儀器設定:

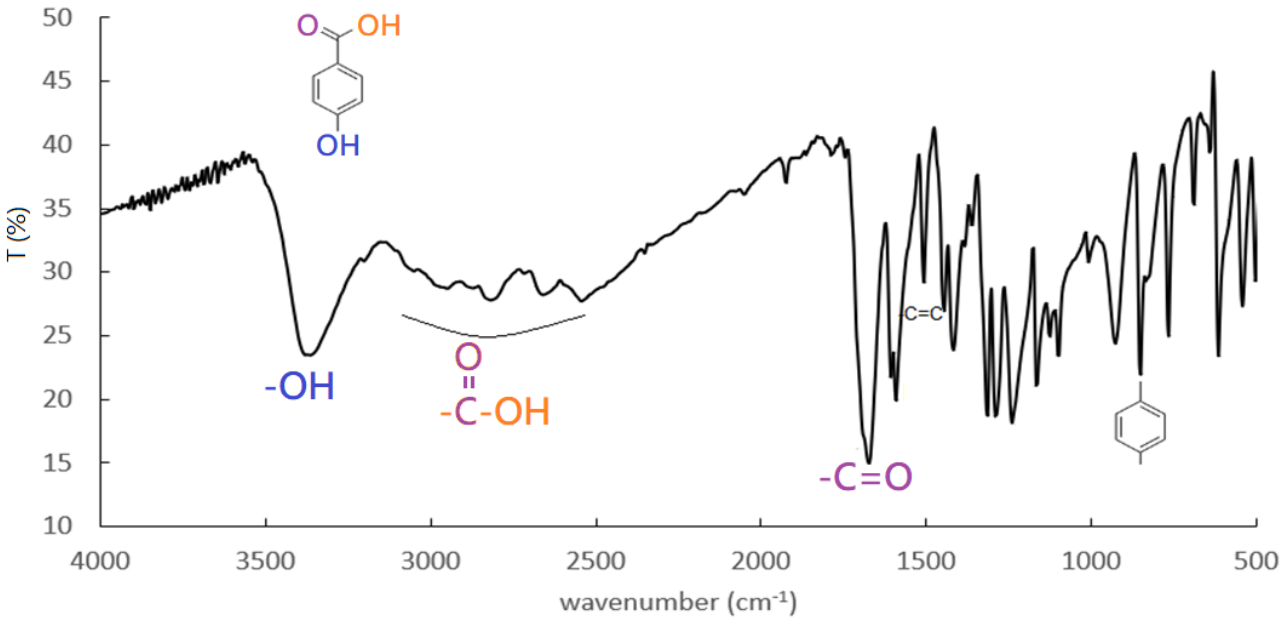
Scan wavenumber：400 ~ 4000 cm^{-1} (以自己的圖為準)

