ORGANIC CHEMISTRY 30B

(Prof. Yves Rubin)

UCLA, FALL 2006

MIDTERM EXAM I

On my honor, I have neither given nor received any aid on this exam (There are no regrades, so you may use pencil or ink):

Signature

I. D. Number

Full Name (<u>Please Print</u> !)

Question	Points
1 (30)	
2 (15)	
3 (15)	
4 (40)	

======

Total (100)

Name

I. SPECTROSCOPY

1. a) (12 points) Give the number of <u>expected signals</u> (*ignore* splittings) in the ¹H and ¹³C NMR spectra of the following compounds:



b) (18 points) Sketch the ¹H NMR spectrum for the compound below. Be sure to consider *chemical shifts, coupling patterns,* and *relative intensities* between each spin system when drawing your spectrum. Label all non-symmetrically related H's on the structure (e.g. a,b,c, etc) and show what peak they correspond to on the spectrum:





Name

2. (15 points) A compound with molecular formula $C_3H_6O_3$ has the following ¹³C NMR spectrum. **Assign** the signals on the spectrum and provide its structure in the box below:

Degree of Unsaturation:_____



Compound C₃H₆O₃

(Assign peaks on or below the spectrum)



Name

3. (15 points) A compound with molecular formula C_6N_4 has the following IR spectrum. Its ¹³C NMR spectrum has only two lines. From this information only, deduce its structure and assign any recognizable peak. Keep in mind that the compound is highly symmetric. *You MUST provide all the relevant information* (peak assignment) to get maximum credit:

Degree of Unsaturation:_____



Compound C₆N₄

IR spectrum:



Name

4. (40 points) A compound has the molecular formula C₁₁H₁₄ClNO. Deduce its structure from the IR, ¹H NMR, and ¹³C NMR spectra given below. *You MUST provide all the relevant information* (peak assignments) to get maximum credit. Draw the structure in the box provided:

Degree of Unsaturation:



Compound C₁₁H₁₄CINO

IR (KBr; assign all recognizable IR stretch frequencies):



Name

¹H NMR: Draw structure here as well and label all non-symmetrically related H's on the structure (e.g. with **a**,**b**,**c**, etc). Show which peak the labels correspond to on the spectrum by drawing arrows to them. Provide labels for integration values (1H, 2H, 3H) and peak multiplicities (splitting type):



Name

¹³C NMR spectrum for question 4. Draw the structure here again and assign the ¹³C signals to specific carbons on the structure. However, aliphatic carbons do not need to be assigned, but you should label the alkene or aromatic peaks as such, but not assign them to specific positions since you cannot calculate precise chemical shifts:



