

Conversion of nuclear spin isomers of water molecules under ultracold conditions of space

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Abstract. The conversion rate of nuclear spin isomers of water molecules in space is calculated using the model of quantum relaxation in the absence of particle collisions. The model is based on the intramolecular mixing of the ortho and para states of H_2O by the spin-rotation interaction and on the interruption of the mixing by radiative transitions of a molecule in a thermal radiation field. The lifetime of water isomers at a thermal radiation temperature $T = 50$ K is $\sim 2 \times 10^7$ years, and at a temperature $T = 100$ K it is 3×10^6 years. The lifetimes of the spin isomers of water molecules are found to be large, but still smaller, for example, than the age of the Solar System. The proposed process of conversion of the spin isomers of water molecules is important for areas of space with low ($n < 1 \text{ cm}^{-3}$) particle concentrations.

Keywords: spin isomers of water molecules, ratio of ortho and para states of molecules in space, Solar System, interstellar space.

1. Introduction

Symmetric molecules exist in nature in the form of nuclear spin isomers, which differ in the states of the spins of identical nuclei [1, 2]. The most known are the nuclear spin isomers of hydrogen molecules: ortho- and para- H_2 molecules. Hydrogen isomers have unique properties, for example, an anomalously long lifetime, which is equal to months at atmospheric pressure of hydrogen and room temperature [3]. Like hydrogen, water molecules (Fig. 1) also have nuclear spin isomers: ortho H_2O (total spin of two protons, $I = 1$; symmetric proton spin wave function) and para H_2O ($I = 0$, antisymmetric proton spin wave function). Quantum statistics requires the antisymmetry of the full wave functions for H_2O relative to permutations of two identical protons (fermions) in a molecule. This leads to certain correlations of rotational and spin states in H_2O molecules [2]. In populating many rotational states of a molecule at high temperatures, the ratio of the concentrations of the H_2O ortho and para isomers (ortho-to-para ratio, OPR) is determined by the nuclear statistical weights of the proton spins in the ortho and para states and is equal to 3. At low temperatures, when only the lower rotational states of H_2O are populated, $\text{OPR} < 3$, and $\text{OPR} \rightarrow 0$ at $T \rightarrow 0$.

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Relaxation (conversion) of the ortho and para states of the isomers of water molecules in the gas phase has not yet been detected in laboratory experiments. These studies have an extensive and long history [4]. The current state of experiments with spin isomers of water is presented in papers [5, 6], devoted to the conversion of water isomers in molecular beams at a low temperature.

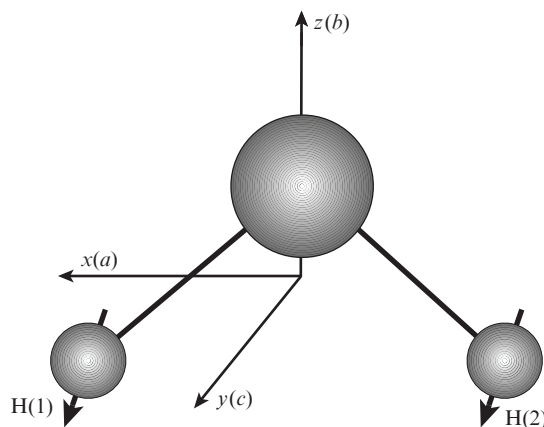


Figure 1. Water molecule and molecular coordinate system. The letters in brackets indicate the directions of the main moments of inertia in decreasing order of the rotational constants, $B_a > B_b > B_c$.

The spectra of molecules serve as a source of important information about the physical conditions in outer space. One of the most common and intensively studied molecules in space is water molecules [7]. Since the 1980s, the OPR of their spin isomers have been measured using both ground-based and space-borne telescopes. At the same time, areas in space have been discovered in which the value of the OPR of water molecules is less than the high-temperature value of 3. Thus, in comas of comets, the OPR of spin isomers of water molecules ranges from 2.0 to 3.0 [8, 9]. The values of $\text{OPR} < 3$ are also observed in interstellar space. Using Herschel observations, Lis et al. [10] derived the OPR of 2.35 ± 0.35 toward the Sagittarius B2(M) gas cloud core, which is situated near the center of our galaxy.

