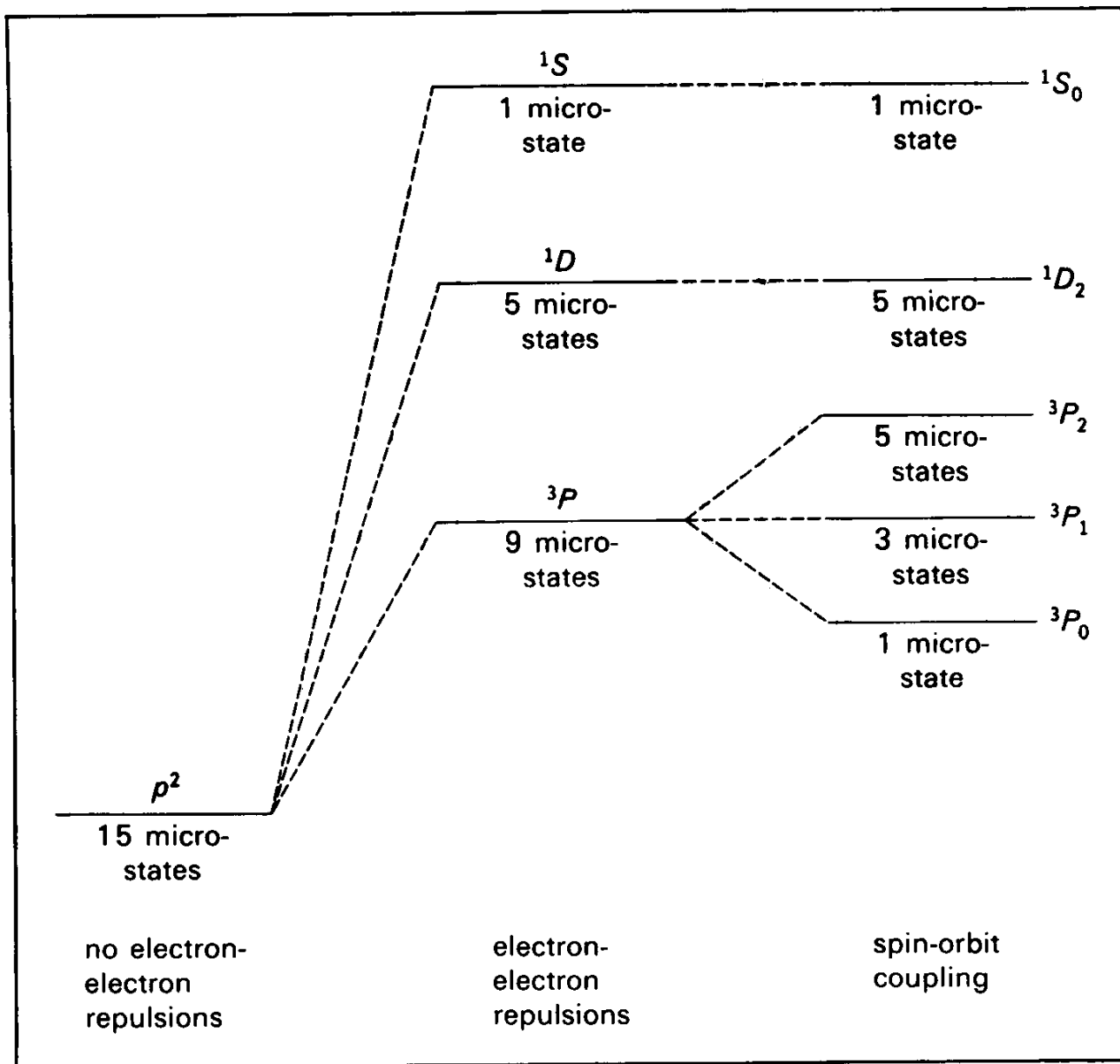


# Regole di Hund per le energie dei termini

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  $l$

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

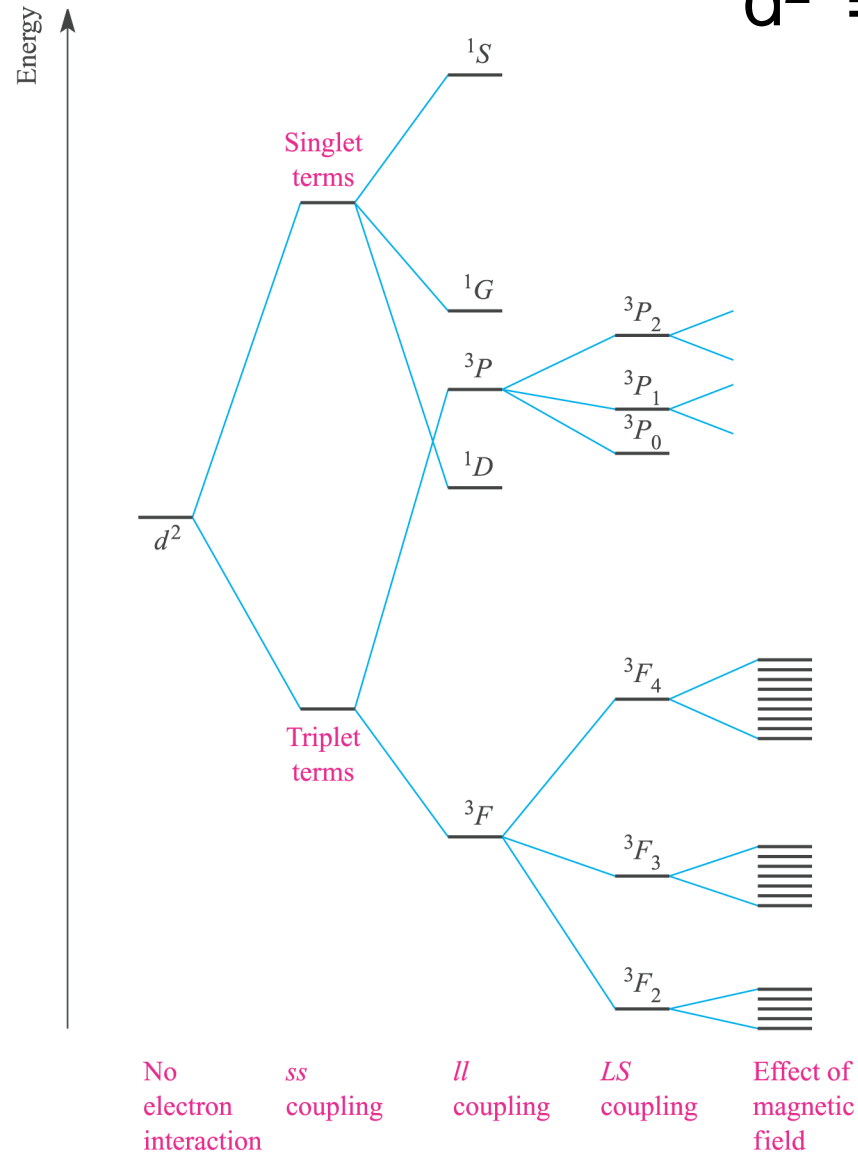


$p^3$   
 $4S, 2P, 2D$

Accoppiamento di Russell-Saunders

$d^2 = 45$  microstati

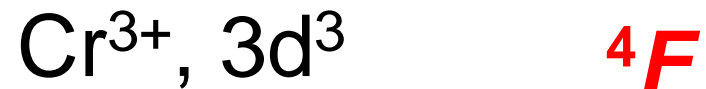
$Ti^{2+}$



$d^2$

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 (cioè delle energie dei termini)

