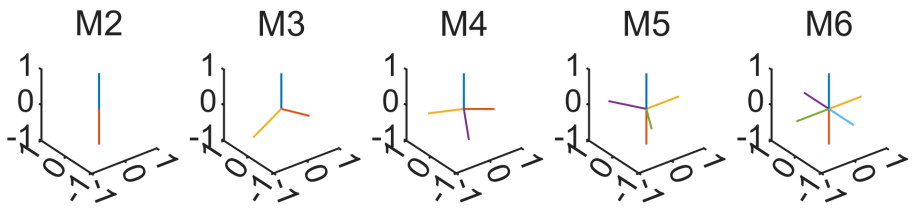
```
clc;
clear;
close all;

msym_tb=readmmffcsv("1_MMFFSYMB.csv");
bs_tb=readmmffcsv("6_MMFFBOND.csv");
ab_tb=readmmffcsv("8_MMFFANG.csv");
sb_tb=readmmffcsv("9_MMFFSTBN.csv");
opb_tb=readmmffcsv("11_MMFFOOP.csv");
ti_tb=readmmffcsv("12_MMFFTOR.csv");
vdw_tb=readmmffcsv("13_MMFFVDW.csv");
```

```
%% 数据表格预处理_Step1_普适

bs_pro_arr=genNDarr(bs_tb,["MTYPE_I" "MTYPE_J"],["R0","KB"]);
ab_pro_arr=genNDarr(ab_tb,["MTYPE_I" "MTYPE_J" "MTYPE_K"],["THETA_0","KA_IJK"]);
[sb_fast_arr,sb_cmpl_arr]=genNDarr_cmpl(sb_tb,["MTYPE_I" "MTYPE_J" "MTYPE_K"],
["KBA_IJK","KBA_KJI"]);
[opb_fast_arr,opb_cmpl_arr]=genNDarr_cmpl(opb_tb,["MTYPE_I" "MTYPE_J" "MTYPE_K"
"MTYPE_L"],"KOOP","Yes");
[ti_fast_arr,ti_cmpl_arr]=genNDarr_cmpl(ti_tb,["MTYPE_I" "MTYPE_J" "MTYPE_K"
"MTYPE_L"],["V1","V2","V3"],"No");
%vdw_pro_arr=genNDarr(vdw_tb,"MTYPE",["ALPHA_I","N_I","A_I","G_I"])


function cmpl_arr=short2cmpl(short_arr)
[isize,jsize]=size(short_arr);
dmax=max(short_arr,[],"all");
cmpl_arr=zeros(isize,dmax);
for i=1:isize
    for j=1:jsize
        mtype=short_arr(i,j);
        if mtype~=0
            cmpl_arr(i,mtype)=j;
        end
    end
end
end
function [arr_nd,cmpl_arr]=genNDarr_cmpl(tb,idname,dimname,is_jl_solid)

dimsize=size(dimname,2);
idsize=size(idname,2);
tbsize=size(tb,1);
arr=tb{:,[idname dimname]};
mshort=cell(idsize,1);
issize=zeros(1,idsize);
for i=1:idsize
    m=sort(unique(arr(:,i), 'rows', 'stable'),1)';
    m(m==0)=[];
    mshort(i,1)={m};
    issize(1,i)=size(m,2);
end
csize=max(arr(:,1:idsize),[],"all");
```

```
short_arr=zeros(idsize,csize);
for i=1:idsize
    short_arr(i,1:issize(1,i))=mshort{i,:};
end
cmpl_arr=short2cmpl(short_arr);

size_arr=[issize,dimsize];
arr_nd=zeros(size_arr);
arr_nd(arr_nd == 0) = NaN;
for k=1:tbsize
    if ~all(arr(k,:),2)
        continue
    end
    for j=1:dimsize
        index=zeros(1,idsize);
        for i=1:idsize
            index(1,i)=cmpl_arr(i,arr(k,i));
        end
        if all(index,1)
            if idsize==3
                arr_nd(index(1,1),index(1,2),index(1,3),j)=arr(k,j+idsize);
                arr_nd(index(1,3),index(1,2),index(1,1),j)=arr(k,j+idsize);
            elseif idsize==4

arr_nd(index(1,1),index(1,2),index(1,3),index(1,4),j)=arr(k,j+idsize);
                if is_jl_solid~="Yes"

arr_nd(index(1,4),index(1,3),index(1,2),index(1,1),j)=arr(k,j+idsize);
                else

arr_nd(index(1,3),index(1,2),index(1,1),index(1,4),j)=arr(k,j+idsize);
                end
            end
        end
    end
end
end
function arr_nd=genNDarr(tb,idname,dimname)
dimsize=size(dimname,2);
idsize=size(idname,2);
tbsize=size(tb,1);
arr=tb{:,[idname dimname]};
max_index=zeros(1,idsize)+max(arr(:,1:idsize),[],"all");
size_arr=[max_index,dimsize];
arr_nd=zeros(size_arr);
arr_nd(arr_nd == 0) = NaN;
for k=1:tbsize
    if ~all(arr(k,:),2)
        continue
    end
    for j=1:dimsize
        if idsize==1
            arr_nd(arr(k,1),j)=arr(k,j+idsize);
        elseif idsize==2
```

```
            arr_nd(arr(k,1),arr(k,2),j)=arr(k,j+idsize);
            arr_nd(arr(k,2),arr(k,1),j)=arr(k,j+idsize);
        elseif idsize==3