Until recently, it was assumed that the spin isomers of water molecules in space have exceptionally large lifetimes. Therefore, small OPR values of water isomers were explained by the specific conditions of their formation, for example, during photodesorption from the ice surface at very low temperatures. However, in recent experiments [8, 11] (see also [12]) it has been shown that water molecules desorbed from

the ice surface at cryogenic temperatures have a high temperature OPR equal to 3. This fact is well consistent with the intuitively expected one, since the formation of water molecules in chemical reactions or during photodesorption requires significantly more energy than the energy difference between the ortho and para states of H₂O.

To explain this phenomenon, one needs to have in space the physical processes that can change the OPR of water molecules from a high-temperature value of OPR = 3, obtained by the molecules during their formation, to lower values, determined by the low temperature of the space medium. In this paper, we propose such a process based on the conversion of the spin isomers of water molecules under the action of thermal radiation in space.

2. Decoherence by thermal radiation

We now turn to laboratory experiments on the conversion of nuclear spin isomers of polyatomic molecules in the gas phase. These studies have begun relatively recently after methods were developed for the enrichment of spin isomers in the gas phase. The most widely used method is based on the effect of light-induced drift [13, 14]. Numerous laboratory experiments with the spin isomers of polyatomic molecules in the gas phase made it possible to reveal that the conversion of isomers is carried out using a specific process, namely, quantum relaxation (see [14–20] and references therein). The process is based on the joint action of two effects: quantum mixing of the ortho and para states of the molecule by intramolecular hyperfine interactions and the interruption of this mixing (decoherence) by collisions with surrounding particles.

Quantum relaxation of spin isomers is the main process in laboratory gas systems in the absence of paramagnetic catalysts for the conversion of isomers, such as Fe(OH)₃. It is important to understand the role of quantum relaxation of spin isomers of water in space, by analogy with the conversion of isomers in the laboratory. However, the direct application of the quantum relaxation model to the conversion of spin isomers in space has led to the conclusion that the rate of decoherence due to collisions in space is too low to ensure the conversion of isomers within astrophysical times [21–24].

It is well known that outer space is filled with electromagnetic radiation. The minimum density of its energy is determined by cosmic microwave background radiation corresponding to the blackbody radiation at 2.725 K. Water molecules interacting with thermal radiation undergo stimulated and spontaneous transitions between rotational states of H₂O (Fig. 2). Due to the stochastic nature of thermal radiation, these processes interrupt the mixing of the ortho and para states of H₂O, similar to interruption of the mixing by collisions. Therefore, intramolecular mixing of the states of the spin isomers of H₂O together with the radiative transitions of the molecule in the thermal radiation field can induce the conversion of the isomers of H₂O. This is the essence of the model proposed in this work.

Consider the interaction of thermal low-temperature radiation with water molecules in the ground electronic and vibrational state. The distribution of the energy density in the spectrum of the equilibrium thermal radiation is described by the Planck law:

$$\varepsilon(\omega) = \frac{\omega^2}{\pi^2 c^3} \frac{\hbar\omega}{\exp(\hbar\omega/k_B T) - 1}. \quad (1)$$

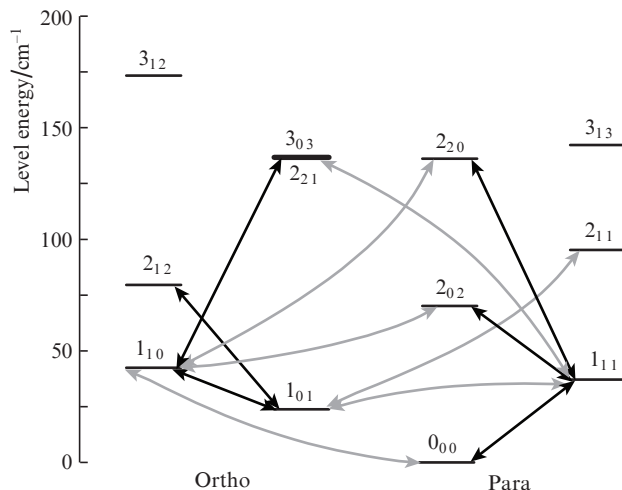


Figure 2. Rotational ortho- and para states of water molecules in the ground electronic and vibrational state. The black arrows indicate the allowed electromagnetic transitions without changing the ortho and para states of the molecule. Grey arrows show the mixing of ortho and para states by intramolecular spin–rotation interaction. Quantum numbers of rotational levels are indicated in the systematics J_{K_a, K_c} [31].

