

Синергетика

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**Коллективные возбуждения,
качественная перестройка
спектров**

"Коллективные" возмущения

$$\hat{H} = \hat{H}_0 + \hat{V}$$

$$\hat{H}_0 \varphi_i^0 = \varepsilon_i^0 \varphi_i^0$$

$$\langle \varphi_i^0 | \hat{H}_0 | \varphi_j^0 \rangle = \varepsilon_i^0 \delta_{ij}$$

$$\langle \varphi_i^0 | \varphi_j^0 \rangle = \delta_{ij}$$

$$\hat{H} \Psi_j = E_j \Psi_j$$

$$\Psi_j = \sum_i A_j^i \varphi_i^0 \quad \sum_i |A_j^i|^2 = 1$$

$$\langle \varphi_k^0 | (\hat{H}_0 + \hat{V} - E_j) \sum_i A_j^i \varphi_i^0 = 0$$

$$\sum_i A_j^i \langle \varphi_k^0 | \hat{H}_0 - E_j | \varphi_i^0 \rangle + \sum_i A_j^i \langle \varphi_k^0 | \hat{V} | \varphi_i^0 \rangle = 0$$

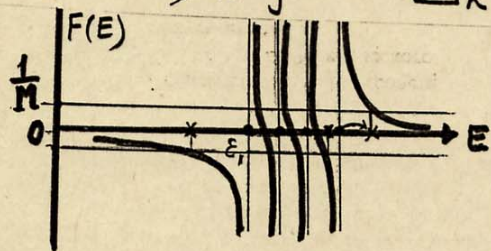
$$\sum_i A_j^i (\varepsilon_k^0 - E_j) \delta_{ik} + \sum_i A_j^i \cdot M = 0$$

