



## Scattering amplitude of C<sub>60</sub> fullerite in the ordered phase. Theory and calculations.

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In solid fullerite C<sub>60</sub> at 250 K, an order-disorder phase transition (first-order transition) occurs, which is inherent in all molecular crystals [1]. The reason for this transition in fullerite is a change in the rotational motion of C<sub>60</sub> molecules [2]. Thus, in the "disordered" phase, C<sub>60</sub> has a cubic lattice Fm3m, with the centers of mass at the sites of molecules that "freely" rotate. The "ordered" phase of C<sub>60</sub> has a cubic Pa3 lattice, in which the fullerene molecules remain in the same positions as in the "disordered". The molecular axes are oriented along the spatial diagonals of the cubic lattice.

One of the features of X-ray diffraction patterns obtained from fullerite C<sub>60</sub> is the absence of reflections of the {h00} type. In [3], a mathematical model was proposed to describe the scattering amplitude for C<sub>60</sub> in the "disordered" phase and it was shown that the intensities of the diffraction lines of the {h00} type are not equal to zero.

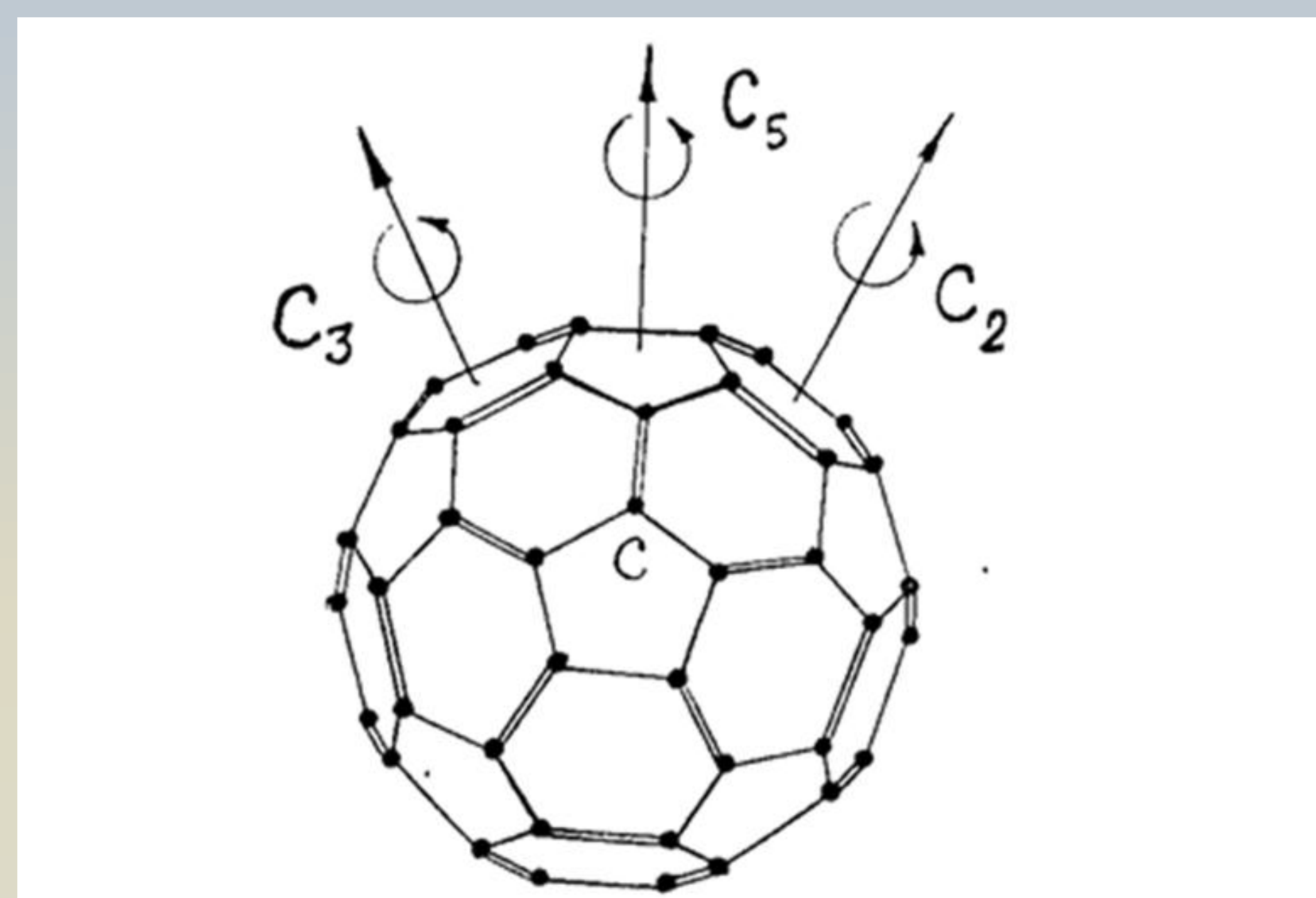
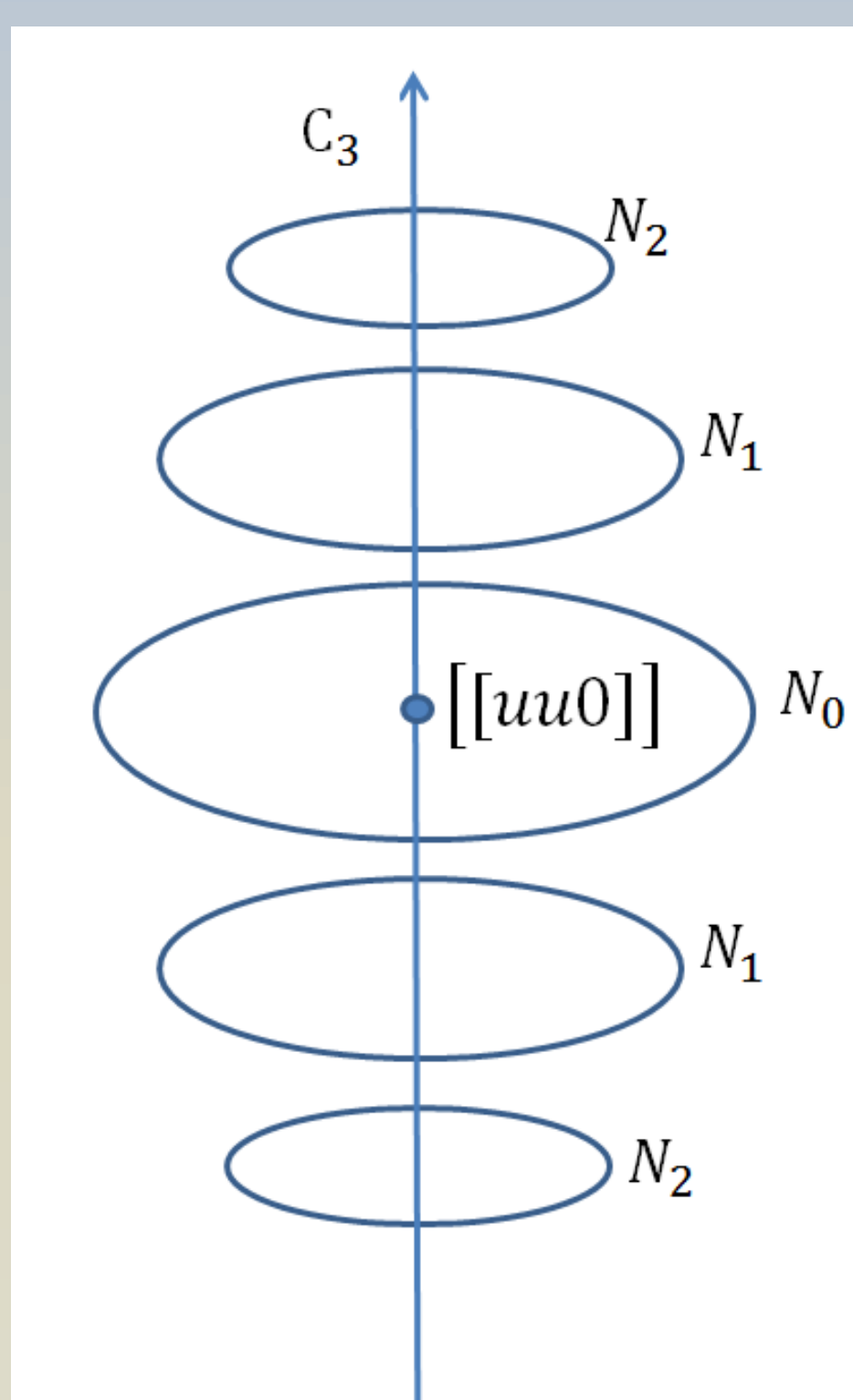