BondingFrequency (cm ⁻¹)Intensity* $(reteching unless no cupolity alkaneC-Halkane2850-3000w-mout-of-plane bending-CH_2-CH_21375 and 1450w-mout-of-plane bending-CH_21450w-mout-of-plane bendingalkene3000-3100w-mout-of-plane bendingalkene3000-3100w-mout-of-plane bendingalkyne3000-3100sout-of-plane bendingalkyne3000-3100sout-of-plane bendingalkyne2900-2900wwalkene1600-1680w-maromatic1450 and 1600w-mc=Calkane(not interpretatively uscful)C=Calkyne1650-1250saromatic1450 and 1600w-mc=C-Oalkyne1650-1250saromatic1705-1250saromatic1705-1260sarotic1700-1750sarotic1700-1760sarotic1700-1760sarotic1700-1760sarotic1300-3500marotic1300-300sarotic1300-300marotic1300-3500marotic1705-1780sarotic1300-3500marotic1300-3500marotic100-300-300marotic100-3200marotic100-3200m<$	BondingFrequency (cm ⁻¹)Intensity*Circling unless not $C -H H$ alkane2850-3000w-mout-of-plane bending $-CH_3$ 1375 and 1450w-mout-of-plane bending $-CH_3$ 3000-31000sout-of-plane bendingalkree3000-31000sout-of-plane bending $alkree3000-31000sout-of-plane bendingalkree3000-31000sout-of-plane bendingalkree3000-31000sout-of-plane bendingalkree2000-2900wwaromatic1450 and 1600wwC=Calkee1050-1250waromatic11600-1250swC=Calkee1050-1250saromatic1705-1740sarid, anhydride1705-1740scerboxlic acid1705-1740sarid, anhydride1705-1740sarid, anhydride1705-1740sarid, anhydride1705-1780sderhyde200-3550mderhyde1705-1740sderhyde1705-1740sderhyde1705-1740sderhyde1705-1740sderhyde1705-1740sderhyde1705-1740s$					Type of Vibration
CHalkane $2850-3000$ w-mout-of-plane bending alkene $-CH_3$ 1450 w-mout-of-plane bending $-CH_3$ 1450 w-mout-of-plane bending $-CH_3$ $3000-3100$ sout-of-plane bending $alkyne$ $3000-3100$ ws $aromatic1460-1880wC=Calkene1600-1680w-mcrictalkene1600-1680wcrictalkene1600-1580wcrictalkene1600-1780scrictalkene1705-1780scrictalkene1705-1780scrictanide1705-1780scrictanide1700-1750scrictanide1700-1780scrictanide1700-1780scrictanide1700-1780scrictanide1700-1780scrictanide1700-300$		Bonding		Frequency (cm^{-1})	Intensity*	(stretching unless not
$\begin{array}{c cccccc} -CH_3 & 1375 \mbox{ and } 1450 & w-m & out-of-plane bending alkene & 5300-3100 & w-m & out-of-plane bending alkyne & 5300-3100 & s & out-of-plane bending alkyne & 3300 & 3100 & s & out-of-plane bending alkyne & 3300-3100 & s & out-of-plane bending alkyne & 2300-2900 & w & w & out-of-plane bending 690-900 & s & out-of-plane bending 690-900 & s & out-of-plane bending 2200-2900 & w & w & w & out-of-plane bending 690-900 & s & out-of-plane bending alkyne & 2200-2900 & w & w & w & out-of-plane bending 690-900 & s & out-of-plane bending 690-900 & s & out-of-plane bending 690-900 & s & out-of-plane bending 690-900 & w & w & w & w & out-of-plane bending 690-900 & w & w & w & w & w & w & w & w & w &$	$\begin{array}{cccc} -CH_{3} & & 1375 \mbox{ and } 1450 & w-m & outofplane bending \\ & -CH_{3} - & 11450 & w-m & outofplane bending \\ & alkene & 300-3100 & w-m & outofplane bending \\ & alsyne & 3300 & s & outofplane bending \\ & aldehyde & 200-3100 & s & outofplane bending \\ & aldehyde & 2700-2800 & w & w & m \\ & 2000-2900 & w & m & m & m & m & m \\ & C-C & alkane & (not interpretatively useful) \\ C=C & alkne & 1600-1680 & w-m & m & m & m & m & m & m & m & m & m &$	C—H	alkane	2850 - 3000	m-m	
CH ₂ -1450mout-of-plane bending alkenealkene $300-3100$ sout-of-plane bendingalkene $300-3100$ sout-of-plane bendingalkene $300-3100$ sout-of-plane bendingaldehyde $2700-2800$ wwCCalkene $200-2900$ walkene $1600-1680$ w-mCCalkene $1600-1680$ w-mCCalkene $1600-1680$ w-mCCalkene $1600-1680$ w-mcid, anhydride 1450 and 1600 w-mcid, anhydride $1700-1250$ scid, anhydride $1700-1250$ scid, anhydride $1700-1250$ sarid, anhydride $1700-1750$ saread 170	$\begin{array}{llllllllllllllllllllllllllllllllllll$		CH ₃	1375 and 1450	m-m	out-of-plane bending
alkene $300-3100$ w-m $650-1000$ s out-of-plane bending alkyne 5300 s $500-3100$ s out-of-plane bending alkyne $3000-3100$ s $3000-3100$ s $3000-3100$ w $200-2900$ w $200-2900$ w $-m$ $2500-2900$ w $-m$ $2100-1680$ w $-m$ $2100-1680$ w $-m$ $2100-2150$ s $-m$ $2100-2250$ w $-m$ $2100-2250$ w $-m$ $2100-2250$ w $-m$ $2100-2250$ w $-m$ $-m$ $2100-2250$ w $-m$ $-m$ $2100-2250$ w $-m$ $2100-2250$ w $-m$ $-m$ $2100-2250$ w $-m$ $-m$ $2100-2250$ w $-m$ $-m$ $-m$ $-m$ $-m$ $-m$ $-m$ $-m$	alkene30003100w-malkene30003100sout-of-plane bendingalkyne30003100sout-of-plane bendingalkyne30003100sout-of-plane bendingaldehyde2700-2800wwC—Calkene(not interpretatively useful)C—Calkene1450 and 1600w-mC—Calkene1450 and 1600w-mC—Calkene1050-11680w-mC—Calkene1050-11500sC—Oalcohol, ether, es-1050-1250sC—Oamonatic1100-1250sC—Oamide1630-1680sC—Oamode1630-1630sC—Oamode1630-1630sC—Oamode1630-1630sC—Oalcohol, ether, es-1050-1250sC—Oamode1630-1630sC—Oamode1630-1630sC—Oamode1705-1730sRetone1705-1730sRetone1705-1730sRetone1705-1730sRetone1705-1740sRetone1705-1740sRetone1705-1740sRetone1705-1740sRetone1705-1740sRetone1705-1740sRetone1705-1740sRetone1705-1740sRetone1705-1740sRetone1706-3650		$-CH_2-$	1450	ш	out-of-plane bending
650-1000sout-of-plane bending a aromaticalkyne 3300 sout-of-plane bendingaldehyde 3300 sout-of-plane bendingaldehyde $2700-2800$ wwC—Calkane(not interpretatively useful)C=Calkene $1600-1680$ w-maromatic 1450 and 1600 w-mC=Oalkyne $2100-2250$ w-maromatic 1450 and 1600 w-mC=Oalkyne $2100-2250$ w-mC=Oalkyne $1050-1250$ saronatic $1700-1750$ scaid, anhydride $1700-1750$ scaid, anhydride $1705-1780$ sacid, anhydride $1700-1750$ sacid, anhydride $1700-1750$ saronatic $1700-1750$ saronatic $1700-1750$ saronatic $1700-1750$ saronatic $1700-1750$ sarohydride $1700-1750$ saroboxylic acid $100-300$ saroboxylic acid $200-3500$ <	Affect650-1000soutofplane bendingalkyne3300soutofplane bendingaromatic3000-3100soutofplane bendingaldehyde2700-2800wwC—Calkene(not interpretatively useful)C=Calkene(not interpretatively useful)C=Calkene(not interpretatively useful)C=Calkene1450 and 1600w-maromatic1450 and 1600w-mC=Calkyne2100-2250w-mc=Calkyne1750-1250sc=Camide1700-1250sc=Canide1700-1250sc=Canide1700-1250sc=Canide1700-1250sc=Canide1700-1250sc=Canide1700-1250sc=Canide1700-1250sc=Canide1700-1250sketone1700-1750sketone1700-1750sketone1700-1750sketone1700-2800mketone1700-1750sketone1700-1750sketone1700-1750sketone1700-1750sketone1700-1750sketone1700-1750sketone1700-1750sketone1700-1750sketone1700-1750sketone1700-1750sketoneani		alkene	3000 - 3100	m-m	
