Measuring chemical evolution and gravitational dependence of α using ultraviolet Fe V and Ni V transitions in white-dwarf spectra

A. Ong,* J. C. Berengut, and V. V. Flambaum
School of Physics, University of New South Wales, Sydney, NSW 2052, Australia
(Received 9 October 2013; published 25 November 2013)

In this paper, we present the details of the *ab initio* high-precision configuration interaction and many-body perturbation theory calculations that were used by Berengut *et al.* [Phys. Rev. Lett. **111**, 010801 (2013)] to place limits on the dependence of the fine-structure constant, α, on the gravitational field of the white-dwarf star G191-B2B. These calculations were combined with laboratory wavelengths and spectra from the Hubble Space Telescope Imaging Spectrograph to obtain the result $\Delta\alpha/\alpha = (4.2 \pm 1.6) \times 10^{-5}$ and $(-6.1 \pm 5.8) \times 10^{-5}$ using Fe V and Ni V transitions, respectively. The uncertainty in these results are dominated by the uncertainty in the laboratory wavelengths. In this work we also present *ab initio* calculations of the isotopic shifts of the Fe V transitions. We show that improved laboratory spectra will enable determination of the relative isotope abundances in Fe V to an accuracy of ∼20%. Therefore this work provides a strong motivation for new laboratory measurements.

DOI: 10.1103/PhysRevA.88.052517 PACS number(s): 31.15.A−, 97.20.Rp, 97.10.Tk, 06.20.Jr

I. INTRODUCTION

The light scalar fields that populate many modern theories of high-energy physics can change parameters of the standard model such as fundamental coupling constants [1]. Near massive bodies the effect of the scalar field can change since, like the gravitational charge, the scalar charge is purely additive. Moreover, the strength of the coupling can increase or decrease near massive gravitating bodies depending on the theoretical model used [2]. For small variations in the fine-structure constant $\alpha = e^2/\hbar c \approx 1/137$, the dependence on the dimensionless gravitational potential $\phi = GM/rc^2$ can be approximately described by the linear relationship [1]

$$\frac{\delta\alpha}{\alpha} \equiv k_\alpha \Delta\phi = k_\alpha \Delta\left(\frac{GM}{rc^2}\right). \tag{1}$$

Here k_α is a sensitivity parameter [3]. This dependence has been investigated in certain theories of varying α, where α is allowed to either increase ($\Delta\alpha/\alpha > 0$) or decrease ($\Delta\alpha/\alpha < 0$) on approach to a massive object [4–7], depending on the balance between electrostatic and magnetic energy in the ambient matter fields [2].

The strongest limit on $k_\alpha = (-5.5 \pm 5.2) \times 10^{-7}$ was obtained by comparing the radio-frequency transitions of two nearly degenerate, opposite-parity excited states in atomic dysprosium [8]. This sensitivity is derived purely from annular changes in the gravitational potential (∼3%) due to the ellipticity of the Earth's orbit around the Sun and the high precision of atomic clocks. The peak-to-trough sinusoidal change in the potential has magnitude $\Delta\phi = 3 \times 10^{-10}$.

A much stronger change in potential can be realized in the atmosphere of white-dwarf stars, where $\Delta\phi$ is 5 orders of magnitude larger than in laboratory-based experiments. This allows us to probe nonlinear coupling of $\Delta\alpha/\alpha$ on $\Delta\phi$. The distance between source and probe is $\sim 10^4$ times smaller than 1 a.u., so we can also test the effect of, for example, a Yukawa-like scalar field $\Phi \sim e^{-mr}/r$, where m is the mass of the light scalar.

High-resolution spectra of Fe^{4+} and Ni^{4+} $4s$-$4p$ transitions in the nearby (≈45 pc [9]) hot, hydrogen-rich (DA) white-dwarf star G191-B2B have been taken using the Hubble Space Telescope Imaging Spectrograph (STIS) [10]. G191-B2B has a mass of $M = 0.51 M_\odot$ and a radius of $R = 0.022 R_\odot$, thus the gravitational potential for ions in the atmosphere of this white dwarf relative to that in the laboratory is $\Delta\phi \approx 4.91 \times 10^{-5}$. The linear sensitivity parameter $k_\alpha = 0.7 \pm 0.3$ obtained from the analysis [17] is not competitive with the limits obtained from atomic clocks, but the white-dwarf result probes a very different field-strength regime.

