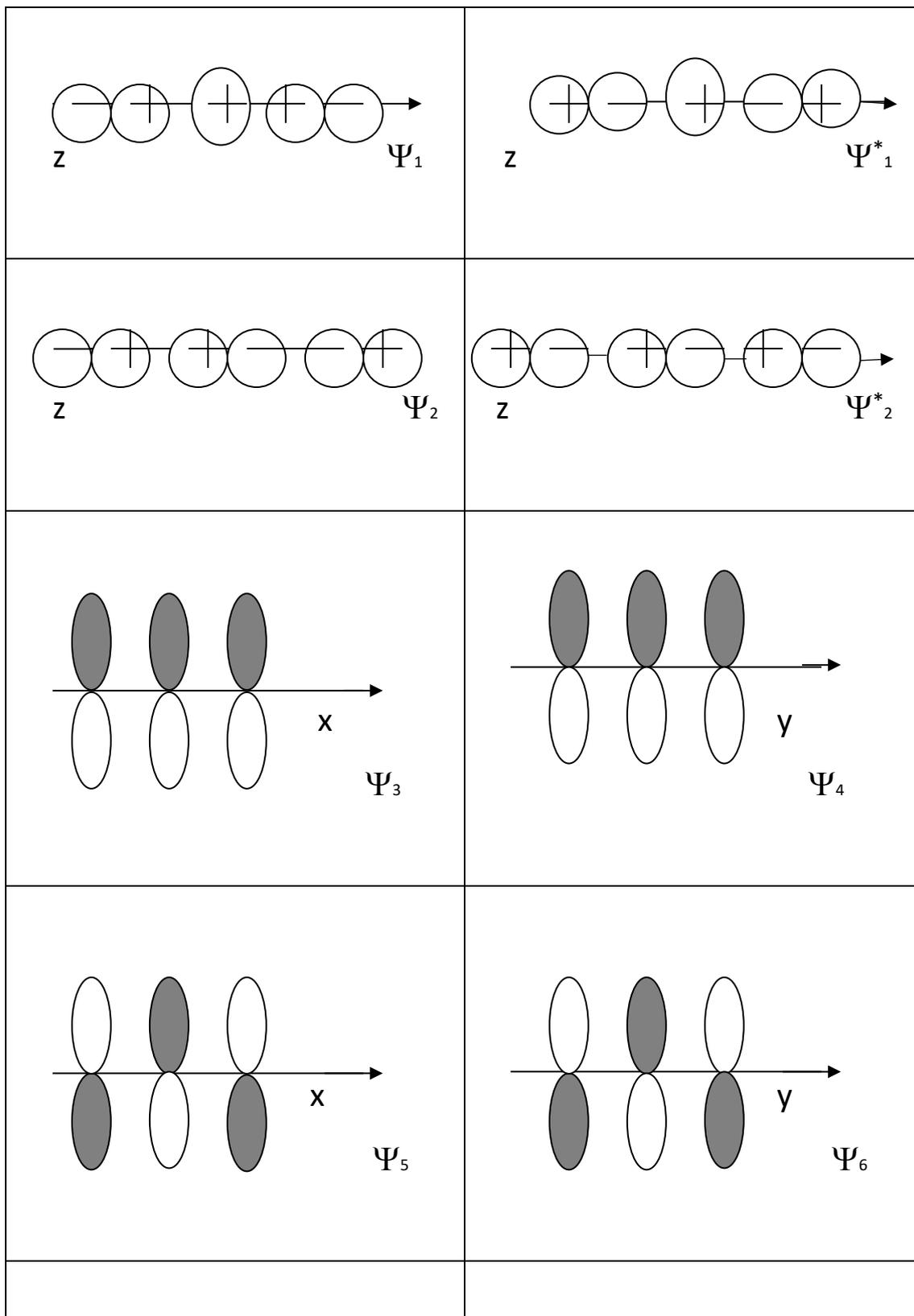
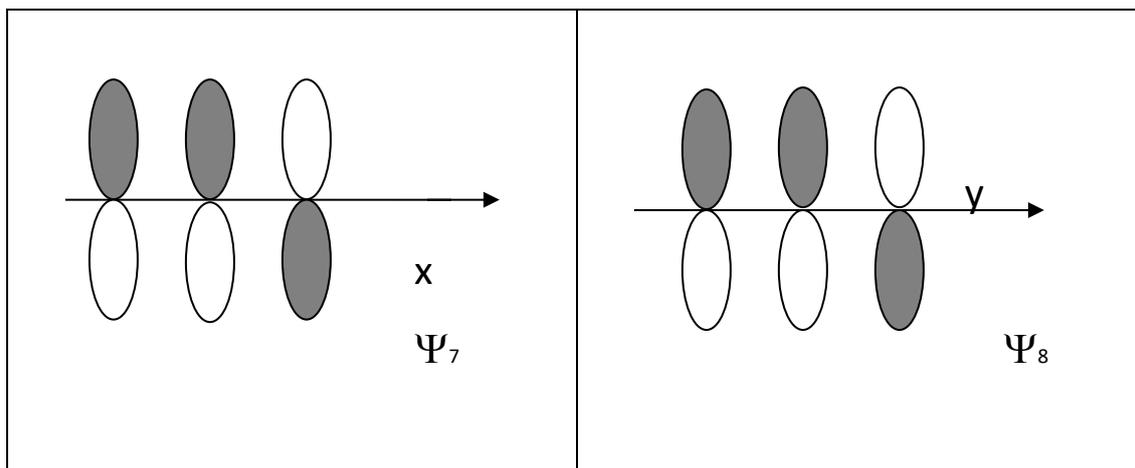