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

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

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

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

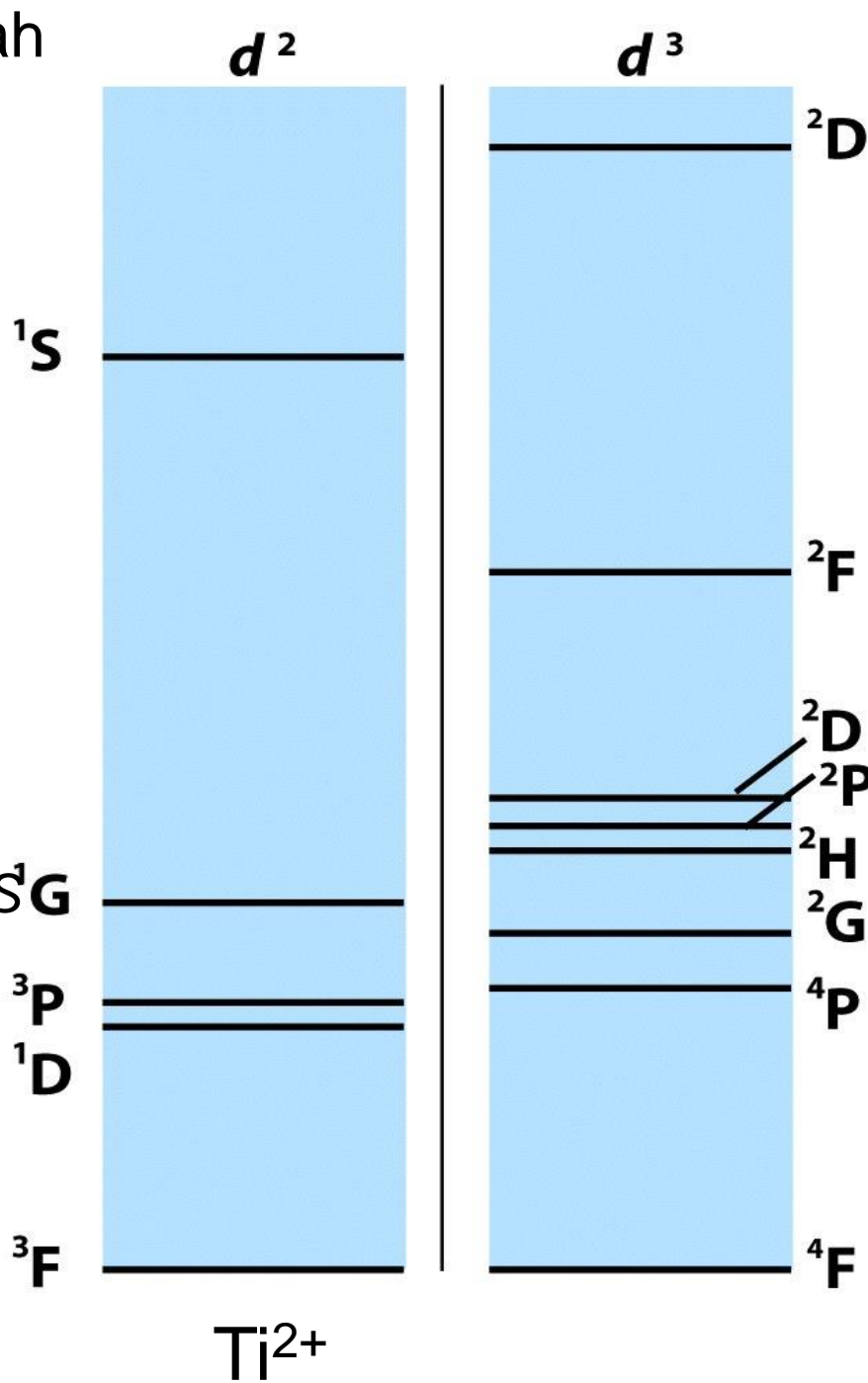
$$E(^3F) = A - 8B$$

$$C > 5B$$

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

$$C < 5B$$

