ISSN 1063-7737, Astronomy Letters, 2020, Vol. 46, No. 4, pp. 224–234. © Pleiades Publishing, Inc., 2020.
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Influence of Radiative Pumping on the HD Rotational Level Populations in Diffuse Molecular Clouds of the Interstellar Medium

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Received March 14, 2020; revised March 14, 2020; accepted March 24, 2020

Abstract—We have performed a theoretical calculation of the influence of radiative pumping on the populations of the rotational levels of the ground vibrational state for HD molecules under conditions of the cold phase of the interstellar medium. Two main excitation mechanisms have been taken into account in our analysis: (i) collisions with atoms and molecules of the interstellar medium and (ii) radiative pumping by the ultraviolet interstellar background. The radiative pumping rate coefficients Γ_{ij} corresponding to the average galactic ultraviolet background in Draine's model have been determined. The influence of HD self-shielding on the radiative pumping rate coefficients has been studied. The population of the first HD rotational level ($J = 1$) is shown to be determined mainly by radiative pumping rather than by collisions if the thermal gas pressure $p_{\rm th} \leq 10^4 \left(\frac{I_{\rm UV}}{1}\right)$ K cm^{-3} and the column density $\log N(\rm HD) < 15$. In such clouds the relative population of the HD levels $N(J = 1)/N(J = 0)$ turns out to be more sensitive to the ultraviolet background intensity than the relative population of the C I fine-structure levels. Thus, an analysis of the relative HD level population can become an important additional source of information about the physical conditions in the interstellar medium both in our Galaxy and in the forming galaxies of the early Universe.

DOI: 10.1134/S1063773720040064

Keywords: *interstellar medium, molecular clouds, early galaxies, quasar spectra.*

1. INTRODUCTION

HD are the next most abundant[1] molecules in the Universe after H_2. Their number density in the cold phase of the neutral interstellar medium (ISM) of our Galaxy is lower than the number density of molecular hydrogen approximately by 5–6 orders of magnitude (Snow et al. 2008). Since the HD lines corresponding to electronic–vibrational–rotational transitions fall into the ultraviolet (UV) wavelength range, they were first detected in our Galaxy only in observations onboard the Copernicus space observatory (Spitzer et al. 1973, 1974) that had a UV telescope and then in observations with the FUSE orbital space telescope (Lacour et al. 2005). By now HD lines have been detected in 41 absorption spectra along the lines of sight toward nearby bright stars in our Galaxy (Snow et al. 2008).

In observations of galaxies in the early Universe the UV HD lines fall into the optical range due to the cosmological redshift z, $\lambda^{\rm obs} = \lambda^{em}(1+z)$, and can be detected by optical ground-based telescopes. HD absorption lines were first detected in the spectrum of the quasar Q 1232+082 in 2001 (Varshalovich et al. 2001). At present, about 20 HD absorption systems have been identified in damped Lyman-alpha (DLA) systems with $z > 1.7$ in the spectra of quasars (see, e.g., Ivanchik et al. 2015; Kosenko and Balashev 2018).

The relative HD/H_2 abundance was investigated by Le Petit et al. (2002), Liszt (2015), Ivanchik et al. (2015), and Balashev and Kosenko (2020). These authors pointed out that the HD/H_2 ratio is an indicator of the physical conditions in the cold ISM phase (the number density, the intensities of the cosmic-ray background and UV radiation, the dust content). An analysis of the populations of the HD rotational levels of the ground vibrational state can be an additional source of information about the physical conditions in the ISM. Like H_2, HD has a system of rotational–vibrational levels that are populated by collisions with atoms and molecules (mostly H, He, H_2, and e^-) and by radiative pumping through the upper electronic levels. At the same time, there is a significant difference in relaxation dynamics between HD and H_2: owing to the higher symmetry of H_2, the lifetime of its excited states is greater than that

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[1] The abundance of CO is approximately the same as that of HD.

in HD by several orders of magnitude. Therefore, the molecular hydrogen transitions in the spectra of quasars can be detected for higher rotational levels, $J = 2 - 8$ (Balashev et al. 2017) ($J = 0$ and 1 are the ground states of para- and ortho-H_2), while only two cases of transitions and only from the first excited rotational level $J = 1$ have been detected so far for HD molecules (no transitions from levels $J \geq 2$ for HD have been observed as yet). They were detected in two absorption systems toward the quasars J 0812+3208 with $z_{\rm abs} = 2.626$ (Balashev et al. 2010) and J 0843+0221 with $z_{\rm abs} = 2.786$ (Balashev et al. 2017). An analysis of the relative HD level population $N(J = 1)/N(J = 0)$ allowed the gas number density to be determined, $n = 240$ cm^{-3} in J 0812+3208A (Balashev et al. 2010; Liszt 2015) and $n = 260-380$ cm^{-3} in J 0843+0221 (Balashev et al. 2017). In these estimates the authors neglected the influence of radiative pumping by assuming that the UV radiation would be shielded in HD lines due to the high column density of molecules.

In this paper we present the results of our calculation of the radiative pumping rate coefficients for the HD rotational levels. We determine the range of physical conditions in the ISM and HD column densities whereby radiative pumping contributes significantly to the HD rotational level populations. Our calculation of the radiative pumping rate coefficients is described in Section 2. In Section 3 we present our calculations of the excitation of HD rotational levels and analyze the effect of self-shielding. In Section 4 we compare the relative population of the HD level $J = 1$ with other indicators of the physical conditions and present our analysis of the physical conditions in two molecular clouds in DLA systems at high redshifts.

2. RADIATIVE PUMPING CALCULATION

The structure of the HD levels is similar to that of the H_2 ones, but there is also a significant difference: since the HD molecule has a dipole moment, the transitions between its levels with $\Delta J = \pm 1$ are permitted and a larger number of levels turn out to be interconnected in the radiative cascade. Following the description of an H_2 radiative pumping calculation (Black and Dolgarno 1976), we calculated the radiative pumping of HD rotational levels. HD molecules absorb UV radiation and populate excited electronic states ($B^1\Sigma_u$ and $C^1\Pi_u$) and then relax to the rotational–vibrational levels of the ground state $X^1\Sigma_g^+$ (subsequently producing a rotational–vibrational cascade).

2.1. Rotational–Vibrational Cascade for the Levels of the Ground Electronic State

The main parameters describing the redistribution of level populations during relaxation to the ground electronic state are the cascade efficiency factors $a(\nu_0, J_0; J)$, which describe the probabilities to occupy a rotational level J of the ground vibrational state $\nu = 0$ through a series of spontaneous transitions from an excited vibrational–rotational state (ν_0, J_0). The scheme described by Black and Dolgarno (1976) was used to calculate $a(\nu_0, J_0, J)$.

