= -5.7822346055407403E-01
w2( 11, 12)= 3.0960755582877799E+00
w2( 12, 12)= -2.8475414967228398E+00
w2( 13, 12)= 2.7536454128187500E+00
w2( 14, 12)= 1.7397333353535600E+00
w2( 15, 12)= -2.3895570507701001E+00
w2( 16, 12)= 2.3932266545918099E+00
w2( 17, 12)= -7.3235999454829304E-01
w2( 18, 12)= -1.0877245087738701E+00
w2( 19, 12)= 7.2263469305564998E-01
w2( 20, 12)= -1.9845846944122301E+00
w2( 21, 12)= 1.3123378390088661E-02
w2( 22, 12)= 1.8098423929279599E+00
w2( 23, 12)= 1.8075943722330301E+00
w2( 24, 12)= 1.6552672338556000E+00
w2( 25, 12)= -4.1324698704700200E+00
w2( 26, 12)= -7.9986331880672701E-01
w2( 27, 12)= -1.5979639769666201E+00
w2( 28, 12)= -8.9601624830845905E-01
w2( 29, 12)= 1.5370746622465101E-01
w2( 30, 12)= 2.3919203641215399E+00
w2( 31, 12)= -2.9816152701504000E+00
w2( 32, 12)= -9.8308600210277897E-01
w2( 33, 12)= 9.1650850299035103E-01
w2( 34, 12)= 1.4278365289453401E+00
w2( 35, 12)= -1.3977759959503400E+00
w2( 36, 12)= 5.6200235205746296E-01
w2( 37, 12)= -5.3498054626711502E+00
w2( 38, 12)= -3.0338643596737400E+00

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w2( 39, 12) = -4.1258046065310499E+00
w2( 40, 12) =  1.7597895876795000E+00
w2(  1, 13) = -4.1487075043230293E-02
w2(  2, 13) =  3.9396682399460299E+00
w2(  3, 13) =  4.1778661616168812E-02
w2(  4, 13) =  7.9484472277026735E-02
w2(  5, 13) =  6.8810956512374974E-03
w2(  6, 13) = -1.7361661278600869E-02
w2(  7, 13) =  9.5916283969000801E-03
w2(  8, 13) = -2.8693962961674502E+00
w2(  9, 13) = -1.9196093785096460E-03
w2( 10, 13) = -4.4917150950147402E+00
w2( 11, 13) =  2.8060783287015251E-02
w2( 12, 13) =  1.2384358779539900E+01
w2( 13, 13) = -4.6015952404626796E+00
w2( 14, 13) =  1.0982307628476619E-03
w2( 15, 13) = -2.9024135544429260E-03
w2( 16, 13) =  1.5107924607912659E-02
w2( 17, 13) = -1.2117502705578600E+01
w2( 18, 13) = -7.3433076753528254E-02
w2( 19, 13) = -7.2067536266602174E-03
w2( 20, 13) =  1.0670362760876801E+01
w2( 21, 13) = -3.1294124536129799E+00
w2( 22, 13) =  5.6594947677973267E-03
w2( 23, 13) =  2.5624229885218401E+00
w2( 24, 13) = -6.4044981670141099E-01
w2( 25, 13) =  1.3302248744846700E+01
w2( 26, 13) =  8.6960207414281196E+00
w2( 27, 13) =  3.8296389653706098E-01
w2( 28, 13) =  1.9515247772084199E-01
w2( 29, 13) =  4.6480574786401819E-03
w2( 30, 13) = -2.9764410631642840E-02
w2( 31, 13) = -1.2558630401455960E-02
w2( 32, 13) =  2.0825652292525308E-03
w2( 33, 13) = -8.5991148583610997E+00
w2( 34, 13) = -7.1025023793746396E+00
w2( 35, 13) = -1.0710642559245301E+01
w2( 36, 13) = -8.0758057856727770E-03
w2( 37, 13) = -1.9599374208144092E-02
w2( 38, 13) =  2.2142367430483001E-01
w2( 39, 13) = -1.0672663659677500E+01
w2( 40, 13) =  1.0005064361399260E-02
w2(  1, 14) =  6.4014594211123499E-01
w2(  2, 14) = -2.0032522345566202E+00
w2(  3, 14) =  2.3629350951101200E-01
w2(  4, 14) = -7.8620615149955997E-01
w2(  5, 14) =  1.1458910769046899E+00
w2(  6, 14) =  1.6750449464448200E-01
w2(  7, 14) = -2.7656768366051301E+00
w2(  8, 14) =  1.4505482364123501E+00
w2(  9, 14) =  4.8782234302607402E-01
w2( 10, 14) = -8.2002375927740601E-01
w2( 11, 14) = -1.2743966778079501E+00
w2( 12, 14) = -5.8921797070149697E+00
w2( 13, 14) = -1.6373991310204099E+00
w2( 14, 14) =  2.0044321222668202E+00
w2( 15, 14) = -4.9178570448968101E-01
w2( 16, 14) =  7.8513832154437802E-01
w2( 17, 14) = -1.1680759240322400E+00
w2( 18, 14) = -7.9423690371065503E-01
w2( 19, 14) =  1.0786985536357101E+00
w2( 20, 14) =  8.4650732772145698E-01
w2( 21, 14) =  3.6623051542237001E-01
w2( 22, 14) = -7.9169208900346499E-01
w2( 23, 14) = -1.5127891185602700E+00
w2( 24, 14) = -2.0771669255448999E+00
w2( 25, 14) =  6.4254695084075300E+00
w2( 26, 14) = -9.8719884840493100E-01
w2( 27, 14) = -3.3534621306452600E-01
w2( 28, 14) =  4.2074896023854902E-01
w2( 29, 14) = -4.4829762042997601E-01
w2( 30, 14) = -9.0345560648393997E-02
w2( 31, 14) = -9.0259548529340194E-01
w2( 32, 14) =  6.7724455442558631E-02
w2( 33, 14) = -2.2317796489371302E+00
w2( 34, 14) =  4.2115285526444701E-01
w2( 35, 14) =  8.0180745850866799E+00
w2( 36, 14) =  6.2071691923193395E-01
w2( 37, 14) =  1.8400262234187399E+00
w2( 38, 14) = -1.9677997677908601E-01
w2( 39, 14) = -2.8473001245530699E-01
w2( 40, 14) = -1.7920855849389400E-01

