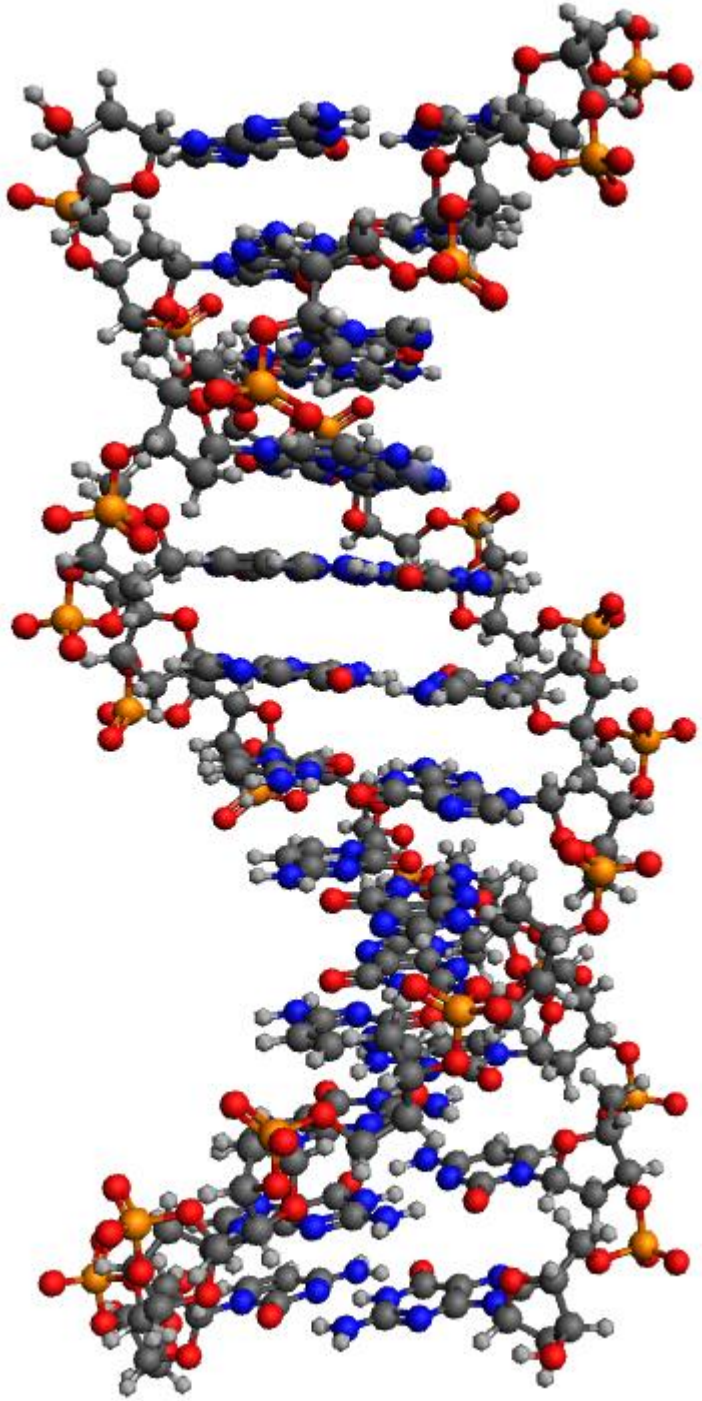
# The symmetry method as a way to visualize the interaction of an ultrashort pulse with matter, using the example of RNA molecules, DNA and diamond crystals



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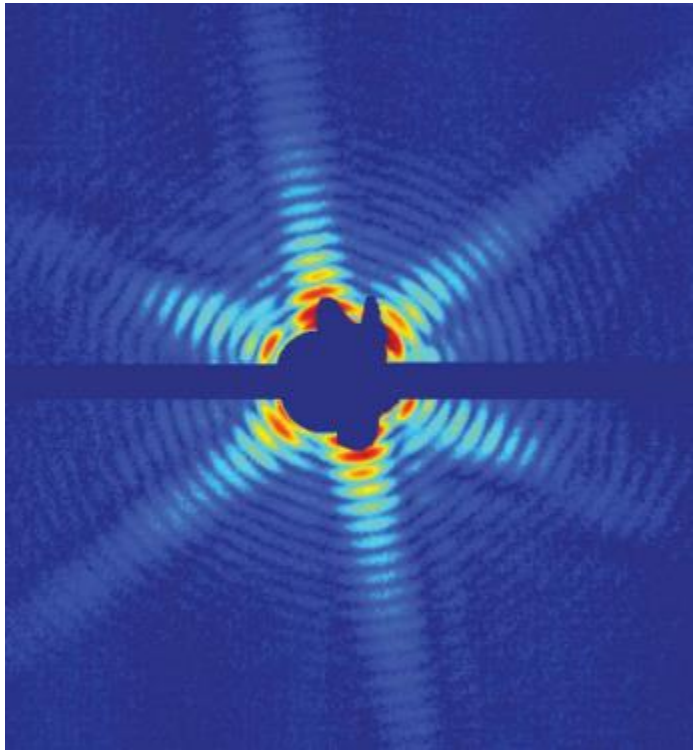
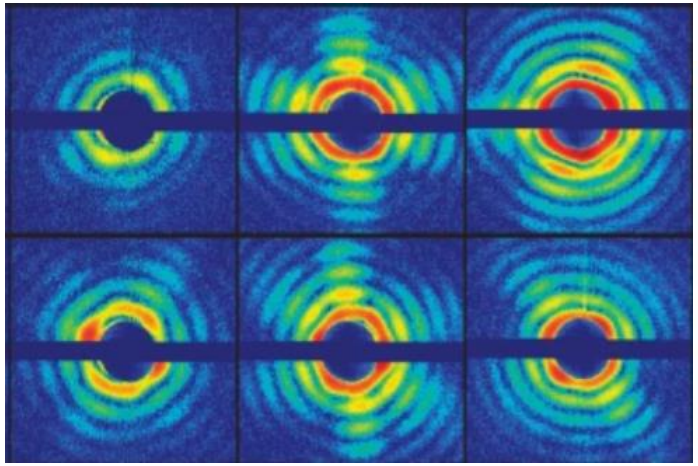
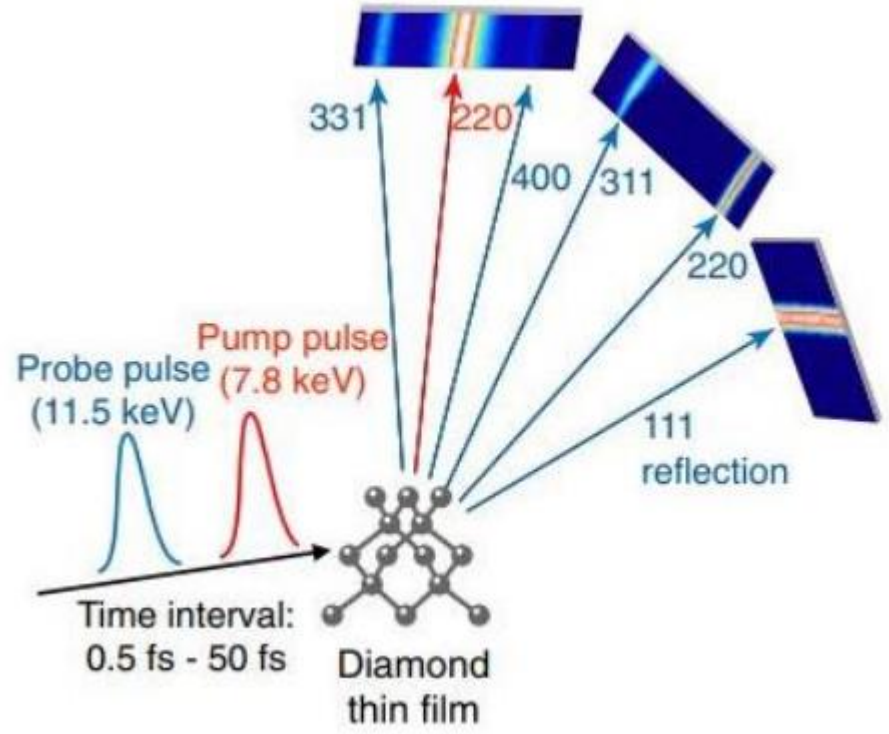
# Introduction

