Clinical Environment to Improve Operations, Medical and Surgical Applications: Study of Alternative Model of Carbon Connection of Diamond

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Abstract

Carbon Materials, especially interesting for practical application in the different areas of science and technique, by virtue of the numerous unique physical and chemical properties. The popular object of researches presently is allotropic modification of carbon – diamond that is examined as a classic model crystal. One of the most effective going near research of physical and chemical properties of diamond is his study by means of preliminary computer design of the studied dielectric descriptions. The authors of the article examine the traditional and alternative mathematical models of the electronic configuration of nonpolar valency chemical connection of diamond. Results over of design of dielectric descriptions of resilient electronic polarization of the examined material are brought on the basis of an offer physical interpretation of electronic structure.

Key words: *carbon, electronic polarization, complex electronic polarizability modeling.*

Introduction.

Diamond and Carbon materials have pulled in broad logical premium because of their superb actual properties, for example, high hardness, low contact and wear rate, optical straightforwardness, and compound idleness [1,2]. Diamond, when embedded with substantial particles to adequately high portions goes through a particular change. Rutherford backscattering [3]. just as electron diffraction tests[4] show that diamond changes from an ideal precious stone to some scattered structure; EPR [5,6]. In recent years, in the physics of a condensed state, research and development in the field of nanomaterials and nanotechnologies have become most popular. The urgency of the problem of production of nanomaterials is determined by the peculiarity of their physico-mechanical properties, which allow creating materials with qualitatively and quantitatively new properties for use in practice The existing methods of calculating these properties are not sufficiently effective, and a large amount of time is required for their implementation. Increasing their effectiveness involves the development of completely new computational methods based on fundamentally different methods of calculation.

Method of computing experiment

In describing the physical process under investigation, it is proposed to use a cybernetic model of the general electronic polarization of a crystal [7, 8]. In this case, the initial dynamics of the elastic deformation of the electron shells of particles can be represented as the following system of linear differential equations of a general type:

$$\frac{d^2\mu_k(t)}{dt^2} + 2\beta_k\frac{d\mu_k(t)}{dt} + \omega_{0k}^2\mu_k(t) = \frac{q_k e^2}{m_e} \quad (1)$$

$$k=l,K$$

where $\mu_k(t)$- functions of the time variation of the induced dipole moments of the electronic orbits of each variety:

β_k and ω_{0k} -are the attenuation coefficients and frequencies of their natural oscillations, respectively;

q_k- is the number of electrons that populate orbits;

e, m_e - charge and mass of electron;

k - numbers of electronic orbitals;

K- is the total number of different electronic orbits;

E (t)- is the effective field strength function;

On the basis of expression (1), the complex electronic polarizability of each individual particle is equal to:

In turn, the complex dielectric permittivity of a condensed material formed by the same type of particles is described by a cybernetic quation of the form:

$$\alpha(j\omega) = \sum_{i=1}^{K}\frac{q_i e^2/m_e}{\omega_{0i}^2 - \omega^2 + j2\beta_i\omega} \quad (2)$$

$$\varepsilon(j\omega) = 1 + \frac{2}{3\varepsilon_0} + N\alpha(j\omega) \quad (3)$$

where **ε_0-** is the electric constant

(the dielectric constant of the vacuum)

N- is the volume concentration of particles, calculated on the basis of the values of the physical density of the sample and its molecular weight.

Taking into account the structure of expressions (2) and (3), it is possible to analyze the effectiveness of the proposed interpretation of the electron configuration of particles, which determines the dynamic features of the initial description of the form (1). This circumstance is due to the fact that the physically measured imaginary frequency response of the complex the permittivity *ε” (ω)*, denoted *ε2 (ω)* in

$$\varepsilon''(\omega) = 1 + \frac{2}{3\varepsilon_0}N\alpha''(\omega)$$

$$\alpha''(\omega) = \sum_{i=l}^{K}\frac{q_i e^2}{m_e}\cdot\frac{2\beta_i\omega}{(\omega_{0i}^2 - \omega^2) + 4\beta_i^2\omega^2} \quad (4)$$