$$A_j^k (\varepsilon_k^0 - E_j) = -M \sum_i A_j^i$$

$$\left(\sum_k \right)$$

$$A_j^k = - \frac{M}{\varepsilon_k^0 - E_j} \sum_i A_j^i \quad (*)$$

$$\sum_k A_j^k = - \sum_k \frac{M}{\varepsilon_k^0 - E_j} \sum_i A_j^i$$



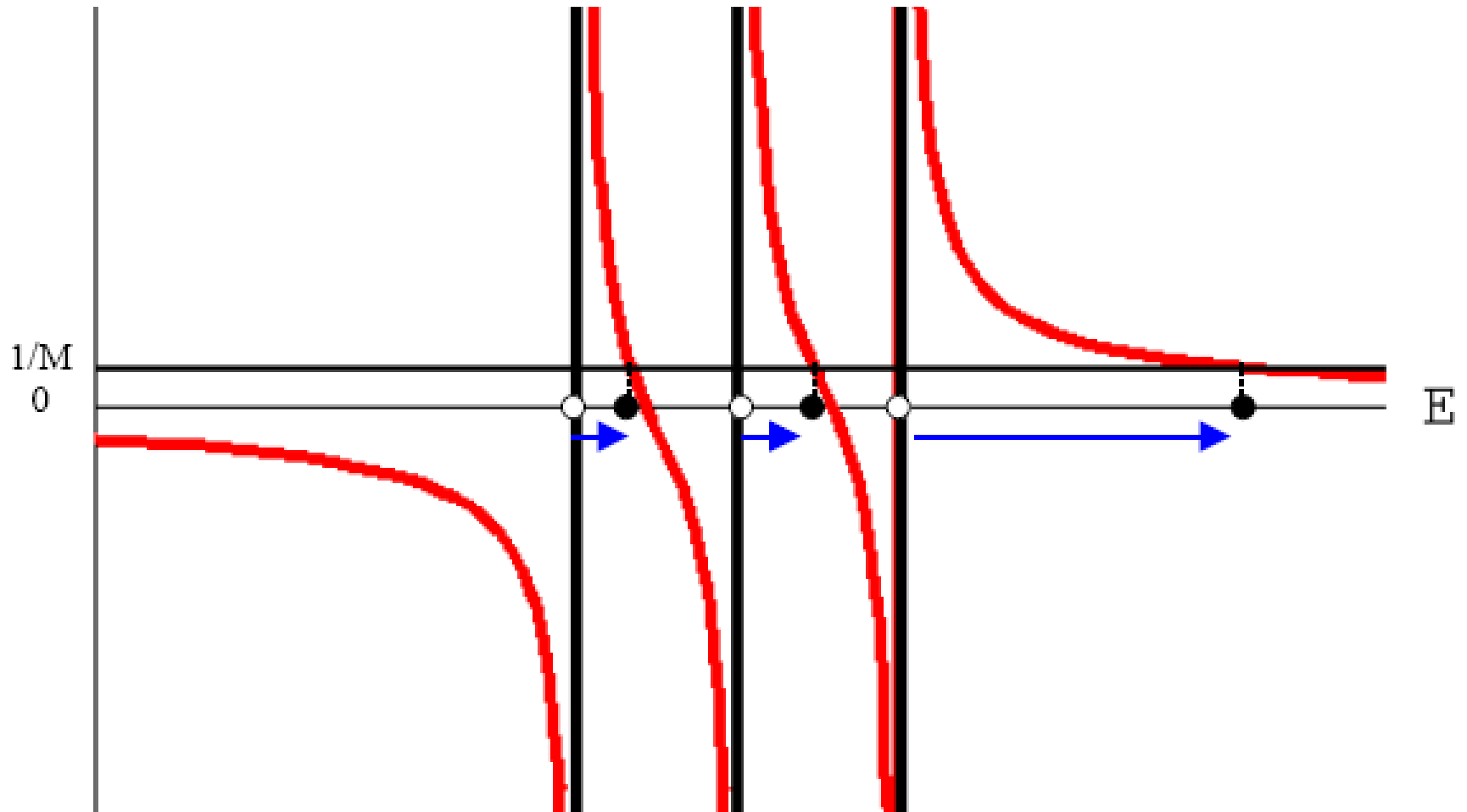
$$- \frac{1}{M} = \sum_k \frac{1}{\varepsilon_k^0 - E_j} = F_j$$

$$\mathcal{D}_j = \langle 0 | \hat{d} | \Psi_j \rangle = \sum_i A_j^i \langle 0 | \hat{d} | \varphi_i^0 \rangle = \sum_i A_j^i \cdot d$$

$$(**) \left(\sum_k \right) A_j^k = - \frac{M}{\varepsilon_k^0 - E_j} \cdot \frac{\mathcal{D}_j}{d}; \quad 1 = + \left(\frac{M \mathcal{D}_j}{d} \right)^2 \sum_k \left(\frac{1}{\varepsilon_k^0 - E_j} \right)^2;$$

$$\mathcal{D}_j^2 = \frac{d^2}{M^2} \frac{1}{\sum_k \left(\frac{1}{\varepsilon_k^0 - E_j} \right)^2} = \frac{d^2}{M^2} \left(\frac{\partial F_j}{\partial E} \right)^{-2};$$