Suppose that some level (ν_0, J_0) is populated at a constant rate $Q(\nu_0, J_0)$ (cm^{-3} s^{-1}). Then, the equilibrium population of the level (ν_0, J_0) is defined as follows:

$$n(\nu_0, J_0) = Q(\nu_0, J_0)/A(\nu_0, J_0), \quad (1)$$

where

$$A(\nu_0, J_0) = \sum_{\nu''=0}^{\nu_0} \sum_{J''=0}^{J_{\rm max}} A(\nu_0, J_0; \nu'', J'') \ ({\rm s}^{-1}) \quad (2)$$

denotes the total probability of spontaneous transitions from the level (ν_0, J_0) to various levels of the ground electronic state. The probabilities of spontaneous dipole and quadrupole transitions $A(\nu_0, J_0; \nu'', J'')$ for the rotational–vibrational levels of the HD ground electronic state were calculated by Abgrall et al. (1982) for vibrational levels $\nu \leq 17$ and rotational levels $J \leq J_{\rm max} = 13$. In this paper we took into account the levels with $J \leq J_{\rm max} = 13$ and $\nu \leq 13$. This is justified by the fact that in molecular clouds, under typical physical conditions, the populations of the overlying levels are negligible and their subsequent inclusion does not affect the radiative pumping rate coefficients for the ground vibrational level. The equilibrium populations of the underlying levels $(\nu, J) < (\nu_0, J_0)$ are determined from the system of equations

$$n(\nu, J)A(\nu, J) = \sum_{\nu''=\nu}^{\nu_0} \sum_{J''=0}^{J_{\rm max}} n(\nu'', J'')A(\nu'', J''; \nu, J). \quad (3)$$

Assuming $Q(\nu_0, J_0) = 1$ cm^{-3} s^{-1} we can calculate the cascade efficiency factors $a(\nu_0, J_0; J)$

$$a(\nu_0, J_0; J) = \sum_{\nu''=1}^{\nu_0} \sum_{J''=0}^{J_{\rm max}} n(\nu'', J'')A(\nu'', J''; 0, J). \quad (4)$$

Table 1. Cascade efficiency factors $a(\nu_0, J_0, J)$ for the population of rotational levels J of the HD ground vibrational state $\nu = 0$. The data for the first four vibrational levels are given

ν_0	J_0	$\nu = 0, J$										
		0	1	2	3	4	5	6	7	8	9	10
1	0	0.00000	0.98813	0.01187	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1	1	0.50542	0.00683	0.48193	0.00582	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1	2	0.00868	0.68212	0.00909	0.29625	0.00386	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1	3	0.00031	0.02783	0.77772	0.01348	0.17807	0.00258	0.00000	0.00000	0.00000	0.00000	0.00000
1	4	0.00002	0.00205	0.06066	0.81772	0.01552	0.10233	0.00170	0.00000	0.00000	0.00000	0.00000
1	5	0.00000	0.00025	0.00732	0.10166	0.82001	0.01433	0.05534	0.00109	0.00000	0.00000	0.00000
1	6	0.00000	0.00004	0.00125	0.01738	0.14244	0.79907	0.01109	0.02804	0.00069	0.00000	0.00000
1	7	0.00000	0.00001	0.00028	0.00386	0.03168	0.17934	0.76388	0.00758	0.01295	0.00043	0.00000
1	8	0.00000	0.00000	0.00008	0.00104	0.00856	0.04847	0.20742	0.72433	0.00461	0.00521	0.00026
1	9	0.00000	0.00000	0.00002	0.00033	0.00270	0.01527	0.06537	0.22859	0.68353	0.00258	0.00161
1	10	0.00000	0.00000	0.00001	0.00012	0.00096	0.00543	0.02326	0.08133	0.24296	0.64456	0.00137
2	0	0.30069	0.40525	0.28838	0.00566	0.00003	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2	1	0.17862	0.50603	0.22670	0.08687	0.00178	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000
2	2	0.21897	0.23825	0.34929	0.16015	0.03262	0.00072	0.00000	0.00000	0.00000	0.00000	0.00000
2	3	0.00847	0.35223	0.26761	0.24523	0.11438	0.01178	0.00029	0.00000	0.00000	0.00000	0.00000
2	4	0.00043	0.02722	0.44704	0.28251	0.15811	0.08070	0.00387	0.00011	0.00000	0.00000	0.00000
2	5	0.00004	0.00261	0.05961	0.50253	0.28344	0.09471	0.05584	0.00117	0.00004	0.00000	0.00000
2	6	0.00000	0.00035	0.00896	0.10051	0.52455	0.27436	0.05283	0.03808	0.00033	0.00001	0.00000
2	7	0.00000	0.00006	0.00168	0.02092	0.14154	0.52238	0.25987	0.02778	0.02566	0.00010	0.00000
2	8	0.00000	0.00001	0.00039	0.00506	0.03766	0.17767	0.50509	0.24311	0.01379	0.01719	0.00004
2	9	0.00000	0.00000	0.00011	0.00142	0.01106	0.05710	0.20486	0.48024	0.22730	0.00659	0.01133
2	10	0.00000	0.00000	0.00003	0.00046	0.00365	0.01967	0.07695	0.22583	0.45512	0.21504	0.00324
3	0	0.31352	0.32714	0.32114	0.03735	0.00084	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000
3	1	0.15907	0.52005	0.20309	0.11003	0.00760	0.00017	0.00000	0.00000	0.00000	0.00000	0.00000
3	2	0.19438	0.26521	0.37865	0.11198	0.04765	0.00208	0.00004	0.00000	0.00000	0.00000	0.00000
3	3	0.08035	0.30363	0.24546	0.28275	0.06696	0.02022	0.00061	0.00001	0.00000	0.00000	0.00000
3	4	0.00490	0.15290	0.37504	0.21850	0.19898	0.04143	0.00804	0.00020	0.00000	0.00000	0.00000
3	5	0.00033	0.01669	0.22275	0.41400	0.18316	0.13334	0.02669	0.00296	0.00007	0.00000	0.00000
3	6	0.00003	0.00195	0.03879	0.28083	0.42467	0.14925	0.08554	0.01793	0.00098	0.00003	0.00000
3	7	0.00000	0.00029	0.00682	0.06917	0.32097	0.41451	0.12186	0.05364	0.01244	0.00028	0.00001
3	8	0.00000	0.00005	0.00140	0.01643	0.10248	0.34411	0.39224	0.10140	0.03295	0.00888	0.00007
3	9	0.00000	0.00001	0.00034	0.00430	0.03050	0.13415	0.35216	0.36469	0.08745	0.02002	0.00638
3	10	0.00000	0.00000	0.00010	0.00129	0.00973	0.04814	0.16214	0.35466	0.34019	0.07683	0.00694

Table 1. (Contd.)

