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New Candidates for Measuring the Primordial Deuterium Abundance: Systematic Analysis of the SQUAD and KODIAQ Spectra

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Abstract—The primordial deuterium abundance is one of the most sensitive observational tests of the standard cosmological model and the primordial nucleosynthesis theory. In this paper we perform a systematic analysis of high-resolution spectra from the SQUAD and KODIAQ catalogs aimed at searching for absorption systems suitable for measuring the D/H ratio. We have analyzed all 767 quasar spectra from these catalogs and, as a result, detected 46 new candidate systems for estimating the deuterium abundance. We have estimated the physical parameters of the medium in the chosen objects and modeled in detail the profiles of H I, D I, and metal absorption lines by the MCMC method for five systems. In contrast to the traditional approach oriented predominantly toward the most metal-poor systems with simple kinematics, the sample spans a wider range of physical characteristics of the interstellar medium. Our preliminary estimates of the D/H ratio confirm that the proposed approach is promising and show that extending the range of conditions under study increases the reliability of cosmological estimates, making it possible to investigate the dependence of the deuterium astration on metallicity and to refine the region where this effect may be neglected.

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INTRODUCTION

Primordial nucleosynthesis is one of the fundamental processes of the standard cosmological model. It describes the formation of the first compound nuclei in the Universe—D, ^{3}He, ^{4}He, ^{7}Li, etc.—within the first minutes after the Big Bang (see, e.g., Weinberg 2008; Gorbunov and Rubakov 2011; Cooke 2026). The observational estimates of their primordial abundances are a direct test of the physical processes occurred in the early Universe.

Deuterium plays a special role among all of the primordial nucleosynthesis products. Its production and destruction in nuclear reactions are sensitive to the baryonic matter density. Primordial nucleosynthesis calculations show that the deuterium abundance exhibits one of the highest sensitivities to the baryon-to-photon ratio $\eta_b = n_b/n_\gamma$. Since observations allow the deuterium abundance to be determined with one-percent precision (Pettini and Cooke 2026; Kislitsyn et al. 2024), it is called the "baryometer of the Universe"—measuring the primordial ratio $(\mathrm{D/H})_\mathrm{p}$ makes it possible to directly determine η_b from which the cosmological parameter Ω_b that characterizes the baryonic matter density is calculated ($\eta_b = 2.74 \times 10^{-8}\Omega_b h^2$, Steigman 2007). The estimated value serves as an independent self-consistency test for the standard cosmological model, since the same parameter can be determined by analyzing the cosmic microwave background (CMB) anisotropy at a considerably later evolutionary stage of the Universe (Aghanim et al. 2020). The agreement between the estimates obtained from primordial nucleosynthesis and the CMB places stringent constraints on the possible deviations from the standard cosmological model and the standard model of particle physics.

At present, the number of reliable D/H measurements remains limited. While hundreds of high-resolution quasar spectra are available, there are only 17 D/H estimates (see Kislitsyn et al. (2024) and references therein). The main difficulty is the rarity of suitable objects and the need to have high-resolution and high-signal-to-noise ratio spectra ($R \gtrsim 30\,000$ and $S/N \gtrsim 10$, Cooke et al. 2014).

Adams (1976) was the first to propose to use the method of absorption spectroscopy to estimate D/H. The spectra of distant quasars containing the damped Lyman-alpha systems (DLAs, see, e.g., Wolfe et al. 2005) that arise in dense HI clouds are the most suitable objects for this task. Metal-poor DLA systems ($[\mathrm{O/H}] = \log(n(\mathrm{O})/n(\mathrm{H})) -$

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$\log(n(\mathrm{O})/n(\mathrm{H}))_\odot \lesssim -2$) have a number of key advantages (Pettini and Cooke 2012).

- *Minimal astration.* A low metallicity points to insignificant stellar reprocessing of matter and, as a consequence, the observed deuterium abundance is close to the primordial one.