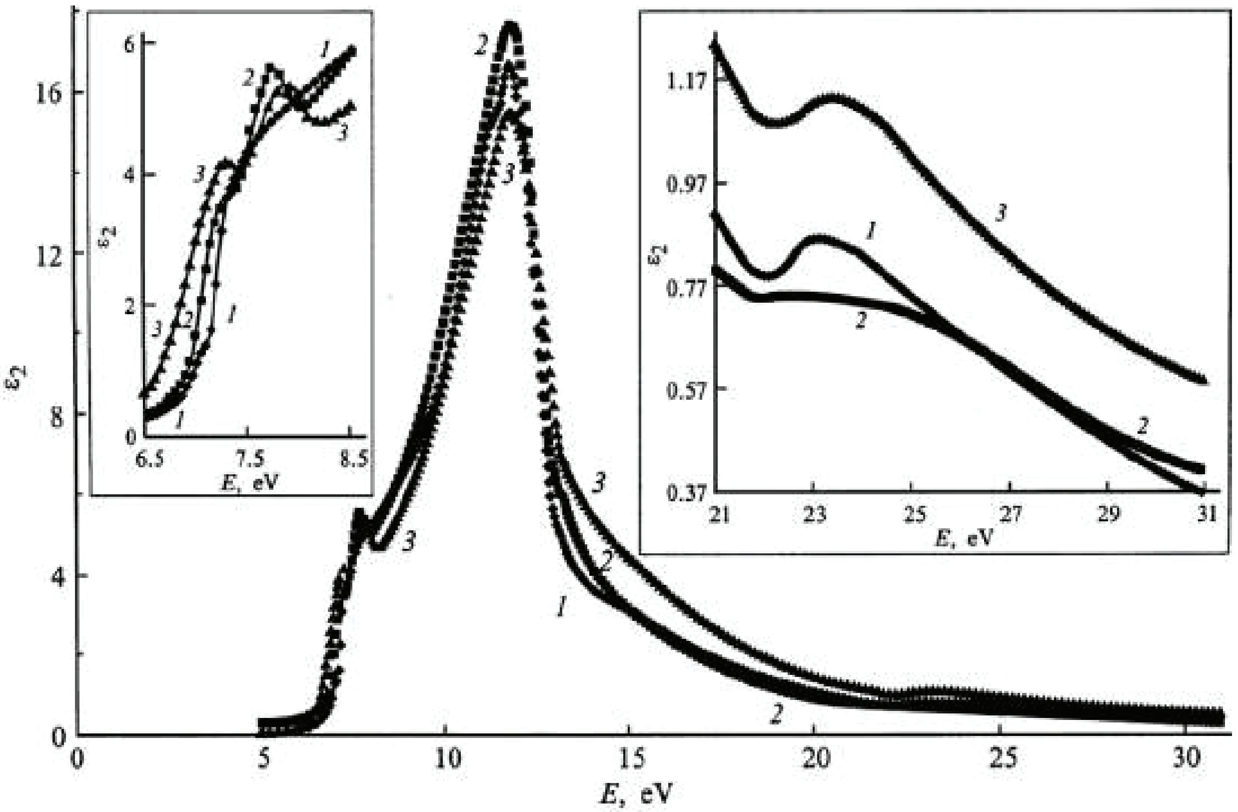


Fig. 1, is the sum of the imaginary parts of the electron polariza of individual particles *α"(ω)*

(Figure.1)shows the reflection spectra of three different samples of diamond(№№. 1, 2, 3), on the insets - spectra in the regions 6.5 - 8.5 and 21-31 eV [9].