            arr_nd(arr(k,1),arr(k,2),arr(k,3),j)=arr(k,j+idsize);
            arr_nd(arr(k,3),arr(k,2),arr(k,1),j)=arr(k,j+idsize);
        end
    end
end
end
```

```
%% 构象坐标转换
m_sphe_arr=zeros(6,4,6)-1;
for i=2:6
    now_sphe_arr=table2array(readspcsv(['M',num2str(i),'.csv']));
    m_sphe_arr(1:i,:,i)=now_sphe_arr;
end

figure;
for i=2:6
now_rect_arr=arr_sphe2rect(m_sphe_arr(:,:,i));
subplot(1,5,i-1);
for j=1:i
    % if now_rect_arr(j,1,i)~=-1
        plot3([now_rect_arr(j,2) 0],[now_rect_arr(j,3) 0],[now_rect_arr(j,4) 0]);
        hold on;
    % end
end
title(['M',num2str(i)])
axis equal
xticks(-1:1)
yticks(-1:1)
zticks(-1:1)
xlim([-1,1])
ylim([-1,1])
zlim([-1,1])
end
```




```
m_sphe_arr
```

```
m_sphe_arr =
m_sphe_arr(:,:,1) =

    -1    -1    -1    -1
    -1    -1    -1    -1
    -1    -1    -1    -1
    -1    -1    -1    -1
    -1    -1    -1    -1
    -1    -1    -1    -1


m_sphe_arr(:,:,2) =

     0     1     0     0
     1     1   180   180
    -1    -1    -1    -1
    -1    -1    -1    -1
    -1    -1    -1    -1
    -1    -1    -1    -1


m_sphe_arr(:,:,3) =

     0     1     0     0
     1     1     0   120
     2     1   180   120
    -1    -1    -1    -1
    -1    -1    -1    -1
    -1    -1    -1    -1


m_sphe_arr(:,:,4) =

         0    1.0000         0         0
    1.0000    1.0000         0  109.5000
    2.0000    1.0000  120.0000  109.5000
```

```
    3.0000    1.0000  240.0000  109.5000
   -1.0000   -1.0000   -1.0000   -1.0000
   -1.0000   -1.0000   -1.0000   -1.0000
```

```
m_sphe_arr(:,:,5) =

     0     1     0     0
     1     1     0   180
     2     1     0    90
     3     1   120    90
     4     1   240    90
    -1    -1    -1    -1
```

```
m_sphe_arr(:,:,6) =

     0     1     0     0
     1     1     0   180
     2     1     0    90
     3     1    90    90
     4     1   180    90
     5     1   270    90
```

```
%% 需要一般化的部分
ori_str="CCC";
nhc=3;
hc=2*nhc+2;
ac=nhc+hc;

%通过一个函数完成 H 的引入
nh_tb=readtable("CCC_TEST/CCC_NH.csv")
```

```
nh_tb = 3×9 table
```

...

	Seq	Element	MType	IsAroma	CCount	CHCount	NHBC
1	0	'C'	1	0	1	3	1
2	1	'C'	1	0	2	2	2
3	2	'C'	1	0	1	3	1

```
h_tb=readtable("CCC_TEST/CCC_H.csv")
```

```
h_tb = 8×3 table
```

	Seq	ParentSeq	MType
1	3	0	5
2	4	0	5
3	5	0	5
4	6	1	5
5	7	1	5
6	8	2	5
7	9	2	5
8	10	2	5

```
mtype_all_arr=[nh_tb{:,"MType"};h_tb{:,"MType"}]
```

```
mtype_all_arr = 11×1
     1
     1
     1
     5
     5
     5
     5
     5
     5
     5
     ⋮
```

```
short_mtype_all_arr=sort(unique(mtype_all_arr(:,1), 'rows', 'stable'),1)';
max_mtype_all=max(mtype_all_arr,[],"all")
```

```
max_mtype_all = 5
```

```
%邻接表
keys={'0','1','2'};
values={[1,3,4,5],[0,2,6,7],[1,8,9,10]};
adj_list=dictionary(keys,values);

%扩展邻接表
big_key=string(0:(ac-1));
big_values={[1,3,4,5],[0,2,6,7],[1,8,9,10],0,0,0,1,1,2,2,2};
big_adj_list=dictionary(big_key,big_values);
```

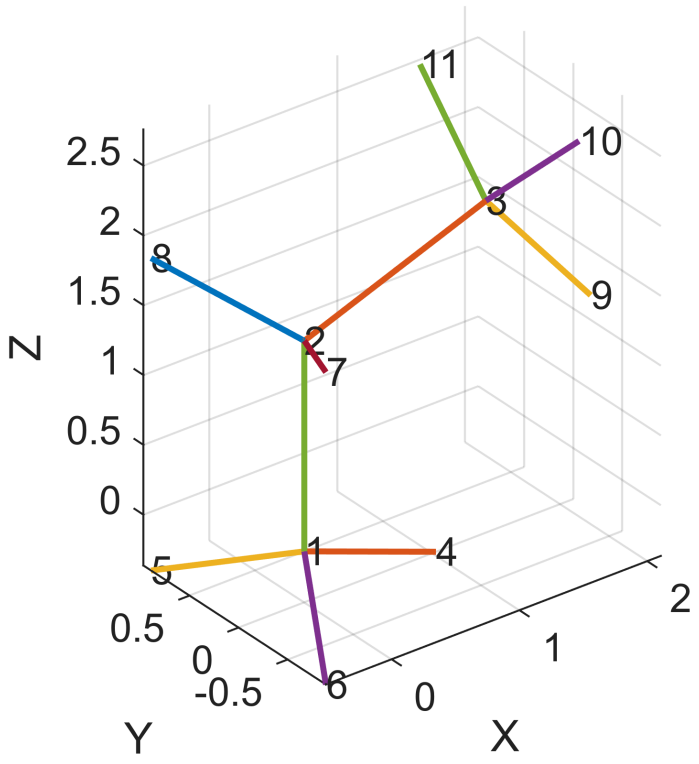
```
%% 数据表格预处理_Step2_针对特定分子
nhc_all_tb=nh_tb{:,"NHBC"}+nh_tb{:,"CHCount"};

bs_procut_arr=bs_pro_arr(1:max_mtype_all,1:max_mtype_all,:);
ab_procut_arr=ab_pro_arr(1:max_mtype_all,1:max_mtype_all,1:max_mtype_all,:);
