CERIC

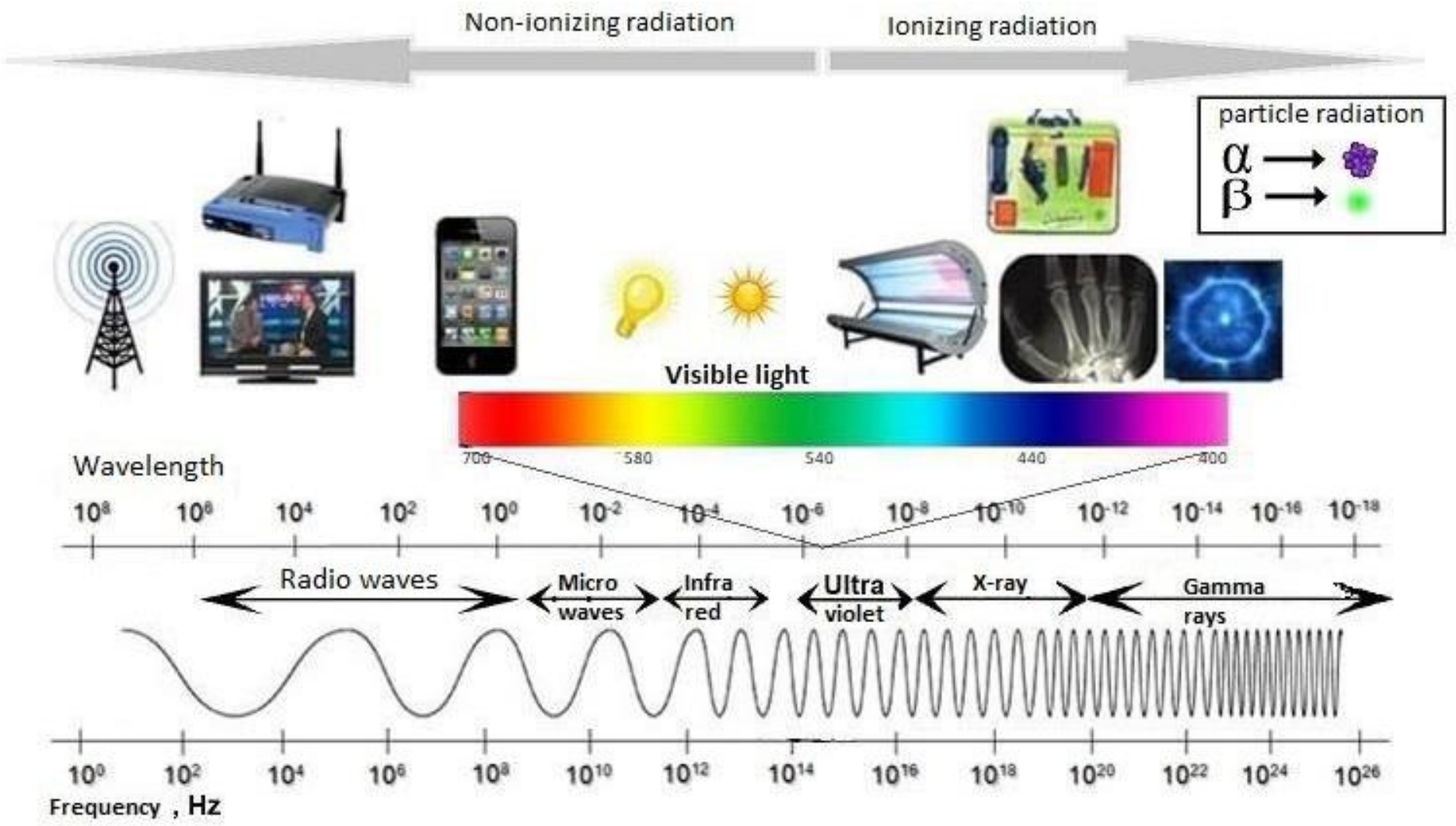
PaGES 8

Planning, Management and Execution of a Scientific Experiment in an international research infrastructure

