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## RADIOACTIVE MOLECULES IN SN1987A REMNANT

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**ABSTRACT.** The investigation of SN1987A remnant is complicated due to absence of the source of ionizing radiation, which should excite the remnant's atoms and molecule. X-ray radiation from the shock wave front and, in accordance with recent observations, the intensity of X-rays significantly decreased during the last year made the backlighting of remnant. At the same time the intensity of molecular lines emission, localized near the front, abruptly increased. The remnant itself can be detected at the longer wavelength due to IR emission of dust component. One of the outburst's results was the synthesis of radioactive isotope  $^{44}_{22}\text{Ti}$ . Its decay time is 85 years, the total mass of synthesized atoms is near the mass of Jupiter. The thermochemical analysis shows that during the last two years the remnant creates a set of diatomic molecules, which will be not a subject of thermal dissociation later. One of these molecules is the radioactive titanium oxide –  $^{44}_{22}\text{Ti}^{16}_8\text{O}$ .

We investigate the properties of diatomic molecules  $^{44}_{22}\text{Ti}^{16}_8\text{O}$  and  $^{44}_{21}\text{Sc}^{16}_8\text{O}$  before and after the radioactive decays of  $^{44}_{22}\text{Ti}$  and  $^{44}_{21}\text{Sc}$ . For oxides  $^{44}_{22}\text{Ti}^{16}_8\text{O}$  and  $^{44}_{21}\text{Sc}^{16}_8\text{O}$  the spectroscopic constants were calculated using the isotopic shifts with respect to well known  $^{48}_{22}\text{Ti}^{16}_8\text{O}$  and  $^{48}_{21}\text{Sc}^{16}_8\text{O}$  molecules. The isotope  $^{44}_{22}\text{Ti}$  captures the electron from internal level. The result is the synthesis of new molecule  $^{44}_{21}\text{Sc}^{16}_8\text{O}$ .  $^{44}_{21}\text{Sc}$  decays after 6 hours and creates the stable isotope  $^{44}_{20}\text{Ca}$ , hard X-ray and  $\gamma$ -quanta and positron ( $e^+$ ). Additional result is the dissociation of molecule and the synthesis of stable neutral isotope  $^{44}_{20}\text{Ca}$  after the sequence of decays  $^{44}_{22}\text{Ti} \rightarrow ^{44}_{21}\text{Sc} \rightarrow ^{44}_{20}\text{Ca}$ .

We found the energetic properties of transient molecules  $^{44}_{22}\text{Ti}^{16}_8\text{O}$  and  $^{44}_{21}\text{Sc}^{16}_8\text{O}$ . We first estimated the probabilities of radioactive transitions in the molecule  $^{44}_{22}\text{Ti}^{16}_8\text{O}$  during its transition to  $^{44}_{21}\text{Sc}^{16}_8\text{O}$ . We calculated the molecular transitions which allow to point the electronic, vibrational and rotational transitions during the decay  $^{44}_{22}\text{Ti} \rightarrow ^{44}_{21}\text{Sc}$ . The obtained results permit us to predict the new spectral lines and bands detection in the spectrum of SN1987A remnant. It will be emitted by transient molecules and can be identified in future observations.

**Keywords:** SN1987A remnant, radioactive molecules.**1. Introduction**

The supernova explosion 1987A in the Magellanic Clouds was the closest type IIb supernova. The availability of this object for a large number of modern ground-based and space telescopes allowed us to stand up its adequate physical model. During the last 30 years, the structure of the shock wave front, created by an asymmetric explosion, is an important source of information on the surrounding supernova interstellar medium. The front of the shock wave formed X-ray radiation, causing the emission of relic cocoon from which the progenitor was formed as well as the dust remnant. Observations of the IR excess of the remnant allowed obtaining the chemical composition, optical characteristics and particle size distribution. Frank et al. (2016) observed a correlation of energy fluxes in the X-ray and IR spectral regions. The chemical composition and optical characteristics of solid particles were found from observations.

Infrared fluxes from the remnant were first observed one year after the explosion, when the temperature of discarded envelope was noticeably decreased. The basic thermodynamic parameters of remnant were described in a simple, Sedov approximation (Zeldovich & Raizer, 1966). Detailed calculations of the reaction rates taking into account the pressure, concentration of the substance, and temperature in the shell have led to the conclusion that the use of the thermochemical equilibrium approximation at the time frames within 360-900 days after the explosion is justified.

The self-consistent scheme of equations of the kinetics of nucleation of the solid phase in the supernova remnant can be solved. It showed that the formation of dust particles is effective when the diatomic molecules are accepted to be condensation centers. That is why with great certainty it can be accepted that the diatomic molecules were formed simultaneously with dust. Unfortunately, the line spectra of molecules during the indicated period of remnant's evolution were not detected because of the strong dominance of other radiation sources. Later the physical conditions of the shell are such that the formation of diatomic molecules and dust becomes not effective.