ν_0	J_0	$\nu=0, J$										
		0	1	2	3	4	5	6	7	8	9	10
4	0	0.25095	0.40008	0.27775	0.06817	0.00300	0.00006	0.00000	0.00000	0.00000	0.00000	0.00000
4	1	0.21629	0.40000	0.28365	0.08385	0.01567	0.00053	0.00001	0.00000	0.00000	0.00000	0.00000
4	2	0.15787	0.34428	0.31837	0.12916	0.04621	0.00401	0.00011	0.00000	0.00000	0.00000	0.00000
4	3	0.11430	0.25709	0.30199	0.23724	0.06699	0.02128	0.00108	0.00003	0.00000	0.00000	0.00000
4	4	0.02680	0.20557	0.30149	0.25207	0.17001	0.03422	0.00954	0.00029	0.00001	0.00000	0.00000
4	5	0.00215	0.06094	0.28266	0.32037	0.19427	0.11776	0.01761	0.00415	0.00009	0.00000	0.00000
4	6	0.00018	0.00838	0.10774	0.35115	0.32582	0.14092	0.05492	0.00955	0.00132	0.00002	0.00000
4	7	0.00002	0.00111	0.02083	0.15014	0.36930	0.29852	0.10082	0.05310	0.00546	0.00069	0.00001
4	8	0.00000	0.00018	0.00409	0.04033	0.19056	0.37920	0.27401	0.07275	0.03526	0.00336	0.00027
4	9	0.00000	0.00004	0.00091	0.01047	0.06441	0.22284	0.37376	0.24868	0.05333	0.02343	0.00213
4	10	0.00000	0.00001	0.00024	0.00299	0.02096	0.09153	0.24894	0.36606	0.22721	0.03518	0.00687

Since the population rate is constant, the normalization condition must be fulfilled: the number of molecules appearing per unit time at the excited level (ν_0, J_0) is equal to the number of molecules arriving at the levels of the ground vibrational state:

$$\sum_{J=0}^{J_{\max}} a(\nu_0, J_0; J) = Q_0 = 1\ \mathrm{cm}^{-3}\,\mathrm{s}^{-1}. \qquad (5)$$

The values of $a(\nu_0, J_0; J)$ were calculated for each pair (ν_0, J_0) of the ground electronic state ($\nu_0 = 1..13$, $J_0 = 0..J_{\max}$) and are given in Table 1 (for the first four vibrational levels).

2.2. Radiative Pumping Rate Coefficients $\Gamma(J_i, J_j)$

To describe the fraction of the molecules at the ground vibrational level $\nu = 0$ passed from a state $(\nu = 0, J_i)$ to a state $(\nu = 0, J_j)$ during radiative pumping, let us introduce the rate coefficients $\Gamma(J_i, J_j)$:

$$\Gamma(J_i, J_j) = \sum_{\nu_0=1}^{13} \sum_{J_0=0}^{J_{\max}} Q^{J_i}(\nu_0, J_0) \times a(\nu_0, J_0; J_j) + Q^{J_i}(\nu = 0, J_j), \qquad (6)$$

where $Q^{J_i}(\nu_0, J_0)$ describes the excitation rate of the levels of the ground electronic state (ν_0, J_0) through spontaneous[2] transitions from the levels of excited HD electronic states and is defined as follows:

$$Q^{J_i}(\nu_0, J_0) = \sum_{B,C} \left[\sum_{\nu'=0}^{40} \sum_{J'=0}^{J'_{\max}} \frac{R(0, J_i; \nu', J')}{A^{\mathrm{tot}}(\nu', J')} A(\nu', J'; \nu_0, J_0) \right], \qquad (7)$$

where $\frac{R(0,J_i;\nu',J')}{A^{tot}(\nu',J')} = \frac{n(\nu',J')}{n(0,J_i)}$ are the relative equilibrium populations of the vibrational–rotational levels (ν', J') of states (B and C) when excited from the level of the ground electronic state $(0, J_i)$, $R(0, J_i; \nu', J')$ is the excitation rate through the absorption of UV radiation, $A^{\mathrm{tot}}(\nu', J') = A_c(\nu', J') + \sum\limits_{\nu_0, J_0} A(\nu', J'; \nu_0, J_0)$ is the total probability of radiative transitions from level (ν', J') of the excited electronic states to the continuum and the rotational–vibrational levels (ν_0, J_0) of the ground electronic state (Abgrall and Roueff 2006). Here and below, the superscript $'$ denotes the populations of the excited HD electronic states and the subscript 0 denotes the levels of the ground electronic state.

[2] The rate of the induced transitions is much lower than the rate of the spontaneous ones and they may be neglected.

The photoabsorption rate is defined by the following expression:

$$R(\nu'', J''; \nu', J') = \int_0^\infty \sigma_{ik}(\nu) c u_\nu(\nu) d\nu \quad (8)$$
$$= f_{ik} \frac{\sqrt{\pi} e^2}{mc} \int_0^\infty H(a, x) c u_\nu(\nu) d\nu$$
$$\simeq f_{ik} \frac{\pi e^2}{m} u_\nu(\nu_{ik}),$$

where f_{ik} is the oscillator strength of the transition between states (ν'', J'') and (ν', J'), $u_\nu(\nu_{ik})$ is the spectral UV radiation density in the cloud at the transition wavelength $\left(\frac{\text{photons}}{\text{cm}^3\ \text{Hz}}\right)$, $H(a, x) = \frac{a}{\pi} \int_{-\infty}^{+\infty} \frac{\exp(-y^2)}{(x-y)^2 + a^2} dy$ is the Voigt function with parameters $a = \Delta\nu_R / \Delta\nu_D$ and $x = \frac{c}{b}\left(\frac{\nu - \nu_{ik}}{\nu_{ik}}\right)$. In the optically thin case, the value of the integral is equal to the value of the function at the transition frequency. Thus, the photoabsorption rate is proportional to the UV photon density in the medium. The influence of shielding in lines is considered in the next section.