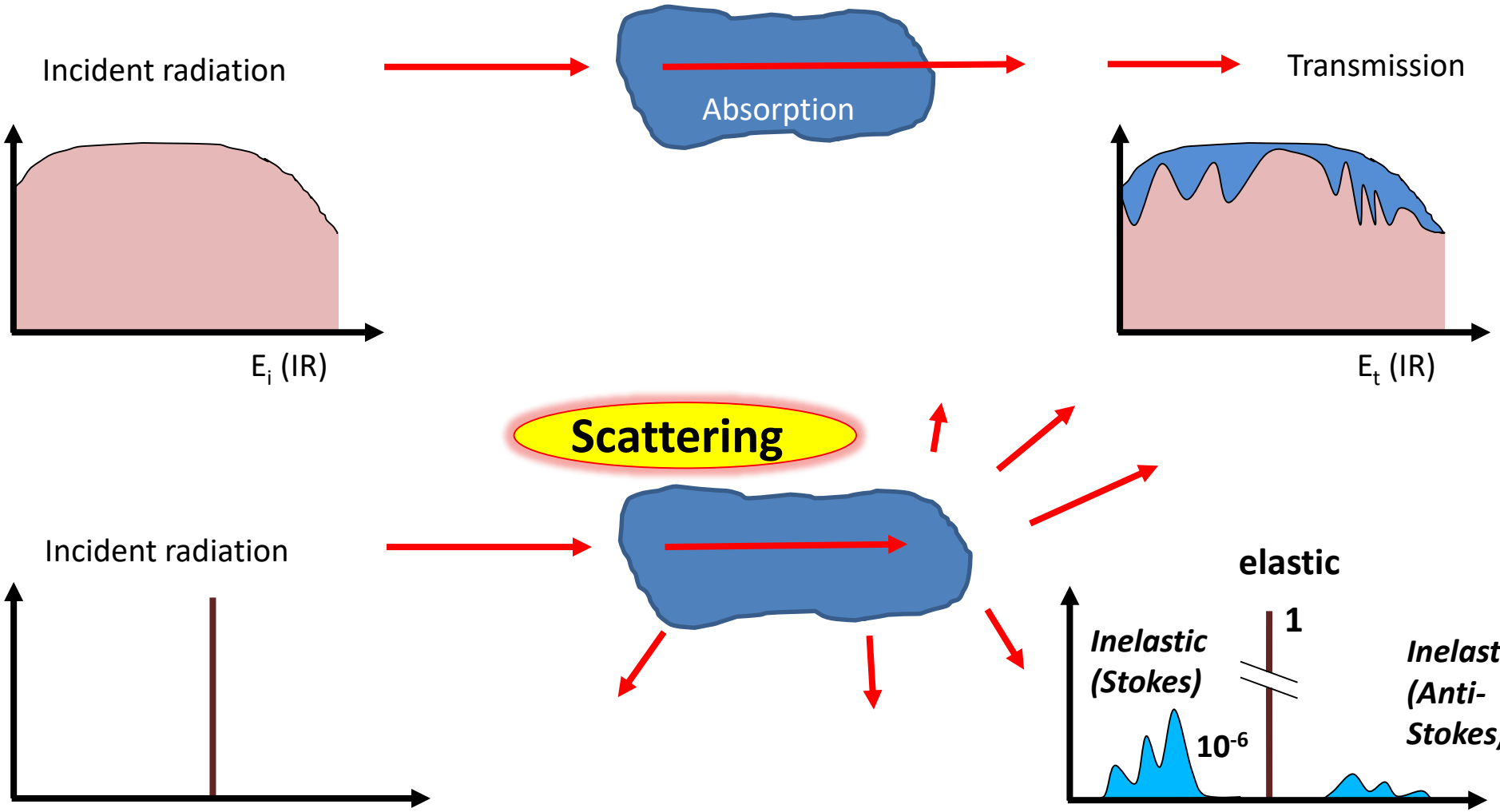
Spettroscopia Raman

Esperimento per progetto PAGES

The electromagnetic spectrum

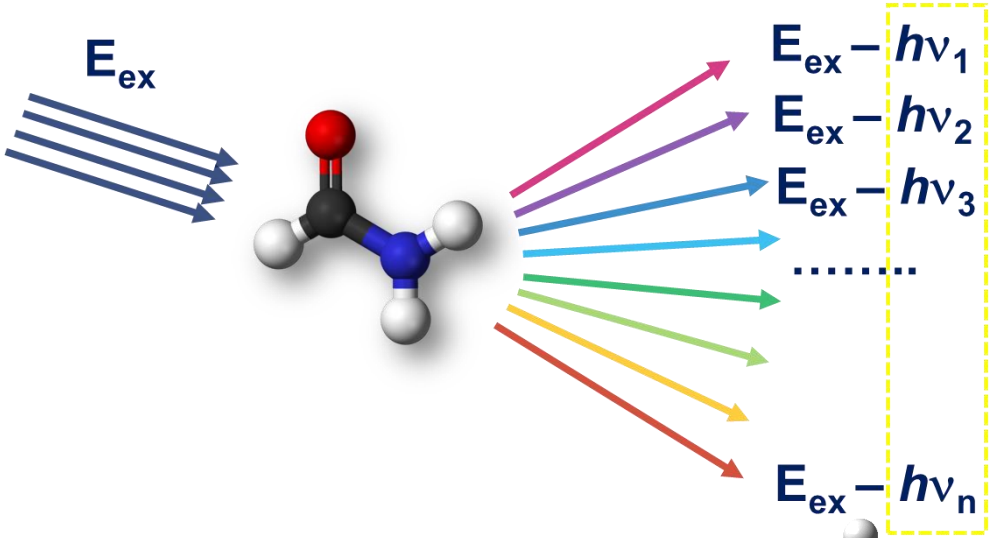


Infrared VS Raman

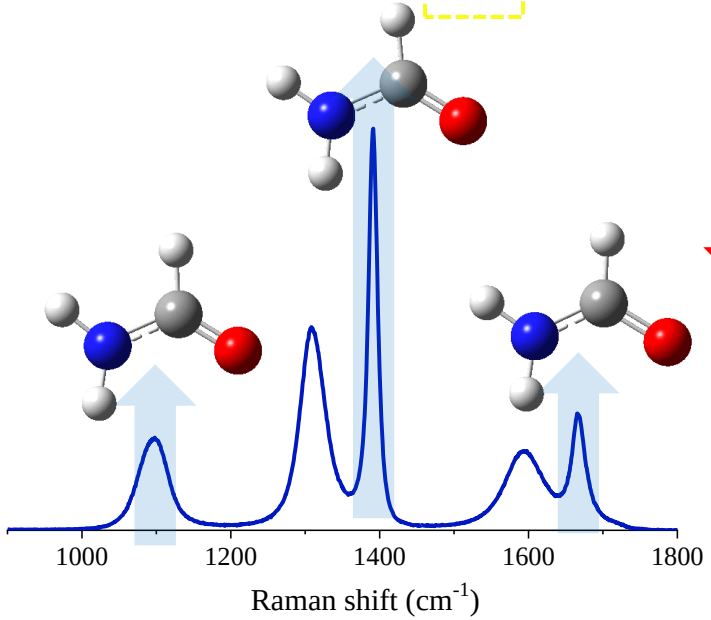


The Raman effect

Sir C. V. Raman
Physics Nobel prize (1930)



shift in photon energy due to excitation of molecular vibrations



vibrational signature of the molecular system

Raman effect: classical model

*Raman bands arise from **changes in the molecular polarizability** during the vibrations*

$$P(t) = \alpha_0 E_0 \cos\omega_0 t + \frac{1}{2}\delta\alpha_k Q_k^0 E_0 \left[\cos(\omega_0 - \omega_k)t - \phi_k + \cos(\omega_0 + \omega_k)t + \phi_k\right]$$

$$= P(\omega_0) + P(\omega_0 - \omega_k) + P(\omega_0 + \omega_k)$$

$P(\omega_0) \propto \cos\omega_0 t$

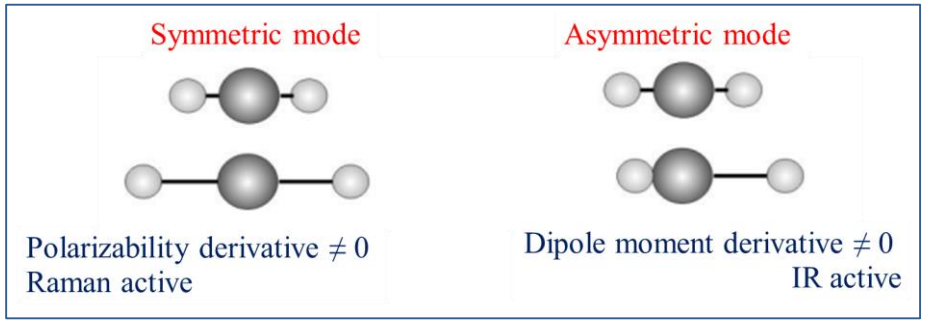
Rayleigh or elastic scattering

$P(\omega_0 - \omega_k) \propto \cos(\omega_0 - \omega_k)t - \phi_k$

Stokes Raman scattering

$P(\omega_0 + \omega_k) \propto \cos(\omega_0 + \omega_k)t + \phi_k$

Anti-Stokes Raman scattering



Raman scattering total intensity:

$$I(\theta)_{av} = B(\nu_0 \pm \nu)^4 I_0 \left(\frac{\partial\alpha_{xx}}{\partial Q_1}\right)_0^2 \sin^2\theta$$

derived polarizability tensor

Molecular vibrations: quantistic model

$$H = T_n + T_e + V_{ne} + V_{nn} + V_{ee}$$

Born-Oppenheimer approximation

$H = \cancel{T_n} + T_e + \cancel{V_{nn}} + V(X_n, x_e)$

$Solve\ [T_e + V(X_n, x_e)]\Psi_e = E_e\Psi_e$

$\Psi_{ei}(X_n)$

$E_{ei}(X_n)$

$H = T_n + V_{nn} + E_e(X_n)$

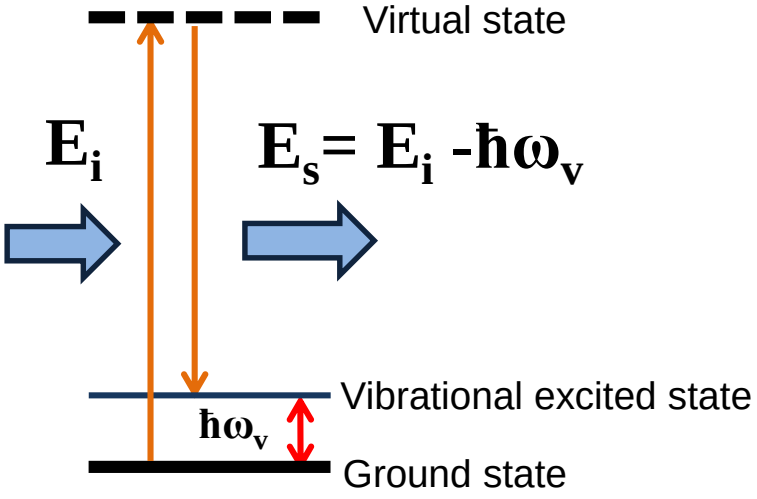
$Solve\ [T_n + V_{nn} + E_e(X_n)]\Psi_n = E_n\Psi_n$