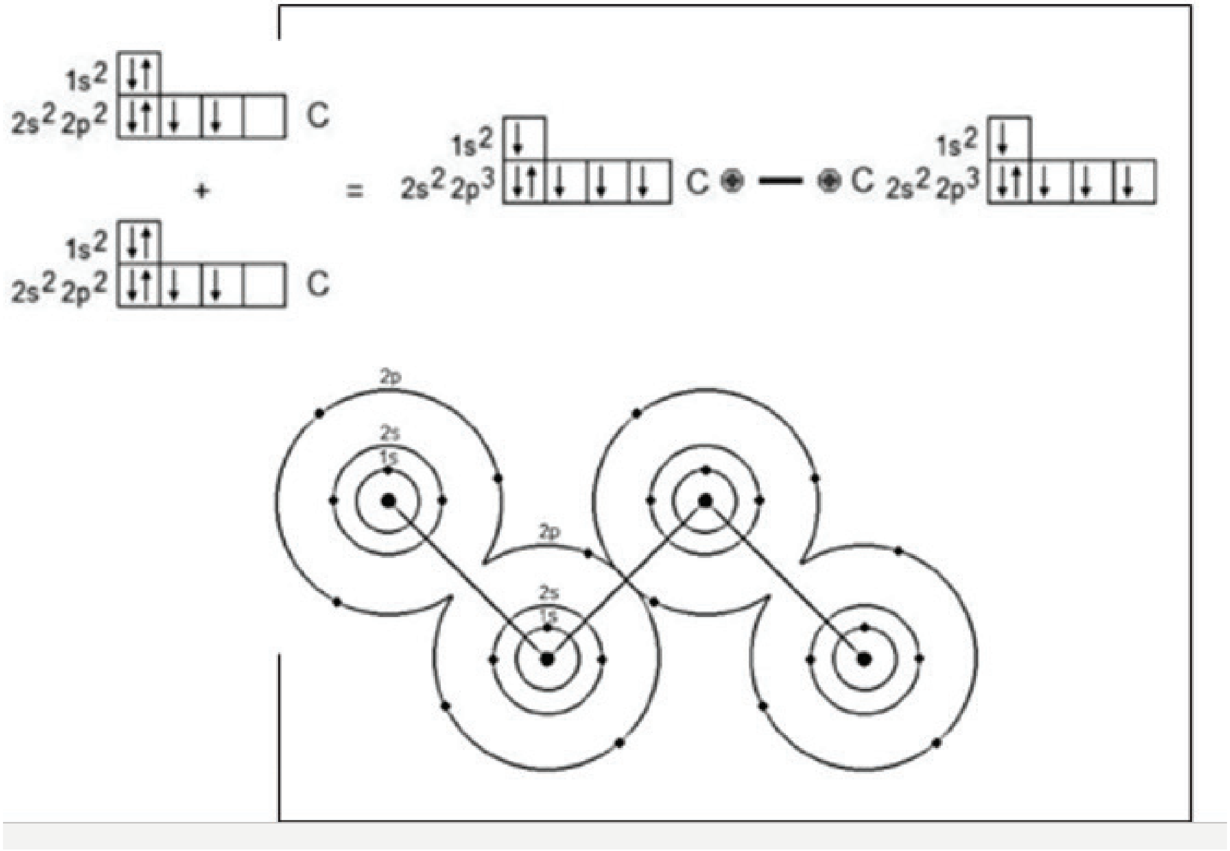
Fig. Electron-volt spectra of the imaginary part of the dielectric permittivity of diamond

Thus, the adequacy of the theoretical model used can be assessed by qualitative comparison of their behavior strata

Traditional treatment of covalent bond of diamond

A diamond crystal can be viewed as a huge molecule in which each carbon atom is surrounded by four neighboring atoms located at the vertices of a regular tetrahedron. Each of them is connected by homeopolar connection It is known that carbon atoms in a diamond crystal that are in chemical bond with other atoms are in an excited state with the configuration $1s^2 2s^1 2p_x 2p_y\ 2p_z$.

Consider the traditional model of the chemical bond of the species, $C^{3+} (3e^-)_2\ C^{3+}$, which contains six electrons, where the pair of electrons corresponds to three electrons in the outer orbitals. The electronic configuration of the crystal in question is shown in Fig. 2



Based on the figure, one electron is found on the inner shell (1-s atomic orbital), and on the outer (optical) shell three electrons, which experience the maximum displacement, and make the main contribution to the electron polarization. On the basis of the scheme, this process can be represented as the following system of linear differential equations, where the first equation of the system describes the electron displacement on the inner shell, and the following equations on 2-s and 2-p atomic orbitals :

$$\frac{d^2\mu_{1s}}{dt^2} + 2\beta_{1s}\frac{d\mu_{1s}}{dt} + \omega_{01s}^2\mu_{1s}(t) = \frac{e^2}{m_e}E(t)$$

$$\frac{d^2\mu_{2s}}{dt^2} + 2\beta_{2s}\frac{d\mu_{2s}}{dt} + \omega_{02s}^2\mu_{2s} = \frac{2e^2}{m_e}E(t) \tag{5}$$

$$\frac{d^2\mu_{2p}}{dt^2} + 2\beta_{2p}\frac{d\mu_{2p}}{dt} + \omega_{02p}^2\mu_{2p} = \frac{3e^2}{m_e}E(t)$$

