

Spectroscopie-générale

- Atkins « 8th edition », pg 432
- Chapitre 13 « MOLECULAR SPECTROSCOPY 1: ROTATIONAL AND VIBRATIONAL SPECTRA”
- 13.2 « The intensities of spectral lines »
- Concepts importante :
- -Absorption / Transmission

$$T = \frac{I}{I_0} \quad [13.1]$$

$$I = I_0 10^{-\epsilon [J] l} \quad (13.2)$$

$$A = \epsilon [J] l \quad (13.4) \quad A = \log \frac{I_0}{I} \quad \text{or} \quad A = -\log T \quad [13.3]$$

Spectroscopie-Rotation

1.
$$E_J = J(J + 1) \frac{\hbar^2}{2I} \quad J = 0, 1, 2, \dots$$

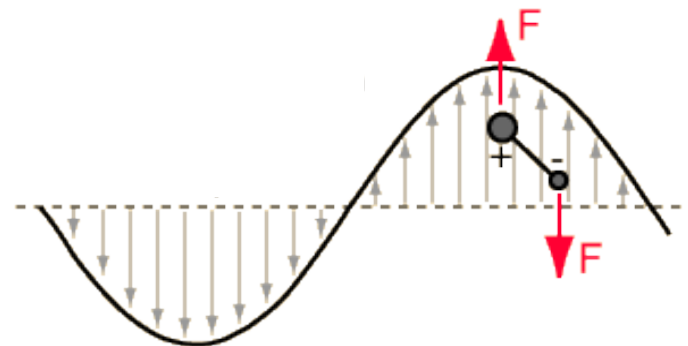
(Atkins: pg 304 sec. 9.7b)

2. Atkins pg 441 spectres de rotation pure.

- moment d'inertie (I)
- constante de rotation (B)
- les règles de sélection
- spectres

3. Causes:

- Dipôle électrique dans champ électrique
- Collision



$$\Delta J = +/\!-1$$

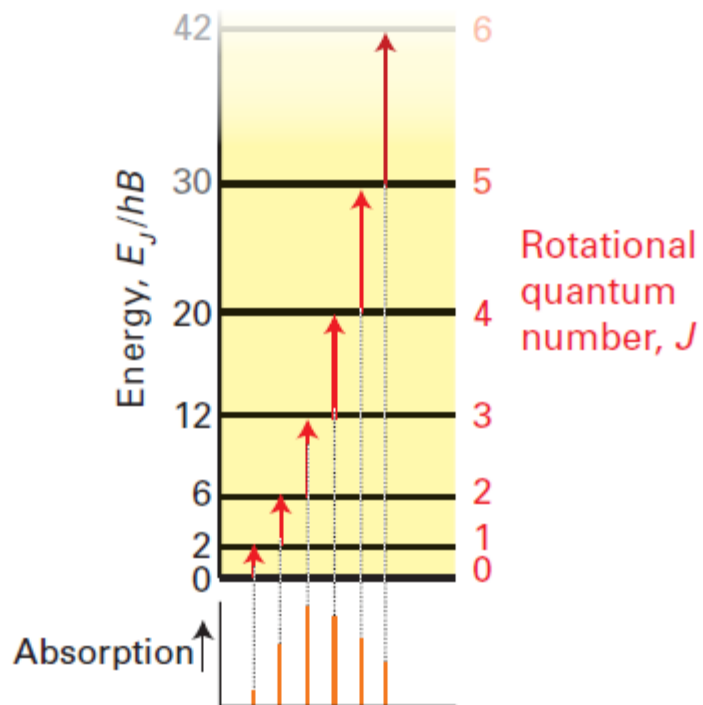


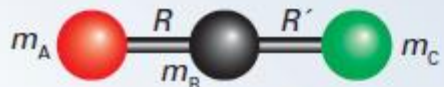
Fig. 19.12 The allowed rotational transitions (shown as absorptions) for a linear molecule.