Ψ_{ni}

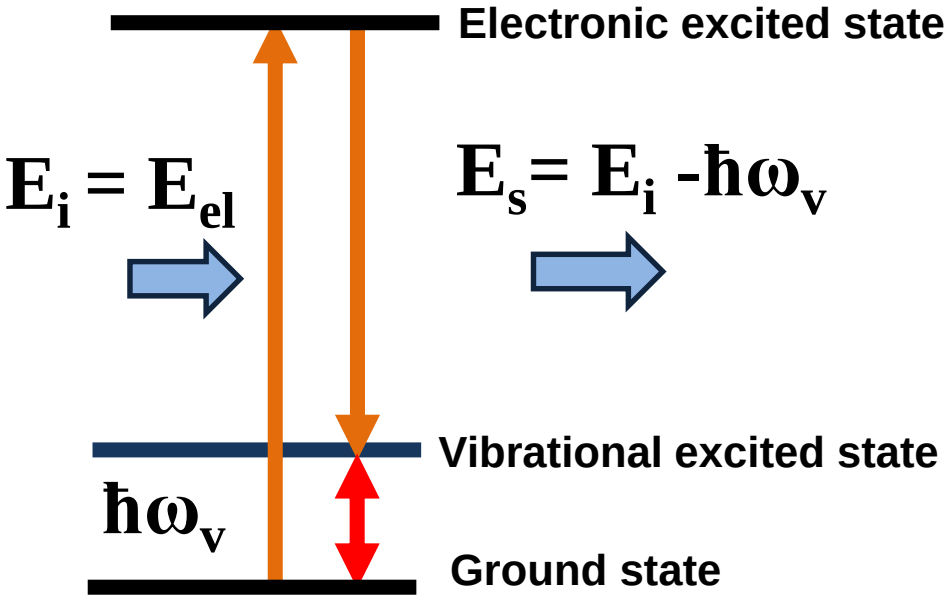
E_{ni}

Raman effect: quantistic model

Spontaneous Raman

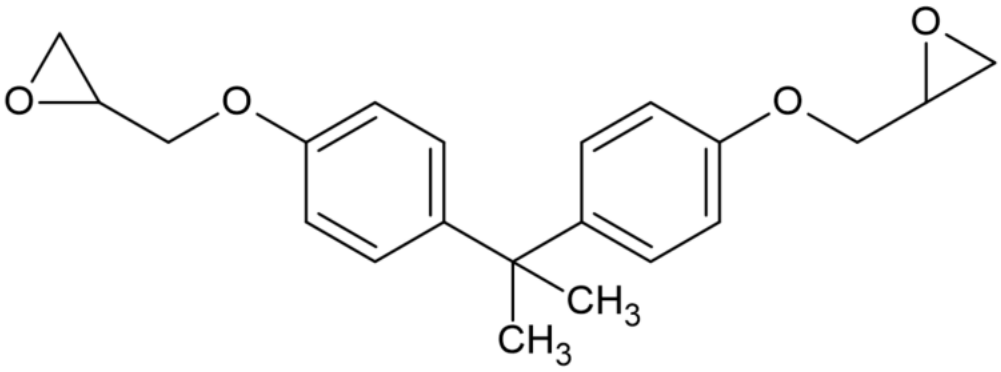


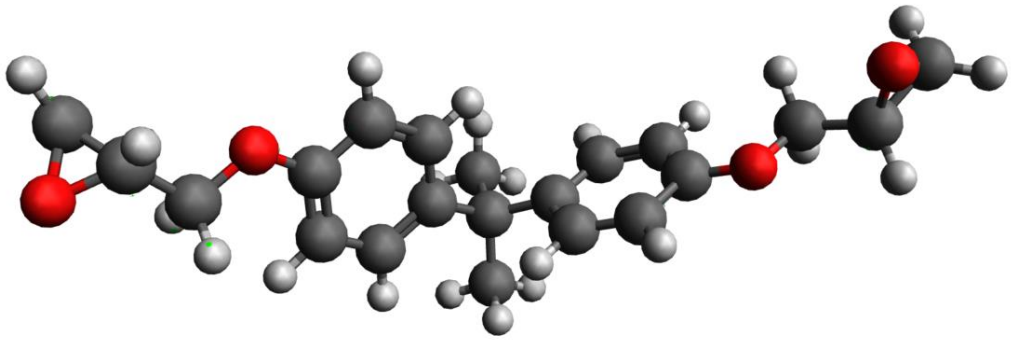