- *Simple kinematic structure.* Low-metallicity absorption systems pertain to low-mass galaxies for which a narrow velocity structure of the absorption system is observed (Ledoux et al. 2006). A small velocity spread facilitates the separation of narrow deuterium lines and stronger hydrogen lines, given their isotopic wavelength shift $\left(\lambda^D - \lambda^H\right)/\lambda^H \times c = -81.6$ km s^{-1}.

- *High column density.* A high abundance of neutral hydrogen allows numerous transitions of the Lyman series to be observed, making multicomponent modeling of the line profiles possible and increasing the accuracy of determining the HI and DI column densities.

Having applied the justified selection criteria, Cooke et al. (2014) compiled a list of the most suitable systems for estimating D/H (precision sample), which was later supplemented (Cooke et al. 2016, 2018) and currently includes only 8 of the 17 systems in which D/H was estimated (Pettini and Cooke 2026).

Each new D/H measurement in such rare systems refines significantly the primordial deuterium abundance and makes it possible to minimize the influence of the systematic uncertainties related to the line profile modeling, the continuum determination, and the influence of the ignored absorption features (Balashev et al. 2016). Kislitsyn et al. (2024) presented a new precision measurement in the sub-DLA system at $z = 3.42$ that together with the previous results gives an estimate of $(\mathrm{D/H})_\mathrm{p} = (2.533 \pm 0.024) \times 10^{-5}$. The estimated value shows moderate ($\approx 2.2\sigma$) disagreement with the predictions of the standard model of primordial nucleosynthesis, where the value obtained by analyzing the CMB anisotropy is taken as η_b, emphasizing the need for a further increase in the precision of observational measurements.

Thus, precision measurements of the primordial deuterium abundance remain among the key directions of modern observational cosmology and an important tool of searching for possible manifestations of new physics beyond the standard model.

THE DATABASES

For our analysis we used the KODIAQ and SQUAD catalogs of high-resolution quasar spectra. Owing to the high quality of the data and their public accessibility, they provide a convenient basis for the statistical studies of absorption systems of various types, including DLA systems and Lyman-limit systems (LLSs), for analyzing the structure of the Lyman-α forest, for studying the lines of neutral hydrogen and metals, and for cosmological problems.

The KODIAQ Catalog of Quasar Spectra

In this paper we use a sample of high-spectral-resolution spectra from the KODIAQ (Keck Observatory Database of Ionized Absorption toward Quasars) survey. The catalog is based on the observations performed with the High-Resolution Echelle Spectrometer (HIRES) mounted at the 10-m Keck I telescope of the Keck Observatory. The original data were retrieved from the Keck Observatory Archive (KOA) and reduced to a uniform form by the authors of the catalog (O'Meara et al. 2015, 2017).

The first data release (KODIAQ DR1) includes the spectra of 170 quasars at redshifts $0.29 < z < 5.29$ observed in the period 2004–2012. The choice of this time interval is related to the upgrade of the HIRES detector in 2004, when the instrument was equipped with a mosaic of three CCD arrays that increased dramatically the sensitivity in the blue spectral range. All of the spectra were reduced to the vacuum wavelength scale and normalized to the continuum.

The second data release (KODIAQ DR2) expanded the sample to include the observations performed before the upgrade of the instrument (1995–2004) using the single-chip Tektronix TK2048 CCD detector. The combined DR1+DR2 catalog contains the spectra of 300 quasars (130 objects were added compared to DR1). The total exposure time reaches $\sim$4.9 Ms. The spectral resolution depends on the slit configuration and, as a rule, lies in the range $R \approx 36\,000$–$50\,000$, corresponding to an instrumental profile width $\sim$6–8 km s^{-1}.

The SQUAD Catalog of Quasar Spectra

For our analysis we also used high-resolution spectra from the first data release of the UVES Spectral Quasar Absorption Database (SQUAD) (Murphy et al. 2019), which is the largest uniformly processed sample of high-resolution quasar spectra to date. The observations were performed with the Ultraviolet and Visual Echelle Spectrograph (UVES) mounted at the Very Large Telescope (VLT) of the European Southern Observatory.

