**For IR, VCD** **!**

Lorentzian fitting function:

v – frequency in computed spectrum (in cm-1) , (f(v) called for each point in spectrum)

vi – frequency of the ith band (in cm-1)

Ii – intensity of the ith band

– half width at half maximum (in cm-1)

Gaussian fitting function:

v – frequency in computed spectrum (in cm-1) , (f(v) called for each point in spectrum)

vi – frequency of the ith band (in cm-1)

Ii – intensity of the ith band

– half width at half maximum (in cm-1)

Dipole strength to IR intensities:

Rotator strength to VCD intensieties:

Oscillator strength to UV intensities:

c = 2.99792458 x 1010 cm/sec (speed of light)

me = 9.10938 × 10-31 kg (electron mass)

e = 4.803204 × 10-10 esu (electron charge)

NA = 6.02214199 × 1023 mol-1 (Avogadro’s constant)

fi – oscillator strength

Rotator strength to ECD intensieties:

h = 6.62606896 x 10-30 kg·cm2·sec-1 (Planck’s constant)

NA = 6.02214199 × 1023 mol-1 (Avogadro’s constant)

Ri – rotator strength

Raman activities (extracted from Gaussian output file) to raman intensieties:

where

h = 6.62606896 x 10-30 kg·cm2·sec-1 (Planck’s constant)

c = 2.99792458 x 1010 cm/sec (speed of light)

K = 1.3806504 x 10-23 Joules/Kelvin (Boltzmann’s constant)

T – temperature (default T = 298.15 K)

Si – raman activities

v0 – frequency of the laser excitation line (default v0 = 532 nm = 18796.99 cm-1)

vi – frequency of the ith band

f – factor for conversion of Si from A4/AMU to s\*m4/kg