Resonant Raman

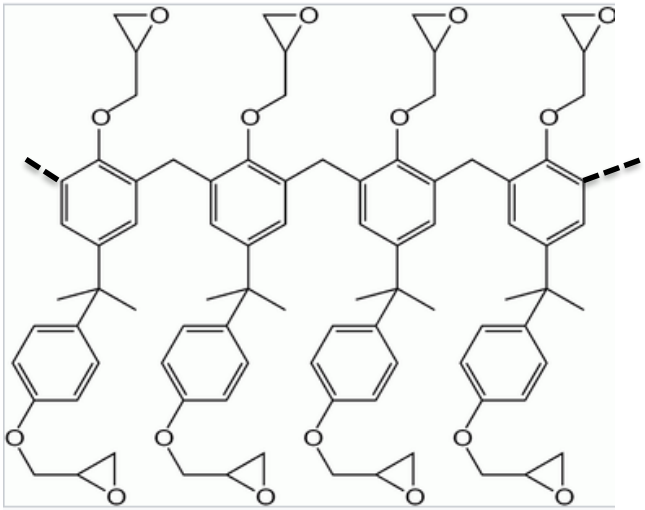


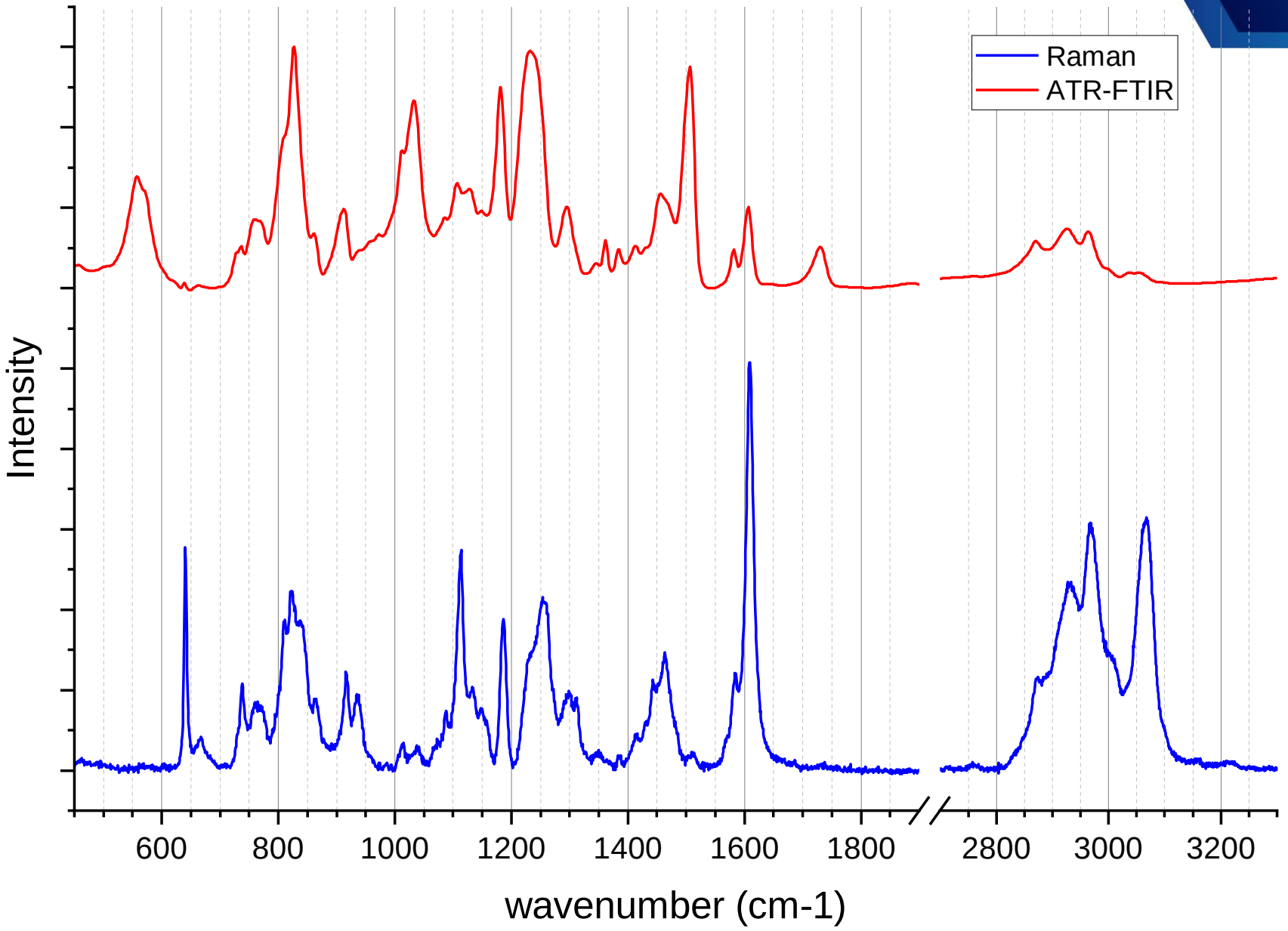
Raman cross section increased

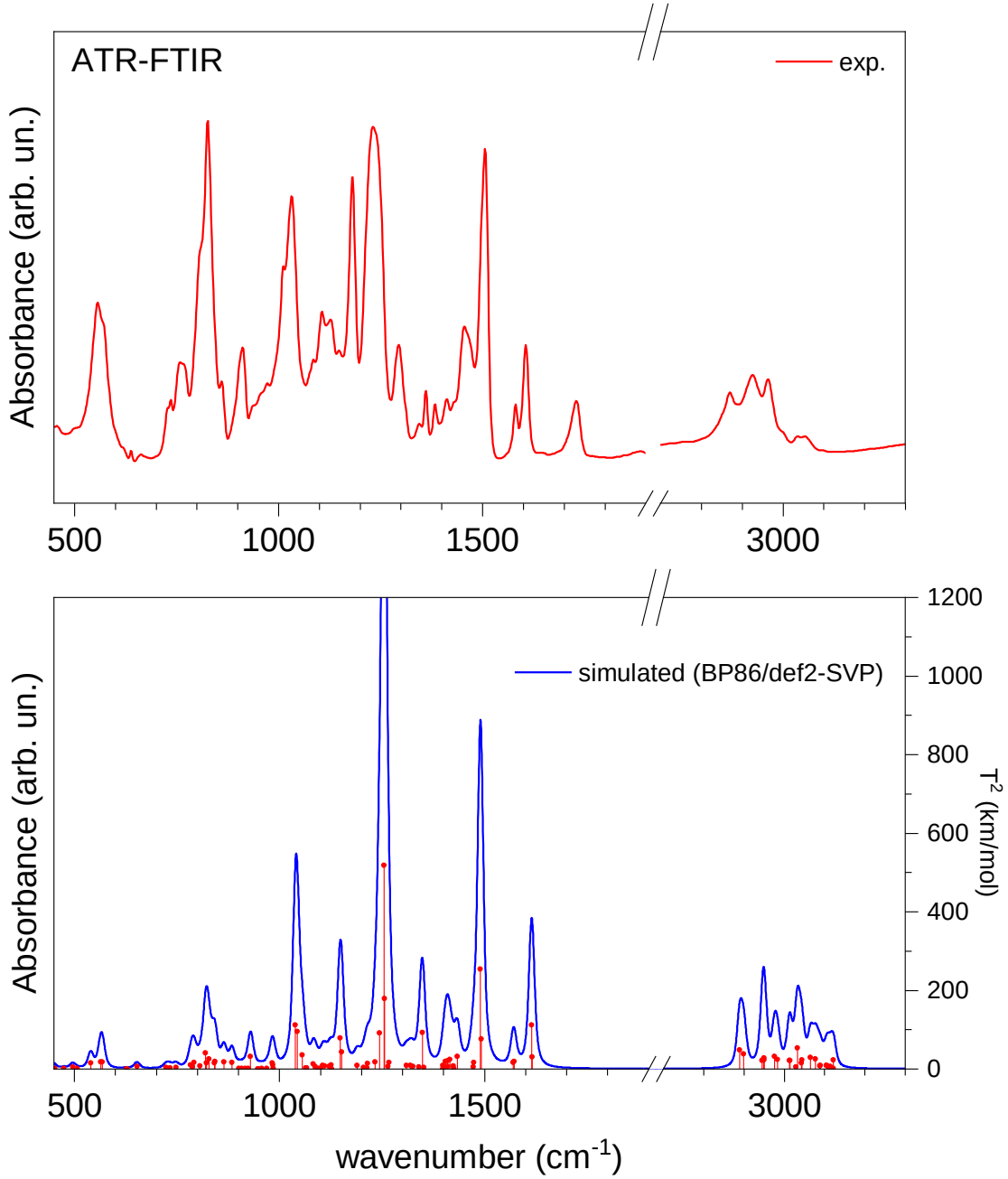
SU8-Basic unit