DR1 contains the final combined spectra of 467 quasars observed since the instrument was put into operation until mid-2008. The total exposure time exceeds ∼1 Ms. The spectra cover the wavelength range ≈3050 – 10 500 Å and have a high spectral resolution ($R \approx 50\,000$).

The key feature of UVES SQUAD is that the data reduction is fully reproducible. All of the reduction steps, from the calibration of the original frames to the construction of the final combined spectrum and the continuum normalization, can be repeated using publicly accessible software (in particular, the `uves_headsort` and `uves_popler` packages). This ensures the transparency of the reduction and allows it to be adapted to the tasks of a specific study.

ANALYSIS OF THE SPECTRA

Each spectrum from both catalogs was visually inspected to reveal the absorption systems in which the deuterium abundance could be potentially estimated. For this purpose, all of the absorption systems in the region of the Lyman-α forest were checked for the presence of deuterium lines located at the expected positions relative to the corresponding hydrogen lines and interpreted as deuterium lines. This and subsequent parts of our analysis were carried out using the SPECTRO[1] software.

Special attention was given to systems with a high hydrogen column density, $\log(N_{\rm HI}) \gtrsim 19$, in which several deuterium lines of the Lyman series could be observed. In such systems the Lyman-α hydrogen line allows the H I column density to be estimated with a relatively high accuracy, reducing the uncertainty of measuring D/H.

If signatures of deuterium lines were detected for the corresponding absorption system, then we constructed a simplified model of the absorption components and fitted the line profiles. This procedure allowed us to check the consistency between the redshift of the putative deuterium lines and the redshifts of the main components determined from the observed metal lines.

Fitting the Absorption Spectra

The goal of our analysis is a precision determination of the deuterium-to-hydrogen density ratio (D/H) in metal-poor absorption systems and the determination of the metallicity boundary at which the ratio (D/H) is not subject to the systematic effects associated with the evolution of the interstellar matter. To achieve the required precision, we used a complex modeling technique that took into account the kinematic structure of the absorbing gas, the characteristics of the spectroscopic data, and the possible sources of systematic errors. The approach is based on fitting the absorption line profiles by a multicomponent Voigt profile for all of the available lines of neutral hydrogen (H I), deuterium (D I), and metals with a low degree of ionization. This approach follows the technique used previously, for example, in Balashev et al. (2016) and Kislitsyn et al. (2024).

The kinematic structure of the absorption system was reconstructed predominantly from the lines of metals with a low ionization potential—O I, Si II, C II, and Fe II. Since these metals are predominantly in a neutral gas, i.e., where H I and D I are located, their profiles allow the number of H I and D I lines, their radial velocities, and the Doppler parameters to be reliably determined.

We modeled the profiles within each component under the assumption of microturbulent broadening, where the Doppler parameter b_s for a species of mass M_s is determined by the gas temperature T and the turbulent component $b_{\rm turb}$:

$$b_s^2 = b_{\rm turb}^2 + \frac{2k_{\rm B}T}{M_s}, \qquad (1)$$

where $k_{\rm B}$ is the Boltzmann constant. This parametric dependence of the broadening of various species ensures a physical consistency of the model and reduces the number of independent parameters.

Special attention was given to determining the continuum in the region of the Lyman lines, where its shape is difficult to determine due to the high density of absorption lines belonging mostly to the Lyman-alpha forest. We fitted the continuum simultaneously with the absorption lines. In the vicinity of the transitions under study it was fitted by a Chebyshev polynomial whose coefficients were optimized together with the parameters of the absorption components. All of the blending absorption lines falling into the spectral intervals being analyzed, including the Lyman-α forest lines, were also included in the model, which prevented the systematic distortions of the H I and D I profiles.

The cloud was assumed to be chemically homogeneous and, as a consequence, the D/H ratio was taken to be the same for all components of the system and was introduced as a single global model parameter.

