Self-assembly of $[PNb_xW_{12-x}O_{40}]^{n-}$ Keggin anions–a simple way to mixed Nb-W polyoxometalates.

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SUPPORTING INFORMATION

SI-1. Matlab code (Topo_MH) to compute isomers in the series $[PNb_xW_{12-x}O_{40}]^{(3+x)-}$.

```
%% topo_MH.m


topology_Keggin_alpha


N= size(topo,1);

temp=zeros(1,N);

temp2= 0;

for in2=1:size(topo,2),

        for in=1:N,  temp(in)= numel(topo{in,in2}); end;

        temp2= [temp2,max(temp)];

end;

N2= 1+ sum(temp2);


N_Niob=7;

wert= [1:N_Niob];  wert(end)=wert(end)-1;


q=[]; while(wert(1)==1), wert= counter( wert ,N); q=[q;wert];end;

liste_start= q(1:end-1,:);

N_liste= size(liste_start,1);


res1= zeros(N_liste,N);

res2= zeros(N_liste,N);

res3= zeros(N_liste,1);

res4= zeros(N,N2,N_liste);

for in1=1:N_liste,


        rang_in= ones(1,N);  rang_in( liste_start(in1,:) )=2;
```

```
        rang_matrix =  topo_extended_ordnen( topo ,rang_in);
        rang_out=      rang_matrix(:,1)';
        rang_sorted=   sort(rang_out);
        N_groups=      numel(unique(rang_out));

        res1(in1,:)=   rang_in;
        res2(in1,:)=   rang_sorted;
        res3(in1,1)=   N_groups;
        %%GF: res4(:,:,in1)= sortrows( rang_matrix );
        res4(:,:,in1)= rang_matrix;
end;

%Finde Wiederholungen:
%---------------------
ist_wiederholung_von= zeros(N_liste,1);
gruppen= cell(0);
count=0;

for in1=1:N_liste-1,
        if( ist_wiederholung_von(in1) ),  continue;  end;
        ;
        count= count+1;
        gruppen{count}= [in1];
        u1= topo_extended_ordnen( topo ,res1(in1,:) ,res1(in1,:));
        for in2= in1+1:N_liste,
                if(     res3(in1)  ~=res3(in2)    ),  continue;  end;
                if(~all(res2(in1,:)==res2(in2,:) )),  continue;  end;
                ;
```

```
                u2=  topo_extended_ordnen( topo ,res1(in1,:) ,res1(in2,:));;
                if(all(u1(1:N,:)==u2(1:N,:))),
                        'identisch';
                        ist_wiederholung_von(in2)= in1;
                        gruppen{count}= [gruppen{count} ,in2];
                else,
                        'unterschiedlich';
                end;
        end;
end;

Ng=numel(gruppen);
anzahl_gruppen_mitglieder=zeros(Ng,1); for in=1:Ng, anzahl_gruppen_mitglieder(in)= numel( gruppen{in}); end;
[anzahl_gruppen_mitglieder ,index]= sort(anzahl_gruppen_mitglieder);
gruppen= gruppen(index);
anzahl= anzahl_gruppen_mitglieder;


%Betrachten einzelner Gruppen:


figure()
posi=[100,100,870,615]; set(gcf,'Position',posi);

if(     size(liste_start,2)==2), felder=4;  anzahl2=anzahl;
elseif( size(liste_start,2)==3), felder=6;  anzahl3=anzahl;
elseif( size(liste_start,2)==4), felder=8;  anzahl4=anzahl;
elseif( size(liste_start,2)==5), felder=12; anzahl5=anzahl;
elseif( size(liste_start,2)==6), felder=12; anzahl6=anzahl;
```

```
else                    felder=16,,
end;

%%%%%%%%
if(true),

for ing=1:Ng,
        clf
        N_molecules= numel(gruppen{ing} );
        for in1=1:N_molecules,
                index_auswahl= find(1<res1(gruppen{ing}(in1) ,:) );

                if(    felder==4), subplot(2,2,in1);
                elseif(felder==6), subplot(2,3,in1);
                elseif(felder==8), subplot(3,3,in1);
                elseif(felder==12),subplot(3,4,in1);
                else,              subplot(4,4,in1);
                end;
                mache_diagram
                title(['Group: ',num2str(ing)]);
        end;
        if(ing<10), filename=['group_0',num2str(ing)];
        else,       filename=['group_',num2str(ing)];
        end;
        print( gcf, '-djpeg' ,filename );
end;

%%%%%%%
end;
```

SI-2. How to use topo_MH.