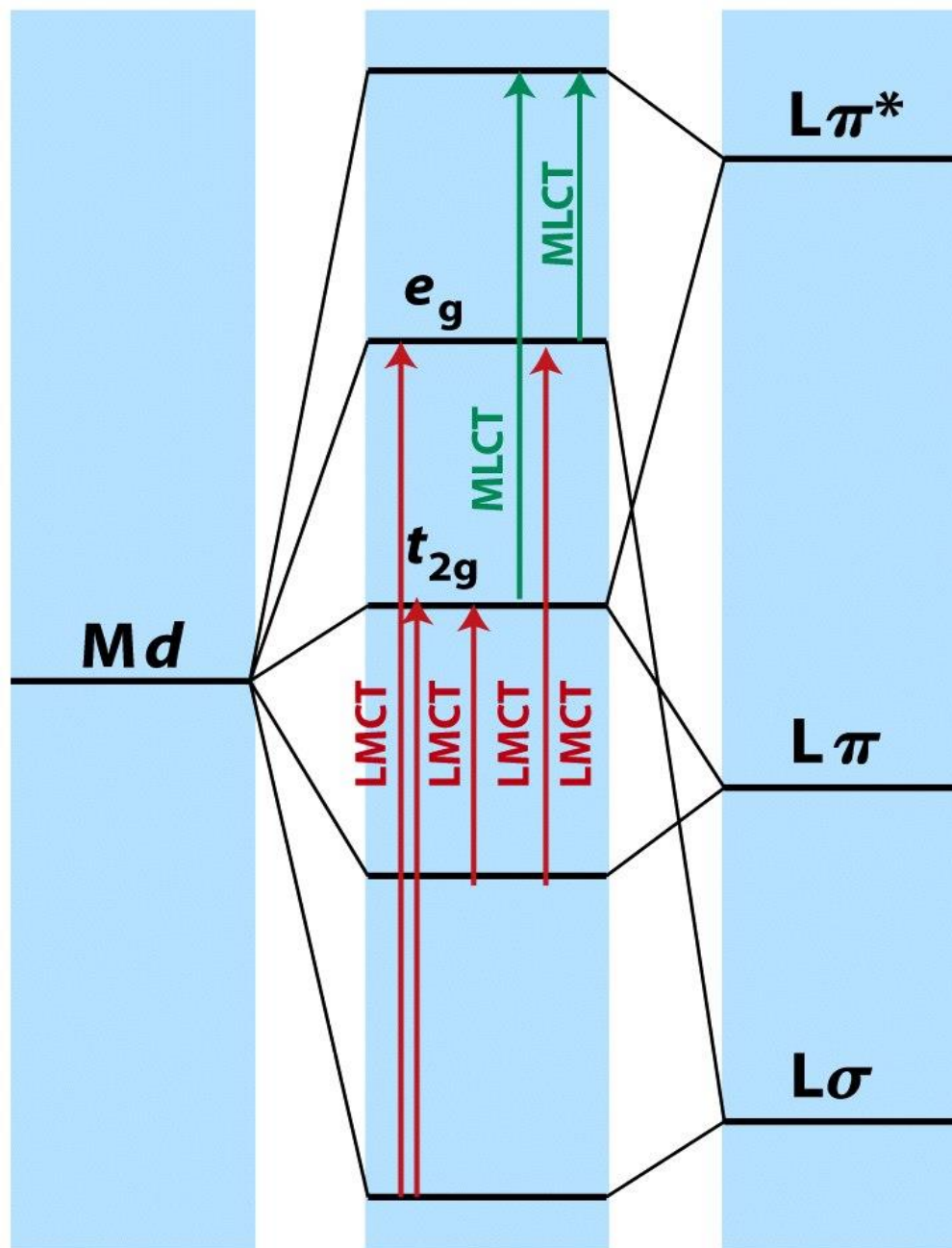
$$^3F < ^1D < ^3P < ^1G < ^1S$$



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

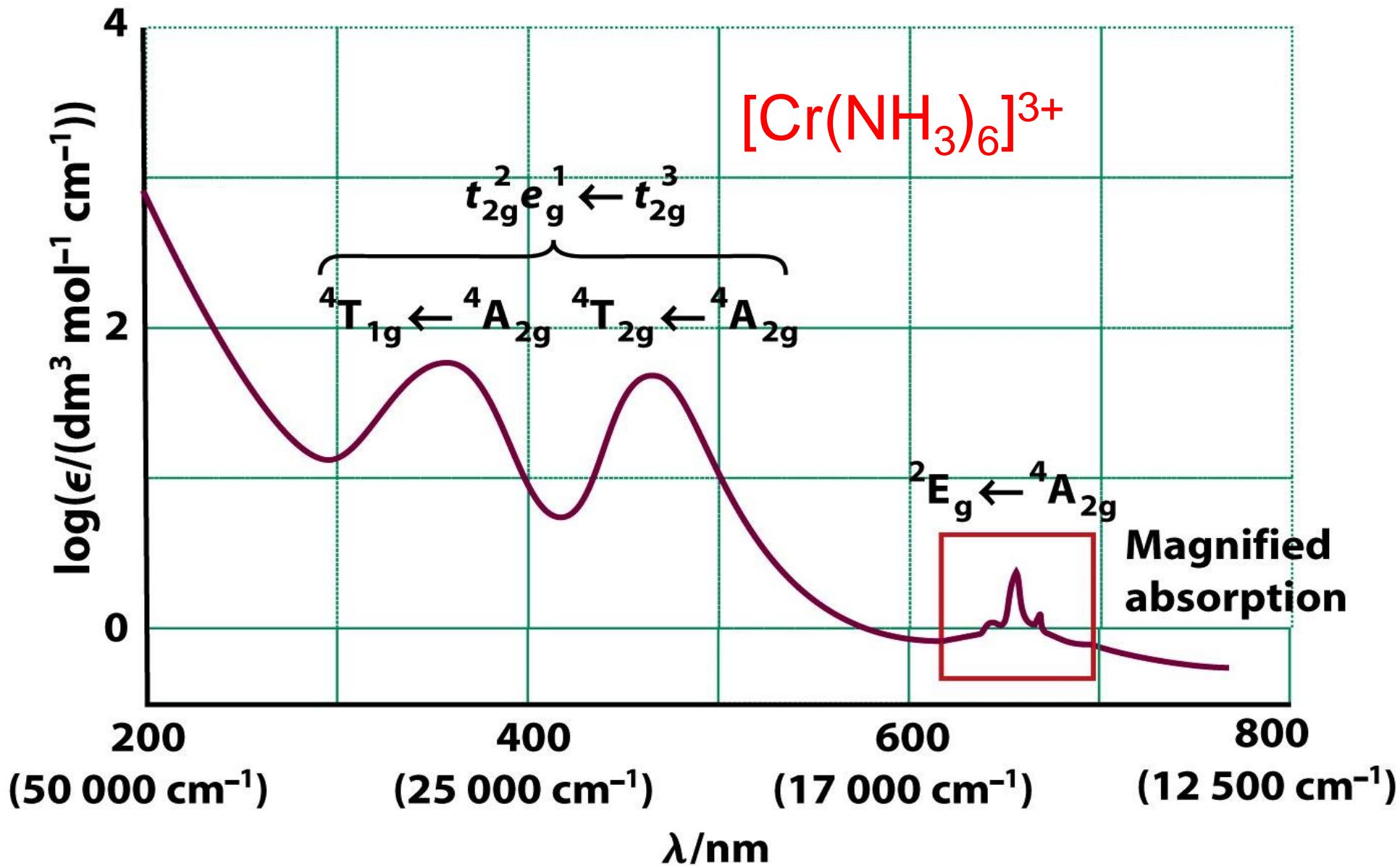
	1+	2+	3+	4+
Ti		720 (3.7)		
V		765 (3.9)	860 (4.8)	
Cr		830 (4.1)	1030 (3.7)	1040 (4.1)
Mn		960 (3.5)	1130 (3.2)	
Fe		1060 (4.1)		
Co		1120 (3.9)		
Ni		1080 (4.5)		
Cu	1220 (4.0)	1240 (3.8)		