blank: air

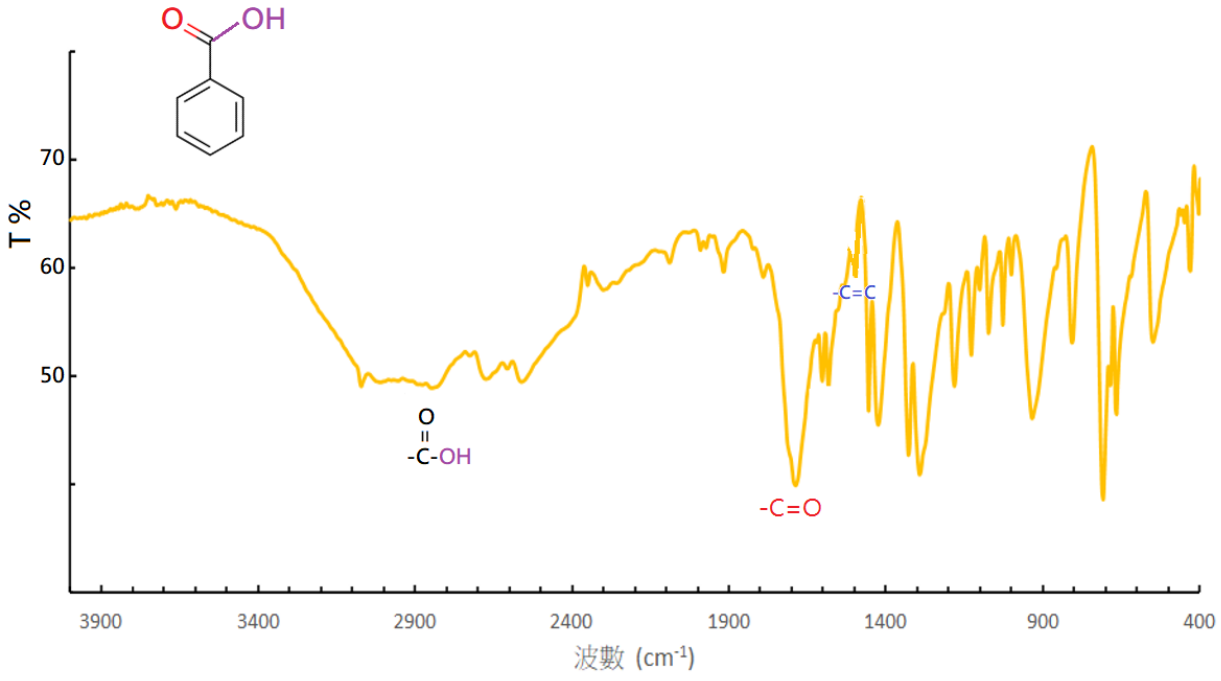
結果: (1)請在**圖上**標示可能的官能基，並繪出可能的結構式。

Example:

(1) $C_7H_6O_3$



(2) $C_7H_6O_2$



推薦網址: https://www.youtube.com/watch?v=hjLqOIN16t4

IR Spectrum Table & Chart

The **IR Spectrum Table** is a chart for use during infrared spectroscopy. The table lists IR spectroscopy frequency ranges, appearance of the vibration and absorptions for functional groups. There are two tables grouped by frequency range and compound class.

IR SPECTRUM TABLE BY FREQUENCY RANGE

Use this table when you already know the frequency of your material. Find the frequency range in the first column on the left side of the chart and corresponding values in adjacent columns.

If you need to find the frequency of a material go to the IR table by compound.

Table 1

Frequency Range	Absorption (cm^{-1})	Appearance	Group	Compound Class	Comments
4000-3000 cm^{-1}	3700-3584	medium, sharp	O-H stretching	alcohol	free
	3550-3200	strong, broad	O-H stretching	alcohol	intermolecular bonded

	3500	medium	N-H stretching	primary amine	
	3400				
	3400-3300	medium	N-H stretching	aliphatic primary amine	
	3330-3250				
	3350-3310	medium	N-H stretching	secondary amine	
	3300-2500	strong, broad	O-H stretching	carboxylic acid	usually centered on 3000 cm^{-1}
	3200-2700	weak, broad	O-H stretching	alcohol	intramolecular bonded
	3000-2800	strong, broad	N-H stretching	amine salt	

3000-2500 cm^{-1}					
3000-2500 cm^{-1}	3333-3267	strong, sharp	C-H stretching	alkyne	
	3100-3000	medium	C-H stretching	alkene	
	3000-2840	medium	C-H stretching	alkane	
	2830-2695	medium	C-H stretching	aldehyde	doublet
	2600-2550	weak	S-H stretching	thiol	
2400-2000 cm^{-1}					
2400-2000 cm^{-1}	2349	strong	O=C=O stretching	carbon dioxide	

	2275-2250	strong, broad	N=C=O stretching	isocyanate	
	2260-2222	weak	C≡N stretching	nitrile	
	2260-2190	weak	C≡C stretching	alkyne	disubstituted
	2175-2140	strong	S-C≡N stretching	thiocyanate	
	2160-2120	strong	N=N=N stretching	azide	
	2150		C=C=O stretching	ketene	
	2145-2120	strong	N=C=N stretching	carbodiimide	
	2140-2100	weak	C≡C stretching	alkyne	monosubstituted

	2140-1990	strong	N=C=S stretching	isothiocyanate	
	2000-1900	medium	C=C=C stretching	allene	
	2000		C=C=N stretching	ketenimine	
2000-1650 cm^{-1}					
2000-1650 cm^{-1}	2000-1650	weak	C-H bending	aromatic compound	overtone
	1870-1540				
	1818	strong	C=O stretching	anhydride	