[sb_fastcut_arr,sb_cmplcut_arr]=cutfastarr(max_mtype_all,sb_fast_arr,sb_cmpl_arr)
;
[opb_fastcut_arr,opb_cmplcut_arr]=cutfastarr(max_mtype_all,opb_fast_arr,opb_cmpl_
arr);
[ti_fastcut_arr,ti_cmplcut_arr]=cutfastarr(max_mtype_all,ti_fast_arr,ti_cmpl_arr)
;
vdw_cut_tb=vdw_tb(vdw_tb.MTYPE<=max_mtype_all,:);


function [arr_cut,cmpl_cut]=cutfastarr(max_mtype_all,arr_nd,cmpl_arr)
cmpl_cut=cmpl_arr(:,1:max_mtype_all);
idsize=size(cmpl_cut,1);
asize=zeros(1,idsize);
for i=1:idsize
    as=find(cmpl_cut(i,:)==max_mtype_all);
    if isempty(as)
        asize(1,i) = max_mtype_all;
    else
        asize(1,i)=find(1,1);
    end
```

```
end
if idsize==2
    arr_cut=arr_nd(1:asize(1,1),1:asize(1,2),:);
elseif idsize==3
    arr_cut=arr_nd(1:asize(1,1),1:asize(1,2),1:asize(1,3),:);
elseif idsize==4
    arr_cut=arr_nd(1:asize(1,1),1:asize(1,2),1:asize(1,3),1:asize(1,4),:);
end
end
```

```
alpha_tb=[0,0,10];
pre_xyz_tb=xyzprecal(alpha_tb,ac,nhc_all_tb,bs_procut_arr,adj_list,mtype_all_arr,
m_sphe_arr)
```

```
pre_xyz_tb = 11×3
         0         0         0
         0         0    1.5080
    1.4215         0    2.0114
    1.0303         0   -0.3649
   -0.5152    0.8923   -0.3649
   -0.5152   -0.8923   -0.3649
   -0.5152   -0.8923    1.8729
   -0.5152    0.8923    1.8729
    2.1041   -0.1789    1.1767
    1.5444   -0.7893    2.7575
      ⋮
```

```
figure;
moledraw(pre_xyz_tb,adj_list)
```



```
[pre_sumE,sumEB,sumEA,sumEBA,sumEOOP,sumET,sumEVDW]=getE(pre_xyz_tb,nhc,bs_procut
_arr,ab_procut_arr,sb_fastcut_arr,sb_cmplcut_arr,opb_fastcut_arr,opb_cmplcut_arr,
ti_fastcut_arr,ti_cmplcut_arr,vdw_tb,big_adj_list,mtype_all_arr);
```

```
accE=1e-4;
accD=1e-2;
alpha_tb=zeros(1,nhc);
apsize=nhc-1;
old_alpha_tb=alpha_tb+360;
sp_tb=[4,4,4];
asep_tb=90./(sp_tb-1);
roundcount=0;
ra=alpha_tb
```

```
ra = 1×3
     0     0     0
```

```
tic
while ~judgestop(old_alpha_tb,alpha_tb,asep_tb)
    old_alpha_tb=alpha_tb;
    for i=2:nhc
        minE=Inf;
        minJ=0;
        now_range=0:asep_tb(1,i):359;
        jsize=size(now_range,2);
        for j=1:jsize
            roundcount=roundcount+1;

            alpha_tb(1,i)=now_range(1,j);
            [sumE,~] =
getoptE(alpha_tb,ac,nhc_all_tb,bs_procut_arr,ab_procut_arr,sb_fastcut_arr,sb_cmpl
cut_arr,opb_fastcut_arr,opb_cmplcut_arr,ti_fastcut_arr,ti_cmplcut_arr,vdw_tb,adj_
list,big_adj_list,mtype_all_arr,m_sphe_arr);
            if minE>sumE
                minE=sumE;
                minJ=j;
            end
        end
        alpha_tb(1,i)=now_range(1,minJ);
    end
end
oldE=Inf;
[newE,~]=getoptE(alpha_tb,ac,nhc_all_tb,bs_procut_arr,ab_procut_arr,sb_fastcut_ar
r,sb_cmplcut_arr,opb_fastcut_arr,opb_cmplcut_arr,ti_fastcut_arr,ti_cmplcut_arr,vd
w_tb,adj_list,big_adj_list,mtype_all_arr,m_sphe_arr);
ratio=0.618;

% rb=alpha_tb
while ~judgestop(newE,oldE,accE)
    oldE=newE;
```

```
    for i=2:nhc

        new_alpha_tb=alpha_tb;

        rmaxD=alpha_tb(1,i)+asep_tb(1,i);
        rminD=alpha_tb(1,i)-asep_tb(1,i);

        new_alpha_tb(1,i)=rmaxD;

[rmaxE,~]=getoptE(new_alpha_tb,ac,nhc_all_tb,bs_procut_arr,ab_procut_arr,sb_fastc
ut_arr,sb_cmplcut_arr,opb_fastcut_arr,opb_cmplcut_arr,ti_fastcut_arr,ti_cmplcut_a