alkyne 3300 saromatic $300-3100$ saromatic $300-3100$ saldehyde $2700-2800$ w CC alkane $(not interpretatively useful)$ $C=-C$ alkane $(not interpretatively useful)$ $C=-C$ alkene $(not interpretatively useful)$ $C=-C$ alkone $(not interpretatively useful)$ $(c-C-C)$ alkone $(not interpretatively useful)$ $(c-C-C)$ alkone $(not interpretatively useful)$ <td>alkyne3300saromatic300-3100saromatic690-900saldehyde2700-2800wC—Calkane(not interpretatively useful)C—Calkane(not interpretatively useful)C—Calkane(not interpretatively useful)C—Calkane(not interpretatively useful)C—Calkane(not interpretatively useful)C—Calkyne1600-1680w-mC—Calkyne2100-2250w-mC—Oalcohol, ether, es1050-1250scmide1600-1860sscmostylicacid, anhydride1700-1750scarboxylic1700-1750ssketone1700-1750sanhydride1700-1750sanhydride1700-1750sKetone1700-1750sN—Halcohol, phenolsanhydride1800sM<h< td="">alcohol, phenolsN—Halcohol, phenolsN—Hanine and anide3100-3500N=Mnitrile200-3500mks acid chloride200-3500mster2100-2250mster3100-3500mster3100-3500mster3100-3500mster2200-2250mstrong, m = medium, w = weak</h<></td> <td></td> <td></td> <td>650 - 1000</td> <td>s</td> <td>out-of-plane bending</td>	alkyne3300saromatic300-3100saromatic690-900saldehyde2700-2800wC—Calkane(not interpretatively useful)C—Calkane(not interpretatively useful)C—Calkane(not interpretatively useful)C—Calkane(not interpretatively useful)C—Calkane(not interpretatively useful)C—Calkyne1600-1680w-mC—Calkyne2100-2250w-mC—Oalcohol, ether, es1050-1250scmide1600-1860sscmostylicacid, anhydride1700-1750scarboxylic1700-1750ssketone1700-1750sanhydride1700-1750sanhydride1700-1750sKetone1700-1750sN—Halcohol, phenolsanhydride1800sM <h< td="">alcohol, phenolsN—Halcohol, phenolsN—Hanine and anide3100-3500N=Mnitrile200-3500mks acid chloride200-3500mster2100-2250mster3100-3500mster3100-3500mster3100-3500mster2200-2250mstrong, m = medium, w = weak</h<>			650 - 1000	s	out-of-plane bending
aromatic $3000-3100$ saldehyde $2700-2900$ w CC alkane $2700-2900$ w CC alkane $(not interpretatively useful)$ $C=-C$ alkane $(not interpretatively useful)$ $C=-C$ alkone $1600-1680$ w-m $C=-C$ alkyne $2100-2250$ w-m $c=-O$ alcohol, ether, es- $1050-1250$ s $c=-O$ alcohol, ether, es- $1050-1250$ s $c=-O$ alcohol, ether, es- $1050-1250$ s $c=-O$ and e $1700-1750$ s $c=-O$ amide $1700-1750$ s $c=-O$ amide $1700-1780$ s $c=-O$ amide $1700-1780$ s $archork1700-1780sarchork1700-1780sc=-Oamide1700-1780sc=-Oamide1700-1780sarchork1700-1780sarchork1700-1780sarchork1700-1780sarchork1700-1780sarchork1700-1780sarchork1700-1780sarchork1700-1780sarchork1700-1780sarchork1700-3100sarchork1700-3100sarchork1700-300marchork1700-300marchork1700-300marchork100-3500m$	aromatic3000-3100sout-of-plane bendingaldehyde $2700-2800$ wsout-of-plane bendingC—Calkane $(not interpretatively useful)$ $w-m$ wC—Calkane $(not interpretatively useful)$ $w-m$ $w-m$ C—Calkene $(not interpretatively useful)$ $w-m$ C—Calkene $1600-1680$ $w-m$ C—Calkyne $1700-1250$ $w-m$ C—Calkyne $1050-1250$ $w-m$ C—Oamide $1630-1680$ s carboxylic $1700-1750$ s carboxylic $1700-1750$ s carboxylic $1700-1750$ s C—Oamide $1700-1750$ s C—Oamide $1700-1750$ s Ketone $1700-1750$ s C—Hamide $1700-1750$ s NerHaldehyde $1700-1750$ s NerHaldehyde $1700-1750$ s nitree $1700-1750$ s actor $1700-1750$ s NerHaldehyde $1700-1750$ s NerHaldehyde $1700-1750$ s NerHanide $1700-1750$ s NerHanine and amide $1700-1250$ m NerHanine and		alkyne	3300	S	
G90-900soutofplane bendingaldehyde $2700-2800$ wC—Calkane(not interpretatively useful)C=Calkene(not interpretatively useful)C=Calkene $1600-1680$ w-maromatic 1450 and 1600 w-mC=Calkyne $2100-2250$ w-maromatic $1160-11250$ sc=Camide $1630-1680$ sc=Canothe $1700-11750$ sc=roboxylic $1700-11750$ sarotid, anhydride $1700-11750$ sc=roboxylic acid $1700-11780$ sactohol, phenol $1700-1780$ sadehyde $1700-1780$ sadehyde $1700-1780$ sactohol, phenol $3800-3650$ mhydrogen bonded $3200-3650$ mN—Hamine and amide $3100-3500$ mN—Hamine and amide $3100-3500$ mN=Nnitrile $2200-2250$ m	690-900soutoof-plane bending 2700-2800wC—Caldehyde2700-2800wC—Calkane(not interpretatively useful)C—Calkene1600-1680w-mC—Calkyne2100-2250w-mC—Oalcohol, ether, es-1050-1250sC—Oalcohol, ether, es-1050-1250sC—Oalcohol, ether, es-1050-1250sC—Oalcohol, ether, es-1050-1250sC—Oand left1700-1750sacid, anhydride1700-1750sketone1700-1750saddehyde1700-1750saddehyde1700-1760saddehyde1700-1750saddehyde1700-1760saddehyde1700-1760shydrogen bonded3200-3650mN—Hanine and amide3100-3500N—Hanine and amide3100-3500hydrogen bonded3200-3500mS = strong.m = medium, w = waks		aromatic	3000 - 3100	s	
aldehyde $2700-2800$ wC—Calkane(not interpretatively useful)C=Calkene(not interpretatively useful)C=Calkene $1600-1680$ w-maromatic 1450 and 1600 w-mC=Calkyne $2100-2250$ w-macid, anhydride $2100-2250$ w-mC=Oalcohol, ether, es $1050-1250$ sc=Canide $1050-1250$ sc=Canide $1700-1750$ scarboxylic $1700-1750$ sacid, anhydride $1705-1740$ scarboxylic acid $1705-1740$ saldehyde 1760 sanddhyde $1705-1740$ saldehyde $1705-1740$ saldehyde $1705-3-1800$ sanhydrode 1800 sactid chloride 1800 sactid chloride 1800 sactid chloride $290-3500$ mhydrogen bonded $2200-3500$ mN—Hannine and amide $3100-3500$ mnitrile $2200-2250$ m	aldehyde2700-2800wC—Calkene2800-2900wC=Calkene(not interpretatively useful)C=Calkene1600-1680w-maromatic1450 and 1600w-mC=Calkyne2100-2250w-mC=Calcohol, ether, es-1050-1250sc=Calcohol, ether, es-1050-1250sc=Calcohol, ether, es-1070-1750sc=Oamide1700-1750scarboxylic acid1705-1740sadehyde1705-1740sacid, chloride1700-3500mfree3200-3500mN—Hanine and amide3100-3500mN—Hamine and amide3100-3500m* s = strong, mstrong, w = strong, ms			006-069	s	out-of-plane bending
