The orientation-averaged classical deflection function for scattering of \( \text{UF}_5^+ \) ions by \( \text{N}_2 \) molecules is calculated in the collision energy range 2–10 keV, using additive interatomic potentials to calculate the anisotropic interaction of the molecular particles. The elastic scattering cross sections are calculated for ions and the interaction potential of the colliding particles is reconstructed using the Firsov method based on classical mechanics.

The results obtained are recommended for determining the isotopic sensitivity of mass spectrometers to be used for analysis of uranium compounds.

To calculate the isotopic sensitivity of mass spectrometers, which is determined by scattering of the beam ions by residual-gas molecules and the walls of the analyzer chamber it is necessary to know the effective cross section for elastic collisions of certain atoms and molecular particles. The experimental cross sections for elastic collisions of \( \text{UF}_5^+ \) ions with nitrogen molecules and iron atoms, necessary for determining the sensitivity of mass spectrometers for investigating the quantitative composition of uranium compounds, are still unknown. They can be estimated by constructing the average (over equally probable orientations) interaction potentials of the molecular particles under study. Such average potentials make it possible to find the classical deflection function for the colliding particles and therefore the differential effective cross section in a prescribed angular range.

We shall use the multicenter representation based on additive interatomic potentials to describe the anisotropic interaction of molecular systems. The assumption that the interatomic potentials are additive is equivalent to the assumption that the total transverse momentum \( \Delta p \) determining the deflection angle is equal to the sum of the impulses obtained by each atom as a result of the interaction.

As shown in [1], to describe the orientations of the colliding particles it is convenient to use the \( xoy \) plane of a coordinate system whose \( z \) axis oriented along the relative velocity vector \( v \). Two angles determine the position of the axisymmetric diatomic nitrogen molecule relative to this plane: the polar angle \( \psi (0–\pi) \) and the azimuthal angle \( \chi (0–2\pi) \). For convenience, we choose the orientation of the “regular hexagon” of \( \text{UF}_5^+ \) such that the fluorine atoms are located at the vertices in a manner so that the three fluorine atoms and the uranium atom are located in this plane, as shown in Fig. 1. We enumerate the atoms as follows: No. 1 – uranium atom, Nos. 2–6 – fluorine atoms, and Nos. 7 and 8 – nitrogen atoms. The positions of the projections of the atoms in \( \text{UF}_5^+ \) will be determined by the azimuthal angles \( \chi_i \) and the projections of the \( \text{U}–\text{F} \) bonds on the \( xoy \) plane. The position of the projections of the nitrogen atoms is determined by the angles \( \chi_j \) and the length of the \( \text{N}–\text{N} \) bond in the nitrogen molecule. Table 1 shows the angles determining the first orientation of the colliding particles.

For small scattering angles, if the projections of the molecules on the \( xoy \) plane (Fig. 2) are known, then the distance \( b_{ij} \) of closest approach of the uranium, fluorine, and nitrogen atoms (interatomic impact parameters) can be found from the...
angles $\varphi_i$ and $\chi_i$, the length of the bonds of the uranium and fluorine atoms $r_2 = 0.1994$ nm and the nitrogen atoms $2r_1 = 0.1094$ nm, and the intermolecular impact parameter $b$:

$$b_{ij} = r_{ij} \left( 1 + 2 \frac{R_i \cos (\gamma_i + \chi_j)}{r_{ij}} + \frac{R_i^2}{R_{ij}} \right)^{1/2}, \quad (1)$$

where

$$R_i = r_{2i} \left( 1 - 2 \frac{b}{r_{2i}} \cos \chi_i + \frac{b^2}{r_{2i}^2} \right)^{1/2},$$

$$r_{2i} = r_2 |\sin \psi_i|; \quad r_{ij} = r_1 |\sin \psi_j|. \quad (2)$$

Here $i = 2, 3, 4; \ j = 7, 8; \ \chi_j$ is the azimuthal angle determining the position of the nitrogen atoms. The coordinates of the uranium and fluorine atoms are determined by the angle $\chi_i$ for finding $R_i$ from Eq. (2). For the atoms $i = 1, 5, 6$ with coordinates $x_i = 0$ and $y_i = 0$ the quantity $b_{ij}$ equals $b_{ij}$:

$$b_{ij} = b \left( 1 + 2 \frac{r_{ij}}{b} \cos \chi_j + \frac{r_{ij}^2}{b^2} \right)^{1/2}. \quad (3)$$

The angle $\gamma_i$ in Eq. (1) is found from the formula

$$\cos \gamma_i = \frac{1}{2} \left( \frac{b}{R_i} + \frac{R_i}{b} - \frac{r_{2i}^2}{bR_i} \right).$$

825