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w2( 1, 15)= 6.9909451292005000E+00
w2( 2, 15)= 3.4798243431657001E+00
w2( 3, 15)= 4.2543573587700800E+00
w2( 4, 15)= -3.2318320558948201E+00
w2( 5, 15)= 5.9960492221151203E+00
w2( 6, 15)= 5.7859483681118000E+00
w2( 7, 15)= 5.1305502468053401E+00
w2( 8, 15)= 1.1030762583445300E-01
w2( 9, 15)= 4.0710313436461902E+00
w2( 10, 15)= -3.0225379957326699E+00
w2( 11, 15)= -5.5548375462218598E+00
w2( 12, 15)= -1.2705893580076100E+00
w2( 13, 15)= 2.8736065017506598E+00
w2( 14, 15)= 2.7296794016066199E+00
w2( 15, 15)= -5.0826815316329599E+00
w2( 16, 15)= 4.1667149123614902E+00
w2( 17, 15)= -3.7276073897053199E+00
w2( 18, 15)= -4.3207848697451201E+00
w2( 19, 15)= 7.0761624770140799E+00
w2( 20, 15)= 3.9259068004282600E+00
w2( 21, 15)= -2.6711407244175400E+00
w2( 22, 15)= -1.7122304027379800E+00
w2( 23, 15)= -1.0339823152154599E+00
w2( 24, 15)= 9.0415605419364393E+00
w2( 25, 15)= 4.6985522422559196E+00
w2( 26, 15)= 6.3375603075086095E-01
w2( 27, 15)= -5.5147357083408597E+00
w2( 28, 15)= -4.6804690230912199E-01
w2( 29, 15)= 3.2933820954019501E+00
w2( 30, 15)= 2.9322163827228498E+00
w2( 31, 15)= 5.2911212887699302E+00
w2( 32, 15)= 5.9860846418657222E-02
w2( 33, 15)= -2.1712797669690800E+00
w2( 34, 15)= -3.7069071820696600E+00
w2( 35, 15)= 1.1769313806564900E-01
w2( 36, 15)= 7.8625812435755704E-01
w2( 37, 15)= 7.6219520969803396E+00
w2( 38, 15)= -7.8047390699895498E+00
w2( 39, 15)= 4.0558675862650800E-01
w2( 40, 15)= 4.8879695829029099E+00
w2( 1, 16)= 1.1158346156323999E+00
w2( 2, 16)= -4.274033942548498E+00
w2( 3, 16)= -2.0427826681607701E+00
w2( 4, 16)= 4.4169909697807003E-01
w2( 5, 16)= 3.0425626648945800E+00
w2( 6, 16)= 3.3282189774925702E-01
w2( 7, 16)= -1.1541154322425500E+00
w2( 8, 16)= 3.8057214782490698E+00
w2( 9, 16)= -8.9703078334842301E-01
w2( 10, 16)= -1.9761305503361699E+00
w2( 11, 16)= -4.2115334581005098E-01
w2( 12, 16)= -1.4679776449179300E+00
w2( 13, 16)= -3.9141051341163000E+00
w2( 14, 16)= 4.1644535190007499E+00
w2( 15, 16)= -1.0022718251851099E+00
w2( 16, 16)= 1.7717871803316201E+00
w2( 17, 16)= 1.1213910179910801E-01
w2( 18, 16)= 1.3145746462116701E+00
w2( 19, 16)= -2.4366053281126701E+00
w2( 20, 16)= -1.9811537148292599E+00
w2( 21, 16)= 1.8212639400473800E+00
w2( 22, 16)= -1.7801871884222000E+00
w2( 23, 16)= -5.6926766203630497E-01
w2( 24, 16)= -1.2113952433496200E+00
w2( 25, 16)= -9.3537776043284104E-01
w2( 26, 16)= -3.2943264792845302E+00
w2( 27, 16)= -4.9967453216993301E+00
w2( 28, 16)= 1.8678720771324799E+00
w2( 29, 16)= 6.0152388812344804E-01
w2( 30, 16)= -1.3445842488132400E+00
w2( 31, 16)= -2.1138541086635798E+00
w2( 32, 16)= -9.1579443498251645E-02
w2( 33, 16)= 5.7414229011159703E+00
w2( 34, 16)= 4.9010602887293304E+00
w2( 35, 16)= 3.2278201540747800E+00
w2( 36, 16)= 7.5614295475822801E-01
w2( 37, 16)= -8.8981076518795499E-01
w2( 38, 16)= -8.6705554995630096E-01
w2( 39, 16)= 4.4465501946579700E+00
w2( 40, 16)= -4.6838761574932999E+00
w2( 1, 17)= 3.5016152475208200E+00
w2( 2, 17)= -2.3387965861214099E+00

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w2( 3, 17)= -9.1911615994305695E-01
w2( 4, 17)= -3.5186367728738701E+00
w2( 5, 17)=  3.9851215306144899E-01
w2( 6, 17)=  1.3012357411448501E+00
w2( 7, 17)=  1.5455707079430900E+00
w2( 8, 17)= -4.5358256268503698E+00
w2( 9, 17)=  1.7770497459423339E-02
w2( 10, 17)= -1.5208212239485600E-01
w2( 11, 17)=  1.1277109694690199E+00
w2( 12, 17)=  7.6946532129736955E-02
w2( 13, 17)= -4.0587489741008600E+00
w2( 14, 17)= -4.0157029222266200E-01
w2( 15, 17)= -4.1334016264279200E-01
w2( 16, 17)=  1.3690516094388401E+00
w2( 17, 17)= -2.8929694639334600E+00
w2( 18, 17)= -5.0725588699423796E-01
w2( 19, 17)= -8.8204526277085277E-02
w2( 20, 17)=  4.3982583180250900E+00
w2( 21, 17)=  1.2997201462589401E+00
w2( 22, 17)=  2.6710906920247401E-01
w2( 23, 17)=  1.5486698636094700E+00
w2( 24, 17)=  4.9142475850811101E-01
w2( 25, 17)= -6.5155324549735730E-02
w2( 26, 17)= -1.8045288420847001E+00
w2( 27, 17)= -3.3378127288505701E+00
w2( 28, 17)=  1.6411407183779001E+00
w2( 29, 17)=  8.3972197176112295E-01
w2( 30, 17)= -1.3160944154311101E+00
w2( 31, 17)=  2.0436950826878002E+00
w2( 32, 17)= -2.3453924780880600E-01
w2( 33, 17)= -1.0575680533185701E+00
w2( 34, 17)= -1.0024875238559201E+00
w2( 35, 17)= -1.8537888564088301E+00
w2( 36, 17)=  1.5752355387365300E+00
w2( 37, 17)= -1.3628627819151000E+00
w2( 38, 17)=  3.1013995289522200E+00
w2( 39, 17)=  7.1529034720283802E-01
w2( 40, 17)= -1.0095294362597400E+00
w2( 1, 18)=  2.1420175696413199E-01
w2( 2, 18)= -1.5825508194731599E+00
w2( 3, 18)= -4.7538455978429500E-01
w2( 4, 18)= -6.3989157941909003E-01
w2( 5, 18)=  1.3559548633961600E+00
w2( 6, 18)=  1.7142236872517599E-01
w2( 7, 18)= -1.1224970750505201E+00
w2( 8, 18)=  8.7777592686151895E-01
w2( 9, 18)=  1.2917528010149399E+00
w2( 10, 18)= -3.4191745237497201E-01
w2( 11, 18)= -9.3250717911032199E-01
w2( 12, 18)=  2.1350827108344599E+00
w2( 13, 18)= -2.3339889084833199E+00
w2( 14, 18)=  2.2035894624541301E+00
w2( 15, 18)= -1.8869060534931001E-01
w2( 16, 18)=  4.1186573261341303E-01
w2( 17, 18)= -1.2173425615433200E+00
w2( 18, 18)=  1.1897867758818600E-01
w2( 19, 18)=  2.2978632402765502E+00
w2( 20, 18)=  3.5012414189214800E+00
w2( 21, 18)=  7.0198847521131102E-01
w2( 22, 18)= -6.3898122253066103E-01
w2( 23, 18)= -1.1709061361277000E+00
w2( 24, 18)=  3.8974348604436599E+00
w2( 25, 18)=  1.3417275851266799E+00
w2( 26, 18)= -6.3061039205236402E-01
w2( 27, 18)= -5.5685318195797595E-01
w2( 28, 18)=  3.8010646938672799E-01
w2( 29, 18)= -1.4572114014620701E+00
w2( 30, 18)=  1.2940327920974100E+00
w2( 31, 18)=  2.5623943642696489E-02
w2( 32, 18)=  3.7590539074970793E-02
w2( 33, 18)= -2.2706047643738748E-03
w2( 34, 18)=  2.5065054923570990E-02
w2( 35, 18)=  3.5712218991726212E-02
w2( 36, 18)= -2.1846129791903719E-02
w2( 37, 18)=  5.8714866670630494E-01
w2( 38, 18)= -2.3118863874710899E-01
w2( 39, 18)=  2.3668311434613201E-01
w2( 40, 18)=  1.500983122222400E-01
w2( 1, 19)=  2.8011003354485903E-01
w2( 2, 19)= -1.1820329688296800E+00
w2( 3, 19)=  1.5720548023133600E+00
w2( 4, 19)=  2.3326929616557601E-01

