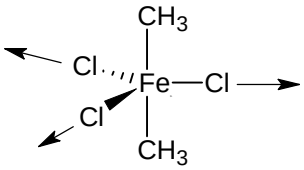
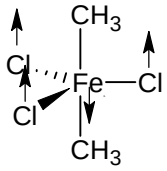
Assignment 2 Solutions (2351 – W11)

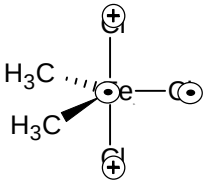
1. The *trans* has D_{3h} and the *cis* has C_{2v} symmetry. Therefore, look up the symmetry elements for those two point groups. Recall that a linear term (any of *x*, *y*, and/or *z*) denotes an IR-active vibration and any quadratic term (any combination of x^2, y^2, z^2, *xz*, *yz*, and/or *xy*) denotes a Ramn-active vibration.



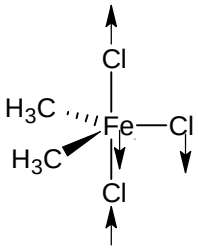
	E	C_3	C_2	σ_h	S_3	σ_v	
	1	1	1	1	1	1	= A_1' (Raman only)



	E	C_3	C_2	σ_h	S_3	σ_v	
	1	1	-1	-1	-1	1	= A_2'' (IR only)

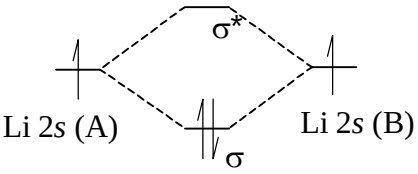


	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$	
	1	-1	1	-1	= B_1 (IR and Raman active)

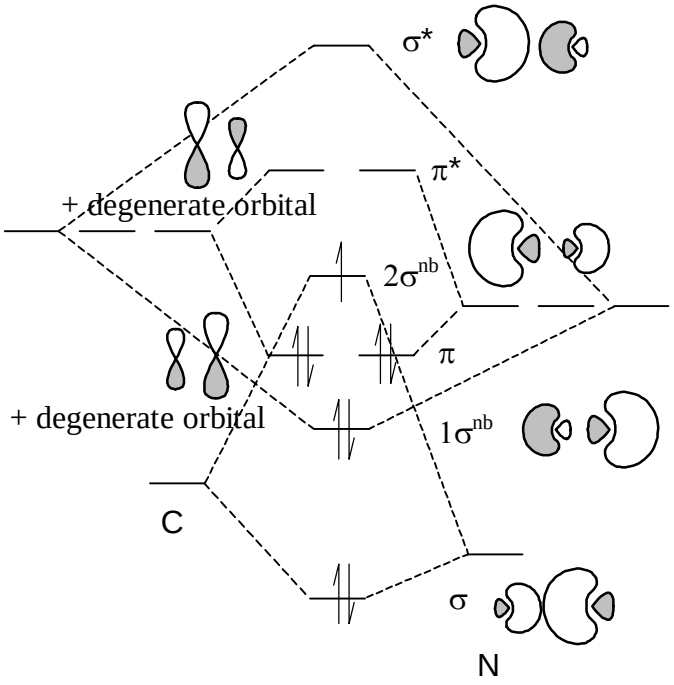


	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$	
	1	-1	-1	1	= B_2 (IR and Raman active)

2. The MO picture for dilithium most resembles H_2, except using the 2*s* orbitals on Li instead of the 1*s* orbitals in H_2. Therefore, it is safe to conclude that dilithium should be a gas-phase diatomic molecule, not a crystalline solid.



3.



(a) the radical CN and CO both have the same electron counts in bonding and antibonding orbitals (6 and 0, respectively); the only difference is in the nonbonding orbitals. Therefore, both molecules should have the same bond strength.

(b) filling all the bonding and nonbonding orbitals requires that one additional electron be added to the 2 σ^{nb} orbital, therefore CN^- is the most stable form.

(c) Looking at the shape of the 2 σ^{nb} orbital, which is the HOMO in this molecule, the wavefunction suggests a greater contribution from the C atom so the H+ should attach there (which verifies the valence bond description).