

# **KÉMIAI ANYAGSZERKEZETTAN**

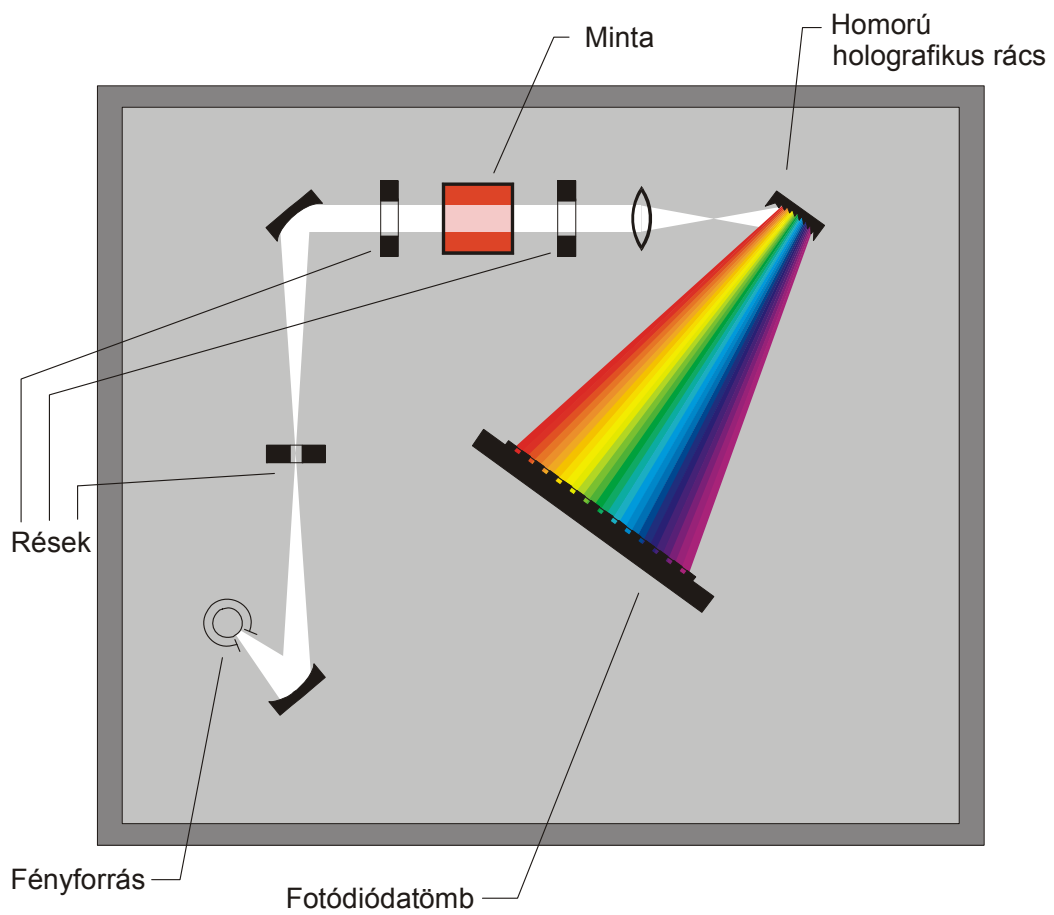
**(Ábragyűjtemény)**

**2010/2011 tanév**

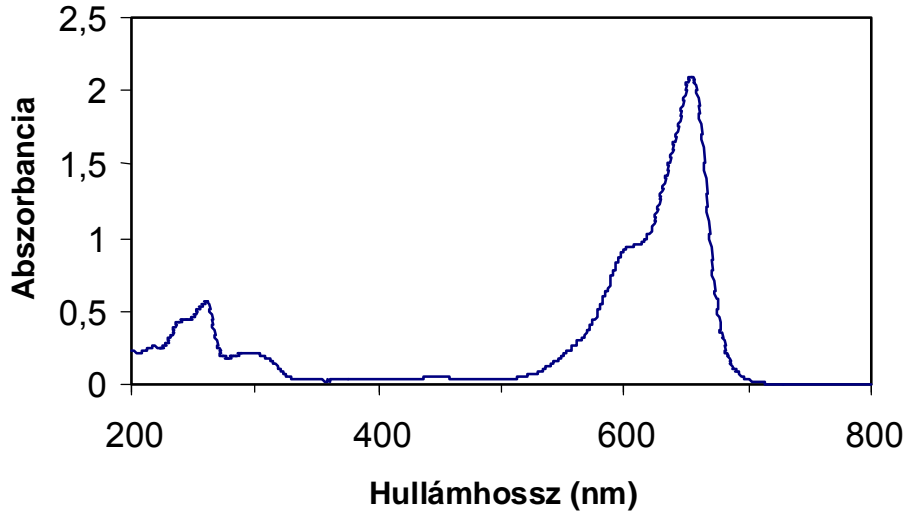
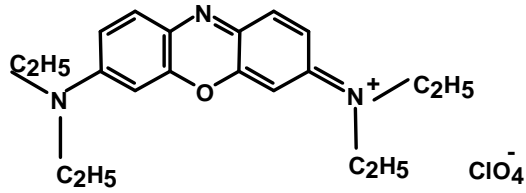
## 1. BEVEZETÉS



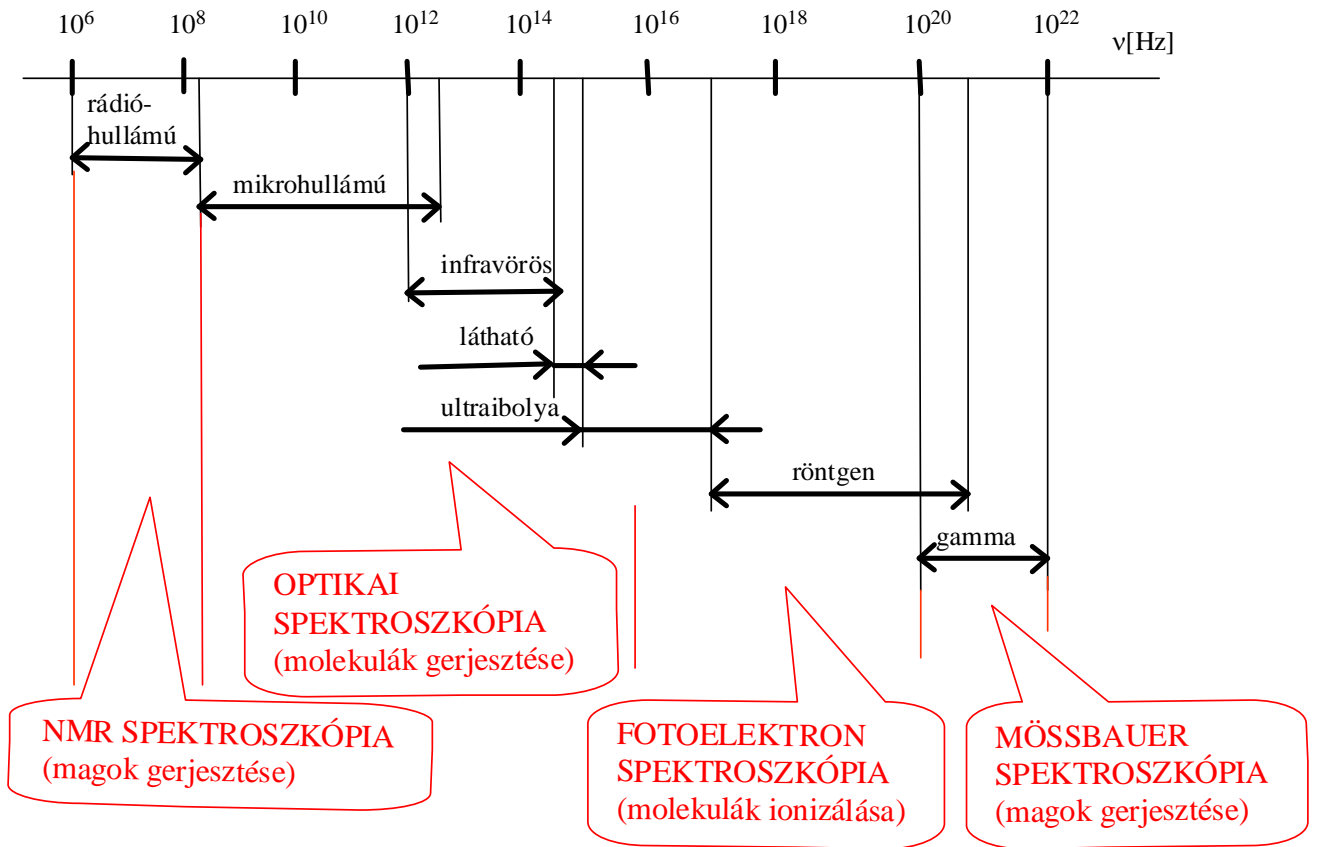
1.1. ábra. A Fraunhofer-vonalak a Nap színekében



1.2. ábra. Egyutas UV-látható abszorpciós spektrométer

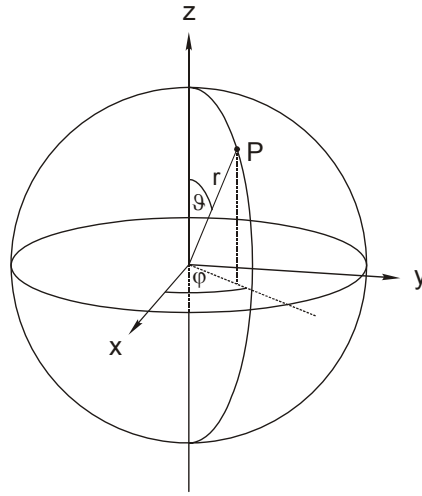


1.3. ábra. Oxazin-1 festék UV-látható abszorpciós színeke



1.4. ábra. Az elektromágneses sugárzás tartományai

### 3. A HIDROGÉNATOM SZERKEZETE



3.1. ábra. A Descartes- és a polárkoordinátarendszer kapcsolata

3.1. táblázat A hidrogénatom komplex hullámfüggvényei

$$a_0 = \frac{h^2}{m_e e^2} \quad \rho = \frac{r}{a_0}$$

$$\psi_{100} = \frac{1}{\sqrt{\pi}} a_0^{-\frac{3}{2}} e^{-\rho}$$

$$\psi_{200} = \frac{1}{4\sqrt{2\pi}} a_0^{-\frac{3}{2}} (2 - \rho) e^{-\frac{\rho}{2}}$$

$$\psi_{210} = \frac{1}{4\sqrt{2\pi}} a_0^{-\frac{3}{2}} \rho e^{-\frac{\rho}{2}} \cos \nu$$

$$\psi_{211} = \frac{1}{8\sqrt{\pi}} a_0^{-\frac{3}{2}} \rho e^{-\frac{\rho}{2}} \sin \nu e^{i\varphi}$$

$$\psi_{21-1} = \frac{1}{8\sqrt{\pi}} a_0^{-\frac{3}{2}} \rho e^{-\frac{\rho}{2}} \sin \nu e^{-i\varphi}$$

$$\psi_{300} = \frac{1}{81\sqrt{3\pi}} a_0^{-\frac{3}{2}} (27 - 18\rho + 2\rho^2) e^{-\frac{\rho}{3}}$$

$$\psi_{310} = \frac{\sqrt{2}}{81\sqrt{\pi}} a_0^{-\frac{3}{2}} (6\rho - \rho^2) e^{-\frac{\rho}{3}} \cos \nu$$

$$\psi_{311} = \frac{1}{81\sqrt{\pi}} a_0^{-\frac{3}{2}} (6\rho - \rho^2) e^{-\frac{\rho}{3}} \sin \nu e^{i\varphi}$$

$$\psi_{31-1} = \frac{1}{81\sqrt{\pi}} a_0^{-\frac{3}{2}} (6\rho - \rho^2) e^{-\frac{\rho}{3}} \sin \nu e^{-i\varphi}$$

$$\psi_{320} = \frac{1}{81\sqrt{6\pi}} a_0^{-\frac{3}{2}} \rho^2 e^{-\frac{\rho}{3}} (3\cos^2 \nu - 1)$$

$$\psi_{321} = \frac{1}{81\sqrt{\pi}} a_0^{-\frac{3}{2}} \rho^2 e^{-\frac{\rho}{3}} \sin \nu \cos \nu e^{i\varphi}$$

$$\psi_{32-1} = \frac{1}{81\sqrt{\pi}} a_0^{-\frac{3}{2}} \rho^2 e^{-\frac{\rho}{3}} \sin \nu \cos \nu e^{-i\varphi}$$

$$\psi_{322} = \frac{1}{162\sqrt{\pi}} a_0^{-\frac{3}{2}} \rho^2 e^{-\frac{\rho}{3}} \sin^2 \nu e^{2i\varphi}$$

$$\psi_{32-2} = \frac{1}{162\sqrt{\pi}} a_0^{-\frac{3}{2}} \rho^2 e^{-\frac{\rho}{3}} \sin^2 \nu e^{-2i\varphi}$$

### 3.2. táblázat A hidrogénatom valós hullámfüggvényei

$$\psi_{1s} = \psi_{100}, \psi_{2s} = \psi_{200}, \psi_{2p_z} = \psi_{210}$$

$$\psi_{2p_x} = \frac{\psi_{211} + \psi_{21-1}}{\sqrt{2}} = \frac{1}{4\sqrt{2}\pi} a_0^{-\frac{3}{2}} \rho e^{-\frac{\rho}{2}} \sin \nu \cos \varphi$$

$$\psi_{2p_y} = \frac{-i(\psi_{211} - \psi_{21-1})}{\sqrt{2}} = \frac{1}{4\sqrt{2}\pi} a_0^{-\frac{3}{2}} \rho e^{-\frac{\rho}{2}} \sin \nu \sin \varphi$$

$$\psi_{3s} = \psi_{300}, \psi_{3p_z} = \psi_{310}$$

$$\psi_{3p_x} = \frac{\psi_{311} + \psi_{31-1}}{\sqrt{2}} = \frac{\sqrt{2}}{81\sqrt{\pi}} a_0^{-\frac{3}{2}} (6\rho - \rho^2) e^{-\frac{\rho}{3}} \sin \nu \cos \varphi$$

$$\psi_{3p_y} = -i \frac{\psi_{311} - \psi_{31-1}}{\sqrt{2}} = \frac{\sqrt{2}}{81\sqrt{\pi}} a_0^{-\frac{3}{2}} (6\rho - \rho^2) e^{-\frac{\rho}{3}} \sin \nu \sin \varphi$$