1. Diatomic molecules

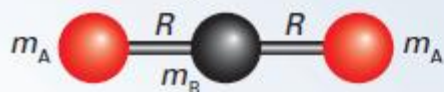


$$I = \mu R^2 \quad \mu = \frac{m_A m_B}{m}$$

2. Triatomic linear rotors

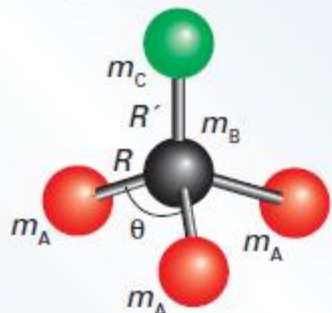


$$I = m_A R^2 + m_C R'^2 - \frac{(m_A R - m_C R')^2}{m}$$



$$I = 2m_A R^2$$

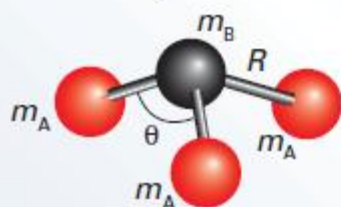
3. Symmetric rotors



$$I_{\parallel} = 2m_A(1 - \cos \theta)R^2$$

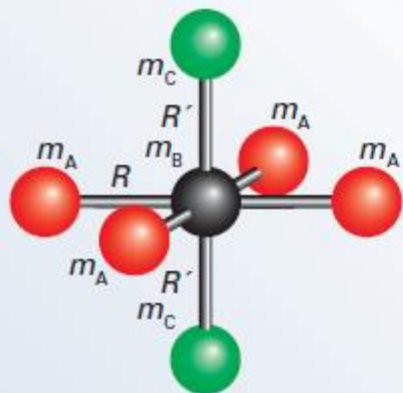
$$I_{\perp} = m_A(1 - \cos \theta)R^2 + \frac{m_A}{m} (m_B + m_C)(1 + 2 \cos \theta)R^2$$

$$+ \frac{m_C}{m} \{ (3m_A + m_B)R' + 6m_A R [\frac{1}{3}(1 + 2 \cos \theta)]^{1/2} \} R'$$



$$I_{\parallel} = 2m_A(1 - \cos \theta)R^2$$

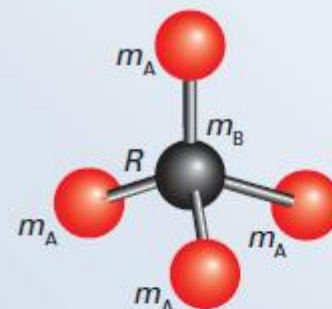
$$I_{\perp} = m_A(1 - \cos \theta)R^2 + \frac{m_A}{m} (m_B + m_C)(1 + 2 \cos \theta)R^2$$