I will attach the wave functions, whose graphical representation is in fig.21:

Fig.21:

T.O.M.





$$\Psi_1 = N \cdot \phi_{C2s} + N' \cdot \phi_{O2pz} + N'' \cdot \phi_{O2pz}$$

$$\Psi_1^* = N \cdot \phi_{C2s} - N' \cdot \phi_{O2pz} - N'' \cdot \phi_{O2pz}$$

$$\Psi_2 = N \cdot \phi_{C2pz} + N' \cdot \phi_{O2pz} + N'' \cdot \phi_{O2pz}$$

$$\Psi_2^* = N \cdot \phi_{C2pz} - N' \cdot \phi_{O2pz} - N'' \cdot \phi_{O2pz}$$

$$\Psi_3 = N \cdot \phi_{C2px} + N' \cdot \phi_{O2px} + N'' \cdot \phi_{O2px}$$

Ψ_4 (the same but with $2p_y$)

$$\Psi_5 = N \cdot \phi_{C2px} - N' \cdot \phi_{O2px} - N'' \cdot \phi_{O2px}$$

Ψ_6 (the same but on the y axis)

$$\Psi_7 = N \cdot \phi_{C2px} + N' \cdot \phi_{O2px} - N'' \cdot \phi_{O2px}$$

$$\Psi_8 = N \cdot \phi_{C2py} + N' \cdot \phi_{O2py} - N'' \cdot \phi_{O2py}$$

And the OM that are left to complete the equality $n^\circ OA = n^\circ OM$ is extracted from the two Ψ_{2s} of the oxygen.

And, put to do, when we are with AB_3 , (for example BCl_3) we have fig.22.

Based on the mathematical expressions of the wave functions (Ψ) of case AB_3 (for example BCl_3) that you have below, I leave for you the graphic representation in Molecular Orbitals (TOM). Keep in mind figures 7 and 8.

$$\Psi_1 = N \cdot \phi_{B2s} + N' \cdot \phi_{Cl\ 2px} + N'' \cdot \phi_{Cl\ 2px} + N''' \cdot \phi_{Cl\ 2px}$$

$$\Psi_1^* = N \cdot \phi_{B\ 2s} - N' \cdot \phi_{Cl\ 2px} - N'' \cdot \phi_{Cl\ 2px} - N''' \cdot \phi_{Cl\ 2px}$$

$$\Psi_2 = N \cdot \phi_{B\ 2px} + N' \cdot \phi_{Cl\ 2px} + N'' \cdot \phi_{Cl\ 2px} + /-N''' \cdot \phi_{Cl\ 2px}$$

$$\Psi_2^* = N \cdot \phi_{B\ 2px} - N' \cdot \phi_{Cl\ 2px} - N'' \cdot \phi_{Cl\ 2px} + /-N''' \cdot \phi_{Cl\ 2px}$$

