

Inorganic 09348 2001

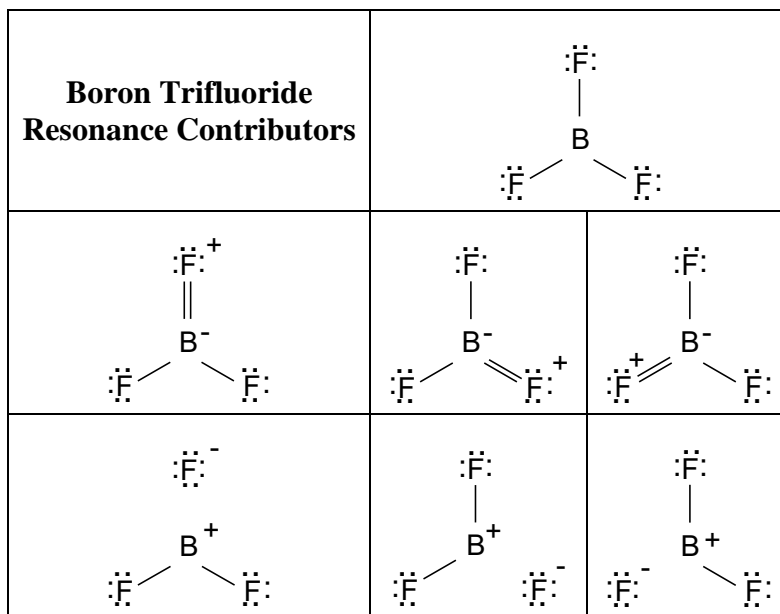
Quiz 2

October 15, 2001

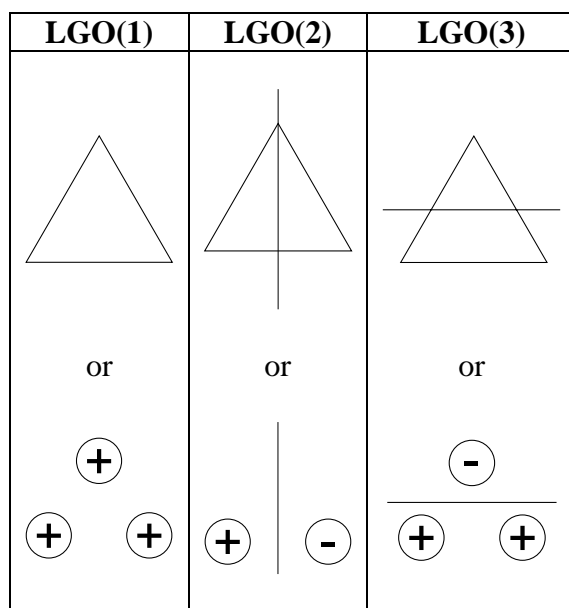
Question 1 – Suggest suitable hybrids for the central atom in each case. Notice that the first one has been done for you.

	Species	Point Group	Hybrids	Specify if needed
(a)	SF_6	O_h	sp^3d^2	$x^2 - y^2$ and z^2
(b)	$\text{N}(\text{CH}_3)_4^+$	T_d	sp^3	not applicable
(c)	BF_3	D_{3h}	sp^2	x, y
(d)	PCl_5	D_{3h}	sp^3d	z^2
(e)	XeF_2	$\text{D}_{\infty h}$	sp^3d	z^2
(f)	$\text{Pt}(\text{CN})_4^{2-}$	D_{4h}	sp^2d	$x^2 - y^2$
(g)	IF_5^{2-}	D_{5h}	sp^3d^3	$z^2, x^2 - y^2, xy$
(h)	TlCl_5^{2-}	C_{4v}	sp^3d	$x^2 - y^2$
(i)	CN_2^{2-}	$\text{D}_{\infty h}$	sp	z

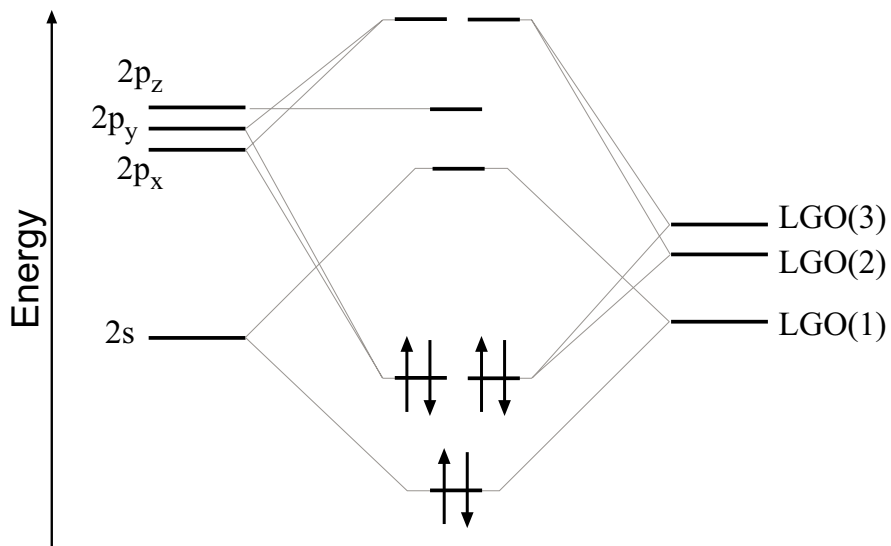
Question 2 – In valence bond theory we often sketch so-called resonance contributors. Sketch the seven most significant contributors to the structure of BF_3 . Put in all lone pairs and formal charges that are not zero.