	1750				
	1815-1785	strong	C=O stretching	acid halide	
	1800-1770	strong	C=O stretching	conjugated acid halide	
	1775	strong	C=O stretching	conjugated anhydride	
	1720				
	1770-1780	strong	C=O stretching	vinyl / phenyl ester	
	1760	strong	C=O stretching	carboxylic acid	monomer
	1750-1735	strong	C=O stretching	esters	6-membered lactone

	1750-1735	strong	C=O stretching	δ-lactone	γ: 1770
	1745	strong	C=O stretching	cyclopentanone	
	1740-1720	strong	C=O stretching	aldehyde	
	1730-1715	strong	C=O stretching	α,β-unsaturated ester	or formates
	1725-1705	strong	C=O stretching	aliphatic ketone	or cyclohexanone or cyclopentenone
	1720-1706	strong	C=O stretching	carboxylic acid	dimer
	1710-1680	strong	C=O stretching	conjugated acid	dimer
	1710-1685	strong	C=O stretching	conjugated aldehyde	

	1690	strong	C=O stretching	primary amide	free (associated: 1650)
	1690-1640	medium	C=N stretching	imine / oxime	
	1685-1666	strong	C=O stretching	conjugated ketone	
	1680	strong	C=O stretching	secondary amide	free (associated: 1640)
	1680	strong	C=O stretching	tertiary amide	free (associated: 1630)
	1650	strong	C=O stretching	δ-lactam	γ: 1750-1700 β: 1760-1730
1670-1600 cm^{-1}					
1670-1600 cm^{-1}	1678-1668	weak	C=C stretching	alkene	disubstituted (trans)

	1675-1665	weak	C=C stretching	alkene	trisubstituted
	1675-1665	weak	C=C stretching	alkene	tetrasubstituted
	1662-1626	medium	C=C stretching	alkene	disubstituted (cis)
	1658-1648	medium	C=C stretching	alkene	vinylidene
	1650-1600	medium	C=C stretching	conjugated alkene	
	1650-1580	medium	N-H bending	amine	
	1650-1566	medium	C=C stretching	cyclic alkene	
	1648-1638	strong	C=C stretching	alkene	monosubstituted

	1620-1610	strong	C=C stretching	α,β-unsaturated ketone	
1600-1300 cm^{-1}					
1600-1300 cm^{-1}	1550-1500	strong	N-O stretching	nitro compound	
	1372-1290				
	1465	medium	C-H bending	alkane	methylene group
	1450	medium	C-H bending	alkane	methyl group
	1375				
	1390-1380	medium	C-H bending	aldehyde	
	1385-1380	medium	C-H bending	alkane	gem dimethyl

	1370-1365			
1400-1000 cm^{-1}				
1400-1000 cm^{-1}	1440-1395	medium	O-H bending	carboxylic acid
	1420-1330	medium	O-H bending	alcohol
	1415-1380	strong	S=O stretching	sulfate
	1200-1185			
	1410-1380	strong	S=O stretching	sulfonyl chloride
	1204-1177			
	1400-1000	strong	C-F stretching	fluoro compound

	1390-1310	medium	O-H bending	phenol	
	1372-1335	strong	S=O stretching	sulfonate	
	1195-1168				
	1370-1335	strong	S=O stretching	sulfonamide	
	1170-1155				
	1350-1342	strong	S=O stretching	sulfonic acid	anhydrous
	1165-1150				hydrate: 1230-1120
	1350-1300	strong	S=O stretching	sulfone	
	1160-1120				

	1342-1266	strong	C-N stretching	aromatic amine
	1310-1250	strong	C-O stretching	aromatic ester
	1275-1200	strong	C-O stretching	alkyl aryl ether
	1075-1020			
	1250-1020	medium	C-N stretching	amine
	1225-1200	strong	C-O stretching	vinyl ether
	1075-1020			
	1210-1163	strong	C-O stretching	ester

	1205-1124	strong	C-O stretching	tertiary alcohol	
	1150-1085	strong	C-O stretching	aliphatic ether	
	1124-1087	strong	C-O stretching	secondary alcohol	
	1085-1050	strong	C-O stretching	primary alcohol	
	1070-1030	strong	S=O stretching	sulfoxide	
	1050-1040	strong, broad	CO-O-CO stretching	anhydride	
1000-650 cm^{-1}					
1000-650 cm^{-1}	995-985	strong	C=C bending	alkene	monosubstituted