$$\Psi_3 = N \cdot \phi_{B\ 2py} + N' \cdot \phi_{Cl\ 2px} + N'' \cdot \phi_{Cl\ 2px} + N''' \cdot \phi_{Cl\ 2px}$$

$$\Psi_3^* = N \cdot \phi_{B\ 2py} - N' \cdot \phi_{Cl\ 2px} - N'' \cdot \phi_{Cl\ 2px} - N''' \cdot \phi_{Cl\ 2px}$$

$$\Psi_4 = N \cdot \phi_{B\ 2s} + /-N' \cdot \phi_{Cl\ 2py} + /-N'' \cdot \phi_{Cl\ 2py} + /-N''' \cdot \phi_{Cl\ 2py}$$

$$\Psi_5 = N \cdot \phi_{B\ 2py} + /-N' \cdot \phi_{Cl\ 2py} + /-N'' \cdot \phi_{Cl\ 2py} + /-N''' \cdot \phi_{Cl\ 2py}$$

$$\Psi_6 = N \cdot \phi_{B\ 2px} + /-N' \cdot \phi_{Cl\ 2py} + /-N'' \cdot \phi_{Cl\ 2py} + /-N''' \cdot \phi_{Cl\ 2py}$$

$$\Psi_7 = N \cdot \phi_{B\ 2pz} + N' \cdot \phi_{Cl\ 2pz} + N'' \cdot \phi_{Cl\ 2pz} + N''' \cdot \phi_{Cl\ 2pz}$$

$$\Psi_7^* = N \cdot \phi_{B\ 2pz} - N' \cdot \phi_{Cl\ 2pz} - N'' \cdot \phi_{Cl\ 2pz} - N''' \cdot \phi_{Cl\ 2pz}$$

$$\Psi_8 = N \cdot \phi_{B\ 2pz} + N' \cdot \phi_{Cl\ 2pz} + N'' \cdot \phi_{Cl\ 2pz} - N''' \cdot \phi_{Cl\ 2pz}$$

$$\Psi_9 = N \cdot \phi_{B\ 2pz} + N' \cdot \phi_{Cl\ 2pz} - N'' \cdot \phi_{Cl\ 2pz} - N''' \cdot \phi_{Cl\ 2pz}$$

The strength of the links σ is greater than that of the links π .

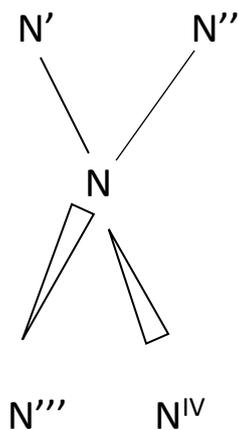
We will see that there are all the options in the links π .

And, finally, we will analyze the representations of the orbitals of AB_4 , located in fig.23.