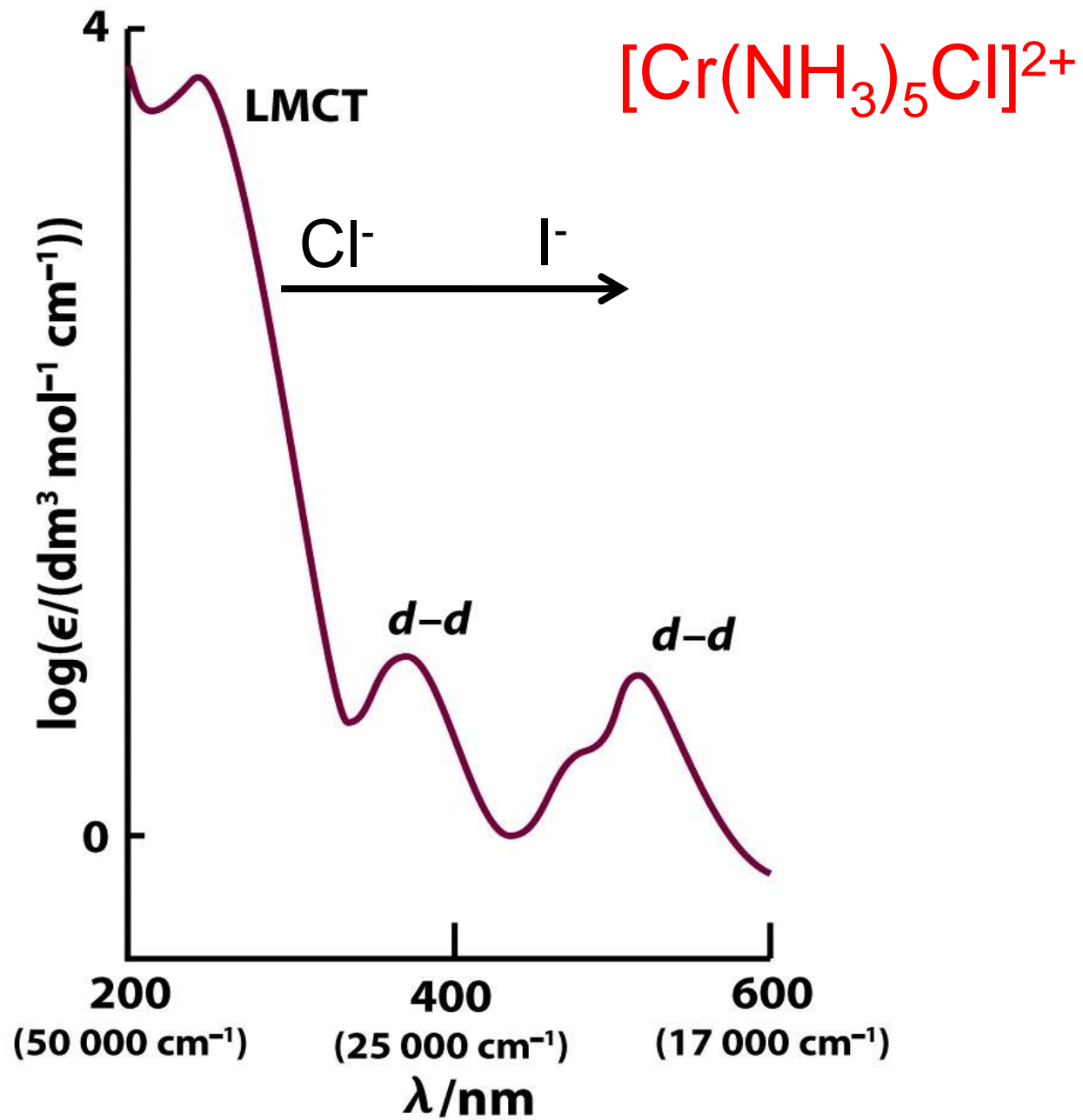
\* The table gives the *B* parameter in  $\text{cm}^{-1}$  with the value of *C/B* in parentheses.



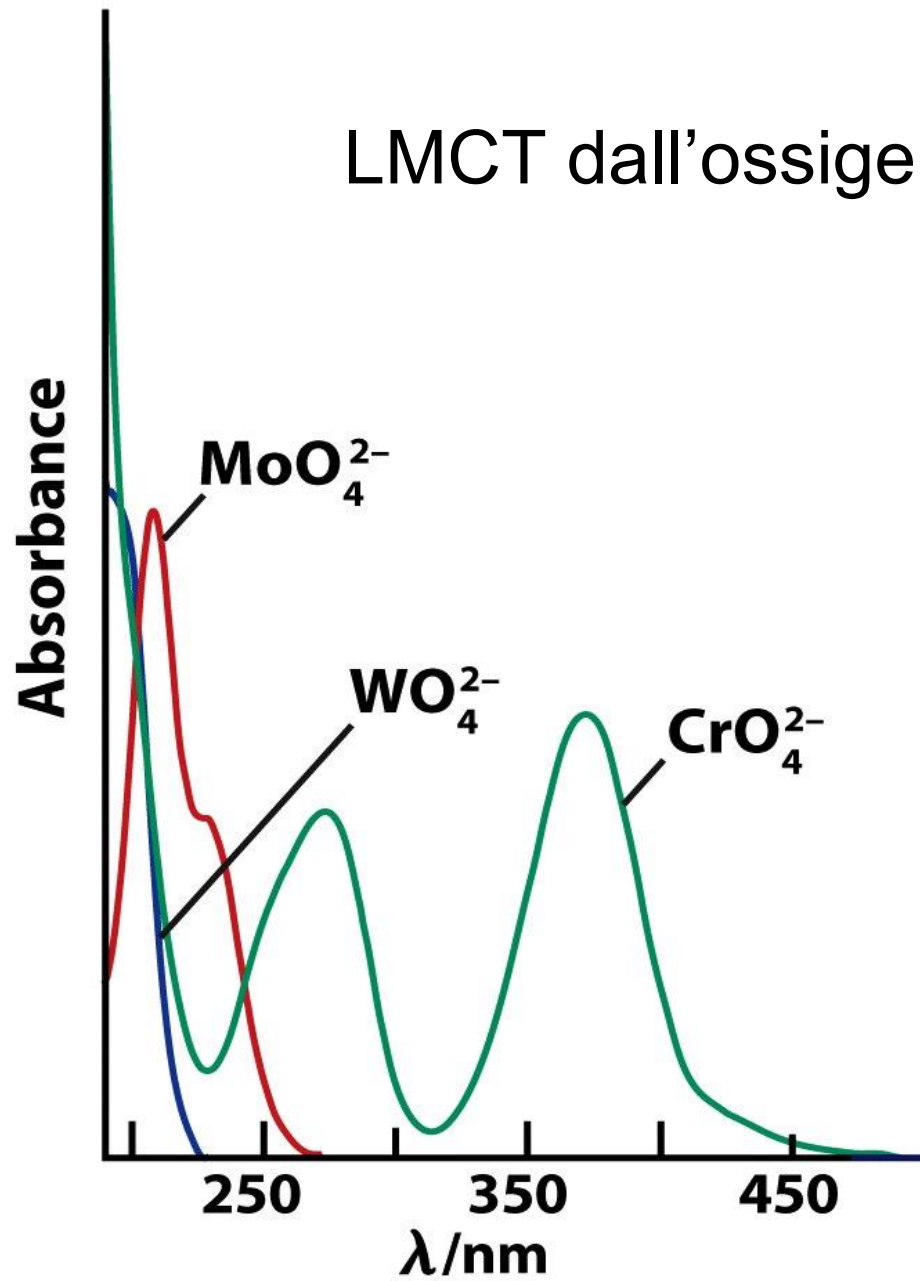
# Regole di selezione e intensità delle transizioni elettroniche