It is instructive to compare the method with previous studies looking at cosmological variation of α using quasar absorption spectra [11–16]. In many ways, we can expect a higher sensitivity from the white-dwarf spectra than the quasar absorption spectra [17] (although we stress, again, that the fundamental physics being tested in these two experiments is quite different). First, there are many more resolved lines per source (about 100 in Fe^{4+} and 50 in Ni^{4+}), which provides a statistical advantage over the typical few narrow lines per absorber in quasar absorption systems. Second, the ionization degrees of the ions available are larger, and thus they are more sensitive to α variation. This is because the sensitivity of an external electron to α variation, q, can be approximated using [18]

$$q \approx -I_n \frac{(Z\alpha)^2}{\nu(j+1/2)}. \tag{2}$$

Here I_n is the ionization energy of the electron (in a.u.; 1 Ry = 1/2), Z is the bare nuclear charge, ν is the noninteger effective principal quantum number, and j is the angular momentum of the external electron. Taken together, from these two advantages we would expect the value of $\Delta\alpha/\alpha$ extracted from the white-dwarf study to be more than an order of magnitude more sensitive (per system) than those in the quasar studies, reaching statistical accuracies below 10^{-6}. However, the work is limited by the relatively poor laboratory wavelengths.

In this paper, we present our calculations of q values for the Fe V and Ni V transitions used in [17]. In addition, we also present an important motivation for remeasurement of their laboratory wavelengths. We calculate the isotope shifts

*ong.andrew@gmail.com

TABLE I. Isotopes of Fe.

Isotope	Mass (amu)	Charge radius (fm)	Abundance (%)
^{54}Fe	53.9396	3.6931 (18)	5.845
^{56}Fe	55.9349	3.7371 (15)	91.754
^{57}Fe	56.9354	3.7534 (17)	2.119
^{58}Fe	57.9333	3.7748 (14)	0.282

in Fe V, which can be used to measure the relative isotope abundances of Fe around G191-B2B and similar white-dwarf stars (relative to a change in the terrestrial abundances, shown in Table I). These isotope abundances can then be used to constrain theories of galactic chemical evolution (see, e.g., [19]). We show that with improved laboratory wavelengths, we could constrain the isotopic abundance ratios in Fe to ∼20%. The method and results of our isotope shift calculations are presented in Sec. III.

II. ENERGY CALCULATION AND RELATIVISTIC SHIFT

When expressed in atomic energy units, the nonrelativistic transition energies are insensitive to α variation. However, the relativistic shifts of atomic energy levels are α dependent. We parametrize the sensitivity of a transition to potential α variation using the q value, defined by

$$q = \left.\frac{d\omega}{dx}\right|_{x=0}, \tag{3}$$

where $x = (\alpha/\alpha_0)^2 - 1$ is the relative change of α^2 from its present-day value of α_0^2. Note that ω here is in atomic units: the nonrelativistic dependence on α cancels when comparing two transitions. In our calculations, q is obtained by taking the gradient of fully relativistic energies with respect to α for a particular configuration by varying the value of α in the calculation. For our Fe^{4+} calculation we used five values of x—i.e., −0.002, −0.001, 0.0, 0.001, and 0.002—to extract q, while for Ni^{4+} we used $x = -0.01$, 0.0, and 0.01 to obtain a three-point fit.

Below we outline our calculations, implementing the configuration interaction with many-body perturbation theory corrections (henceforth, the CI + MBPT method). Full details of the theory behind this method are presented in [20] (more details on our particular implementation are provided in [21]). Briefly, our calculations begin by computing the Dirac-Fock energies of core orbitals in a chosen starting potential. This provides a "frozen-core" potential from which to generate a basis and perform CI. Our CI basis is formed from a set of between 40 and 70 B splines [22,23], which we diagonalize over the Dirac-Fock potential and select those orbitals with the lowest energy eigenvalues. A larger selection of these virtual orbitals is used to formMBPT corrections to the potential, Σ.

The ions Fe^{4+} and Ni^{4+} are four- and six-valence electron ions, respectively. The use of the CI + MBPT method to obtain energies, q values, and isotope shifts in many-valence-electron systems is justified by past work (see, for example, Cr II [24]). Due to the large number of valence electrons, the size of the CI matrix grows beyond the limit of available computer memory before a fully converged result can be reached. This is particularly true for Ni^{4+}, which has two additional valence electrons over Fe^{4+}. Therefore, it becomes necessary to truncate the calculation and/or to adjust the parameters in order to make the calculation manageable. We used the available experimental data [25] as a benchmark to judge the "correctness" of calculations and thus decide on the most suitable set of parameters.