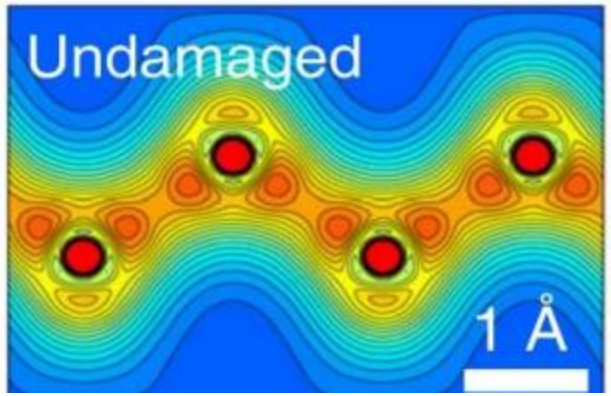
- Theory of calculation of the polyatomic structure
- The model under study
- Parameters of the mathematical model
- Simulation results - Spectrum graphs
- Conclusions

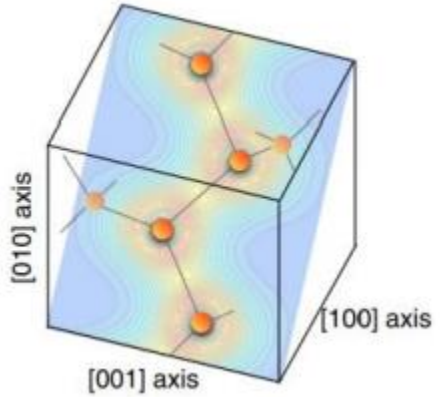
# Modern experiments

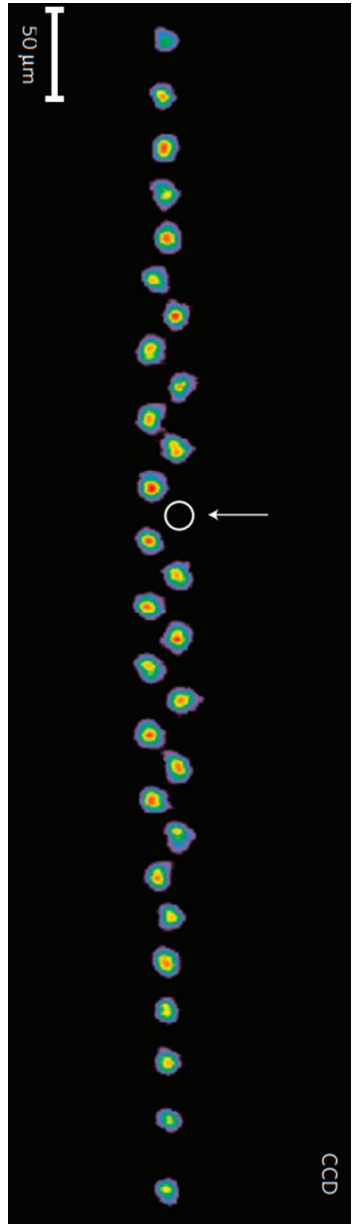






# Theory

$$\frac{d\varepsilon}{d\Omega_k} = \frac{[\mathbf{E_0 n}]^2}{8c^3\alpha\sqrt{2\pi}}\left[\sum_{i=1}^{s} N_{e,i}N_{A,i}\left(1-\left|F_i\right|^2\right)+\sum_{i,j=1}^{s}\delta_{i,j}\beta N_{e,i}N_{e,j}F_iF_j\right]$$

$\mathbf{E_0}$ electromagnetic field strength USPs

$\delta_{i,j}$ interference factor

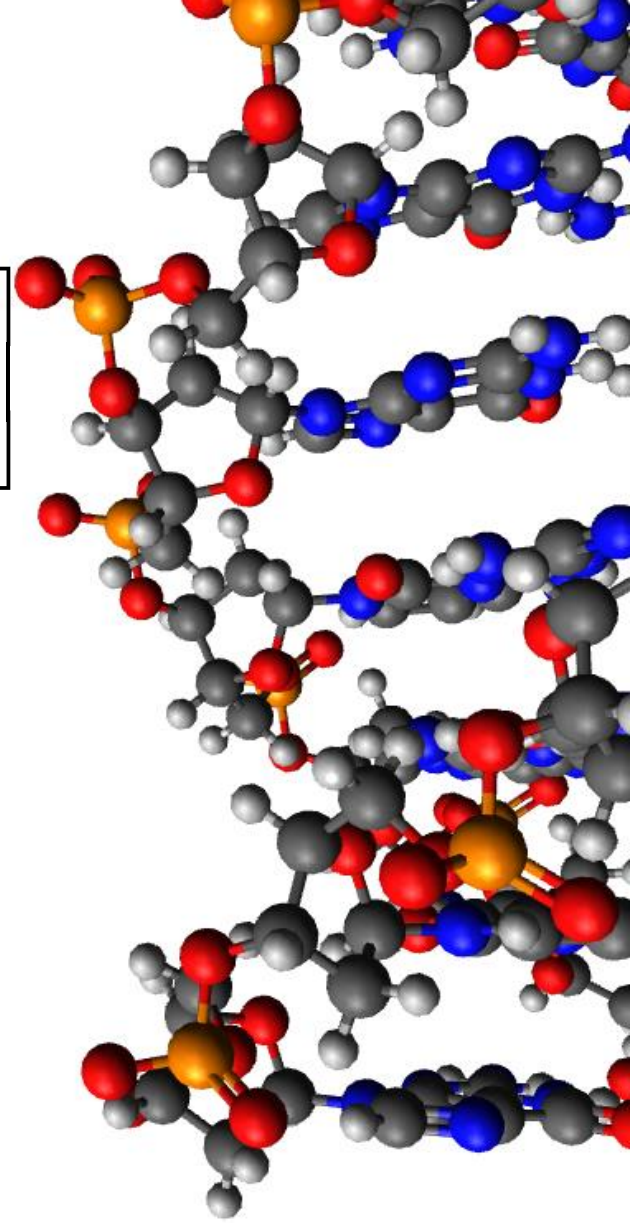
$N_{e,i}$ number of electrons in the atom of the i - grade

$N_{A,i}$ number of atoms of the i - grade

$F_i$ form factor of the atom of the i - grade with the corresponding electron density

$$H_e = 1$$

$$H_A = 80$$



D.N.Makarov, A.A.Kharlamova, “Scattering of X-ray Ultrashort Pulses by Complex Polyatomic Structures,” International Journal of Molecular Sciences, Vol 163, December 2021.