Fig.2. Symmetry axes and bond types of the C<sub>60</sub> molecule

Fig.1. C<sub>60</sub> molecule in the ordered phase is represented as a multilayer model, where the layers are strung on a molecular axis. The axis of the 2nd, 3rd or 5th order molecule coincides with the crystallographic axes (directions) [111]:  $[\bar{1}11]$ ,  $[1\bar{1}1]$  and  $[11\bar{1}]$ , respectively (Fig.2).

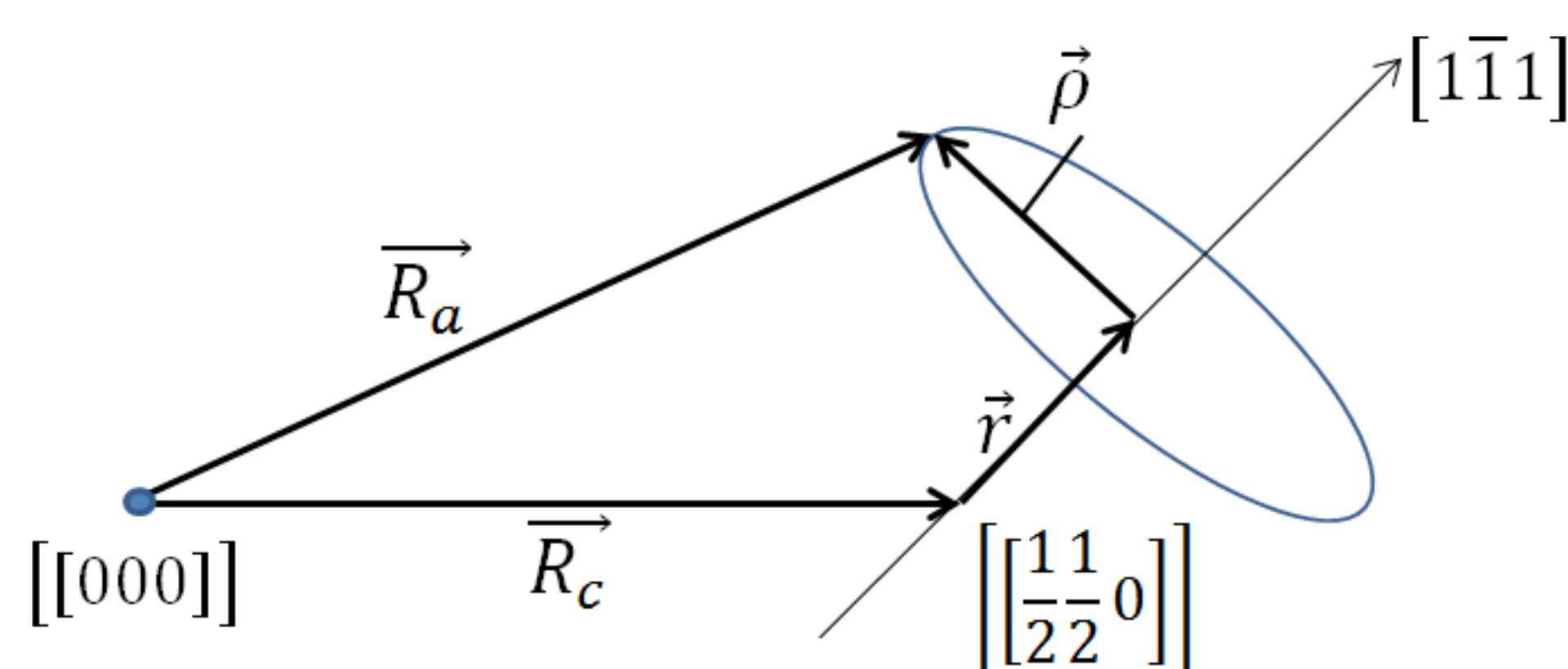


Fig. 4. Vector representation of the position of each atom

$$\vec{R}_a = \vec{R}_c + b\vec{r} + \vec{\rho}$$

$\vec{R}_c$  – position of the mass center of the molecule (fcc lattice unit):

$$[000], \left[\frac{1}{2}\frac{1}{2}0\right], \left[0\frac{1}{2}\frac{1}{2}\right], \left[\frac{1}{2}0\frac{1}{2}\right]$$

