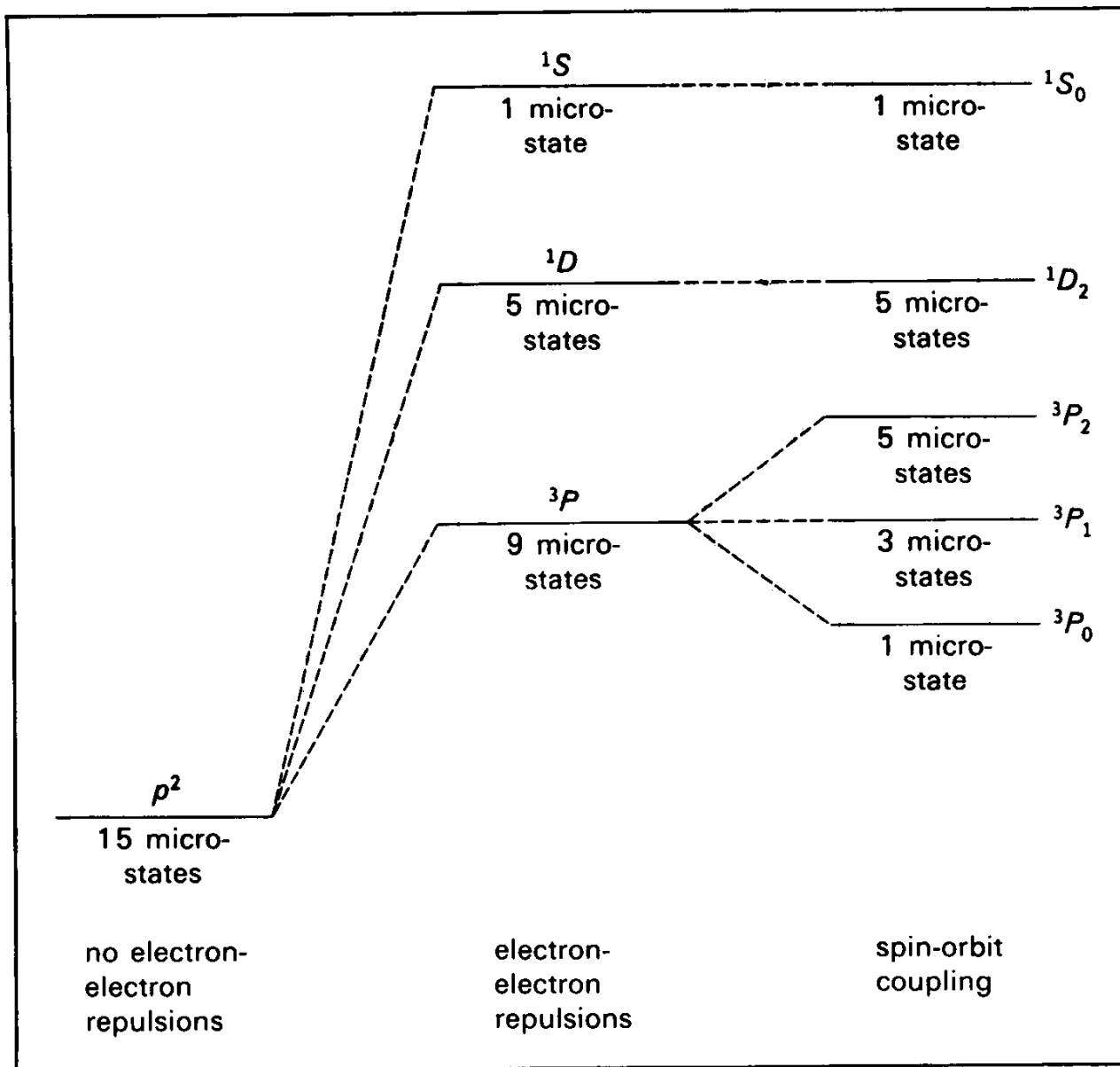


Regole di Hund per le energie dei termini

1. Il termine con la più elevata molteplicità di spin ha l'energia minore.
2. Se due o più termini hanno la stessa molteplicità di spin (e.g. 3F e 3P), il termine con il più alto valore di L ha energia minore (e.g. 3F ha energia inferiore a 3P). In realtà questa seconda regola funziona bene solo per trovare il **ground term**.
3. Per termini con la stessa molteplicità di spin e lo stesso valore di L (e.g. 3P_0 e 3P_1) **se il sotto-livello è meno che mezzo pieno** (e.g. p^2) il livello più basso in energia è quello con il più piccolo valore di J , mentre **se il sotto-livello è più che mezzo pieno** (e.g. p^4) il livello più stabile è quello con il più alto valore di J . Se il sotto-livello è mezzo pieno con la massima molteplicità di spin (e.g. p^3 con $S = 3/2$), L deve essere 0, e $J = S$ (**serie di Clebsch-Gordan**).