C—C alkane 2800–2900 w C—C alkane (not interpretatively useful) C=C alkene 1600 w-m aromatic 1450 and 1600 w-m C≡C alkyne 2100–2250 w-m C=C alcohol, ether, es 1050–1250 s ter, carboxylic acid, anhydride 1630–1680 s ter, carboxylic acid 1700–1750 s ketone 1705–1740 s anhydride 1700 s anhydride 1700 m free 300–3650 m N—H amine and amide 3100–3500 m N—H amine and amide 3100–3500 m N—H amine and amide 3100–3500 m	CC alkane (not interpretatively useful) C=-C alkene (not interpretatively useful) C=C alkene 1600 w-m aromatic 1450 and 1600 w-m C=C alkyne 2100-2250 w-m C=-O alcohol, ether, es- 1050-1250 s ter, carboxylic acid 1700-1750 s ketone 1705-1740 s ketone 1705-1740 s ketone 1705-1740 s addehyde 1705-1740 s ketone 1705-1740 s addehyde 1705-1740 s addehyde 1705-1740 s ketone 1705-1740 s addehyde 1705-1740 s hydrogen bonded 2400-3650 m hydrogen bonded 2400-3650 m NH amine and amide 2400-3650 m NH amine and amide 2400-3650 m s = strong, m = medium, w = weak		aldehyde	2700 - 2800	Μ	
C—Calkane(not interpretatively useful)C=Calkene1600–1680w-maromatic1450 and 1600w-mC=Calkyne2100–2250w-mC=Oalcohol, ether, es-1050–1250saris, anhydride2100–2250w-mC=Oalcohol, ether, es-1050–1250scarboxylic1700–1750saridé1700–1750scarboxylic acid1700–1760sketone1705–1740sanhydride1705–1740sanhydride1705–1740sanhydride1705–1740sarid chloride1800sarid chloride1800shydrogen bonded3200–3650mN—Hamine and amide3100–3500mN—Hamine and amide3100–3500mN—Hamine and amide3100–3500m	CCalkane(not interpretatively useful)C=-Calkene1600-1680w-maromatic1450 and 1600w-mC=-Oalkyne2100-2250w-mC=-Oalcohol, ether, es-1050-1250sc=-Oalcohol, ether, es-1050-1250sc=-Oalcohol, ether, es-1050-1250sc=-Oanide1630-1680sc=-Oamide1700-1750scarboxylic acid1700-1750sketone1705-1740sadehyde1705-1740sadehyde1705-1740sadidehyde1705-1740sadidehyde1705-1740sacid chloride1700-1750sacid chloride1700-1750sfree300-3650mN-Hanine and amide3100-3650hydrogen bonded3200-3650mN-Hanine and amide3100-3500*s = strong, m = medium, w = weak2200-2250			2800 - 2900	Μ	
C=C alkene 1600–1680 w-m aromatic 1450 and 1600 w-m C≡C alkyne 2100–2250 w-m C=O alcohol, ether, es- 1050–1250 s ter, carbosylic acid, anhydride 1630–1680 s ter, carbosylic acid 1700–1750 s ketone 1705–1740 s ketone 1705–1740 s anhydride 1705–1740 s anhydride 1705–1740 s acid chloride 1705–1740 s arid chloride 1705–1740 s arid chloride 1705–1740 s arid chloride 1705–1740 s arid chloride 2400–3650 m hydrogen bonded 3200–3650 m hydrogen bonded 3100–3500 m hydrogen bonded 3100–3500 m hydrogen bonded 3100–3500 m hydrogen bonded 2400–3400 m nitrile 2200–2250 m	C=-Calkene1600-1680w-maromatic1450 and 1600w-mC=-Calkyne2100-2250w-mCOalcohol, ether, es-1050-1250scOalcohol, ether, es-1050-1250scOalcohol, ether, es-1050-1250scOalcohol, ether, es-1050-1250scOanide1600-1550scarboxylic acid1700-1750sketone1700-1750sadehyde1705-1740sadehyde1705-1740sadehyde1705-1740sadehyde1705-1740sacid chloride1700-3500mfree3200-3650mNHanine and amide3200-3650mNHanine and amide2400-3650mNHanine and amide3100-3550m*s = strong, m = medium, w = weakscolor-2250m	C-C	alkane	(not interpretative	ely useful)	
aromatic1450 and 1600w-mC \equiv Calkyne2100-2250w-mC $-$ Oalcohol, ether, es-1050-1250ster, carboxylicter, carboxylicsacid, anhydride1630-1680sc=Oamide1630-1680sacid, anhydride1700-1750scarboxylic acid1700-1750sketone1705-1740saldehyde1705-1740sanhydride1705-1740sacid chloride1705-1740sared chloride1705-1740sared chloride1705-1740sared chloride1705-1740sared chloride1705-1740sared chloride1705-1770sared chloride1705-1770sN-Halcohol, phenolshydrogen bonded3200-3550mN-Hamine and amide3100-3500mN-Hamine and amide3100-3500mN-Hamine and amide2200-2250m	aromatic1450 and 1600w-mC \equiv Calkyne2100-2250w-mC $-$ Oalcohol, ether, es-1050-1250ster, carboxylicter, carboxylicsacid, anhydride1630-1680sc=Oamide1630-1680sacid, anhydride1700-1750scarboxylic acid1700-1750sketone1705-1740saddehyde1705-1740sadidhyde1705-1740sadidhyde1765-1740sacid chloride1705-1740sacid chloride1700-3500mhydrogen bonded3200-3650mN-Hamine and amide3100-3550mN-Hamine and amide3100-3550m*s = strong, mnitrile2200-2250m	C=C	alkene	1600 - 1680	m-m	
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	C \equiv Calkyne2100-2250w-mCOalcohol, ether, es-1050-1250ster, carboxylicter, carboxylicsacid, anhydride1630-1680sC=-Oamide1630-1680scarboxylic acid1700-1750sketone1700-1750saddehyde1705-1740saddehyde1705-1740saddehyde1705-1740saddehyde1705-1740saddehode1705-1740saddehode1700-3500macid chloride1800sacid chloride1800shydrogen bonded3200-3650mNHamine and amide3100-3650mNHamine and amide3100-3550mNHamine and amide3100-3550m* s = strong, m = medium, w = weak2200-2250m		aromatic	1450 and 1600	m-m	
C—O alcohol, ether, es- 1050–1250 s ter, carboxylic acid, anhydride $1630-1680$ s acid, anhydride $1630-1680$ s carboxylic acid $1700-1750$ s ketone $1705-1740$ s aldehyde $1705-1740$ s anhydride $1705-1740$ s arboxylic acid chloride $1700-1750$ s anhydride $1705-1740$ s acid chloride $1705-1740$ s arboxylic acid $1705-1740$ s arboxylic acid $1700-3500$ m hydrogen bonded $3200-3550$ m N—H amine and amide $3100-3500$ m N—s C≡N nitrile $2200-2250$ m	COalcohol, ether, es- ter, carboxylic1050-1250ster, carboxylicter, carboxylicter, carboxylicacid, anhydride1680sacid, anhydride1670-1750scarboxylic acid1700-1750sketone1705-1740saldehyde1705-1740saddehyde1705-1740saddehyde1705-1740saddehyde1705-1740saddehyde1705-1740saddehyde1705-1740saddehyde1760 and 1810sacid chloride1800sacid chloride1800shydrogen bonded3200-3650mhydrogen bonded3200-3650mNHamine and amide3100-3550mNHamine and amide3100-3550m $x s = strong, m = medium, w = weak2200-2250m$	C≡C	alkyne	2100 - 2250	m-m	