Here, the first and second factors determine the density of photon states in the phase space and their average energy in one state at a temperature T , respectively; and k_B is the Boltzmann constant.

The interaction of a molecule with thermal radiation is described by Einstein's theory. The relaxation rate of the ortho state (α) of water molecules due to radiative transitions to other ortho states i with lower energy ($E_i < E_\alpha$) and to the ortho state j with higher energy ($E_j > E_\alpha$) is

$$\Gamma_\alpha = \sum_{i < \alpha} [A_{\alpha i} + B_{\alpha i} \varepsilon(\omega_{\alpha i})] + \sum_{j > \alpha} B_{\alpha j} \varepsilon(\omega_{j\alpha}). \quad (2)$$

Here, A and B are the Einstein coefficients for radiation spontaneous and stimulated transitions along the $\alpha \rightarrow i$ and $\alpha \rightarrow j$ channels. Between the coefficients A and B there are known relations:

$$B_{\alpha i} g_\alpha = B_{i\alpha} g_i, \quad B_{\alpha i} = A_{\alpha i} \frac{\pi^2 c^3}{\hbar\omega_{\alpha i}^3}, \quad E_\alpha > E_i, \quad (3)$$

where g_α and g_i are the statistical weights of the ortho levels α and i , respectively. Formulae, similar to relations (2) and (3), also hold for the para-state relaxation rate (α') $\Gamma_{\alpha'}$ of the H₂O molecule. The decoherence rate at the transition $\alpha - \alpha'$ is given by the expression [25]:

$$\Gamma_{\alpha\alpha'} = 0.5(\Gamma_\alpha + \Gamma_{\alpha'}). \quad (4)$$

Thus, the calculation of the decoherence rate $\Gamma_{\alpha\alpha'}$ under the action of thermal radiation requires the knowledge of the frequencies of all allowed ortho–ortho and para–para transitions, the rate of radiation relaxation, and the statistical weights of the ortho and para states.

The rotational spectra of water molecules are well studied theoretically and experimentally. Water absorption spectra in the THz region are measured, for example, by pulsed THz spectrometers under the laboratory conditions [26]. Electrodiode rotational transitions in water molecules are

allowed with a change in the spatial parity of the molecule and its angular momentum by $0, \pm 1$. The HITRAN database contains the frequencies of rotational transitions in the ground electronic and vibrational state, the Einstein coefficients A of these transitions, and the statistical weights of the states [27].

Radiation relaxation of the rotational states of water molecules under the action of thermal radiation turns out to be quite fast. For example, the ortho state 1_{10} (see Fig. 2) has a radiation relaxation rate of $3 \times 10^{-3} \text{ s}^{-1}$ in the field of cosmic microwave background radiation with a temperature $T = 2.725 \text{ K}$ and $1 \times 10^{-2} \text{ s}^{-1}$, if the radiation temperature is $T = 30 \text{ K}$. Relaxation of the states of water molecules by collisions in space is significantly slower. For example, the relaxation rate of $1 \times 10^{-2} \text{ s}^{-1}$ due to collisions is reached at a very high particle density of 10^8 cm^{-3} for open space, if we assume the collision cross section to be $\sigma = 10^{-14} \text{ cm}^2$ and the gas temperature to be $T = 30 \text{ K}$.

3. Conversion of spin isomers of water molecules

Let us now calculate the rate of conversion of the ortho and para states of the spin isomers of water molecules in the case of intramolecular mixing of the ortho and para states and interruption of the mixing by thermal radiation. The Hamiltonian of the molecule can be expressed as

$$\hat{H} = \hat{H}_0 + \hbar \hat{V}. \quad (5)$$

Here, \hat{H}_0 is the main part of the Hamiltonian of an isolated molecule, which has pure ortho and para states of H_2O as its eigenstates (see Fig. 2); and $\hbar \hat{V}$ is the hyperfine intramolecular interaction mixing ortho and para states of H_2O with each other. The spatial structure of the H_2O molecule and the molecular coordinate system are shown in Fig. 1. The quantization axis z is directed along the symmetry axis of the molecule (as in Ref. [2]). This choice differs from the traditional one used in spectroscopy of water molecules [27, 28], but makes the analysis of their spin isomers more illustrative [29]. It is convenient to perform the calculation of the energies and wave functions of the rotational states of the asymmetric top of H_2O using a modified Wang basis [2, 30]:

$$\begin{aligned} |a, p\rangle &= \frac{1}{\sqrt{2}} [|a\rangle + (-1)^{J+K+p} |\bar{a}\rangle], \quad 0 < K \leq J, \\ |a_0, p\rangle &= \frac{1 + (-1)^{J+p}}{2} |a_0\rangle, \quad K = 0. \end{aligned} \quad (6)$$

Here, the quantum number is $p = 0, 1$; $|a\rangle$ are the rotational states of the symmetric top; sets of quantum numbers are expressed as $a \equiv \{J, K, M\}$, $\bar{a} \equiv \{J, -K, M\}$, $a_0 \equiv \{J, K = 0, M\}$; and J, K and M are the angular momentum of the molecule (in units of \hbar) and its projection onto the molecular and laboratory quantization axes, respectively. Depending on the parity of the quantum numbers K and p , states (6) generate four different irreducible representations of the molecular symmetry group $C_{2v}(M)$.

Each rotational state of the asymmetric top of H_2O is characterised by quantum numbers J, M , and p , as well as by a set of amplitudes in the expansion of the wave function over states (6) with different numbers K . In each such decomposition there are only states $|a, p\rangle$ of one symmetry. Thus, the

rotational states of the asymmetric top of H_2O can be presented in the form

$$|\beta, p\rangle = \sum_K A_K |a, p\rangle. \quad (7)$$

Here, for the coefficients of the A_K expansion, only the summation index K is indicated, although A_K also depends on other quantum numbers.

It is convenient to accept the following notations on the systematics of rotational states of the H_2O molecule. We arrange all rotational states (7) belonging to each of the sets of quantum numbers J, M , and p , in ascending order of their energy and enumerate them with odd numbers $\mathcal{K} = 1, 3, \dots, J$ or even numbers $\mathcal{K}' = 0, 2, 4, \dots, J$, depending on which the K , odd or even, are present in the expansion of the wave function over states (6). Then, each rotational term of H_2O will be completely determined by a set of quantum numbers $\beta \equiv \{J, \mathcal{K}, M, p\}$. The clarity of this classification can be explained by the fact that for an elongated symmetric top with the $C_{2v}(M)$ symmetry, $\mathcal{K} = K$ should be satisfied.

Note that the choice of basic rotational states (6) and molecular axes, as in Fig. 1, makes the relation between the quantum number p and the spatial parity of states very simple: even states have $p = 0$, and odd states have $p = 1$. For convenience, we express the relation of the adopted quantum numbers of rotational states with the quantum numbers K_a and K_c frequently used for water molecules (see, for example, [31]) in the form:

$$p = 0.5(1 - (-1)^{K_c}), \quad \mathcal{K} = K_a + (-1)^{J+K_a+K_c} p. \quad (8)$$

Thus, the parities of the quantum numbers p and K_c coincide with each other. For the quantum number \mathcal{K} , a more complicated relation (8) is valid.

Tennyson et al. [31] presented exact experimental values of the rotational levels of H_2O . We used these data to calculate the energies and wave functions $|\beta, p\rangle$ in the molecular coordinate system of Fig. 1. To this end, the rotational Hamiltonian of the water molecule, which contains expansion in the angular momentum operators up to the 10th degree [32], was diagonalised in basis (6), and the rotational constants of this Hamiltonian were then found from the approximation of the experimental energy values [31] using the least squares method. The energies of the rotational levels of the ground vibrational state are shown in Fig. 2. The energy gap between the lower ortho state and the lower para state of the H_2O molecule is 23.8 cm^{-1} .

The allowed symmetries of the coordinate and spin functions in the full wave function of H_2O can be set as follows. Since the full wave function of H_2O must change the sign when two protons (fermions) are permuted, states with odd \mathcal{K} and an even spin function under permutation (total spin of two protons $I = 1$, ortho modification of the molecule) or even \mathcal{K} and an odd spin function under permutation ($I = 0$, para modification of the molecule) are allowed. These correlations of the rotational numbers \mathcal{K} and the spin I of protons take place for arbitrary quantum numbers J, M , and p .