We estimated the parameters and their uncertainties within the Bayesian approach using the Markov-chain Monte Carlo (MCMC) method. This method allows one to efficiently study the multidimensional parameter space by obtaining the a posteriori probability distributions from which the statistical errors

[1] https://github.com/balashev/spectro

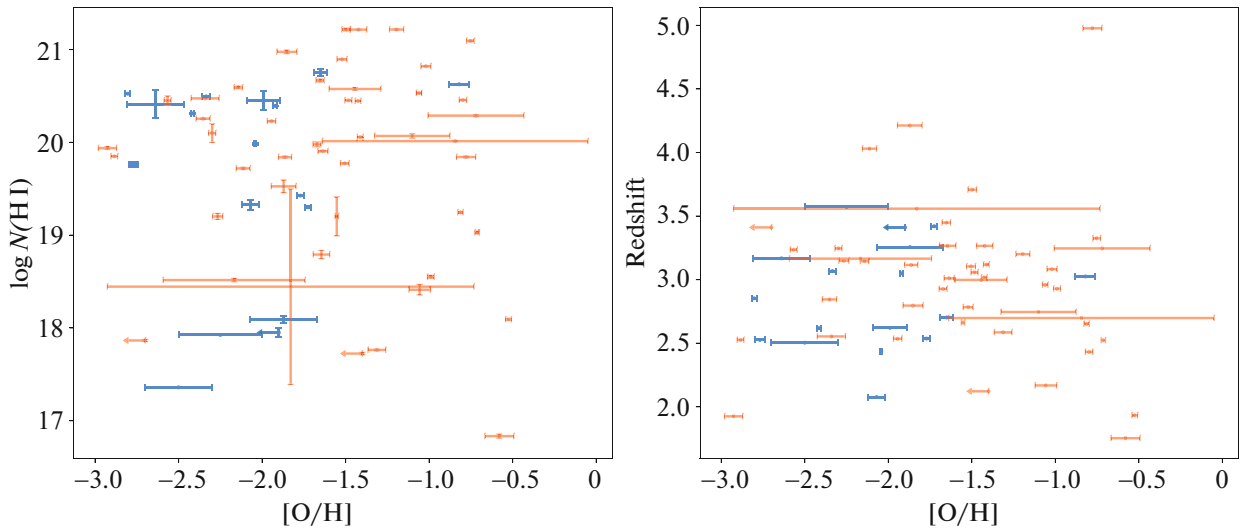


Fig. 1. Estimates of physical parameters in the new absorption systems that can be used to estimate the deuterium abundance. The published observations are indicated by the blue color; the estimates of physical conditions in the candidates found are indicated by the orange color.