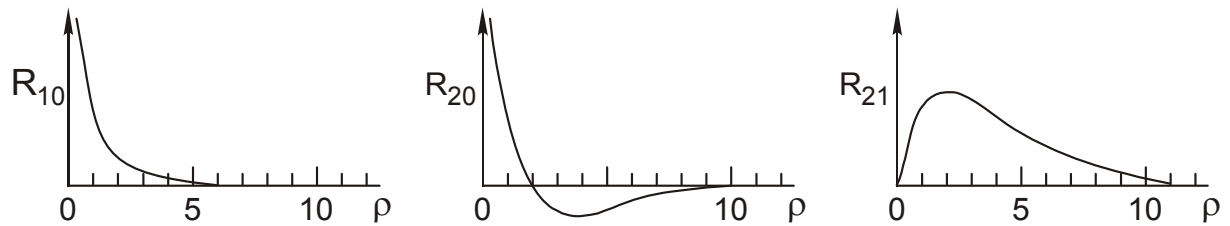
$$\psi_{3s} = \psi_{300}, \psi_{3p_z} = \psi_{310}$$

$$\psi_{3d_{xz}} = \frac{\psi_{321} - \psi_{32-1}}{\sqrt{2}} = \frac{\sqrt{2}}{81\sqrt{\pi}} a_0^{-\frac{3}{2}} \rho^2 e^{-\frac{\rho}{3}} \sin \nu \cos \nu \cos \varphi$$

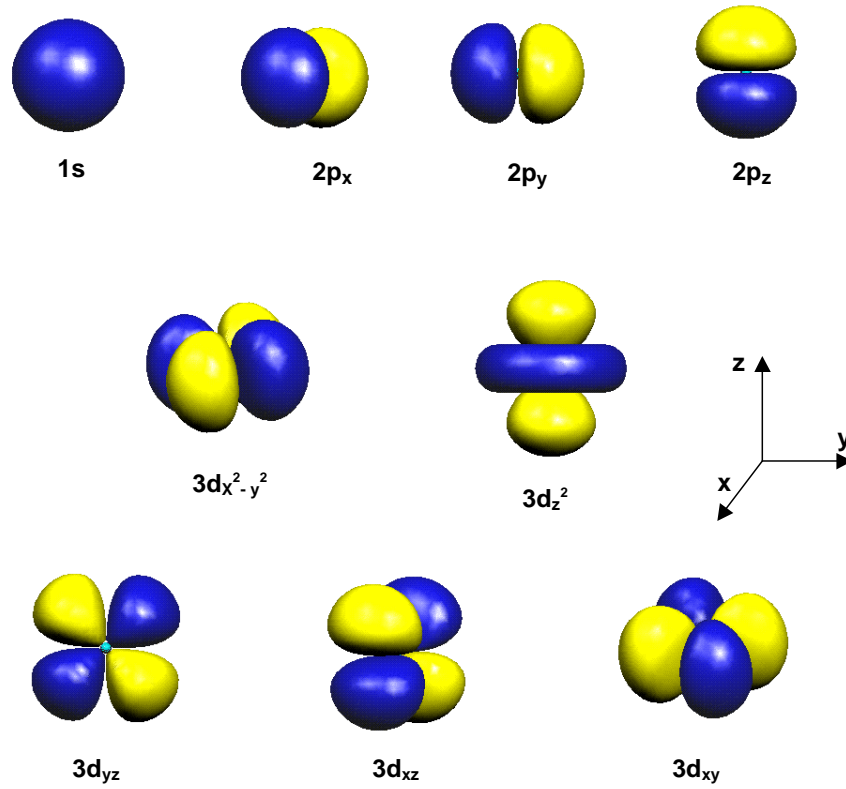
$$\psi_{3d_{yz}} = -i \frac{\psi_{321} - \psi_{32-1}}{\sqrt{2}} = \frac{\sqrt{2}}{81\sqrt{\pi}} a_0^{-\frac{3}{2}} \rho^2 e^{-\frac{\rho}{3}} \sin \nu \cos \nu \sin \varphi$$

$$\psi_{3d_{x^2-y^2}} = \frac{\psi_{322} + \psi_{32-2}}{\sqrt{2}} = \frac{1}{81\sqrt{2}\pi} a_0^{-\frac{3}{2}} \rho^2 e^{-\frac{\rho}{3}} \sin^2 \nu \cos 2\varphi$$

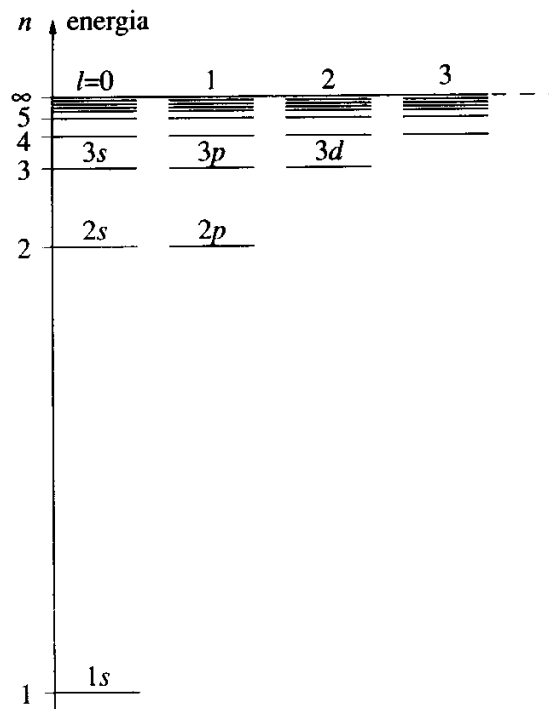
$$\psi_{3d_{z^2-r^2}} = \psi_{320}$$



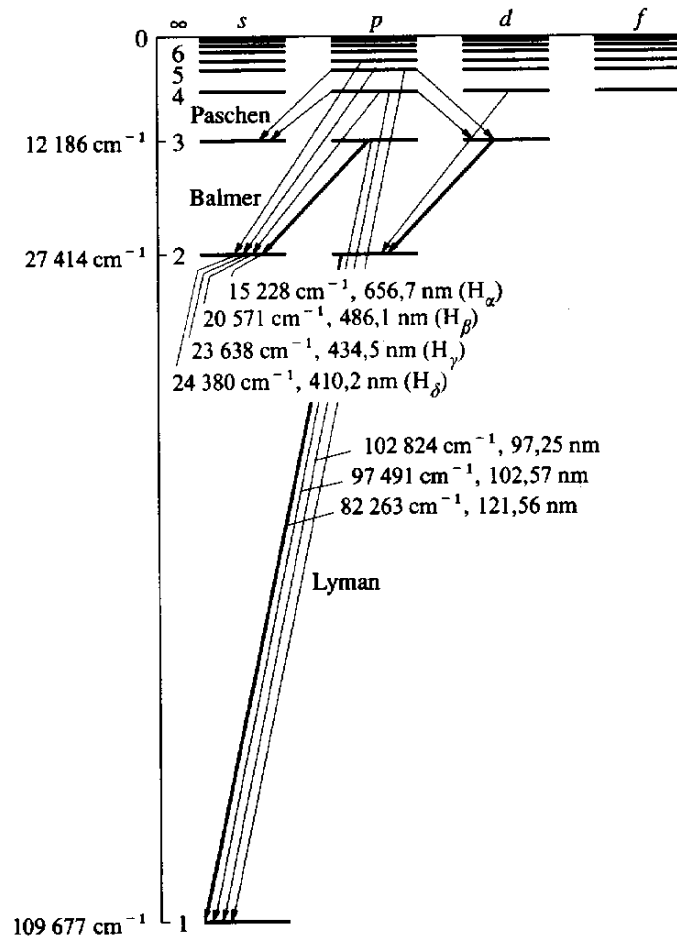
3.2. ábra. A hidrogénatom  $R_{n\ell}$  radiális hullámfüggvényei



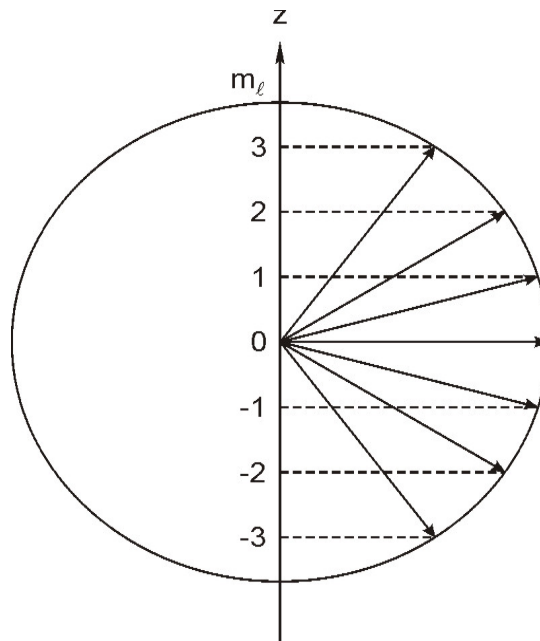
3.3. ábra. A hidrogénatom anguláris hullámfüggvényei

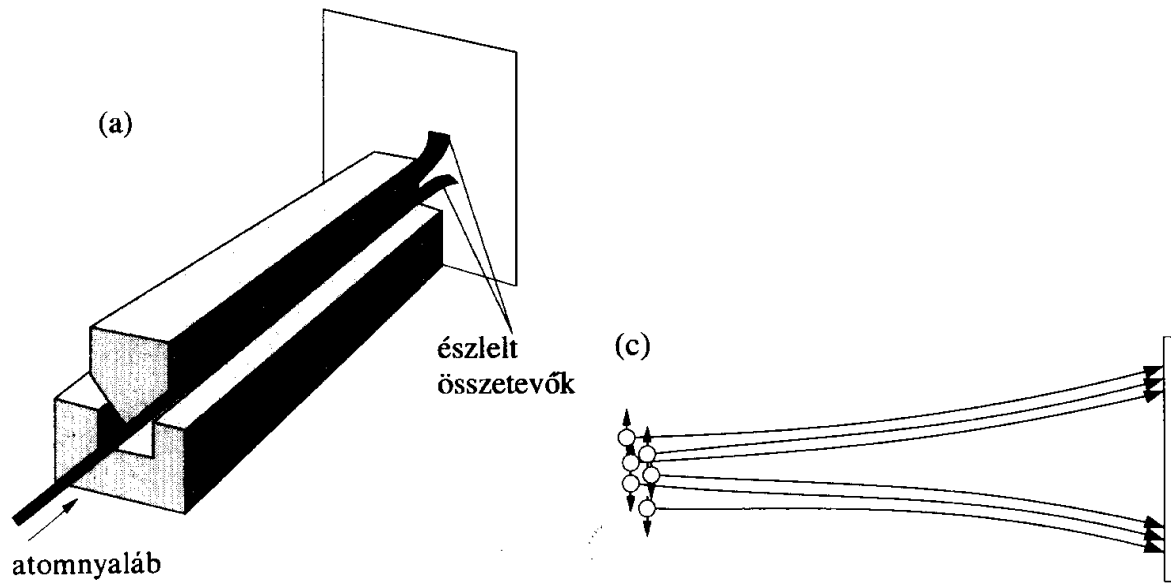


3.4. ábra. A hidrogénatom energiaszintjei



3.5. ábra. A hidrogénatom megengedett átmenetei

3.6. ábra. Az  $\ell=3$ -hoz tartozó pályaimpulzusmomentum térbeli kvantáltsága



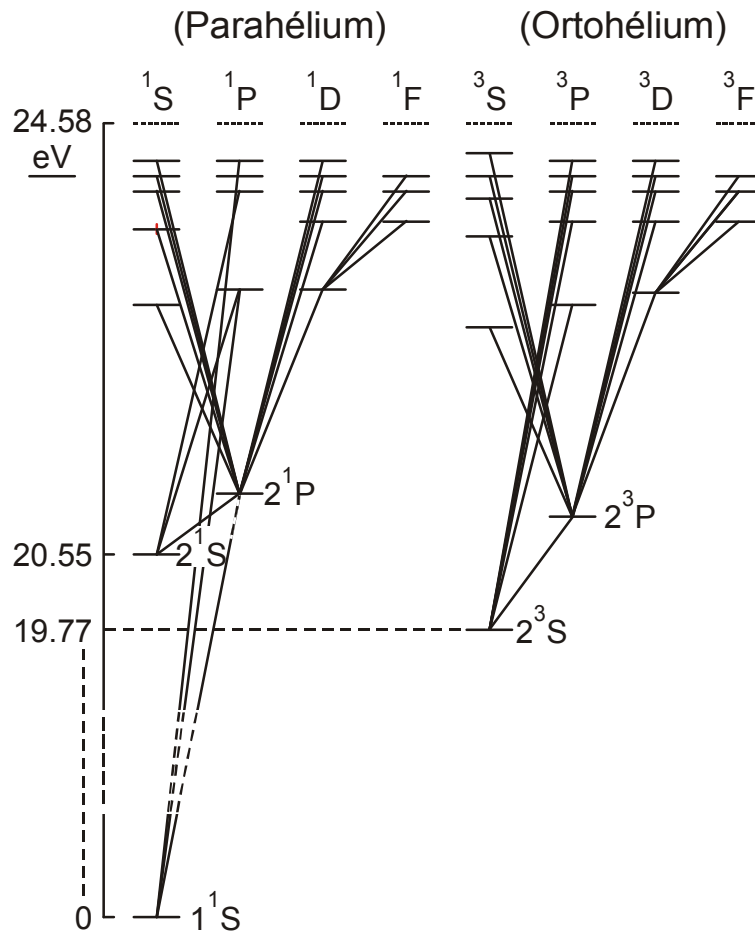
3.7. ábra. Stern-Gerlach-kísérlet



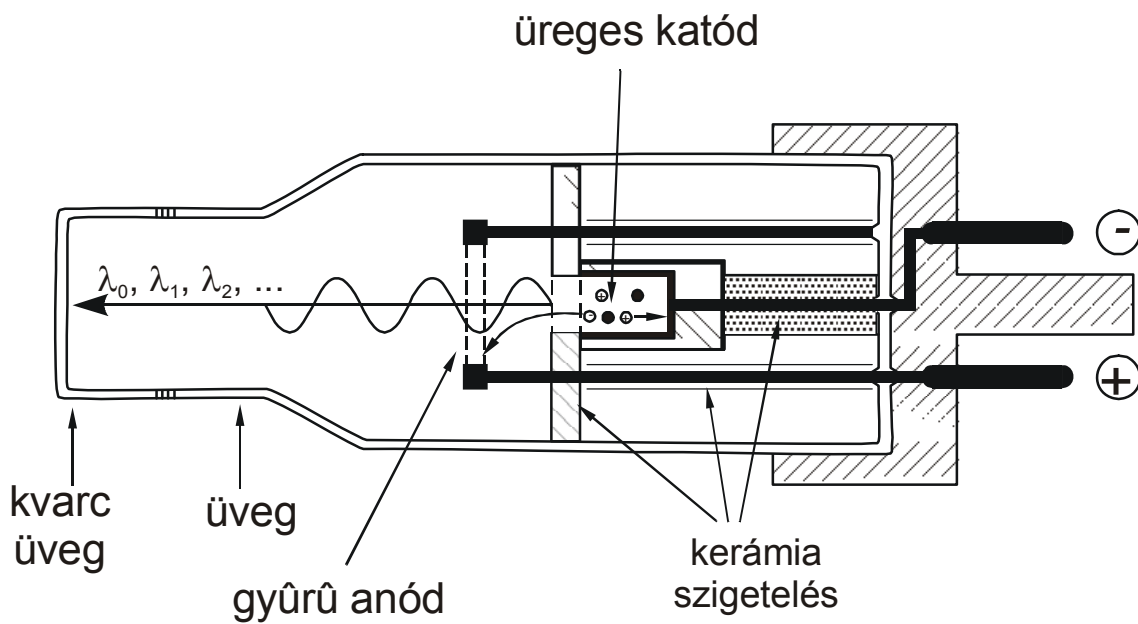
## 4. A TÖBBELEKTRONOS ATOMOK SZERKEZETE