ter, carboxylicacid, anhydride1630–1680sacid, anhydride1700–1750scarboxylic acid1700–1750sketone1705–1780saddehyde1705–1740sanhydride1755–1740sanhydride1760 and 1810sacid chloride1800sfree3200–3550mhydrogen bonded3200–3500mN—Hamine and amide3100–3500mC≡Nnitrile2200–2250m	ter, carboxylicacid, anhydride1630-1680sacid, anhydride1630-1680scarboxylic acid1700-1750sketone1705-1780saldehyde1705-1780saldehyde1705-1780saddehyde1705-1780saddehyde1705-1780saddehyde1705-1780saddehyde1705-1780saddehyde1705-1780saddehyde1705-1780saddehyde1705-1780saddehyde1700-3650mhydrogen bonded3200-3650mhydrogen bonded3200-3650mN-Hamine and amide3100-3550mN-Hamine and amide3100-3550m $C \equiv N$ nitrile2200-2250m	C-0	alcohol, ether, es-	1050 - 1250	s	
acid, anhydride $acid, anhydrideC=Oamide1630-1680scarboxylic acid1700-1750sketone1705-1740sketone1705-1740saldehyde1705-1740saldehyde1705-1740saldehyde1705-1740saldehyde1760 and 1810sacid chloride1800sacid chloride1800sfree3600-3650mhydrogen bonded2200-3500mNHamine and amide3100-3500mC=Nnitrile2200-2250m$	acid, anhydrideC=Oamide1630-1680sketone1700-1750sketone1700-1750sketone1705-1740saldehyde1705-1740sanhydride1760 and 1810sanhydride1760 and 1810sacid chloride1800sfree3600-3650mhydrogen bonded3200-3500mNHamine and amide3100-3500ms = strong, mscidom, w = weaks		ter, carboxylic			
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	$C=O amide \qquad 1630-1680 \qquad s \\ carboxylic acid \qquad 1700-1750 \qquad s \\ ketone \qquad 1705-1780 \qquad s \\ aldehyde \qquad 1705-1740 \qquad s \\ ester \qquad 1735-1800 \qquad s \\ anhydride \qquad 1735-1800 \qquad s \\ arid chloride \qquad 1760 and 1810 \qquad s \\ arid chloride \qquad 1760 and 1810 \qquad s \\ arid chloride \qquad 1760 and 1810 \qquad s \\ arid chloride \qquad 1760 and 1810 \qquad s \\ nhydrogen bonded \qquad 3200-3650 \qquad m \\ hydrogen bonded \qquad 3200-3650 \qquad m \\ N-H \qquad amine and amide \qquad 3100-3500 \qquad m \\ N-H \qquad amine and amide \qquad 3100-3500 \qquad m \\ *s = strong, m = medium, w = weak$		acid, anhydride			
carboxylic acid1700-1750sketone1705-1780sketone1705-1740saldehyde1705-1740sanhydride1735-1800sanhydride1760 and 1810sacid chloride1800sbydrogen3600-3650mhydrogen bonded3200-35500mNHamine and amide3100-3500mC=Nnitrile2200-2250m	carboxylic acid1700-1750sketone1705-1780saldehyde1705-1740saldehyde1705-1740sanhydride1735-1800sarid chloride1760 and 1810sarid chloride1800shydrogen3600-3650mhydrogen bonded3200-3650mNHamine and amide3100-3550mNHamine and amide3100-3550ms = strong, m = medium, w = weak2200-2250m	C=0	amide	1630 - 1680	s	
ketone 1705-1780 s aldehyde 1705-1740 s aldehyde 1705-1740 s ester 1735-1800 s anhydride 1760 and 1810 s acid chloride 1800 s acid chloride 1800 s free 3600-3650 m hydrogen bonded 3200-3500 m NH amine and amide 3100-3500 m C=N nitrile 2200-2250 m	ketone 1705–1780 s aldehyde 1705–1740 s ester 1705–1740 s ester 1735–1800 s acid chloride 1706 and 1810 s acid chloride 1800 s O—H alcohol, phenol $3000-3650$ m hydrogen bonded 3200–3650 m n N—H amine and amide 3100–3500 m SC=N nitrile 2200–2250 m * s = strong, m = medium, w = weak		carboxylic acid	1700-1750	s	
aldehyde 1705-1740 s aldehyde 1735-1800 s ester 1735-1800 s anhydride 1760 and 1810 s acid chloride 1800 s O-H alcohol, phenol 3600-3650 m free 3200-3550 m N-H amine and amide 3100-3500 m C≡N nitrile 2200-2250 m	$\begin{tabular}{ccc} & 1705-1740 & s \\ \mbox{ester} & 1735-1800 & s \\ \mbox{ester} & 1735-1800 & s \\ \mbox{acid chloride} & 1760 \mbox{and }1810 & s \\ \mbox{acid chloride} & 1760 \mbox{acid chloride} & 1800 & s \\ \mbox{acid chloride} & 1800 & m \\ \mbox{acid chloride} & 3200-3650 & m \\ \mbox{acrboxylic acid} & 2400-3400 & m \\ \mbox{amine and amide} & 3100-3500 & m \\ \box{cmbox} & m \mbox{amine and amide} & 2200-2250 & m \\ \end{tabular} * s = strong, m = medium, w = weak \\ \end{tabular}$		ketone	1705 - 1780	s	
ester 1735-1800 s anhydride 1760 and 1810 s acid chloride 1760 and 1810 s acid chloride 1800 s O—H alcohol, phenol s free 3600-3650 m hydrogen bonded 3200-35500 m N—H annine and amide 3100-3500 m C≡N nitrile 2200-2550 m	$\begin{tabular}{c c c c c c c c c c c c c c c c c c c $		aldehyde	1705 - 1740	s	
anhydride1760 and 1810sacid chloride1800sacid chloride1800sO—Halcohol, phenol3600–3650mfree3200–3500mhydrogen bonded3200–3500mN—Hamine and amide3100–3500mC≡Nnitrile2200–2250m	$\begin{tabular}{c c c c c c c c c c c c c c c c c c c $		ester	1735 - 1800	s	
acid chloride 1800 s OH alcohol, phenol $3600-3650$ m free $3200-3500$ m hydrogen bonded $3200-3500$ m carboxylic acid $2400-3400$ m NH amine and amide $3100-3500$ ms C \equiv N nitrile $2200-2250$ m	$\begin{array}{llllllllllllllllllllllllllllllllllll$		anhydride	1760 and 1810	s	
O—H alcohol, phenol free 3600–3650 m hydrogen bonded 3200–3500 m carboxylic acid 2400–3400 m N—H amine and amide 3100–3500 m–s C≡N nitrile 2200–2250 m	$\begin{array}{llllllllllllllllllllllllllllllllllll$		acid chloride	1800	s	
free 3600–3650 m hydrogen bonded 3200–3500 m carboxylic acid 2400–3400 m N—H amine and amide 3100–3500 m–s C≡N nitrile 2200–2250 m	$\label{eq:constraint} \begin{array}{llllllllllllllllllllllllllllllllllll$	H-0	alcohol, phenol			
hydrogen bonded 3200–3500 m carboxylic acid 2400–3400 m N—H amine and amide 3100–3500 m–s C \equiv N nitrile 2200–2250 m	hydrogen bonded3200-3500mcarboxylic acid2400-3400mNHamine and amide3100-3500m-s $C \equiv N$ nitrile2200-2250m* s = strong, m = medium, w = weak		free	3600 - 3650	ш	
carboxylic acid 2400–3400 m NH amine and amide 3100–3500 m-s $C\equiv N$ nitrile 2200–2250 m	carboxylic acid2400-3400mNHamine and amide $3100-3500$ m-sC=Nnitrile $2200-2250$ m* s = strong, m = medium, w = weak		hydrogen bonded	3200-3500	ш	
N—H amine and amide $3100-3500$ m–s C \equiv N nitrile 2200-2250 m	$\label{eq:N-H} \begin{array}{ll} \mbox{amine and amide} & 3100-3500 & m-s \\ \hline \mbox{C=N} & \mbox{nitrile} & 2200-2250 & m \\ \mbox{*} s = \mbox{strong}, m = \mbox{medium}, w = \mbox{weak} \end{array}$		carboxylic acid	2400 - 3400	ш	
C≡N nitrile 2200–2250 m	$C \equiv N \text{nitrile} 2200-2250 \text{m}$ * s = strong, m = medium, w = weak	H—N	amine and amide	3100 - 3500	m-s	
	* s = strong, m = medium, w = weak	C≡N	nitrile	2200 - 2250	Ш	
		C	c	C	C	C
)—)—)—) —)—
0= 0= 0= 0=	0= 0= 0=	$\left\langle \right\rangle$	\langle	\prec	<	۳
			\supset	>]	
		ò				/-funnal
		1715	1745	1780	1850	16E0_1E00 cm-