# Theory

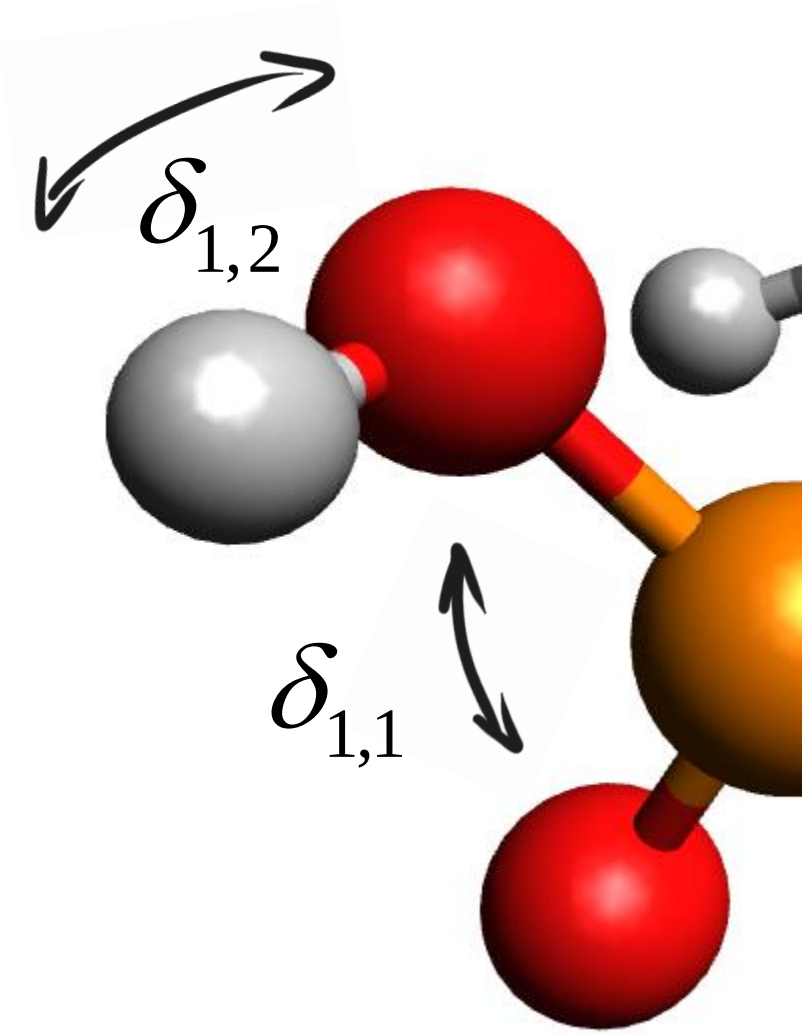
$$\delta_{i,j} = \sum_{A_{i,j}} e^{-i\mathbf{p}(\mathbf{R_i}-\mathbf{R_j})}$$

$A_{i,j}$ number of atoms of the i - grade

$\mathbf{R_i}$ radius vector specifying the position of the atoms of the corresponding variety

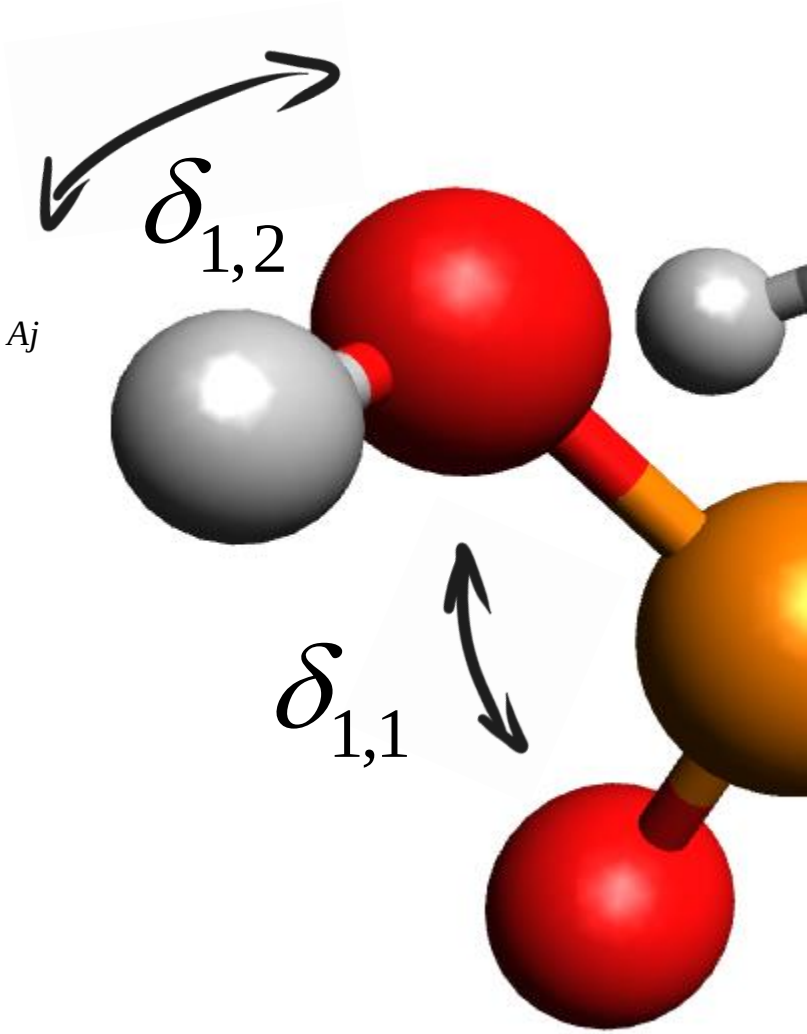
$\mathbf{R_j}$

$\mathbf{p}$ momentum vector of the USPs falling on the multi-atom system



# Theory

$$\delta_{i,j} = \sum_{\alpha=1}^{S} \sum_{n_\alpha=0}^{N_\alpha} e^{i\mathbf{pR}_{n_\alpha}} \sum_{A_i \in R_{\alpha,1}} e^{i\mathbf{pR}_{A_i}} \sum_{\beta=1}^{S} \sum_{n_\beta=0}^{N_\beta} e^{-i\mathbf{pR}_{n_\beta}} \sum_{A_j \in R_{\beta,1}} e^{-i\mathbf{pR}_{Aj}}$$




$\alpha, \beta$ some asymmetry in the system

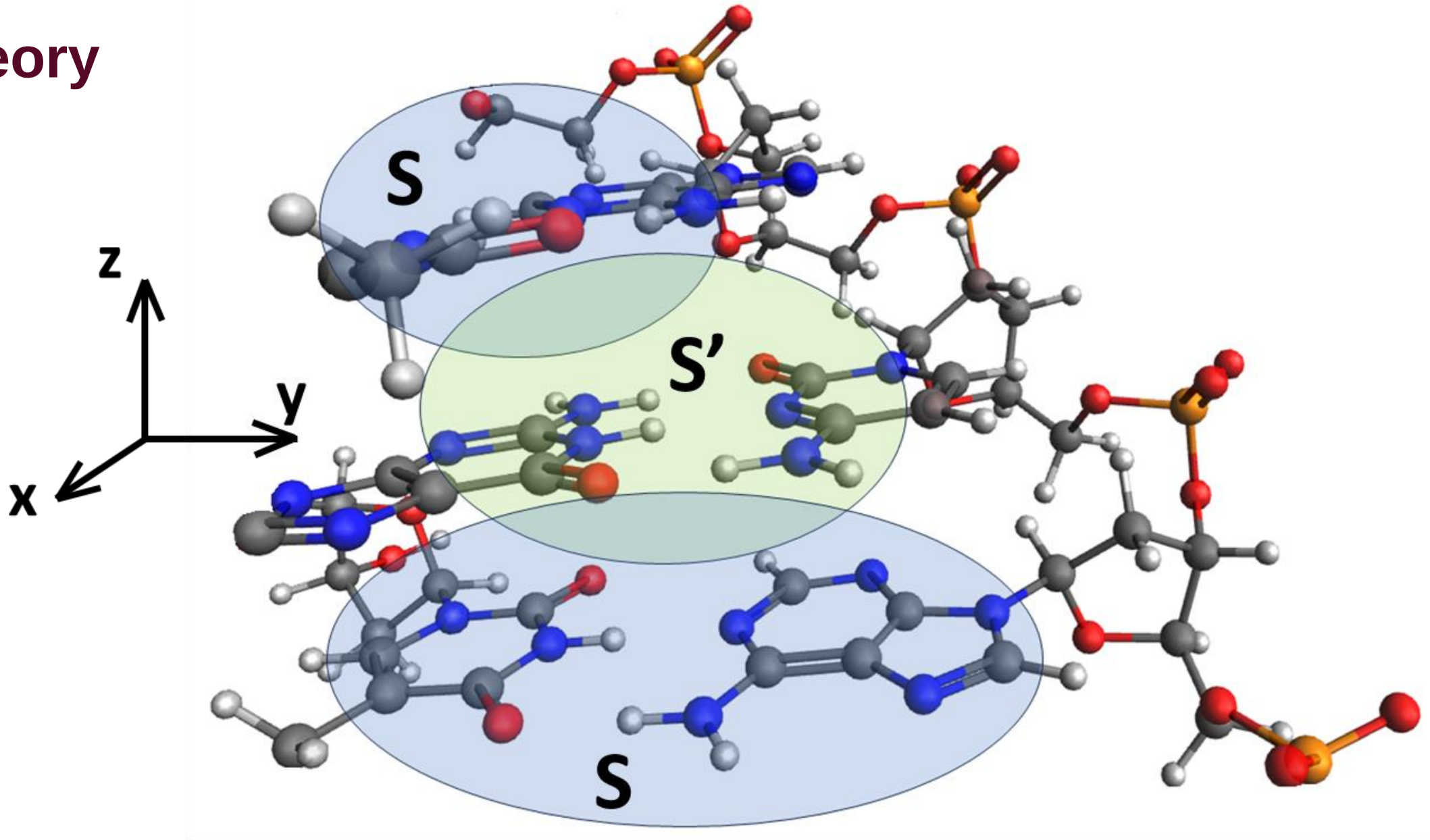
$S$ the number of symmetries in the system