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w2( 5, 19)= 9.2707662280080705E-01
w2( 6, 19)= -1.6394295581888501E+00
w2( 7, 19)= -3.2727014873925397E-01
w2( 8, 19)= 9.2703731801229206E-01
w2( 9, 19)= 1.9140790472286799E+00
w2( 10, 19)= 1.5142148702625899E-01
w2( 11, 19)= 1.2702088625538199E-01
w2( 12, 19)= -7.4522417784275496E-01
w2( 13, 19)= -1.0725082754480200E+00
w2( 14, 19)= -1.0337349701811800E+00
w2( 15, 19)= 6.2662144527944297E-01
w2( 16, 19)= 1.4854308341566499E-01
w2( 17, 19)= -8.7934379952526298E-01
w2( 18, 19)= -1.0692240765031999E+00
w2( 19, 19)= 2.8167815707544399E+00
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w2( 22, 19)= -5.7802324719703901E-01
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w2( 26, 19)= -5.7768309610778001E-01
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w2( 30, 19)= -3.5145224142414002E+00
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w2( 33, 19)= -2.4415703329321201E-01
w2( 34, 19)= 1.6862638497667699E+00
w2( 35, 19)= -2.1989159981687498E+00
w2( 36, 19)= -2.6060943757745197E-01
w2( 37, 19)= -5.8357480498511505E-01
w2( 38, 19)= 5.2296860238998999E-01
w2( 39, 19)= -1.6356029681173301E+00
w2( 40, 19)= 2.4811020626661402E+00
w2( 1, 20)= -2.1602847252540900E+00
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w2( 3, 20)= 4.2512057643332204E+00
w2( 4, 20)= -5.8169966129103901E-01
w2( 5, 20)= -3.3392550848282001E+00
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w2( 8, 20)= -7.9708700936081902E+00
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w2( 11, 20)= 6.4704430829557502E-01
w2( 12, 20)= 5.2124790408961497E+00
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w2( 14, 20)= -6.0460811769418603E+00
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w2( 16, 20)= -4.0175563201688602E+00
w2( 17, 20)= 2.2503352705644999E+00
w2( 18, 20)= -3.5706465127100402E+00
w2( 19, 20)= -2.2500299282700902E+00
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w2( 21, 20)= -1.1865237869035099E+00
w2( 22, 20)= 2.4965261186285499E+00
w2( 23, 20)= 1.1508561913511599E+00
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w2( 25, 20)= -2.9700281748381201E+00
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w2( 27, 20)= -5.0915738594984905E-01
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w2( 29, 20)= 1.5020520610553700E+00
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w2( 39, 20)= -2.0341072910796001E+00
w2( 40, 20)= 4.8190862870410101E+00
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w2( 3, 21)= -2.7406538360173802E+00
w2( 4, 21)= 5.7243667139385002E-01
w2( 5, 21)= -1.2591247438046400E+00
w2( 6, 21)= -1.3531456228172900E-01

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w2( 7, 21)= 3.5621116444363699E-01
w2( 8, 21)= -1.8730621088731001E+00
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w2( 10, 21)= 2.7108778658354599E-01
w2( 11, 21)= 2.5846730463145100E+00
w2( 12, 21)= 2.0123815787141401E+00
w2( 13, 21)= 1.8413116673159899E+00
w2( 14, 21)= 5.5838684197045596E-01
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w2( 16, 21)= -6.3996232262454000E-01
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w2( 31, 21)= -2.8777836113678501E-01
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w2( 34, 21)= 1.1621518208220700E+00
w2( 35, 21)= 2.7807034134945701E+00
w2( 36, 21)= -3.9750215826126800E-01
w2( 37, 21)= -4.0559181997478202E+00
w2( 38, 21)= 1.8022216637004900E+00
w2( 39, 21)= -1.5331720300817799E+00
w2( 40, 21)= 1.0245295185044001E+00
w2( 1, 22)= -1.0490965421201499E+00
w2( 2, 22)= -6.9140103612440995E-01
w2( 3, 22)= -5.6198177728826904E-01
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w2( 5, 22)= -5.1787376642487004E-01
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w2( 13, 22)= -3.0413335524224800E+00
w2( 14, 22)= -3.0039569129262900E-01
w2( 15, 22)= 1.2696763925073100E+00
w2( 16, 22)= 4.2860464836812717E-02
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w2( 18, 22)= 8.8717759156164006E-02
w2( 19, 22)= 1.8511703130291199E+00
w2( 20, 22)= 5.3417657877064895E-01
w2( 21, 22)= -1.3761742836671800E-01
w2( 22, 22)= 1.1308277396364200E-01
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w2( 24, 22)= -3.0261672885344302E+00
w2( 25, 22)= -4.3122617568240401E-01
w2( 26, 22)= 2.1309971343520400E+00
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w2( 29, 22)= -5.0097612373290301E-01
w2( 30, 22)= 5.4302725519203898E-01
w2( 31, 22)= 1.1944997815677501E+00
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w2( 5, 23)= 1.5878078666356401E+00
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w2( 8, 23)= 2.6188991179218699E+00