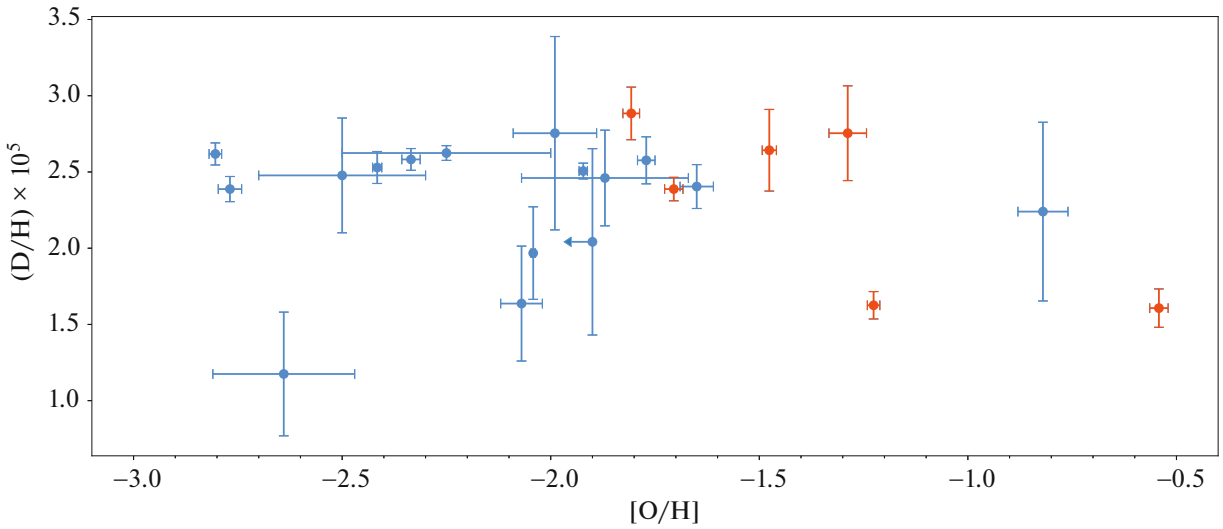


Fig. 2. Preliminary estimates of the D/H ratio. The published measurements are indicated by the blue color; the new estimates made for five random candidates to estimate the deuterium abundance are indicated by the red color. Only the statistical errors are shown for the new measurements.

were determined. For this purpose, we used the 68.3% confidence intervals of the maximum a posteriori probability.

RESULTS

Within our study we analyzed all of the accessible quasar spectra from the UVES SQUAD and KODIAQ catalogs that include 767 high-spectral-resolution spectra in total. Based on our visual and quantitative analysis of the absorption features, we produced a list of 46 new candidate systems potentially suitable for a precision determination of the deuterium-to-hydrogen density ratio. The summary results of our analysis are presented in Fig. 1 and Table 1.

For five systems from our sample we modeled in detail the line profiles by the MCMC method. The preliminary estimates of the D/H ratio obtained through our modeling are presented in Fig. 2.

Despite the fact that these five measurements are yet to be carefully checked, including checking whether the number of free parameters is sufficient, whether the kinematic structure is properly described, and whether all of the blending Lyman-alpha forest lines are properly taken into account, one might

Table 1. The list of candidates selected from the SQUAD and KODIAQ catalogs that can be used to estimate D/H