To calculate the photoabsorption rate, we use the standard model of an isotropic free-space galactic interstellar UV background by Draine (1978). In the wavelength range <2000 Å corresponding to the HD transition wavelengths the UV radiation intensity by the number of photons $\left(\text{photons}/(\text{s cm}^2\ \text{Hz sr})\right)$ is described by the following expression from Sternberg and Dalgarno (1995):

$$I_\nu^{\text{Draine}}(\nu) = \frac{1}{4\pi} \times \left[1.068 \times 10^{-3} \left(\frac{1\ \text{Å}}{\lambda}\right) \right. \quad (9)$$
$$\left. -1.719 \left(\frac{1\ \text{Å}}{\lambda}\right)^2 + 6.853 \times 10^2 \left(\frac{1\ \text{Å}}{\lambda}\right)^3 \right].$$

In the case of an isotropic background, the spectral density is related to the intensity as $u_\nu = 4\pi I_\nu / c$; the total radiation density in the range 912–1108 Å is then $6.9 \times 10^{-4}\ \text{cm}^{-3}$. We introduce the scale factor I_{UV} to take into account the stronger radiation fields, $I_\nu = I_{\text{UV}} I_\nu^{\text{Draine}}(\nu)$. The scale factor I_{UV} appears linearly in Eqs. (6)–(9) and, therefore, the radiative pumping rate coefficients $\Gamma(J_i, J_j)$ depend linearly on I_{UV}. The values of $\Gamma(J_i, J_j)$ calculated for the standard galactic background radiation ($I_{\text{UV}} = 1$) are given in Table 2.

2.3. Self-shielding

HD and H_2 molecules, along with atomic hydrogen H I, in molecular clouds are known to absorb UV radiation in lines, thereby shielding the interior of the cloud from radiation at the frequencies of the corresponding transitions (see, e.g., Draine and Bertoldi 1996; Wolcott-Green and Haiman 2011). In these papers the self-shielding factor is calculated as the ratio of the total dissociation rates of molecules deep in the cloud and at the cloud boundary, $f_{\text{shield}}(N_{\text{HD}}) = \xi_{\text{diss}}(N_{\text{HD}}) / \xi_{\text{diss}}(N_{\text{HD}} = 0)$; here (and below) N is the column density expressed in cm^{-2}. The dissociation of molecules occurs as a process accompanying radiative pumping, so that some of the excited molecules relax to the continuum (about 15%) and are destroyed, while the other ones (about 85%) pass to the excited levels of the ground electronic state. Thus, as a result of self-shielding, the dissociation rate of molecules (ξ_{diss}), along with the excitation rate of the ground state levels $Q^{J_i}(\nu_0, J_0)$, weaken in the same way. We used the expression for the shielding factor from Draine and Bertoldi (1996). It gives zero shielding at the cloud boundary, in contrast to the approximation proposed by Wolcott-Green and Haiman (2011):

$$f_{\text{shield}}(x, D) = \frac{0.965}{(1 + x/D)^2} \quad (10)$$
$$+ \frac{0.035}{\sqrt{1+x}} \exp\left(-8.5 \times 10^{-4} \sqrt{1+x}\right),$$

where $x = N(\text{HD}) / 8.465 \times 10^{13}\ \text{cm}^{-2}$ is the normalized column density and $D = b / 10^5\ \text{cm s}^{-1}$ is the Doppler parameter.

In our model the molecular cloud is described by a plane-parallel slab irradiated by a uniform interstellar radiation background on both sides. We assume the radiation flux to be uniform and incident normally to the cloud surface. The flux density on each of the cloud sides is $F_\nu = 2\pi I_\nu I_{\text{UV}}$. The cloud is divided into parallel layers in each of which the UV radiation density $u_\nu(x)$ is calculated by taking into account the shielding of the radiation coming from each of the cloud sides:

$$u_\nu(x) = \frac{2\pi I_\nu I_{\text{UV}}}{c} \Big(f_{\text{shield}}[N_{\text{HD}}(x)] \quad (11)$$
$$+ f_{\text{shield}}[N_{\text{HD}}(l_c - x)] \Big),$$

where l_c is the cloud size, x is the coordinate along the line of sight (normally to the layer), and $N_{\text{HD}}(x)$ is the column density of molecules on the line of sight between the cloud edge and the layer x being investigated. In the absence of shielding, the radiation density $u_\nu(x) = 4\pi I_\nu I_{\text{UV}} / c$ is constant and does not depend on x. Thus, the radiative pumping

Table 2. Radiative pumping rate coefficients for HD molecules $\Gamma(J_i, J_j)$ $(10^{-10}\ \mathrm{s}^{-1})$ calculated for the standard average galactic UV background in Draine's model with $I_{\mathrm{UV}} = 1$

J_i	J_j										
	0	1	2	3	4	5	6	7	8	9	10
0	0.839	1.323	1.109	0.358	0.077	0.010	0.001	0.000	0.000	0.000	0.000
1	0.423	1.029	0.772	0.482	0.112	0.018	0.002	0.000	0.000	0.000	0.000
2	0.374	0.787	0.915	0.481	0.289	0.047	0.006	0.000	0.000	0.000	0.000
3	0.249	0.665	0.749	0.711	0.312	0.202	0.021	0.002	0.000	0.000	0.000
4	0.160	0.468	0.711	0.652	0.609	0.220	0.148	0.011	0.001	0.000	0.000
5	0.095	0.322	0.569	0.713	0.566	0.519	0.161	0.142	0.006	0.000	0.000
6	0.049	0.202	0.433	0.613	0.664	0.478	0.468	0.117	0.133	0.003	0.000
7	0.022	0.113	0.298	0.500	0.614	0.630	0.436	0.451	0.099	0.128	0.002
8	0.008	0.054	0.179	0.374	0.557	0.631	0.611	0.397	0.428	0.087	0.117
9	0.002	0.021	0.090	0.223	0.388	0.493	0.495	0.425	0.208	0.318	0.004
10	0.001	0.008	0.038	0.114	0.230	0.326	0.342	0.289	0.256	0.095	0.164

rate coefficients $\Gamma(J_i, J_j)$ for molecules deep the cloud decrease by a factor

$$f_{\mathrm{sh}}(x) = \frac{1}{2}\Big(f_{\mathrm{shield}}[N_{\mathrm{HD}}(x)] + f_{\mathrm{shield}}[N_{\mathrm{HD}}(l_c - x)]\Big), \tag{12}$$

compared to the unshielded case.