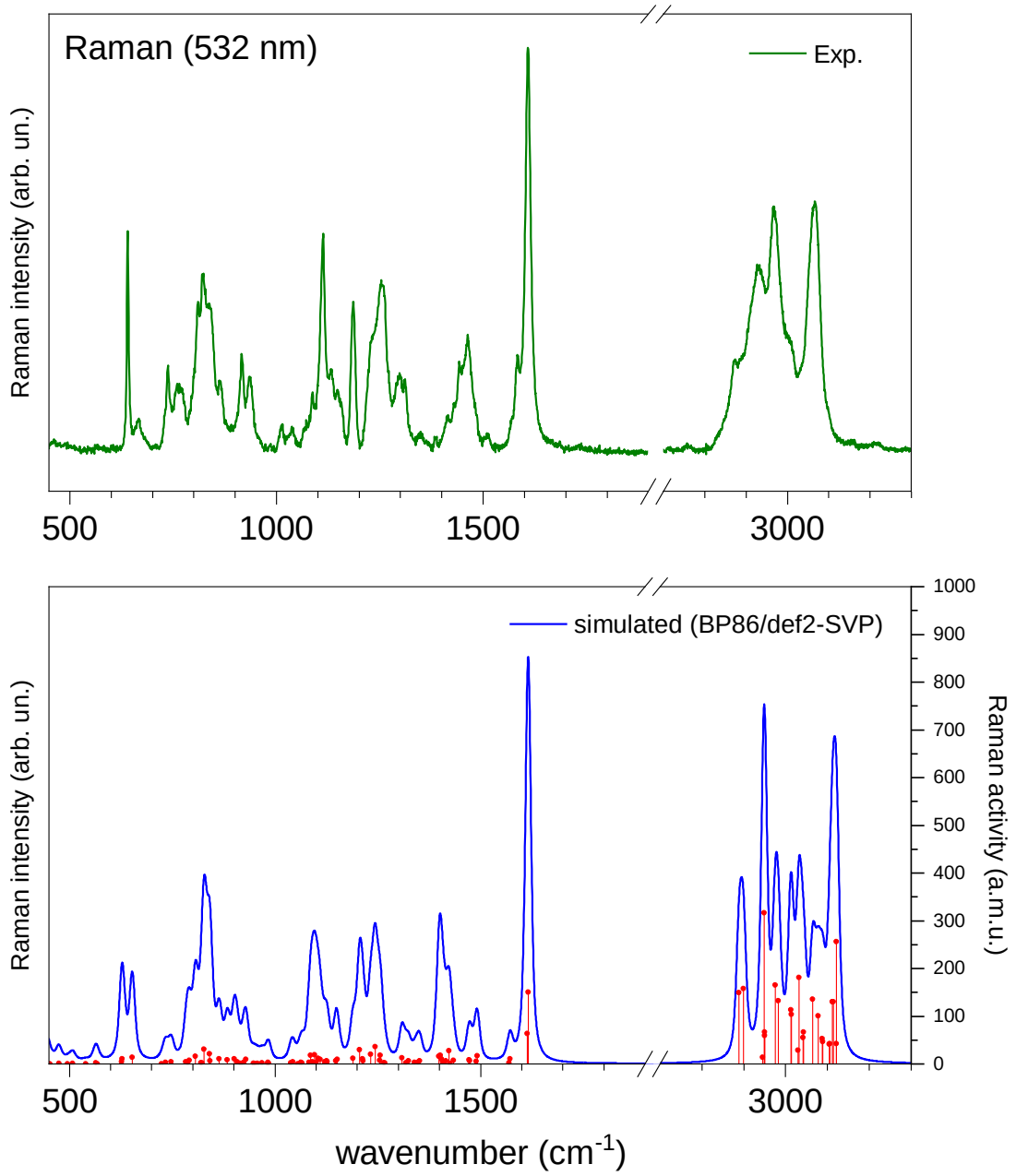






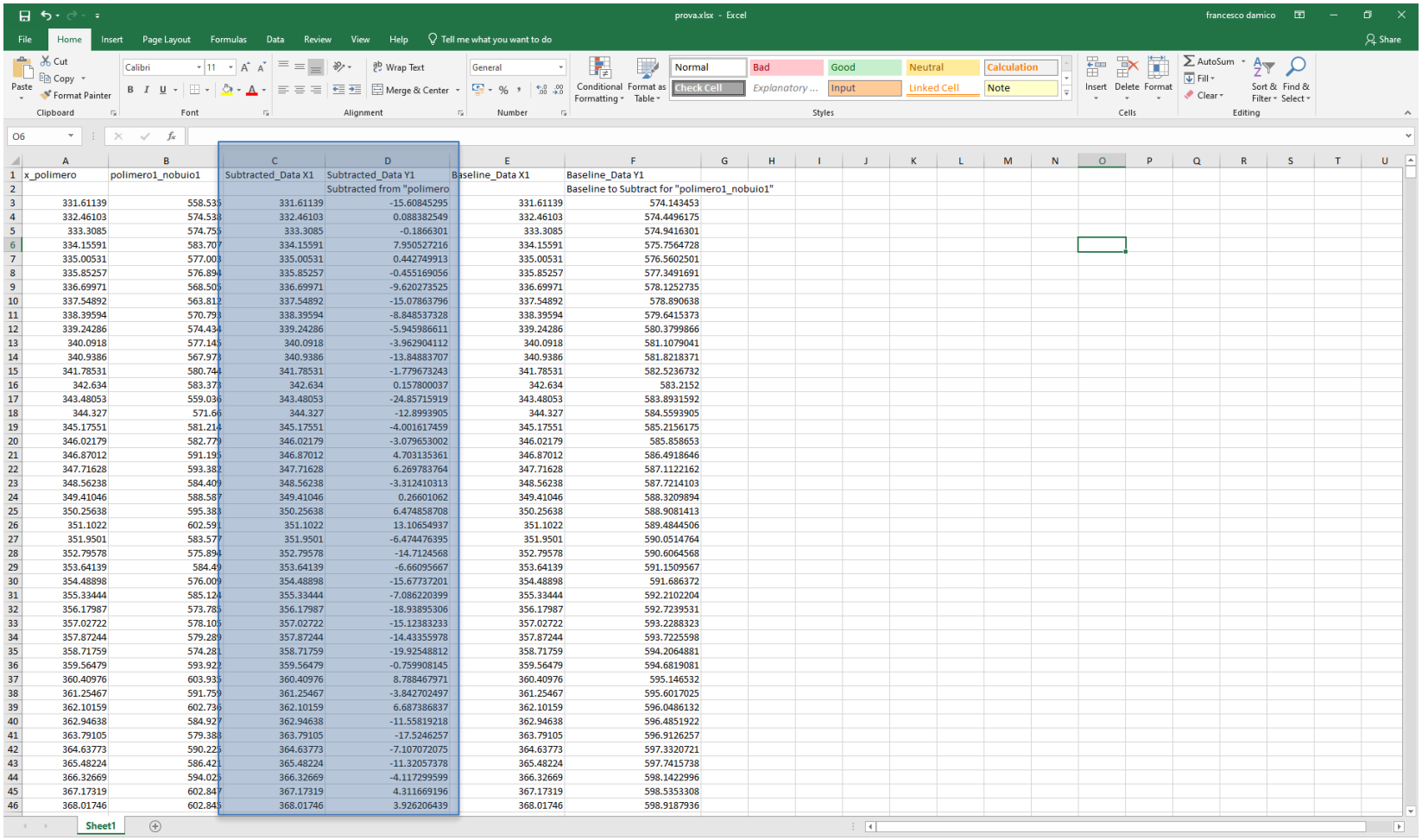

Raman
ATR-FTIR
Intensity
600
800
1000
1200
1400
1600
1800
2800
3000
3200
wavenumber (cm-1)