rr,vdw_tb,adj_list,big_adj_list,mtype_all_arr,m_sphe_arr);

        new_alpha_tb(1,i)=rminD;

[rminE,~]=getoptE(new_alpha_tb,ac,nhc_all_tb,bs_procut_arr,ab_procut_arr,sb_fastc
ut_arr,sb_cmplcut_arr,opb_fastcut_arr,opb_cmplcut_arr,ti_fastcut_arr,ti_cmplcut_a
rr,vdw_tb,adj_list,big_adj_list,mtype_all_arr,m_sphe_arr);
        rmidE=Inf;
        while ~judgestop(rmaxE,rminE,accE)&&~judgestop(rminD,rmaxD,accD)
            roundcount=roundcount+1;
            sepD=rmaxD-rminD;
            midD_left=rminD+ratio*sepD;
            midD_right=rmaxD-ratio*sepD;
            mid_alpha_tb=alpha_tb;

            mid_alpha_tb(1,i)=midD_left;

midE_left=getoptE(mid_alpha_tb,ac,nhc_all_tb,bs_procut_arr,ab_procut_arr,sb_fastc
ut_arr,sb_cmplcut_arr,opb_fastcut_arr,opb_cmplcut_arr,ti_fastcut_arr,ti_cmplcut_a
rr,vdw_tb,adj_list,big_adj_list,mtype_all_arr,m_sphe_arr);

            mid_alpha_tb(1,i)=midD_right;

midE_right=getoptE(mid_alpha_tb,ac,nhc_all_tb,bs_procut_arr,ab_procut_arr,sb_fast
cut_arr,sb_cmplcut_arr,opb_fastcut_arr,opb_cmplcut_arr,ti_fastcut_arr,ti_cmplcut_
arr,vdw_tb,adj_list,big_adj_list,mtype_all_arr,m_sphe_arr);
            if midE_left<midE_right
                rmaxD=midD_left;
                rmaxE=midD_left;
            else
                rminD=midD_right;
                rminE=midE_right;
            end
        end
        alpha_tb(1,i)=(rmaxD+rminD)/2;
    end

[newE,~]=getoptE(alpha_tb,ac,nhc_all_tb,bs_procut_arr,ab_procut_arr,sb_fastcut_ar
r,sb_cmplcut_arr,opb_fastcut_arr,opb_cmplcut_arr,ti_fastcut_arr,ti_cmplcut_arr,vd
w_tb,adj_list,big_adj_list,mtype_all_arr,m_sphe_arr);

end
```

```
elapsedTime = toc;
disp(['运行时间: ', num2str(elapsedTime),'s']);
```

```
运行时间: 0.26815s
```

```
rc=alpha_tb
```

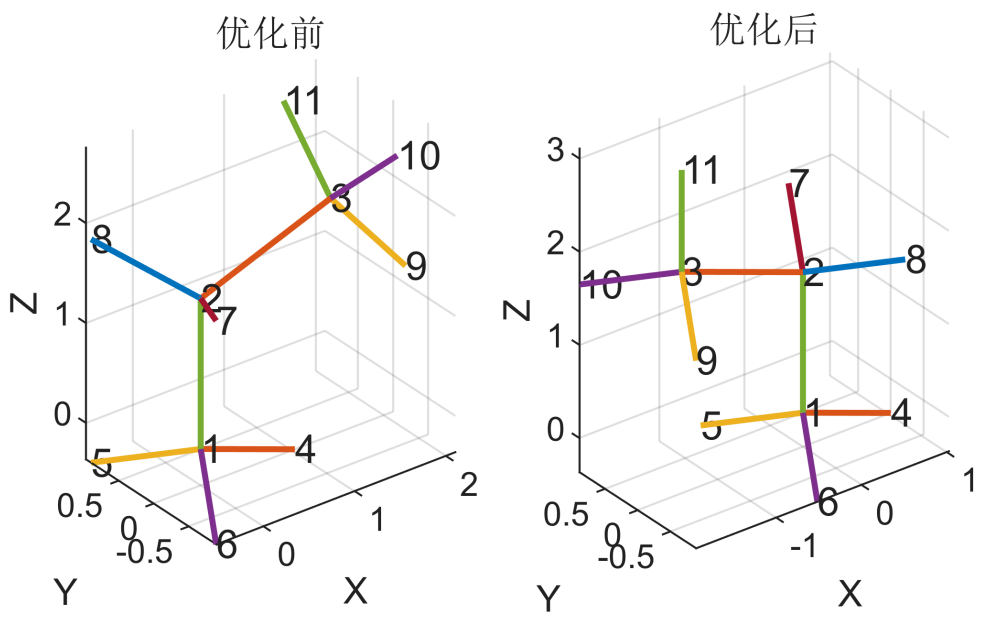
```
rc = 1×3
     0   180   120
```

```
roundcount
```

```
roundcount = 24
```

```
opt_xyz_tb=xyzprecal(alpha_tb,ac,nhc_all_tb,bs_procut_arr,adj_list,mtype_all_arr,
m_sphe_arr);

function judge=judgestop(old_tb,new_tb,sep_tb)
osize=size(old_tb,2);
for i=1:osize
    if abs(new_tb(1,i)-old_tb(1,i))<=sep_tb(1,i)
        judge=true;
        return
    end
end
judge=false;
end

function [sumE,mid_xyz_tb] =
getoptE(alpha_tb,ac,nhc_all_tb,bs_procut_arr,ab_procut_arr,sb_fastcut_arr,sb_cmpl
cut_arr,opb_fastcut_arr,opb_cmplcut_arr,ti_fastcut_arr,ti_cmplcut_arr,vdw_tb,adj_
list,big_adj_list,mtype_all_arr,m_sphe_arr)

mid_xyz_tb=xyzprecal(alpha_tb,ac,nhc_all_tb,bs_procut_arr,adj_list,mtype_all_arr,
m_sphe_arr);
nhc=size(nhc_all_tb,1);
[sumE,~,~,~,~,~,~]=getE(mid_xyz_tb,nhc,bs_procut_arr,ab_procut_arr,sb_fastcut_arr
,sb_cmplcut_arr,opb_fastcut_arr,opb_cmplcut_arr,ti_fastcut_arr,ti_cmplcut_arr,vdw
_tb,big_adj_list,mtype_all_arr);
end
```

```
figure;
subplot(1,2,1)
moledraw(pre_xyz_tb,adj_list)
title("优化前")

subplot(1,2,2)
moledraw(opt_xyz_tb,adj_list)
title("优化后")
```




```
[sumE,sumEB,sumEA,sumEBA,sumEOOP,sumET,sumEVDW]=getE(opt_xyz_tb,nhc,bs_procut_arr
,ab_procut_arr,sb_fastcut_arr,sb_cmplcut_arr,opb_fastcut_arr,opb_cmplcut_arr,ti_f
astcut_arr,ti_cmplcut_arr,vdw_tb,big_adj_list,mtype_all_arr)
```

```
sumE = -1.0054
sumEB = 0