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w2( 10, 23)= 1.1203755635911099E+00
w2( 11, 23)= -1.8289893951272800E+00
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w2( 40, 23)= -6.1826283067745003E-01
w2(  1, 24)= -1.8565964863969799E+00
w2(  2, 24)= 6.7442587169085433E-03
w2(  3, 24)= 1.3296489444708901E+00
w2(  4, 24)= -1.3699284207533700E+00
w2(  5, 24)= -1.7612737449001301E-01
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w2(  5, 25)= 7.0347759935173604E-01
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w2(  8, 25)= 4.0603298611062497E+00
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w2( 12, 25)= -1.4829388179183101E+00
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w2( 19, 28)= -1.5082980066355200E-01
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w2( 30, 28)= 1.7106881888660500E-02
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w2( 32, 28)= 8.3989351256680600E-01
w2( 33, 28)= -2.2680792899618898E+00
w2( 34, 28)= -1.7615232926446101E+00
w2( 35, 28)= 2.1078479735408600E+00
w2( 36, 28)= -1.1031400246585700E-01
w2( 37, 28)= -4.5535680836123409E-02
w2( 38, 28)= -8.9391924051222105E-01
w2( 39, 28)= -8.5930749810754703E-01
w2( 40, 28)= -2.3797748235233701E-01
w2( 1, 29)= 1.5580121328885901E+00
w2( 2, 29)= -3.9745030918639201E-01
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w2( 4, 29)= 1.6970152540896200E-01
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w2( 6, 29)= -2.8703987211964509E-02
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w2( 8, 29)= 1.6986528861379599E+00
w2( 9, 29)= -1.3693819836286900E+00
w2( 10, 29)= -8.7795149102468495E-01
w2( 11, 29)= 9.8673917164524305E-01
w2( 12, 29)= 2.7081742602593900E-01
w2( 13, 29)= 1.8266080053877300E+00
w2( 14, 29)= 1.8610790593129301E+00

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w2( 15, 29)= -6.8290063545009805E-01
w2( 16, 29)= 4.8571794595083900E-01
w2( 17, 29)= 2.9237640012788502E-01
w2( 18, 29)= -1.9123901970582700E+00
w2( 19, 29)= -1.0592670757343301E+00
w2( 20, 29)= -2.6814227487897302E+00
w2( 21, 29)= -1.6011218525776301E+00
w2( 22, 29)= 4.6986342030985501E-01
w2( 23, 29)= -3.7332130667556201E-01
w2( 24, 29)= 2.5120544525780000E+00
w2( 25, 29)= -1.2047757986190999E+00
w2( 26, 29)= 1.2254472365806000E-01
w2( 27, 29)= -2.7471979047701600E+00
w2( 28, 29)= 2.1719940466974701E+00
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w2( 32, 29)= 1.0258001800165430E-02
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w2( 34, 29)= 2.1284284593887302E+00
w2( 35, 29)= 2.2053370998663999E-01
w2( 36, 29)= 5.1106803230145903E-01
w2( 37, 29)= -5.5080070939965392E-02
w2( 38, 29)= 7.0008880803193196E-01
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w2( 40, 29)= 5.2327950430840298E-01
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w2( 2, 30)= 6.7500543249961198E-01
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w2( 5, 30)= 1.0014247837377399E+00
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w2( 8, 30)= -6.8788861377457000E-01
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w2( 10, 30)= 1.9345013524783099E+00
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w2( 19, 30)= -1.0949680058110001E+00
w2( 20, 30)= -1.7307497835608201E+00
w2( 21, 30)= 5.6424530335081802E-01
w2( 22, 30)= 1.6334598898898400E+00
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w2( 33, 30)= 2.1193047823936501E-01
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w2( 35, 30)= 1.3401020260169101E+00
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w2( 38, 30)= -9.0401359159932604E-01
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w2( 13, 31)= 1.0679470062008400E+00
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w2( 15, 31)= 1.6342142734840959E-02
w2( 16, 31)= 1.4886068003018900E+00

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w2( 18, 31)= -8.3610339852634996E-01
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w2( 36, 31)= 4.7374105863082799E-01
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w2( 11, 32)= 2.1546424803906099E+00
w2( 12, 32)= -2.5440089530303598E+00
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w2( 15, 32)= -2.3478211239809901E+00
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w2( 25, 32)= 1.1664986034704801E+00
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w2( 7, 33)= 7.1120425500105717E-03
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w2( 32, 33)= -1.5022650066243790E-03
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w2( 5, 35)= 1.5137345693606901E+00
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w2( 18, 35)= -3.4063780470288498E+00
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w2( 20, 35)= -5.1614654326824301E+00

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w2( 11, 38)= -5.8941759702128105E-01
w2( 12, 38)= -3.2697783306078498E-01
w2( 13, 38)= 5.9899642207828596E-01
w2( 14, 38)= 3.7729472701479599E-01
w2( 15, 38)= -3.7390354979383100E-01
w2( 16, 38)= -2.3693986016047300E-01
w2( 17, 38)= 4.5391273930104203E+00
w2( 18, 38)= 2.1045149468907620E-02
w2( 19, 38)= -9.0243707514905103E-01
w2( 20, 38)= -1.8332190238561199E+00
w2( 21, 38)= -1.3016918794479300E+00
w2( 22, 38)= 1.6826500913391201E-01
w2( 23, 38)= 3.5924269880488802E-01
w2( 24, 38)= -1.7580917355009701E-01
w2( 25, 38)= 1.1083535837186800E-01
w2( 26, 38)= 6.3099628702257504E-01
w2( 27, 38)= -1.8842701388548200E+00
w2( 28, 38)= 1.2684978482206499E+00
w2( 29, 38)= -1.9925722895850700E-01
w2( 30, 38)= 2.0970174722999699E+00
w2( 31, 38)= -4.0711085337958602E-01
w2( 32, 38)= -1.8076789531470899E-01
w2( 33, 38)= 1.0111819115646301E+00
w2( 34, 38)= 9.1122735983445002E-01
w2( 35, 38)= -1.2741448853017301E+00
w2( 36, 38)= 6.5687414420787710E-02
w2( 37, 38)= -1.8517643991192601E-01
w2( 38, 38)= 5.3854632453040496E-01
w2( 39, 38)= 2.7580956117991001E-01
w2( 40, 38)= 5.3832602937578400E-01
w2( 1, 39)= 1.7156656422249299E+00
w2( 2, 39)= -4.9743803697319100E-01
w2( 3, 39)= 1.3422154678636000E-01
w2( 4, 39)= 1.0941363122914600E+00
w2( 5, 39)= 5.6582417920795502E-01
w2( 6, 39)= 3.4224535754589098E+00
w2( 7, 39)= -6.4117339999243494E-01
w2( 8, 39)= 4.0245216379846198E+00
w2( 9, 39)= 4.1798273565247601E-01
w2( 10, 39)= 1.2288995818990101E+00
w2( 11, 39)= 5.8456668806518097E-01
w2( 12, 39)= -8.2020204504404903E-01
w2( 13, 39)= 2.4320493027884602E+00
w2( 14, 39)= 3.3023832568531403E-01
w2( 15, 39)= -1.8532796001430201E+00
w2( 16, 39)= 5.5083165007268828E-02
w2( 17, 39)= 9.3114831701303802E-01
w2( 18, 39)= -3.1438083784647449E-03
w2( 19, 39)= -3.0052226071207500E+00
w2( 20, 39)= -3.0899219079921201E+00
w2( 21, 39)= -1.0175921949346700E+00
w2( 22, 39)= -1.5511560413103501E-01
w2( 23, 39)= 1.9040833664934900E-01
w2( 24, 39)= 1.1718892937001100E+00