numero di microstati per x
elettroni in un guscio con
numero quantico angolare l

$$= \frac{[2(2l + 1)]!}{x! \times [2(2l + 1) - x]!}$$

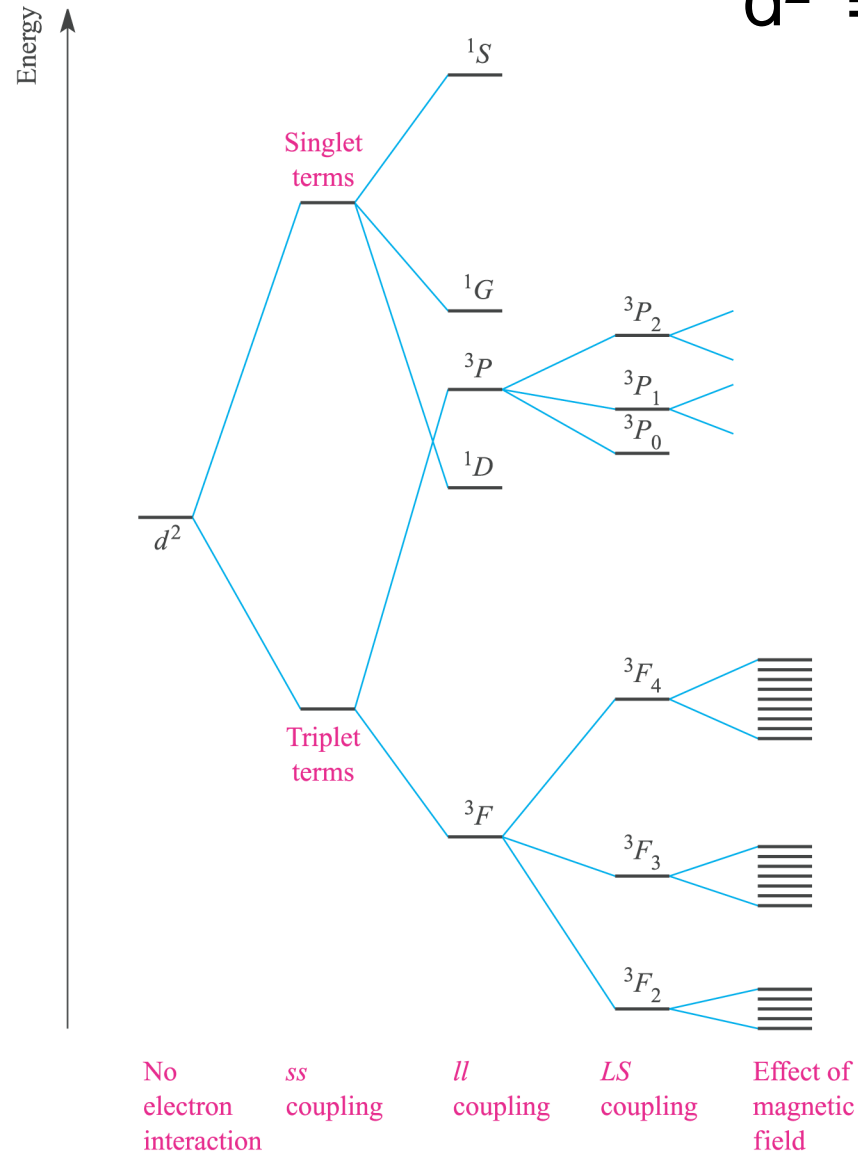


p^3
 $4S, 2P, 2D$

Accoppiamento di Russell-Saunders

$d^2 = 45$ microstati

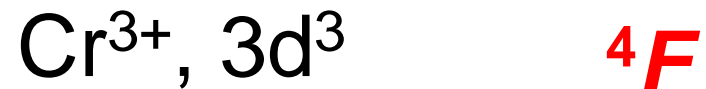
Ti^{2+}



d^2

Term	Number of states
1G	$9 \times 1 = 9$
3F	$7 \times 3 = 21$
1D	$5 \times 1 = 5$
3P	$3 \times 3 = 9$
1S	$1 \times 1 = 1$
Total:	45

Definizione del *ground term* secondo le regole di Hund