3. EXCIATION OF HD LEVELS

In equilibrium the populations of the HD rotational levels in the ground vibrational state are described by a system of linear equations:

$$\sum_{i\neq j} N_i \left(\sum_q n_q k_{ij}^q + A_{ij} + \Gamma_{ij}\right) = N_j \sum_{i\neq j}\left(\sum_q n_q k_{ji}^q + A_{ji} + \Gamma_{ji}\right), \tag{13}$$

where the indices i and j are the HD rotational level numbers, q are the particles involved in the collision (H I, pH_2, oH_2, He, and electrons), n_q are the particle number densities, and k_{ij}^q are the collisional rate coefficients that are functions of the kinetic temperature. The particle–HD collisional rate coefficients were taken from Flower et al. (2000) and Dickinson and Richards (1975). The particle number densities with respect to the total hydrogen number density ($n_H^{\mathrm{tot}} = n_{\mathrm{H}} + n_{\mathrm{H}_2} + n_{\mathrm{H}^+}$) were assumed to be equal to their typical values measured in diffuse molecular clouds of our Galaxy: $n_{\mathrm{He}}/n_H^{\mathrm{tot}} = 0.085$ (Asplund et al. 2009), the electron number density $n_e/n_H^{\mathrm{tot}} = 10^{-4}$ (in molecular clouds, as a rule, it corresponds to the abundance of ionized carbon, $\mathrm{n_C/n_H^{tot}} \sim 2\times10^{-4}\times Z$, where Z is the metallicity of the medium), $n_{H_2}/n_H^{\mathrm{tot}} = 0.2$ (a typical molecular fraction of the gas in clouds with a high column density of molecular hydrogen $\log N_{\mathrm{H}_2} > 19$ (see, e.g., Balashev et al. 2019), the ortho-to-para hydrogen ratio was assumed to be equal to the equilibrium one $9\times\exp(-E_{10}/kT_{\mathrm{kin}})$.

The populations of the first and second HD rotational levels as functions of the number density, temperature, and UV background intensity are shown in Fig. 1. Radiative pumping increases (by more than 10%) the population of the first HD rotational level with $J = 1$ in molecular clouds with a thermal ISM gas pressure

$$p_{\mathrm{th}} = nT_{\mathrm{kin}} < 10^4\left(\frac{I_{\mathrm{UV}}}{1}\right)\mathrm{K\,cm^{-3}}. \tag{14}$$

This constraint can hold for diffuse molecular clouds in our Galaxy, the Magellanic Clouds, and galaxies at high redshifts observed in absorption as DLA systems in the spectra of quasars with $z = 2$–4. The thermal gas pressure in the cold ISM phase was estimated by analyzing the relative populations of the rotational H_2

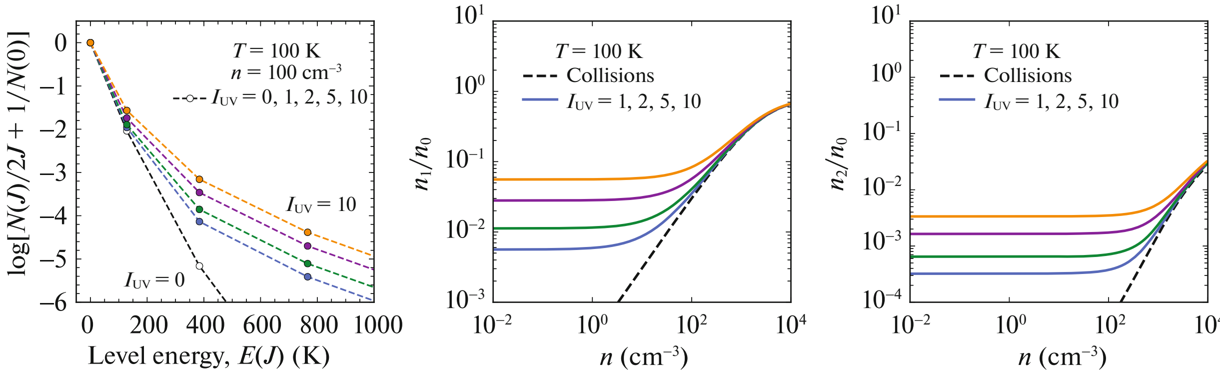

Fig. 1. Relative populations of the HD rotational levels $J = 1$ and $J = 2$ with respect to the ground state $n_J/n_0 = n(J)/n(J = 0)$ calculated for various physical conditions.

levels and the fine-structure levels of atomic carbon C I to be $\sim 10^{3.5}$–$10^{4.5}$ K cm^{-3}: $\log p_{\rm th} = 3.58 \pm 0.18$ in our Galaxy (Jenkins and Tripp 2011), the Large and Small Magellanic Clouds (Welty et al. 2016), and $\log p_{\rm th} = 4.0 \pm 0.5$ in DLA systems (see, e.g., Balashev et al. 2019). At the same time, the intensity of the background interstellar UV radiation and, consequently, the constraint on the thermal pressure (according to Eq. (14)) in distant galaxies can be higher by an order of magnitude. An enhanced intensity of the interstellar UV radiation in galaxies at $z \sim 2$ is partly confirmed by observations (for example, for some DLA systems, e.g., Wolfe 2003; Noterdaeme et al. 2007, 2015; Klimenko et al. 2016; Balashev et al. 2017).

3.1. Self-Shielding Effect

The self-shielding of HD molecules reduces the radiative pumping rate deep in the cloud by the factor $f_{\rm sh}(x)$. We calculated the ratio of the HD column densities at the first and second rotational levels for various gas number densities and UV background intensities by taking into account the shielding effect. The gas temperature was assumed to be 100 K, corresponding to a typical kinetic temperature in diffuse molecular clouds (see, e.g., Balashev et al. 2019). The results are shown in Fig. 2. The color gradient indicates the relative population of the first rotational level. The contours indicate the isolines corresponding to 1/100, 1/30, and 1/10. Thus, at column densities $\log N_{\rm HD} < 15$ pumping by UV radiation can contribute significantly to the HD rotational level populations even if the self-shielding of molecules is taken into account.

4. PHYSICAL CONDITIONS IN A MOLECULAR GAS

The population of the first HD rotational level can serve as an indicator of physical conditions in a gas, such as the kinetic temperature, the gas number density, and the interstellar UV radiation intensity. The same parameters can be measured using other indicators, for example, the fine-structure level populations of atoms and ions (Silva and Viegas 2002). The most useful indicator of the gas density and UV background intensity in the diffuse cold ISM phase is neutral carbon C I (for a review of the C I absorption systems in our Galaxy, see, e.g., Jenkins and Tripp 2011).

