Orbitales Moleculares

Moléculas con más de dos átomos
H$_2$O (C$_{2v}$)

Three a$_1$ atomic orbitals give three a$_1$ molecular orbitals.

Predicts that the properties of water should be dominated by this lone pair, i.e., that it’s a good nucleophile.

Central oxygen atom’s atomic orbitals

LGO orbitals of terminal atoms H$_1$ + H$_2$
<table>
<thead>
<tr>
<th>Energías</th>
<th>1 ( a_1 )</th>
<th>1 ( b_2 )</th>
<th>2 ( a_1 )</th>
<th>1 ( b_1 )</th>
<th>3 ( a_1^* )</th>
<th>2 ( b_2^* )</th>
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<tbody>
<tr>
<td>( s )</td>
<td>( O ) 1 0.8779</td>
<td>0.0000</td>
<td>0.3331</td>
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<td>( p_z )</td>
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<td>( p_y )</td>
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<tr>
<td>( s )</td>
<td>( H ) 2 0.3304</td>
<td>0.4529</td>
<td>-0.3100</td>
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<tr>
<td>( s )</td>
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<td>-0.3100</td>
<td>0.0000</td>
<td>-0.5429</td>
<td>0.5431</td>
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Energías:

- \( 1 \ a_1 \): -36.828
- \( 1 \ b_2 \): -17.582
- \( 2 \ a_1 \): -14.523
- \( 1 \ b_1 \): -12.317
- \( 3 \ a_1^* \): 4.061
- \( 2 \ b_2^* \): 5.333
Etileno

- Construir combinaciones lineales adaptadas por simetría (CLAS) con los orbitales s de los 4 átomos de hidrógeno

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<tr>
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<th>$C_2(z)$</th>
<th>$C_2(y)$</th>
<th>$C_2(x)$</th>
<th>i</th>
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