The standard transformations of the presented system of equations make it possible to obtain the imaginary frequency characteristics of the electron polarizability in the investigated material of the form:

$$\begin{aligned}
\overset{''}{\alpha}_{1s}(\omega) &= \frac{e^2}{m_e}\cdot\frac{2\beta_{1s}\omega}{(\omega_{01s}^2-\omega^2)^2+4\beta_{1s}^2\omega^2} \\
\overset{''}{\alpha}_{2s}(\omega) &= \frac{2e^2}{m_e}\cdot\frac{2\beta_{2s}\omega}{(\omega_{02s}^2-\omega^2)^2+4\beta_{2s}^2\omega^2} \\
\overset{''}{\alpha}_{2p}(\omega) &= \frac{3e^2}{m_e}\cdot\frac{2\beta_{1s}\omega}{(\omega_{02s}^2-\omega^2)^2+4\beta_{2p}^2\omega^2}
\end{aligned} \tag{6}$$

On the basis of the mathematical model under consideration, a computational experiment was carried out aimed at modeling the continuous frequency spectrum of the imaginary component of the complex electron polarizability of the crystal, within which the numerical values of the dynamic parameters were set of abstract values, starting from the mutual ratio of the radii of the corresponding electron orbits .

The results of the simulation performed in MatLAB on the basis of equations (4) and (5) are shown in Fig.3. Comparing the general form of the absorption bands of the electronic orbitals that occur on the theoretical curve with their physically observable analogs (Fig.1.) note that:

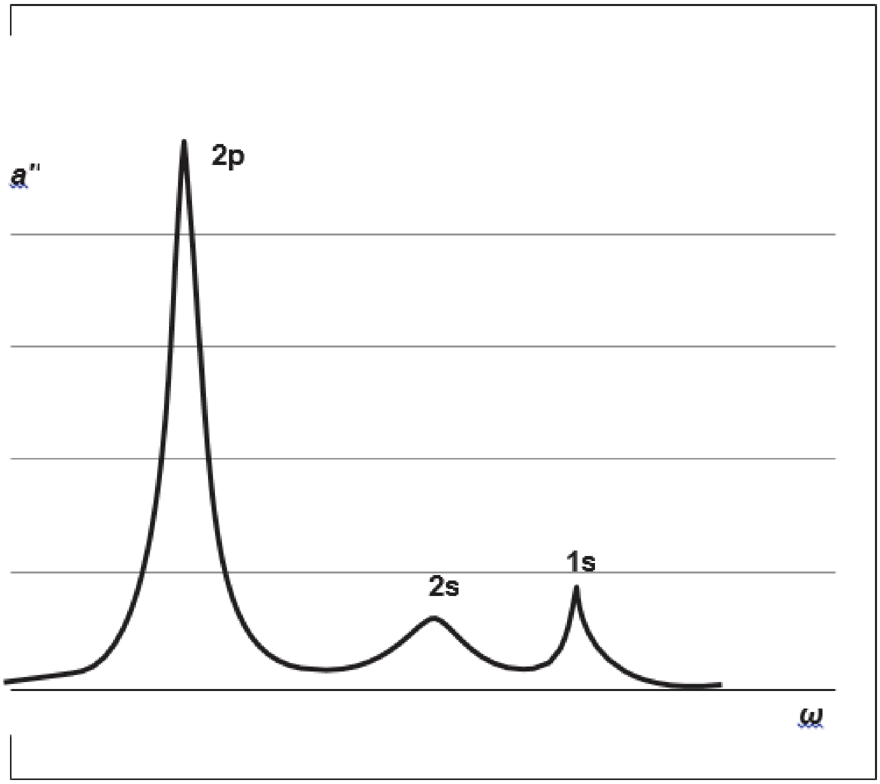


Fig. 3. Imitation spectrum of the electron polarizability of a diamond corresponding to the model (5).