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w2( 25, 39)= -3.2477176824251401E+00
w2( 26, 39)= -7.4831693711774105E-01
w2( 27, 39)= -1.6868700289073699E+00
w2( 28, 39)= -2.1274905026913902E+00
w2( 29, 39)=  7.3867851623516700E-01
w2( 30, 39)= -2.3776250154709300E-01
w2( 31, 39)= -1.1073003562046300E+00
w2( 32, 39)=  2.1783309240752950E-02
w2( 33, 39)=  5.0173483156456899E-01
w2( 34, 39)=  9.6362681188025900E-01
w2( 35, 39)=  1.5364189288516501E+00
w2( 36, 39)=  1.0572066040873900E-01
w2( 37, 39)= -9.3026672034604796E-01
w2( 38, 39)= -2.0529193621932600E+00
w2( 39, 39)=  3.2631236254216698E+00
w2( 40, 39)=  1.0992867893397300E+00
w2( 1, 40)=  9.9668209469106706E-01
w2( 2, 40)= -7.4227210202935301E-01
w2( 3, 40)= -5.4636924420477202E+00
w2( 4, 40)=  1.0978677970773700E+00
w2( 5, 40)= -8.7453055806279600E-01
w2( 6, 40)= -7.0311593629470404E-01
w2( 7, 40)= -3.2144739893119301E+00
w2( 8, 40)=  4.8436894329078800E-01
w2( 9, 40)=  1.1429283784149400E+00
w2( 10, 40)= -2.0137608530281699E+00
w2( 11, 40)= -1.1925632951202401E+00
w2( 12, 40)=  4.0203822152990598E-01
w2( 13, 40)= -2.8349303781999899E+00
w2( 14, 40)=  1.1567819687052400E-01
w2( 15, 40)=  3.1391691066645802E+00
w2( 16, 40)= -2.8556991251885799E+00
w2( 17, 40)= -1.7304686333902299E+00
w2( 18, 40)=  9.7347379554713498E-01
w2( 19, 40)=  6.0958940756160196E-01
w2( 20, 40)=  1.0876812080110101E+00
w2( 21, 40)= -1.0065644214772800E+00
w2( 22, 40)= -1.5360810558861000E+00
w2( 23, 40)=  1.2170647855242400E+00
w2( 24, 40)= -3.3714694386351098E+00
w2( 25, 40)=  1.3633214158650599E+00
w2( 26, 40)= -1.0786225669667100E-01
w2( 27, 40)=  4.2286754716197397E+00
w2( 28, 40)=  2.5076956197086702E+00
w2( 29, 40)= -1.8040412881586700E+00
w2( 30, 40)= -4.9309237018163898E-01
w2( 31, 40)= -8.9736469631457511E-02
w2( 32, 40)= -7.0998617823656296E-01
w2( 33, 40)=  6.5616394083958896E-01
w2( 34, 40)=  1.6611209381415999E+00
w2( 35, 40)= -1.7974619198424200E+00
w2( 36, 40)= -3.1971463602482803E-01
w2( 37, 40)=  7.2149757693345296E-01
w2( 38, 40)=  3.5509094436303601E-01
w2( 39, 40)=  8.5875982410245216E-02
w2( 40, 40)= -6.7135358491921804E-01
b2( 1)=  3.7233698224670699E+00
b2( 2)= -5.5595679644379103E+00
b2( 3)= -1.0130684300306300E-01
b2( 4)= -1.4425995713635000E+00
b2( 5)=  2.6536347302076799E+00
b2( 6)=  2.4126331682713101E-01
b2( 7)=  6.4407034920795703E-01
b2( 8)=  5.2157747706787505E-01
b2( 9)= -7.5669140789146805E-01
b2( 10)= 5.3260646700739500E-01
b2( 11)= 4.7284340665053497E+00
b2( 12)= -2.6938507647906200E+00
b2( 13)= 1.5515096285576499E+01
b2( 14)= 1.9882553640102600E+00
b2( 15)= 2.4877485139532500E+00
b2( 16)= -8.1808551989812495E-01
b2( 17)= 5.6021706591366904E-01
b2( 18)= 6.3600955590585595E-01
b2( 19)= -1.0333157999091800E+00
b2( 20)= -5.7527088139301359E-02
b2( 21)= -8.8120902329786299E-01
b2( 22)= 1.5781902977466700E+00
b2( 23)= -3.5257471233690700E+00
b2( 24)= 1.5318900378006101E-01
b2( 25)= 1.7531372212402501E+00
b2( 26)= -1.5402021451673200E+00

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b2( 27)= 2.4422242514949000E+00
b2( 28)= -2.3744882846476698E+00
b2( 29)= -1.3580931098611999E+00
b2( 30)= -1.1977470941529400E+00
b2( 31)= -3.6562395089104598E+00
b2( 32)= -2.6404092382536200E+00
b2( 33)= -4.2655723203724296E+00
b2( 34)= -4.6891647640849001E+00
b2( 35)= -3.1504981299259800E+00
b2( 36)= -9.7272364218894902E-01
b2( 37)= -5.5733258180326697E+00
b2( 38)= 1.0081691020975201E+00
b2( 39)= -5.7766735660400004E+00
b2( 40)= 2.8316961717469100E+00
w3( 1)= -1.0645305406409100E+00
w3( 2)= -5.4747363558228301E-01
w3( 3)= 8.6541620567173307E+00
w3( 4)= -4.4376474316605199E+00
w3( 5)= 1.6612037427321400E+01
w3( 6)= -2.2155594721528601E+01
w3( 7)= 1.6744737269962201E+01
w3( 8)= -3.2779922421347498E+00
w3( 9)= -3.6484379428217600E-01
w3( 10)= 1.6857103127609701E+00
w3( 11)= -8.9727461266406239E-02
w3( 12)= -7.5387012419410704E+00
w3( 13)= -6.9366398345211294E+01
w3( 14)= 1.5057598004538701E+01
w3( 15)= 1.3552680668025900E+01
w3( 16)= 2.6273451273521897E-01
w3( 17)= 1.6169252674987600E-01
w3( 18)= -1.0486741855626400E+01
w3( 19)= 1.7104820829626401E+01
w3( 20)= -7.1932956944838300E-01
w3( 21)= -9.7189032736724492E+00
w3( 22)= 2.6861227917335700E-01
w3( 23)= -1.4151224844265100E+01
w3( 24)= 2.8638255257053402E-01
w3( 25)= 1.6358580757937999E+00
w3( 26)= 1.3212483373779600E+01
w3( 27)= -7.5076410191247500E-01
w3( 28)= -1.8933527672982000E+00
w3( 29)= -3.0279131335818699E+00
w3( 30)= -3.2795157747956400E+00
w3( 31)= 1.9827515081113700E+00
w3( 32)= -1.7255927062334301E+01
w3( 33)= -4.9566880945312697E+00
w3( 34)= 5.4334985891419700E+00
w3( 35)= -1.0486799564566500E+01
w3( 36)= 1.0678252413906399E+01
w3( 37)= 3.9667692256108800E+00
w3( 38)= 6.4231907686458101E+00
w3( 39)= 2.1299522738003299E-01
w3( 40)= -5.2699805942847897E+00
b3= 2.0622087228094099E+01
rg( 1, 1)= -5.8130000000000000004E-01
rg( 2, 1)= 2.183303000000000000E+00
rg( 1, 2)= -6.925810000000000000E-01
rg( 2, 2)= 1.948760000000000000E+00
rg( 1, 3)= 9.36213999999999999E-01
rg( 2, 3)= 8.20169100000000003E+00
rg( 1, 4)= -6.410799999999998E-01
rg( 2, 4)= 2.22774200000000001E+00
rg( 1, 5)= -6.7870200000000003E-01
rg( 2, 5)= 2.0312190000000001E+00
rg( 1, 6)= 1.1146920000000000E+00
rg( 2, 6)= 8.2412089999999996E+00
vg( 1)= -1.9187155000000001E+02
vg( 2)= -1.8650091000000000E+02
endif

