

- (b). Calculate M_L for each of the states.
 (c). Find $L = |M_L|_{\max}$. Remove the M_L states from the list from part (b) corresponding to this L .
 (d). Find $L = |M_L|_{\max}$ for the remaining states. Remove the M_L states from the list corresponding to this L .
 (e). Repeat part (d) until all the M_L states are accounted for. Write the term symbols for each of the different L values that you have found (for example, 1D or 3P).
 (f). Repeat steps (a) through (e) for all possible explicit triplet states. For example, one of the explicit triplet states is:
- $\uparrow \square \square \square \square \square \square \square$ $\uparrow \square \square \square \square \square \square \square$
- (g). Verify that the Clebsch-Gordon series applied to the total orbital angular momentum gives the same results.

Answer: (a). and (b). The explicit configurations and M_L values are:

$+3 +2 +1 0 -1 -2 -3$ $\uparrow \square \square \square \square \square \square \square$	$+3 +2 +1 0 -1 -2 -3$ $\square \uparrow \square \square \square \square \square \square$	$+3 +2 +1 0 -1 -2 -3$ $\square \square \uparrow \square \square \square \square \square$	$+3 +2 +1 0 -1 -2 -3$ $\square \square \square \uparrow \square \square \square \square$
with one of:	with one of:	with one of:	with one of:
$+1 0 -1 M_L$ $\downarrow \square \square \square$ 4 $\square \downarrow \square \square$ 3 $\square \square \downarrow \square$ 2	$+1 0 -1 M_L$ $\downarrow \square \square \square$ 3 $\square \downarrow \square \square$ 2 $\square \square \downarrow \square$ 1	$+1 0 -1 M_L$ $\downarrow \square \square \square$ 2 $\square \downarrow \square \square$ 1 $\square \square \downarrow \square$ 0	$+1 0 -1 M_L$ $\downarrow \square \square \square$ 1 $\square \downarrow \square \square$ 0 $\square \square \downarrow \square$ -1
$+3 +2 +1 0 -1 -2 -3$ $\square \square \square \square \uparrow \square \square \square$	$+3 +2 +1 0 -1 -2 -3$ $\square \square \square \square \square \uparrow \square \square$	$+3 +2 +1 0 -1 -2 -3$ $\square \square \square \square \square \square \uparrow \square$	
with one of:	with one of:	with one of:	
$+1 0 -1 M_L$ $\downarrow \square \square \square$ 0 $\square \downarrow \square \square$ -1 $\square \square \downarrow \square$ -2	$+1 0 -1 M_L$ $\downarrow \square \square \square$ -1 $\square \downarrow \square \square$ -2 $\square \square \downarrow \square$ -3	$+1 0 -1 M_L$ $\downarrow \square \square \square$ -2 $\square \downarrow \square \square$ -3 $\square \square \downarrow \square$ -4	

(b). The full list is then:

$$M_L = \{4, 3, 3, 2, 2, 2, 1, 1, 1, 0, 0, 0, -1, -1, -1, -2, -2, -2, -3, -3, -4\}$$

(c). With $L = |M_L|_{\max} = 4$, the first term is a G term based on the definitions of the term symbols:

L:	0	1	2	3	4
Term:	S	P	D	F	G

Removing $M_L = \{4, 3, 2, 1, 0, -1, -2, -3, -4\}$ from the full list leaves:

$$M_L = \{3, 2, 2, 1, 1, 0, 0, -1, -1, -2, -2, -3\}$$

(d). Repeating the process, $L = |M_L|_{\max} = 3$ and the second term is an F term. Removing $M_L = \{3, 2, 1, 0, -1, -2, -3\}$ leaves: $M_L = \{2, 1, 0, -1, -2, -3\}$.

(e). The last term is a D term. The final singlet terms are 1G , 1F , 1D .

(f). The possible triplet arrangements are the same as the singlet terms except that the electron spins are parallel. The resulting terms are, taken together: 1G , 1F , 1D , 3G , 3F , 3D :

(g). Using the Clebsch-Gordan series for the total orbital angular momentum for a p^1f^1 configuration corresponds to $l_1 = 3$ and $l_2 = 1$ so that:

$$L = l_1 + l_2, l_1 + l_2 - 1, \dots, |l_1 - l_2| = 4, 3, 2$$

giving G, F, D terms as listed above.

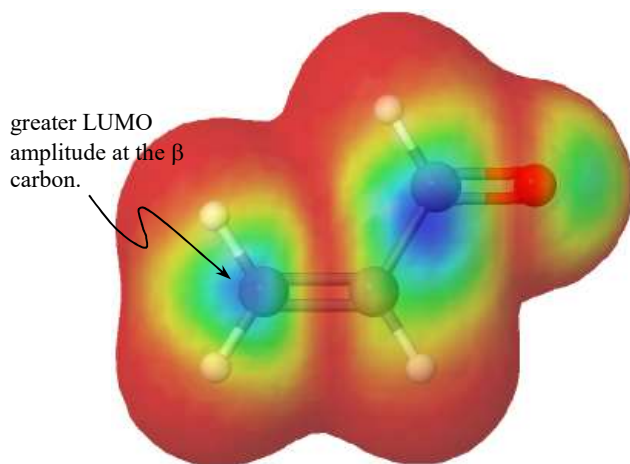
(3). For *trans*-Acrolein:

1. Is the LUMO of acrolein consistent with experimental evidence for reactivity of α,β -unsaturated carbonyl compounds?

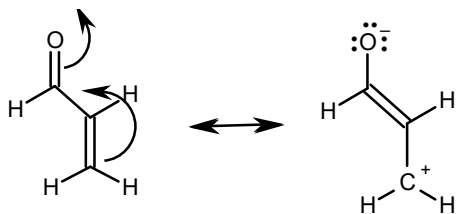
2. Draw the resonance structure that predicts the position of nucleophilic attack on the alpha or beta carbon of the C=C double bond. Show the shifts in the electron pairs with arrows.

3. Does this resonance structure agree with the LUMO map intensity distribution? Explain how you know that they agree or disagree with reference to attack at the alpha or beta carbon of the C=C double bond.

Answer: 1. The LUMO intensity is greater above the β -carbon than the α , which is consistent with the preference for Michael addition at the β -olefin position.



2. The resonance structure that predicts the position of nucleophilic attack on the beta carbon of the C=C double bond is:



3. This resonance structure agrees with the LUMO map intensity distribution. The resonance structure predicts nucleophilic attack at the β -carbon of the C=C double bond, since the β -carbon develops a partial positive charge.