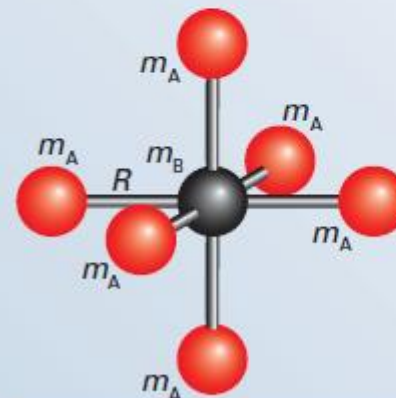
$$I_{\parallel} = 4m_A R^2$$

$$I_{\perp} = 2m_A R^2 + 2m_C R'^2$$

4. Spherical rotors



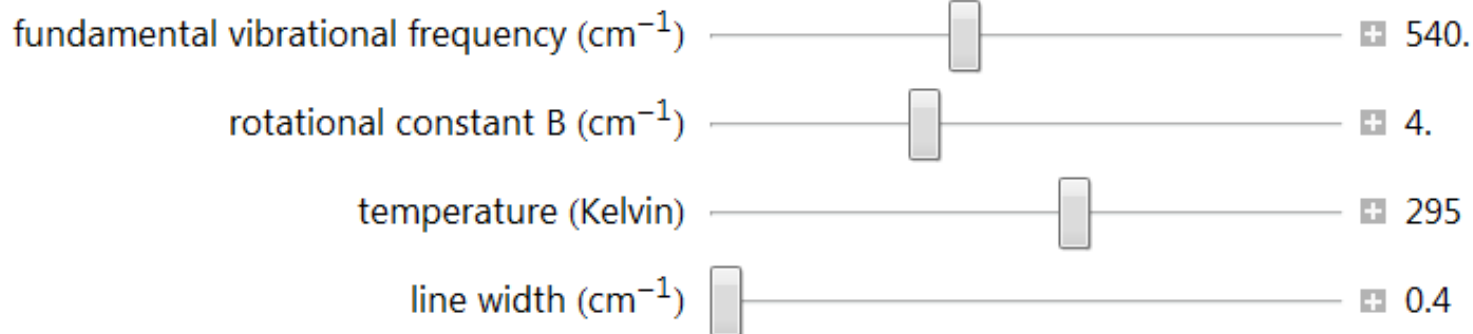
$$I = \frac{8}{3} m_A R^2$$



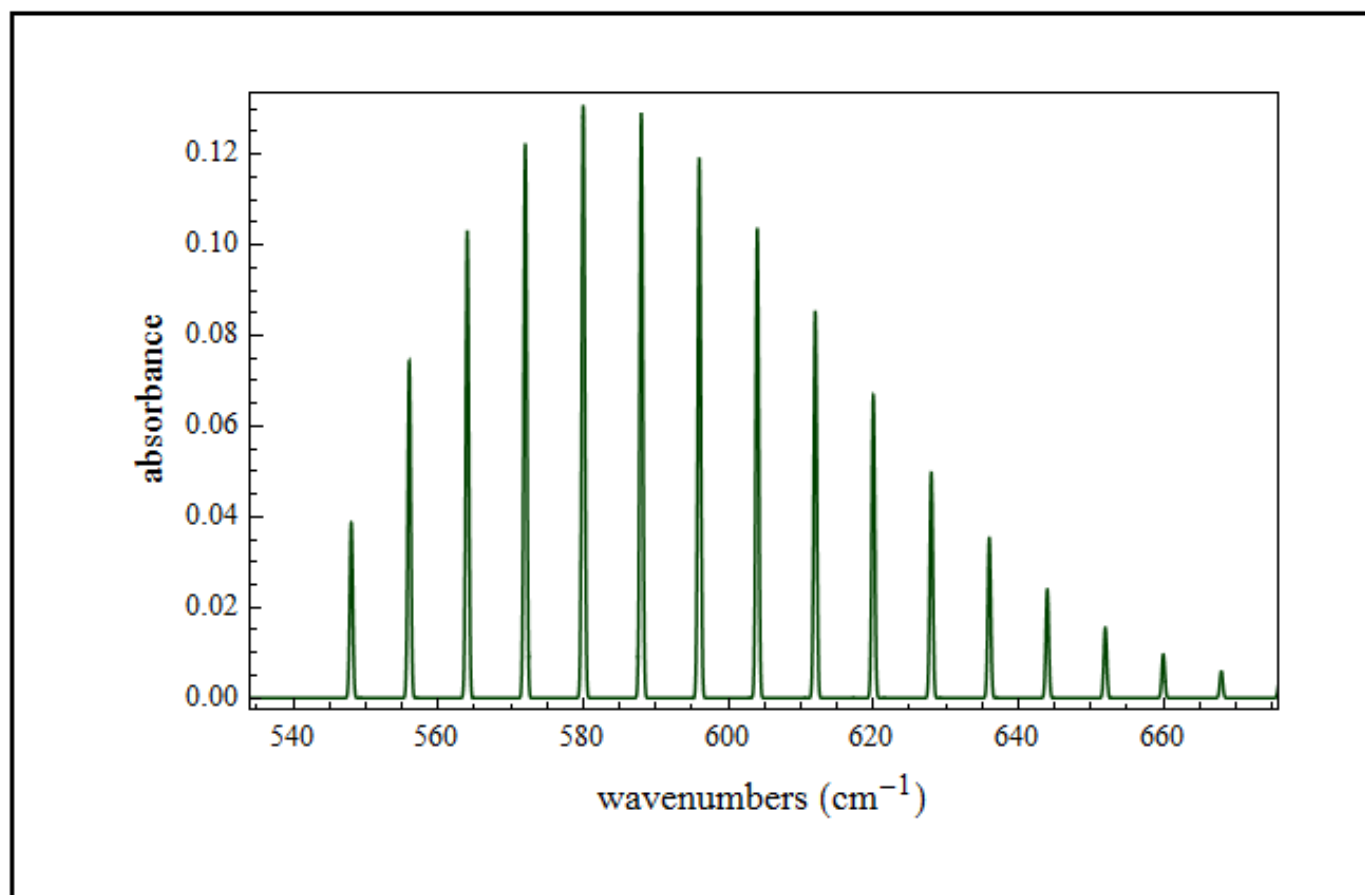
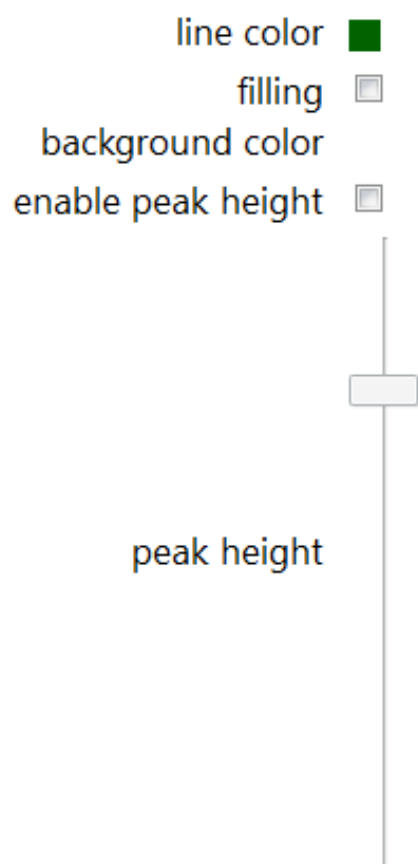
$$I = 4m_A R^2$$