$\mathbf{R}_{n\alpha}$ radius is a vector specifying the position of the symmetry α or β

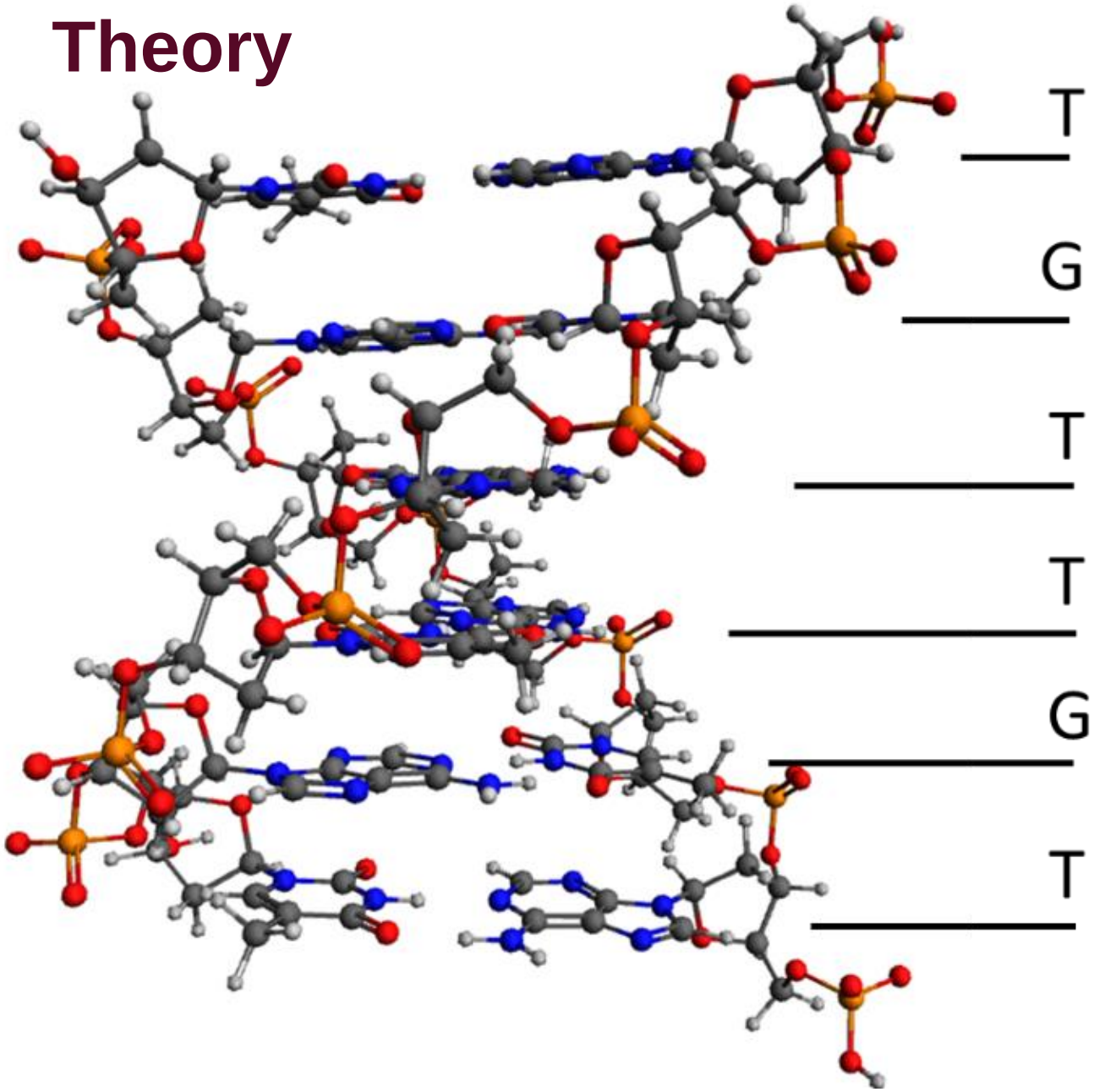
$\mathbf{p}$ momentum vector of the USPs falling on the multi-atom system

$\mathbf{R}_{Ai}$ radius is a vector specifying the position of atoms of grade i in symmetry