sumEA = 5.6726e-05
sumEBA = 0
sumEOOP = 0
sumET = -13.1459
sumEVDW = 12.1404
```

```
S=strings(ac,1);
for i=1:ac
    if i<=nhc
        S(i,1)=nh_tb{i,"Element"};
    else
        S(i,1)="H";
    end
end
SXYZ=array2table([S,opt_xyz_tb],"VariableNames",["Symbol","X","Y","Z"]);
writetable(SXYZ, "CCC_TEST/SXYZ.csv");

T2=[];
for j=1:nhc
    now_parent_j=j-1;
    nb_node=big_adj_list({num2str(now_parent_j)});
    nb_node=sort(nb_node{:});
    nsize=size(nb_node,2);
```

```
    for i=1:nsize
        if j<nb_node(1,i)+1
            T2=[T2;j nb_node(1,i)+1];
        end
    end
end
ADJT=array2table(T2,"VariableNames",["A","B"]);
writetable(ADJT, "CCC_TEST/ADJ_AB.csv");
```

```
% pre_xyz_tb
% opt_xyz_tb
```

```
function tb=readmmffcsv(csv_filename)
csv_folder = "../Values/MMFF94_CSV";
tb = readtable(fullfile(csv_folder,csv_filename));
end
function tb=readspcsv(csv_filename)
csv_folder = "../Values/C_SP_CSV";
tb = readtable(fullfile(csv_folder,csv_filename));
end

function rect=sphe2rect(r,theta,varphi)
x=r*sind(varphi)*cosd(theta);
y=r*sind(varphi)*sind(theta);
z=r*cosd(varphi);
rect=[x,y,z];
end

function [vec_ox,vec_oy,vec_oz]=gencoosys(xyz_tb,now_parent,now_child)
% 求解 oz
vec_oz=xyz_tb(now_child+1,:)-xyz_tb(now_parent+1,:);
vec_oz=vec_oz/norm(vec_oz);

%求解 ox
%vec_ox=genvec_xyz(zeros(1,3));
vec_ox=zeros(1,3);
if sum(vec_oz(1,2:3))==0
vec_ox(1,1)=0;
vec_ox(1,2)=1;
else
vec_ox(1,1)=1;
vec_ox(1,2)=0;
end
c_xz=dot(vec_ox,vec_oz);
if c_xz~=0
    vec_ox(1,3)=-c_xz/vec_oz(1,3);
end
vec_ox=vec_ox/norm(vec_ox);
%% 求解 oy
vec_oy=cross(vec_oz,vec_ox);
vec_oy=vec_oy/norm(vec_oy);
end
```

```
function [Rv_ij,epsilon_ij]=precalEVDWParam(vdw_tb,mtype_arr)
mi=mtype_arr(1,1);
mj=mtype_arr(1,2);
A_i=vdw_tb{mi,"A_I"};
A_j=vdw_tb{mj,"A_I"};
G_i=vdw_tb{mi,"G_I"};
G_j=vdw_tb{mj,"G_I"};
N_i=vdw_tb{mi,"N_I"};
N_j=vdw_tb{mj,"N_I"};
alpha_i=vdw_tb{mi,"ALPHA_I"};
alpha_j=vdw_tb{mj,"ALPHA_I"};
B=0.2;
beta=12;
Rv_ii=A_i*alpha_i^0.25;
Rv_jj=A_j*alpha_j^0.25;
gamma_ij=(Rv_ii-Rv_jj)/(Rv_ii+Rv_jj);
Rv_ij=0.5*(Rv_ii+Rv_jj)*(1+B*(1-exp(-beta*gamma_ij^2)));
epsilon_ij=181.16*G_i*G_j*alpha_i*alpha_j/((alpha_i/N_i)^0.5+(alpha_j/N_j)^0.5)/
Rv_ij^6;
end
```

```
function m_rect_arr=arr_sphe2rect(m_sphe_arr)
m_rect_arr=zeros(size(m_sphe_arr));
for i=1:size(m_sphe_arr,1)
    rect=sphe2rect(m_sphe_arr(i,2),m_sphe_arr(i,3),m_sphe_arr(i,4));
    m_rect_arr(i,:)=[m_sphe_arr(i,1),rect];
end
end
```

```
function r=xyz2r(xyz_ij)
r=sqrt(sum((xyz_ij(1,:)-xyz_ij(2,:)).^2));
end

function vartheta=xyz2vartheta(xyz_ijk)
a=xyz_ijk(1,:)-xyz_ijk(2,:);
b=xyz_ijk(3,:)-xyz_ijk(2,:);
vartheta=acosd(dot(a,b)/(norm(a)*norm(b)));
end

function phi=xyz2phi(xyz_ijkl)
a=xyz_ijkl(1,:)-xyz_ijkl(2,:);
b=xyz_ijkl(3,:)-xyz_ijkl(2,:);
c=xyz_ijkl(4,:)-xyz_ijkl(3,:);

n_ab=cross(a,b);
n_bc=cross(b,c);
```

```
phi_1=acosd(dot(n_ab,n_bc)/norm(n_ab)/norm(n_bc));
k=-dot(a,b)/dot(b,b);
d=a+k*b;
judge=dot(d,c)<0;
if judge
    phi=180-phi_1;
else
    phi=phi_1;
end
end

function chi=xyz2chi(xyz_ijkl)
a=xyz_ijkl(1,:)-xyz_ijkl(2,:);
b=xyz_ijkl(3,:)-xyz_ijkl(2,:);
c=xyz_ijkl(4,:)-xyz_ijkl(2,:);
n=cross(a,b);
chi=abs(90-acosd(dot(c,n)/norm(c)/norm(n)));
end

