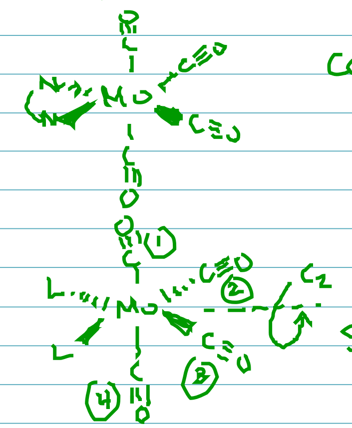
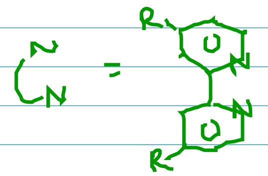
Find the IR and Raman-active M-C≡O stretches

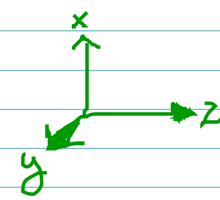


$CO_2 + 2e^- + 2H^+ \longrightarrow CO + H_2O$

Chem. Sci., 2014, 5, p1894



R: H, tBu



Symmetry Operations
$E,\ C_2,\ \sigma_{xz},\ \sigma_{yz}$

octahedral geometry $\quad C_{2v}$

C_{2v}	E	C_2	σ_{xz}	σ_{yz}
Γ	4	0	2	2

reducible representation (Γ)

C_{2v}	E	C_2	σ_{xz}	σ_{yz}		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz

irr. rep

Mulliken symbols $\qquad$ IR (x,y,z) $\qquad$ Raman active

# of irr. reps in $\Gamma = \frac{1}{\text{order}} \Sigma (\text{\# of elements})(\chi \text{ of element in } \Gamma)(\chi \text{ element irr. rep})$

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

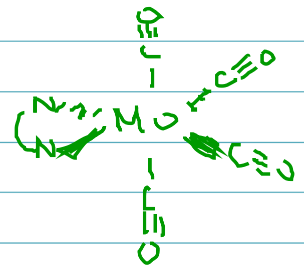
$\# A_2 = \frac{1}{4}[(1)(4)(1) + (1)(0)(1) + (1)(2)(-1) + (1)(2)(-1)] = 0A_2$

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

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

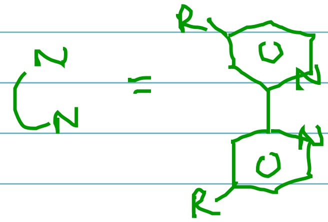
$\Gamma = 2A_1 + B_1 + B_2$

Find the IR and Raman-active M–C≡O stretches

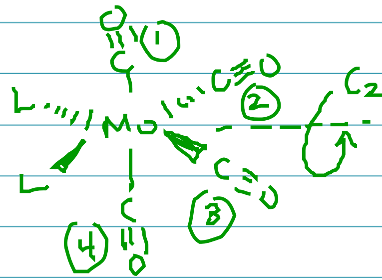


$CO_2 + 2e^- + 2H^+ \longrightarrow CO + H_2O$

Chem. Sci., 2014, 5, p 1894

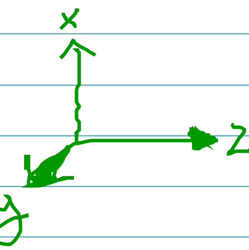


R = H, tBu



Symmetry Operations

$E, C_2, \sigma_{xz}, \sigma_{yz}$



octahedral geometry

C_{2v}

C_{2v}	E	C_2	σ_{xz}	σ_{yz}
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B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

irr. rep

Mulliken symbols

IR (x, y, z)

Raman active

$$\#\text{ of irr. reps in } \Gamma = \frac{1}{\text{order}} \sum (\#\text{ of elements})(\chi \text{ of element in } \Gamma)(\chi \text{ element in irr. rep})$$

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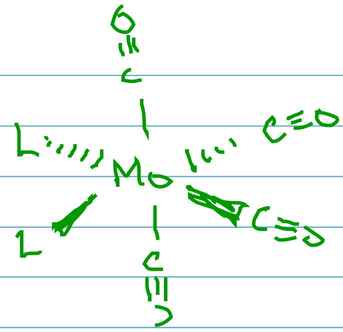
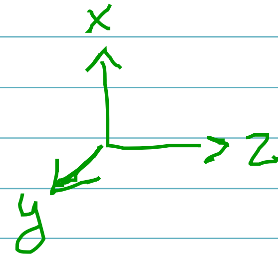
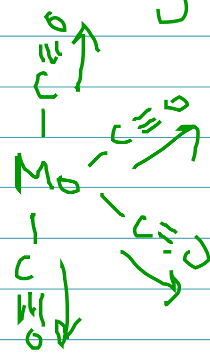
$$\Gamma = 2A_1 + B_1 + B_2$$

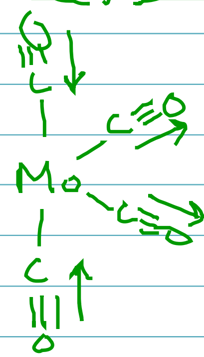




$2A_1 \rightarrow (z,\ x^2 y^2 z^2) \rightarrow$ Both IR and Raman Active

A_1 is totally symmetric w/ C_2, σ_{xz}, σ_{yz}

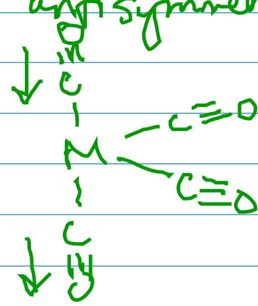




C_2
σ_{xz}
σ_{yz}

$B_1 \rightarrow (x,\ xz) \rightarrow$ Both IR and Raman Active

B_1 is antisymmetric w/ C_2 and $\sigma(yz)$



$B_2 \rightarrow (y,\ yz) \rightarrow$ Both IR and Raman Active

B_2 is antisymmetric w/ C_2 and $\sigma(xz)$