Table	
oectroscopy	ohn Mouser)
Infrared Sp	l, vd)

or (u)		
Functional Group	Frequency (cm ⁻¹)	intensity
water OH Stretch	3700-3100	strong
alcohol OH stretch	3600-3200	strong, broad
carboxylic acid OH stretch	3600-2500	strong, broad
N-H stretch	3500-3350 ^{(1 for NH} , 2 for NH ₂)	strong
≡C-H stretch	~3300	strong
=C-H stretch	3100-3000	variable
-C-H stretch	2950-2840	variable
-C-H aldehydic	2850-2750	variable
C≡N stretch	~2250	strong
C≡C stretch	2260-2100	variable
C=O aldehyde	1740-1720	strong
C=O anhydride	1840-1800, 1780-1740	weak, strong
C=O ester	1750-1720	strong
C=O ketone	1745-1715	strong
C=O amide	1700-1500	strong
C=C alkene	1680-1600	variable
C=C aromatic	1600-1400	variable
CH ₂ bend	1480-1440	medium
CH ₃ bend	1465-1440, 1390- 1365	medium
C-O-C stretch	1250-1050 several	strong
C-OH stretch	1200-1020	strong
C-F	1400-1000	strong
C-CI	800-600	strong
C-Br	750-500	strong
Ċ	~500	strong