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

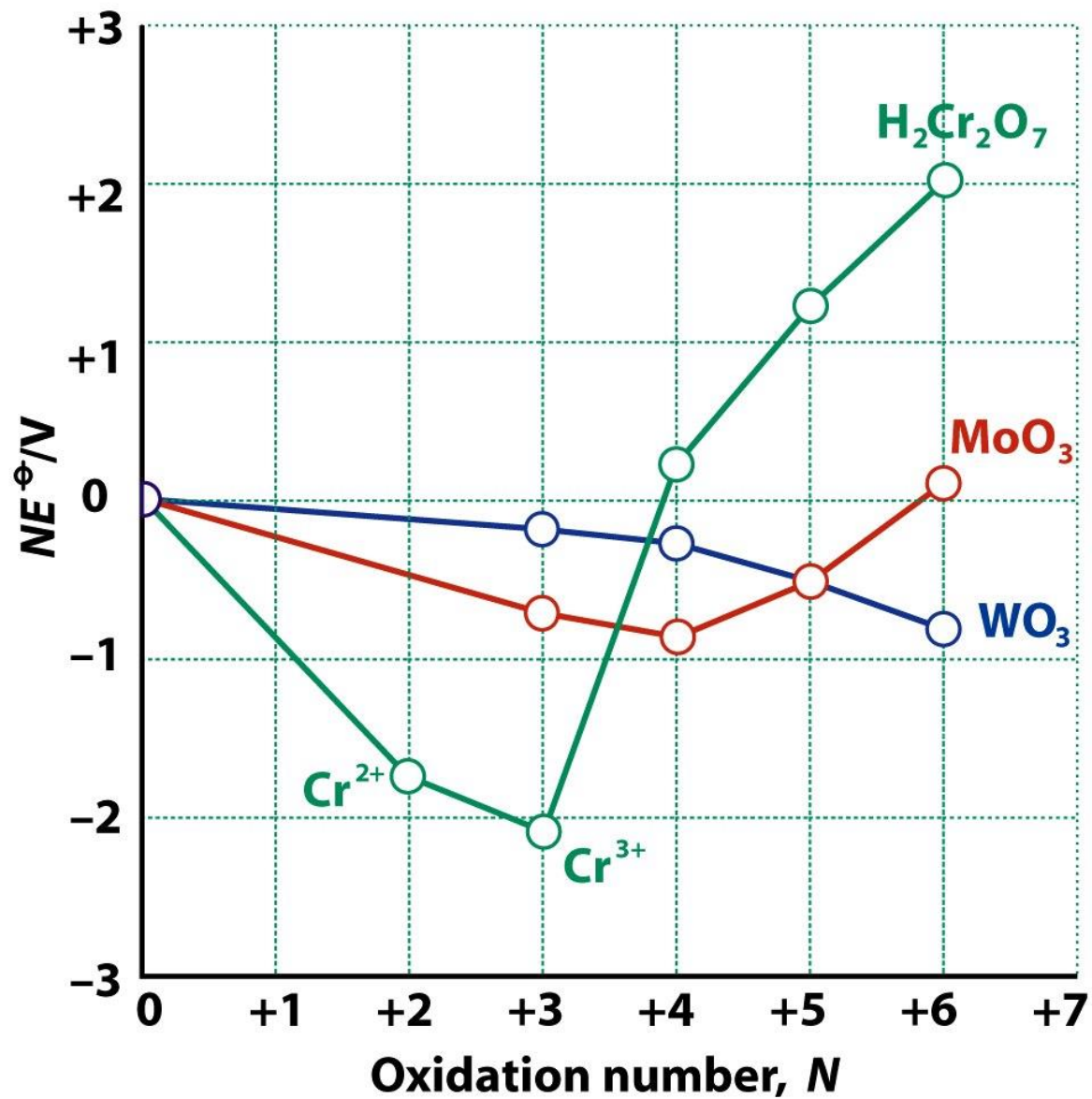




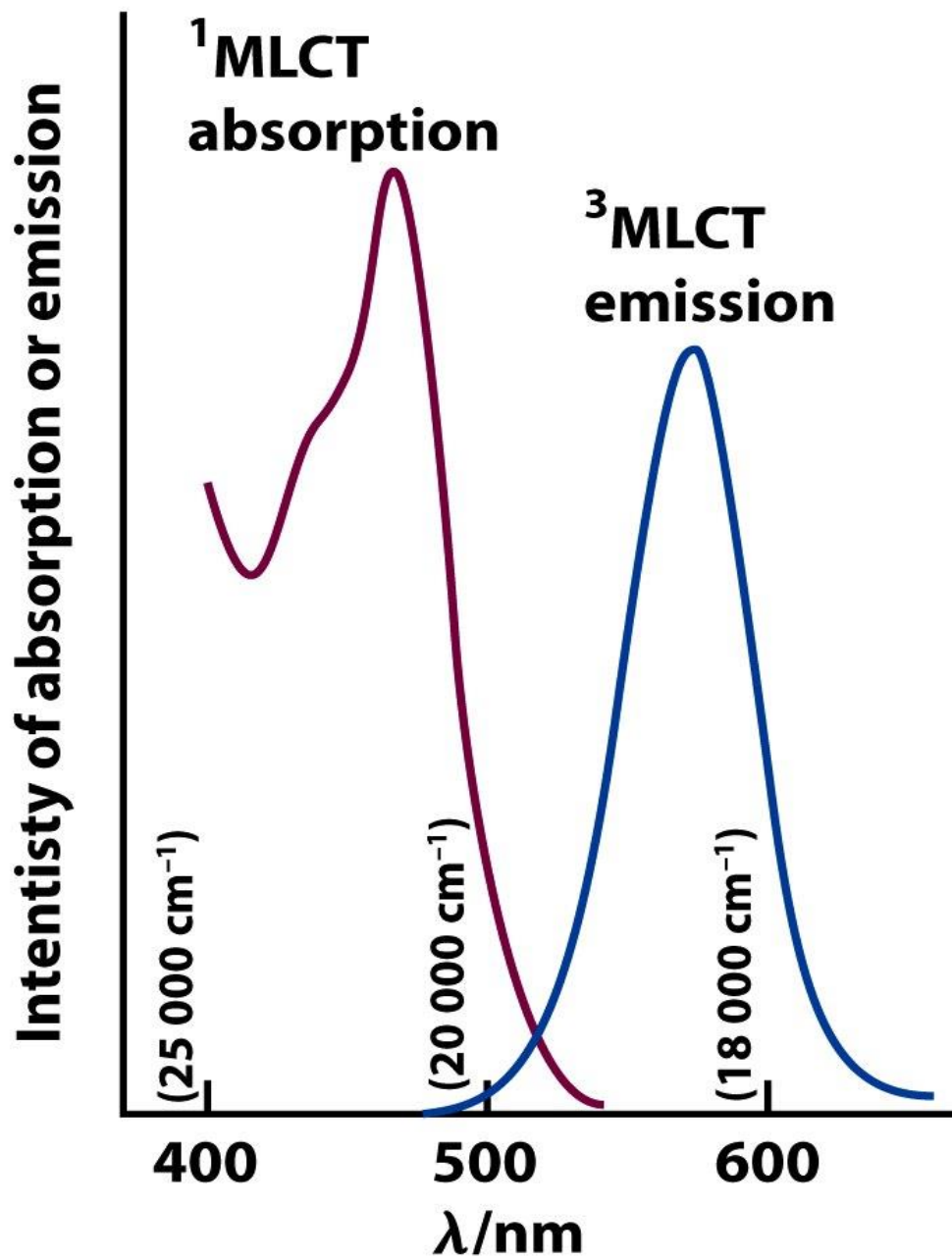
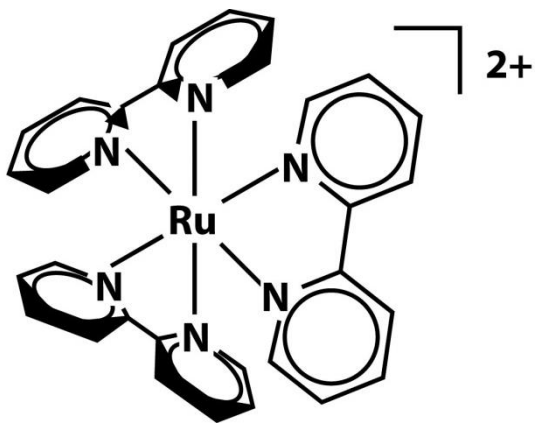
# LMCT dall'ossigeno al metallo