function rec_node=bfs_finddepth(adj_list,start_pos,depth)
adj_key={num2str(start_pos)};
if depth==0 || ~isKey(adj_list,adj_key)
    rec_node= start_pos;
    return
else
    now_node_arr=adj_list(adj_key);
    now_node_arr=now_node_arr{:};
    rec_node=start_pos;
    for i=1:size(now_node_arr,2)
        rec_node=[rec_node, bfs_finddepth(adj_list,now_node_arr(1,i),depth-1)];
    end
end
end
```

```
%% 初始三维坐标生成
function
xyz_tb=xyzprecal(alpha_tb,ac,nhc_all_tb,bs_pro_arr,adj_list,mtype_all_arr,m_sphe_
arr)


nhc=size(nhc_all_tb,1);
xyz_tb=zeros(ac,3);

rec_xyz=[1 zeros(1,ac-1)];
for j=1:nhc
    now_parent=j-1;
    m=nhc_all_tb(j,1);
    if m~=4
        disp(m)
        continue
    end
    nb_node=adj_list({num2str(now_parent)});
    nb_node=nb_node{:};
```

```
    nsize=size(nb_node,2);

    new_m_arr=m_sphe_arr(1:m,:,m);
    new_m_arr(:,3)=mod(new_m_arr(:,3)+alpha_tb(1,j),360);
    m_rect_arr=arr_sphe2rect(new_m_arr);
    B=[];
    for i=1:nsize
        now_child=nb_node(1,i);
        index_ij=[now_child,now_parent]+1;
        mtype_ij=mtype_all_arr(index_ij,1)';
        r0=bs_pro_arr(mtype_ij(1,1),mtype_ij(1,2),1);
        if i==1
            %% 第二个原子
            if j==1
                xyz_tb(now_child+1,:)=[0,0,r0];
                rec_xyz(1,now_child+1)=1;
            end
            %% 确定坐标系 II 基矢 ox,oy,oz
            [vec_ox,vec_oy,vec_oz]=gencoosys(xyz_tb,now_parent,now_child);

            B=[vec_ox; vec_oy; vec_oz];
        elseif now_child>now_parent &&rec_xyz(1,now_child+1)==0
            %% 向量旋转公式
            adot=m_rect_arr(i,2:end)*B;
            xyz_i=(r0*adot)+xyz_tb(now_parent+1,:);
            xyz_tb(now_child+1,:)=xyz_i;
            rec_xyz(1,now_child+1)=1;
        end
    end

end

end
```

```
function moledraw(xyz_tb,adj_list)
nhc=size(keys(adj_list),1);
for j=1:nhc
    nb_node=adj_list({num2str(j-1)});
    nb_node=sort(nb_node{:});
    nsize=size(nb_node,2);
    for i=1:nsize
        line_parent_child(xyz_tb,j,nb_node(1,i)+1);
        hold on;
    end
end
for i=1:size(xyz_tb,1)
    text(xyz_tb(i,1),xyz_tb(i,2),xyz_tb(i,3),num2str(i));
end
axis equal
grid on
box off
xlabel("X")
ylabel("Y")
```

```
zlabel("Z")

end
```

```
function
[sumE,sumEB,sumEA,sumEBA,sumEOOP,sumET,sumEVDW]=getE(xyz_tb,nhc,bs_pro_arr,ab_pro
_arr,sb_fast_arr,sb_cmpl_arr,opb_fast_arr,opb_cmpl_arr,ti_fast_arr,ti_cmpl_arr,vd
w_tb,big_adj_list,mtype_all_arr)

ac=size(xyz_tb,1);

max_m=6;
r_ij_tb=zeros(ac,ac);
dr_ij_tb=zeros(size(r_ij_tb));

var_ijk_tb=zeros(nhc,max_m,max_m);
var_ijk_tb(var_ijk_tb==0)=NaN;
dvar_ijk_tb_rad=var_ijk_tb;

mtype_short = sort(unique(mtype_all_arr, 'rows', 'stable'),1);
max_mtype_count=size(mtype_short,1);
max_mtype=max(mtype_short,[],"all");
mtype_2_mid=zeros(max_mtype,1);
for i=1:max_mtype_count
    mt=mtype_short(i,1);
    mtype_2_mid(mt,1)=i;
end

Rv_ij_mid_tb=zeros(max_mtype_count,max_mtype_count);
epsilon_ij_mid_tb=zeros(max_mtype_count,max_mtype_count);

Rv_ij_tb=zeros(ac,ac);
epsilon_ij_tb=zeros(ac,ac);

% Rv_ij 表坐标变换
for i=1:max_mtype_count
    for j=1:max_mtype_count

[Rv_ij_mid_tb(i,j),epsilon_ij_mid_tb(i,j)]=precalEVDWParam(vdw_tb,mtype_all_arr(m