We compared the radiative pumping efficiencies (or the level population sensitivities to the UV background) for the fine-structure levels of carbon (C I*) and the first HD rotational level ($J = 1$) as a function of the gas number density.[3] The gas temperature was assumed to be 100 K, a typical temperature in the cold ISM phase. The results of our comparison are shown in Fig. 3. The isolines indicate the physical conditions under which the relative level population increases by 10 and 100% (or 0.04 and 0.3 units in a logarithmic scale) of the population produced only by collisions.

It is usually believed that self-shielding strongly suppresses the radiative pumping of HD molecules. To verify this assertion, we presented the results of our calculation performed for three values of the total HD column density in the cloud, $\log N(\rm HD) = 14, 15, 16$. Because of a typically low C I column density in molecular clouds, the self-shielding of C I atoms is usually neglected when calculating the radiative pumping. At a column density $\log N(\rm HD) \leq 14$ the HD ($J = 1$) level population is seen to be several times more sensitive to the UV background intensity than the population of the first C I* level. In other words, the influence of radiative pumping on the HD level populations is much stronger than on the C I level populations. In this case, HD are a

[3] The population of the second C I** level shows approximately the same sensitivity as C I*.

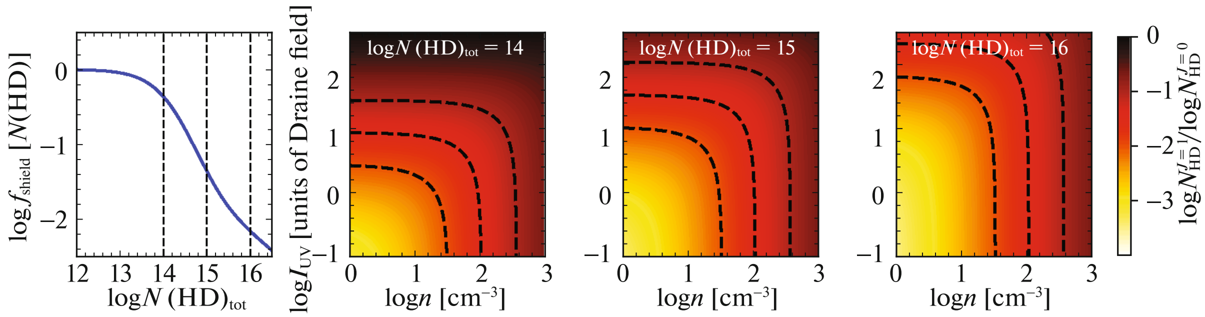

Fig. 2. Left panel: HD self-shielding function as a function of the column density along the line of sight. Right panels: the color indicates the logarithm of the relative HD $J = 1$ level population (integrated along the line of sight $N_{\rm HD}(J = 1)/N_{\rm HD}(J = 0)$) in clouds with various total column densities of HD molecules as a function of the gas number density and UV background intensity. The dashed lines indicate the isolines of the relative HD ($J = 1$) level population corresponding to $N_{\rm HD}(J = 1)/N_{\rm HD}(J = 0) = 1/100$, $1/30$, $1/10$.

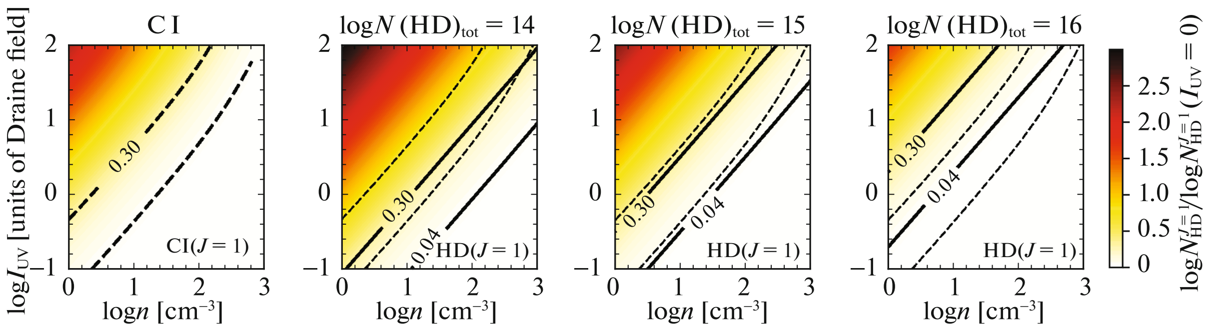

Fig. 3. Comparison of the sensitivities of the C I* fine-structure level and HD $J = 1$ level populations to the UV background intensity and gas number density. The calculation was performed at $T = 100$ K. The dashed and solid lines indicate the isolines corresponding to a change in the C I* and HD ($J = 1$) level populations by 10 and 100% of the population produced only by collisions (at $I_{\rm UV} = 0$). The color gradient indicates the logarithm of the change in the C I* and HD ($J = 1$) level populations. For HD molecules the calculation was performed for clouds with column densities $\log N(\rm HD) = 14, 15, 16$.

better indicator of the UV background and a poorer indicator of the gas number density than C I. As $N(\rm HD)$ increases, the shielding of molecules suppresses the radiative pumping efficiency. At HD column densities $\log N(\rm HD) \sim 15$ the HD ($J = 1$) and C I* level populations have a similar sensitivity to the UV background. In clouds with a greater column density $\log N(\rm HD) > 15$ the radiative pumping of the HD ($J = 1$) level is suppressed.

At the same time, as was shown in Section 3, the upper HD rotational levels with $J \geq 2$ have a higher sensitivity to the UV background intensity than $J = 1$ and could be a good indicator of the UV radiation intensity. However, at present, the lines of HD transitions from levels $J \geq 2$ have not yet been detected in absorption in our Galaxy (see, e.g., Snow et al. 2008) and high-redshift galaxies (see, e.g., Ivanchik et al. 2015). Measuring the populations of HD levels with $J \geq 2$ would allow the UV intensity in a molecular cloud to be measured with a high accuracy. This problem can become possible when future observatories, such as the Extremely Large Telescope (ELT) with the HIRES spectrograph (Oliva et al. 2018) and Spectrum-UV (Shustov et al. 2018), will be put into operation.