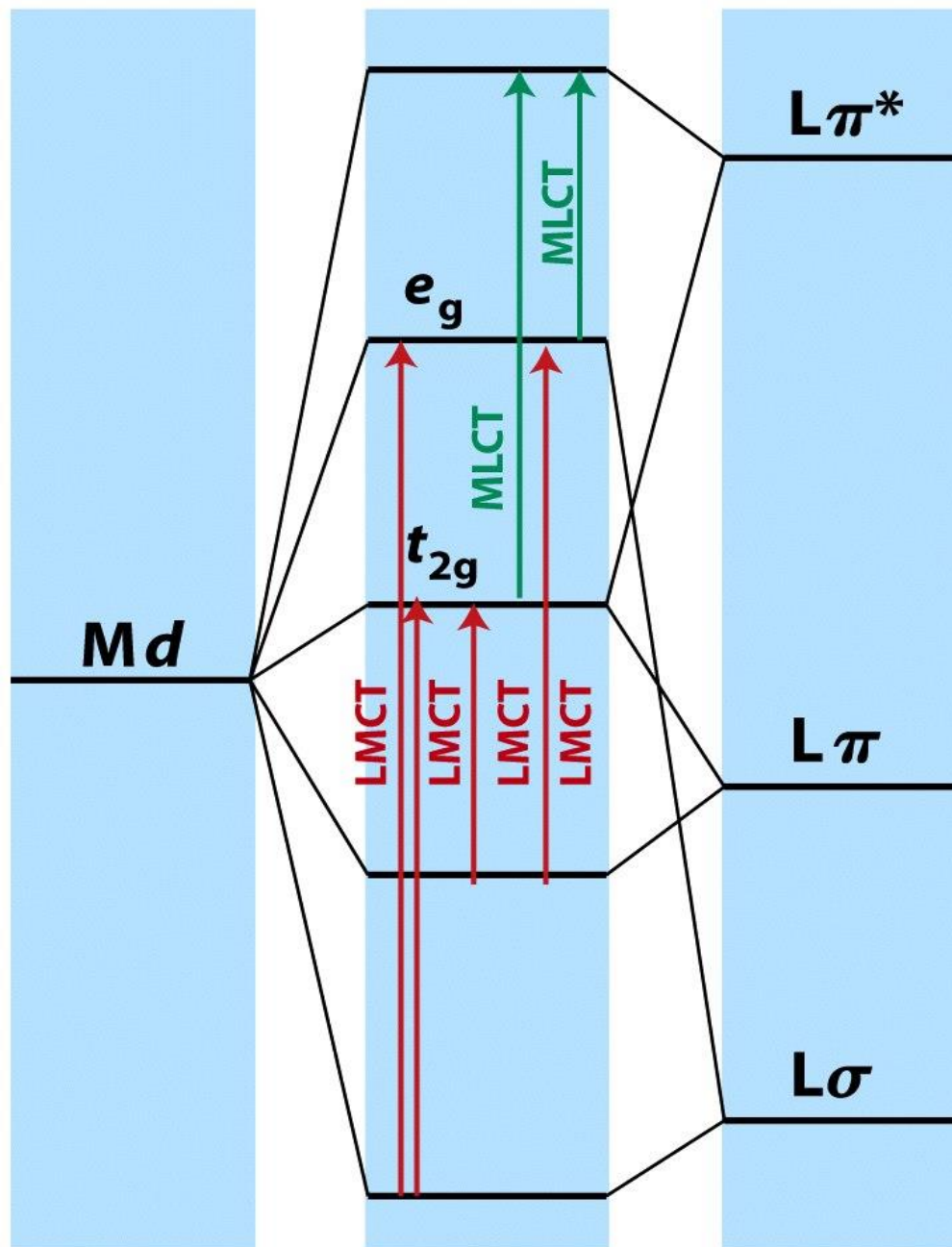


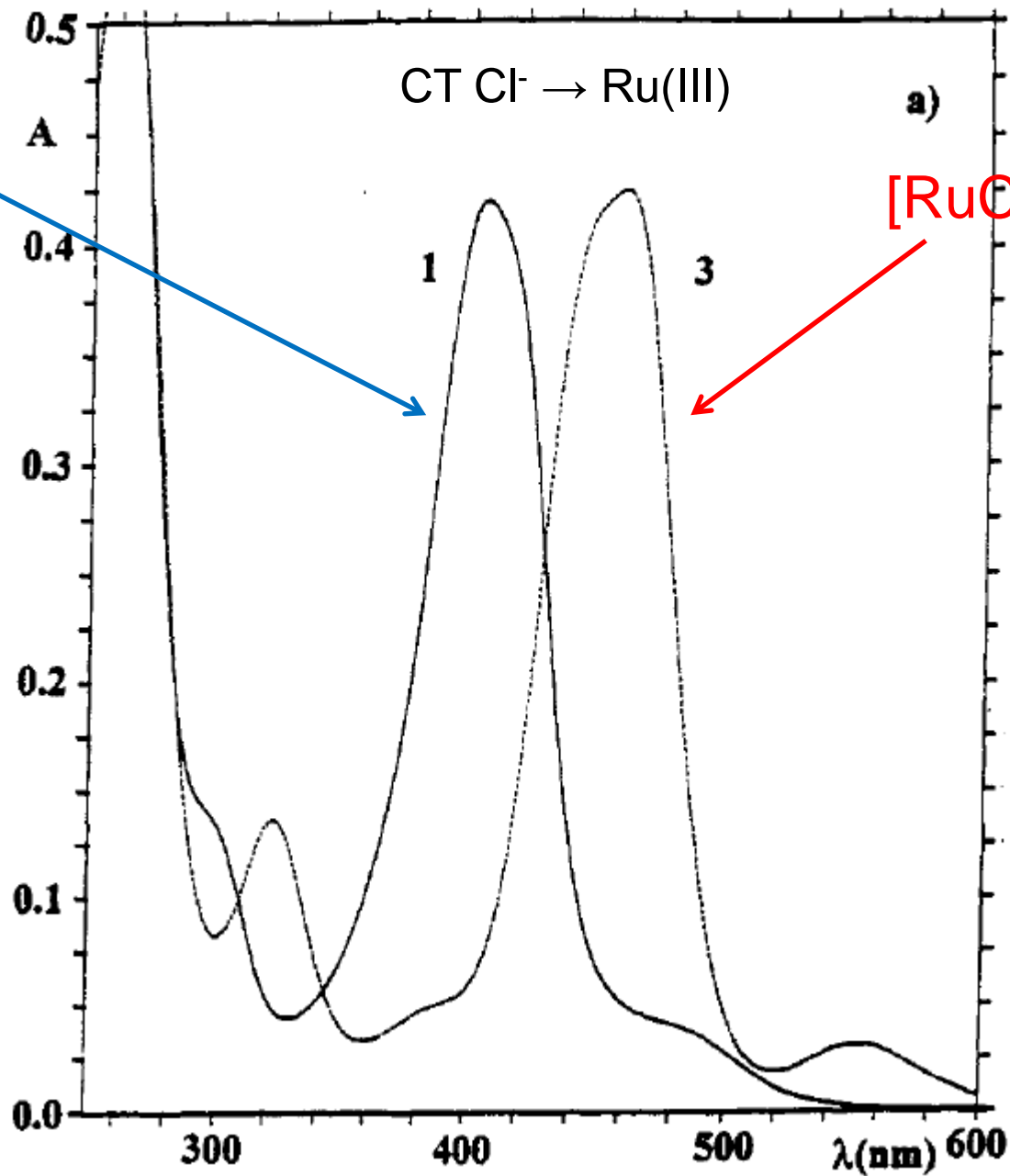
# Correlazione fra $\lambda$ LMCT e potenziale redox