Rough estimates show that the total mass of the dust in SN1987A residue until recently was no more than one solar mass, and the mass of the molecular component can be as high as several solar masses. According to the solution of the thermochemical equilibrium equations for the gas mixture in the remnant, virtually all metals are first

linked into diatomic molecules and then are condensed to the dust (Kozasa et al., 1989). In an atomic form, they can be observed only near the remnant's surface, where due to X-ray illumination, the presence of a shock front, the dissociation of molecules and the evaporation of dust are more intense than inside it. At present time, according to the Sedov's equations and the observations of IR radiation of dust, the average thermodynamic temperature of the remnant is not higher than 100 K, and the concentration of molecules and particles reaches  $10^6$ - $10^8$   $\text{cm}^{-3}$  and below. Under such conditions, only rotational levels can be excited in diatomic molecules, the intensity of which sharply increases against the significant recent drop of the X-ray and IR radiation.

The absence of a high temperature compact source in the remnant's center makes it impossible to excite the vibrational-rotational electronic transitions in diatomic molecules located inside the shell. Purely rotational transitions of molecules can be intensive only under the specific ratios between the Franck-Condon and Henle-London factors. Such conditions are rarely satisfied and are valid only for molecules in which the dipole moment is sufficiently small or zero.

The physical conditions for intense rotational transitions of molecules arise near the shock wave front of and near the surface of the remnant. In these cases, the conditions for shock excitation of the rotational levels of diatomic molecules exist. The similar physical conditions are also valid for regions of the interstellar medium behind the shock wave front.

The probabilities of radiative and impact transitions are high in the regions near the remnant's surface. It is caused by its high intrinsic speed in the interstellar space. Such physical conditions exist at all stages of the remnant's evolution. In this regard, it is clear that the radioastronomical observations will be always important for determining the location of supernova remnants, the shock waves generated by them, and the relict cocoon, which in the past led to the formation of a progenitor star. To perform the spectral diagnostics and to determine the chemical composition of the cold remnant, it is necessary to use the lines of atomic transitions as well as the lines of vibrational-rotational transitions of diatomic molecules.

The only source of excitation of various electronic states of atoms and molecules can be the decay of radioactive isotopes. Modern satellite observations revealed the significant enrichment of supernova remnants of type II with radioactive isotopes – the products of asymmetric supernova explosions. In particular, a significant content of the isotope  ${}^{44}_{22}\text{Ti}$  was found.

This review is devoted to the physical signs of the presence of radioactive isotopes in supernova remnants, which can manifest themselves in the form of atomic and molecular lines and bands, and can be observed. Here after we give the review and the new results obtained by authors are presented. Conclusions are drawn about the future observations of supernova remnants. We introduce a new type of molecules and call it Radioactive Molecules.

## 2. Radioactive Molecules

Molecules in which the nucleus of at least one of the atoms is unstable will be called radioactive. In the overwhelming majority of cases, the radioactive decay of atoms entering the molecule does not give any spectroscopic manifestations, characteristic of diatomic molecules. The molecular spectra are not observed. The decaying nucleus acquires a recoil energy that is many orders of magnitude higher than the energy of the molecular bond, namely several electron volts. That is why the products of such decays exist in an atomic form and increase the fraction of the atomic component in the remnant's chemical composition. However, there is a small group of radioactive nucleus that can carry out electronic capture and do not acquire recoil energy at the time of capture.

In this case, the molecule's internal structure changes. The nucleus of a lower atomic number and charge appears. Here after we will be interested in such changes in the structure of diatomic molecules, for which an electronic transition is allowed and the selection rules are satisfied. In the case of electron K-capture by the nucleus of a radioactive isotope, first the redistribution of electronic and nuclear states occurs in the initial molecule, second a finite diatomic molecule is formed. Depending on the characteristic times of these processes, electronic transitions occur, in particular, similar to vibrational-rotational transitions in usual (non-radioactive) molecules.

For experimental spectroscopy of radioactive diatomic molecules, it is important to know the location of the lines and bands in the emission spectrum. Absorption spectra in this paper are not considered because of the physical and astrophysical features of the objects studied, noted in the previous section.

### 2.1. Radioactive Molecules in SNR1987A

The information about the initial and boundary conditions of the explosion of the progenitor star allowed to carry out quantitative calculations of the main average thermodynamic quantities, the chemical composition of gas and dust in SNR1987A. A sharp increase in the sensitivity threshold of the recording equipment in the x-ray and gamma wavelength regions made it possible to detect the quanta responsible for the radioactive decay of the isotope of titanium in the chain of radioactive transformations of the type  ${}^{44}_{22}\text{Ti} \xrightarrow{85\text{y}} {}^{44}_{22}\text{Co} \xrightarrow{6\text{h}} {}^{44}_{22}\text{Ca}$  (Grebenev et al., 2012). In this chain of decays, the radioactive isotope of titanium  ${}^{44}_{22}\text{Ti}$  forms diatomic molecules:  ${}^{44}_{22}\text{Ti}{}^{16}_8\text{O}$ ,  ${}^{44}_{22}\text{Ti}{}^{12}_6\text{C}$ ,  ${}^{44}_{22}\text{Ti}{}^{14}_7\text{N}$ ,  ${}^{44}_{22}\text{Ti}{}^1_1\text{H}$ .

