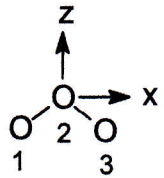
1. Refer to the molecular orbitals for ozone in the table below by number and:
a) Assign each a symmetry label (Mulliken symbol in first column for its irreducible representation) in the C_{2v} point group.



b) Classify each orbital as having σ or π symmetry (this is done relative to the bond axis, not the point group symmetry

c) Use the wave functions below to determine whether each orbital is fully bonding (F), mixed bonding and antibonding (M), non-bonding (N) or fully antibonding (A).
Fully bonding orbitals will have no contribution from an orbital on a terminal atom that is opposite in phase to that of the orbital used by the center atom. Mixed bonding and antibonding will have a contribution from an orbital on a terminal atom with opposite phase to that of the orbital used by the center atom, but also a contribution from an orbital with the same phase.

	MO#	1	2	3	4	5	6	7	8	9	10	11	12
	E, eV	-42.7	-34.0	-25.3	-16.9	-17.9	-17.1	-10.8	-10.2	-8.4	2.7	13.6	16.5
Atomic orbital	O 1 s	0.32	0.60	0.61	0.40	0.28	0.00	-0.06	-0.05	0.00	0.00	-0.31	0.33
	O 1 px	0.09	0.07	-0.06	-0.22	-0.35	0.00	0.51	-0.14	0.00	0.00	-0.67	0.52
	O 1 py	0.00	0.00	0.00	0.00	0.00	0.37	0.00	0.00	0.71	-0.61	0.00	0.00
	O 1 pz	0.05	0.06	-0.10	-0.35	0.16	0.00	-0.50	0.64	0.00	0.00	-0.28	0.43
	O 2 s	0.68	0.00	-0.69	0.00	0.08	0.00	0.00	-0.20	0.00	0.00	0.72	0.00
	O 2 px	0.00	-0.32	0.00	0.58	0.00	0.00	-0.15	0.00	0.00	0.00	0.00	0.95
	O 2 py	0.00	0.00	0.00	0.00	0.00	0.76	0.00	0.00	0.00	0.67	0.00	0.00
	O 2 pz	-0.13	0.00	-0.23	0.00	0.69	0.00	0.00	-0.45	0.00	0.00	-0.64	0.00
	O 3 s	0.32	-0.60	0.61	-0.40	0.28	0.00	0.06	-0.05	0.00	0.00	-0.31	-0.33
	O 3 px	-0.09	0.07	0.06	-0.22	0.35	0.00	0.51	0.14	0.00	0.00	0.67	0.52
	O 3 py	0.00	0.00	0.00	0.00	0.00	0.37	0.00	0.00	-0.71	-0.61	0.00	0.00
	O 3 pz	0.05	-0.06	-0.10	0.35	0.16	0.00	0.50	0.64	0.00	0.00	-0.28	-0.43

d) Draw a schematic diagram of MO #11 showing the orientations, appropriate relative phases and rough relative sizes of the composite atomic orbitals on each atom as they would combine to form the molecular orbital. Example to right: MO #4 (shading indicates positive phase – drawing done with ChemDraw)