if(ntot.ge.24) then
  call nsimx(ntot,r0,vx,idv,dv,s0,s1,s2,rg,w1,b1,w2,b2,w3,b3,vg)
else
  do i=1,ntot
    call nsim(r0(1,i),vx(i),idv,dv(:,i),s0,s1,s2,rg,w1,b1,w2,b2,w3,b3,vg)
  enddo
endif

return
end subroutine

```

```

! -----
subroutine nsim(r0,v,idv,dv,n0,n1,n2,rg,w1,b1,w2,b2,w3,b3,vg)
! ---- simulate a neural network with two hidden layers
! ---- n0-n1-n2-1
! ---- blas routines used in this subroutine: dgemv, ddot
implicit none
integer,intent(in) :: n0,n1,n2,idv
real*8,intent(in) :: r0(n0),rg(2,n0),vg(2)
real*8,intent(in) :: w1(n0,n1),b1(n1)
real*8,intent(in) :: w2(n1,n2),b2(n2)
real*8,intent(in) :: w3(n2),b3
real*8,intent(out) :: v,dv(n0)
integer :: i,j,k
real*8 :: r(n0),rgg(n0),vgg,ax(n1),bx(n2)
real*8 :: dvtm,rtmp,rt1(n1),rt2(n2)
real*8,external :: ddot
v=0.d0
r=r0
vgg=vg(2)-vg(1)
! mapminmax [-1,1]
do i=1,n0
    rgg(i)=rg(2,i)-rg(1,i)
    r(i)=2.d0*(r(i)-rg(1,i))/rgg(i)-1.d0
end do
! 1st layer
rt1=b1
call dgemv('t',n0,n1,1.d0,w1,n0,r,1,1.d0,rt1,1)
ax=dtanh(rt1)
! 2nd layer
rt2=b2
call dgemv('t',n1,n2,1.d0,w2,n1,ax,1,1.d0,rt2,1)
bx=dtanh(rt2)
! output layer
v=b3+ddot(n2,w3,1,bx,1)
!reverse map
v=vgg*(v+1.d0)/2+vg(1)
if(idv.ne.1) return
! calculate first derivatives, dv(i)=dv/dr(i)
dv=0.d0
do i=1,n0
    do k=1,n2
        dvtm=0.d0
        do j=1,n1
            dvtm=dvtm+w2(j,k)*w1(i,j)*(1-ax(j)**2)
        enddo
        dv(i)=dv(i)+w3(k)*dvtm*(1-bx(k)**2)
    enddo
    dv(i)=dv(i)*vgg/rbg(i)
enddo
return
end subroutine nsim
! -----
subroutine nsimx(nt,r,v,idv,dv,n0,n1,n2,rg,w1,b1,w2,b2,w3,b3,vg)
! ---- simulate a neural network with two hidden layers
! ---- n0-n1(tansig)-n2(tansig)-1(pureline)
! ---- blas routines used in this subroutine: dgemm, dgemv
! ---- the syntax keeps the same with nsim, except input nt at first
! ---- Chen Jun, 2013/11/26
!
! ---- description of parameters
! ---- nt : total number of points in r,v and dv
! ---- r : input of nn, r(n0,nt), r(1:n0,i) is the i-th input
! ---- v : output of nn, v(nt), v(i) is the i-th input
! ---- idv : if idv==0, calc. v only, else calc. v and derivatives dv
! ---- dv : derivatives of dv/dr, dv(n0,nt), dv(j,i)=d v(i) / d r(j,i)
! ---- n0 : neurons of the input layer, dimension of r
! ---- n1 : neurons of the first hidden layer
! ---- n2 : neurons of the second hidden layer
! ---- rg : input ranges of the training set, rg(2,n0)
! ---- w1 : weights connect input layer with 1-st hidden layer
! ---- b1 : biases of 1-st hidden layer
! ---- w2 : weights connect 1-st hidden layer with 2-nd hidden layer
! ---- b2 : biases of 2-nd hidden layer
! ---- w3 : weights connect 2-nd hidden layer with output layer
! ---- b3 : bias of output layer
! ---- vg : output range of the training set, vg(2)
implicit none
integer,intent(in) :: nt,idv,n0,n1,n2
real*8,intent(in) :: r(n0,nt)
real*8,intent(out) :: v(nt),dv(n0,nt)
real*8,intent(in) :: w1(n0,n1),b1(n1),w2(n1,n2),b2(n2),w3(n2),b3
real*8,intent(in) :: rg(2,n0),vg(2)

```

```

real*8 :: x0(n0,nt),x1(nt,n1),x2(nt,n2),tmp,rgg(n0),vgg
integer :: i,j,k,n

v=0.d0
do i=1,n0
  rgg(i)=rg(2,i)-rg(1,i)
enddo
vgg=vg(2)-vg(1)

x0=r

do i=1,n0
  x0(i,1:nt)=(x0(i,1:nt)-rg(1,i))/rgg(i)*2.d0-1.d0
enddo

do i=1,n1
  x1(1:nt,i)=b1(i)
enddo

! ---- x1=trans(x0(n0,nt))*w1(n0,n1)+x1(nt,n1)
!call gpu_dgemm('t','n',nt,n1,n0,1.d0,x0,n0,w1,n0,1.d0,x1,nt)
call dgemm('t','n',nt,n1,n0,1.d0,x0,n0,w1,n0,1.d0,x1,nt)

x1=dtanh(x1)

do i=1,n2
  x2(1:nt,i)=b2(i)
enddo

! ---- x2=x1(nt,n1)*w2(n1,n2)+x2(nt,n2)
!call gpu_dgemm('n','n',nt,n2,n1,1.d0,x1,nt,w2,n1,1.d0,x2,nt)
call dgemm('n','n',nt,n2,n1,1.d0,x1,nt,w2,n1,1.d0,x2,nt)

x2=dtanh(x2)

v(1:nt)=b3

! ---- v=x2(nt,n2)*w3(n2)+v(nt)
call dgemv('n',nt,n2,1.d0,x2,nt,w3,1,1.d0,v,1)

v=(v+1.d0)/2.d0*vgg+vg(1)

if (idv.ne.1) return
! ---- calculate first derivatives
dv=0.d0
do n=1,nt
  do i=1,n0
    do k=1,n2
      tmp=0.d0
      do j=1,n1
        tmp=tmp+w2(j,k)*w1(i,j)*(1-x1(n,j)**2)
      enddo
      dv(i,n)=dv(i,n)+w3(k)*tmp*(1-x2(n,k)**2)
    enddo
    dv(i,n)=dv(i,n)*vgg/(rgg(i))
  enddo
enddo
return
end subroutine nsimx
! -----
```

---