The main part of  ${}^{44}_{22}\text{Ti}$  is bound by these diatomic molecules and does not occur in free form. Here after we begin with the molecule  ${}^{48}_{22}\text{Ti}{}^{16}_8\text{O}$ . In spectroscopy of stellar atmospheres this molecule is known for more than 60 years. Its molecular constants were determined by experimental methods and theoretical ab initio calculations. The most studied titanium isotope  ${}^{48}_{22}\text{Ti}$  is stable to radioactive decays. To determine the molecular constants of the radioactive molecule of interest, namely  ${}^{44}_{22}\text{Ti}{}^{16}_8\text{O}$ , we use the results obtained by Hertzberg (1949), formulas and data on them. Jorgensen (1994) & Dobrodey (2001) refined the

molecular data and used them to calculate the molecular lines of different titanium isotopes.

Titanium isotopes that we are interested in, namely those with an excess of protons in the nucleus, were not considered earlier. Titanium molecules were important to determine the average absorption coefficient in the atmospheres of cold stars. Molecular bands and lines with the isotope of interest to us,  ${}^{44}\text{Ti}$ , in stellar atmospheres are not found. It is radioactive and can be formed effectively only during strong asymmetrical supernova explosions. The planning of observations of molecular bands and their lines in the SN1987A remnant requires the consideration of state of the remnant at present time and in the forthcoming years.

There are no specific sources of excitation of molecular bands and lines. There is no central source of energy in the form of a relativistic object that pushes the widening remnant with a wide range of photons. External illumination by hard radiation from the front of the shock wave only leads to partial dissociation of diatomic molecules in the near surface layer of the residue and does not excite the molecules that are of interest to us. The average thermodynamic temperature of the remnant is 30-60 K. This value was found using IR observations of the dust in remnant. Under these conditions, practically all diatomic molecules under discussion are in the main "frozen" state.

Under these physical conditions, we have an initial radioactive molecule in the ground state. The values of vibrational quantum numbers are zero and the rotational lines can be calculated from the isotopic shift of molecular vibrations inside the vibrational bands for molecules with stable isotopes of titanium ( ${}^{44}\text{Ti}$ ). It will be shown that the radioactive processes associated with the isotope of titanium lead to a significant change in the quantum state of the molecules.

## 2.2. Electronic capture in radioactive molecules

The physical phenomena considered below are valid for all molecules which include radioactive isotopes experiencing electron capture at the time of nuclear transformation. From the point of view of future spectroscopic observations, the most interesting isotopes are those with a half-life period much longer than the characteristic time of the electronic transition of the molecule from the excited state to the ground one. As it was noted in the previous section, there are no sources of external excitation in the SN1987A remnant due to low average thermodynamic temperatures. The infrared field of radiation caused by dust particles can only affect the formation of weak rotational lines.

The total Coulomb energy of an atom (or a molecule) will decrease because of a decrease in the charge of the nucleus – the product of the nuclear transformation. The stored potential energy of the molecule is comparable to the molecular binding energy and to the energies of all types of electronic molecular transitions. The excess of the Coulomb potential energy leads to the fact that the state of the initial molecule proves to be unstable and the transition to the stable state of the daughter molecule is forced.

Following the previous sections, the initial radioactive molecule is  ${}^{44}\text{Ti}^{16}\text{O}$ , and the daughter radioactive mole-

cule is  ${}^{44}\text{Sc}^{16}\text{O}$ . The half-life of scandium is  $T_{1/2} = 6^{\text{h}}$ , the molecule will exist during the time sufficient to emit a certain number of emission quanta. To date, there is no reliable data on recombination transitions to a hole in a 1s shell of titanium and then scandium, which are part of different molecules. Under low temperatures and low concentrations of the remnant's substance, the probability of such recombination is comparable to the probabilities of purely molecular emission transitions.

The main part of the energy of the radioactive transition accompanying the electron capture in the marked titanium molecules is estimated from the mass difference between  ${}^{44}\text{Ti}$  and  ${}^{44}\text{Sc}$ , taking into account the total energy of the captured electron (0.512 MeV) minus the ionization energy 1s of the level  ${}^{44}\text{Ti}$ , the total energy of the emitted neutrino (0.1 MeV) and the recoil energy of the nucleus of the newly formed  ${}^{44}\text{Sc} - E_{\text{Sc}}$ .

$$E_{\text{Sc}} = \frac{(hv)^2}{2Mc^2} \approx 2 - 4 \text{ eV} \quad (1)$$

Until recently, it was believed that all types of neutrinos do not have a rest mass like quanta of electromagnetic radiation. The observed oscillations of the energy of these particles led to the understanding that they have infinitesimal rest masses at the upper threshold of the sensitivity of the our hardware. In this case, the formula for  $E_{\text{Sc}}$  remains valid, taking into account the small correction for the rest mass of the electron neutrino.