$F(E)$



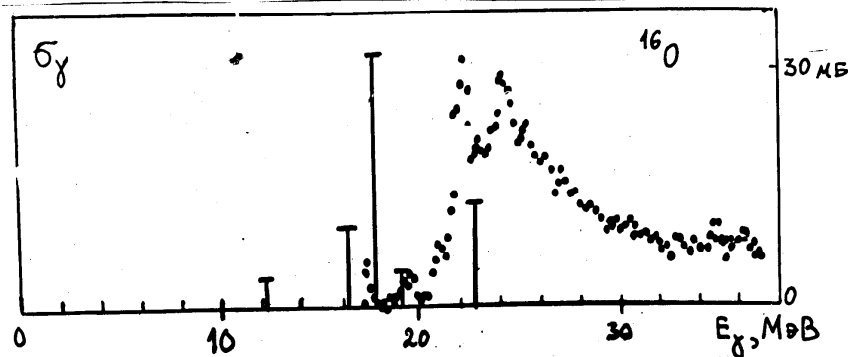
РОТОРАСЩЕПЛЕНИЕ ^{16}O

$$^{16}\text{O} \quad |1s_{1/2}^4 1p_{1/2}^4 1p_{3/2}^8 : J=0 T=0\rangle$$

	E _{св} , MeV		E, MeV
(n)	{	1p _{1/2} ⁻¹ 15.65	2s _{1/2} - 3.27
		1p _{3/2} ⁻¹ 21.81	1d _{3/2} 0.94
			1d _{5/2} - 4.14
(p)	{	1p _{1/2} ⁻¹ 12.11	2s _{1/2} - 0.1
		1p _{3/2} ⁻¹ 18.44	1d _{3/2} 4.5
			1d _{5/2} - 0.6

$$^{16}\text{O}^* : |J=1^-$$

n ⁻¹ n>		p ⁻¹ p>	
конфигур.	E, МэВ	конфигур.	E, МэВ
1p _{1/2} ⁻¹ 2s _{1/2}	12.38	1p _{1/2} ⁻¹ 2s _{1/2}	12.01
1p _{1/2} ⁻¹ 1d _{3/2}	16.59	1p _{1/2} ⁻¹ 1d _{3/2}	16.66
1p _{3/2} ⁻¹ 2s _{1/2}	18.54	1p _{3/2} ⁻¹ 2s _{1/2}	18.34
1p _{3/2} ⁻¹ 1d _{3/2}	22.75	1p _{3/2} ⁻¹ 1d _{3/2}	22.89
1p _{3/2} ⁻¹ 1d _{5/2}	17.67	1p _{3/2} ⁻¹ 1d _{5/2}	17.84