Question 3 – a) Sketch the set of three LGO's suitable for the construction of a simple MO diagram for BH_3 . LGO(1) has no nodes.



b) Complete the MO diagram and put in the electrons.



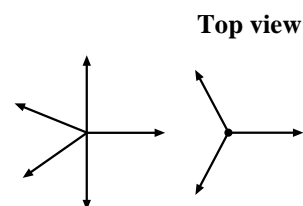
Question 4 – Assign the correct point groups to each of the following objects.

Object	Point Group
(a) T-Shirt (assume flat)	C_{2v}
(b) Wine glass	$C_{\infty v}$
(c) Cheerleader (assume flat with no eyes in back of head)	C_s
(d) Regular pentagonal prism	D_{5h}
(e) Two wine glasses – one on top of the other	$D_{\infty h}$

Question 5 – (a) Use the D_{3h} character table in order to obtain a reducible representation (Γ_r) for the C-O stretching modes in $F(CO)_5$.

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A'_1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A'_2	1	1	-1	1	1	-1	R_z	
E'	2	-1	0	2	-1	0	(x, y)	$(x^2 - y^2, xy)$
A''_1	1	1	1	-1	-1	-1		
A''_2	1	1	-1	-1	-1	1	z	
E''	2	-1	0	-2	1	0	(R_x, R_y)	(xz, yz)

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$
Γ_r	5	2	1	3	0	3



(b) Decompose Γ_r into its irreducible components.

$$\text{Order} = h = 1 + 2 + 3 + 1 + 2 + 3 = 12$$

$$\#A'_1 = \frac{1}{12} [(1 \times 1 \times 5) + (1 \times 2 \times 2) + (1 \times 3 \times 1) + (1 \times 1 \times 3) + (1 \times 2 \times 0) + (1 \times 3 \times 3)] = 2$$

$$\#A'_2 = \frac{1}{12} [(1 \times 1 \times 5) + (1 \times 2 \times 2) + (-1 \times 3 \times 1) + (1 \times 1 \times 3) + (1 \times 2 \times 0) + (-1 \times 3 \times 3)] = 0$$

$$\#E' = \frac{1}{12} [(2 \times 1 \times 5) + (-1 \times 2 \times 2) + (0 \times 3 \times 1) + (2 \times 1 \times 3) + (-1 \times 2 \times 0) + (0 \times 3 \times 3)] = 1$$

$$\#A''_2 = \frac{1}{12} [(1 \times 1 \times 5) + (1 \times 2 \times 2) + (-1 \times 3 \times 1) + (-1 \times 1 \times 3) + (-1 \times 2 \times 0) + (1 \times 3 \times 3)] = 1$$

$$\#E'' = \frac{1}{12} [(2 \times 1 \times 5) + (-1 \times 2 \times 2) + (0 \times 3 \times 1) + (-2 \times 1 \times 3) + (1 \times 2 \times 0) + (0 \times 3 \times 3)] = 0$$

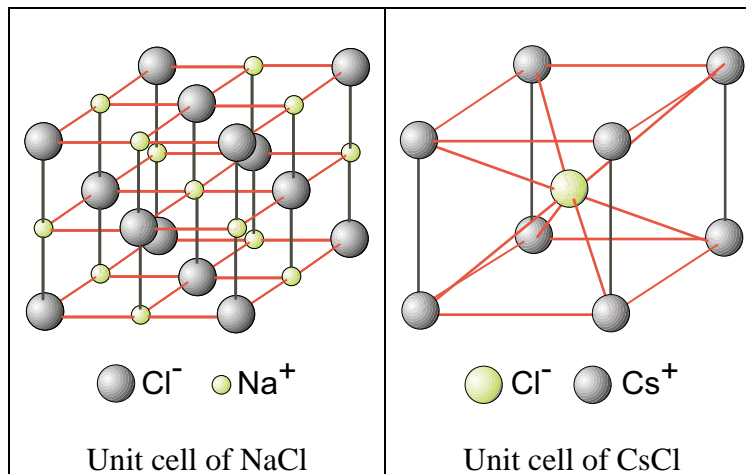
$$\#A_1'' = \frac{1}{12} [(1 \times 1 \times 5) + (1 \times 2 \times 2) + (1 \times 3 \times 1) + (-1 \times 1 \times 3) + (-1 \times 2 \times 0) + (-1 \times 3 \times 3)] = 0 \text{ not asked}$$

$$\Gamma_r = 2A_1' + E' + A_2''$$

(c) Decide on the number of IR and Raman absorptions.

	Origin		
	A_1'	E'	A_2''
Infra Red		one line	one line
Raman	two lines	one line	

Question 6 – Sketch the unit cells for both sodium chloride and cesium chloride.



Show that these unit cells are consistent with the formulae NaCl and CsCl.

For NaCl

$$\# \text{ of } \text{Na}^+ = (1 \times 1) + \left(12 \times \frac{1}{4}\right) = 4$$

The relation is one to one

$$\# \text{ of } \text{Cl}^- = \left(6 \times \frac{1}{2}\right) + \left(8 \times \frac{1}{8}\right) = 4$$

For CsCl

$$\# \text{ of } \text{Cs}^+ = (1 \times 1) = 1$$

The relation is one to one

$$\# \text{ of } \text{Cl}^- = \left(8 \times \frac{1}{8}\right) = 1$$