4.1. táblázat. A héliumatom elektronállapotai

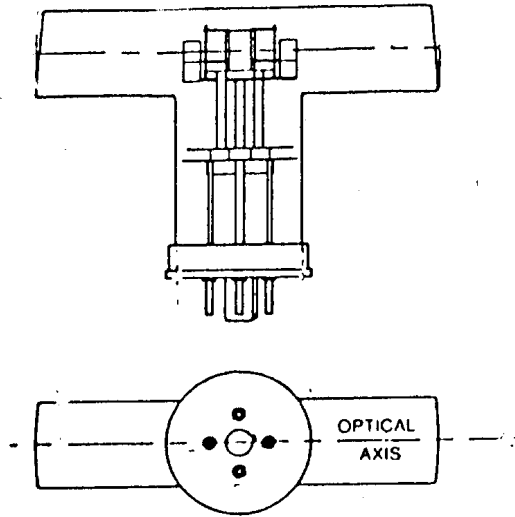
Konfiguráció	$n_{\max}$	$l_1$ $l_2$	$l_{s1}$ $l_{s2}$	$L$	$S$	$J$	Állapot
$1s^2$	1	0 0	+1/2 +1/2	0	0	0	$1^1S_0$
$1s^12s^1$	2	0 0	+1/2 +1/2	0	0	0	$2^1S_0$
	2	0 0	+1/2 +1/2	0	1	1	$2^3S_0$
$1s^12p^1$	2	0 1	+1/2 +1/2	1	0	1	$2^1P_1$
	2	0 1	+1/2 +1/2	1	1	2	$2^3P_2$
	2	0 1	+1/2 +1/2	1	1	1	$2^3P_1$
	2	0 1	+1/2 +1/2	1	1	0	$2^3P_0$



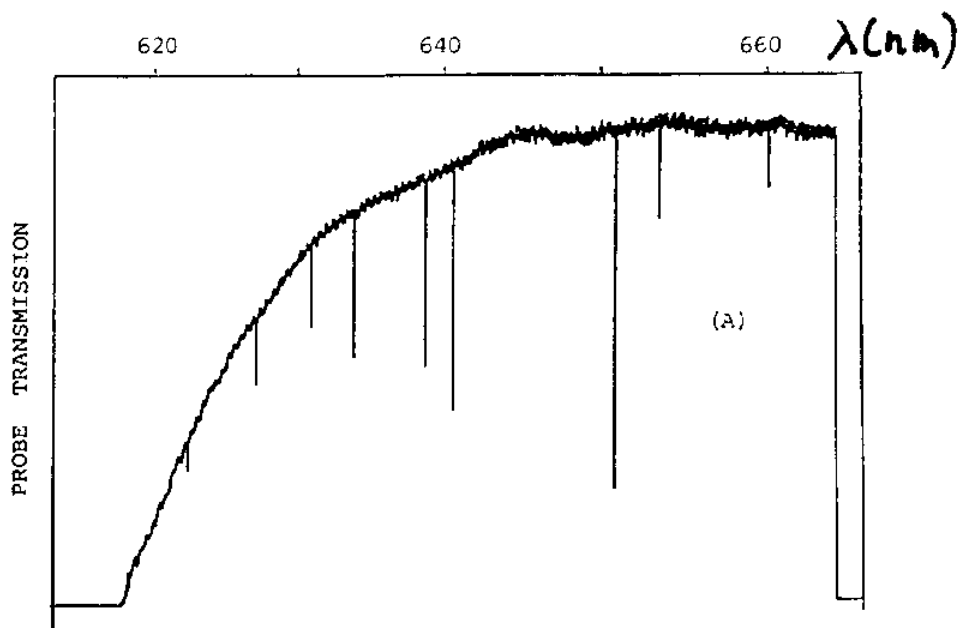
4.1. ábra. A héliumatom energiaszint-diagramja



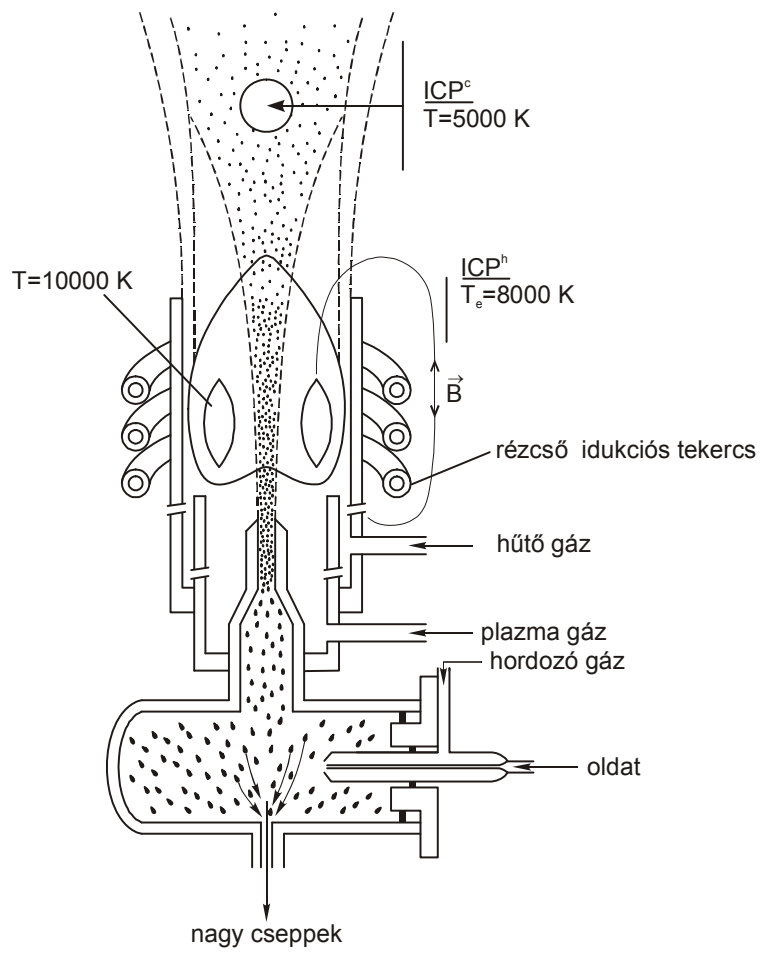
4.2. ábra. Katódüreglámpa emissziós méréshez



4.3. ábra. Katódüreglámpa abszorpciós méréshez

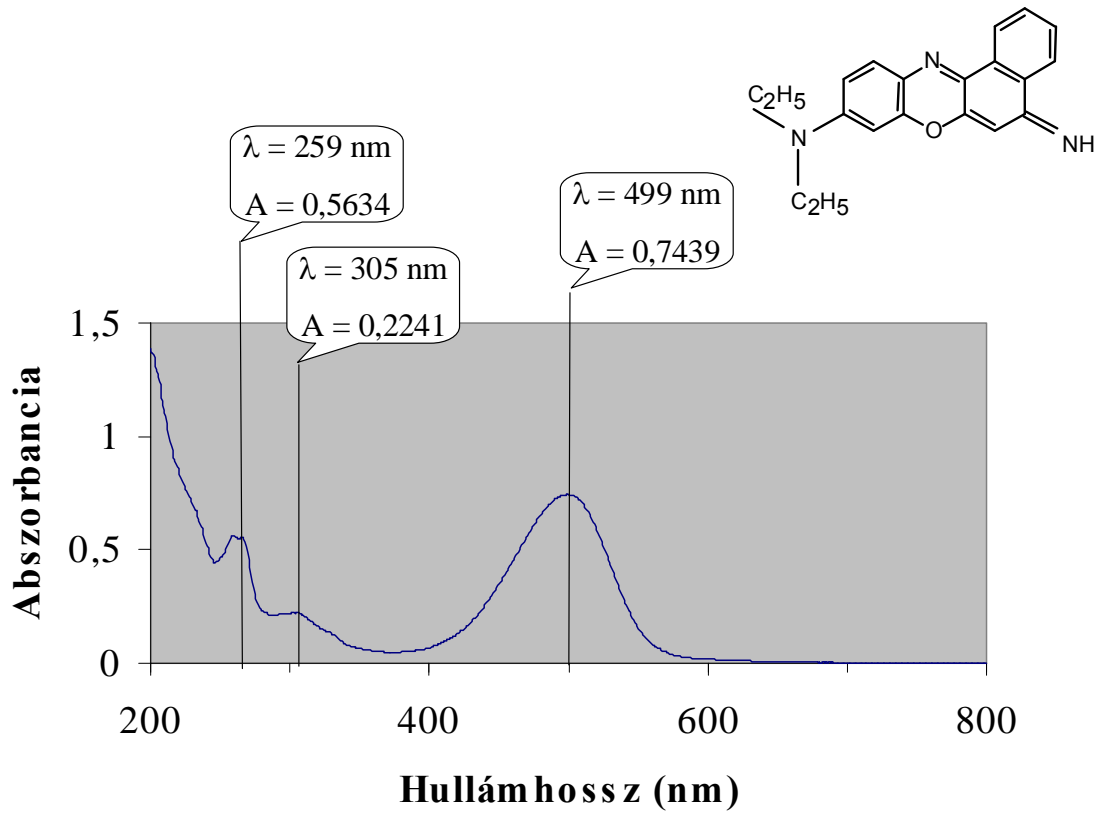


4.4. ábra. Neonnal töltött katódüreglámpa elnyelési színepe

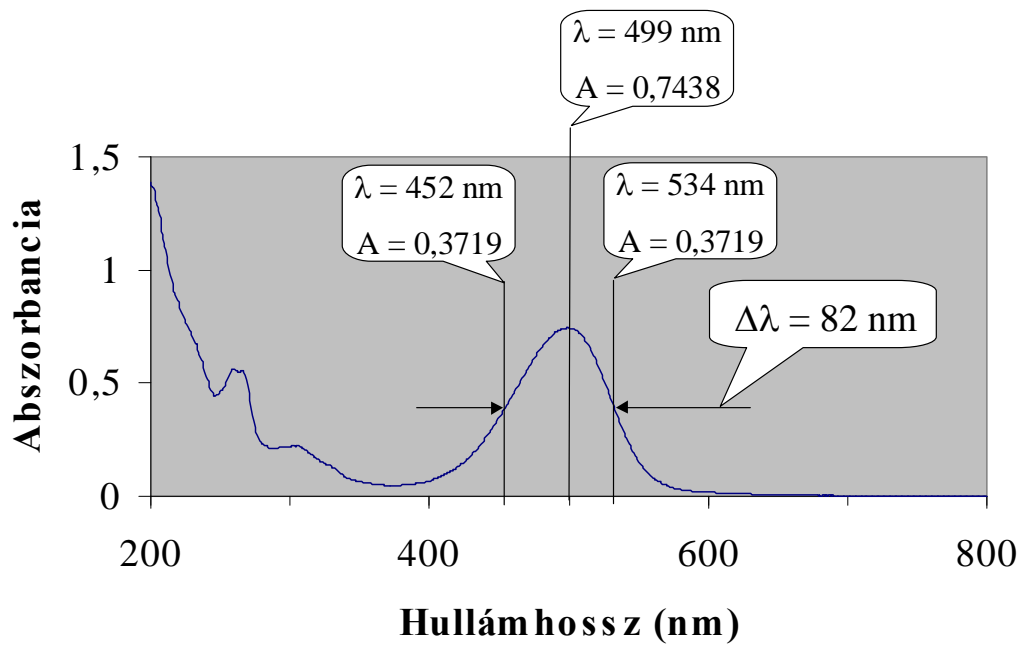


4.5. ábra. Indukciósan csatolt plazma égő (ICP-égő)

## 5. OPTIKAI SPEKTROSZKÓPIA

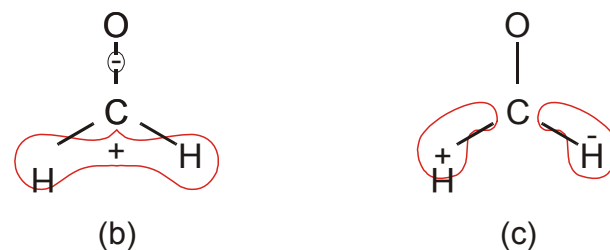
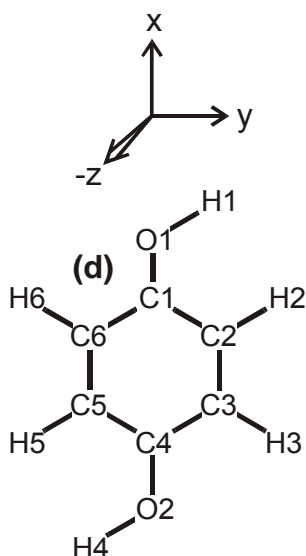
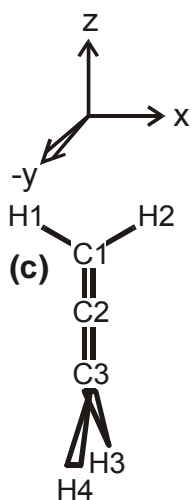
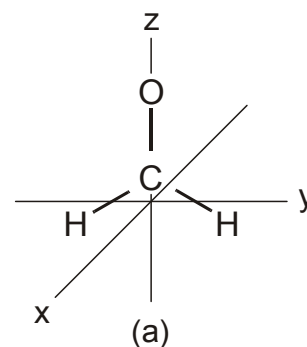
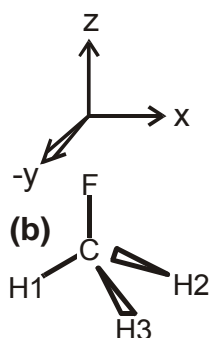
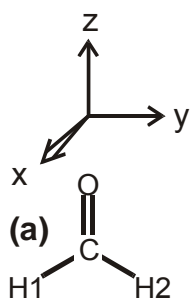


5.1. ábra. Niluskék-A festék UV-látható abszorpciós színe



5.2. ábra Félértékszélesség meghatározása

$C_{2v}$	E	$C_2^1(z)$	$\sigma_v(xz)$	$\sigma_v(yz)$	
$A_1$	+1	+1	+1	+1	$T_z, \alpha_{xx}, \alpha_{yy}, \alpha_{zz}$
$A_2$	+1	+1	-1	-1	$R_x, \alpha_{xy}$
$B_1$	+1	-1	+1	-1	$T_x, R_y, \alpha_{xz}$
$B_2$	+1	-1	-1	+1	$T_y, R_z, \alpha_{yz}$