* In each case, m is the total mass of the molecule.

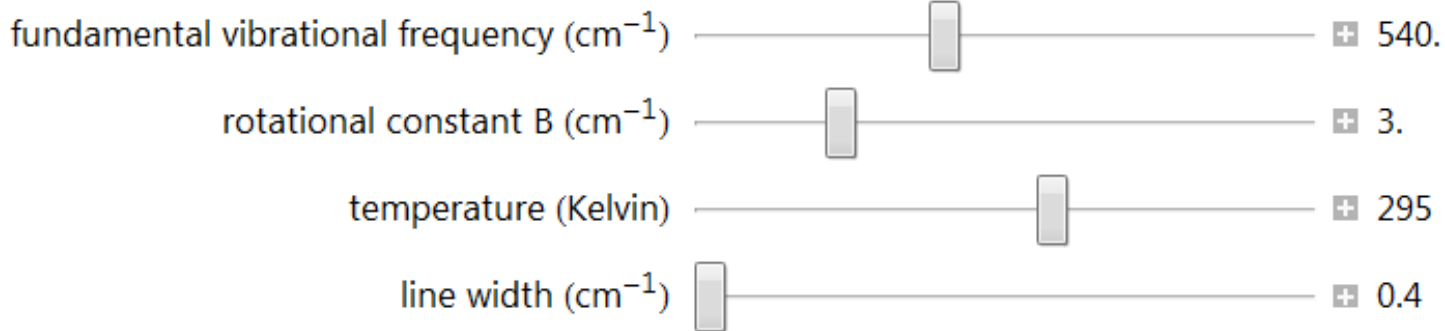
parameters



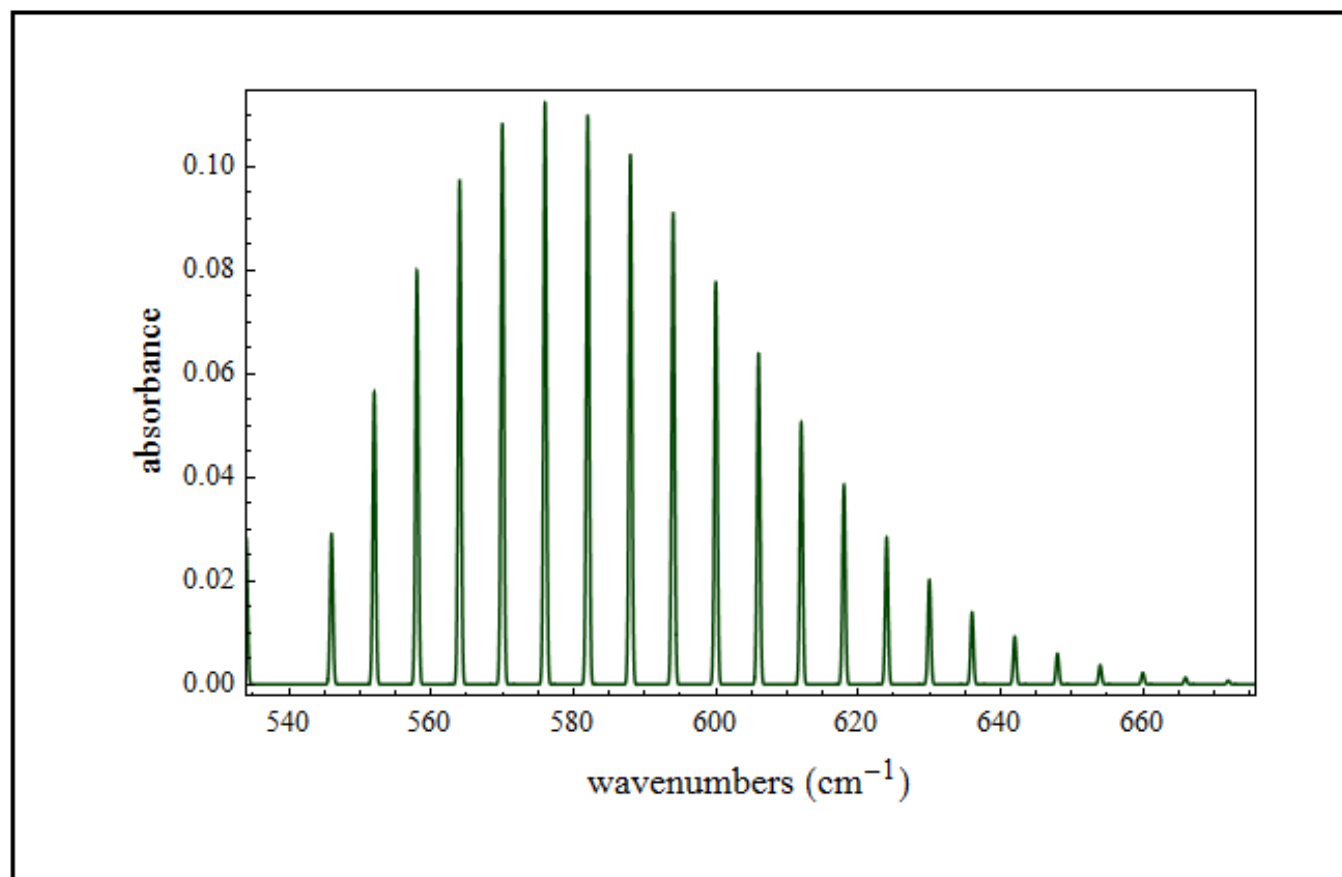
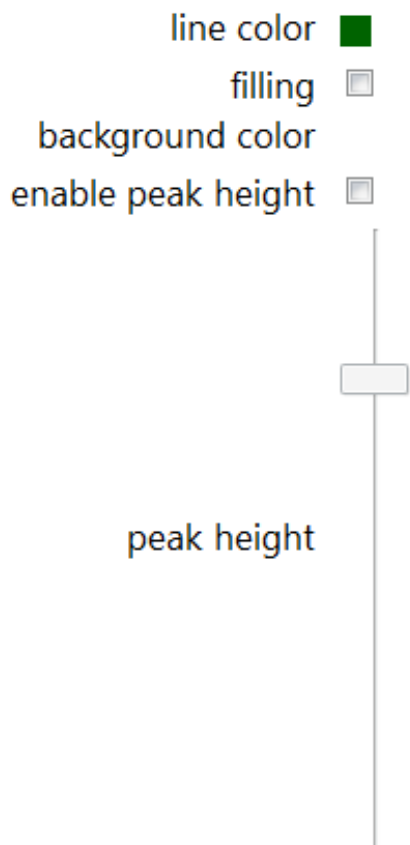
spectrum display