The quantum kinetic equation for the density matrix of a system with Hamiltonian (5) in the representation of the eigenstates of the operator H_0 has the standard form [25]:

$$\frac{\partial \hat{\rho}}{\partial t} = -i[\hat{V}, \hat{\rho}] + \hat{R}. \quad (9)$$

The matrix of radiative transitions \hat{R} describes the interaction of a water molecule with radiation. It is assumed in (9) that there are no collisions between particles. Since the electromagnetic field does not produce transitions between the pure ortho and para states of H₂O, the relation

$$\sum R_{\alpha\alpha} = \sum R_{\alpha'\alpha'} = 0, \quad \alpha \in \text{ortho}, \quad \alpha' \in \text{para} \quad (10)$$

holds for the matrix \hat{R} . Such properties of the radiation matrix \hat{R} allow us to obtain from the kinetic equation (9) an equation describing the change in time of the total concentration of ortho molecules, $\rho_o = \sum \rho_{\alpha\alpha}$, $\alpha \in \text{ortho}$:

$$\frac{\partial \rho_o}{\partial t} = 2 \operatorname{Re} \sum i \rho_{\alpha\alpha'} V_{\alpha'\alpha}, \quad \alpha \in \text{ortho}, \quad \alpha' \in \text{para}. \quad (11)$$

The off-diagonal elements of the density matrix (coherences) $\rho_{\alpha\alpha'}$ necessary for the calculation of ρ_o are found from the equation, which also follows from (9):

$$\frac{\partial \rho_{\alpha\alpha'}}{\partial t} = -\Gamma_{\alpha\alpha'} \rho_{\alpha\alpha'} - i V_{\alpha\alpha'} (\rho_{\alpha'\alpha} - \rho_{\alpha\alpha}). \quad (12)$$

In this equation, the relaxation rate $\Gamma_{\alpha\alpha'}$ of the off-diagonal element of the density matrix $\rho_{\alpha\alpha'}$ is introduced. For thermal radiation, $\Gamma_{\alpha\alpha'}$ is defined by equation (4).

The intramolecular interaction \hat{V} does not explicitly depend on time. Therefore, $V_{\alpha\alpha'} = \bar{V}_{\alpha\alpha'} \exp(i\omega_{\alpha\alpha'} t)$, where $\bar{V}_{\alpha\alpha'}$ is a time-independent factor, and $\omega_{\alpha\alpha'} = (E_\alpha - E_{\alpha'})/\hbar$. The conversion of the H₂O isomers is accompanied by the rapid relaxation of molecules over the rotational states inside the ortho and para families of states and exhibits a significantly slower conversion of the ortho and para states. This allows the use of two important simplifications in equation (12). First, it can be assumed that $\rho_{\alpha\alpha'} = \bar{\rho}_{\alpha\alpha'} \exp(i\omega_{\alpha\alpha'} t)$, with the time-independent factor $\bar{\rho}_{\alpha\alpha'}$. Secondly, it is possible to make use of the equilibrium Boltzmann distributions over the rotational levels of ortho and para molecules with current total concentrations of ortho (ρ_o) and para (ρ_p) isomers of H₂O. As a result, from (12) we obtain

$$\bar{\rho}_{\alpha\alpha'} = \frac{i \bar{V}_{\alpha\alpha'}}{\Gamma_{\alpha\alpha'} + i\omega_{\alpha\alpha'}} (\rho_o W_\alpha - \rho_p W_{\alpha'}). \quad (13)$$

Here

$$W_\alpha = Z_o^{-1} \exp(-E_\alpha/k_B T), \quad W_{\alpha'} = Z_p^{-1} \exp(-E_{\alpha'}/k_B T) \quad (14)$$

are the Boltzmann factors; and Z_o and Z_p are the partition functions for the ortho and para states, respectively.