type_short([i,j],1),1)');
        Rv_ij_mid_tb(j,i)=Rv_ij_mid_tb(i,j);
        epsilon_ij_mid_tb(j,i)=epsilon_ij_mid_tb(i,j);
    end
end

for j=1:nhc
    now_parent_j=j-1;
    nb_node=big_adj_list({num2str(now_parent_j)});
    nb_node=sort(nb_node{:});
    nsize=size(nb_node,2);
    for i=1:nsize
        for k=(i+1):nsize
```

```
            now_child_i=nb_node(1,i);
            now_child_k=nb_node(1,k);
            index_ijk=[now_child_i,now_parent_j,now_child_k]+1;

            xyz_ijk=xyz_tb(index_ijk,:);
            var_ijk_tb(j,i,k)=xyz2vartheta(xyz_ijk);

            mtype_ijk=mtype_all_arr(index_ijk,1)';
            dvar_ijk_tb_rad(j,i,k)=deg2rad(var_ijk_tb(j,i,k)-
ab_pro_arr(mtype_ijk(1,1),mtype_ijk(1,2),mtype_ijk(1,3),1));
            dvar_ijk_tb_rad(j,k,i)=dvar_ijk_tb_rad(j,i,k);
        end
    end
end

for j=1:ac
    for i=j:ac

        index_ij=[i,j];
        mtype_ij=mtype_all_arr(index_ij,1)';
        new_id=mtype_2_mid(mtype_ij,1)';
        Rv_ij_tb(i,j)=Rv_ij_mid_tb(new_id(1,1),new_id(1,2));
        Rv_ij_tb(j,i)=Rv_ij_tb(i,j);
        epsilon_ij_tb(i,j)=epsilon_ij_mid_tb(new_id(1,1),new_id(1,2));
        epsilon_ij_tb(j,i)=epsilon_ij_tb(i,j);
        if i~=j
            xyz_ij=xyz_tb([i j],:);
            r_ij_tb(i,j)=xyz2r(xyz_ij);
            r_ij_tb(j,i)=r_ij_tb(i,j);
            dr_ij_tb(i,j)=r_ij_tb(i,j)-bs_pro_arr(mtype_ij(1,1),mtype_ij(1,2));
            dr_ij_tb(i,j)=dr_ij_tb(j,i);
        end
    end
end

%% 总势能计算
sumEB=0;
sumEA=0;
sumEBA=0;
sumEOOP=0;
sumET=0;
sumEVDW=0;

%% 计算各个能量
for j=1:nhc
    now_parent_j=j-1;
    nb_node=big_adj_list({num2str(now_parent_j)});
    nb_node=nb_node{:};
    nsize=size(nb_node,2);

    %% EB：对第 i 个原子只遍历编号比 i 大的相邻节点
    for i=1:nsize
        now_child=nb_node(1,i);
        if now_child>now_parent_j
```

```
            index_ij=[now_child,now_parent_j]+1;
            mtype_ij=mtype_all_arr(index_ij,1)';
            mi=mtype_ij(1,1);
            mj=mtype_ij(1,2);
            sumEB=sumEB+newgetEB(dr_ij_tb(i,j),bs_pro_arr(mi,mj,2));
        end
    end

    %% EA：遍历中心原子
    %% EBA：同 EA
    for i=1:nsize
        for k=(i+1):nsize
            ci=nb_node(1,i)+1;
            cj=now_parent_j+1;
            ck=nb_node(1,k)+1;

            mtype_ijk=mtype_all_arr([ci,cj,ck],1)';

            mi=mtype_ijk(1,1);
            mj=mtype_ijk(1,2);
            mk=mtype_ijk(1,3);

            ti=sb_cmpl_arr(1,mi);
            tj=sb_cmpl_arr(2,mj);
            tk=sb_cmpl_arr(3,mk);

            sumEA=sumEA+newgetEA(dvar_ijk_tb_rad(j,i,k),ab_pro_arr(mi,mj,mk,2));

sumEBA=sumEBA+newgetEBA(dr_ij_tb(j,i),dr_ij_tb(j,k),dvar_ijk_tb_rad(j,i,k),sb_fas
t_arr(ti,tj,tk,1),sb_fast_arr(ti,tj,tk,2));
            % sumEBA=sumEBA+newgetEBA(dr_ij,dr_kj,dvar,kba_ijk,kba_kji);
        end
    end
    %% EOOP：仅 AllBond=3 时
    if nsize==3
        for l=1:nsize
            now_child_l=nb_node(1,l);
            now_node_arr=nb_node;
            now_node_arr(1,l)=[];
            now_child_i=now_node_arr(1,1);
            now_child_k=now_node_arr(1,2);

            index_ijkl=[now_child_i,now_parent_j,now_child_k,now_child_l]+1;
            xyz_ijkl=xyz_tb(index_ijkl,:);