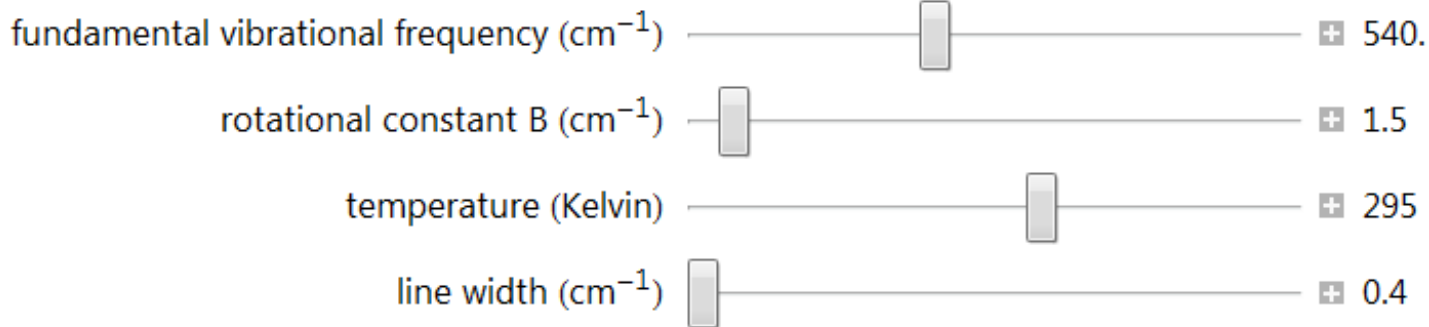
parameters



spectrum display



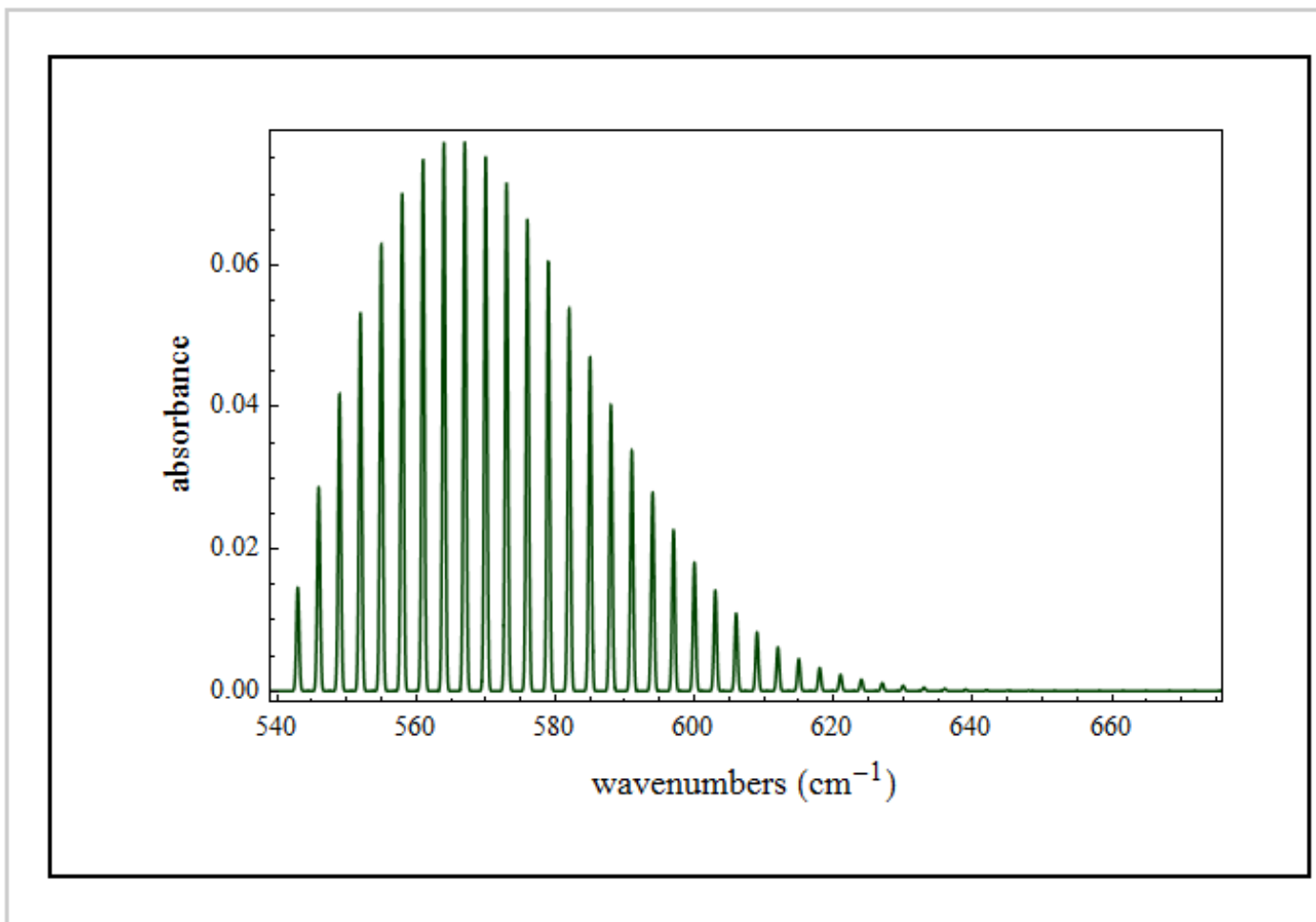
parameters



spectrum display

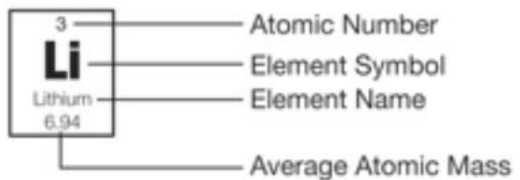
- line color
- filling
- background color
- enable peak height

peak height



The Periodic Table of the Elements

1 H Hydrogen 1.01																	2 He Helium 4.00
3 Li Lithium 6.94	4 Be Beryllium 9.01																
11 Na Sodium 22.99	12 Mg Magnesium 24.31																
19 K Potassium 39.10	20 Ca Calcium 40.08	21 Sc Scandium 44.96	22 Ti Titanium 47.87	23 V Vanadium 50.94	24 Cr Chromium 52.00	25 Mn Manganese 54.94	26 Fe Iron 55.85	27 Co Cobalt 58.93	28 Ni Nickel 58.69	29 Cu Copper 63.55	30 Zn Zinc 65.39	31 Ga Gallium 69.72	32 Ge Germanium 72.61	33 As Arsenic 74.92	34 Se Selenium 78.96	35 Br Bromine 79.90	36 Kr Krypton 83.80
37 Rb Rubidium 85.47	38 Sr Strontium 87.62	39 Y Yttrium 88.91	40 Zr Zirconium 91.22	41 Nb Niobium 92.91	42 Mo Molybdenum 95.94	43 Tc Technetium (98)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.91	46 Pd Palladium 106.42	47 Ag Silver 107.87	48 Cd Cadmium 112.41	49 In Indium 114.82	50 Sn Tin 118.71	51 Sb Antimony 121.76	52 Te Tellurium 127.60	53 I Iodine 126.90	54 Xe Xenon 131.29