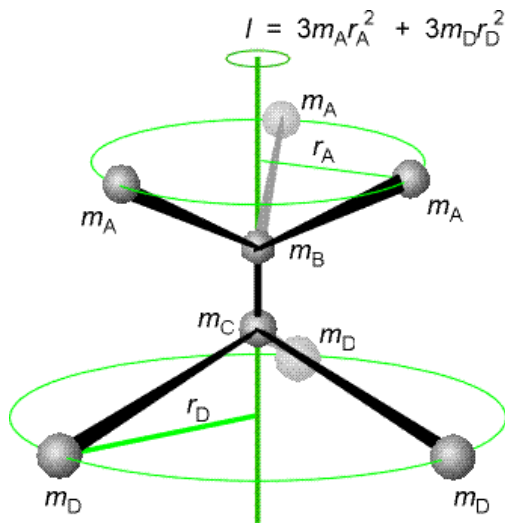
5.1. táblázat. A  $C_{2v}$  csoport karaktertáblázata

5.4. ábra. A formaldehid két molekulapályája

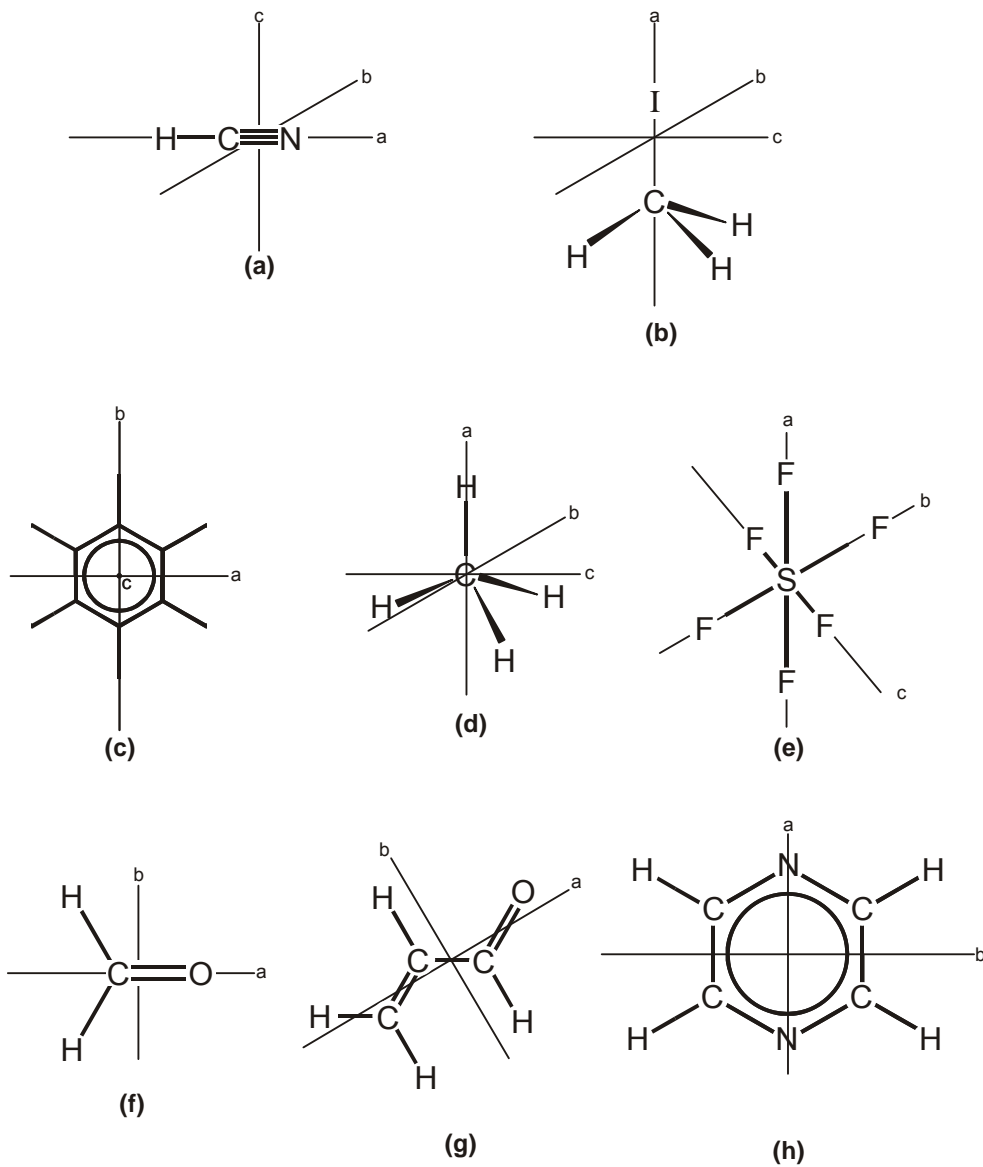
5.3. ábra. Molekulák térszerkezete

- (a) formaldehid
- (b) metilfluorid
- (c) allén
- (d) hidrokinon (anti-konformer)

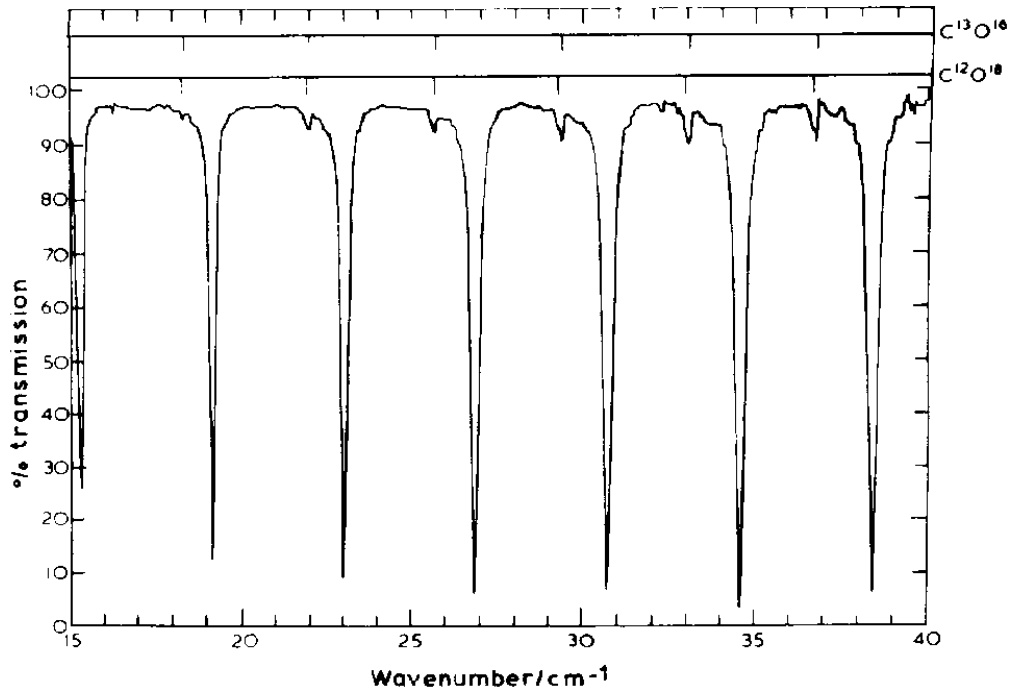
## 6. A MOLEKULÁK FORGÓMOZGÁSA



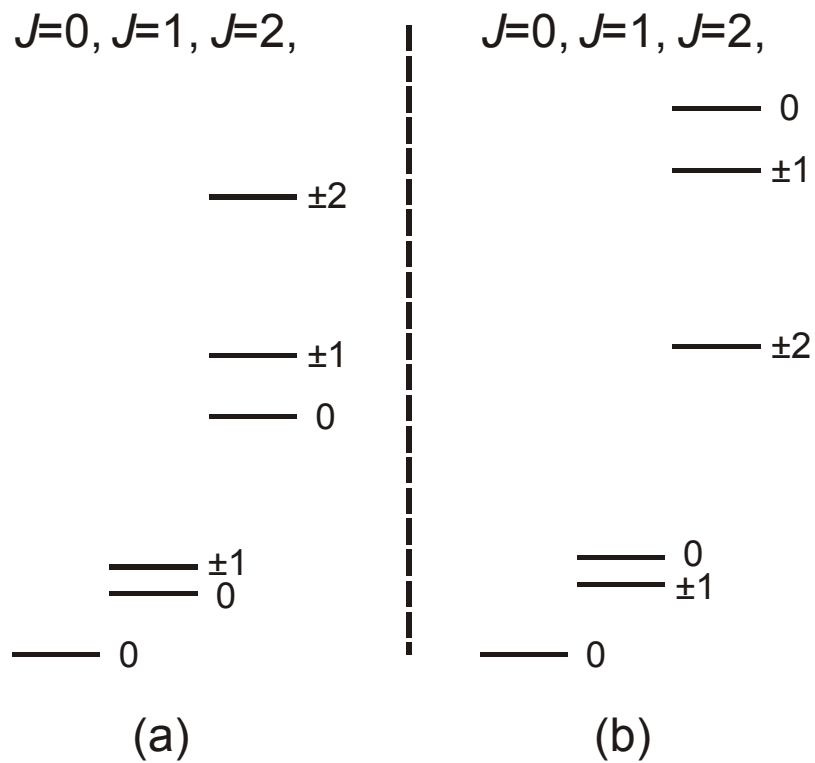
6.1. ábra. A tehetetlenségi nyomaték számítása



6.2. ábra. Molekulák fő tehetetlenségi tengelyei

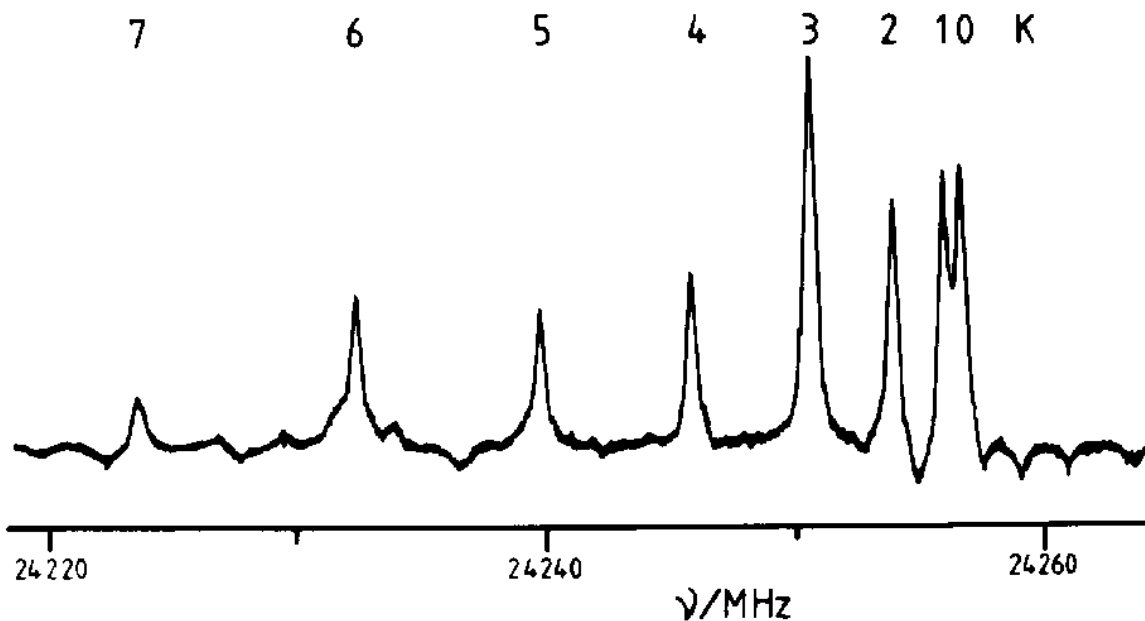


6.3. ábra. A CO molekula forgási szinképe

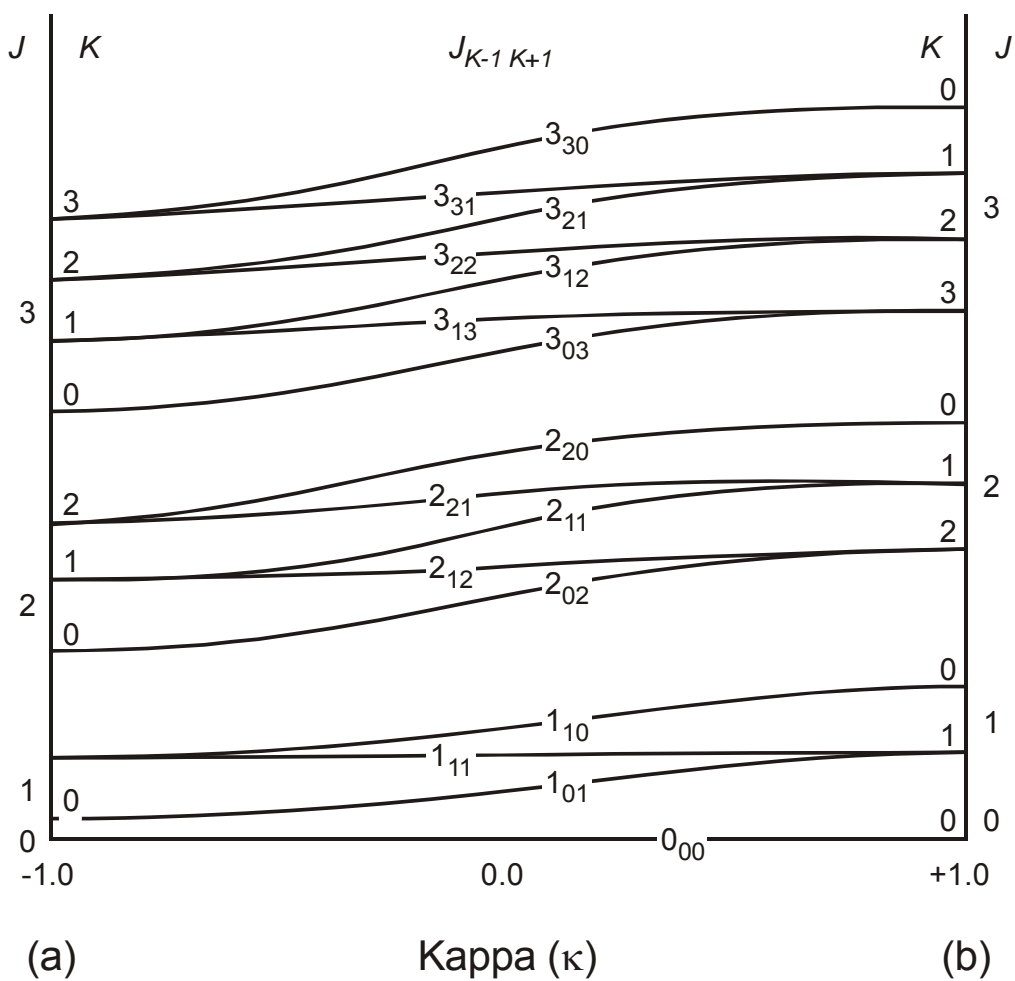


6.4. ábra. Nyújtott (a) és lapított (b) szimmetrikus pörgettyű forgási energiaszintjei.