The Dirac-Fock calculation that we start with allows for a few different sensible choices of starting potentials (mean field of all electrons). In a completely converged CI calculation, the effect of choosing the starting potential will be negligible; however, the choice of potential can make a significant difference in a truncated computation. As a specific example, in Fe^{4+} we could reasonably expect to choose between a V^N or a V^{N-1} starting potential by varying the number of electrons to be used. Furthermore, after choosing one of these, we are free to choose the distribution of the electrons among the available valence orbitals. For Fe^{4+}, we compared the results obtained using $3d^2 4s^2$ (V^N), $3d^4$ (V^N), and $3d^3$ (V^{N-1}) potentials and found those produced from a $3d^4$ V^N potential to be the best. However, we note that there was good agreement among calculations performed using the three potentials. A similar result was obtained for Ni^{4+}, with the $3d^6$ V^N potential found to give results closest to experimental data.

The next set of parameters we can vary affects the CI calculation. It consists of the leading configurations, the number of electron excitations taken from these leading configurations, and the number of virtual orbitals included at which the CI valence basis is truncated for the generation of electron excitations. The number of leading configurations included significantly influences the overall size of the CI matrix. For Fe^{4+}, we tested the ($3d^4$, $3d^2 4s^2$) and the ($3d^4$, $3d^3 4s$, $3d^3 4p$) sets and found the latter to give better results. Again, the results produced by the other set of leading configurations were still reasonably close to the experimental results. For Ni^{4+}, the ($3d^6$, $3d^5 4s$, $3d^5 4p$) leading configuration set was found to give the best agreement with experiment, although we suspect that the ($3d^6$, $3d^5 4s$, $3d^5 4p$, $3d^4 4s^2$, $3d^4 4p^2$) superset of leading configurations would have improved the agreement if not for computer memory limitations.

For the number of electron excitations, we can choose either to include a large number of single-electron excitations from the leading configurations, at the cost of some double-electron excitations, by choosing different CI valence basis sets for each or to include single- and double-electron excitations to the same CI valence basis. For Fe^{4+}, we were able to include both single- and double-electron excitations to the $11spdf7g$ valence orbitals, and this provided a better agreement with experiment than including single-electron excitations to $15spdf$ and double-electron excitations to $9spdf$. The resulting energy levels in both these cases are within 5% of their experimental values [25].

For Ni^{4+}, the number of valence orbitals we can use for the CI calculation is markedly smaller due to the two additional valence electrons. In this case, our calculations reveal that taking a large number of single-electron excitations to $12spdf$ and a smaller number of double-electron excitations to $5spdf$ produced a better result than taking single and double excitations to the $7s6pdf$ level. Once again, the level energies are within 5% of their experimental values.

MBPT corrections using a valence basis of $35spdfghi$ for Fe^{4+} and $30spdfgh$ for Ni^{4+} were then added to the CI calculation. We included one-body, two-body, and three-body MBPT diagrams to second order in the residual Coulomb interaction. The final energies were improved by the addition of MBPT; agreement with experimental values was at the level of ∼2%. Tables II and III illustrate the effect of the addition of MBPT corrections. The q values are stable with the addition of MBPT corrections: one can be certain that the MBPT q values would differ by, at most, 5% (see Table II) from their CI-only values when differences in configuration mixing are not significant.

A. Error estimates and state mixing

In the results we present, some energy levels that were mixed in the CI calculation (that is, states that included a significant percentage of more than one term) become separated in the CI + MBPT calculation, and vice versa. In such cases, the presented g factors of the two calculations differ significantly. This can pose an issue when the q values for the two levels are different; a strong mixing would imply that the q values of the two levels move towards the average of the two q values, whereas less mixed states would have rather different q values. In the absence of additional information, we are unable to decide which of these cases more closely represents the physical reality of the picture. In Table IV we have marked with asterisks, the levels that may have underestimated errors in q as a result of the uncertainty in the true physical mixing. Table V contains the CI + MBPT energy levels used to obtain the result for nickel ions in the original paper [17] and a comparison with experimental values.

For levels that do not demonstrate notable differences in mixing between calculations, we estimate our uncertainties in q using the difference in values computed using the CI versus the CI + MBPT for energy levels. The errors in q values in Table IV were computed similarly by taking the difference between the final CI and the final CI + MBPT q values of the transitions.