55 Cs Cesium 132.91	56 Ba Barium 137.33	57 La Lanthanum 138.91	72 Hf Hafnium 178.49	73 Ta Tantalum 180.95	74 W Tungsten 183.84	75 Re Rhenium 186.21	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.97	80 Hg Mercury 200.59	81 Tl Thallium 204.38	82 Pb Lead 207.2	83 Bi Bismuth 208.98	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)
87 Fr Francium (223)	88 Ra Radium (226)	89 Ac Actinium (227)	104 Rf Rutherfordium 178.49	105 Db Dubnium (262)	106 Sg Seaborgium (266)	107 Bh Bohrium (264)	108 Hs Hassium (269)	109 Mt Meitnerium (268)	110 Ds Darmstadtium (281)	111 Rg Roentgenium (272)	112 Cn Copernicium (285)						



58 Ce Cerium 140.12	59 Pr Praseodymium 140.91	60 Nd Neodymium 144.24	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.96	64 Gd Gadolinium 157.25	65 Tb Terbium 158.93	66 Dy Dysprosium 162.50	67 Ho Holmium 164.93	68 Er Erbium 167.26	69 Tm Thulium 168.93	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.97
90 Th Thorium 232.04	91 Pa Protactinium 231.04	92 U Uranium 238.03	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium 168.93	102 No Nobelium (259)	103 Lr Lawrencium (262)