ATR-FTIR
exp.
Absorbance (arb. un.)
500
1000
1500
3000
simulated (BP86/def2-SVP)
Absorbance (arb. un.)
1200
1000
800
600
400
200
0
T² (km/mol)
500
1000
1500
3000
wavenumber (cm-1)


Raman (532 nm)
Exp.
Raman intensity (arb. un.)
500
1000
1500
3000
simulated (BP86/def2-SVP)
Raman intensity (arb. un.)
Raman activity (a.m.u.)
1000
900
800
700
600
500
400
300
200
100
0
500
1000
1500
3000
wavenumber (cm-1)

Analis dati

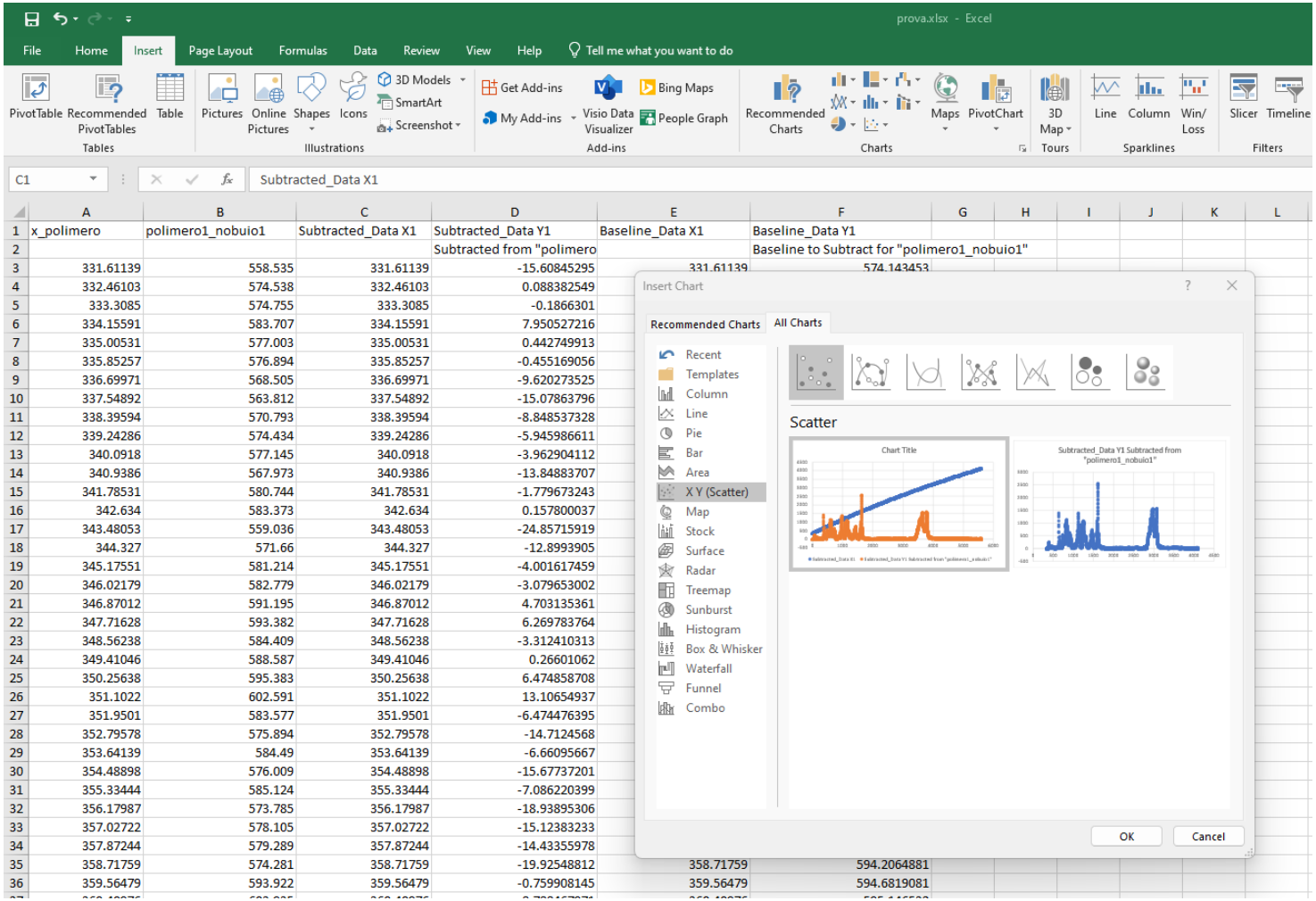
Creare uno spettro con Excel



	A	B	C	D	E	F
1	x_polimero	polimero1_nobuio1	Subtracted_Data X1	Subtracted_Data Y1	Baseline_Data X1	Baseline_Data Y1
2				Subtracted from "polimero		Baseline to Subtract for "polimero1_nobuio1"
3	331.61139	558.535	331.61139	-15.60845295	331.61139	574.143453
4	332.46103	574.538	332.46103	0.088382549	332.46103	574.4496175
5	333.3085	574.755	333.3085	-0.1866301	333.3085	574.9416301
6	334.15591	583.707	334.15591	7.950527216	334.15591	575.7564728
7	335.00531	577.003	335.00531	0.442749913	335.00531	576.5602501
8	335.85257	576.894	335.85257	-0.455169056	335.85257	577.3491691
9	336.69971	568.505	336.69971	-9.620273525	336.69971	578.1252735
10	337.54892	563.812	337.54892	-15.07863796	337.54892	578.890638
11	338.39594	570.793	338.39594	-8.848537328	338.39594	579.6415373
12	339.24286	574.434	339.24286	-5.945986611	339.24286	580.3799866
13	340.0918	577.145	340.0918	-3.962904112	340.0918	581.1079041
14	340.9386	567.973	340.9386	-13.84883707	340.9386	581.8218371
15	341.78531	580.744	341.78531	-1.779673243	341.78531	582.5236732
16	342.634	583.373	342.634	0.157800037	342.634	583.2152
17	343.48053	559.036	343.48053	-24.85715919	343.48053	583.8931592
18	344.327	571.66	344.327	-12.8993905	344.327	584.5593905
19	345.17551	581.214	345.17551	-4.001617459	345.17551	585.2156175
20	346.02179	582.779	346.02179	-3.079653002	346.02179	585.858653
21	346.87012	591.196	346.87012	4.703135361	346.87012	586.4918646
22	347.71628	593.382	347.71628	6.269783764	347.71628	587.1122162
23	348.56238	584.409	348.56238	-3.312410313	348.56238	587.7214103
24	349.41046	588.587	349.41046	0.26601062	349.41046	588.3209894
25	350.25638	595.383	350.25638	6.474858708	350.25638	588.9081413
26	351.1022	602.591	351.1022	13.10654937	351.1022	589.4844506
27	351.9501	583.577	351.9501	-6.474476395	351.9501	590.0514764
28	352.79578	575.894	352.79578	-14.7124568	352.79578	590.6064568
29	353.64139	584.49	353.64139	-6.66095667	353.64139	591.1509567
30	354.48898	576.009	354.48898	-15.67737201	354.48898	591.686372
31	355.33444	585.124	355.33444	-7.086220399	355.33444	592.2102204
32	356.17987	573.785	356.17987	-18.93895306	356.17987	592.7239531
33	357.02722	578.106	357.02722	-15.12383233	357.02722	593.2288323
34	357.87244	579.289	357.87244	-14.43355978	357.87244	593.7225598
35	358.71759	574.281	358.71759	-19.92548812	358.71759	594.2064881
36	359.56479	593.922	359.56479	-0.759908145	359.56479	594.6819081
37	360.40976	603.935	360.40976	8.788467971	360.40976	595.146532
38	361.25467	591.759	361.25467	-3.842702497	361.25467	595.6017025
39	362.10159	602.736	362.10159	6.687386837	362.10159	596.0486132
40	362.94638	584.927	362.94638	-11.55819218	362.94638	596.4851922
41	363.79105	579.388	363.79105	-17.5246257	363.79105	596.9126257
42	364.63773	590.225	364.63773	-7.107072075	364.63773	597.3320721
43	365.48224	586.421	365.48224	-11.32057378	365.48224	597.7415738
44	366.32669	594.025	366.32669	-4.117299599	366.32669	598.1422996
45	367.17319	602.847	367.17319	4.311669196	367.17319	598.5353308
46	368.01746	602.845	368.01746	3.926206439	368.01746	598.9187936