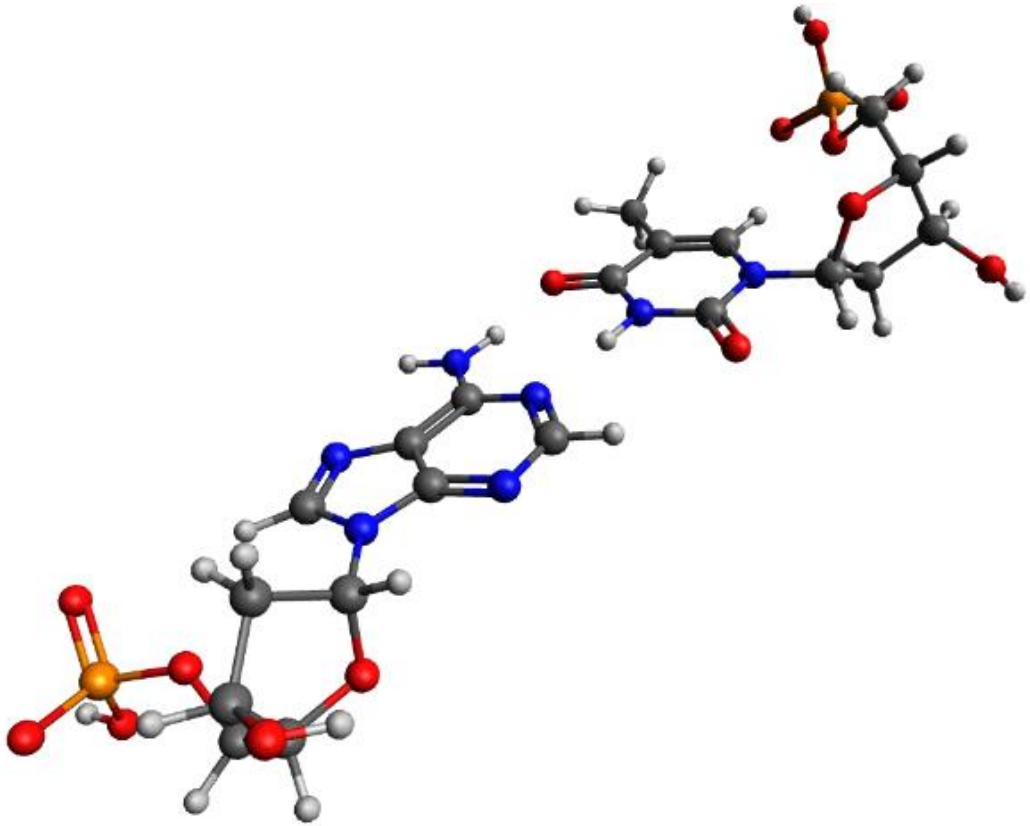
# Theory



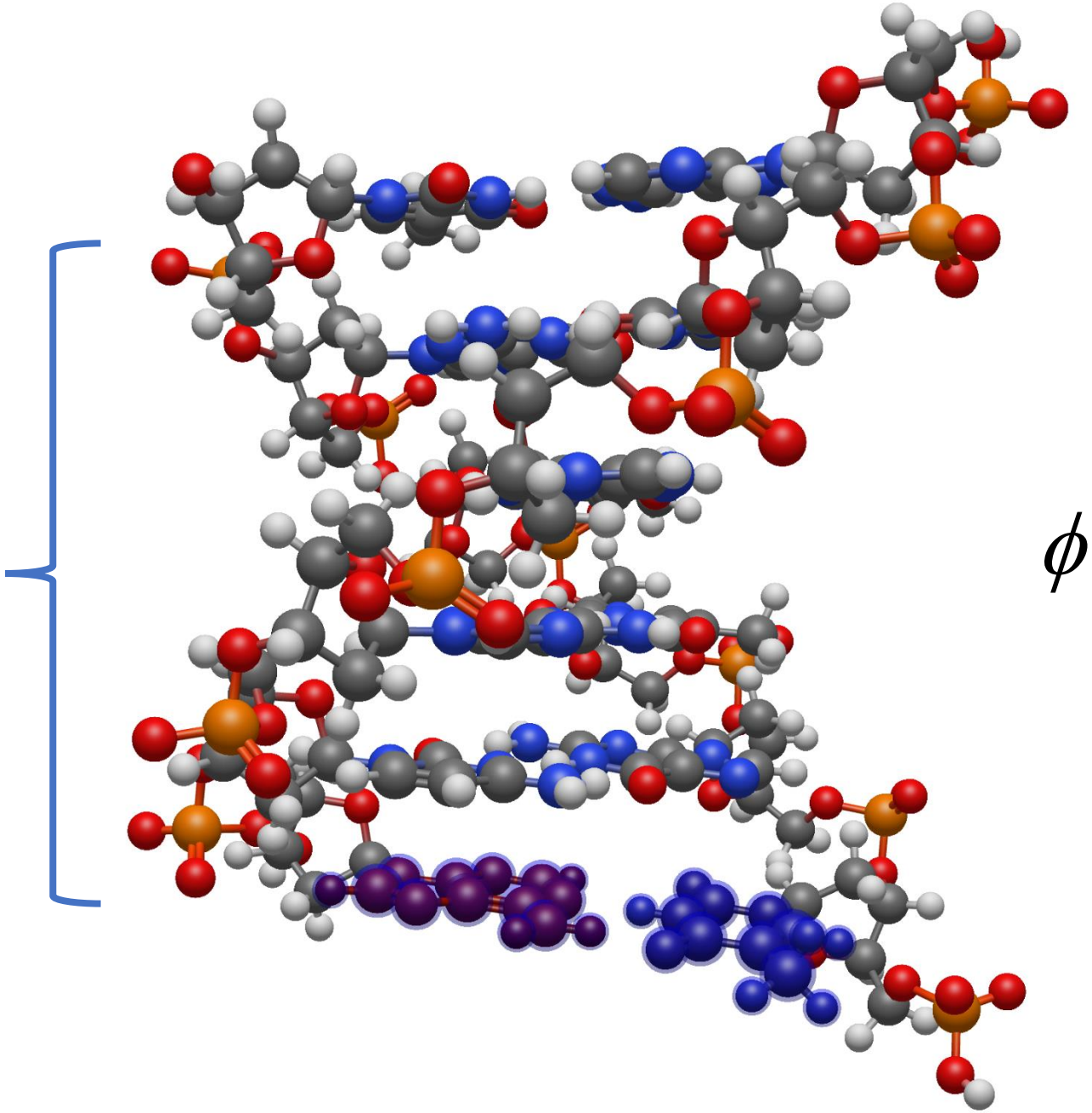
# Theory

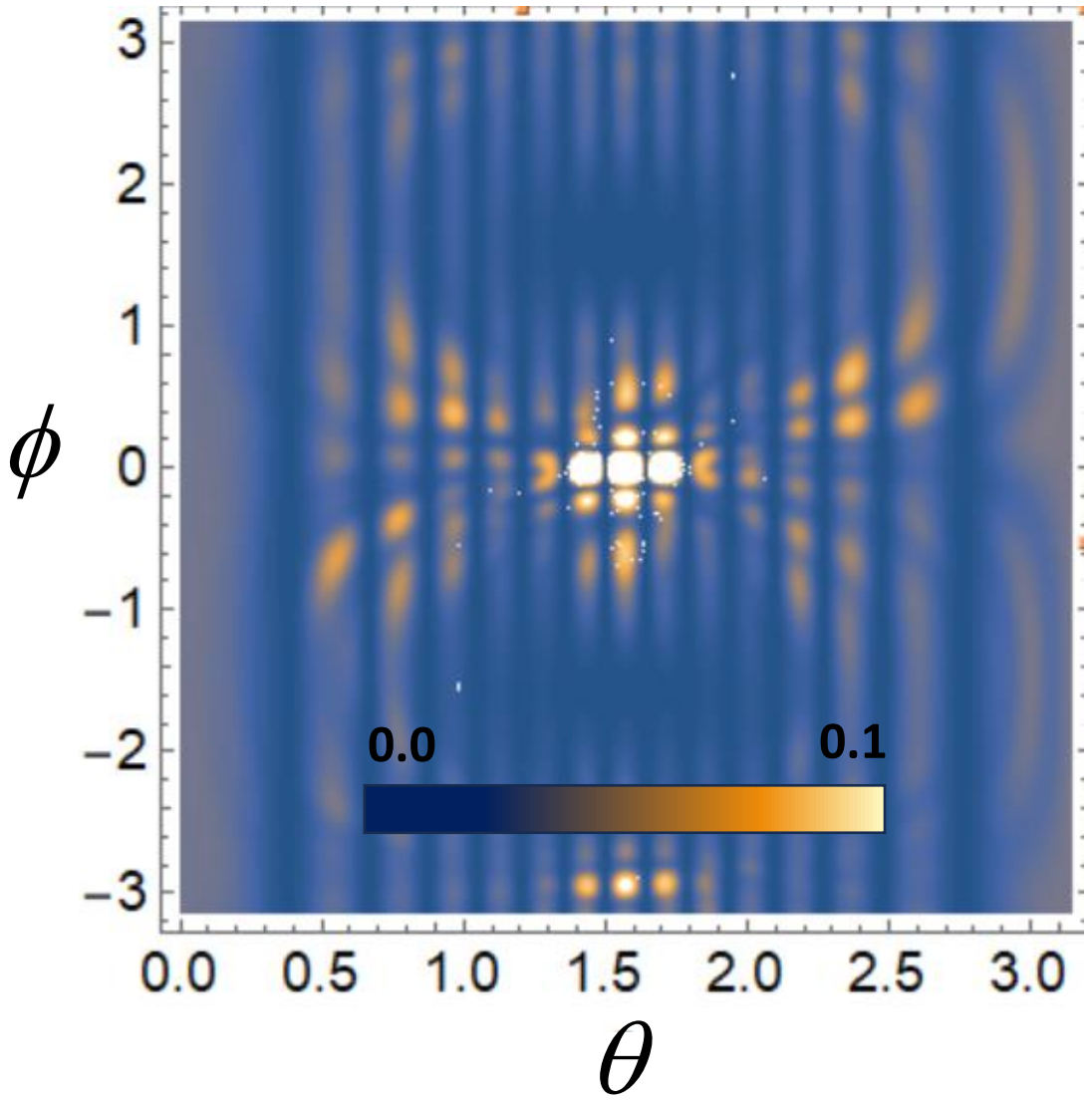