## 3. Electronic transitions in radioactive molecules

The calculation of electronic transitions in diatomic radioactive molecules is to find the wave functions of the initial and final states of two radioactive diatomic molecules, one of whose nuclei participates in the radioactive transformation. For example,  ${}^{44}\text{Ti}^{16}\text{O} \rightarrow {}^{44}\text{Sc}^{16}\text{O}$ . The method to choose or calculate molecular constants consists in taking into account the kinematic features and quantum characteristics of the excited and ground levels of radioactive diatomic molecules before and after their excitation in the cold supernova remnant.

In some cases it is convenient to carry out calculations of the spectroscopic properties of titanium oxide on the basis of previously chosen molecular constants (Herzberg, 1949; Huber and Herzberg, 1979; Jorgensen, 1994; Dobrodey, 2001). To implement the electronic transition, the selection rules and statistical sums must be taken into account. Here after we shall consider only allowed dipole transitions.

### 3.1. Emission characteristics of transition molecules.

The molecule  ${}^{44}\text{Ti}^{16}\text{O}$

The molecule  ${}^{48}\text{Ti}^{16}\text{O}$  will become the starting point of our analysis of the spectroscopic properties of the molecule  ${}^{44}\text{Ti}^{16}\text{O}$ . In laboratory experiments, as well as in spectroscopy of stellar and planetary atmospheres, the molecular spectra of  ${}^{48}\text{Ti}^{16}\text{O}$  have been studied in detail. Laboratory experiments on the measurement of spectroscopic constants are also known. Following the method proposed by Jorgensen (1994), we will search the emission properties of  ${}^{44}\text{Ti}^{16}\text{O}$  using the known parameter of isotopic shift between the  ${}^{48}\text{Ti}$  and  ${}^{44}\text{Ti}$  nuclei in the indi-

cated oxides  $\rho$  according to the formula  $\rho = \frac{\mu_{48}}{\mu_{44}} = 1.011075$ , where  $\mu_{48}$  and  $\mu_{44}$  are the specific masses of the molecules  ${}^{48}\text{Ti}{}^{16}\text{O}$  and  ${}^{44}\text{Ti}{}^{16}\text{O}$ , respectively.

As a first step, we find an isotopic shift of the rotational line when the isotope  ${}^{48}\text{Ti}$  is replaced by the isotope  ${}^{44}\text{Ti}$  in the titanium oxide.

$$\begin{aligned} \Delta v_r J'' &= v_{44} v, J'' - v_{44} v, 0 - v_{48} v'', J'' - \\ &\quad v_{48} v'', 0 \\ &= F_v^{44} J' - F_v^{44} J'' - F_v^{48} J' - F_v^{48} J'' \\ &= \Delta F_v^{48} J' - \Delta F_v^{48} J'' \\ &= \rho^2 - 1 B_e' - \rho^3 - 1 \alpha' u' J' J' + 1 \\ &\quad + \rho^4 - 1 D_e' - \rho^5 - 1 \beta' u' J'^2 (J' + 1)^2 \\ &\quad - \rho^2 - 1 B_e'' - \rho^3 - 1 \alpha'' u'' J' J' + 1 \\ &\quad + \rho^4 - 1 D_e'' - \rho^5 - 1 \beta'' u'' J''^2 (J'' + 1)^2 \end{aligned}$$

The isotopic shift  $\Delta v_v(v'')$  relative to the center of the vibrational band for these molecule depends on the molecular constants and the displacements relative to the upper  $\Delta G_v(v')$  and the lower  $\Delta G_v(v')$  states of the vibrational levels in the molecule  ${}^{48}\text{Ti}{}^{16}\text{O}$

$$\begin{aligned} \Delta v_v(v'') &= \Delta G_v(v') - \Delta G_v v'' \\ &= \rho - 1 u^1 \omega_e' - u'' \omega_e'' \\ &\quad - \rho^2 - 1 u'^2 x_e \omega_e' - u''^2 x_e \omega_e'' \\ &\quad + \rho^3 - 1 u'^3 y_e \omega_e' - u''^3 y_e \omega_e'' \end{aligned}$$

Thus, we find the true position of the line (its wave number) in the molecule  ${}^{44}\text{Ti}{}^{16}\text{O}$  using the expression

$$v' v'', J'' = v v'', J'' + \Delta v_v(v'') + \Delta v_r(J'').$$

In this paper we consider cold remnants, and therefore we will only be interested in transitions that lead to the emission of photons. Small values of emission fluxes from cold gas-dust formations are caused by remoteness of the studied objects or by a small concentration of the molecules studied. We will search for possible intense bands in which the molecules emit with higher probability and energy. In order to relate the quantum transitions in the radioactive decay under consideration to emission, the upper limit of the population of the upper excited levels is assumed equal to N.