As an example, we compared the constraints on the physical conditions that can be obtained using HD molecules or C I atoms. In Fig. 4 we present

Table 3. Column densities of HD molecules at the ground and first rotational levels in the DLA systems in the spectra of the quasars J 0812+3208 (Balashev et al. 2010) and J 0843+0221 (Balashev et al. 2017)

Parameter	J 0812+3208	J 0843+0221
HD ($J = 0$)	$15.70^{+0.07}_{-0.07}$	$17.34^{+0.13}_{-0.37}$
HD ($J = 1$)	$13.77^{+0.15}_{-0.15}$	$15.87^{+0.72}_{-0.49}$

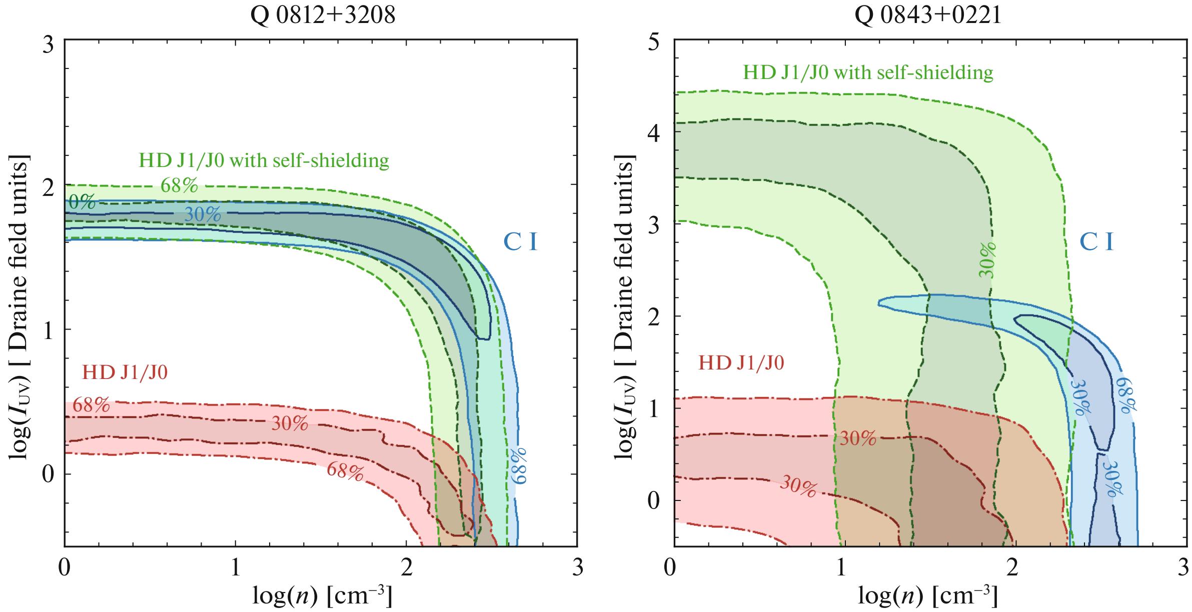

Fig. 4. The constraint on the gas number density and UV radiation intensity obtained by analyzing the relative population of the HD $J = 1$ level (with and without self-shielding) and the fine-structure levels of C I in the DLA system with $z = 2.626$ in the spectrum of the quasar Q 0812+3208 (a) and in the DLA system with $z = 2.786$ in the spectrum of the quasar Q 0843+0221 (b). The contours indicate the probability density corresponding to 30% and 68% confidence levels. Even if the self-shielding effect is taken into account ($\log N(\mathrm{HD}) = 15.7$ and 17.3 in Q 0812+3208 and Q 0843+0221, respectively), the constraint from the ratio $N(J = 1)/N(J = 0)$ for HD turns out to be comparable to the constraint from the fine-structure levels of C I.

our estimates of the gas number density and UV intensity in two DLA systems with high redshifts $z > 2$ in the spectra of the quasars Q 0812+3208A (Balashev et al. 2010) and J 0843+0221 (Balashev et al. 2017), in which the lines of HD transitions from the $J = 1$ level were found. The HD column density is $\log N(\mathrm{HD}) = 15.70 \pm 0.07$ for Q 0812+3208A and $17.35^{+0.15}_{-0.34}$ for J 0843+0221. The HD column densities for the rotational levels are given in Table 3. For J 0812+3208A an analysis of the ratio of the HD and C I level populations gives identical constraints on the number density and the UV background intensity. The kinetic temperature of the gas was assumed to be equal to the excitation temperature of the first H_2 rotational level (T_{01}). With additional constraints (see, e.g., Balashev et al. 2019), these parameters can be determined unambiguously. If we assume that the UV background intensity in a DLA system does not exceed the intensity of the background interstellar UV radiation in our Galaxy by more than a factor of 10, then the gas number density in a molecular cloud can be estimated, $\sim$240 cm^{-3}. On the other hand, we can set an upper limit on the UV background intensity in the system. An analysis of the excitation of C I and HD gives the same constraint: $I_{\mathrm{UV}} < 60$ Draine field units. This means that even at a high HD column density the influence of radiative pumping on the HD ($J = 1$) level population can be as significant as that for the fine-structure levels of C I. For comparison, we also presented the constraint on the UV radiation intensity obtained without HD self-shielding. The difference is almost one and a half orders of magnitude; consequently, HD has a high sensitivity to the UV background intensity and the self-shielding effect should be taken into account in such calculations.

For the system in the spectrum of J 0843+0221 the population of the first HD level is determined only by collisions due to the high HD column density. The radiative pumping rate is suppressed by more than three orders of magnitude through self-shielding. The gas number density estimates obtained with HD and C I agree within the statistical uncertainties.

5. CONCLUSIONS

We considered the influence of radiative pumping by UV radiation on the populations of the lower rotational levels of the ground electronic state in HD molecules under conditions of the diffuse cold ISM phase. We calculated the rate coefficients for radiative pumping of molecules by background UV radiation in Draine's model. The radiative pumping rate coefficients for the first 11 ($J = 0$–10) rotational levels of the ground HD vibrational state are given in Table 2.

We showed that near the molecular cloud boundary, when the self-shielding of HD molecules may be neglected, the population of the first HD rotational level with $J = 1$ is determined mainly by radiative pumping rather than by collisions if the thermal gas pressure satisfies the condition $p_{\rm th} \leq 10^4 \left(\frac{I_{\rm UV}}{1}\right)$ K cm^{-3}. Such conditions correspond to typical physical conditions of the cold ISM phase in our Galaxy (Jenkins and Tripp 2011) and in DLA systems at high redshifts (Balashev et al. 2019). The populations of the upper HD rotational levels with $J \geq 2$ are almost entirely determined only by radiative pumping (the contribution of collisional pumping does not exceed 10%). Measuring the populations of these levels would allow the UV background intensity in a molecular cloud to be determined with a high accuracy.

