1. Multiplication table: (don’t confuse it with character table!)

<table>
<thead>
<tr>
<th>×</th>
<th>-1</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td>1</td>
</tr>
</tbody>
</table>

It is a group:
1. it’s closed (see multiplication table)
2. multiplication is associative
3. identity=1. identity * 1 = 1, identity * -1 = -1
4. inverse of 1 is 1: 1 * 1 = 1 = identity; inverse of -1 is -1: -1 * -1 = 1 = identity.

order: 2 (2 elements) (The table is not a character table, don’t use Eq. 17.6)

identity: 1

Another thing that you should be aware is that the group (-1,1) is NOT a point group. Don’t try to associate it with symmetry operations and molecules. The operator here is multiplication, and the operator in point groups is to do symmetry operations one after another. And group members in point groups are symmetry operations.

2. 2d ops: E, C4, C4, C4, C4, 2σ, 2σ', i (C2, σh, S4 are not 2d ops, so the two set of mirror planes can’t be addressed as σv and σd)

3. (a) (1*3)+8*(1*0)+3*(1*-1)+6*(-1*1)+6*(-1*-1) = 3+0-3-6+6 = 0 (don’t forget the weights)
(b) Raman activity: x^2, y^2, z^2, xy, yz, xz. 1 for A1, 2 for E, and 3 for T2. The 2 Es and 3 T2s are degenerate respectively.

Make-up:
1. Errors of wavefunction methods (HF and MP2) are not systematic(some errors >0 and others <0). HF result doesn’t follow expectations that the result should always be larger than experimental values, while MP2 result is okay. CO is most difficult to get the property right.
2. Errors of DFT methods (LDA, GGA and B3LYP) are not systematic. Generally the results follow expectations, but it’s surprising to learn that GGA are not always better than LDA (since they are dealing with polar molecules). CO is most difficult to get the property right.