Here N is the number of decaying isotopes in the given molecules. Without the loss of physical meaning, the population of the excited level can be assumed equal to the number of decaying atoms  ${}^{44}\text{Ti}$ . In order to quantitatively determine the number of  ${}^{44}\text{Ti}{}^{16}\text{O}$  molecules, after determining the position of the center of the vibrational band  $v' v'', J''$  it is necessary to calculate the integral emission coefficient of the electron-vibrational band (Kuznetsova, 1980; Kuzmenko, 1984)

$$k v', v'' = \frac{h c v_{v'v''}}{4\pi} A_{v'v''}^{nm} N_{nv'} \quad (2)$$

$$A_{v'v''}^{nm} = \frac{64\pi^4 v_{v'v''}^3 S_e(r_{v'v''}) q_{v'v''}}{3h (2-\delta_{0,\lambda'})} \quad (3)$$

We take into account that this process is going only in one direction and the use of local thermodynamic equilibrium for the calculation of populations is not required in

the problem under consideration. In this case,  $N_{nv'}$  will be considered equal to N. The coefficients of spontaneous, electron-vibrational transitions with emission  $A_{v'v''}^{nm}$  are taken into account without the discussion of induced transitions.

Let us calculate the wave numbers of the lines  $\nu$  in the electron-vibrational-rotational spectrum arising during the transition from one quantum state to another:

$$\nu = T_e' - T_e'' + G v' - G v'' + F J' - F J'' \quad (4)$$

The first term is called the wave number  $\nu_e$  of the electronic transition and has a dimension of  $\text{cm}^{-1}$ . Accordingly, the first two summands are called the beginning of the strip and are denoted as  $\nu v', v'' = \nu_e + G v' - G v''$ . The initial point of this will be levels with zero rotational energy, i.e.  $J^{\lambda'}=0, J^{\lambda''}=0$ . The substitution of the values of molecular constants in the formula (4) makes it possible to calculate the wave number  $\nu$  for the quanta created by the radioactive  $\beta$  process in the transition like  ${}^{44}\text{Ti}{}^{16}\text{O} \rightarrow {}^{44}\text{Sc}{}^{16}\text{O}$ .

Using the molecular constants for the well-studied molecules  ${}^{48}\text{Ti}{}^{16}\text{O}$  and  ${}^{48}\text{Sc}{}^{16}\text{O}$  according to Jorgensen (1994) & Herzberg (1949) it is possible to estimate the positions of head's bands and lines of  ${}^{44}\text{Ti}{}^{16}\text{O}$  and  ${}^{44}\text{Sc}{}^{16}\text{O}$  molecules as a result of the isotopic shift.

### 3.2. Selection of excited and ground states in radioactive molecules

The transition of initial radioactive molecule to the excited state before the subsequent radiative transition in the newly formed daughter molecule will be considered in three steps. During the first step, the original molecule with a radioactive core resides in the frozen ground state with zero values of the vibrational quantum number. As noted in the introduction, this is due to the fact that at present time the remnant has a molecular-dust component with an average thermodynamic temperature of the order of 30-60 K.

One-third of the original radioactive titanium  ${}^{44}\text{Ti}$  has already turned into the isotope  ${}^{44}\text{Ca}$ , existed in an atomic form. The remaining two-thirds are represented as diatomic molecules. In particular,  ${}^{44}\text{Ti}{}^{16}\text{O}$ . During the second step, at the moment of K-electron capture by a nucleus  ${}^{44}\text{Ti}$  with a filled 1s molecular orbital, the total quantum number J changes by one, the electron shells are rearranged almost instantaneously, simultaneously with this the electronic dipole moment changes. At time intervals in order of magnitude equal to or shorter by 2-3 orders of magnitude, the charge of the titanium nucleus decreases, A nucleus  ${}^{44}\text{Sc}$ , whose lifetime is  $6^h$ , arises.

It is obvious that for radiative transitions we have sufficient time. Quantum electronic transitions arise. Electronic transitions can be divided into molecular and cascade-recombination to 1s level. At the same time, the lifetime of molecular transitions can take  $10^{-8}$  seconds to reach the main level of the newly formed molecules  ${}^{44}\text{Sc}{}^{16}\text{O}$ . That is why the molecular transition succeeds either during or

after the cascade recombination transition to the 1s-vacancy.

Direct spectroscopic measurements of the recombination transition in a given molecule gave a value of 2478 eV and a dissociation energy of  $D_0 = 9.5$  eV (Dobrodey 2001). The last, third step is the destruction of the molecule  ${}^{44}_{21}\text{Sc}^{16}_8\text{O}$ , obtaining a significant recoil energy from the positron emitted from the nucleus  ${}^{44}_{21}\text{Sc}$  and the formation of the atom  ${}^{44}_{20}\text{Ca}$ . During the third step, the movement of the atom  ${}^{44}_{20}\text{Ca}$  in the remnant at high speed causes the ionization losses in it.