$\vec{r}$  – unit vector directed along the spatial diagonals of the cube

$b$  – distance from a lattice unit to a layer in a multilayer model

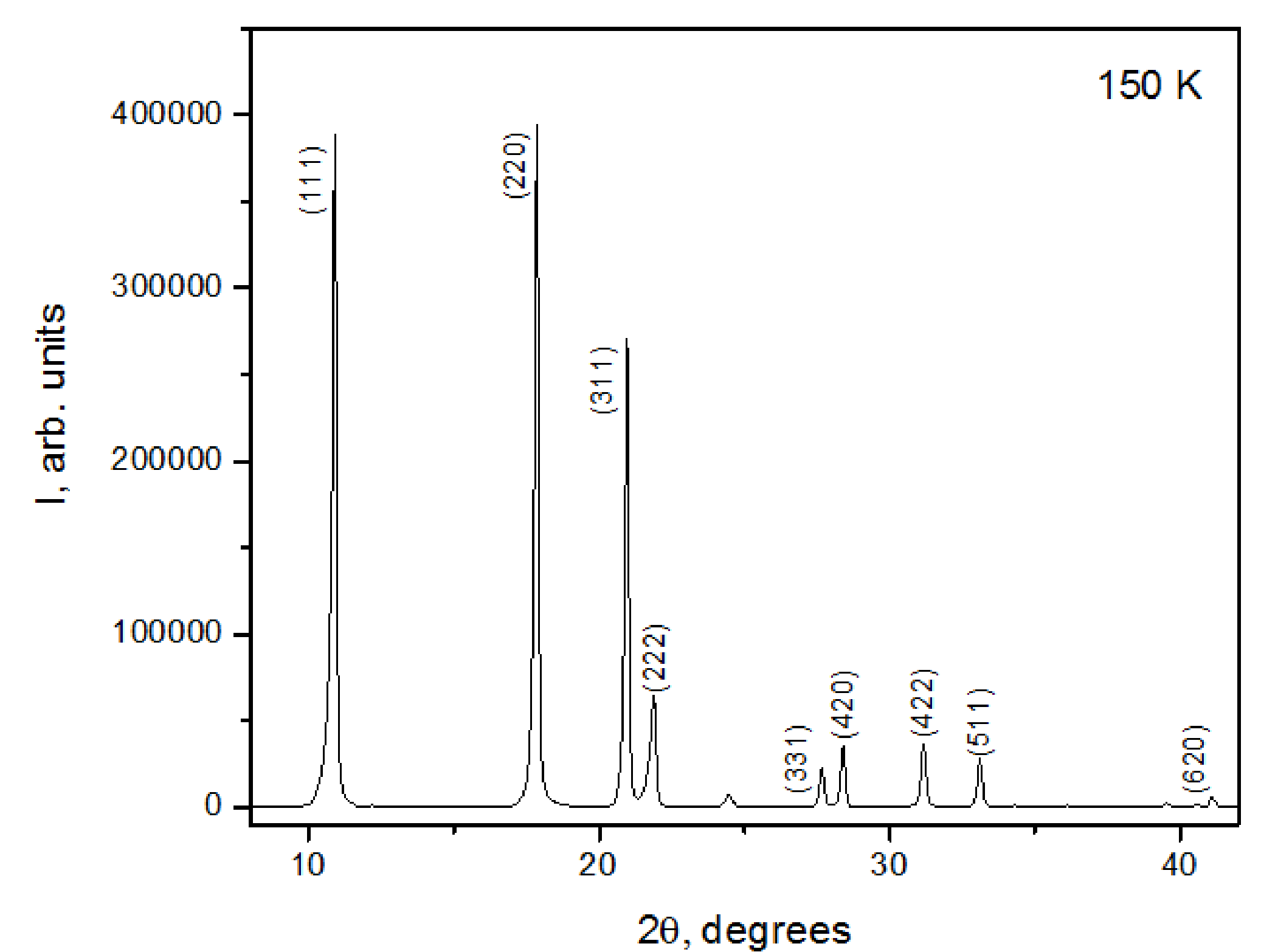


Fig.3. Typical powder X-ray pattern for C<sub>60</sub> at 150K (ordered phase)

Scattering amplitude for fullerite C<sub>60</sub>

$$F(\vec{S}) = \sum f(\vec{S}) \exp[2\pi i \vec{S} \vec{R}_a]$$

$\vec{R}_a$  – carbon atom position

$$F(\vec{S}) = f(\vec{S}) \sum \exp[2\pi i \vec{R}_c \vec{S}] \sum \exp[2\pi i b_k \vec{r}_{ck} \vec{S}] \exp[2\pi i \vec{\rho}_{ck} \vec{S}]$$

Due to the fact that the C<sub>60</sub> molecule rotates freely around the molecular axis C<sub>n</sub> (n-order), the atoms of N-number are uniformly distributed (smeared) over the ring of  $\rho$  radius.

$$\langle \exp[2\pi i \vec{\rho} \vec{S}] \rangle = \frac{N}{2\pi} \oint d\varphi \exp[2\pi i \rho S \cos\varphi \cdot \sin\varphi]$$

averaging over a ring

$N$  - number of atoms in the ring of the corresponding layer.

$$\oint d\varphi \exp[i A \cos\varphi] = 2\pi J_0(A)$$

$$\frac{N}{2\pi} 2\pi J_0(2\pi \rho S \sin\theta) = N J_0(2\pi \rho S \sin\theta)$$

The spreading function of  $N$  carbon atoms over a ring of radius  $\rho$

## Main results

The results of processing the experimental X-ray diffraction pattern (Fig. 3) for fullerite C<sub>60</sub> in the "ordered" phase were compared with the results of calculations using the proposed model (Figs. 1, 4). It was found that both for the experiment and in the calculation, the intensities of both "forbidden" and "allowed" ((111), (220), (311)) diffraction lines of the crystal lattice differ by two orders of magnitude.

The calculations carried out according to our model also showed that the intensity of diffraction peaks of the type ( $hk0$ ), for which  $h+k=2n+1$  will be equal to zero. This can be considered as an addition to the extinction law, taking into account the almost spherical symmetry of the molecule.

Also, X-ray diffraction patterns will not show reflections from lines ( $h00$ ) if  $h=2n+1$ .

[1] V.G. Manzhelei and Yu.A. Freiman, Physics of Cryocrystals, AIP Press, New York, 1996.

[2] P.H.M. van Loosdrecht at all, PRL, v. 68, 1176, 1992

[3] A.I. Prokhvatilov at all, LTP, 31, 445, 2005