Analis dati

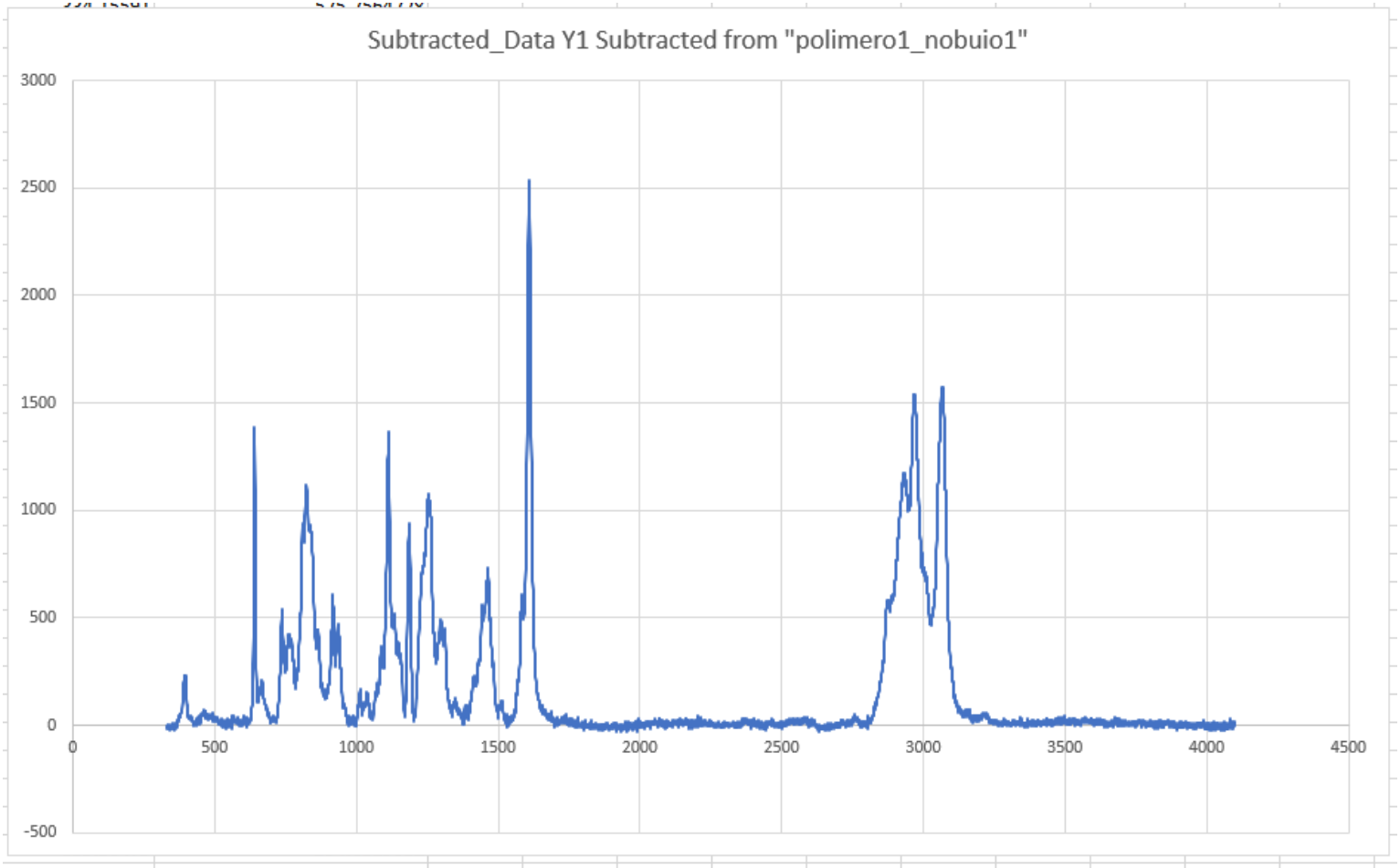
Creare uno spettro con Excel



	A	B	C	D	E	F
1	x_polimero	polimero1_nobuio1	Subtracted_Data X1	Subtracted_Data Y1	Baseline_Data X1	Baseline_Data Y1
2				Subtracted from "polimero		Baseline to Subtract for "polimero1_nobuio1"
3	331.61139	558.535	331.61139	-15.60845295	331.61139	574.143453
4	332.46103	574.538	332.46103	0.088382549		
5	333.3085	574.755	333.3085	-0.1866301		
6	334.15591	583.707	334.15591	7.950527216		
7	335.00531	577.003	335.00531	0.442749913		
8	335.85257	576.894	335.85257	-0.455169056		
9	336.69971	568.505	336.69971	-9.620273525		
10	337.54892	563.812	337.54892	-15.07863796		
11	338.39594	570.793	338.39594	-8.848537328		
12	339.24286	574.434	339.24286	-5.945986611		
13	340.0918	577.145	340.0918	-3.962904112		
14	340.9386	567.973	340.9386	-13.84883707		
15	341.78531	580.744	341.78531	-1.779673243		
16	342.634	583.373	342.634	0.157800037		
17	343.48053	559.036	343.48053	-24.85715919		
18	344.327	571.66	344.327	-12.8993905		
19	345.17551	581.214	345.17551	-4.001617459		
20	346.02179	582.779	346.02179	-3.079653002		
21	346.87012	591.195	346.87012	4.703135361		
22	347.71628	593.382	347.71628	6.269783764		
23	348.56238	584.409	348.56238	-3.312410313		
24	349.41046	588.587	349.41046	0.26601062		
25	350.25638	595.383	350.25638	6.474858708		
26	351.1022	602.591	351.1022	13.10654937		
27	351.9501	583.577	351.9501	-6.474476395		
28	352.79578	575.894	352.79578	-14.7124568		
29	353.64139	584.49	353.64139	-6.66095667		
30	354.48898	576.009	354.48898	-15.67737201		
31	355.33444	585.124	355.33444	-7.086220399		
32	356.17987	573.785	356.17987	-18.93895306		
33	357.02722	578.105	357.02722	-15.12383233		
34	357.87244	579.289	357.87244	-14.43355978		
35	358.71759	574.281	358.71759	-19.92548812	358.71759	594.2064881
36	359.56479	593.922	359.56479	-0.759908145	359.56479	594.6819081