Parametri di Racah

per il calcolo parametrizzato della repulsione inter-elettronica in ogni termine di una **configurazione elettronica d^n** (cioè delle energie dei termini). Per d^2 :

$$E(^1S) = A + 14B + 7C$$

$$E(^1G) = A + 4B + 2C$$

$$E(^1D) = A - 3B + 2C$$

$$E(^3P) = A + 7B$$

$$E(^3F) = A - 8B$$

$$C > 5B$$

$$^3F < ^3P < ^1D < ^1G < ^1S$$

$$C < 5B$$

$$^3F < ^1D < ^3P < ^1G < ^1S$$

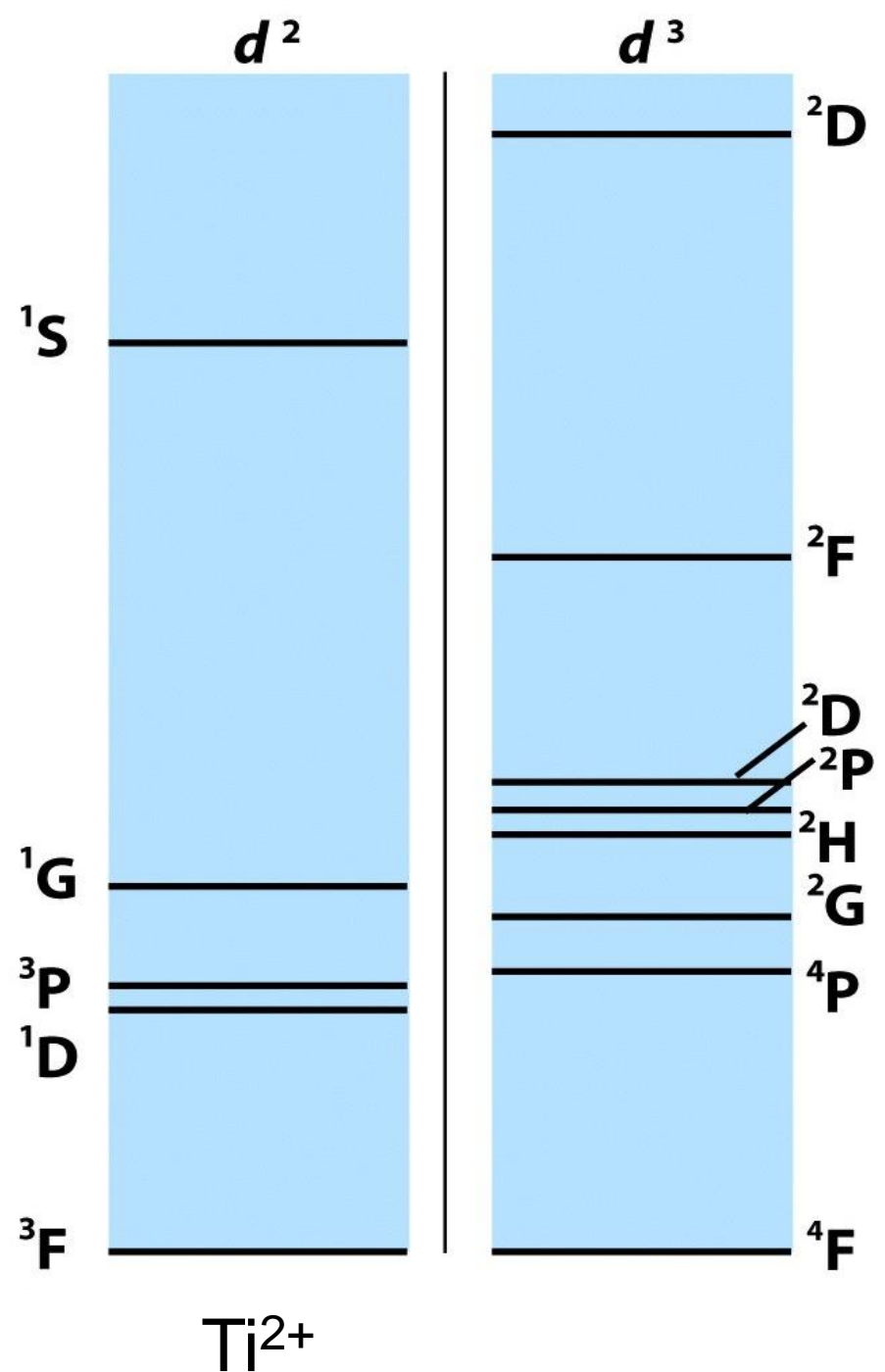
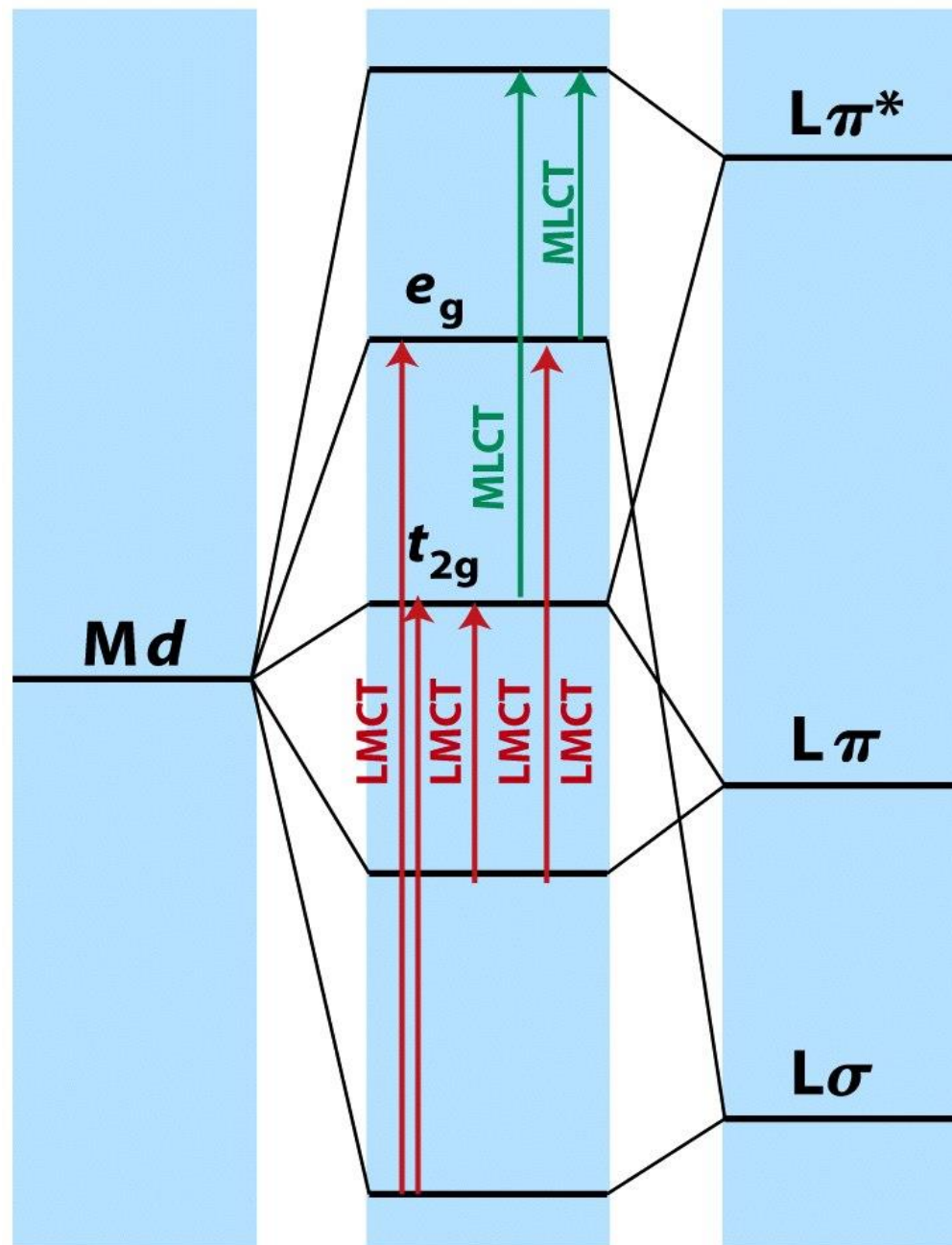


