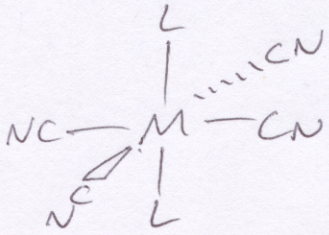
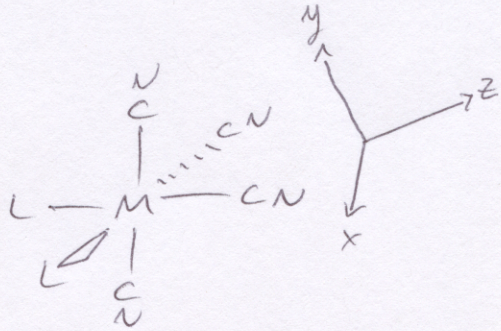
Show how you can use vibrational Spectroscopy (IR/Raman) to determine which of the following two isomers you have.



D_{4h}

vs.



C_{2v}

down band / between bands

D_{4h}	E	$2C_4(z)$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$
Γ_{CN}	4	0	0	2	0	0	0	4	2	0

C_{2v}	E	$C_2(z)$	$\sigma_v(xz)$	$\sigma_v(yz)$
Γ_{CN}	4	0	2	2

$\#A_{1g} = \frac{1}{16}(4+0+0+4+0+0+0+4+4+0) = 1$

$\#B_{1g} = \frac{1}{16}(4+0+0+4+0+0+0+4+4+0) = 1$

$\#B_{2g} = \frac{1}{16}(4+0+0-4+0+0+0+4-4+0) = 0$

$\#E_g = \frac{1}{16}(8+0+0+0+0+0+0-8+0+0) = 0$

$\#A_{2u} = \frac{1}{16}(4+0+0-4+0+0+0-4+4) = 0$

$\#E_u = \frac{1}{16}(8+0+0+0+0+0+0+8+0+0) = 1$

$\Gamma_{CN} = \underbrace{A_{1g} + B_{1g}}_{\text{Raman}} + \underbrace{E_u}_{\text{IR}}$

2 Raman active CN stretches

1 IR active CN stretch

$\#A_1 = \frac{1}{4}(4+0+2+2) = 2$

$\#A_2 = \frac{1}{4}(4+0-2-2) = 0$

$\#B_1 = \frac{1}{4}(4+0+2-2) = 1$

$\#B_2 = \frac{1}{4}(4+0-2+2) = 1$

$\Gamma_{CN} = \underbrace{2A_1 + B_1 + B_2}_{\text{Raman \& IR active}}$

4 Raman active stretches

4 IR active stretches