Analis dati

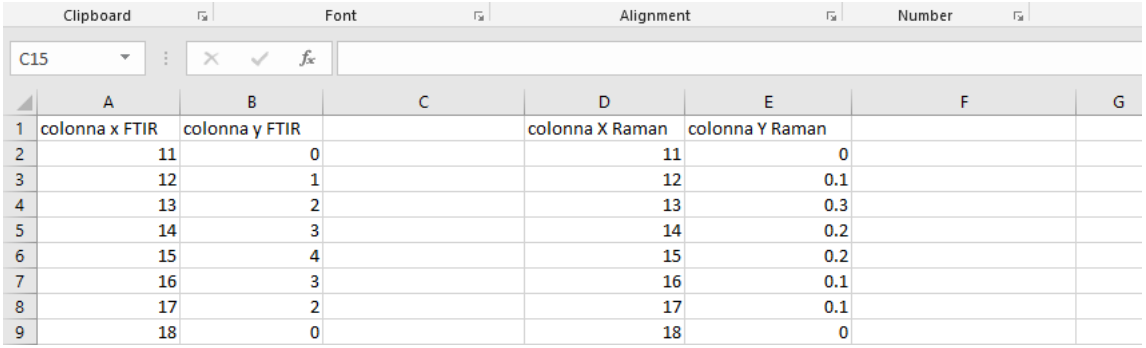
Creare uno spettro con Excel



Analisi dati

Creare le colonne su excel

Normalizzare e graficare gli spettri



Clipboard | Font | Alignment | Number

C15

	A	B	C	D	E	F	G
1	colonna x FTIR	colonna y FTIR		colonna X Raman	colonna Y Raman		
2	11	0		11	0		
3	12	1		12	0.1		
4	13	2		13	0.3		
5	14	3		14	0.2		
6	15	4		15	0.2		
7	16	3		16	0.1		
8	17	2		17	0.1		
9	18	0		18	0		

Analisi dati

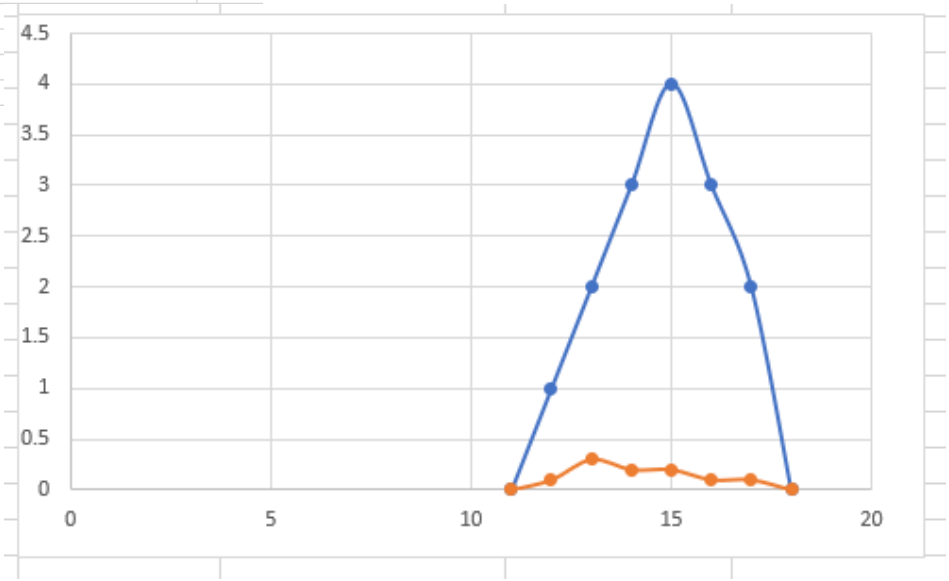
Creare le colonne su excel

Normalizzare e graficare gli spettri

Clipboard | Font | Alignment | Number

C15

	A	B	C	D	E	F	G
1	colonna x FTIR	colonna y FTIR		colonna X Raman	colonna Y Raman		
2	11	0		11	0		
3	12	1		12	0.1		
4	13	2		13	0.3		
5	14	3		14	0.2		
6	15	4		15	0.2		
7	16	3		16	0.1		
8	17	2		17	0.1		
9	18	0		18	0		



Analisi dati

Creare le colonne su excel

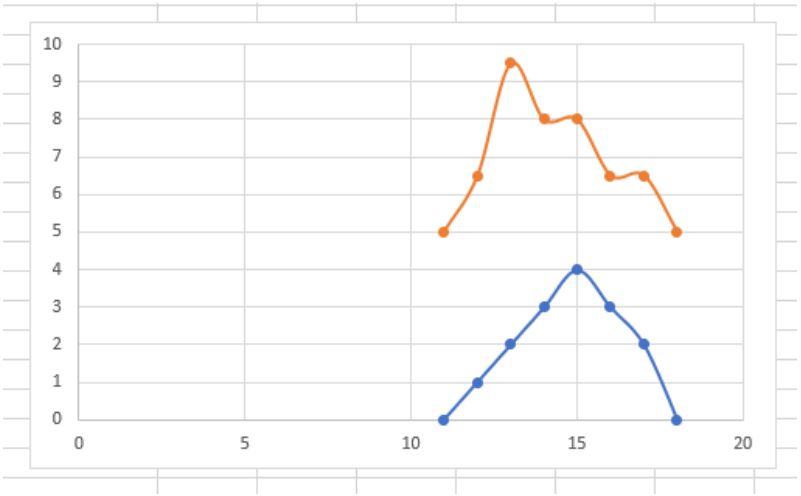
Normalizzare e graficare gli spettri

SUM | =0+1*B2

	A	B	C	D	E	F
1	colonna x FTIR	colonna y FTIR	colonna y FTIR corretta	colonna X Raman	colonna Y Raman	colonna Y Raman corretta
2	11	0	=0+1*B2	11	0	1
3	12	1	1	12	0.1	2
4	13	2	2	13	0.3	4
5	14	3	3	14	0.2	3
6	15	4	4	15	0.2	3
7	16	3	3	16	0.1	2
8	17	2	2	17	0.1	2
9	18	0	0	18	0	1

SUM | =5+15*E2

	A	B	C	D	E	F
1	colonna x FTIR	colonna y FTIR	colonna y FTIR corretta	colonna X Raman	colonna Y Raman	colonna Y Raman corretta
2	11	0	0	11	0	=5+15*E2
3	12	1	1	12	0.1	6.5
4	13	2	2	13	0.3	9.5
5	14	3	3	14	0.2	8
6	15	4	4	15	0.2	8
7	16	3	3	16	0.1	6.5
8	17	2	2	17	0.1	6.5
9	18	0	0	18	0	5



Thank you

Contact details