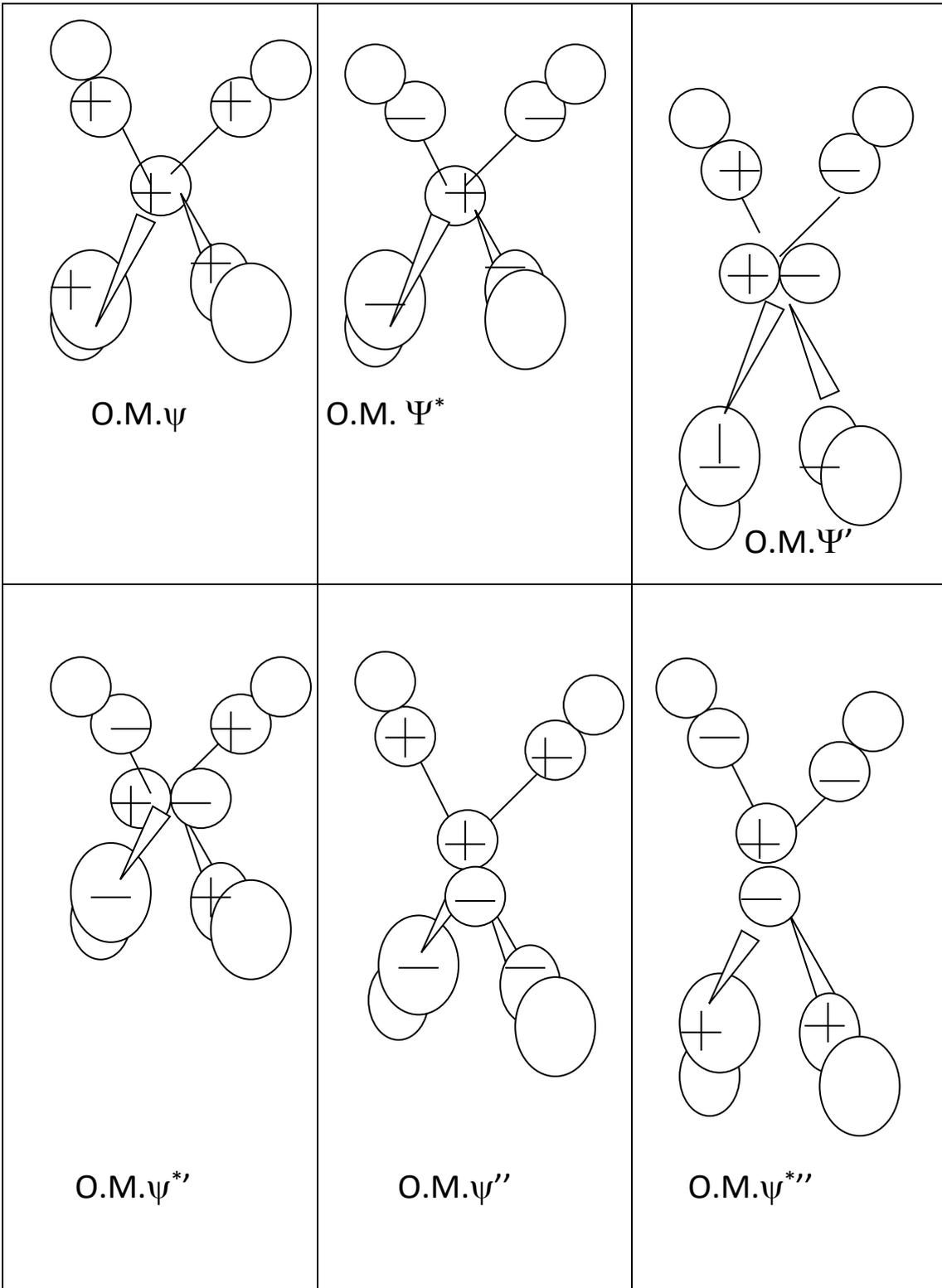
Fig. 23:

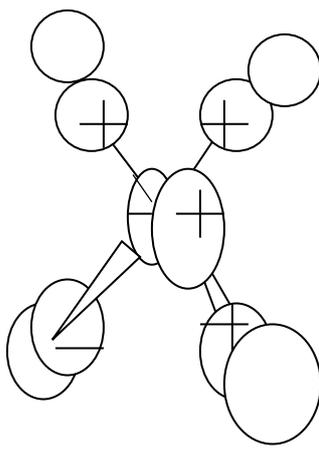
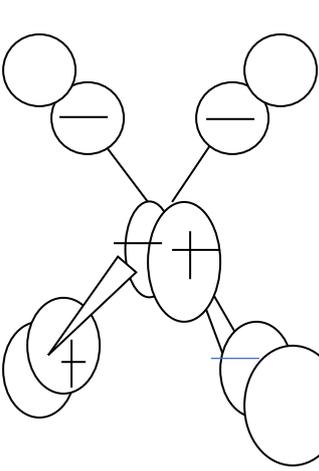
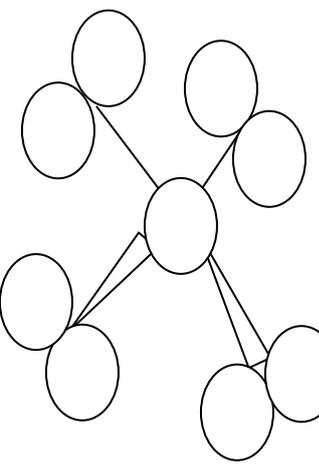
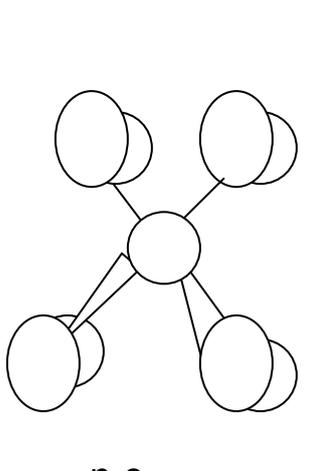
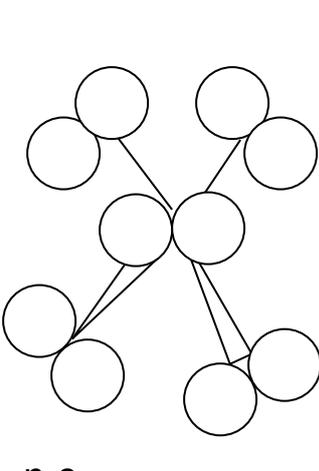
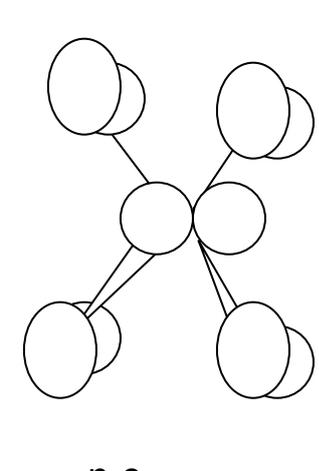
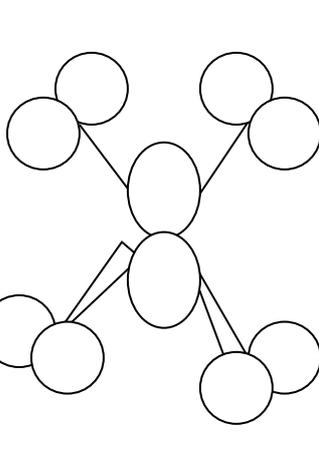
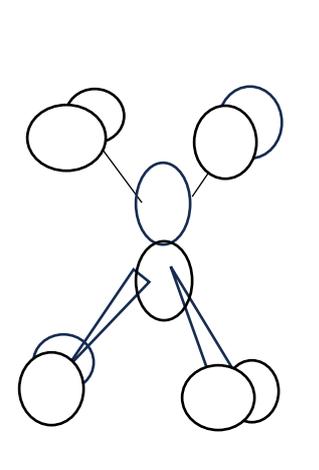
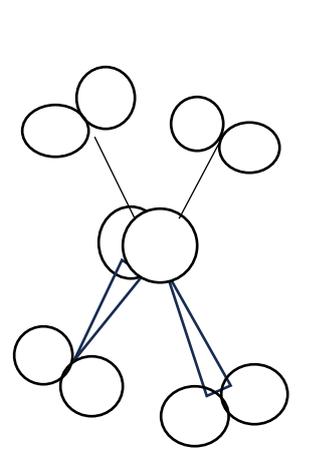
As we have seen in fig.19, we start from the shape of the tetrahedron.

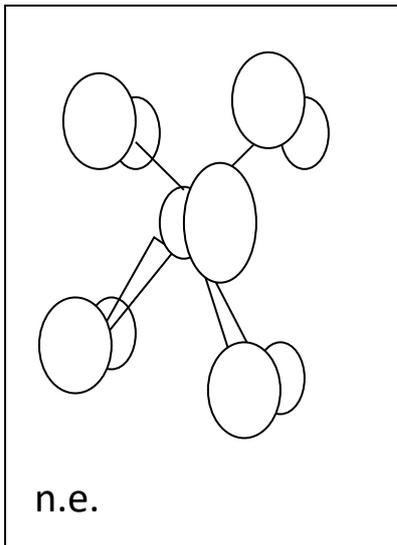
I also show the order of the normalization factors I have taken in such a tetrahedron; Let's remember that the representation of the Ψ is in the "repeca". I care that "n.e" \equiv nonbonding.