III. ISOTOPE SHIFTS

The addition of neutrons to or removal of neutrons from the nucleus causes a change in both the nuclear mass and the nuclear charge distribution, both of which in turn cause measurable shifts in the positions of energy levels. These shifts can be parametrized, for two isotopes with mass number A and A', using the equation

$$\delta\nu_{A,A'} = \left(\frac{1}{A} - \frac{1}{A'}\right)(k_{\mathrm{NMS}} + k_{\mathrm{SMS}}) + F\delta\langle r^2\rangle_{A,A'}, \tag{4}$$

where k_{NMS} is the normal mass shift constant, k_{SMS} is the specific mass shift constant, and F is the field shift constant. k_{NMS} is related to the transition frequency ν by

$$k_{\mathrm{NMS}} = -\frac{\nu}{1823}. \tag{5}$$

k_{SMS} is more difficult to obtain; it can be calculated through the addition of a new term to the Coulomb potential and variation of a parameter related to the nuclear inverse mass, as described below. F can be similarly obtained by instead varying the nuclear charge radius. Our calculations reveal that k_{SMS} can be quite different with the inclusion of MBPT corrections, as shown in Table III. On the other hand, F does not change much between CI and CI + MBPT calculations.

A. Finite-field method

To calculate k_{SMS}, the all-order finite-field method is used [21,24,26–28]. A two-body SMS operator is added to the Coulomb potential to form an effective potential which can be written as

$$\tilde{Q} = \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} + \lambda\mathbf{p}_1 \cdot \mathbf{p}_2, \tag{6}$$

and the CI + MBPT energy calculation is performed for several values of λ. The SMS constant is then calculated using

$$k_{\mathrm{SMS}} = \left.\frac{d\omega}{d\lambda}\right|_{\lambda=0}. \tag{7}$$

TABLE II. Energy levels relative to the $3d^4\ {}^5D_0$ ground state and Landé g factors of $4s$ and $4p$ levels in Fe^{4+}. CI: quantities obtained using the configuration interaction. CI + Σ: quantities obtained using the configuration interaction plus many-body perturbation theory.

		Energy (cm^{-1})			g factor		
Level		CI	CI + Σ	Expt. [25]	CI	CI + Σ	LS
$3d^4$	${}^5D_0$	0	0	0	0	0	
$3d^4$	${}^5D_1$	159	165	142	1.4999	1.4999	1.5
$3d^4$	${}^5D_2$	468	484	417	1.4998	1.4998	1.5
$3d^4$	${}^5D_3$	912	942	803	1.4997	1.4996	1.5
$3d^4$	${}^5D_4$	1475	1523	1283	1.4995	1.4995	1.5
$3d^4$	${}^3P2_0$	28652	27027	24055			
$3d^4$	${}^3H_4$	26985	26756	24933	0.8031	0.8061	0.8
$3d^4$	${}^3P2_1$	29590	28043	24973	1.4988	1.4981	1.5
$3d^4$	${}^3H_5$	27335	27129	25226	1.0348	1.0359	1.033
$3d^4$	${}^3H_6$	27721	27541	25529	1.1662	1.1661	1.167
$3d^4$	${}^3P2_2$	31229	29733	26468	1.4980	1.4978	1.5
$3d^4$	${}^3F2_2$	31055	29397	26761	0.6684	0.6681	0.667
$3d^4$	${}^3F2_3$	31139	29462	26842	1.0658	1.0617	1.083

TABLE II. (*Continued*.)