Table 19.6 Racah parameters for some *d*-block ions*

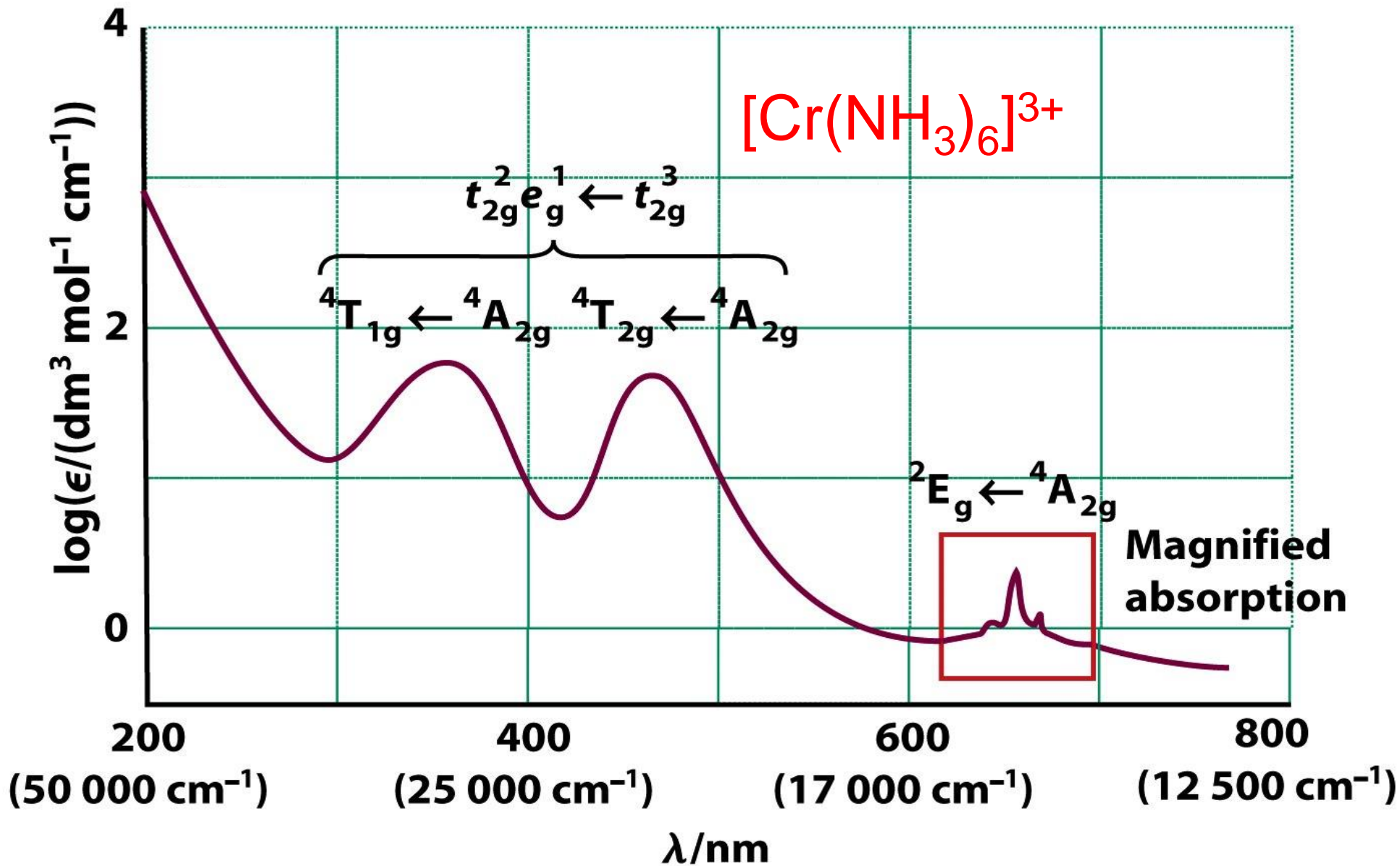
	1+	2+	3+	4+
Ti		720 (3.7)		
V		765 (3.9)	860 (4.8)	
Cr		830 (4.1)	1030 (3.7)	1040 (4.1)
Mn		960 (3.5)	1130 (3.2)	
Fe		1060 (4.1)		
Co		1120 (3.9)		
Ni		1080 (4.5)		
Cu	1220 (4.0)	1240 (3.8)		