-the resonant emission of the **1s** orbitals included in the composition of the atomic residue should be located in the X-ray spectral range, therefore, when analyzing the general adequacy of the model under study, it can not be taken into account, since the control data cover only the region of ultraviolet frequencies;

-the traditional interpretation of hybridized orbitals (Fig. 2) makes it practical to model a single clearly pronounced resonant ejecta characterizing the elastic deformations of the 2p orbitals. In this case, the physical experiment indicates the presence of a more complex spectral picture.

-the existence of yet another small absorption band, observed in the region of 7.5 electron-volts.-

Alternative treatment of diamond carbon bond

The results of earlier applied research [10, 11] have shown that the efficiency of mathematical modeling of optical and dielectric spectra of substances possessing a polar covalent type of chemical bond can be significantly increased due to its purely ionic interpretation. Thus, within the framework of the modified interpretation of the mechanism for realizing the nonpolar covalent bond arising for each pair of neighboring diamond atoms, it is assumed that one half goes to the cation state C4 +, and the other to the anion state C4- [12]. The main advantage of the changes lies in the fact that on their basis it becomes possible to consider carbon particles in the form of incompressible ion balls [6], which have a complex electronic structure, depicted in Fig. 4.In addition, analyzing the optical characteristics of crystalline substances (for example, the long-wave spectrum of the refractive index of a quartz crystal [7], one can note the presence of several absorption bands, which, in accordance with the Pauli exclusion principle, agrees well with the electronic structure of the outer shells of anions.

Thus, on the basis of the physical interpretation of the diamond carbon bond shown in Figure 4, taking into account the proportions of electron pairs that populate the electron orbitals, it becomes possible to describe this process mathematically:

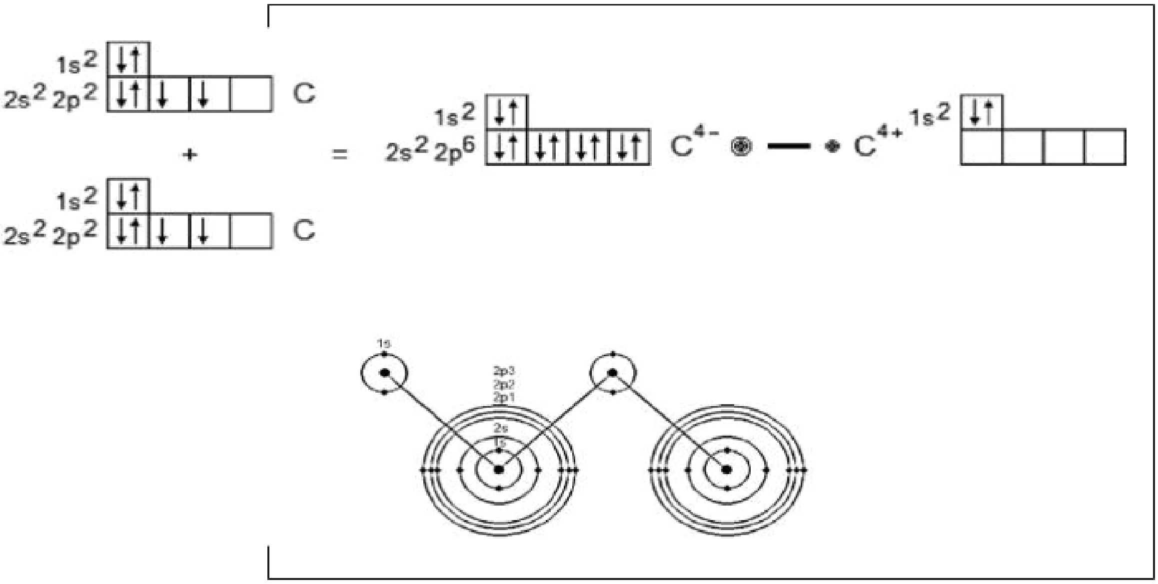


Fig. 4. Diagram of the ionic interpretation of the electronic configuration of diamond.