### 3.3. Preliminary calculations

The calculation of quantum transitions in radioactive molecules should be started with the determination of molecular constants of the excited  ${}^{44}_{22}\text{Ti}^{16}_8\text{O}$  and of the basic  ${}^{44}_{21}\text{Sc}^{16}_8\text{O}$  molecules. All molecular constants for the main lower levels of  ${}^{48}_{22}\text{Ti}^{16}_8\text{O}$  were revised by Dobrodey (2001). To the lowest singlet states are  $a^1\Delta$ ,  $d^1\Sigma^+$ , and the triplet  $-X^3\Delta$ ,  $E^3\Pi$ . The energies of the electronic terms are:  $T_e = 3565, 3435, 0$ , and  $13713$ , respectively. For the molecule  ${}^{44}_{21}\text{Sc}^{16}_8\text{O}$  the doublet transitions  $A^2\Pi \rightarrow X^2\Sigma$  (574-730 nm) and  $B^2\Sigma \rightarrow X^2\Sigma$  (450-577 nm) are well known. The chemical ties in  ${}^{44}_{22}\text{Ti}^{16}_8\text{O}$  and  ${}^{44}_{21}\text{Sc}^{16}_8\text{O}$  molecules are created by configurations formed by the interaction of valence P and D oxygen shells ( $2p^4$ ), titanium ( $3d^2$ ) and scandium ( $3d^1$ ) shells.

In this case, a large number of quantum states of a diatomic molecule arise as a whole, with different values of the projection of the orbital angular momentum onto its internuclear axis. Namely,  $\Sigma^+$ ,  $\Sigma^\pm$ ,  $\Sigma^-$ ,  $\Pi^+$ ,  $\Pi^\pm$ ,  $\Pi^-$ ,  $\Delta^+$ ,  $\Delta^-$ , and  $\Phi$  terms. To determine the configuration of the excited and ground levels in a radioactive molecule, it is also necessary to be guided by the rules for selecting the molecular transitions.

These selection rules are formally analogous to the rules for individual atoms and their ions, in fact supplemented by the projections of the angular and spin moments on the nuclear axis of the diatomic molecule. For the basic and nearest excited molecular levels, we can restrict ourselves to the following rules:

$\Delta S = 0$ . Molecular transitions of different multiplicity are forbidden.

$\Delta \Sigma = 0$ . The projection of the spin on the internuclear axis of the molecule should not change.

$\Delta \Omega = 0, \pm 1$  The sum of the projections on the internuclear axis of the spin and orbital angular momentum can vary only in this ratio.

$\Delta A = 0, \pm 1$  The projection of the orbital angular momentum on the internuclear axis varies within the framework of this equation.

The application of selection rules for radioactive molecules is difficult because of the fact that only singlet and triplet multiplets appear in titanium oxide, while they are doublets in scandium oxide. Those either transitions will be forbidden, or after electron capture by a titanium nucleus 1s-electron, the electron configuration changes so rapidly that the electron from the initial electronic configuration find its position in the newly formed molecule  ${}^{44}_{21}\text{Sc}^{16}_8\text{O}$ .

According to the law of energy conservation, the nearest electronic configuration of this molecule must have the energy of the electronic term  $T_e$  of the original molecule  ${}^{44}_{22}\text{Ti}^{16}_8\text{O}$ . The use of the molecular constants of diatomic molecules permits to find the energy characteristics of all types of allowed transitions. Then the value of the initial energy of the electronic term of the excited state, together with the molecular constants, is chosen for  ${}^{44}_{22}\text{Ti}^{16}_8\text{O}$ . And the ground lower state corresponds to the basic doublet level  ${}^{44}_{21}\text{Sc}^{16}_8\text{O}$ .

### 3.4. Selection of molecular constants

Molecular constants of the excited state are chosen in accordance with the ground state of titanium oxide using the physically valid value of the electron term  $T_e$ . The used values are pointed in Table 1.

Usually, the electronic structure of a molecule changes almost instantly in comparison with the vibration and rotation of nuclei. This can lead, in our case, to a ban on dipole and rotational transitions in accordance with the above selection rules and to the appearance of purely rotational transitions. In our case, at least, the transition from the triplet to the doublet states is forbidden. Then rotational energy is calculated using the formulas:

$$E'_j = hB_{e1}j(j-1) - hD_{e1}j^2(j-1)^2 \quad (5)$$

$$E''_j = hB_{e2}j(j+1) - hD_{e2}j^2(j+1)^2 \quad (6)$$

Here the anharmonicity of the rotation of diatomic molecules is taken into account. The rule for selecting rotational levels is written as  $\Delta j = \pm 1$ . In the case of radiation as a result of rotational transitions, we have  $\Delta j = 1$ . This means the replacement of the rotational quantum number  $j$  by  $j-1$ . Then the energy of quantum emitted as a result of radioactive transformation of these molecules is:

$$\Delta E = hB_{e2}j(j+1) - hD_{e2}j^2(j+1)^2 - hB_{e1}j(j-1) + hD_{e1}j^2(j-1)^2 \quad (7)$$