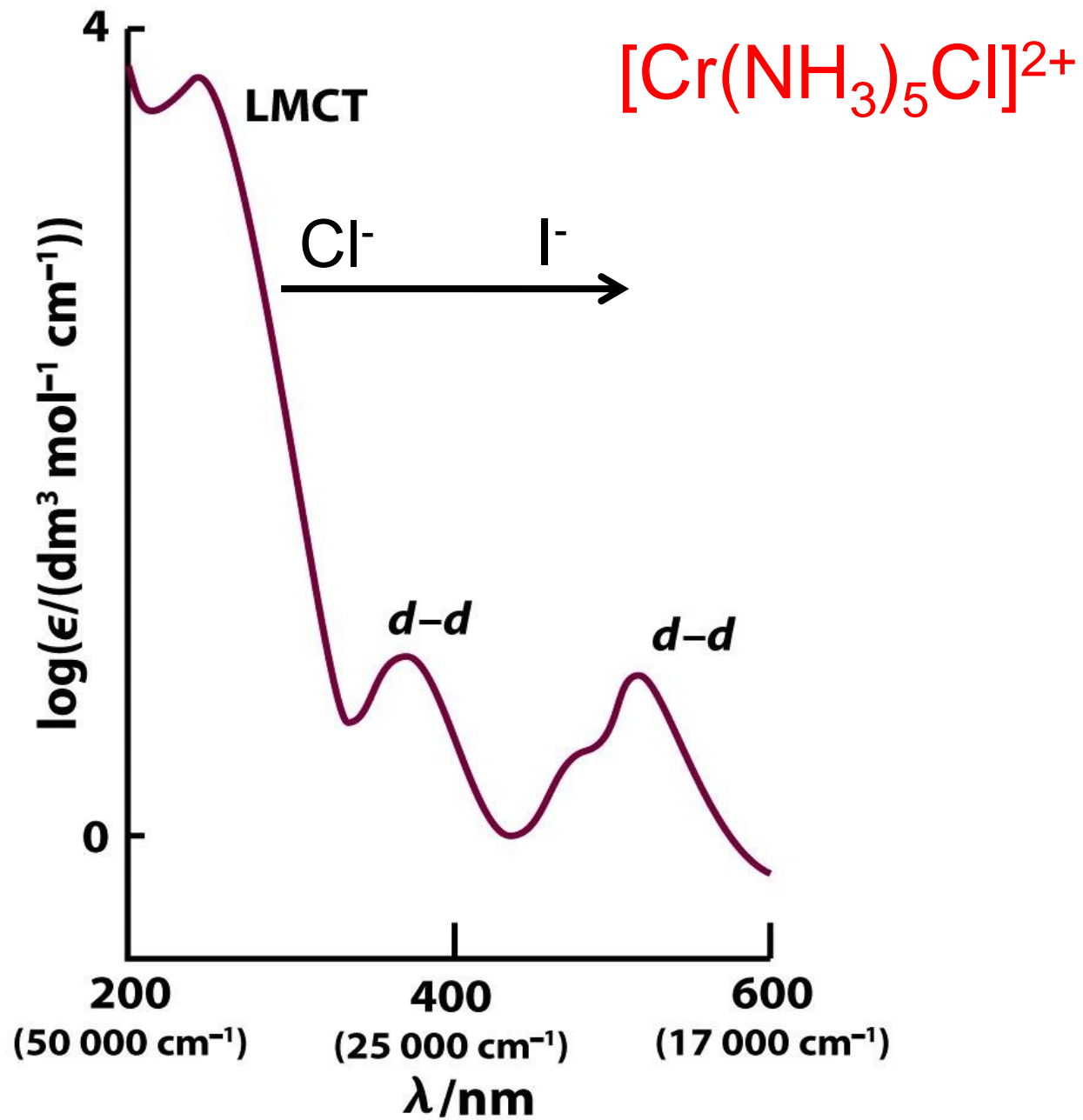
* The table gives the *B* parameter in cm^{-1} with the value of C/B in parentheses.



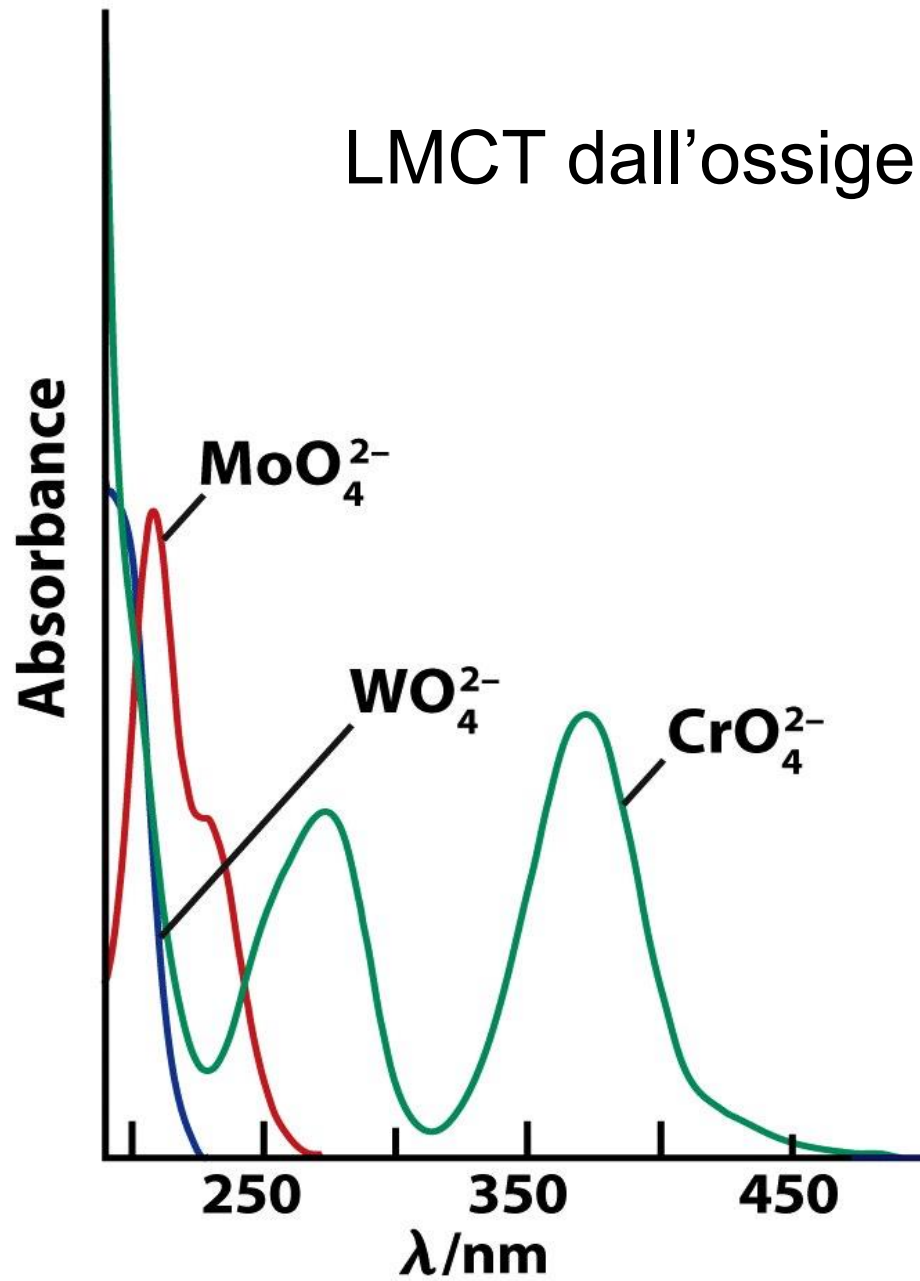
Regole di selezione e intensità delle transizioni elettroniche