Source	z	$\log N(\mathrm{H\,I})$	[O/H]	Source	z	$\log N(\mathrm{H\,I})$	[O/H]
J0109−2102	3.145	20.592 ± 0.014	-2.143 ± 0.025	J1646+5514	4.030	19.719 ± 0.011	-2.113 ± 0.042
J0121+1448	2.662	19.203 ± 0.210	-1.553 ± 0.010	J1944+7705	2.844	20.255 ± 0.007	-2.353 ± 0.042
J0209−0005	2.523	19.028 ± 0.014	-0.713 ± 0.013	J2206−1818	2.698	20.013 ± 0.006	-0.844 ± 0.795
J0339−0133	3.115	19.840 ± 0.011	-1.863 ± 0.039	J2346+1248	2.431	20.456 ± 0.003	-0.798 ± 0.022
J1421−0643	3.448	20.666 ± 0.015	-1.653 ± 0.025	J2348−1041	2.998	20.575 ± 0.014	-1.444 ± 0.155
J0745+4734	3.017	20.446 ± 0.003	-1.426 ± 0.017	J0004−4157	2.168	18.412 ± 0.056	-1.057 ± 0.064
J0814+5029	3.707	21.215 ± 0.014	-1.498 ± 0.025	J0105−1846	2.927	19.978 ± 0.026	-1.672 ± 0.024
J0821+3107	2.535	20.228 ± 0.004	-1.944 ± 0.025	J0108+0623	1.933	18.092 ± 0.010	-0.525 ± 0.017
J0831+5245	3.558	18.445 ± 1.053	-1.829 ± 1.097	J0946+1251	3.010	19.905 ± 0.008	-1.636 ± 0.030
J0851+1612	1.925	19.938 ± 0.014	-2.926 ± 0.054	J1113−1533	3.265	21.215 ± 0.005	-1.423 ± 0.049
J0900+4215	3.246	20.288 ± 0.011	-0.720 ± 0.287	J0338−0005	2.746	20.069 ± 0.024	-1.101 ± 0.225
J0933+2845	3.235	20.450 ± 0.050	-2.566 ± 0.021	J1111+1336	3.200	21.216 ± 0.008	-1.195 ± 0.042
J0933+2845	3.246	20.100 ± 0.100	-2.299 ± 0.021	J1155+0530	3.325	21.093 ± 0.008	-0.753 ± 0.023
J1014+4300	2.959	20.531 ± 0.006	-1.061 ± 0.016	J1211+0902	3.165	18.516 ± 0.018	-2.167 ± 0.425
J1040+5724	3.266	18.791 ± 0.044	-1.645 ± 0.049	J1340+1106	2.796	20.975 ± 0.019	-1.852 ± 0.060
J1135+2227	2.783	20.895 ± 0.004	-1.522 ± 0.030	J1342−1355	3.118	20.056 ± 0.004	-1.413 ± 0.017
J1134+5742	3.411	17.865 ± 0.011	$\lesssim -2.7$	J1350−2512	1.753	16.834 ± 0.022	-0.580 ± 0.087
J1202+3235	4.977	19.842 ± 0.009	-0.779 ± 0.057	J1621−0042	3.104	19.773 ± 0.006	-1.505 ± 0.026
J1246+3031	2.526	19.849 ± 0.004	-2.885 ± 0.020	J2102−3553	3.082	20.820 ± 0.004	-1.020 ± 0.030
J1304+2953	2.122	17.724 ± 0.013	$\lesssim -1.4$	J2155+1358	4.213	19.526 ± 0.068	-1.871 ± 0.074
J1433+3131	2.585	17.763 ± 0.009	-1.313 ± 0.053	J2234+0000	2.652	19.245 ± 0.010	-0.813 ± 0.016
J1512+4652	3.148	19.202 ± 0.032	-2.266 ± 0.030	J2334−0908	3.057	20.452 ± 0.003	-1.484 ± 0.021
J1558+4053	2.553	20.474 ± 0.005	-2.341 ± 0.084	J2350−0052	2.929	18.551 ± 0.016	-0.990 ± 0.020

expect that the order of magnitude of the errors will not change significantly. This means that any new measurements will have a comparable statistical significance with the previous ones, while the data at a high metallicity can observationally constrain the deuterium astration (Dvorkin et al. 2016) from the analysis of absorption systems at redshifts $z \sim 2-3$.

CONCLUSIONS

In this paper we performed a systematic search for absorption systems suitable for precision measurements of the primordial deuterium-to-hydrogen density ratio based on high-resolution spectra from the SQUAD and KODIAQ catalogs. We analyzed 767 quasar spectra, which allowed us to produce a sample of 46 new candidate systems potentially suitable for a reliable determination of the D/H ratio, and estimated their basic parameters. The distribution of these parameters shows that the D/H ratio can be measured in a wider range of physical characteristics than has been assumed previously. In particular, higher-metallicity systems can be used to directly estimate the deuterium astration, as predicted, for example, by Dvorkin et al. (2016). This will allow

one to make more reliable assumptions about the systematic influence of this effect on the primordial deuterium abundance estimate.

For five systems we modeled in detail the line profiles using the Bayesian approach and the Markov-chain Monte Carlo method. Our preliminary estimates of the D/H ratio show that the expansion of the current sample of high-precision primordial deuterium abundance measurements is promising, since the errors of these measurements are of the same order of magnitude as those of the published estimates.

The results of our five new measurements confirm that the systematic analysis of archival high-resolution spectroscopic data is highly efficient in searching for new objects suitable for cosmological measurements. The measurements of the remaining selected candidates will be published as the estimates are obtained. Extending the statistics of $(D/H)_p$ measurements and the range of physical conditions under study helps to reduce the influence of possible systematic effects and increases the reliability of determining the primordial deuterium abundance.

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CONFLICT OF INTEREST

The authors of this work declare that they have no conflicts of interest.

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