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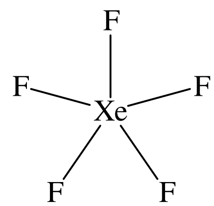
Chem 370 - Spring, 2018
Test II - Part 2
April 9, 2018

4. (42 points) The pentafluoroxenate(IV) anion, XeF_5^-, was the first example of a pentagonal planar AX_5 species.[1]



a. (16 points) Using the template below and the character table on the last page, generate a reducible representation for the five fluorine σ-SALCs of XeF_5^-, Γ_{SALC}, and carry out the systematic reduction into its component irreducible representations to show the symmetries of the individual SALCs.

D_{5h}	E	$2C_5$	$2C_5^2$	$5C_2$	σ_h	$2S_5$	$2S_5^3$	$5\sigma_v$		
Γ_{SALC}									Σ	Σ/h
A_1'										
A_2'										
E_1'										
E_2'										
A_1''										
A_2''										
E_1''										
E_2''										

Γ_{SALC} =

b. (6 points) Give the symmetries of the individual *s*, *p*, and *d* orbitals on the central Xe atom.

[1]K. O. Christe, E. C. Curtis, D. A. Dixon, H. P. Mercier, J. C. P. Sanders, G. J. Schrobilgen, *J. Am. Chem, Soc.* **1991**, *113*, 3351-3361.

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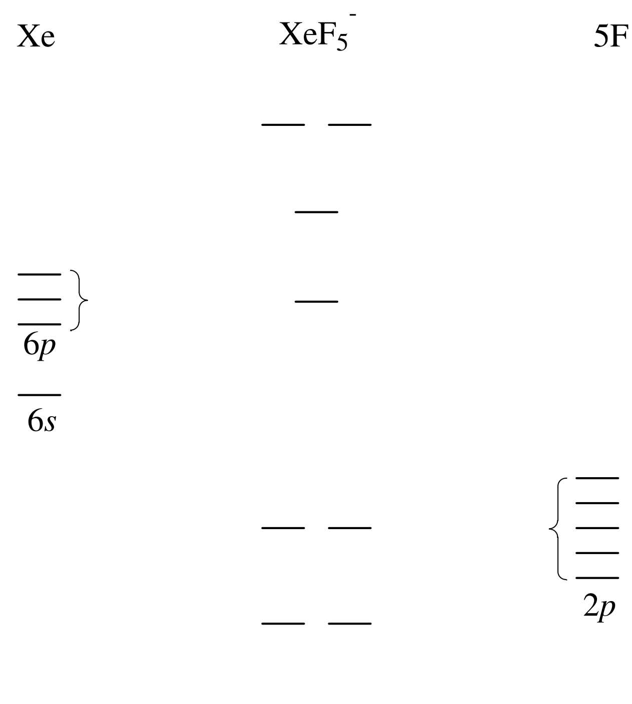
c. (12 points) Assume that Xe only uses *s* and *p* orbitals for bonding in XeF_5^-. Using the skeletal MO scheme below, connect the SALC and AO levels with the MOs to which they contribute. Label all levels with the appropriate Mulliken symbols (lower case), and indicate the bond type of every MO level (σ, σ*, or σ^n). Show the filling of electrons in the MO scheme, assuming that Xe contributes its eight valence electrons, each F contributes one electron, and there is an extra electron for the negative charge.



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d. (8 points) On the basis of symmetry, which specific combinations of *s*, *p*, and *d* orbitals could be combined to form sets of hybrid orbitals to account for pentagonal planar geometry about a central atom? [Hint: The reducible representation Γ_{SALC}, which you generated in part a, would be the same as Γ_{hybrid} for five hybrid orbitals in a pentagonal planar arrangement.]

e. (BONUS - 5 points) No pentagonal planar transition metal complex has yet been reported. Nonetheless, suppose that a planar complex, ML_5 were prepared. Show the CFT splitting of *d* orbitals expected for such a complex, labeled with the Mulliken symbols and specific *d* orbitals for each level.

D_{5h}	E	$2C_5$	$2C_5^2$	$5C_2$	σ_h	$2S_5$	$2S_5^3$	$5\sigma_v$		
A_1'	1	1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	1	-1	1	1	1	-1	R_z	
E_1'	2	2 cos 72°	2 cos 144°	0	2	2 cos 72°	2 cos 144°	0	(x, y)	
E_2'	2	2 cos 144°	2 cos 72°	0	2	2 cos 144°	2 cos 72°	0		$(x^2 - y^2, xy)$
A_1''	1	1	1	1	-1	-1	-1	-1		
A_2''	1	1	1	-1	-1	-1	-1	1	z	
E_1''	2	2 cos 72°	2 cos 144°	0	-2	-2 cos 72°	-2 cos 144°	0	(R_x, R_y)	(xz, yz)
E_2''	2	2 cos 144°	2 cos 72°	0	-2	-2 cos 144°	-2 cos 72°	0		

Note: Feel free to detach this page for use in working through the problems, but please do not write anything on this that you wish to have graded.