$$\frac{d^2\mu_{1s}}{dt^2}+2\beta_{1s}\frac{d\mu_{1s}(t)}{dt}+\omega_{01s}^2\mu_{1s}=\frac{2e^2}{m_e}E(t)$$

$$\frac{d^2\mu_{2s}}{dt^2}+2\beta_{2s}\frac{d\mu_{2s}}{dt}+\omega_{02s}^2\mu_{2s}={}^1\!/_2\frac{2e^2}{m_e}E(t) \qquad (7)$$

$$\frac{d^2\mu_{2p1}}{dt^2}+2\beta_{2p1}\frac{d\mu_{2p1}}{dt}+\omega_{02p1}^2\mu_{2p1}={}^1\!/_2\frac{2e^2}{m_e}E(t)$$

$$\frac{d^2\mu_{2p2}}{dt^2}+2\beta_{2p2}\frac{d\mu_{2p2}}{dt}+\omega_{02p2}^2\mu_{2p2}={}^1\!/_2\frac{2e^2}{m_e}E(t)$$

$$\frac{d^2\mu_{2p3}}{dt^2}+2\beta_{2p3}\frac{d\mu_{2p3}}{dt}+\omega_{02p3}^2\mu_{2p3}(t)={}^1\!/_2\frac{2e^2}{m_e}E(t)$$

On the basis of expression (7), the imaginary frequency characteristic of the complex electron polarizability takes the form:

$$\alpha''_{1s}(\omega)=\frac{2e^2}{m_e}\cdot\frac{2\beta_{1s}\omega}{(\omega_{01s}^2-\omega^2)^2+4\beta_{1s}^2\omega^2}$$

$$\alpha''_{2s}(\omega)=\frac{e^2}{m_e}\cdot\frac{2\beta_{2s}\omega}{(\omega_{02s}^2-\omega^2)^2+4\beta_{2s}^2\omega^2} \qquad (8)$$

$$\alpha''_{2p2}(\omega)=\frac{e^2}{m_e}\cdot\frac{2\beta_{2p2}\omega}{(\omega_{01s}^2-\omega^2)^2+4\beta_{2p2}^2\omega^2}$$

$$\alpha''_{2p1}(\omega)=\frac{e^2}{m_e}\cdot\frac{2\beta_{2p1}\omega}{(\omega_{02p1}^2-\omega^2)^2+4\beta_{2p1}^2\omega^2}$$

$$\alpha''_{2p3}(\omega)=\frac{e^2}{m_e}\cdot\frac{2\beta_{2p3}\omega}{(\omega_{02p3}^2-\omega^2)^2+4\beta_{2p3}^2\omega^2}$$

simulation results on the basis of equations (4) and (7) are shown in Fig. 5. The

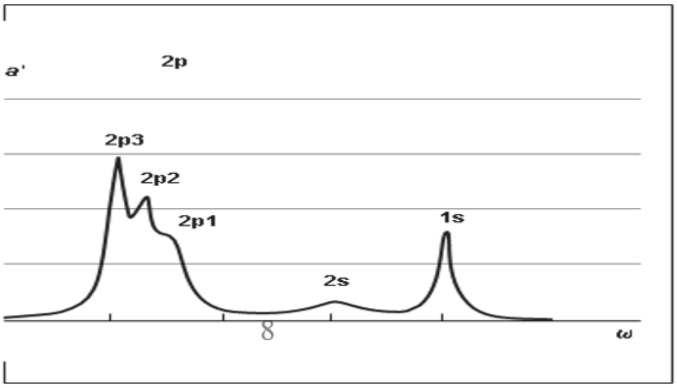


Fig. 5. Imitation spectrum of the electron polarizability of a diamond corresponding to the model (7)

Comparing the general form of the absorption bands of specific electronic orbitals that occur on the theoretical curve with their physically observable analogs, it should be noted that the ionic treatment of the formation of the carbon bond considered above, on the one hand, retains the previously indicated merits of the model of hybridized orbitals concerning arrangement of resonance emissions of 1s and 2s electrons; on the other hand, it also corrects the revealed shortcoming of the traditional interpretation, since it allows one to simulate a complex spectral picture of the electron polarization of 2p orbitals.

Conclusions

The theoretical models of elastic electronic polarization of diamond described above make it possible to simulate the polarization characteristics of a dielectric, which turn out to be sufficiently effective. In addition, the proposed modified diamond carbon bond model allows the most accurate study of its optical properties. Consequently, its practical use in the study of the internal structure of crystalline substances can be useful for the further evolution of the theoretical principles of condensed-state physics.

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Conflict of Interest: None to declare.

Ethical Clearance: All experimental protocols were approved under the College of Education for Pure Sciences and all experiments were carried out in accordance with approved guidelines.

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