Escherichia coli str. K-12 substr. MG1655

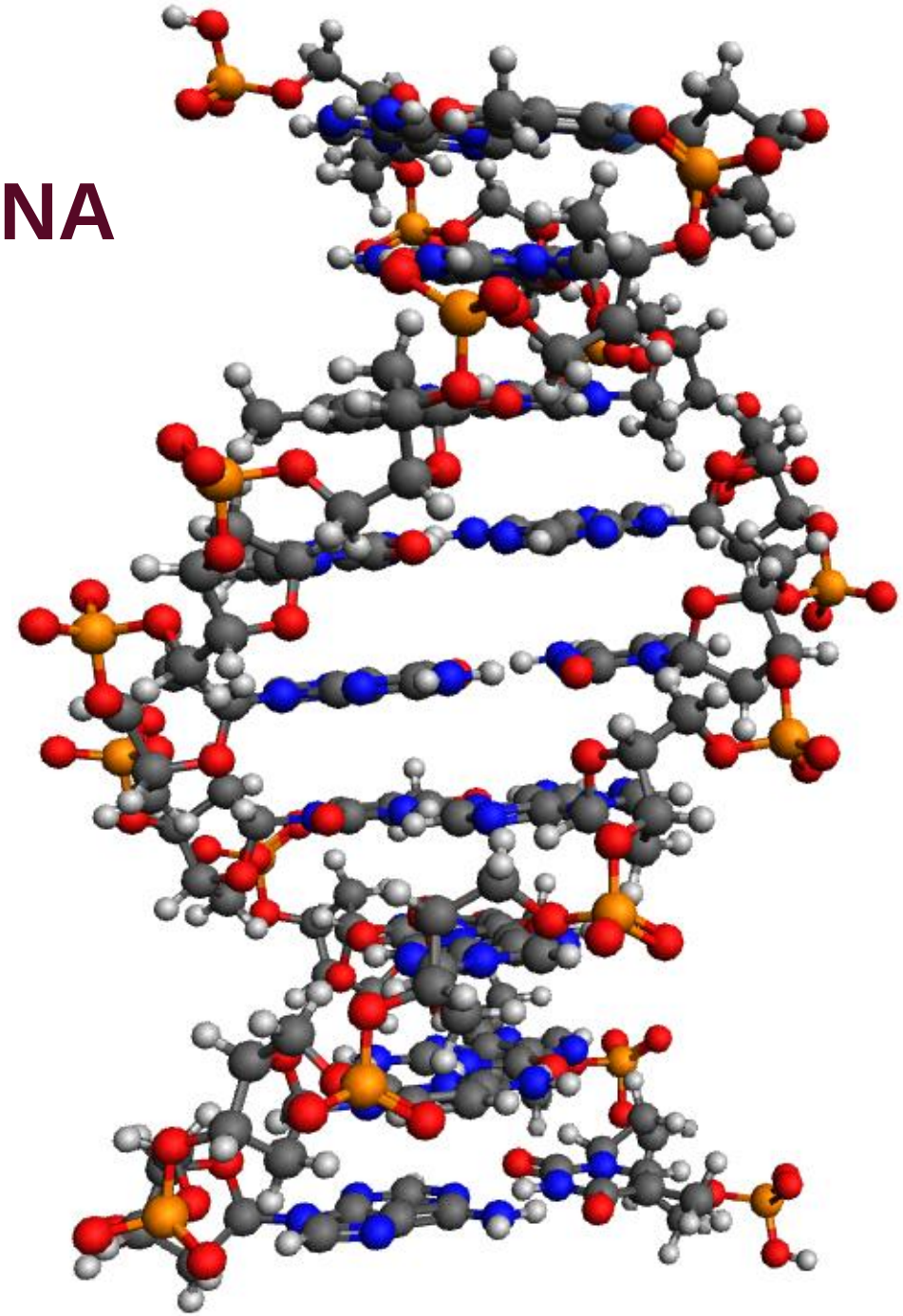


# Object for Modeling





DNA



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