The equation for ρ_o now has the form

$$\frac{\partial \rho_o}{\partial t} = -\gamma_{op} \rho_o + \gamma_{po} \rho_p, \quad (15)$$

$$\gamma_{op} = \sum \gamma_{\alpha\alpha'}, \quad \gamma_{po} = \sum \gamma_{\alpha'\alpha'}, \quad \alpha \in \text{ortho}, \quad \alpha' \in \text{para}.$$

The rates $\gamma_{\alpha\alpha'}$ and $\gamma_{\alpha'\alpha}$ have the meaning of partial isomer conversion rates through the channels $\alpha \rightarrow \alpha'$ and $\alpha' \rightarrow \alpha$, respectively:

$$\gamma_{\alpha\alpha'} = \frac{2\Gamma_{\alpha\alpha'} |V_{\alpha\alpha'}|^2}{\Gamma_{\alpha\alpha'}^2 + \omega_{\alpha\alpha'}^2} W_\alpha, \quad \gamma_{\alpha'\alpha} = \frac{2\Gamma_{\alpha'\alpha} |V_{\alpha'\alpha}|^2}{\Gamma_{\alpha'\alpha}^2 + \omega_{\alpha'\alpha}^2} W_{\alpha'}. \quad (16)$$

Concentrations of ortho and para isomers are related to each other by the relation $\rho_p = N - \rho_o$, where N is the total concentration of water molecules. Using this relation, we obtain from (15)

$$\frac{\partial \rho_o}{\partial t} = -\gamma \rho_o + \gamma_{po} N, \quad \gamma = \gamma_{op} + \gamma_{po}. \quad (17)$$

The concentration of ortho isomers can be presented as $\rho_o = \bar{\rho}_o + \delta\rho_o(t)$, where $\bar{\rho}_o$ and $\delta\rho_o(t)$ are the equilibrium and time-dependent parts of the ortho-molecule concentration, respectively. These values are found from equation (17):

$$\delta\rho_o(t) = \delta\rho_o(0) e^{-\gamma t}, \quad \bar{\rho}_o = \frac{\gamma_{po} N}{\gamma_{op} + \gamma_{po}}, \quad (18)$$

where $\delta\rho_o(0)$ is the nonequilibrium part of the concentration of ortho molecules at $t = 0$.

Solution (18) allows us to express the ratio of equilibrium concentrations of ortho and para molecules through the rates of conversion of the ortho and para states:

$$\bar{\rho}_o/\bar{\rho}_p = \gamma_{po}/\gamma_{op}. \quad (19)$$

An analysis of this relationship reveals an interesting feature of the quantum relaxation of spin isomers. Suppose, for simplicity, that the conversion of spin isomers is essentially dependent on the mixing of only two states: m (ortho) and n (para). Then from (19) we obtain

$$\frac{\bar{\rho}_o}{\bar{\rho}_p} = \frac{Z_o}{Z_p} \exp\left(\frac{E_m - E_n}{k_B T}\right). \quad (20)$$

This expression differs from the generally accepted expression $\bar{\rho}_o/\bar{\rho}_p = Z_o/Z_p$ (see, for example, [11]). Note that both formulae for $\bar{\rho}_o/\bar{\rho}_p$ give similar results in the high-temperature limit at $k_B T \gg (E_m - E_n)$. At present, it remains unclear how fair our relation (19) is. Therefore, in the present work, the calculations were performed for not too low temperatures.

There are two types of hyperfine interactions in the H₂O molecule: the magnetic spin-spin interaction between the protons, \hat{V}_{SS} , and the spin-rotation interaction of the proton spins with the magnetic field caused by the rotation of the molecule, \hat{V}_{SR} . It can be shown that the \hat{V}_{SS} interaction does not mix the ortho and para states of H₂O [30], and the spin-rotation interaction mixes them. In general, this interaction can be represented as [33]:

$$\hat{V}_{SR} = \frac{1}{2} \left(\sum_k \hat{I}^{(k)} \cdot C^{(k)} \cdot \hat{J} + \text{h.c.} \right), \quad k = 1, 2. \quad (21)$$