Band type	$\epsilon_{\max}/$ ($\text{dm}^3 \text{ mol}^{-1} \text{ cm}^{-1}$)
Spin-forbidden	< 1
Laporte-forbidden <i>d-d</i>	20–100
Laporte-allowed <i>d-d</i>	<i>ca</i> 250
Symmetry-allowed (e.g. CT)	1000–50 000

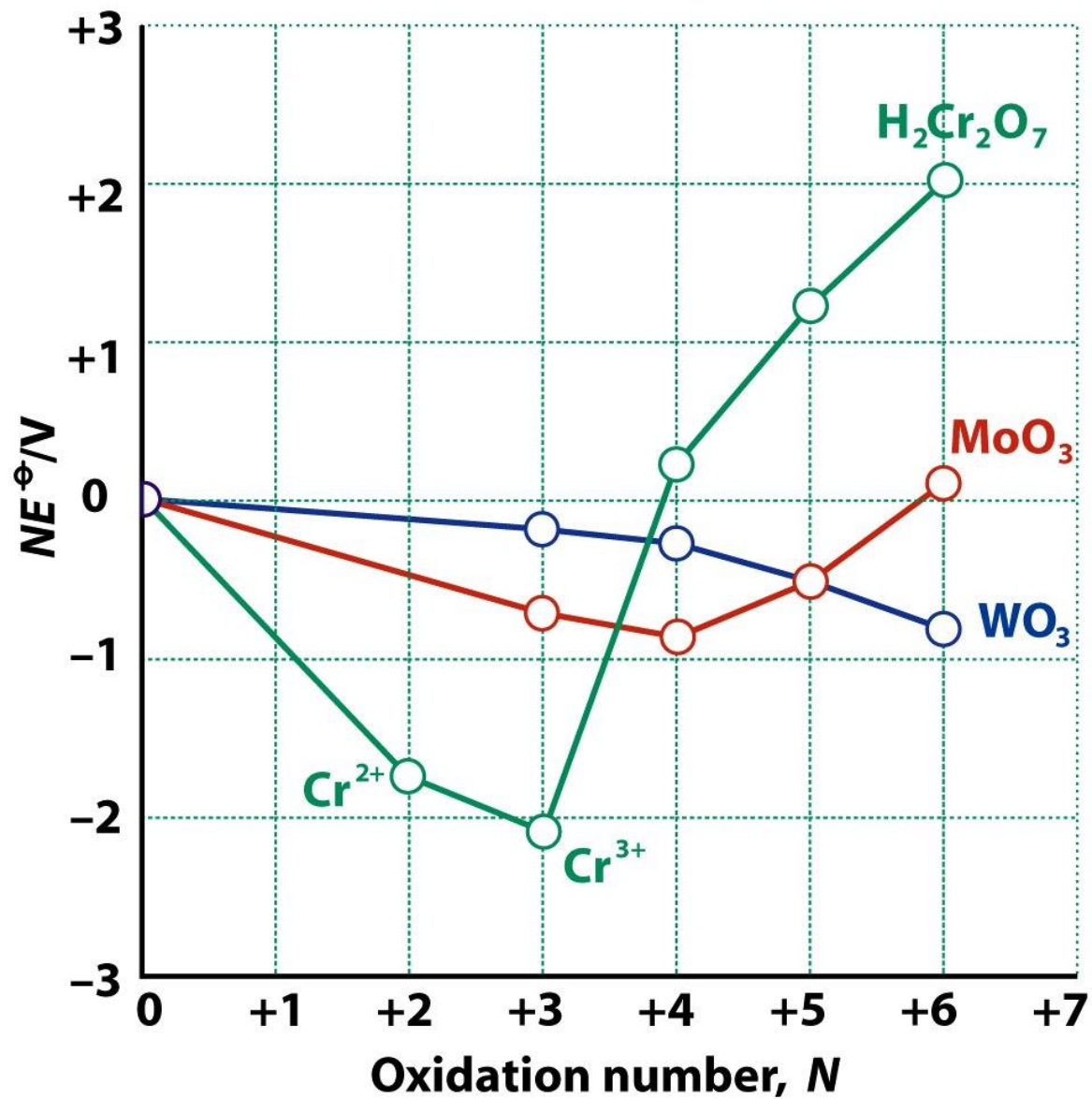


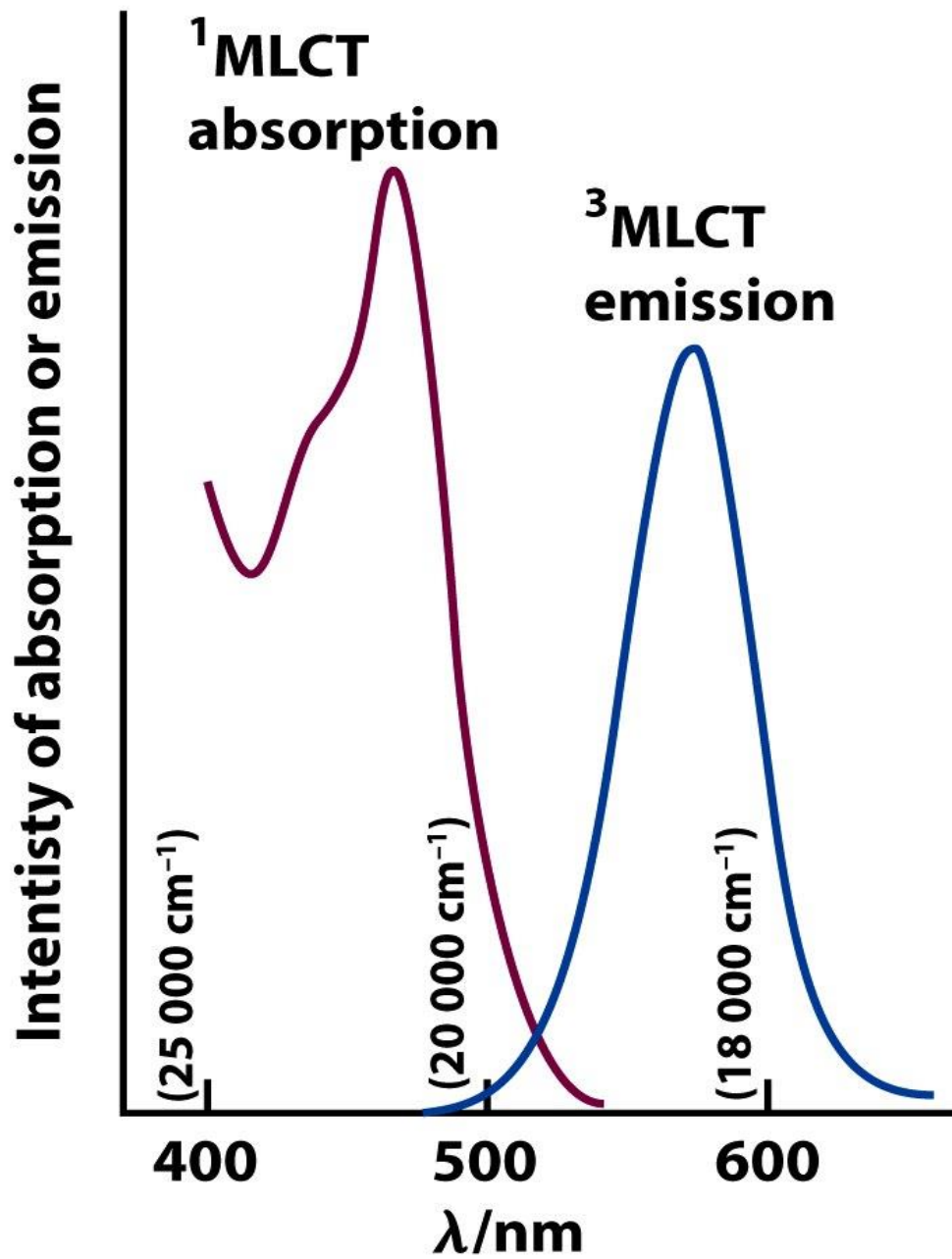
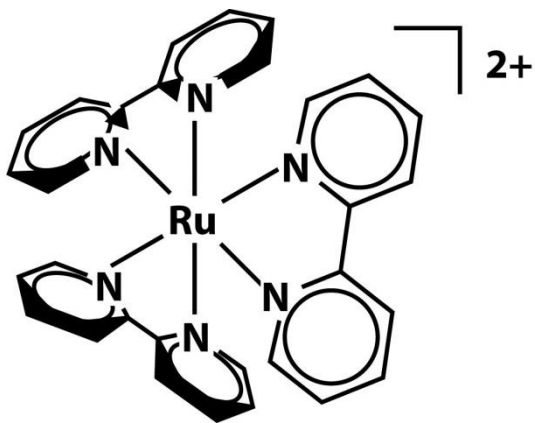