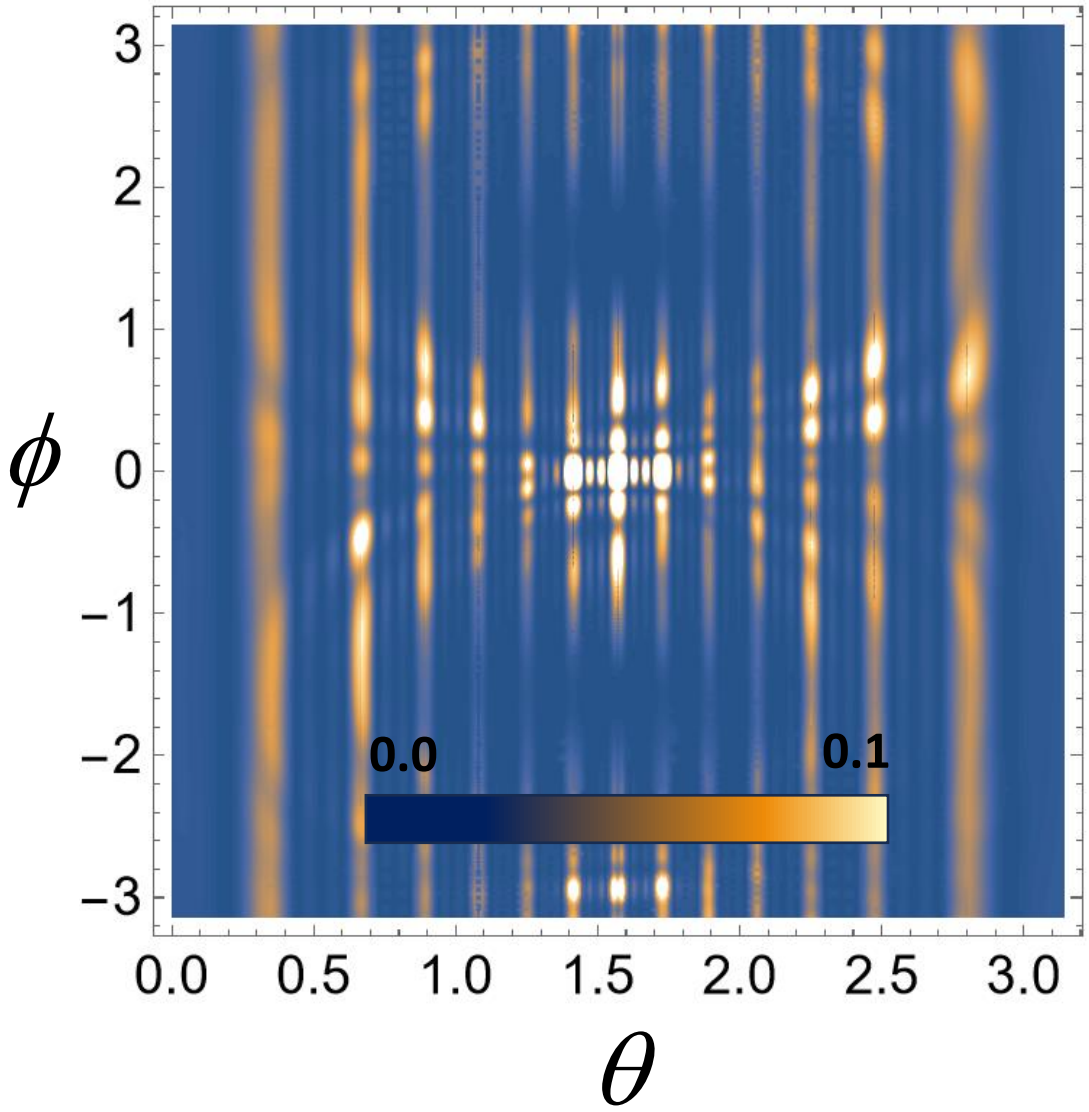
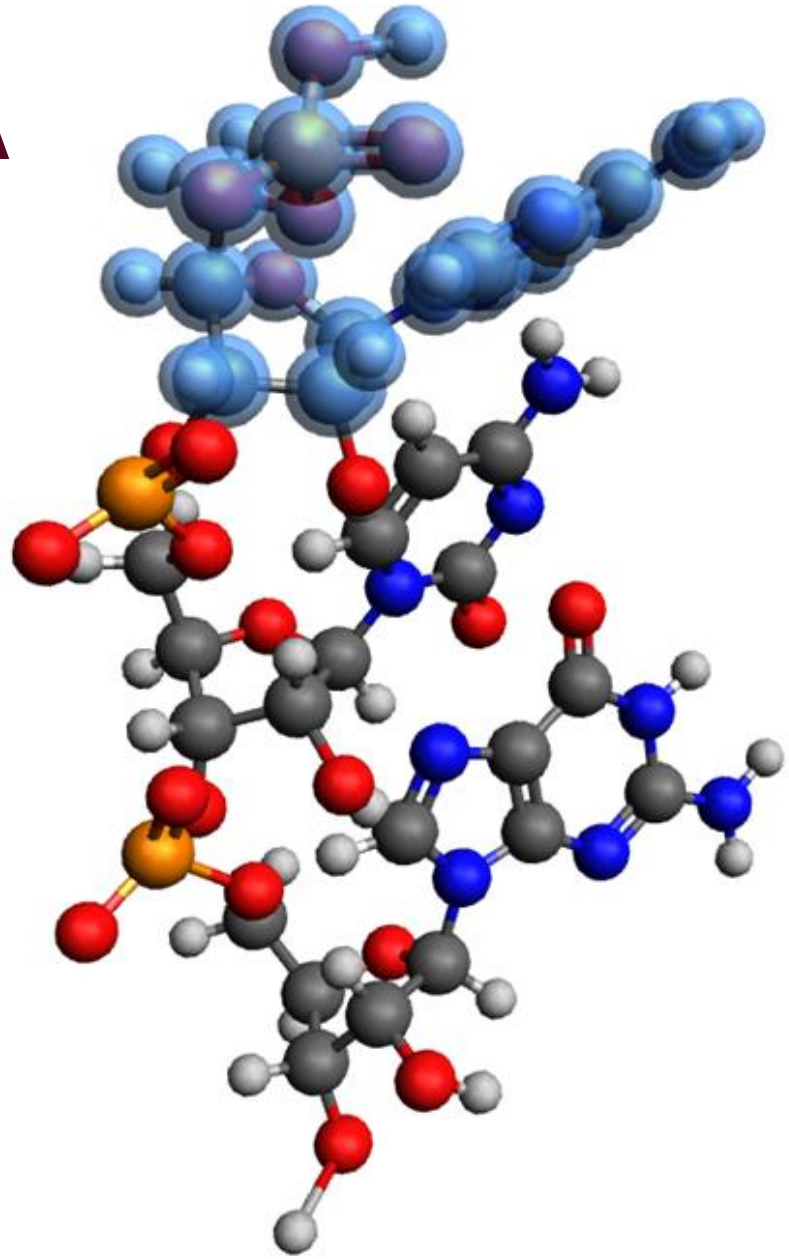
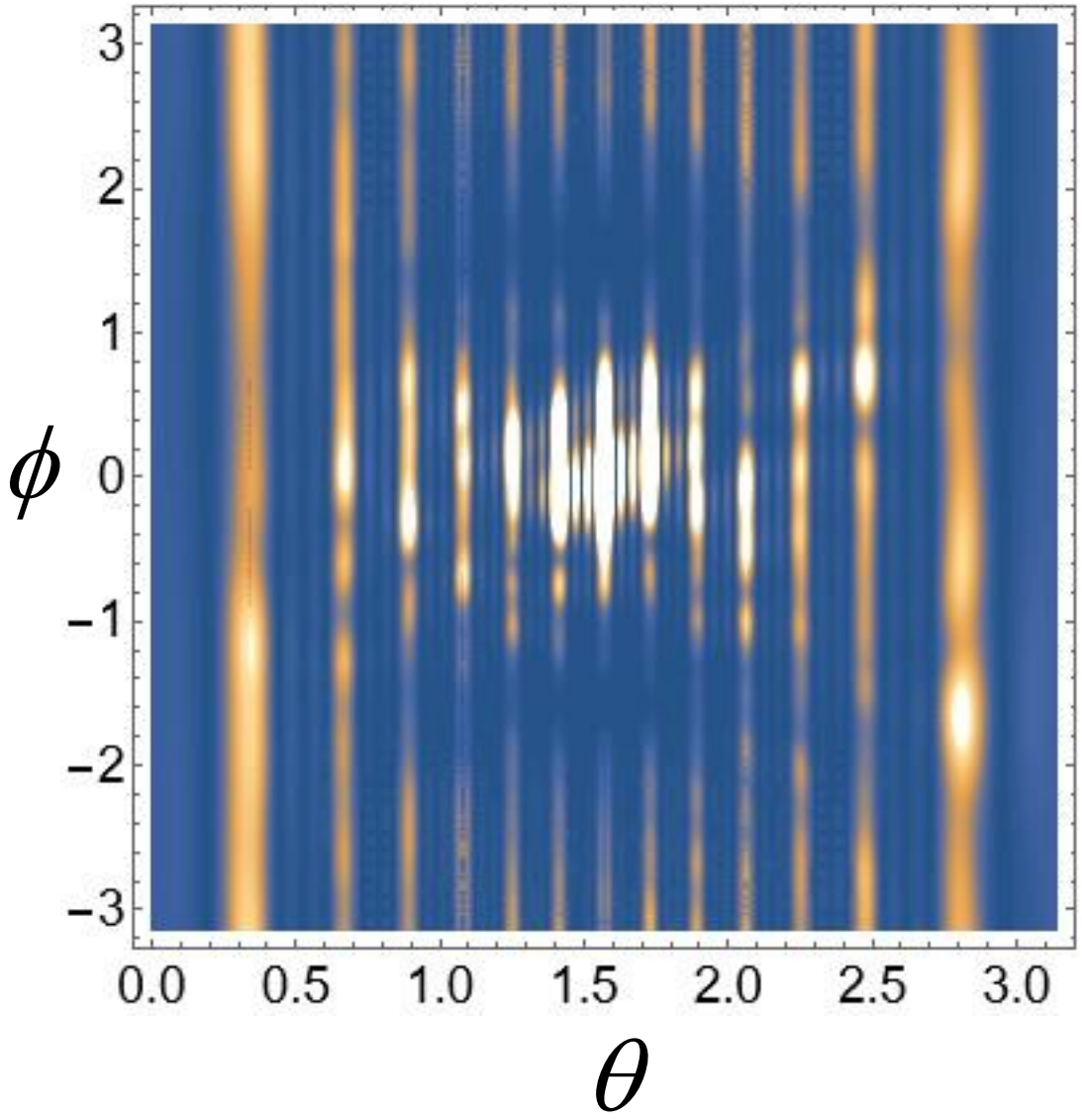