Tables for IR and NMR data:

Type of Hydrogen (R = alkyl, Ar = aryl)	Chemical Shift (δ)*	Type of Hydrogen (R = alkyl, Ar = aryl)	Chemical Shift (δ)*
(C <mark>H</mark> ₃) ₄ Si	0 (by definition)	Q	
RCH ₃	0.8 - 1.0	RCOCH ₃	3.7 - 3.9
RC <mark>H</mark> 2R	1.2 - 1.4	O U	
R ₃ C <mark>H</mark>	1.4-1.7	RCOC <mark>H</mark> 2R	4.1 - 4.7
$R_2C = CRCHR_2$	1.6 - 2.6	RC <mark>H</mark> 2I	3.1-3.3
RC≡C <mark>H</mark>	2.0 - 3.0	RC <mark>H</mark> 2Br	3.4 - 3.6
ArC <mark>H</mark> 3	2.2 - 2.5	RC <mark>H</mark> 2Cl	3.6 - 3.8
ArC <mark>H</mark> 2R	2.3 - 2.8	RC <mark>H</mark> ₂ F	4.4 - 4.5
ROH	0.5 - 6.0	ArOH	4.5 - 4.7
RC <mark>H</mark> 2OH	3.4-4.0	$R_2C = CH_2$	4.6 - 5.0
RC <mark>H</mark> 2OR	3.3-4.0	$R_2C = CHR$	5.0 - 5.7
R_2NH	0.5 - 5.0	Ar <mark>H</mark>	6.5 - 8.5
O II		O II	
RCC <mark>H</mark> 3	2.1-2.3	RCH	9.5-10.1
O II			
RCC <mark>H</mark> 2R	2.2-2.6	RCOH	10-13

