

Model -113: Raman intensity for the Stokes and Anti-Stokes response, excluding the Rayleigh peak. The excitations are modelled using a Breit Wigner Fano line shape.

#	Wo	Wp	G
1	--	T (K)	Δ (cm ⁻¹) (not fittable)
2	--	C_A	C_B
3	C	--	--
4	$\omega_{0,1}$ (cm ⁻¹)	A_1	γ_1 (cm ⁻¹)
5	p_1	--	--
6	$\omega_{0,2}$ (cm ⁻¹)	A_2	γ_2 (cm ⁻¹)
7	p_2	--	--
--	--	--	--
3+N	$\omega_{0,N}$ (cm ⁻¹)	A_N	γ_N (cm ⁻¹)
3+N+1	p_N	--	--

E1	Raman Intensity: $\omega + \Delta < 0$: Anti-Stokes, $\omega - \Delta > 0$: Stokes
S1	Camera correction
N1	Bose-factor

If $\omega > \Delta$, the Raman intensity corresponds to the Stokes response:

$$I_{Stokes}(\omega') = C + (1 + n(\omega')) * CC(\omega') * \sum_{i=1}^N \frac{A_i \left(1 + \frac{\omega' - \omega_{0,i}}{\gamma_i q_i}\right)^2}{1 + \left(\frac{\omega' - \omega_{0,i}}{\gamma_i}\right)^2},$$

where $\omega' = \omega - \Delta$.

If $\omega < \Delta$, the Raman intensity corresponds to the Anti-Stokes response:

$$I_{Anti-Stokes}(\omega') = C + n(\omega') * CC(\omega') * \sum_{i=1}^N \frac{A_i \left(1 + \frac{\omega' - \omega_{0,i}}{\gamma_i q_i}\right)^2}{1 + \left(\frac{\omega' - \omega_{0,i}}{\gamma_i}\right)^2},$$

where $\omega' = \Delta - \omega$.

C = constant, can be used to account for black noise

$n(\omega)$ = Bose-Factor

$CC(\omega)$ = function for camera correction

$q_i = 1/p_i$ = Breit Wigner Fano factor ($p = 0$: fully symmetric)

Δ = Shift of the Rayleigh peak from 0.

Bose-factor:

$$n(\omega) = \frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1}$$

Camera correction:

$$CC(\omega) = 1.0 + C_A * \omega + C_B * \omega^2$$