We considered the influence of HD self-shielding on the radiative pumping efficiency of the first HD rotational level ($J = 1$). We showed that in clouds with a column density $\log N(\rm HD) < 15$ radiative pumping by a UV background of average galactic intensity ($I_{\rm UV} = 1$) could change significantly the population of the first HD level ($J = 1$) at gas number densities $n < 50$ cm^{-3} and a temperature ∼100 K. The additional excitation of HD molecules can be important in calculating the cooling of primordial plasma behind the shock fronts at the galaxy formation epoch. For example, the ionizing radiation of the first stars can increase the HD rotational level populations and, as a consequence, increase the primordial plasma cooling rate.

The HD level population ratio $N(J = 1)/N(J = 0)$ in molecular clouds can be used to estimate the physical conditions in the ISM, both the gas number density and the UV radiation intensity. At a column density $\log N(\rm HD) < 15$ the HD level population ratio J1/J0 turns out to be more sensitive to the UV background intensity and less sensitive to the gas number density than the the fine-structure level population ratio for atomic carbon (C I*/C I and C I**/C I). As an example, we estimated the physical conditions in two DLA systems at high redshifts in the spectra of the quasars Q 0812+3208A ($\log N(\rm HD) = 15.7$) and Q 0843+0221 ($\log N(\rm HD) = 17.3$), in which the lines of HD transitions from $J = 1$ were detected (Balashev et al. 2010, 2017). In the system of Q 0812+3208A we determined the gas number density in the molecular cloud, ∼240 cm^{-3}, and constrained the UV radiation intensity, $I_{\rm UV} <$ 60 Draine field units.

ACKNOWLEDGMENTS

This work was supported by the Russian Science Foundation (project no. 18-12-00301).

REFERENCES

1. H. Abgrall and E. Roueff, Astron. Astrophys. **445**, 361 (2006).
2. H. Abgrall, E. Roueff, and Y. Viala, Astron. Astrophys. Suppl. Ser. **50**, 505 (1982).
3. M. M. Asplund, N. Grevesse, A. J. Sauval, and P. Scott, Ann. Rev. Astron. Astrophys. **47**, 481 (2009).
4. S. A. Balashev, A. V. Ivanchik, and D. A. Varshalovich, Astron. Lett. **36**, 761 (2010).
5. S. A. Balashev and D. N. Kosenko, Mon. Not. R. Astron. Soc. **492**, L45 (2020).
6. S. A. Balashev, P. Noterdaeme, H. Rahmani, V. V. Klimenko, C. Ledoux, P. Petitjean, R. Srianand, A. V. Ivanchik, et al., Mon. Not. R. Astron. Soc. **470**, 2809 (2017).
7. S. A. Balashev, V. V. Klimenko, P. Noterdaeme, J.-K. Krogager, D. A. Varshalovich, A. V. Ivanchik, P. Petitjean, R. Srianand, et al., Mon. Not. R. Astron. Soc. **490**, 2668 (2019).
8. J. H. Black and A. Dolgarno, Astrophys. J. **203**, 132 (1976).
9. A. S. Dickinson and D. Richards, J. Phys. B: At. Mol. Phys. **8**, 2846 (1975).
10. B. T. Draine, Astrophys. J. Suppl. Ser. **36**, 595 (1978).
11. B. T. Draine and F. Bertoldi, Astrophys. J. **468**, 269 (1996).
12. D. R. Flower, J. Le Bourlot, G. Pineau des Forets, and E. Roueff, Mon. Not. R. Astron. Soc. **314**, 753 (2000).
13. A. V. Ivanchik, S. A. Balashev, D. A. Varshalovich, and V. V. Klimenko, Astron. Rep. **59**, 100 (2015).
14. E. B. Jenkins and T. M. Tripp, Astrophys. J. **734**, 32 (2011).
15. V. Klimenko, S. A. Balashev, A. V. Ivanchik, and D. A. Varshalovich, Astron. Lett. **42**, 137 (2016).
16. D. N. Kosenko and S. A. Balashev, J. Phys.: Conf. Ser. **1135**, 012009 (2018). doi 10.1088/1742-6596/1135/1/012009
17. S. Lacour, M. K. Andre, P. Sonnentrucker, F. Le Petit, D. E. Welty, J.-M. Desert, R. Ferlet, E. Roueff, et al., Astron. Astrophys. **430**, 967 (2005).
18. H. S. Liszt, Astrophys. J. **799**, 11 (2015).
19. P. Noterdaeme, C. Ledoux, P. Petitjean, F. Le Petit, R. Srianand, and A. Smette, Astron. Astrophys. **474**, 393 (2007).
20. P. Noterdaeme, R. Srianand, H. Rahmani, P. Petitjean, I. Paris, C. Ledoux, N. Gupta, and S. Lopez, Astron. Astrophys. **577**, 24 (2015).
21. E. Oliva, A. Tozzi, D. Ferruzzi, M. Riva, M. Genoni, A. Marconi, R. Maiolino, and L. Origlia, Proc. SPIE **10702**, 18 (2018).
22. F. le Petit, E. Roueff, and J. le Bourlot, Astron. Astrophys. **390**, 369 (2002).
23. B. Shustov, A. I. Gomez de Castro, M. Sachkov, J. C. Vallejo, P. Marcos-Arenal, E. Kanev, I. Savanov, A. Shugarov, et al., Astrophys. Space Sci. **363**, 62 (2018).
24. A. I. Silva and S. M. Viegas, Mon. Not. R. Astron. Soc. **329**, 135 (2002).

25. T. P. Snow, T. L. Ross, J. D. Destree, M. M. Drosback, A. G. Jensen, B. L. Rachford, P. Sonnentrucker, and R. Ferlet, Astrophys. J. **688**, 1124 (2008).
26. L. Spitzer, J. F. Drake, E. B. Jenkins, D. C. Morton, J. B. Rogerson, and D. G. York, Astrophys. J. **181**, L116 (1973).
27. L. Spitzer, W. D. Cochran, and A. Hirshfeld, Astrophys. J. Suppl. Ser. **28**, 373 (1974).
28. A. Sternberg and A. Dalgarno, Astrophys. J. Suppl. Ser. **99**, 565 (1995).
29. D. A. Varshalovich, A. V. Ivanchik, P. Petitjean, R. Srianand, and C. Ledoux, Astron. Lett. **27**, 683 (2001).
30. D. E. Welty, J. T. Lauroesch, T. Wong, and D. G. York, Astrophys. J. **821**, 118 (2016).
31. J. Wolcottgreen and Z. Haiman, Mon. Not. R. Astron. Soc. **412**, 2603 (2011).
32. A. M. Wolfe, E. Gawiser, and J. X. Prochaska, Astrophys. J. **593**, 215 (2003).

Translated by V. Astakhov