Characteristic ¹H-NMR Chemical Shifts

* Values are approximate. Other atoms within the molecule may cause the signal to appear outside these ranges.

Characteristic ¹³C-NMR Chemical Shifts

Type of Carbon	Chemical Shift (δ)	Type of Carbon	Chemical Shift (δ)
R <mark>C</mark> H ₃	0-40		110 160
R <mark>C</mark> H ₂ R	15 - 55	C-K	110-100
R₃ <mark>C</mark> H	20-60	O II	
R <mark>C</mark> H ₂ I	0 - 40	R <mark>C</mark> OR	160 - 180
R <mark>C</mark> H ₂ Br	25 - 65	O II	
R <mark>C</mark> H ₂ Cl	35-80	R <mark>C</mark> NR ₂	165 - 180
R₃ <mark>C</mark> OH	40-80	O II	
R ₃ COR	40-80	R <mark>С</mark> ОН	175 - 185
R <mark>C</mark> ≡CR	65 - 85	0 0	
$R_2 C = CR_2$	100 - 150	R <mark>C</mark> H, R <mark>C</mark> R	180 - 210

CHEM 30C, COMMON ¹H NMR CHEMICAL SHIFT RANGES



CHEM 30B, COMMON ¹³C NMR CHEMICAL SHIFT RANGES

