Fancy a functional group? Usual Raman vibrational frequencies

Introduction

SPELEC RAMAN is a compact instrument that allows to perform Raman spectroelectrochemical experiments in a simple and elegant way. This instrument integrates in only one box: a high-resolution spectrometer, a laser source (785 nm) and a bipotentiostat/galvanostat, and it can be controlled by an excellent spectroelectrochemical software.

Although the SPELEC RAMAN will facilitate the Raman spectroelectrochemical measurements, the interpretation of data should be performed by you. In this Application Note, we describe the main vibrational frequencies for different functional groups and a probable intensity of the signal. It must be considered that these properties could vary significantly according to the structural atomic environment of the functional groups of the complete molecules or by strong interaction with surfaces as it happens with the SERS effect.

Vibrational frequencies

Functional group	Region (cm^{-1})	Signal
Lattice vibrations	100 - 210	strong
Metal-O	150 - 450	strong
C-C aliphatic chain	250 - 400	strong
Se-Se	290 - 330	strong
S-S	430 - 550	strong
$S_2O_3^{2-}$	430 - 470	strong
Si-O-Si	450 - 550	strong
C-I	480 - 660	strong
C-Br	500 - 700	strong
C-Cl	550 - 800	strong
C=S	580 - 680	strong
C-C aliphatic chain	600 - 1300	medium
C-S aliphatic	630 - 790	strong
C-F	720 - 800	strong
IO_3^-	740 - 760	very strong
BrO_3^-	780 - 805	strong
C-O-C	800 - 970	medium
O-O	845 - 900	strong
ClO_4^-	920 - 935	strong
ClO_3^-	930 - 940	strong
PO_4^{3-}	940 - 960	medium
SO_4^{2-}	965 – 1035	strong
SO_3^{2-}	970 - 990	strong
$S_2O_3^{2-}$	985 - 1015	medium
C-C aromatic ring	990 - 1100	medium/strong
C-C aliphatic chain	1000 - 1250	strong
NO_3^-	1020 - 1070	strong
C=S	1020 - 1225	strong
HCO_3^-	1025 - 1045	strong
C-O-C asym.	1060 - 1150	weak
CO_3^{2-}	1075 - 1095	strong
C-S aromatic	1080 - 1100	strong

Functional group	Region (cm^{-1})	Signal
R-SO_3H	1145 - 1240	weak
R-CO_2^-	1315 - 1435	medium
NO_2^-	1320 - 1330	strong
C-NO_2 asym.	1340 - 1380	strong
N=N aromatic	1365 - 1450	very strong
C-C aromatic ring	1370 - 1400	medium
CH_2, CH_3 bending	1380 - 1470	medium
C-C aromatic ring	1450 - 1500	medium
C=C	1500 - 1900	strong
C-NO_2 asym.	1530 - 1590	medium
N=N aliphatic	1550 - 1580	medium
HN-C=O (amide)	1550 - 1700	strong
C-C aromatic ring	1580 - 1600	strong
R-CO-R (ketone)	1600 - 1710	medium
R-COOH (acid)	1610 - 1740	medium
C=N	1610 - 1680	strong
H_2O bending	1640	weak
R-(CO)-H (aldehyde)	1710 - 1725	medium
R-(CO)O-R (ester)	1710 - 1745	medium
R-(CO)-O-(CO)-R	1740 - 1830	medium
R-N=C=S	2020 - 2100	medium
C≡C	2070 - 2250	strong
R-N≡C	2090 - 2170	medium
R-S-C≡N	2100 - 2170	medium
N_3^-	2110 - 2160	medium
R-N≡N	2200 - 2280	medium
C≡N	2200 - 2260	medium
R-N=C=O	2230 - 2270	weak
R-S-H	2530 – 2610	strong
OC-H (aldehyde)	2680 - 2740	weak
N-CH_3	2750 - 2800	weak
CH_2	2700 - 2800	strong

References

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