```

subroutine frac2unit(frac0,cart,zmat,level,vasp)
!! level 0: move C and O atoms into a same 2x2 cell, then trans to Cartesian only.
!! level 1: move CO into the 1x1 cell, then trans to Cartesian.
!! level 2: symmetrize the Cartesian to the minimum triangle

implicit none
real*8,parameter :: pi=dacos(-1.d0)
real*8,intent(in) :: frac0(3,2)
real*8,intent(out) :: cart(3,2),zmat(6)
integer,intent(in) :: level,vasp
real*8 :: frac(3,2),comc(3),dist2d,comc(3),tmpx,tmpy,tmpa,phi,alpha

real*8 :: a(3),b(3),c(3),a0
integer :: i,j

data a/4.7463322314000056d0,-2.7402961914621891d0, 0.0000000000000000d0/
data b/0.0000000000000000d0, 5.4805923829243808d0, 0.0000000000000000d0/
data c/0.0000000000000000d0, 0.0000000000000000d0,23.5301296545844991d0/
data a0/5.4805923829243808d0/

frac=frac0
```

```

frac(1,:)=frac(1,:)-0.16669d0
frac(2,:)=frac(2,:)-0.02782d0
frac(3,:)=frac(3,:)-0.36005d0

!! move C and O to the same 2x2 cell, only for vasp results
if(vasp.eq.1) then
dist2d=dsqrt(dot_product(frac(1:2,1)-frac(1:2,2),frac(1:2,1)-frac(1:2,2)))
if(dist2d.gt.0.5d0) then
  if(frac(1,1)-frac(1,2).gt. 0.5d0) frac(1,2)=frac(1,2)+1.d0
  if(frac(1,1)-frac(1,2).lt.-0.5d0) frac(1,1)=frac(1,1)+1.d0
  if(frac(2,1)-frac(2,2).gt. 0.5d0) frac(2,2)=frac(2,2)+1.d0
  if(frac(2,1)-frac(2,2).lt.-0.5d0) frac(2,1)=frac(2,1)+1.d0
endif
endif

com(1:3)=(frac(1:3,1)+frac(1:3,2))*0.5d0

if(level.eq.0) goto 990 !! translate to cartesian directly

!! move all poins to a unit cell
!! move com(1) to [0.0,0.5)
!! move com(2) to [0.0,0.5)
do while(com(1).ge.0.5d0)
  com(1)=com(1)-0.5d0
  frac(1,:)=frac(1,:)-0.5d0
enddo
do while(com(1).lt.0.0d0)
  com(1)=com(1)+0.5d0
  frac(1,:)=frac(1,:)+0.5d0
enddo
do while(com(2).ge.0.5d0)
  com(2)=com(2)-0.5d0
  frac(2,:)=frac(2,:)-0.5d0
enddo
do while(com(2).lt.0.0d0)
  com(2)=com(2)+0.5d0
  frac(2,:)=frac(2,:)+0.5d0
enddo

990 continue

!! translate to cartesian coordinate, assuming a0=1
do i=1,2
  cart(1,i)=sqrt(3.d0)/2.d0*frac(1,i)
  cart(2,i)=-0.5d0*frac(1,i)+frac(2,i)
  cart(3,i)=frac(3,i)*c(3)
enddo
comc(1)=sqrt(3.d0)/2.d0*com(1)
comc(2)=-0.5d0*com(1)+com(2)
comc(3)=com(3)*c(3)

if(level.eq.0 .or. level.eq.1) goto 991 !! have moved all poins to a unit cell

!! move CO to a minimum triangle through Cs symmetries
! Cs-1: y=0.d0
if(comc(2).lt.0.d0) then
  cart(2,:)=cart(2,:)
  comc(2)=comc(2)
endif

! CS-2: y=sqrt(3.d0)*x
if(comc(2).gt.sqrt(3.d0)*comc(1)) then
  !write(91,'(3f10.5)') comc(1)*a0,comc(2)*a0,comc(3)
  ttmpx=comc(1); ttmpy=comc(2)
  comc(1)=-0.5d0*ttmpx + 0.5d0*sqrt(3.d0)*tmpy
  comc(2)= 0.5d0*sqrt(3.d0)*ttmpx + 0.5d0*tmpy
  do i=1,2
    ttmpx=cart(1,i); ttmpy=cart(2,i)
    cart(1,i)=-0.5d0*ttmpx + 0.5d0*sqrt(3.d0)*tmpy
    cart(2,i)= 0.5d0*sqrt(3.d0)*ttmpx + 0.5d0*tmpy
  enddo
  !write(92,'(3f10.5)') comc(1)*a0,comc(2)*a0,comc(3)
endif

! CS-3: y=0.25d0 !! remind that the vasp use 2x2 supercell
if(comc(2).gt.0.25d0) then
  !write(91,'(3f10.5)') comc(1)*a0,comc(2)*a0,comc(3)
  comc(2)=0.5d0-comc(2)
  cart(2,:)=0.5d0-cart(2,:)
  !write(92,'(3f10.5)') comc(1)*a0,comc(2)*a0,comc(3)
endif

```

```

! CS-4: y=sqrt(3.d0)*x-0.5d0 !! remind that the vasp use 2x2 supercell
if(comc(2).lt.(sqrt(3.d0)*comc(1)-0.5d0)) then
!write(91,'(3f10.5)') comc(1)*a0,comc(2)*a0,comc(3)
tmpx=comc(1); tmpy=comc(2); !tmpa=sqrt(3.d0)*tmpx-tmpy-0.5d0
!! x' = x - sqrt(3)*0.5*a; y' = y + 0.5*a
comc(1)=-0.5d0*tmpx + 0.5d0*sqrt(3.d0)*tmpy + 0.25d0*sqrt(3.d0)
comc(2)= 0.5d0*sqrt(3.d0)*tmpx + 0.5d0*tmpy - 0.25d0
do i=1,2
  tmpx=cart(1,i); tmpy=cart(2,i); !tmpa=sqrt(3.d0)*tmpx-tmpy-0.5d0
  cart(1,i)=-0.5d0*tmpx + 0.5d0*sqrt(3.d0)*tmpy + 0.25d0*sqrt(3.d0)
  cart(2,i)= 0.5d0*sqrt(3.d0)*tmpx + 0.5d0*tmpy - 0.25d0
enddo
!write(92,'(3f10.5)') comc(1)*a0,comc(2)*a0,comc(3)
endif

