

Characteristic Raman Vibrational Frequencies of Organic Groups

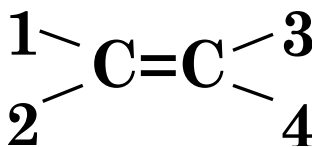
Raman Products Technical Note

Number 1103

Frequency, cm ⁻¹	Vibration	Compound
480-510	SS stretch	dialkyl disulfides
615-630	ring deformation	monosubstituted benzenes
650-660	CCI stretch	primary chloroalkanes
620-715	CS stretch	dialkyl disulfides
585-740	CS stretch	alkyl sulfides
820-825	C ₃ O skeletal stretch	secondary alcohols
720-830	ring vibration	para-disubstituted benzenes
749-835	skeletal stretch	isopropyl group
877	OO stretch	hydrogen peroxide
850-900	symmetric CNC stretch	secondary amines
837-905	CC skeletal stretch	n-alkanes
830-930	symmetric COC stretch	aliphatic ethers
990-1010	trigonal ring breathing	mono-substituted benzenes
990-1010	trigonal ring breathing	meta-substituted benzenes
1015-1030	in-plane CH deformation	mono-substituted benzenes
1020-1060	ring vibration	ortho-disubstituted benzenes
950-1150	CC stretches	n-alkanes
1188-1196	symmetric SO ₂ stretch	alkyl sulfates
1205	C ₆ H ₅ -C vibration	alkyl benzenes
1200-1230	ring vibration	para-disubstituted benzenes
1251-1270	in-plane CH deformation	cis-dialkyl ethylenes
1295-1305	CH ₂ in-phase twist	n-alkanes
1175-1310	CH ₂ twist and rock	n-alkanes
1290-1314	in-plane CH deformation	trans-dialkyl ethylenes
1330-1350	CH deformation	isopropyl group
1368-1385	CH ₃ symmetric deformation	n-alkanes
1370-1390	ring stretch	naphthalenes
1385-1415	ring stretch	anthracenes
1465-1466	CH ₃ deformation	n-alkanes
1446-1473	CH ₃ , CH ₂ deformations	n-alkanes
1550-1630	ring stretches (doublet)	benzene derivatives
1590-1650	NH ₂ scissors	primary amines
1649-1654	symmetric C=O stretch	carboxylic acids (cyclic dimer)
1700-1725	C=O stretch	aliphatic ketones
1720-1740	C=O stretch	aliphatic aldehydes
2100-2160	C≡C stretch	alkyl acetylenes
2232-2251	C≡N stretch	aliphatic nitriles
2231-2301	C≡C stretch	dialkyl acetylenes
2560-2590	SH stretch	thiols
2849-2861	symmetric CH ₂ stretch	n-alkanes
2883-2884	symmetric CH ₃ stretch	n-alkanes
2912-2929	anti-symmetric CH ₂ stretch	n-alkanes
2965-2969	anti-symmetric CH ₃ stretch	n-alkanes
3000-3100	aromatic CH stretch	benzene derivatives
3330-3400	bonded antisymmetric NH ₂ stretch	primary amines

Reference: Lin-Vien, D.; Colthup, N.B.; Fateley, W.B. and Graselli, J.G. *The Handbook of Infrared and Raman Characteristic Frequencies of Organic Molecules*. Academic Press: Boston, 1991.

Raman Characteristic Frequencies of Vinyl Groups



1,3 = H (cis isomers)		
2	4	Frequency, cm ⁻¹
CH ₃ -	CH ₃ -	1662
CH ₃ CH ₂ -	CH ₃ -	1658
(CH ₃) ₂ CH-	(CH ₃) ₂ CH-	1649
CH ₃ CH ₂ -	C(CH ₃) ₃ -	1650
C ₆ H ₅ -	C ₆ H ₅ -	1629
OCH ₃ -	OCH ₃ -	1672
Cl-	Cl-	1591
Br-	Br-	1587
COOH	COOH	1631, 1697
CH ₃ -	CH ₃ (CH ₂) ₄ -	1655
CH ₃ -	CH ₃ CH ₂ SS-	1612
1,4 = H (trans isomers)		
2	3	Frequency, cm ⁻¹
CH ₃ -	CH ₃ -	1676
CH ₃ CH ₂ -	CH ₃ -	1673
(CH ₃) ₂ CH-	(CH ₃) ₂ CH-	1663
CH ₃ CH ₂ -	C(CH ₃) ₃ -	1659
C ₆ H ₅ -	C ₆ H ₅ -	1648
OCH ₃ -	OCH ₃ -	1666
Cl-	Cl-	1579
Br-	Br-	1582
COOH	COOH	1683

1	2	3	4	Frequency, cm ⁻¹
H-	H-	CH ₃ -	CH ₃ -	1658
H-	H-	CH ₃ -	CH ₃ CH ₂ -	1649
H-	H-	CH ₃ -	CH ₃ CH ₂ CH ₂ -	1649
H-	H-	CH ₃ -	C ₆ H ₅ -	1634
H-	H-	C ₆ H ₅ -	C ₆ H ₅ -	1610
H-	H-	Cl-	Cl-	1612
H-	Cl-	Cl-	Cl-	1582
H-	CH ₃ -	CH ₃ -	CH ₃ CH ₂ -	1669
H-	CH ₃ -	CH ₃ -	CH ₃ -	1680
CH ₃ -	CH ₃ -	CH ₃ -	CH ₃ -	1676
Cl-	Cl-	Cl-	Cl-	1572
CN-	CN-	CN-	CN-	1567

1, 2, 3 = H	
4	Frequency, cm ⁻¹
C ₆ H ₅ -	1625
C ₆ H ₅ CH ₂ -	1635
C ₆ H ₅ CH ₂ CH ₂ -	1648
CN-	1607
CNCH ₂ -	1646
Cl-	1607
Br-	1601
I-	1581
CH ₂ Cl-	1650
CH ₂ Br-	1630
HOCH ₂ -	1644
CH ₃ CHOHCH-	1644
OCNCH ₂ -	1645
(CH ₃) ₃ C-	1641
CH ₃ COO-	1635
1, 2, 3 = H 4 = unbranched alkane	
C's in 4	Frequency, cm ⁻¹
0	1623
1	1651
2	1645
3	1641
4	1638
5	1640
6	1642
7	1641
10	1641
11	1637
14	1642
16	1641

Selected from:

- Schrader, B. *Raman / Infrared Atlas of Organic Compounds*, 2nd ed. VCH-Verl.-Ges.: Weinheim, 1989.
- Lin-Vien, D.; Colthup, N.B.; Fateley, W.B.; and Grasselli, J.B. *The Handbook of Infrared and Raman Characteristic Frequencies of Organic Molecules*, Academic Press: Boston, 1991.
- Freeman, S.K. *Applications of Laser Raman Spectroscopy*, Wiley: New York, 1974.



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