T.O.M



 <p>Ψ'''</p>	 <p>$\Psi^{*'''}$</p>	 <p>n.e.</p>
 <p>n.e.</p>	 <p>n.e.</p>	 <p>n.e.</p>
 <p>n.e.</p>	 <p>n.e.</p>	 <p>n.e.</p>



While in terms of TEV, we have already analyzed it at the beginning, they are hybrids. We have left the AB case that is easy to deduce:

$$\Psi_{sp} = \sqrt{1/2} \cdot \varphi_s + \sqrt{1/2} \cdot \varphi_{px}$$

$$\Psi_{sp} = \sqrt{1/2} \cdot \varphi_s - \sqrt{1/2} \cdot \varphi_{px}$$

“REPESCA”:

TOM AB₄:

$\Psi = N.\phi A_{2s+N'}.\phi B_{2px+N''}.\phi B_{2px+N'''}.\phi B_{2px+N^{IV}}.\phi B_{2px}$

$\Psi^* = N.\phi A_{2s-N'}.\phi B_{2px-N''}.\phi B_{2px-N'''}.\phi B_{2px-N^{IV}}.\phi B_{2px}$

$\Psi' = N.\phi A_{2px+N'}.\phi B_{2px+N''}.\phi B_{2px+N'''}.\phi B_{2px+N^{IV}}.\phi B_{2px}$

$\Psi^{*'} = N.\phi A_{2px-N'}.\phi B_{2px-N''}.\phi B_{2px-N'''}.\phi B_{2px-N^{IV}}.\phi B_{2px}$

$\Psi_1 = N.\phi A_{2s+/-N'}.\phi B_{2py+/-N''}.\phi B_{2py+/-N'''}.\phi B_{2py+/-N^{IV}}.\phi B_{2py}$

$\Psi_2 = N.\phi A_{2s+/-N'}.\phi B_{2pz+/-N''}.\phi B_{2pz+/-N'''}.\phi B_{2pz+/-N^{IV}}.\phi B_{2pz}$

$\Psi_3 = N.\phi A_{2px+/-N'}.\phi B_{2py+/-N''}.\phi B_{2py+/-N'''}.\phi B_{2py+/-N^{IV}}.\phi B_{2py}$

$\Psi_4 = N.\phi A_{2px+/-N'}.\phi B_{2pz+/-N''}.\phi B_{2pzy+/-N'''}.\phi B_{2pz+/-N^{IV}}.\phi B_{2pz}$

$\Psi_5 = N.\phi A_{2py+/-N'}.\phi B_{2py+/-N''}.\phi B_{2py+/-N'''}.\phi B_{2py+/-N^{IV}}.\phi B_{2py}$

$\Psi_6 = N.\phi A_{2py+/-N'}.\phi B_{2pz+/-N''}.\phi B_{2pz+/-N'''}.\phi B_{2pz+/-N^{IV}}.\phi B_{2pz}$

$\Psi_7 = N.\phi A_{2pz+/-N'}.\phi B_{2py+/-N''}.\phi B_{2py+/-N'''}.\phi B_{2py+/-N^{IV}}.\phi B_{2py}$

$\Psi_8 = N.\phi A_{2pz+/-N'}.\phi B_{2pz+/-N''}.\phi B_{2pz+/-N'''}.\phi B_{2pz+/-N^{IV}}.\phi B_{2pz}$

$\Psi'' = N.\phi A_{2py+N'}.\phi B_{2px+N''}.\phi B_{2px+/-N'''}.\phi B_{2px+/-N^{IV}}.\phi B_{2px}$

$\Psi^{*''} = N.\phi A_{2py-N'}.\phi B_{2px-N''}.\phi B_{2pz-/-N'''}.\phi B_{2pz-/-N^{IV}}.\phi B_{2pz}$

$\Psi''' = N.\phi A_{2pz+/-N'}.\phi B_{2px+/-N''}.\phi B_{2px+N'''}.\phi B_{2px+N^{IV}}.\phi B_{2px}$

$\Psi^{*'''} = N.\phi A_{2pz+/-N'}.\phi B_{2px+/-N''}.\phi B_{2px-N'''}.\phi B_{2px-N^{IV}}.\phi B_{2px}$

On de Ψ_1 a Ψ_8 són no enllaçants