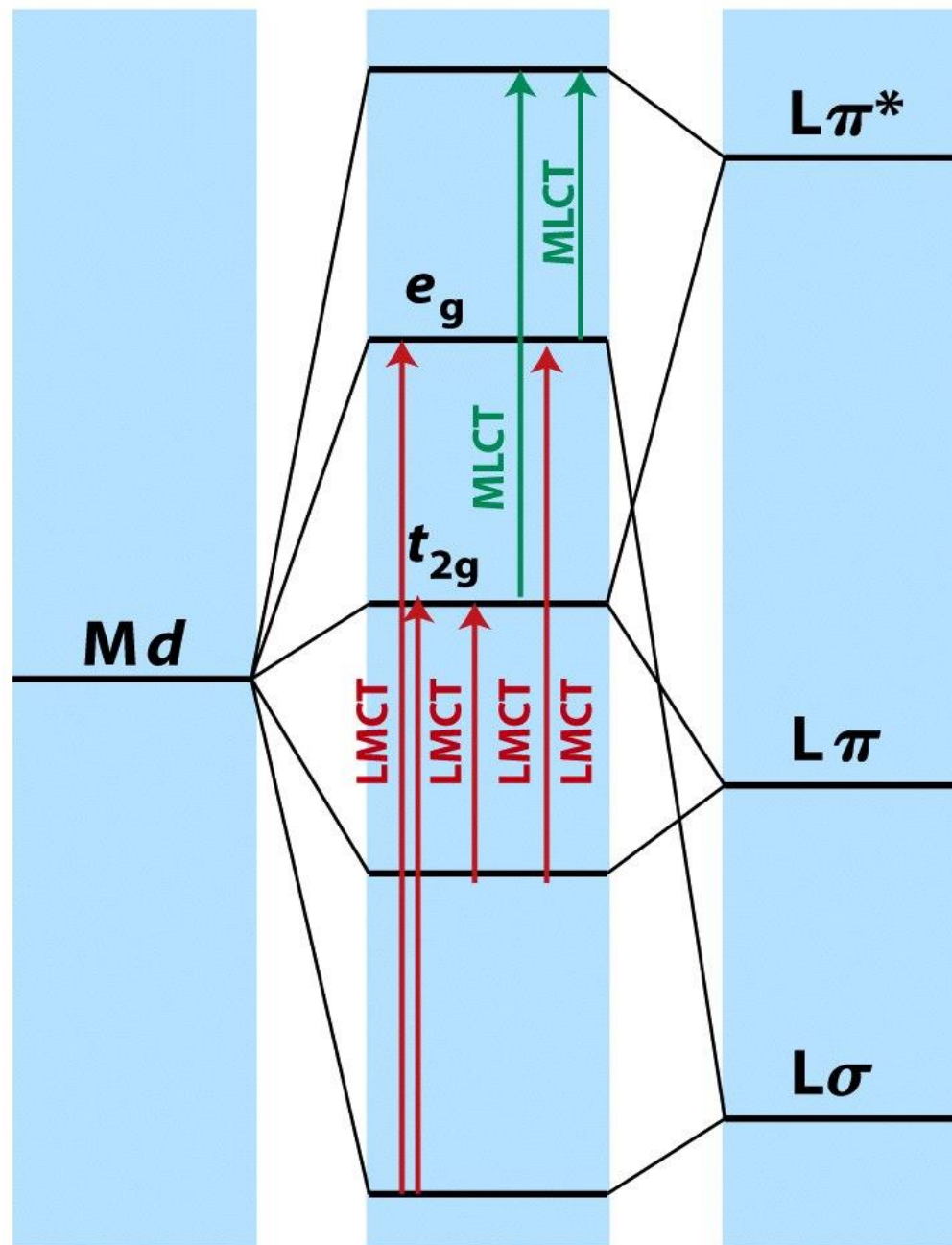
LMCT dall'ossigeno al metallo

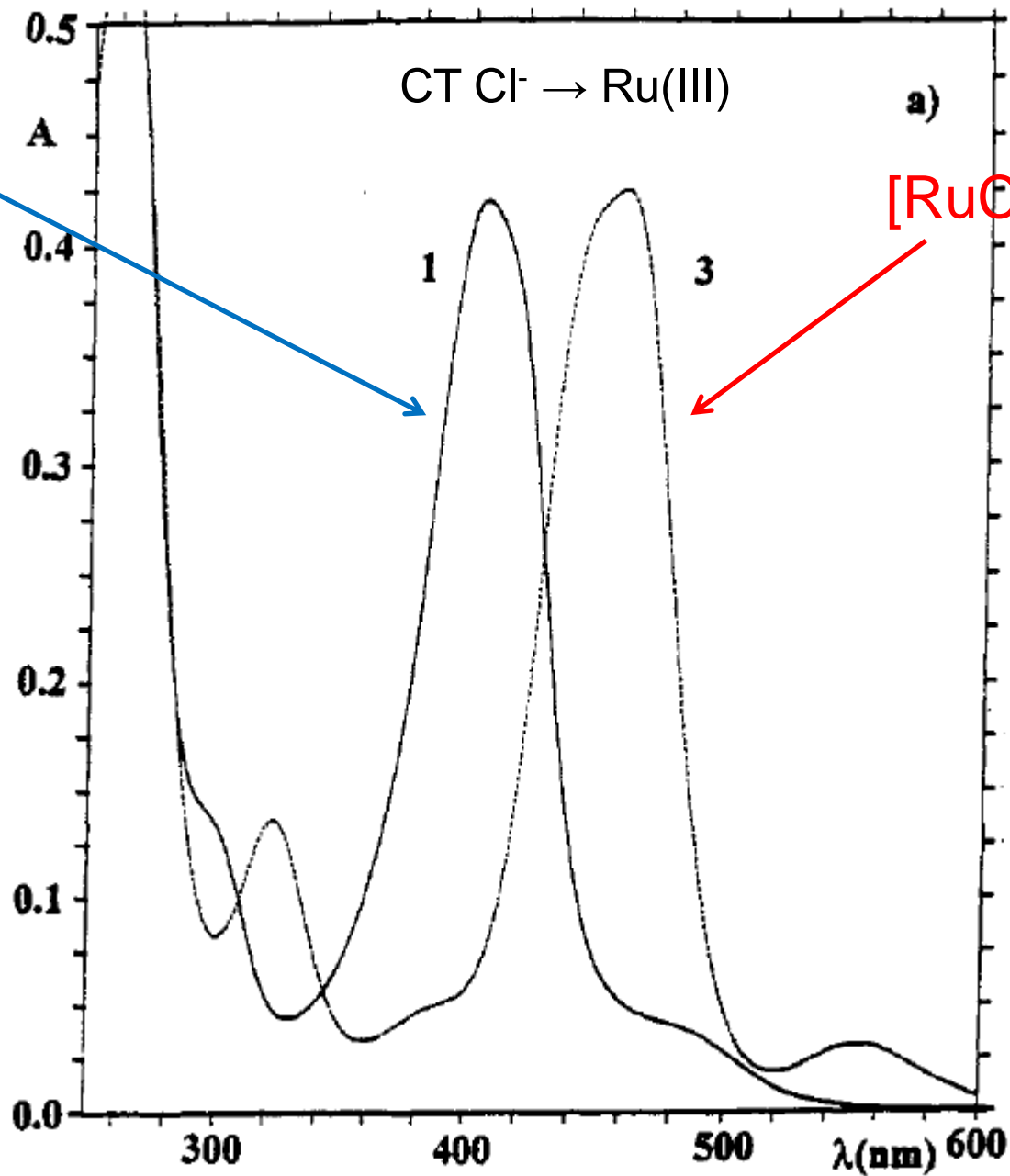


Correlazione fra λ LMCT e potenziale redox



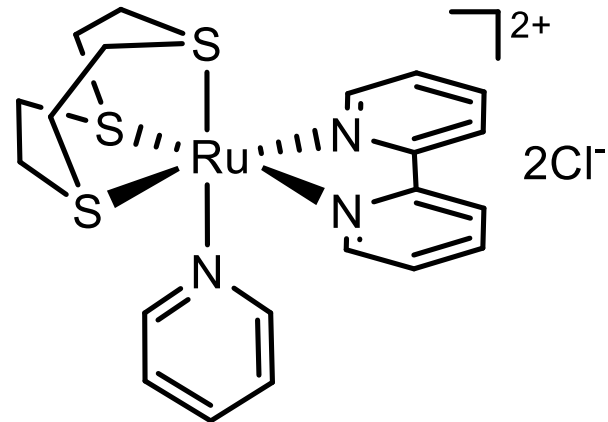
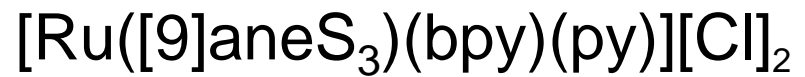
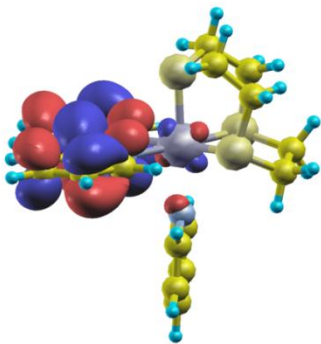
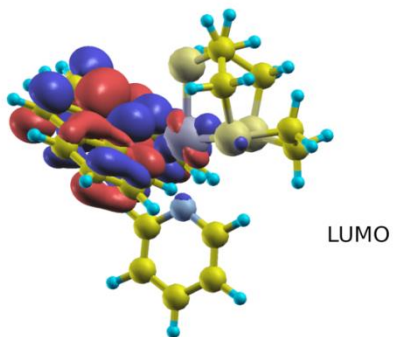
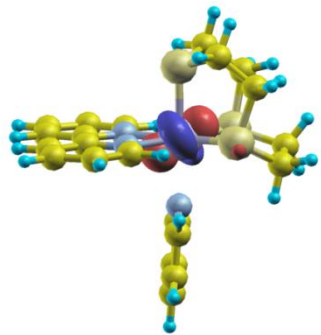
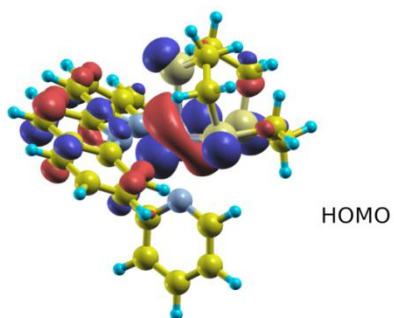
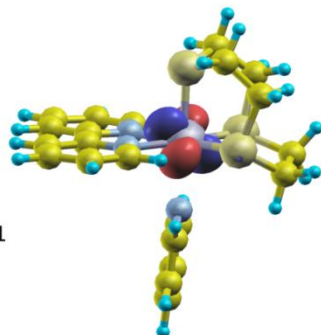
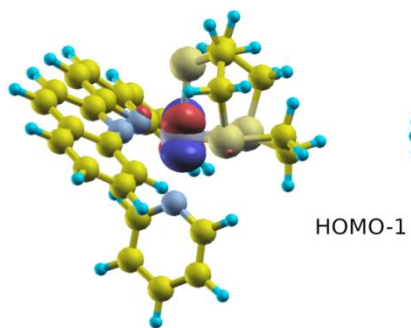
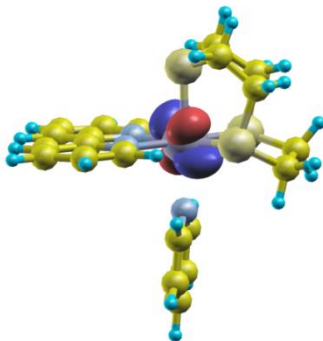
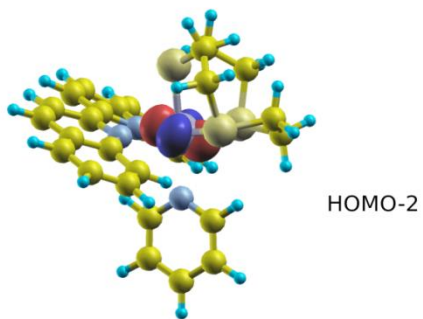