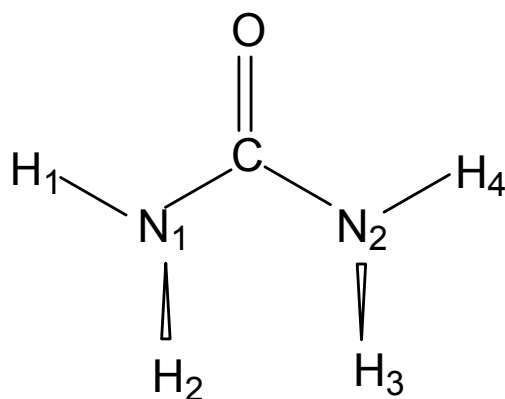
6.5. ábra. A  $J=7 \rightarrow J=8$  átmenet  $K$ -szerinti felhasadása az  $\text{SiH}_3\text{NCS}$  forgási szinképében.



6.6. ábra. Aszimmetrikus pörgettyű forgási energiaszintjei (a) nyújtott pörgettyű, (b) lapított pörgettyű,  $\kappa$  szimetriaparaméter.



6.7. ábra. A mikrohullámú spektrométer vázlatja

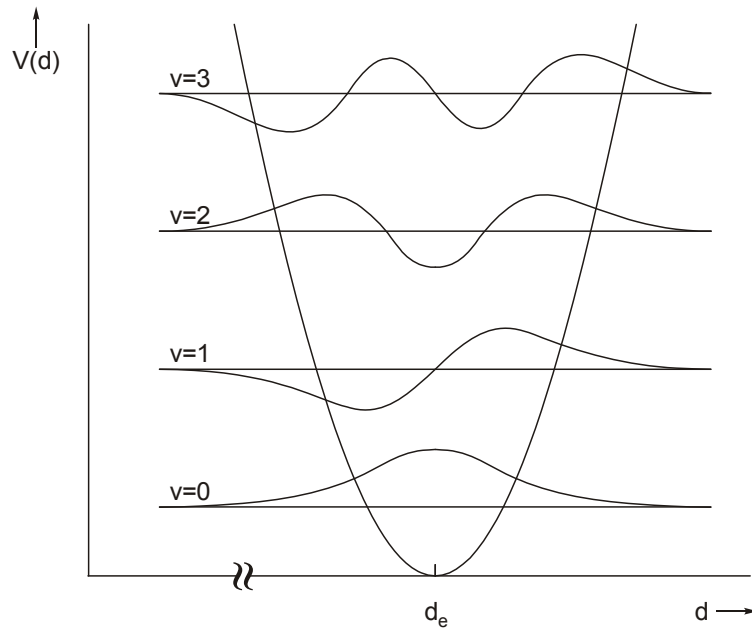


Izotópok
$\text{H}_2\text{N-CO-NH}_2$
$\text{H}_2\text{N-CO-NHD}$
$\text{H}_2\text{ }^{15}\text{N-CO- }^{15}\text{NH}_2$
$\text{H}_2\text{N-C }^{18}\text{O-NH}_2$

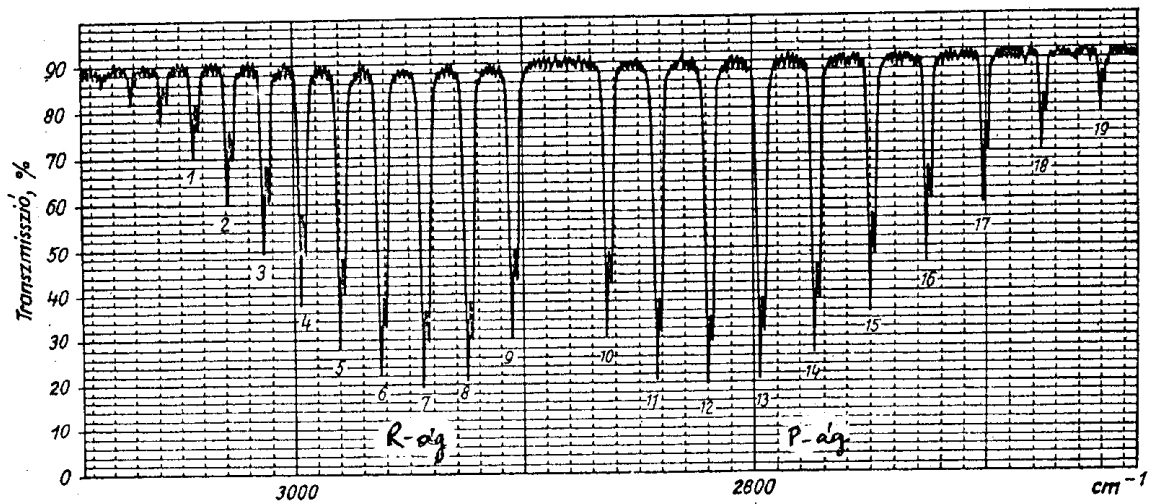
Kötéstávolság (Å)		Kötésszög (°)		Diéderes szög	
C-O	1,2211	O-C-N <sub>1</sub>	122,64	.	.
C-N <sub>1</sub>	1,3779	N <sub>1</sub> -C-N <sub>2</sub>	114,71	.	.
N <sub>1</sub> -H <sub>1</sub>	0,9978	C-N <sub>1</sub> -H <sub>1</sub>	119,21	.	.
N <sub>1</sub> -H <sub>2</sub>	1,0212	C-N <sub>1</sub> -H <sub>2</sub>	112,78	.	.
		H <sub>1</sub> -N <sub>1</sub> -H <sub>2</sub>	118,61		

6.8. ábra. Karbamid molekulageometrijának meghatározása mikrohullámú spektrumból

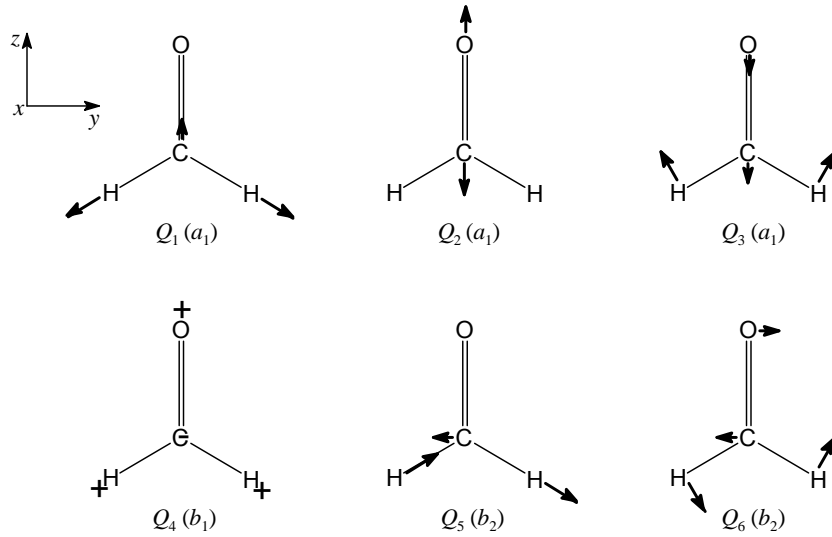
## 7. MOLEKULÁK REZGŐMOZGÁSA



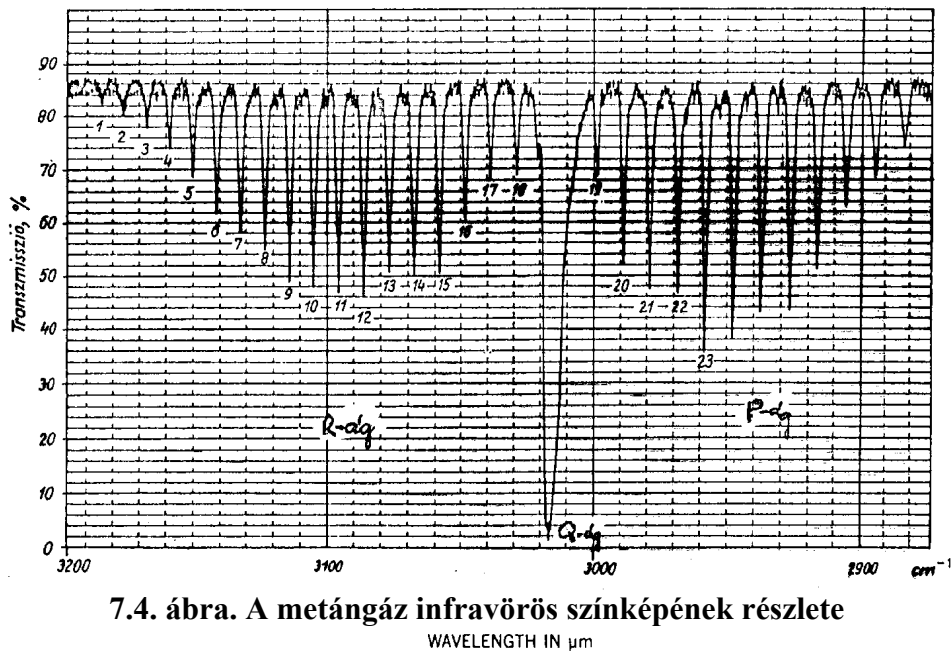
7.1. ábra. Kéttomos oszcillátor potenciálgörbéje, energiaszintjei és hullámfüggvényei.



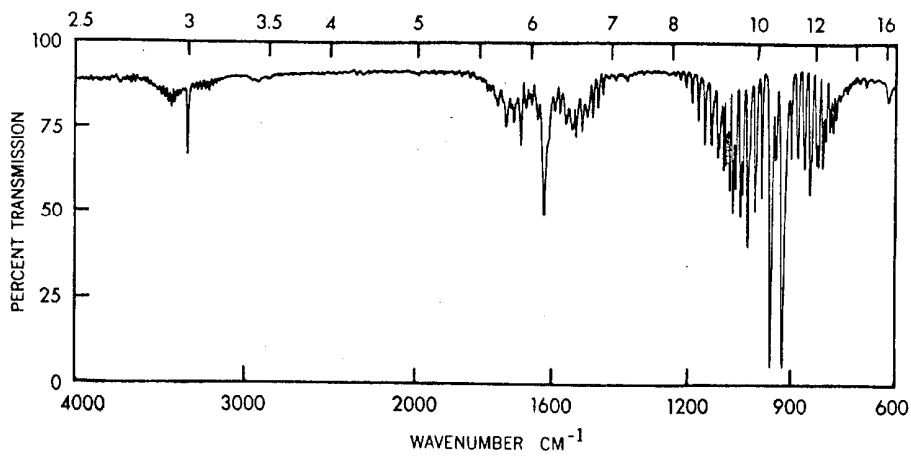
7.2. ábra. A HCl-gáz rezgési-forgási spektruma



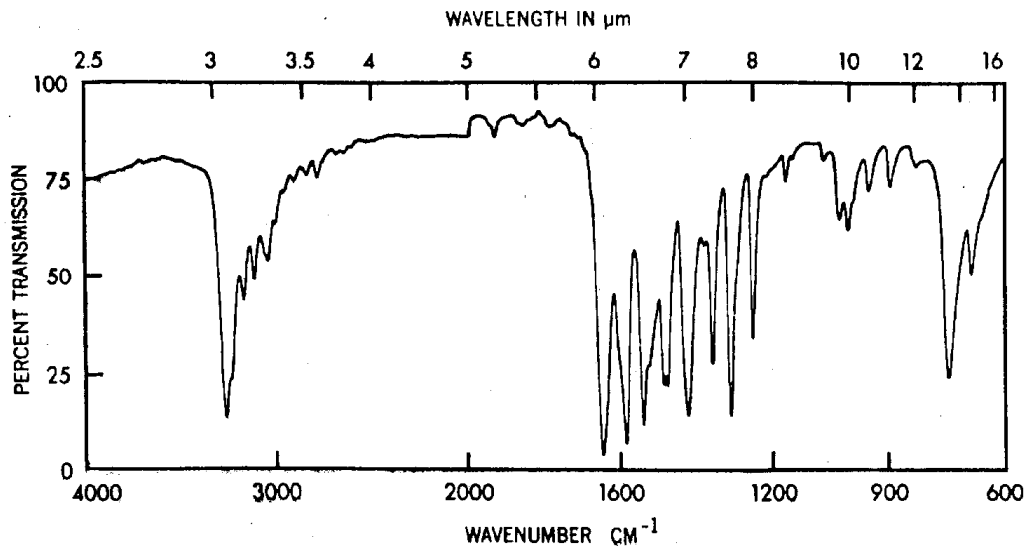
7.3. ábra. A formaldehid molekula normálrezgéseit



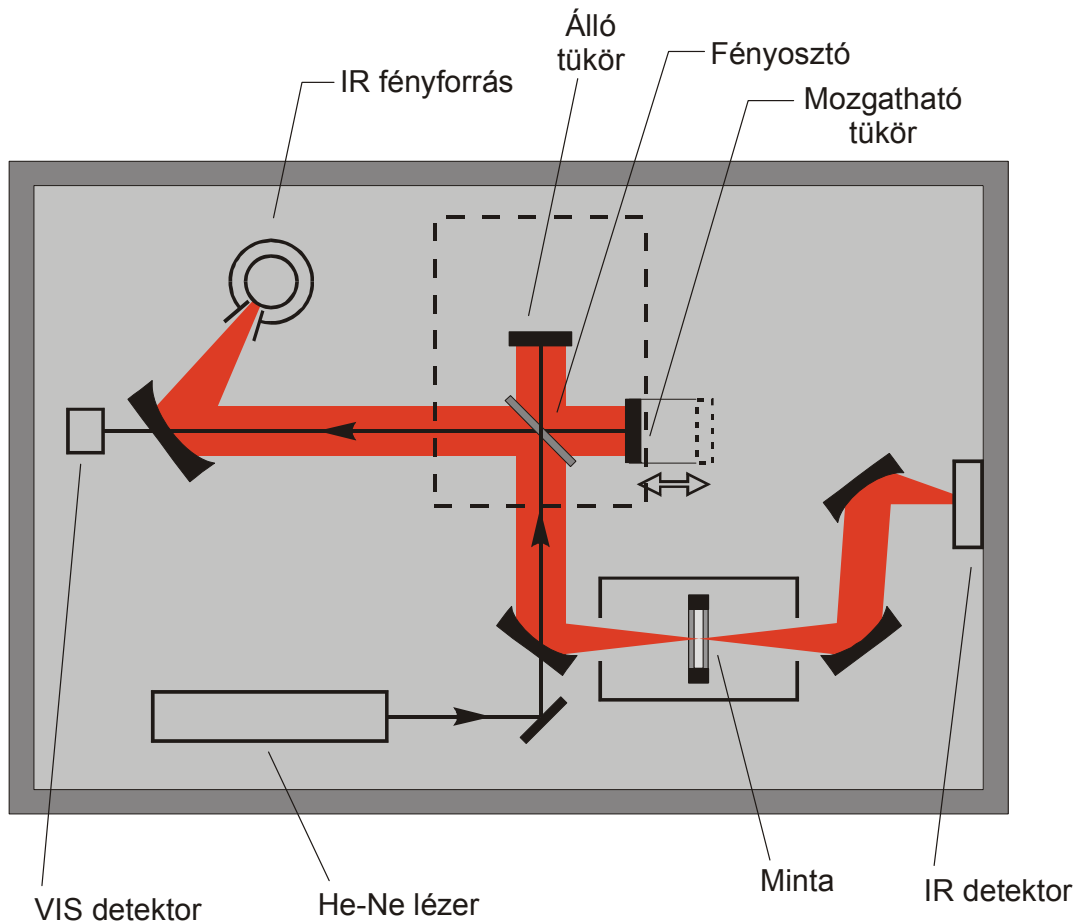
7.4. ábra. A metángáz infravörös színekének részlete