1- open matlab sofware and go to the program location (For example C:\Programs\Matlab7\work\Topo)

2- Edit the program ("edit topo_MH") and enter the Nb of Nb atom line 14: "N_Niob=n" and then save the file

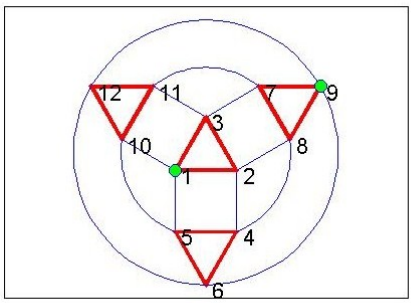
3- run the program ("topo_MH")

4- As a result (output) figures (jpeg) will be created in the folder (C:\Programs\Matlab7\work\Topo) have to be moved (overwise will be erased next time !!) and some figures will appear (2 in all the first and the last results)

5- To obtain the multiplicity tape "gruppen"

SI-3. Example for x = 2, $[PNb_2W_{10}O_{40}]^{5-}$.

Group: 1



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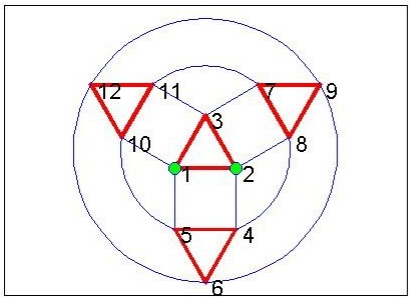

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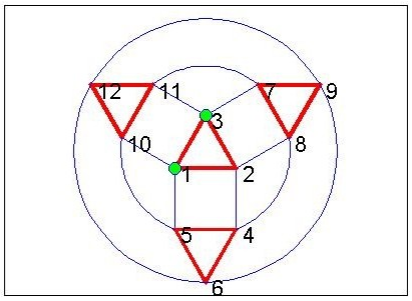

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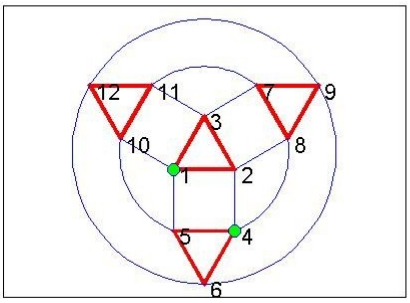

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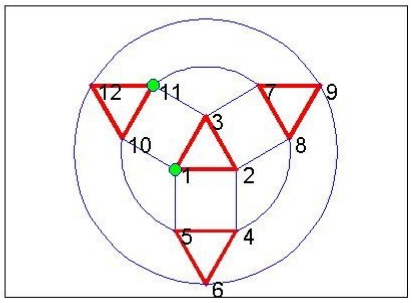

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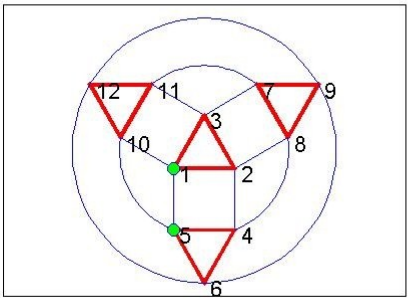

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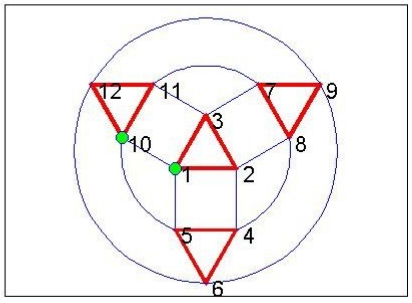

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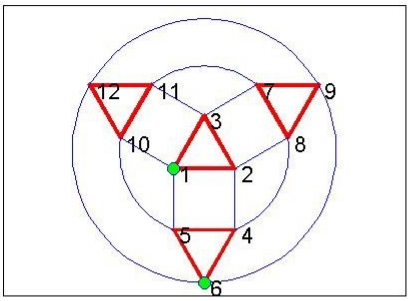

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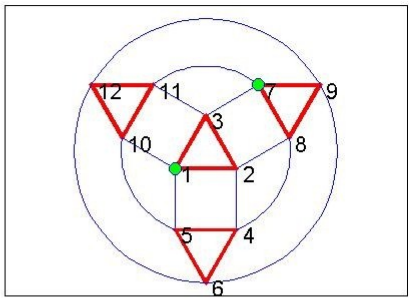

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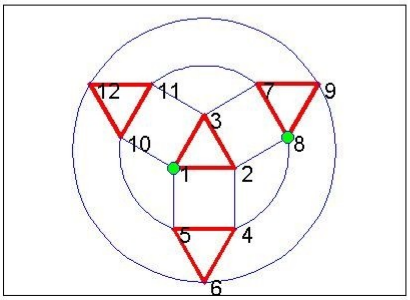

Group: 5