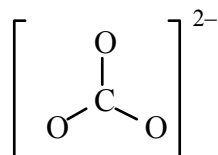


## CHEMISTRY 273

### PROBLEMS

21. Carter, p. 65, 2.8 and  
(c) Using (Lowe, p. 405, flowchart handout; Carter pp. 60-61; Cotton p. 90) give the Mulliken symbols for each of  $\Gamma_1, \dots, \Gamma_5$  assuming  $A=C_4, B=C_4^2, C=C_2', D=C_2''$ . [no peeking at the character tables!!]
22. What irreducible representations span the following direct product representations:  
(a)  $E \times E$  in  $C_{4v}$       (b)  $E_1 \times E_1$  in  $D_{4d}$       (c)  $T_2 \times T_2$  in  $T_d$
23. For formaldehyde,  $H_2CO$ :  
(a) What are the symmetries of the 12 m.o.'s which arise from the valence a.o. basis set ( $H_A 1s; H_B 1s; C 1s, 2s, 2p_x, 2p_y, 2p_z; O 1s, 2s, 2p_x, 2p_y, 2p_z$ )?  
(b) Using the output of the G94 calc indicate the symmetry of each m.o. (1  $\rightarrow$  12). The relevant section of this output is included as an appendix to the problem set.
24. (a) What are the symmetries of the 10  $\pi$ -electron m.o.'s in naphthalene (use geometry convention on page 129 of Cotton).  
(b) Write the SALCS for naphthalene.  
(c) Using nodal concepts, make a guess on how the SALCS will combine to form m.o.'s and what the energy ordering of m.o.'s will be.  
(d) What is the state symmetry of naphthalene in open shell configuration  $b_{1u} b_{2g}$ ?
25. Consider the planar molecule  $CO_3^{2-}$ . The oxygen atoms are at the corners of an equilateral triangle.



- (a) What is the point group of this molecule?

- (b) Using the appropriate character table, assign a symmetry symbol to each of the following m.o.s (1-4 are from 2p a.o.s; 5 is from 2s a.o.s).