### 3.5. Radiation in the vibrational bands

Another variant of the transition state of the radioactive molecule will be the presence of vibrational transitions. In practice, they are allowed within any permitted electronic transition. Any excited electronic state is associated with a change (most often an increase) of the distance between the nuclei  $r_e$ . The values of the potential energy for vibrational motion of nuclei near the equilibrium points for better physical clarity will be first written as the Morse potential:

$$E(r) = D_e \{1 - e^{-\alpha(r-r_e)}\}^2 \quad (8)$$

Where  $D_e$  is the dissociation potential of the molecule,  $r_e$  is the equilibrium distance between the nuclei of molecule,  $\beta$  is the conditional force constant determined by the known values of the molecular constants using the formula  $\alpha = 2\pi\nu_e \frac{\mu}{2D_e}$ ,  $\mu$  is the reduced mass of the radioactive molecule. In the case of the  $\beta$ -decay processes under con-

Table 1. Molecular constants of the molecules  ${}^{44}_{22}\text{Ti}{}^{16}_8\text{O}$  and  ${}^{44}_{21}\text{Sc}{}^{16}_8\text{O}$  in the ground state in accordance with Dobrodey (2001) & Jorgensen (1994).

Molecule	State	$T_e$	$\omega_e$	$\omega_e x_e$	$B_e$	$\alpha_e$	$D_e 10^{-7}$	$\beta_e 10^{-9}$	$r_e$	$\nu_{00}$	$D_0$
${}^{44}_{22}\text{Ti}{}^{16}_8\text{O}$	$X^3\Delta$		1009	4.2	0.53	0.033	6.03	3.4			55413.42
${}^{44}_{21}\text{Sc}{}^{16}_8\text{O}$	$X^2\Sigma$	0	964.9	4.5	0.52	0.00034	5.8	1.67			56266.73

sideration as an electron capture by a radioactive titanium atom, in the first approximation the reduced mass remains unchanged. The mass change does not exceed the electron mass. The difference of the vibrational energies within the electronic transition in the first approximation is represented in the form:

$$E_{v'} - E_{v''} = D'_e \left[ 1 - e^{-\alpha'(r_{v'v''} - r_{e'})} \right]^2 - D''_e \left[ 1 - e^{-\alpha''(r_{v'v''} - r_{e''})} \right]^2 \quad (9)$$

Assuming that  $\alpha = \alpha' = \alpha'' = \frac{\alpha' + \alpha''}{2}$ , and making the substitutions  $F_1 = e^{\alpha r_{e'}}$ ,  $F_2 = e^{\alpha r_{e''}}$ ,

$$\begin{aligned} P &= F_1^2 D'_e - F_2^2 D''_e, \\ Q &= F_1 D'_e - F_2 D''_e, \\ R_{v'v''} &= D'_e - D''_e - E_{v'} - E_{v''}, \quad x = e^{-\alpha r_{v'v''}} \end{aligned}$$

we obtain a quadratic equation in which  $x$  is unknown:

$$Px^2 - 2Qx + R_{v'v''} = 0 \quad (10)$$

The roots of this quadratic equation obtained can be written as the following values of  $r_{v'v''}$ :

$$r_{v'v''} = -\frac{1}{\alpha} \ln x \quad (11)$$

The simplest estimate of the molecular transition can be the difference in the energies of the lower zero states in molecules  ${}^{44}_{22}\text{Ti}{}^{16}_8\text{O}$  and  ${}^{44}_{21}\text{Sc}{}^{16}_8\text{O} - \Delta E_0$ :

$$\frac{\Delta E_0}{hc} = \frac{1}{2} \omega'_e - \omega''_e - \frac{1}{4} (\omega'_e x'_e - \omega''_e x''_e) \quad (12)$$

Substitution of molecular constants from Table 1 gives a value  $\frac{\Delta E_0}{hc} = 43.8 \text{ cm}^{-1}$  which corresponds to a wavelength  $\lambda = 2.287983 \text{ cm}$ . This wavelength is available for observation by radio telescopes. Let us find the necessary Morse potentials of the initial excited state from the molecular data of the ground state of  ${}^{44}_{22}\text{Ti}{}^{16}_8\text{O}$  and the final ground state of  ${}^{44}_{21}\text{Sc}{}^{16}_8\text{O}$ .

Calculations of the vibrational structure of  $E(r)$  are usually considered in the form of a Rydberg-Klein-Riesch potential (the so-called RKR potential). Let  $E(r)$  be determined by the Morse potential. The energy difference between the vibrational levels of the molecule is comparable to the calculated recoil energies of the  $E_R$  nucleus. Then the source of excitation of the vibrational levels of the molecule is the transfer of kinetic energy to the scandium nucleus at the moment of radioactive transformation of titanium.