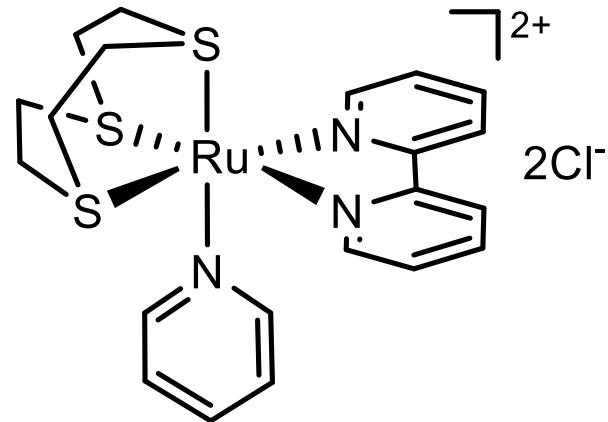
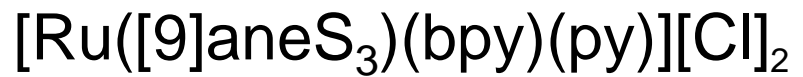
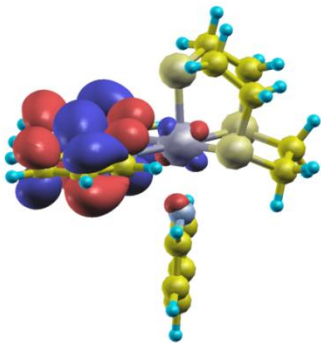
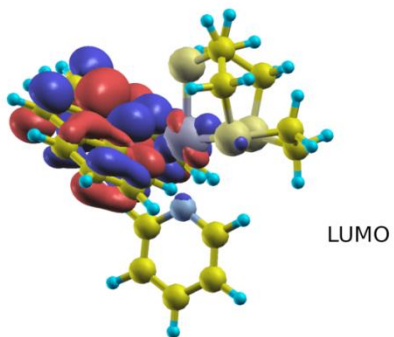
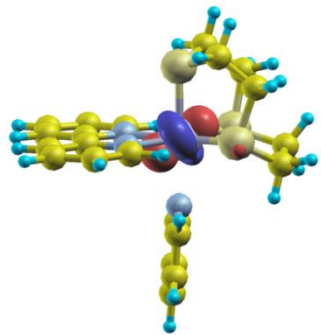
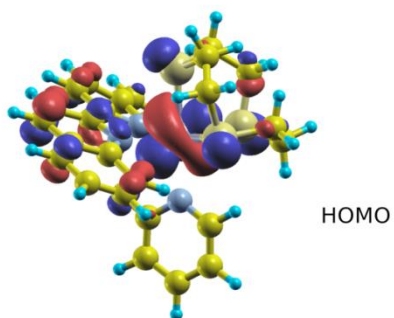
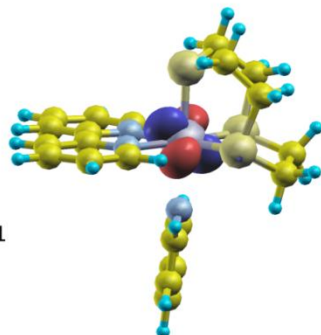
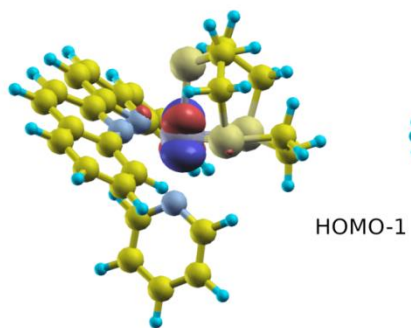
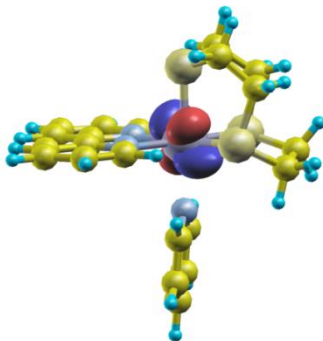
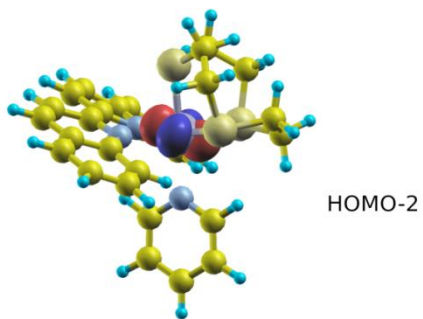