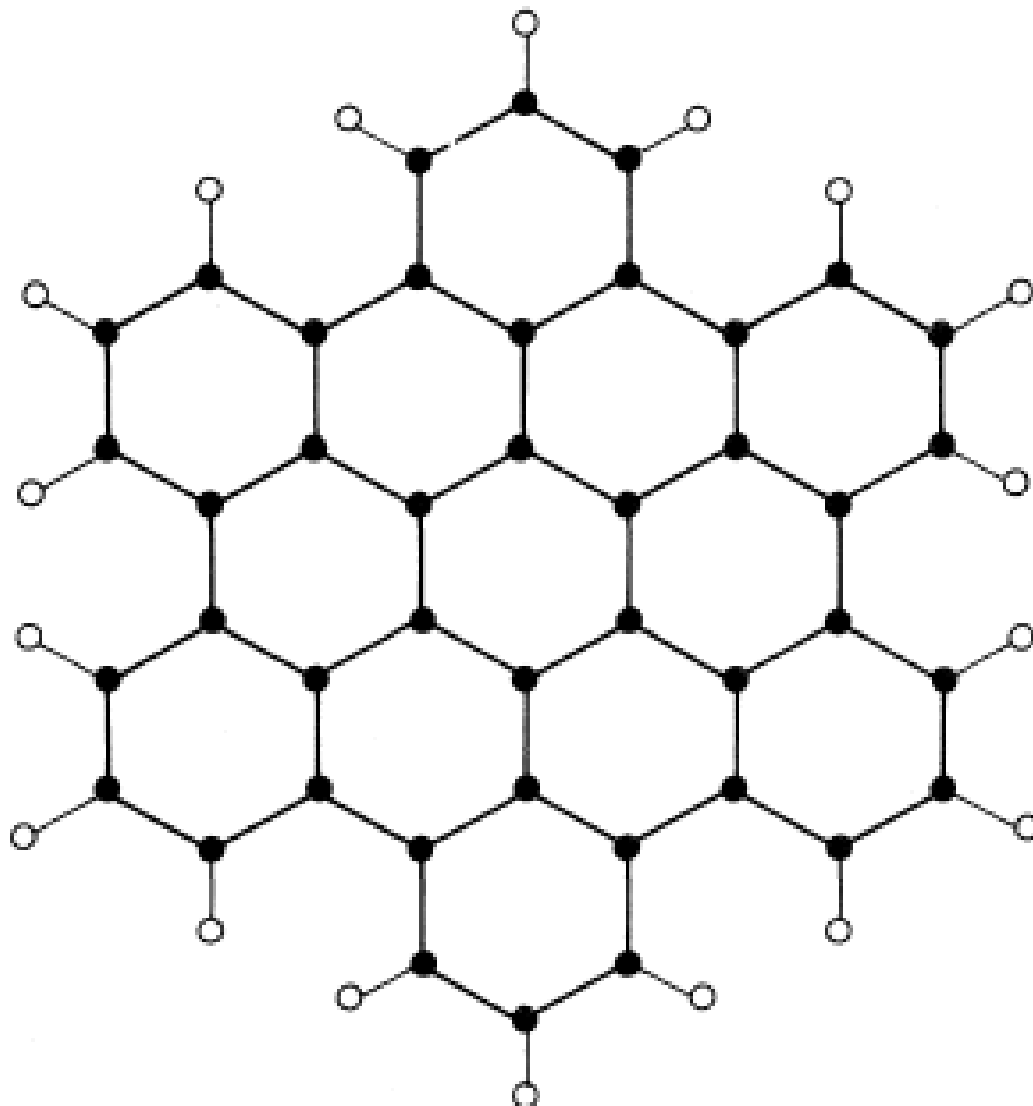


FIG. 1. Schematic representation of the hexabenzocoronene molecule. Full circles represent carbon atoms, empty circles, hydrogen atoms.

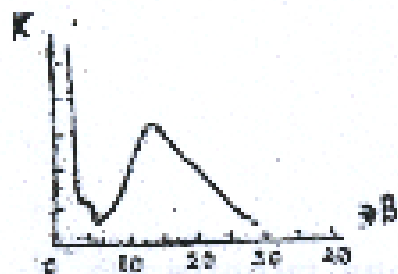
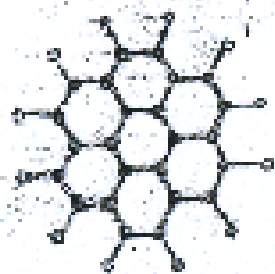


Рис. Слева схематическое представление молекулы коронена. Сплошные кружки представляют атомы углерода, пустые - атомы водорода. Справа представлен спектр потерь при рассеянии фотонов на молекуле коронена.