#### 4. M-L-K emission in radioactive atoms and molecules

Let us consider such a process in the first approximation of a hydrogen-like atom. Namely, the energy difference between the electrons of the first ground level in  ${}^{44}_{22}\text{Ti}$  and  ${}^{44}_{21}\text{Sc}$ . In the atomic system of units, we can write down that the energy of electron at the first quantum level is the function of atomic number:

$$E = -\frac{1}{2} \frac{Z^2}{n^2}, \Delta E = -20.5 \text{ eV} \quad (13)$$

Thus, during the radioactive transition, the formed daughter molecule  ${}^{44}_{21}\text{Sc}{}^{16}_8\text{O}$  receives an additional energy of the electrostatic field equal to 20.5 eV. Part of this energy is sufficient for quantum transitions in the formation of a daughter molecule. We can also estimate the closest position of the first level in  ${}^{44}_{21}\text{Sc}$  atom:

$$\langle r \rangle = \frac{1}{2Z} (3n^2 - l(l+1)) = 0.36 \text{ \AA} \quad (14)$$

As it was noted above, the description of the localization of the  $1s^1$  orbital near the titanium nuclei and also the scandium gives a relatively accurate value of  $\Delta E$ . However, the observed wavelength of the recombination X-ray line  ${}^{44}_{21}\text{Sc}$  does not correspond to formula (10) and requires the consideration of various types of molecular interactions. The titanium atom and then scandium atom after electron capture in a highly excited ionized states. It leads to cascade of X-ray transitions between the following levels: L-K, M-K, H-L.

The average probabilities of L-K transitions are 68.4%, M-L – 22.2%, and H-K – 2%. In some cases, for light nuclei, the energy of these transitions is not transferred to quanta corresponding for the indicated transitions, but are spent on the extraction of one or more electrons out of the molecule. This process is called the Auger effect. The probability of this effect is small in the discussed process. We note only that in some cases the result of Auger effect is the ionization of molecule, in others the molecule dissociates due to the detachment of the valence electrons participating in the molecular interactions.

X-ray quanta, after their emission, also transmit a certain kinetic energy to the nucleus of the recoil of radioactive scandium, sufficient for excitation of the vibrational levels of the scandium oxide  ${}^{44}_{21}\text{Sc}{}^{16}_8\text{O}$ .

#### 5. Conclusion

The effective pollution of cold gas-dust nebulae can be associated with their enrichment in radioactive isotopes of

chemically active elements produced by remnants of supernovae, stellar winds of giants, supergiants and cosmic rays. The important feature of explosive processes in type II supernovae is the asymmetry. It was first proposed by Zeldovich and Chechetkin (Popov et al., 2014). Numerous theoretical models for calculating the abundances of chemical elements as a result of asymmetric explosions were proposed.

These calculations found that one of the manifestations of the asymmetric explosion is the presence of specific isotopes:  $^{44}_{22}\text{Ti}$  and other. The pointed titanium isotope forms diatomic molecules. The registration of radioactive species in cold supernova remnants is a new task for molecular spectroscopy. In this review the possibility of detection of isotopic nuclei on molecules during radioactive decays was shown. It should be noted that in earlier investigations the supernova remnants were studied mainly using the radiation of shock-wave fronts.

Taking into account the remoteness of shock wave fronts from actual remnants, for several decades the shock waves highlighted the gas and dust in supernova remnant and gave us the possibility of diagnosis of interstellar medium. The registration of traces of radioactive emissions is associated exclusively with the presence of nonstable isotopes in supernova remnants. Therefore, together with dust particles analysis, the radioactivity is the only source of information about the chemical composition of cold remnants.

The radioactivity of  $^{44}_{22}\text{Ti}$  is manifested in the form of emission of specific quanta, some of them are similar to those emitted by individual atoms in the  $\gamma$  and X-ray energy diapasons. This review shows that the remaining quanta are of a molecular nature. Namely, they are formed as a result of cascade transitions, after K-capture by the nucleus  $^{44}_{22}\text{Ti}$  of the 1s electron in the molecule as a result of its strong excitation. We give the set of energy intervals of the emission lines:

1. Cascade transitions 3-4 keV
2. Cascade transitions 30-40 eV;
3. Molecular transitions caused by the presence of recoil energy of the nucleus  $^{44}_{21}\text{Sc}$  2-4 eV;
4. Transitions in molecules during the radioactive decay of  $^{44}_{22}\text{Ti}$  isotope ( $^{44}_{22}\text{Ti}^{16}\text{O} - ^{44}_{21}\text{Sc}^{16}\text{O}$ ). The wavelengths of these lines are close to 2 cm;
5. Radiation due to ionization losses as a result of the motion of  $^{44}_{20}\text{Ca}$  atom, whose nucleus is the end of a chain of radioactive decays similar to  $^{44}_{22}\text{Ti} \rightarrow ^{44}_{21}\text{Sc} \rightarrow ^{44}_{20}\text{Ca}$ .

Thus, the very fact of detection of emission transitions in the spectral ranges listed above will be the basis for identifying this type of radioactive decay. The determination of the activity of these radioactive elements and their effective amount, and also the time series observations, allows us to reconstruct the physical picture of stellar explosion. The detection of CaI and CaII recombination lines arising during the ionization losses makes it possible the precise identification of atoms and ions of  $^{44}_{20}\text{Ca}$  isotope in cold remnants.

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