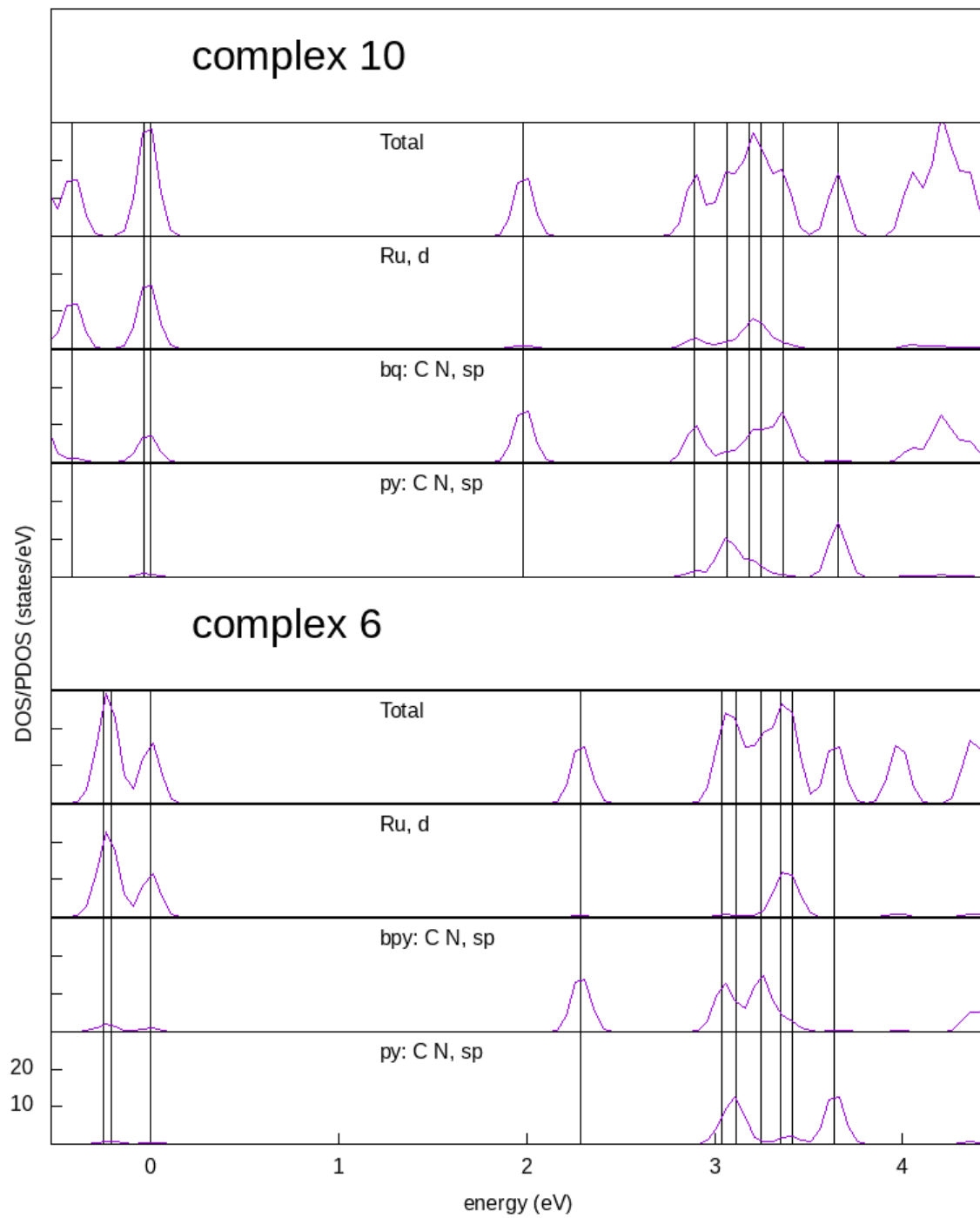


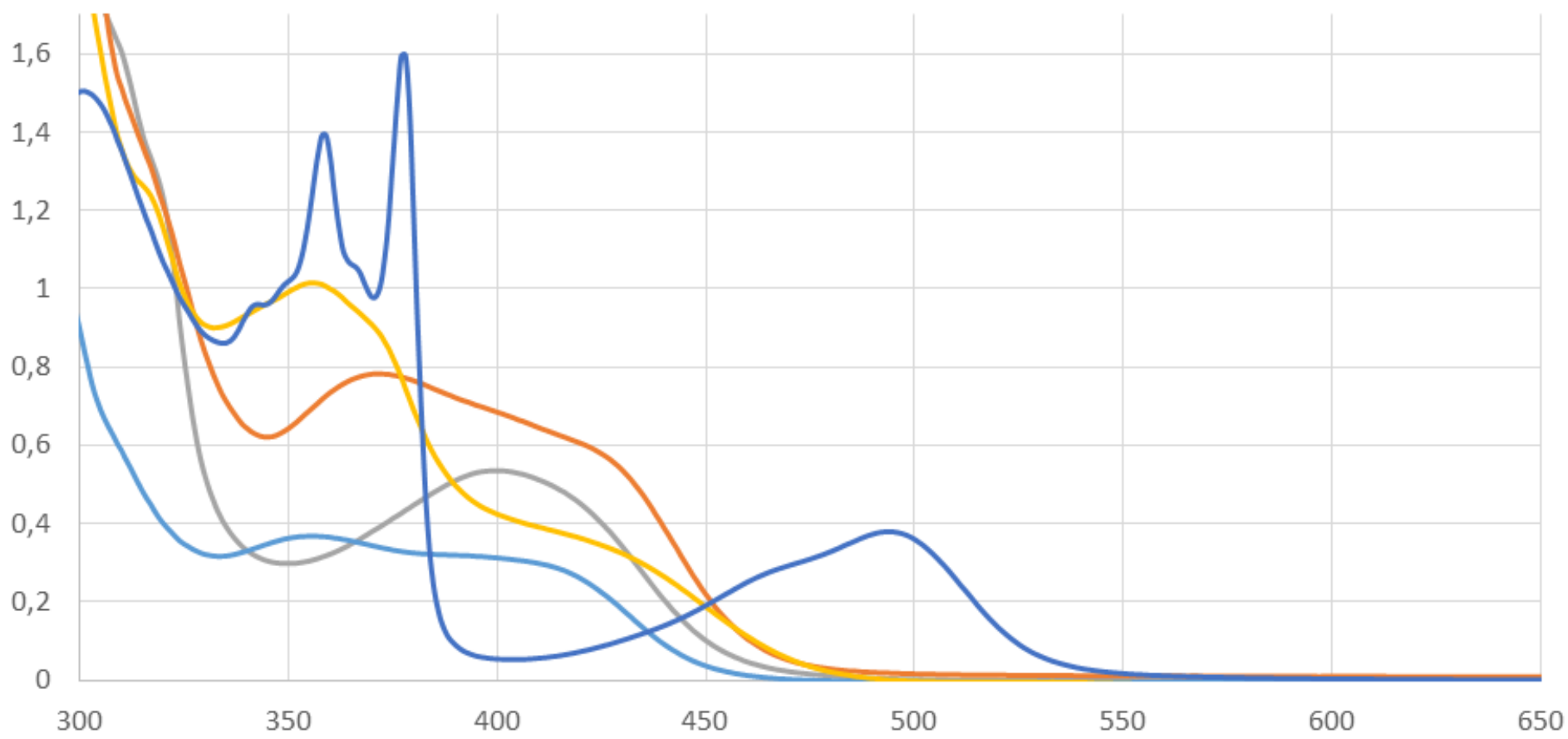


complex 10

complex 6







— 6 — 7 — 8 — 9 — 10