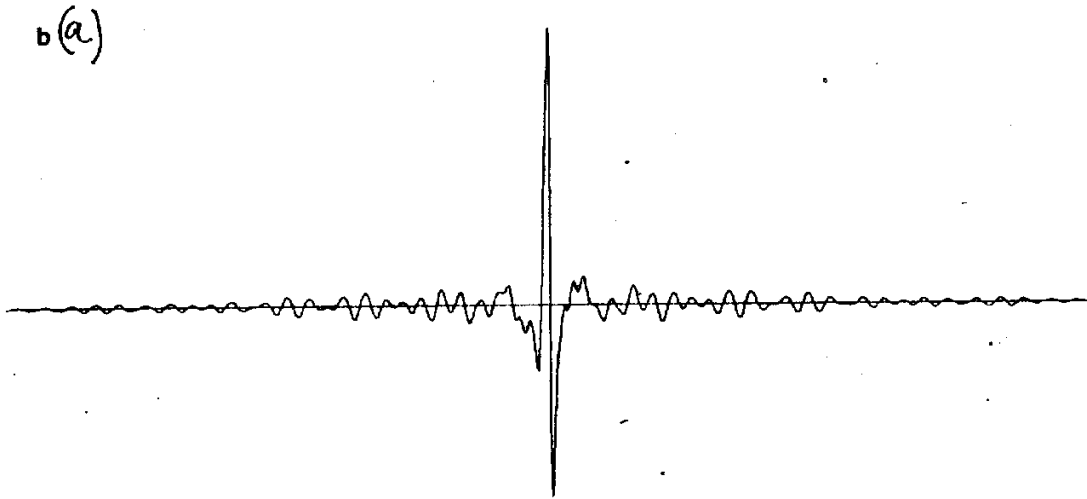
7.5. ábra. Az ammóniagáz infravörös színeké



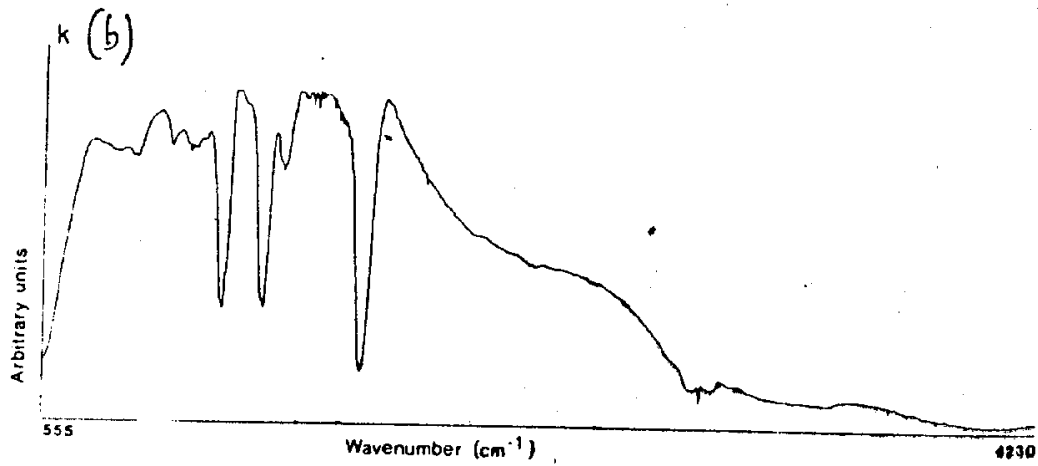
7.6. ábra. Kristályos acetanilid infravörös szinképe KBr pasztillában



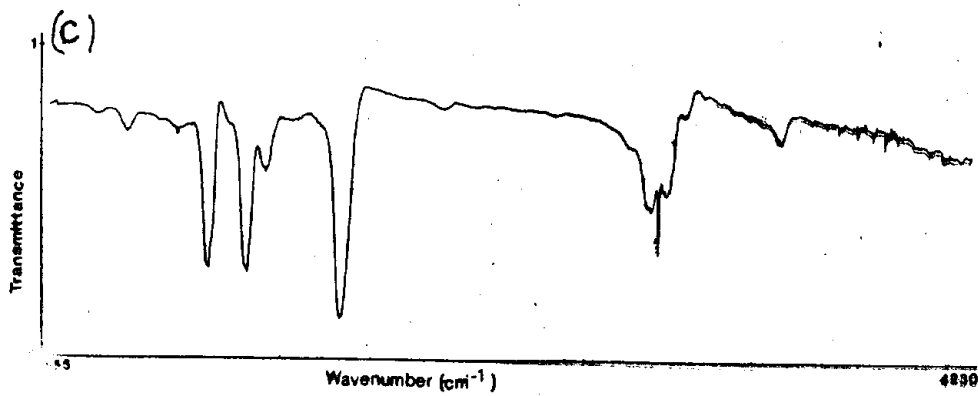
7.7. ábra. Fourier-transzformációs infravörös spektrométer



7.8a. ábra. Acetongőzről készült interferogram

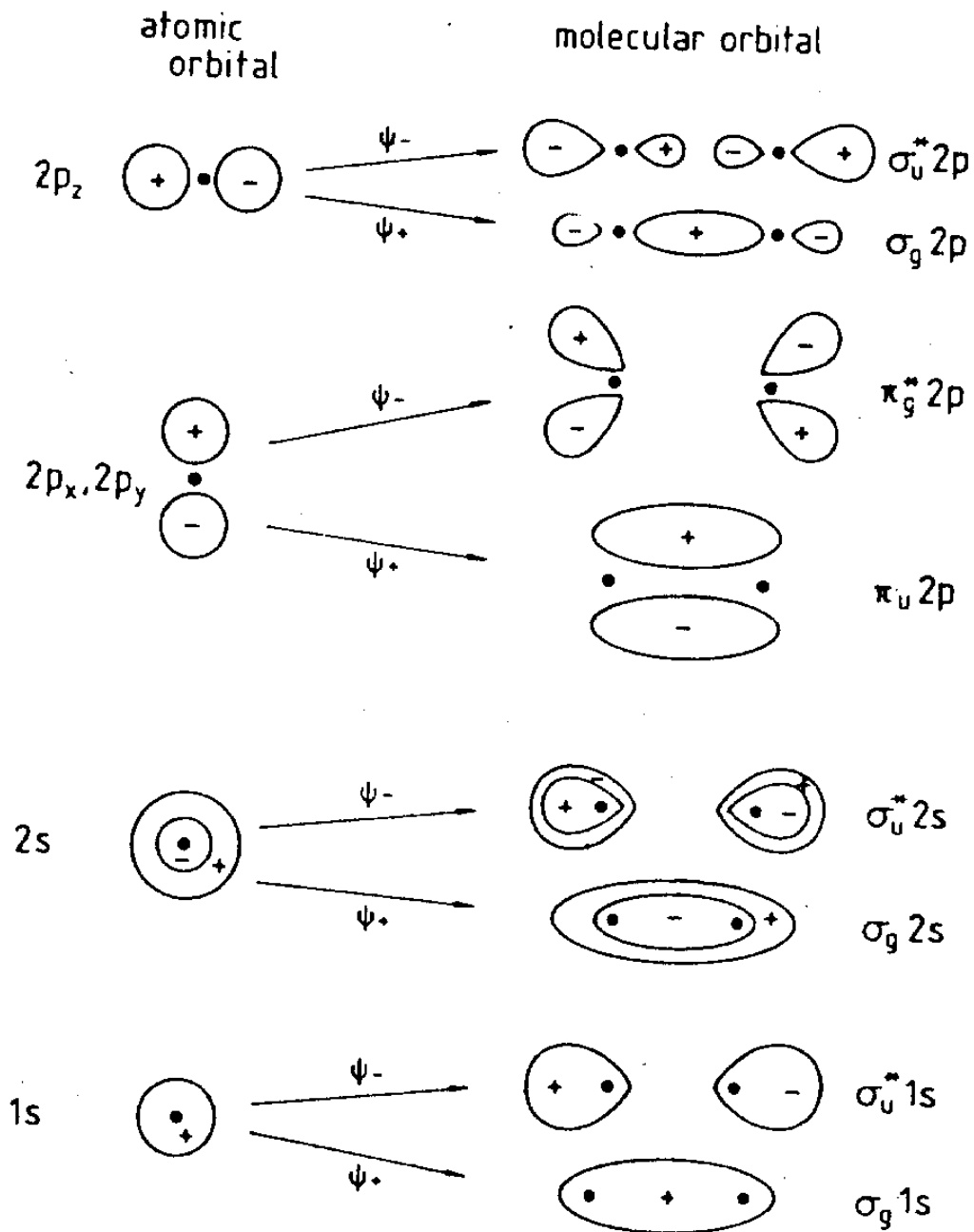


7.8b. ábra. A Fourier-transzformációval kapott spektrum

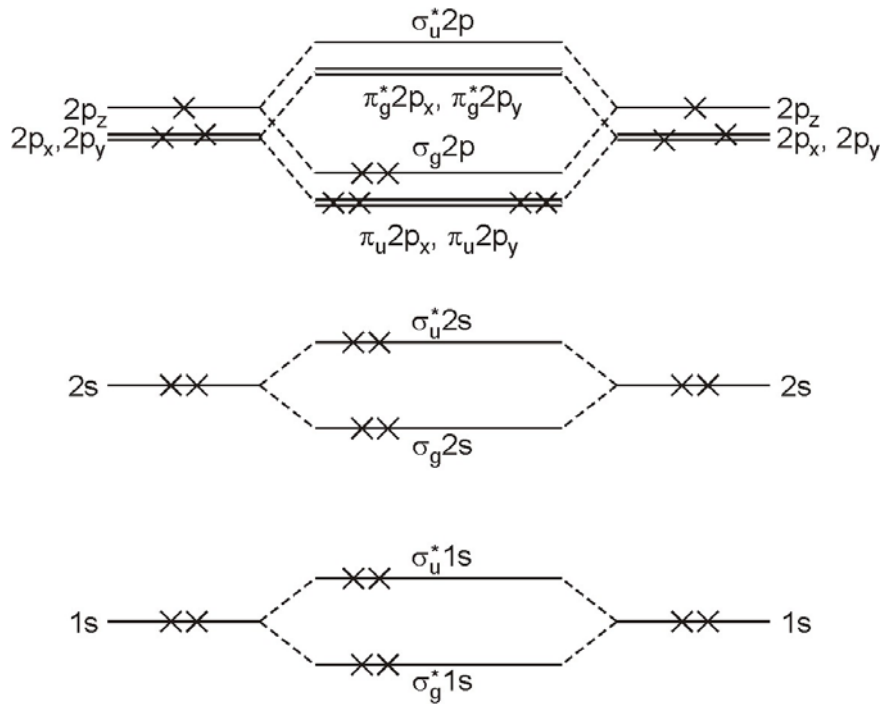


7.8c. ábra. A spektrum a háttérrel történő osztás után

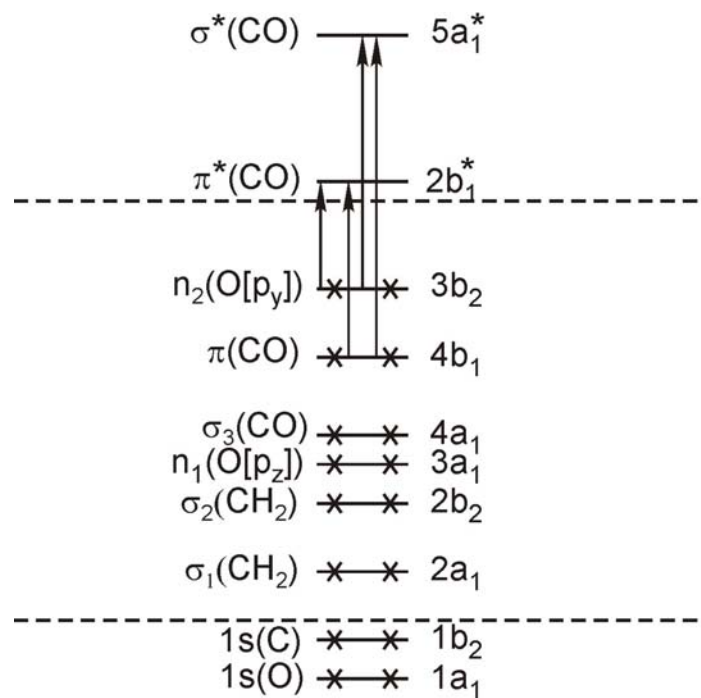
## 8. MOLEKULÁK ELEKTRONSZERKEZETE



8.1. ábra Molekulapályák előállítása atompályákból

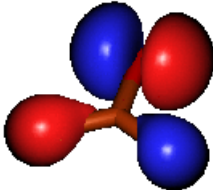
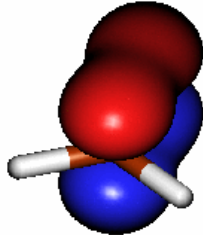
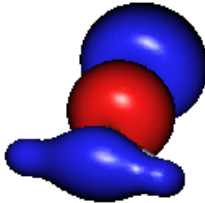
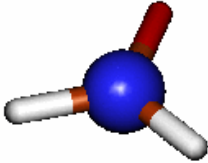
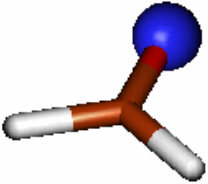


8.2. ábra. A nitrogénmolekula molekulapályaenergia-diagramja



8.3. ábra. A formaldehid molekulapályaenergia-diagramja

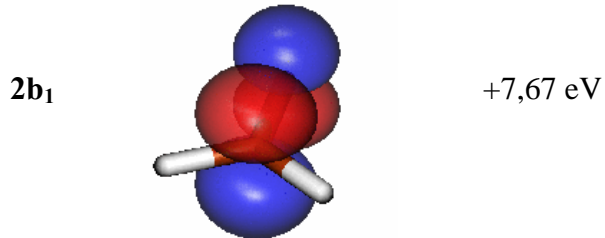
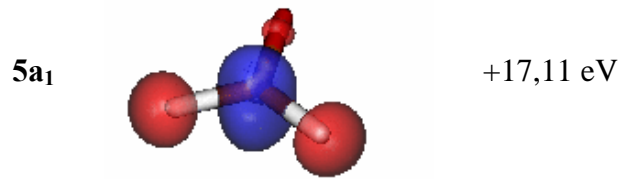