	915-905				
	980-960	strong	C=C bending	alkene	disubstituted (trans)
	895-885	strong	C=C bending	alkene	vinylidene
	850-550	strong	C-Cl stretching	halo compound	
	840-790	medium	C=C bending	alkene	trisubstituted
	730-665	strong	C=C bending	alkene	disubstituted (cis)
	690-515	strong	C-Br stretching	halo compound	
	600-500	strong	C-I stretching	halo compound	
900-700 cm^{-1}					

900-700 cm^{-1}	880 ± 20	strong	C-H bending	1,2,4-trisubstituted
	810 ± 20			
	880 ± 20	strong	C-H bending	1,3-disubstituted
	780 ± 20			
	(700 ± 20)			
	810 ± 20	strong	C-H bending	1,4-disubstituted or
				1,2,3,4-tetrasubstituted
	780 ± 20	strong	C-H bending	1,2,3-trisubstituted
	(700 ± 20)			
	755 ± 20	strong	C-H bending	1,2-disubstituted

	750 ± 20	strong	C-H bending	monosubstituted
	700 ± 20			benzene derivative

IR TABLE BY COMPOUND CLASS

If you are looking up the absorption of a particular compound class, use this IR spectrum chart. If you already know the frequency, use the IR frequency table above.

Table 2

Compound Class	Group	Absorption (cm^{-1})	Appearance	Comments
acid halide	C=O stretching	1815-1785	strong	
alcohols	O-H stretching	3700-3584	medium, sharp	free
	O-H stretching	3550-3200	strong, broad	intermolecular bonded

	O-H stretching	3200-2700	weak, broad	intramolecular bonded
	O-H bending	1420-1330	medium	
aldehyde	C-H stretching	2830-2695	medium	doublet
	C=O stretching	1740-1720	strong	
	C-H bending	1390-1380	medium	
aliphatic ether	C-O stretching	1150-1085	strong	
aliphatic ketone	C=O stretching	1725-1705	strong	or cyclohexanone or cyclopentenone
aliphatic primary amine	N-H stretching	3400-3300	medium	
alkane	C-H stretching	3000-2840	medium	
	C-H bending	1465	medium	methylene group

	C-H bending	1450	medium	methyl group
	C-H bending	1385-1380	medium	gem dimethyl
	C-H stretching	3100-3000	medium	
	C=C stretching	1678-1668	weak	disubstituted (trans)
	C=C stretching	1675-1665	weak	trisubstituted
	C=C stretching	1675-1665	weak	tetrasubstituted
	C=C stretching	1662-1626	medium	disubstituted (cis)
	C=C stretching	1658-1648	medium	vinylidene
	C=C stretching	1648-1638	strong	monosubstituted
	C=C bending	995-985	strong	monosubstituted
	C=C bending	980-960	strong	disubstituted (trans)

	C=C bending	895-885	strong	vinylidene
	C=C bending	840-790	medium	trisubstituted
	C=C bending	730-665	strong	disubstituted (cis)
alkyl aryl ether	C-O stretching	1275-1200	strong	
alkyne	C-H stretching	3333-3267	strong, sharp	
	C≡C stretching	2260-2190	weak	disubstituted
	C≡C stretching	2140-2100	weak	monosubstituted
allene	C=C=C stretching	2000-1900	medium	
amine	N-H bending	1650-1580	medium	
	C-N stretching	1250-1020	medium	
amine salt	N-H stretching	3000-2800	strong, broad	

anhydride	C=O stretching	1818	strong	
	CO-O-CO stretching	1050-1040	strong, broad	
aromatic amine	C-N stretching	1342-1266	strong	
aromatic compound	C-H bending	2000-1650	weak	overtone
aromatic ester	C-O stretching	1310-1250	strong	
azide	N=N=N stretching	2160-2120	strong	
benzene derivative		700 ± 20		
carbodiimide	N=C=N stretching	2145-2120	strong	
carbon dioxide	O=C=O stretching	2349	strong	
carboxylic acid	O-H stretching	3300-2500	strong, broad	usually centered on 3000 cm^{-1}