            chi_ijkl=deg2rad(xyz2chi(xyz_ijkl));
            mtype_ijkl=mtype_all_arr(index_ijkl,1)';

            ti=opb_cmpl_arr(1,mtype_ijkl(1,1));
            tj=opb_cmpl_arr(2,mtype_ijkl(1,2));
            tk=opb_cmpl_arr(2,mtype_ijkl(1,3));
            tl=opb_cmpl_arr(2,mtype_ijkl(1,4));

            sumEOOP=sumEOOP+newgetEOOP(chi_ijkl,opb_fast_arr(ti,tj,tk,tl,1));
        end
```

```
    end

    %% ET：同 EB
    for k =j:nsize
        now_parent_k=nb_node(1,k);
        if now_parent_k<nhc
            node_i_arr=sort(cell2mat(big_adj_list({num2str(now_parent_j)})));
            node_l_arr=sort(cell2mat(big_adj_list({num2str(now_parent_k)})));
            insize=size(node_i_arr,2);
            lnsize=size(node_l_arr,2);
            for i=1:insize
                for l=1:lnsize
                    now_child_i=node_i_arr(1,i);
                    now_child_l=node_l_arr(1,l);
                    if now_child_l~=now_parent_j&&now_parent_k~=now_child_i

index_ijkl=[now_child_i,now_parent_j,now_parent_k,now_child_l]+1;
                        xyz_ijkl=xyz_tb(index_ijkl,:);
                        mtype_ijkl=mtype_all_arr(index_ijkl,1)';

                        ti=ti_cmpl_arr(1,mtype_ijkl(1,1));
                        tj=ti_cmpl_arr(2,mtype_ijkl(1,2));
                        tk=ti_cmpl_arr(3,mtype_ijkl(1,3));
                        tl=ti_cmpl_arr(4,mtype_ijkl(1,4));

                        phi=xyz2phi(xyz_ijkl);
                        %ET=newgetET(phi,V1,V2,V3)

sumET=sumET+newgetET(phi,ti_fast_arr(ti,tj,tk,tl,1),ti_fast_arr(ti,tj,tk,tl,2),ti
_fast_arr(ti,tj,tk,tl,3));
                    end
                end
            end
        end
    end
end
for j=1:ac
    %% EVDW：BFS
    rec_node=bfs_finddepth(big_adj_list,j-1,2);
    rec_node_arr=zeros(1,ac);
    rnsize=size(rec_node,2);
    for ii=1:rnsize
        rec_node_arr(1,1+rec_node(1,ii))=true;
    end
    for bi=j:ac
        if rec_node_arr(1,bi)
            continue
        end
        index_ij=[j,bi];
        %mtype_ij=mtype_all_arr(index_ij,1)';
        R_ij=r_ij_tb(index_ij(1,1),index_ij(1,2));

EVDW=newgetEVDW(R_ij,Rv_ij_tb(index_ij(1,1),index_ij(1,2)),epsilon_ij_tb(index_i
j(1,1),index_ij(1,2)));
```

```
        sumEVDW=sumEVDW+EVDW;
    end
end
sumE=sumEB+sumEA+sumEBA+sumEOOP+sumET+sumEVDW;
end

function p=line_parent_child(xyz_tb,parent,child)
p=plot3([xyz_tb(child,1),xyz_tb(parent,1)], ...
    [xyz_tb(child,2),xyz_tb(parent,2)], ...
    [xyz_tb(child,3),xyz_tb(parent,3)],"-",LineWidth=1.5);
end

function EB=newgetEB(dr_ij,kb)
cs=-2;
EB=143.9525*kb/2*dr_ij^2*(1+cs*dr_ij+7/12*cs^2*dr_ij^2);
end

function EA=newgetEA(dvar,ka)
cb=-0.000122;
EA=0.043844*ka/2*dvar^2*(1+cb*dvar);
end

function EBA=newgetEBA(dr_ij,dr_kj,dvar,kba_ijk,kba_kji)
EBA=2.51210*(kba_ijk*dr_ij+kba_kji*dr_kj)*dvar;
end

function EOOP=newgetEOOP(chi_ijkl,koop)
EOOP=0.034844*koop/2*chi_ijkl^2;
end

function ET=newgetET(phi,V1,V2,V3)
ET=0.5*(V1*(1+cosd(phi))+V2*(1-cosd(2*phi)+V3*(1+cosd(3*phi))));
end

function EVDW=newgetEVDW(R_ij,Rv_ij,epsilon_ij)
EVDW=epsilon_ij*(1.07*Rv_ij/(R_ij+0.07*Rv_ij))^7*(1.12*Rv_ij^7/
(R_ij+0.12*Rv_ij^7)-2);
end
```