Molekulapályák		IE [eV]
<b>5a<sub>1</sub></b>	•	<b>+17,11 eV</b>
<b>2b<sub>1</sub></b>	•	<b>+7,67 eV</b>
----- 0 eV		
<b>3b<sub>2</sub></b>		-9,64 eV
<b>1b<sub>1</sub></b>		-12,06 eV
<b>4a<sub>1</sub></b>		-14,84 eV
<b>3a<sub>1</sub></b>	•	<b>-17,22 eV</b>
<b>2b<sub>1</sub></b>	•	<b>-21,98 eV</b>
<b>2a<sub>1</sub></b>	•	<b>-36,39 eV</b>
<b>1b<sub>2</sub></b>		-302,73 eV
<b>1a<sub>1</sub></b>		-552,74 eV

8.4a. ábra. A formaldehid betöltött molekulapályái

Molekulapályák

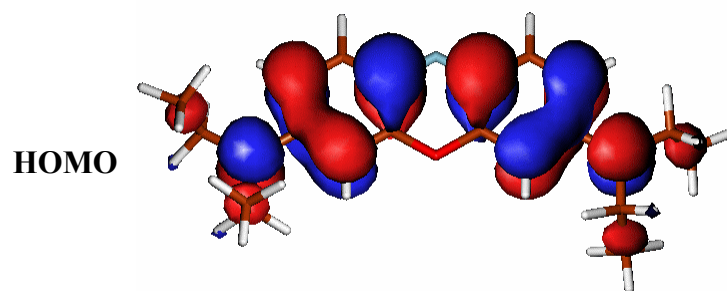
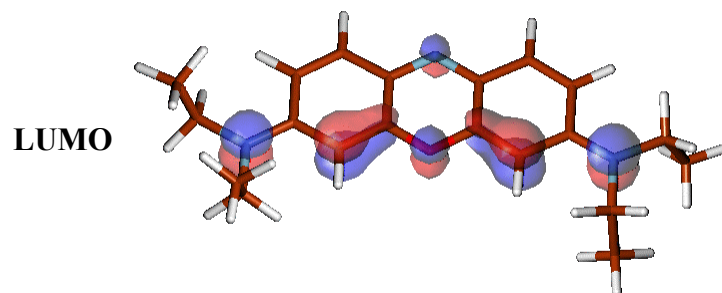
IE [eV]



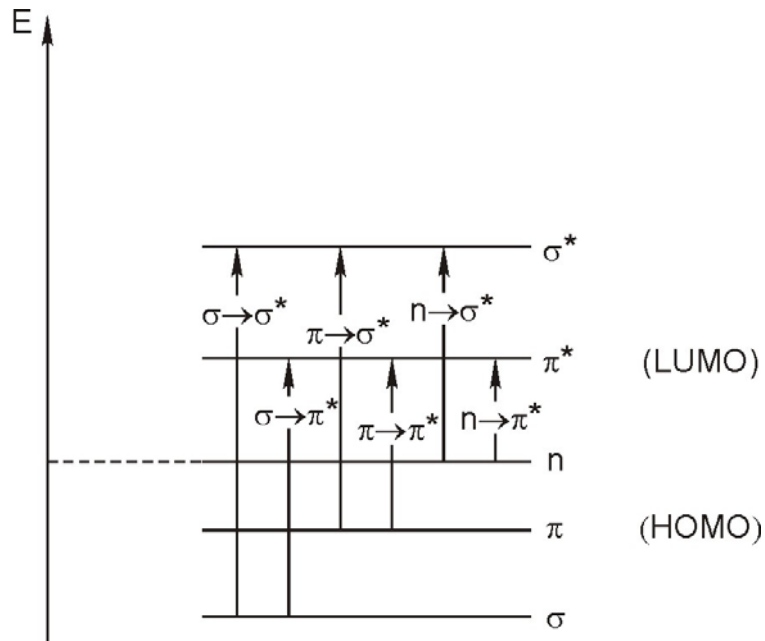

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3b <sub>2</sub>	•	-9,64 eV	0 eV
1b <sub>1</sub>	•	-12,06 eV	
4a <sub>1</sub>	•	-14,84 eV	
3a <sub>1</sub>	•	-17,22 eV	
2b <sub>1</sub>	•	-21,98 eV	
2a <sub>1</sub>	•	-36,39 eV	
1b <sub>2</sub>	•	-302,73 eV	
1a <sub>1</sub>	•	-552,74 eV	

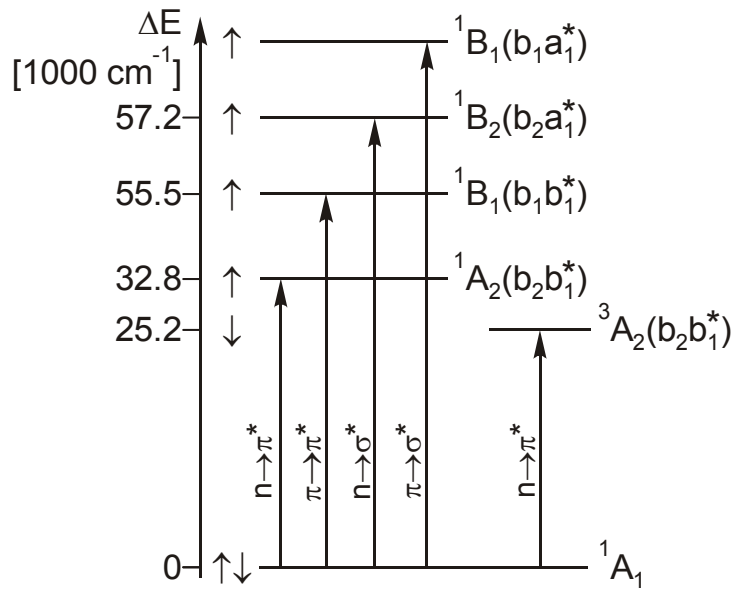
8.4b. ábra. A formaldehid betöltetlen molekulapályái



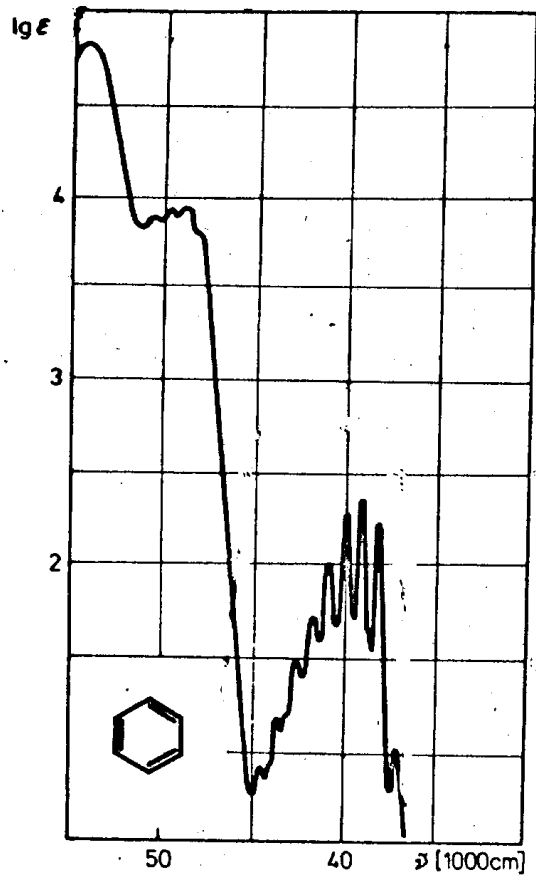
8.5. ábra. Az oxazin-1 kation két molekulapályája



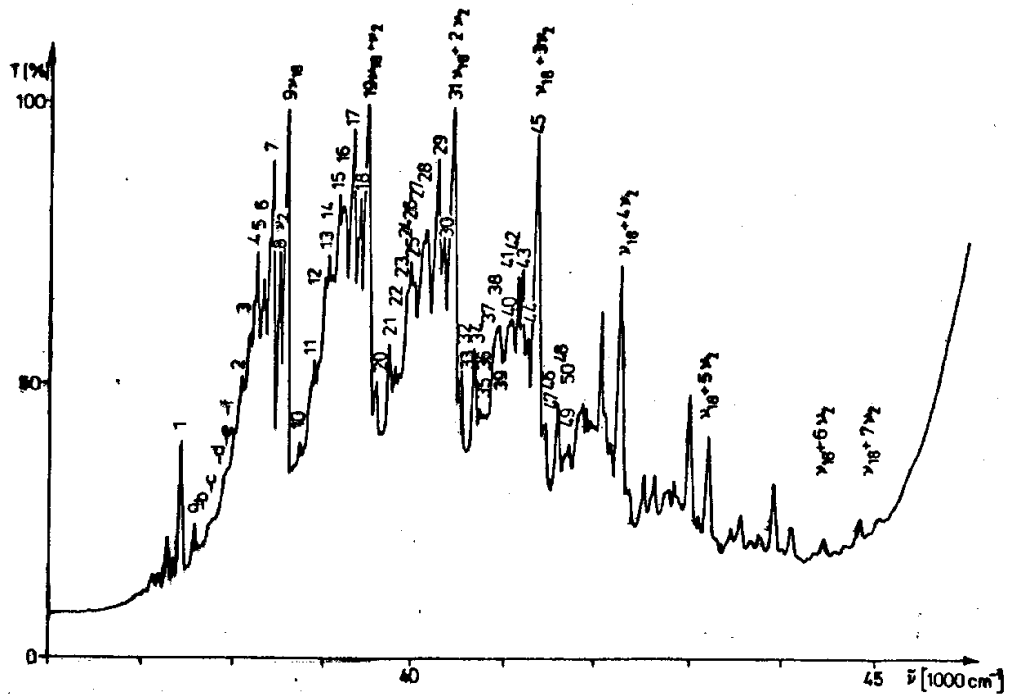
8.6. ábra. Elektronátmenetek és jelöléseik



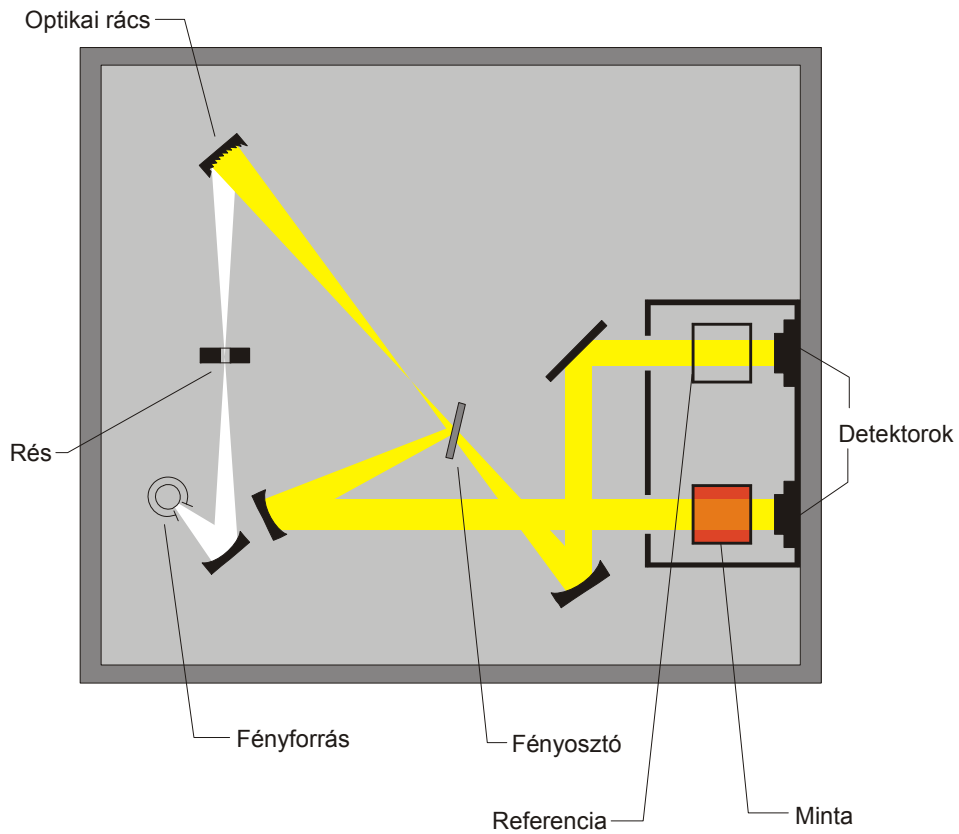
8.7. ábra. A formaldehid elektronátmenetei



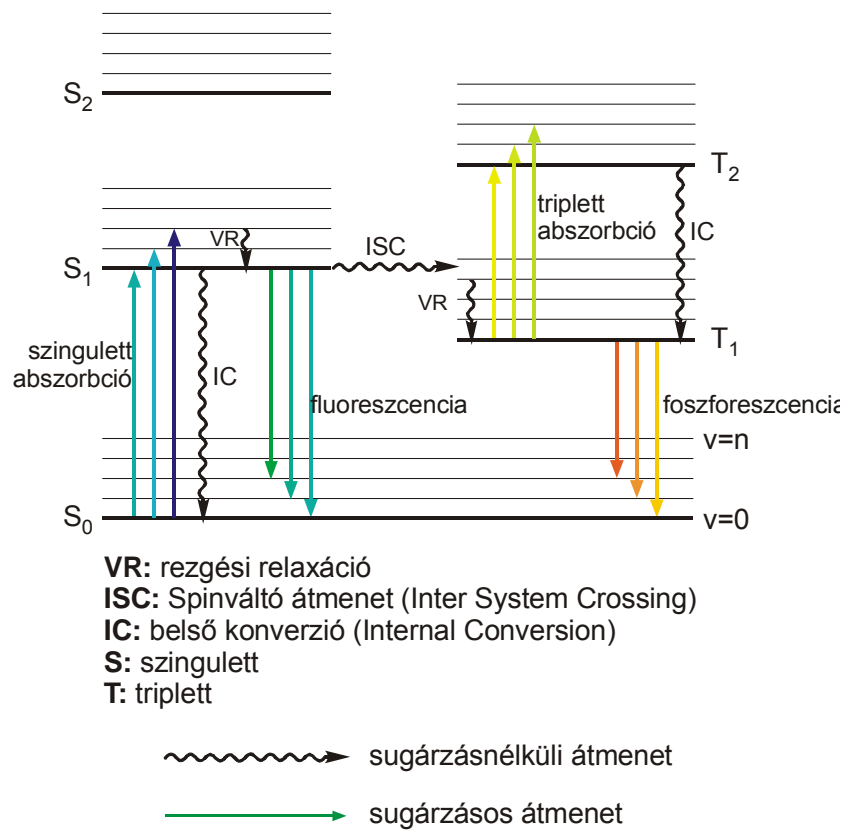
8.8. ábra. A benzol elektronszínképe (etanolos oldat)