# RNA

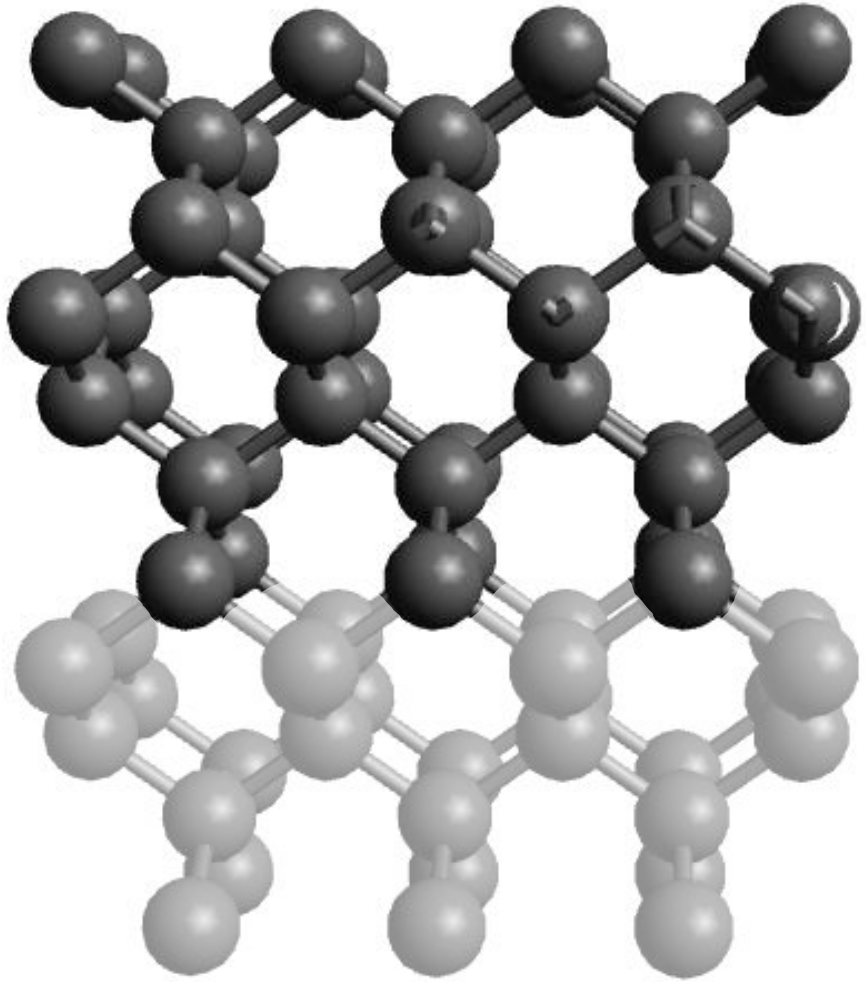


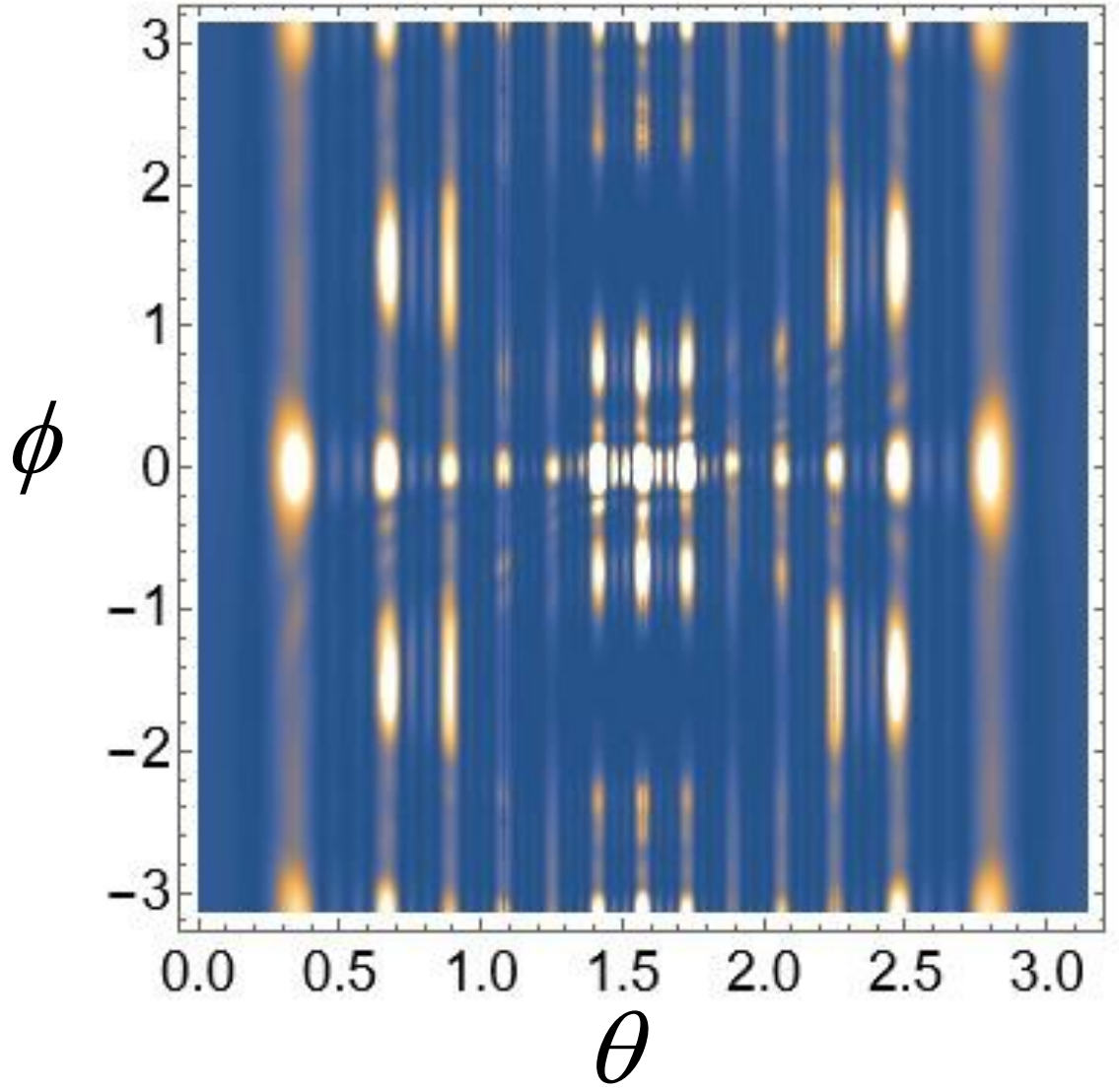
# Object for Modeling



# Object for Modeling

## Diamond plate

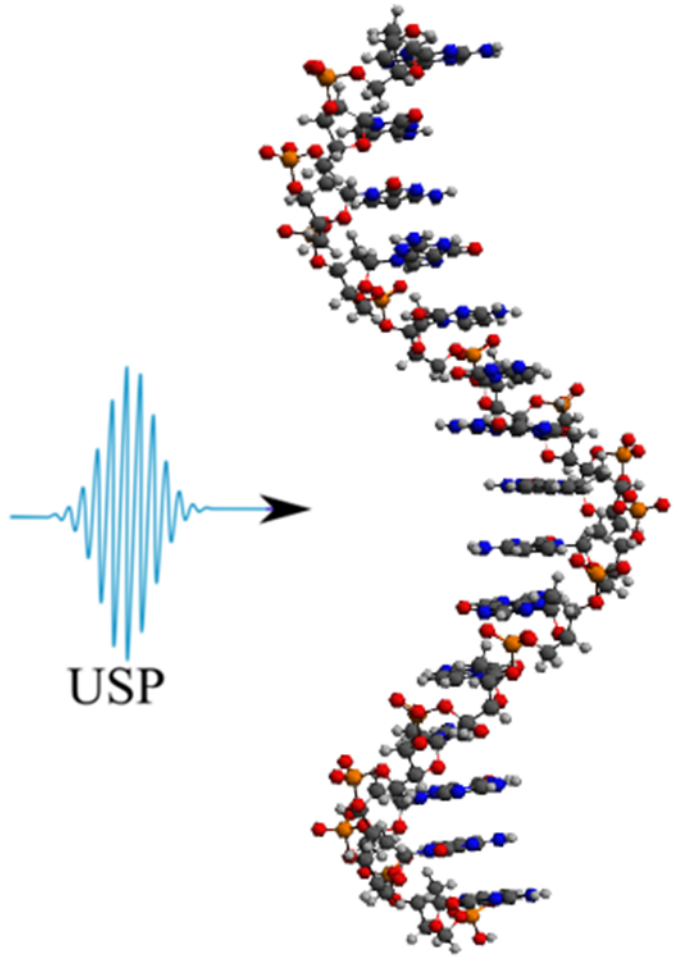




# Object for Modeling

The following parameters were used in the simulation:

- The main axis of DNA runs along the molecule, perpendicular to its bases
- The pulse falls on the system at an angle of 90 degrees to the main axis, system parameter
- Θ angle between the helix axis and the scattering direction
- ϕ angle between the x-axis and the projection on the plane perpendicular to the helix axis, the calculations were performed in spherical coordinates
- The results in all figures are normalized to the maximum value of the scattering spectrum.
- The value $\omega_0$= 2c, which corresponds to the photon energy 7.46 keV



# Conclusions

The scattering spectra of ultrashort laser pulses are mathematically modeled based on the theory of sudden disturbances.

An analytical formula is presented and the principle of calculating a polyatomic structure using atomic coordinates is explained.

As a result, mathematical models of USPs spectra were performed for three types of models.

The results show that the models give an idea of the structure of the sample, and the graphs obtained differ from each other.

# Thanks for your attention