! CS-5: y=-sqrt(3.d0)*x+0.5d0 !! remind that the vasp use 2x2 supercell
if(comc(2).gt.(-sqrt(3.d0)*comc(1)+0.5d0)) then
!write(91,'(3f10.5)') comc(1)*a0,comc(2)*a0,comc(3)
tmpx=comc(1); tmpy=comc(2); tmpa=sqrt(3.d0)*tmpx+tmpy-0.5d0
!! x' = x - sqrt(3)*0.5*a; y' = y - 0.5*a
comc(1)=tmpx-0.5d0*sqrt(3.d0)*tmpa
comc(2)=tmpy-0.5d0*tmpa
do i=1,2
  tmpx=cart(1,i); tmpy=cart(2,i); tmpa=sqrt(3.d0)*tmpx+tmpy-0.5d0
  cart(1,i)=tmpx-0.5d0*sqrt(3.d0)*tmpa
  cart(2,i)=tmpy-0.5d0*tmpa
enddo
!write(92,'(3f10.5)') comc(1)*a0,comc(2)*a0,comc(3)
endif

991 continue
cart(1,:)=cart(1,:)*a0
cart(2,:)=cart(2,:)*a0
comc(1)=comc(1)*a0
comc(2)=comc(2)*a0

!! translate cartesian to zmat
zmat(1:3)=comc
zmat(4)=dsqrt(dot_product(cart(:,1)-cart(:,2),cart(:,1)-cart(:,2)))

! phi: angle between C0 and z axis
phi=acos(max(-1.d0,min(1.d0,((cart(3,2)-cart(3,1))/zmat(4))))/pi*180.d0
zmat(5)=phi

! alpha: angle between (C0's projection on xy plane) and y axis
dist2d=dsqrt(dot_product(cart(1:2,1)-cart(1:2,2),cart(1:2,1)-cart(1:2,2)))
alpha=acos(max(-1.d0,min(1.d0,((cart(2,2)-cart(2,1))/dist2d))))/pi*180.d0
if(cart(1,1).gt.cart(1,2)) alpha=-alpha
zmat(6)=alpha

return
end subroutine

subroutine trans2cart(n,frac,cart)
implicit none
integer,intent(in) :: n
real*8,intent(in) :: frac(3,n)
real*8,intent(out) :: cart(3,n)

real*8 :: a(3),b(3),c(3)
integer :: i,j

data a/4.7463322314000056d0,-2.7402961914621891d0, 0.0000000000000000d0/
data b/0.0000000000000000d0, 5.4805923829243808d0, 0.0000000000000000d0/
data c/0.0000000000000000d0, 0.0000000000000000d0,23.5301296545844991d0/

do i=1,n
  cart(1:3,i)=(frac(1,i)-0.16669d0)*a&
    +(frac(2,i)-0.02782d0)*b&
    +(frac(3,i)-0.36005d0)*c
enddo
return
end subroutine

subroutine rotate(xyz,axis,direction,degree)
!! examples:
!! call rotate(x(1:3,2),"y","a",45.d0)
!! call rotate(x(1:3,4),"z","c",120.d0)
implicit none
real(kind=8),intent(inout) :: xyz(3)
character(kind=1,len=1),intent(in) :: axis
character(kind=1,len=1),intent(in) :: direction

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real(kind=8),intent(in) :: degree
real(kind=8),parameter :: pi=3.14159265358979323846d0
real*8 :: tx,ty,tz,ta
tx=xyz(1)
ty=xyz(2)
tz=xyz(3)
ta=degree/180.d0*pi
if(direction.ne."a" .and. direction.ne."c") stop "direction = a or c"
if(axis.ne."x" .and. axis.ne."y" .and. axis.ne."z") stop "axis = x y z"
if(direction.eq."c") ta=-ta
if(axis.eq."x") then
  xyz(2)=cos(ta)*ty-sin(ta)*tz
  xyz(3)=sin(ta)*ty+cos(ta)*tz
elseif(axis.eq."y") then
  xyz(3)=cos(ta)*tz-sin(ta)*tx
  xyz(1)=sin(ta)*tz+cos(ta)*tx
elseif(axis.eq."z") then
  xyz(1)=cos(ta)*tx-sin(ta)*ty
  xyz(2)=sin(ta)*tx+cos(ta)*ty
endif
return
end subroutine

subroutine cart2frac(cart,frac)
implicit none
real*8,intent(in) :: cart(3,2)
real*8,intent(out) :: frac(3,2)
real*8 :: a(3),b(3),c(3),a0
integer :: i,j

data a/4.7463322314000056d0,-2.7402961914621891d0, 0.0000000000000000d0/
data b/0.0000000000000000d0, 5.4805923829243808d0, 0.0000000000000000d0/
data c/0.0000000000000000d0, 0.0000000000000000d0,23.5301296545844991d0/
data a0/5.4805923829243808d0/

frac(1,:)=cart(1,:)/a0*2.d0/sqrt(3.d0)
frac(2,:)=cart(2,:)/a0+0.5d0*frac(1,:)
frac(3,:)=cart(3,:)/c(3)

frac(1,:)=frac(1,:)+0.16669d0
frac(2,:)=frac(2,:)+0.02782d0
frac(3,:)=frac(3,:)+0.36005d0

return
end subroutine

subroutine zmat2cart(zmat,cart)
implicit none
real*8,intent(in) :: zmat(6)
real*8,intent(out) :: cart(3,2)
real*8 :: comc(3),phi,dist2d,alpha,distco
comc=zmat(1:3)
distco=zmat(4)
phi=zmat(5)
alpha=zmat(6)
! put CO along y axis
cart=0.d0
cart(2,1)=-distco/2.d0
cart(2,2)=distco/2.d0
! rotate around x axis for (90-phi) anticlockwisely
call rotate(cart(:,1),'x','a',90.d0-phi)
call rotate(cart(:,2),'x','a',90.d0-phi)
! rotate around z axis for alpha clockwise
call rotate(cart(:,1),'z','c',alpha)
call rotate(cart(:,2),'z','c',alpha)
! move the COM
cart(:,1)=cart(:,1)+comc
cart(:,2)=cart(:,2)+comc
return
end subroutine

subroutine cart2zmat(cart,zmat)
implicit none
real*8,intent(in) :: cart(3,2)
real*8,intent(out) :: zmat(6)
real*8 :: comc(3),phi,dist2d,alpha
real*8,parameter :: pi=dacos(-1.d0)

comc=(cart(:,1)+cart(:,2))/2.d0
!! translate cartesian to zmat
zmat(1:3)=comc
zmat(4)=dsqrt(dot_product(cart(:,1)-cart(:,2),cart(:,1)-cart(:,2)))

```

```
! phi: angle between C0 and z axis
phi=acos(max(-1.d0,min(1.d0,((cart(3,2)-cart(3,1))/zmat(4))))/pi*180.d0
zmat(5)=phi

! alpha: angle between (C0's projection on xy plane) and y axis
dist2d=dsqrt(dot_product(cart(1:2,1)-cart(1:2,2),cart(1:2,1)-cart(1:2,2)))
alpha=acos(max(-1.d0,min(1.d0,((cart(2,2)-cart(2,1))/dist2d)))/pi*180.d0
if(cart(1,1).gt.cart(1,2)) alpha=-alpha
zmat(6)=alpha
return
end subroutine
```