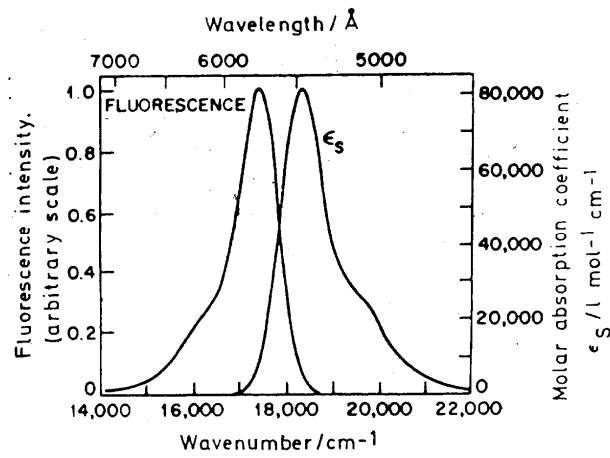
8.9. ábra. A benzol elektronszínképe (gőz)



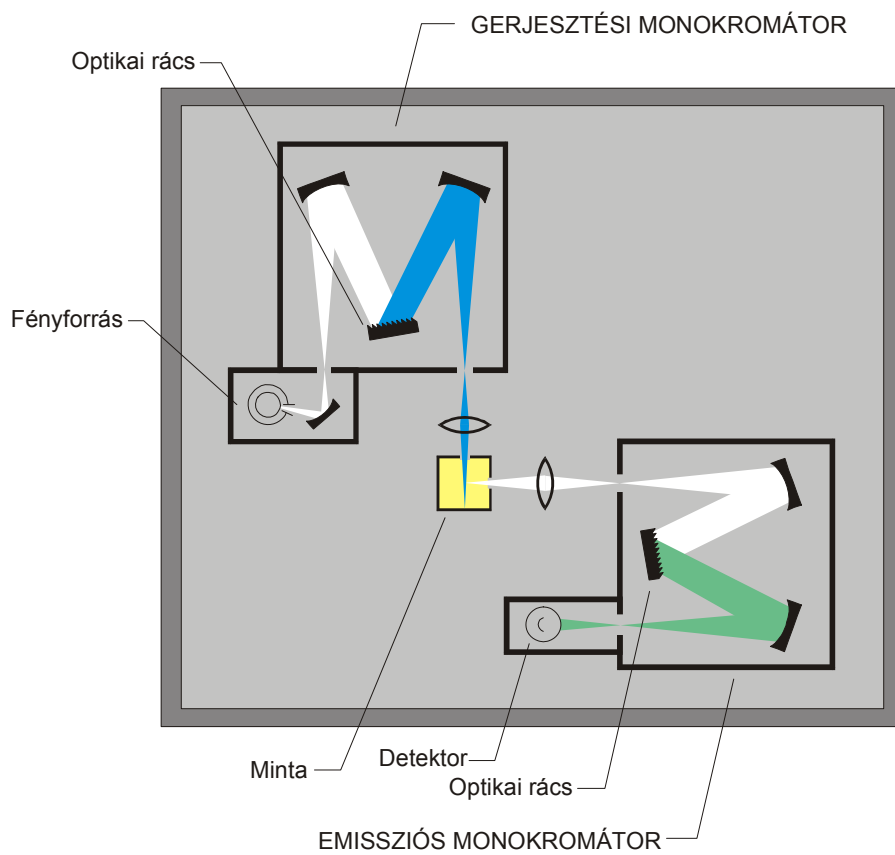
8. 10. ábra. Kétutas UV-látható abszorpciós spektrométer



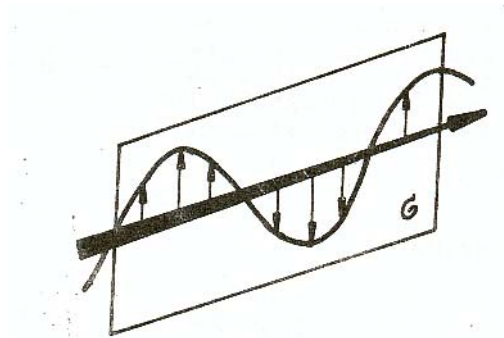
8.11. ábra. Jablonski-diagram



8.12. ábra. Rodamin-B festék abszorpciós és emissziós színepe

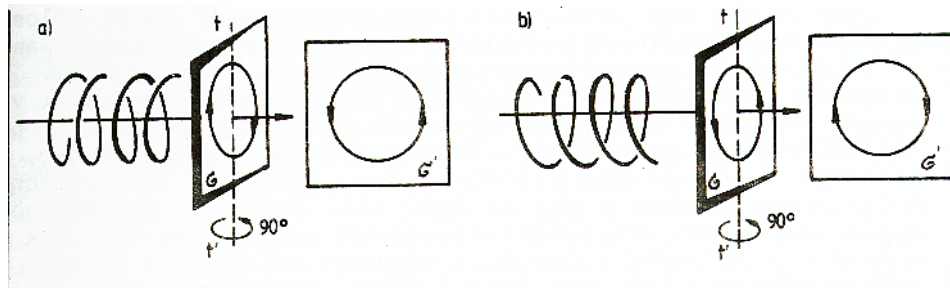


8.13. ábra Spektrofluoriméter

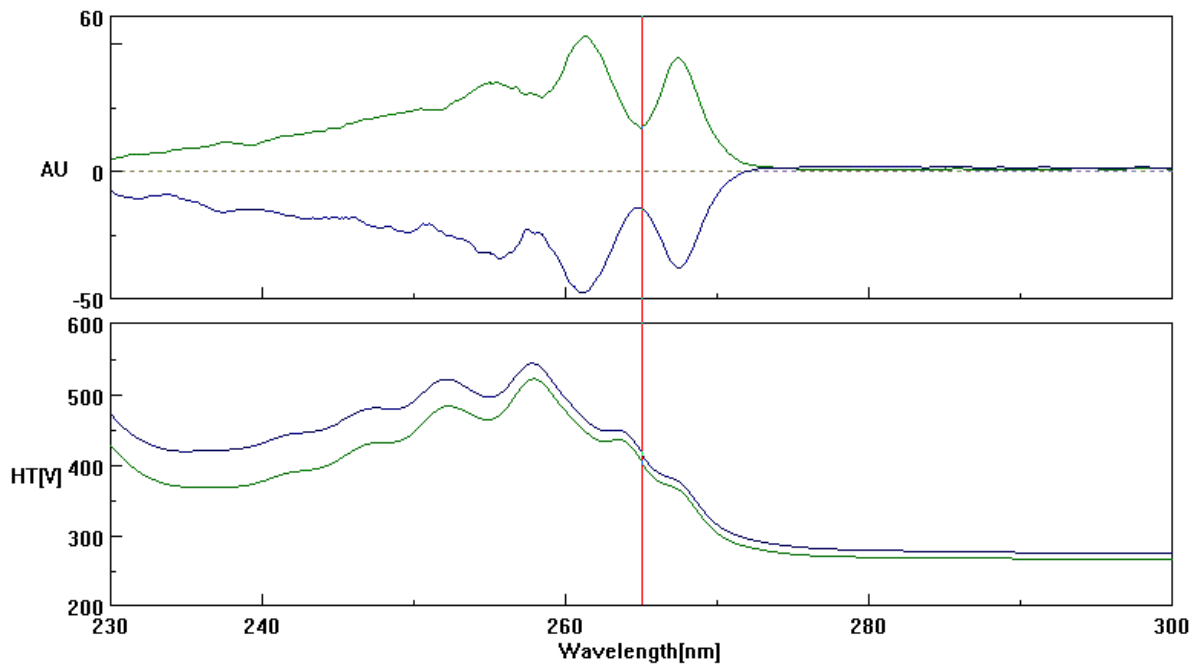


a fény terjedési iránya: a vékonyodó nyíl iránya,  
 $\sigma$ : a polarizáció síkja.

8.14. ábra. Lineárisan polarizált fény

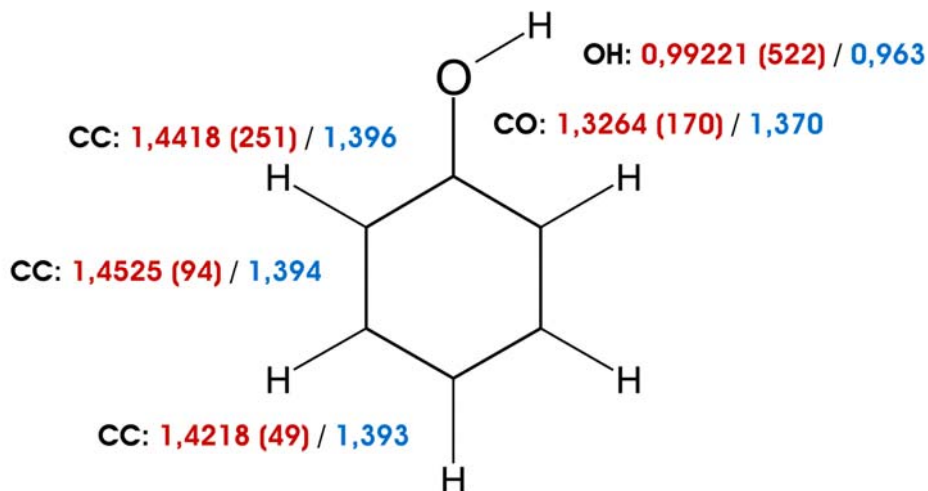


8.15. ábra. Jobbra és balra körülarisan polarizált fény



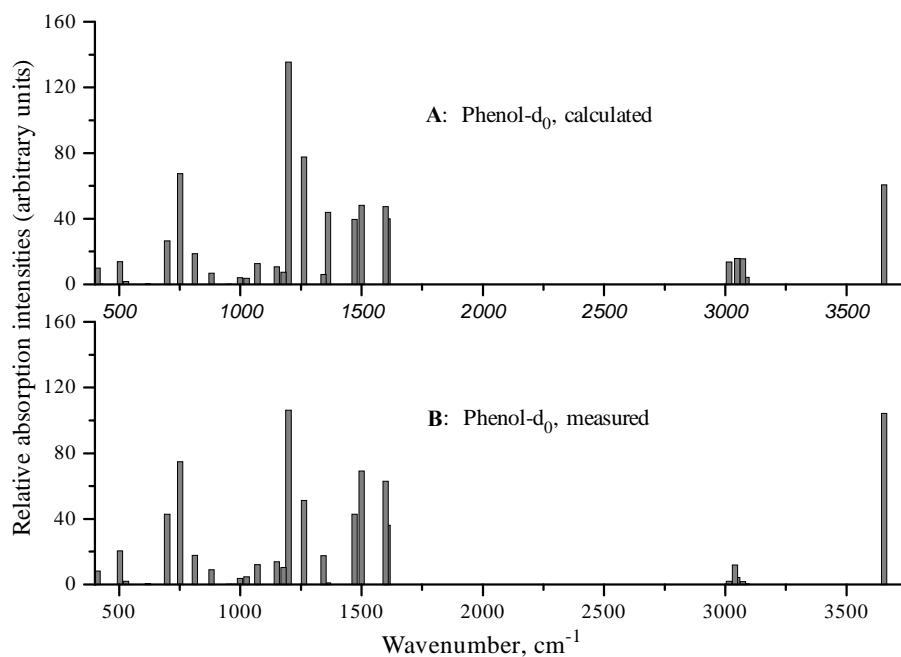
8.16. ábra. (R)- és (S)-fenil-etil-amin CD-spektruma

## Fenol gázfázisú mért és számított szerkezete (kötéshosszak Angstrom-ben)



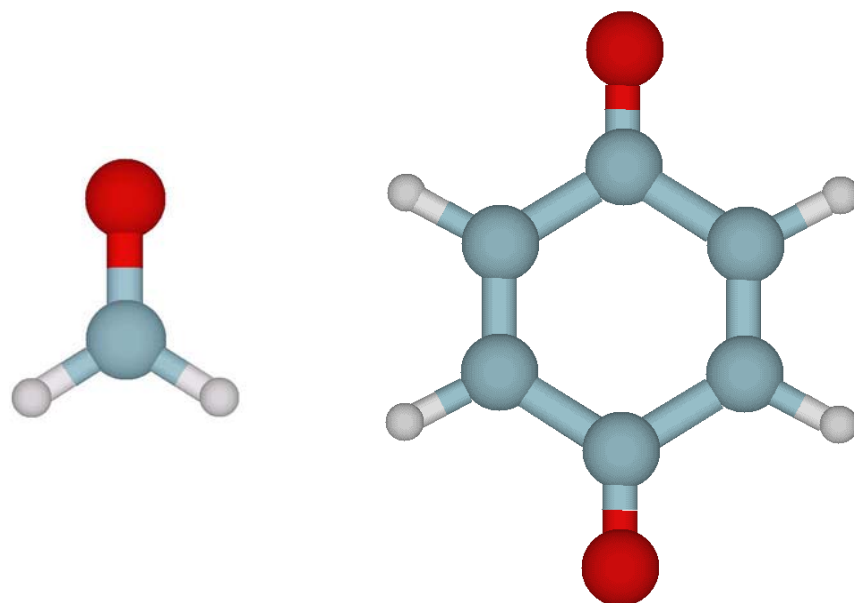
Jelölés: **MW adat**  $r_0$  (hiba) / **B3LYP/6-311+G(d,p) adat**  
Forrás: *Chem. Phys.* 2002, **283**, 153.

### 8.17. A fenolmolekula geometriája

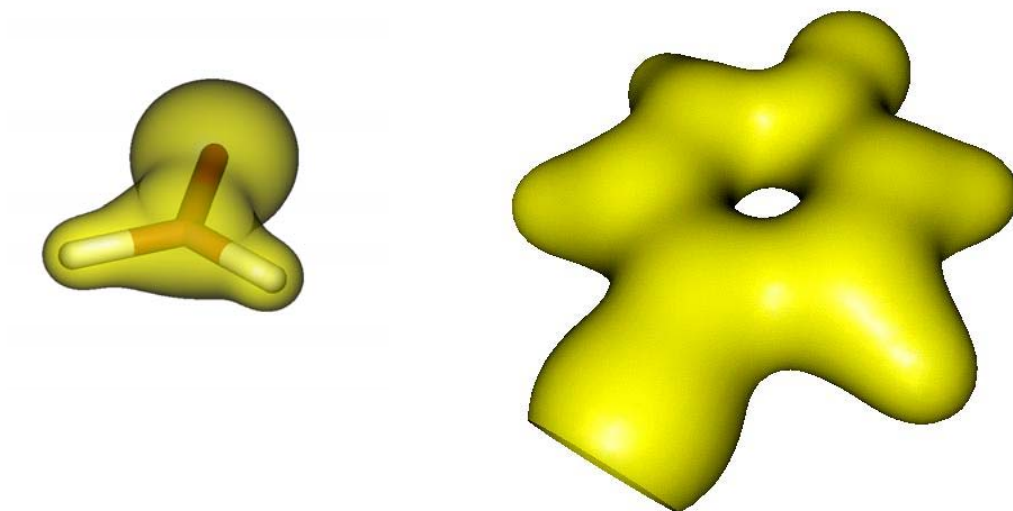


### 8.18. ábra. A fenolmolekula számított és mért rezgési színepe





8.19. ábra. Formaldehid és p-benzokinon pálcikamodellje



8.20. ábra. Formaldehid és p-benzokinon elektronfelhője