	C=O stretching	1760	strong	monomer
	C=O stretching	1720-1706	strong	dimer
	O-H bending	1440-1395	medium	
conjugated acid	C=O stretching	1710-1680	strong	dimer
conjugated acid halide	C=O stretching	1800-1770	strong	
conjugated aldehyde	C=O stretching	1710-1685	strong	
conjugated alkene	C=C stretching	1650-1600	medium	
conjugated anhydride	C=O stretching	1775	strong	
conjugated ketone	C=O stretching	1685-1666	strong	
cyclic alkene	C=C stretching	1650-1566	medium	

cyclopentanone	C=O stretching	1745	strong	
ester	C-O stretching	1210-1163	strong	
esters	C=O stretching	1750-1735	strong	6-membered lactone
fluoro compound	C-F stretching	1400-1000	strong	
halo compound	C-Cl stretching	850-550	strong	
	C-Br stretching	690-515	strong	
	C-I stretching	600-500	strong	
imine / oxime	C=N stretching	1690-1640	medium	
isocyanate	N=C=O stretching	2275-2250	strong, broad	
isothiocyanate	N=C=S stretching	2140-1990	strong	
ketene	C=C=O stretching	2150		

ketenimine	C=C=N stretching	2000	
monosubstituted	C-H bending	750 ± 20	strong
nitrile	C≡N stretching	2260-2222	weak
nitro compound	N-O stretching	1550-1500	strong
none		3330-3250	
none		1870-1540	
none		1750	
none		1720	
none		1372-1290	
none		1375	
none		1370-1365	

none	1200-1185	
none	1204-1177	
none	1195-1168	
none	1170-1155	
none	1165-1150	hydrate: 1230-1120
none	1160-1120	
none	1075-1020	
none	1075-1020	
none	915-905	
none	810 ± 20	
none	780 ± 20	

none		(700 ± 20)		
none		(700 ± 20)		
phenol	O-H bending	1390-1310	medium	
primary alcohol	C-O stretching	1085-1050	strong	
primary amide	C=O stretching	1690	strong	free (associated: 1650)
	N-H stretching	3500	medium	
secondary alcohol	C-O stretching	1124-1087	strong	
secondary amide	C=O stretching	1680	strong	free (associated: 1640)
secondary amine	N-H stretching	3350-3310	medium	
sulfate	S=O stretching	1415-1380	strong	
sulfonamide	S=O stretching	1370-1335	strong	

sulfonate	S=O stretching	1372-1335	strong	
sulfone	S=O stretching	1350-1300	strong	
sulfonic acid	S=O stretching	1350-1342	strong	anhydrous
sulfonyl chloride	S=O stretching	1410-1380	strong	
sulfoxide	S=O stretching	1070-1030	strong	
tertiary alcohol	C-O stretching	1205-1124	strong	
tertiary amide	C=O stretching	1680	strong	free (associated: 1630)
thiocyanate	S-CΞN stretching	2175-2140	strong	
thiol	S-H stretching	2600-2550	weak	
vinyl / phenyl ester	C=O stretching	1770-1780	strong	
vinyl ether	C-O stretching	1225-1200	strong	

α,β-unsaturated ester	C=O stretching	1730-1715	strong	or formates
α,β-unsaturated ketone	C=C stretching	1620-1610	strong	
δ-lactam	C=O stretching	1650	strong	γ: 1750-1700 β: 1760-1730
δ-lactone	C=O stretching	1750-1735	strong	γ: 1770
1,2,3,4-tetrasubstituted				
1,2,3-trisubstituted	C-H bending	780 ± 20	strong	
	C-H bending	880 ± 20	strong	
1,2-disubstituted	C-H bending	755 ± 20	strong	
	C-H bending	880 ± 20	strong	
1,4-disubstituted or	C-H bending	810 ± 20	strong	

HOW TO READ AN IR SPECTRUM TABLE

To use an IR spectrum table, first find the frequency or compound in the first column, depending on which type of chart you are using. Then find the corresponding values for absorption, appearance and other attributes. The value for absorption is usually in cm^{-1}.

Note that not all frequencies have a related compound.

取自: https://www.sigmaaldrich.com/TW/en/technical-documents/technical-article/analytical-chemistry/photometry-and-reflectometry/ir-spectrum-table