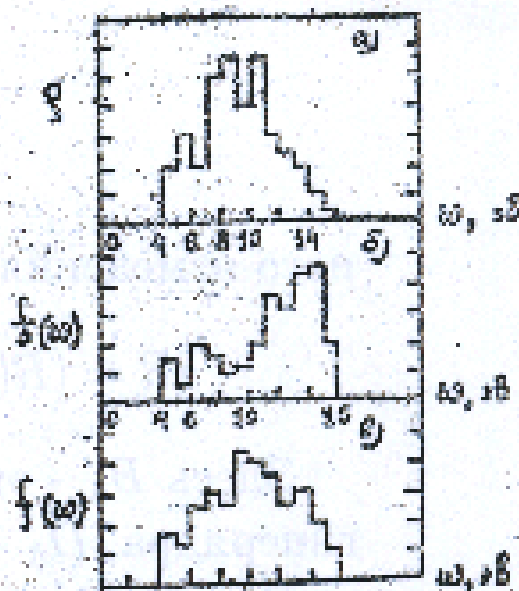
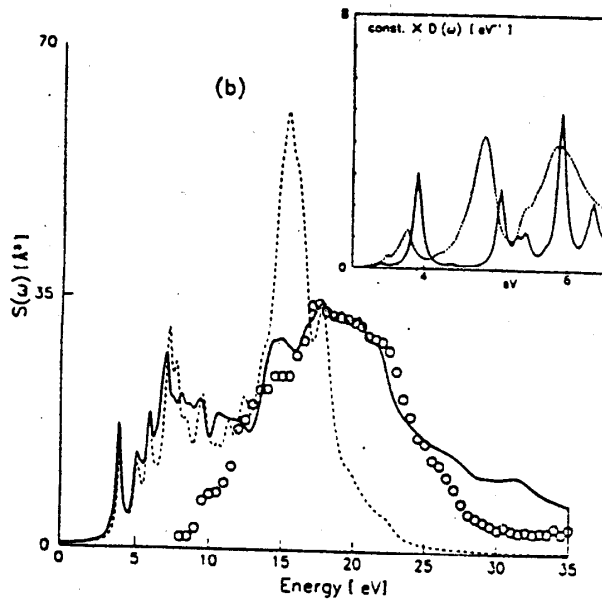
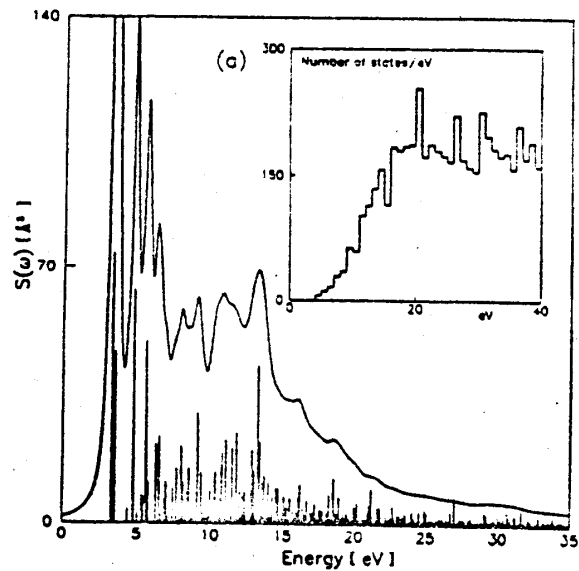


Рис. а) - распределение плотности частично-дырочных возбуждений в молекуле коронена; б) - расчет распределения сил осциллятора перехода в коронене с учетом частично-дырочного взаимодействия; в) - распределение сил осциллятора перехода в коронене без учета частично-дырочного взаимодействия.



ЭКОН.		TEOPUS	
$E, \text{эВ}$	f	$E, \text{эВ}$	f
3.04	0.005	3.4	0.048
3.30	—	3.91	0.53
3.78	0.37	4.38	0.941
4.06	0.10	5.05	0.51
4.35	0.10	5.30	0.14
4.84	2.27	5.42	0.21
5.46	0.22	5.70	0.021
5.88	3.09	5.92	0.31
6.36	—	6.35	0.42
	6.07		3.1

($f_0 = 3.34$)

Figure 1. Dipole strength function of the C_{60} molecule. (a) The free response $S^{(0)}(\omega)$. Making use of this result, the density of states has been calculated and is displayed in the inset. Also shown is the unperturbed strength function averaged with Lorentzian functions having widths $\Gamma = 0.06\omega$ (full curve). (b) The RPA response (full curve). $S(\omega)$ is displayed and compared with experimental data [2] (circles). The RPA results have been averaged with Lorentzian functions having widths $\Gamma = 0.06\omega$. The broken curve represents the RPA result obtained by keeping only those particle-hole transitions which contribute more than 0.1% to the EWSR. In the inset details are given of the optical/UV response of the system ($\text{const} = 2m/\hbar^2 e^2$) in comparison with the experimental findings [1] (broken curve).