Here, $\hat{I}^{(k)}$ and $C^{(k)}$ are the spin operator and the tensor of the spin-rotation interaction of the k th proton, respectively; and \hat{J} is the angular momentum operator of the molecule. The components of the spin-rotation tensor of water molecules are calculated in [23, 34]. The spherical components of the spin-rotation interaction tensor, which mix the ortho and para states of H₂O, have the following values (according to the definition [2] of the relationship between Cartesian and spherical components of the second rank tensor):

$$C_{2,\pm 1} = \mp 35.2 \text{ kHz}, \quad C_{1,\pm 1} = 14.1 \text{ kHz}.$$

The calculation of the mixing of the ortho- and para states by the spin–rotation interaction in the H₂O molecule formally coincides with the analogous calculation for the formaldehyde molecule, H₂CO [30]. Therefore, we can employ the relations obtained in [30] using the above values of the components of the spin–rotation tensor. The selection rules for mixing the ortho and para states of H₂O by the spin–rotation interaction have the form

$$\Delta J = 0, \pm 1, \quad \Delta K = \pm 1, \quad \Delta p = 0. \quad (22)$$

Mixed states of the water molecule are shown in Fig. 2 by grey arrows.

The results of the calculation of the lifetime $\tau = \gamma^{-1}$ of the spin isomers of H₂O at various temperatures of thermal radiation are presented in Fig. 3. Calculations were performed only for moderately low temperatures ($T > 25$ K) due to the above-discussed problem of the validity of the theory in the low-temperature limit.

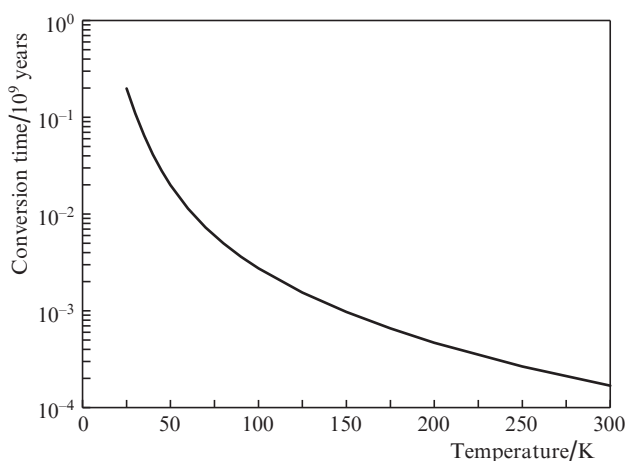


Figure 3. Lifetimes of nuclear spin isomers of water molecules at various temperatures of equilibrium thermal radiation in space.

4. Discussion and conclusions

We have calculated the rate of conversion of nuclear spin isomers of water molecules in space within the framework of a quantum relaxation model based on the intramolecular mixing of the ortho and para states of H₂O by the spin–rotation interaction and the interruption of the mixing by radiative transitions of a molecule in a thermal radiation field. At a thermal radiation temperature $T = 50$ K, the lifetime of water isomers is $\sim 2 \times 10^7$ years, and at a temperature $T = 100$ K it is $\sim 3 \times 10^6$ years. The lifetimes of the spin isomers of water molecules turned out to be smaller than the age of the Solar System.

Of course, the mechanism of water isomer conversion proposed in this work should be taken into account if there are no faster, alternative processes, such as chemical reactions or proton exchange. In paper [10], for a gas density of 10^4 cm⁻³ in the Sagittarius B2(M) cloud, the lifetime of water isomers was estimated to be 3×10^5 years under the action of proton exchange. The mechanism proposed in this work gives significantly longer times. However, the estimation of the conversion time in [10] was made for a very dense gas by cosmic

standards. In areas with a density of less than 1 cm⁻³, the proposed mechanism for the conversion of water isomers seems to be more important than proton exchange.

An attractive feature of the proposed model is that it is based on reliably established effects, such as hyperfine mixing of spin isomers, the distribution of thermal radiation in space, and the spectral properties of water molecules. The proposed model can be applied to calculate the properties of spin isomers of other molecules in space: rare isotopes of water molecules, ammonia, methane, formaldehyde, and many other molecules abundant in space [7, 24].

It is clear what needs to be done next. It is necessary to detect and study the conversion of nuclear spin isomers of H₂O in the gas phase in laboratory experiments. Equally important is the continuation of the theory to the domain of low temperatures. In the future, when the theory of spin isomers of molecules in space is developed in detail, the conversion processes of nuclear spin isomers of water molecules and other molecules can be used to design astrophysical clocks of a new type.

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