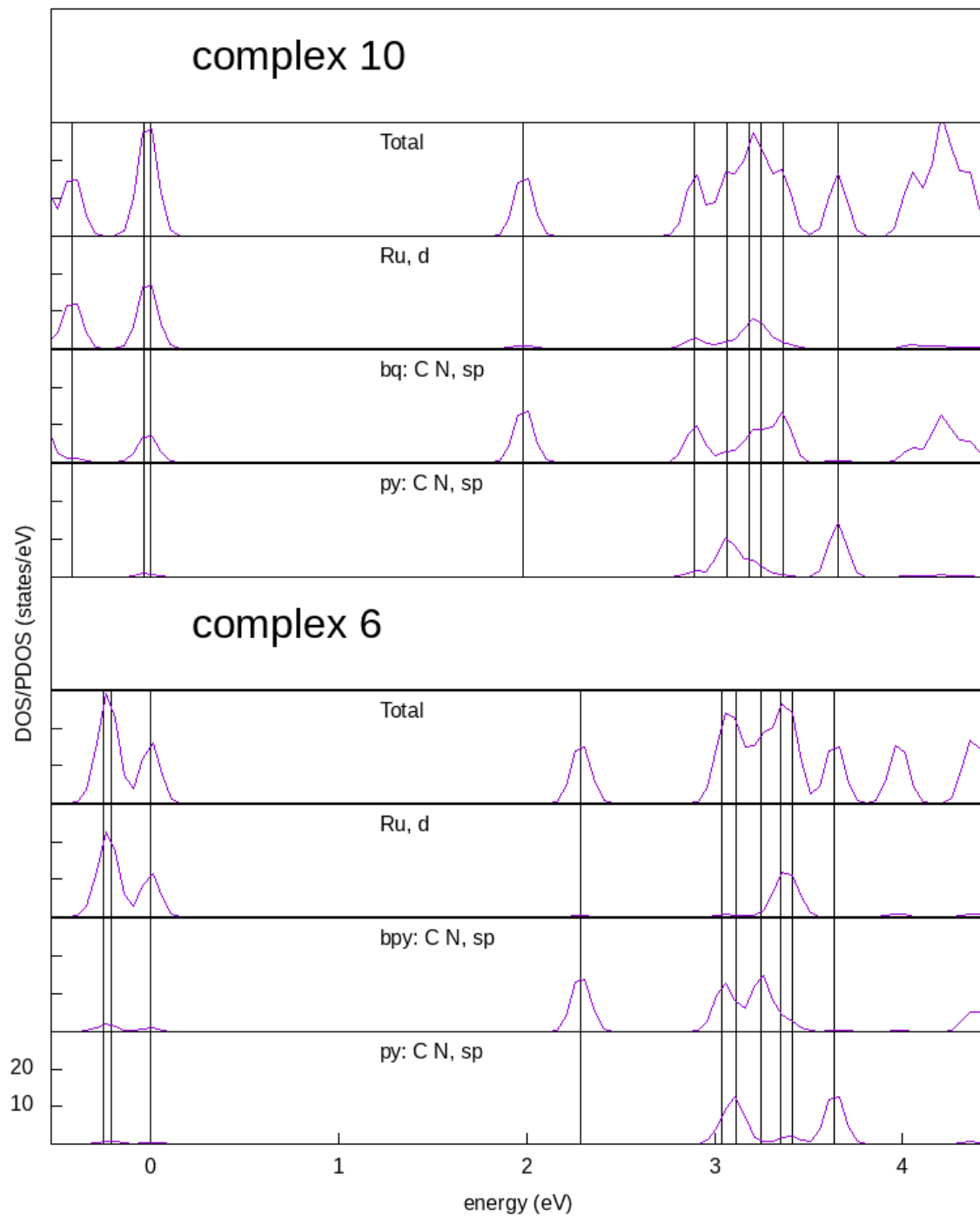


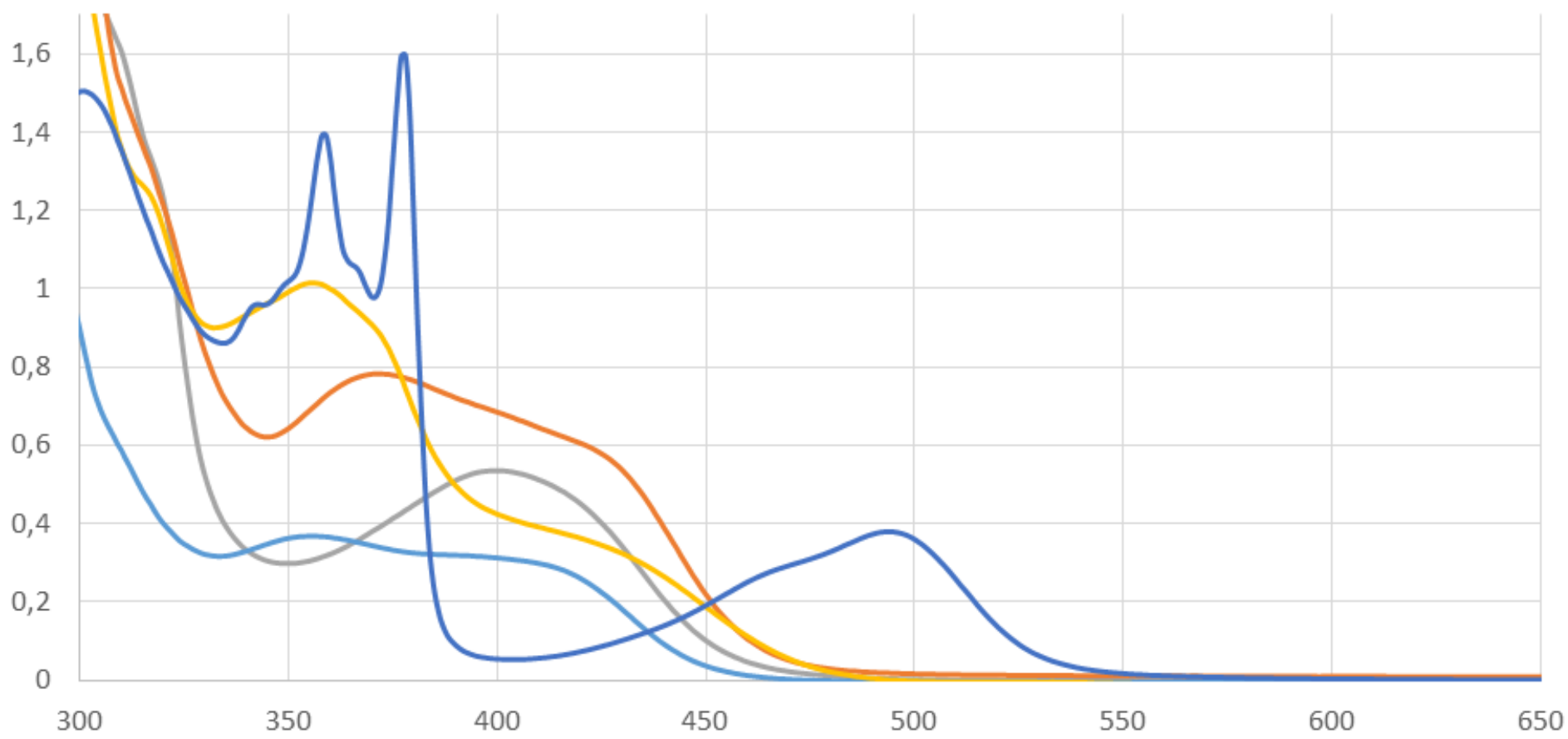


complex 10

complex 6







— 6 — 7 — 8 — 9 — 10