Level		Energy (cm^{-1})			g factor		
		CI	CI + Σ	Expt. [25]	CI	CI + Σ	LS
$3d^4$	$^3F2_4$	31315	29625	26974	1.2373	1.2337	1.25
$3d^4$	$^3G_3$	34027	32147	29817	0.7681	0.7723	0.75
$3d^4$	$^3G_4$	34434	32564	30147	1.0588	1.059	1.05
$3d^4$	$^3G_5$	34753	32895	30430	1.1985	1.1974	1.2
$3d^4$	$^1G2_4$	43009	39814	36586	1.0014	1.0018	1
$3d^4$	$^3D_3$	43968	39668	36630	1.3327	1.3327	1.333
$3d^4$	$^3D_2$	44079	39809	36759	1.1661	1.167	1.167
$3d^4$	$^3D_1$	44224	39937	36925	0.5015	0.5023	0.5
$3d^4$	$^1I_6$	40841	40241	37512	1.0005	1.0006	1
$3d^4$	$^1S2_0$	49881	43418	39633			
$3d^4$	$^1D2_2$	53243	51089	46291	1.0011	1.0009	1
$3d^4$	$^1F_3$	61424	57246	52733	1.0008	1.0008	1
$3d^4$	$^3P1_2$	72538	67756	61854	1.4991	1.499	1.5
$3d^4$	$^3F1_4$	72001	68224	62238	1.2494	1.2494	1.25
$3d^4$	$^3F1_2$	72032	68222	62321	0.6674	0.6674	0.667
$3d^4$	$^3F1_3$	72093	68307	62364	1.0830	1.0830	1.083
$3d^4$	$^3P1_1$	73614	68866	62914	1.4998	1.4997	1.5
$3d^4$	$^3P1_0$	74162	69431	63420			
$3d^4$	$^1G1_4$	81641	77831	71280	1.0006	1.0006	1
$3d^4$	$^1D1_2$	109739	102229	93832	1.0000	1.0000	1
$3d^4$	$^1S1_0$	141458	133273	121130			
$3d^3(^4F)4s$	$^5F_1$	194157	185985	186434	0.0011	0.0013	0
$3d^3(^4F)4s$	$^5F_2$	194503	186323	186726	0.9998	0.9999	1
$3d^3(^4F)4s$	$^5F_3$	195021	186831	187158	1.2496	1.2497	1.25
$3d^3(^4F)4s$	$^5F_4$	195703	187501	187719	1.3496	1.3496	1.35
$3d^3(^4F)4s$	$^5F_5$	196538	188318	188395	1.3995	1.3995	1.4
$3d^3(^4F)4s$	$^3F_2$	203002	195431	195196	0.6679	0.6680	0.667
$3d^3(^4F)4s$	$^3F_3$	203886	196280	195933	1.0835	1.0834	1.083
$3d^3(^4F)4s$	$^3F_4$	204993	197365	196839	1.2494	1.2492	1.25
$3d^3(^4P)4s$	$^5P_1$	216371	205239	204730	2.4909	2.4927	2.5
$3d^3(^4P)4s$	$^5P_2$	216641	205515	204975	1.8271	1.8283	1.833
$3d^3(^4P)4s$	$^5P_3$	217310	206157	205536	1.6660	1.6661	1.667
$3d^3(^2G)4s$	$^3G_3$	219245	209658	208838	0.7506	0.7507	0.75
$3d^3(^2G)4s$	$^3G_4$	219555	209965	209110	1.0478	1.0484	1.05
$3d^3(^2G)4s$	$^3G_5$	220043	210454	209524	1.1969	1.1976	1.2
$3d^3(^4P)4s$	$^3P_0$	224416	213930	212542	0	0	
$3d^3(^4P)4s$	$^3P_1$	224720	214180	212818	1.4624	1.4598	1.5
$3d^3(^2G)4s$	$^1G_4$	223887	214643	213534	0.9806	0.9855	1
$3d^3(^4P)4s$	$^3P_2$	225598	215038	213649	1.4981	1.4981	1.5
$3d^3(^2P)4s$	$^3P_2$	226717	216232	214526	1.4433	1.3843	1.5
$3d^3(^2P)4s$	$^3P_1$	226612	216267	214611	1.4364	1.2592	1.5
$3d^34s$	$_0$	226814	216626	—[a]			
$3d^3(^2D2)4s$	$^3D_1$	228639	217569	215783	0.6570	0.8015	0.5
$3d^3(^2D2)4s$	$^3D_3$	229870	218368	216538	1.3336	1.3335	1.333
$3d^3(^2D2)4s$	$^3D_2$	229721	218549	216593	1.2219	1.2774	1.167
$3d^3(^2H)4s$	$^3H_4$	226810	217829	216779	0.8227	0.8175	0.8
$3d^3(^2H)4s$	$^3H_5$	226872	217917	216860	1.0359	1.0354	1.033
$3d^3(^2H)4s$	$^3H_6$	227205	218266	217123	1.1667	1.1667	1.167
$3d^3(^2P)4s$	$^1P_1$	231796	221770	219487	0.9522	0.9854	1
$3d^3(^2D2)4s$	$^1D_2$	233909	222735	220621	1.0081	1.0102	1
$3d^3(^2H)4s$	$^1H_5$	231287	222634	221305	1.0010	1.0008	1
$3d^3(^2F)4s$	$^3F_4$	248021	235784	233634	1.2498	1.2498	1.25
$3d^3(^2F)4s$	$^3F_3$	248221	235976	233849	1.0833	1.0833	1.083
$3d^3(^2F)4s$	$^3F_2$	248388	236145	234027	0.6674	0.6674	0.667
$3d^3(^2F)4s$	$^1F_3$	252318	240350	237730	1.0004	1.0004	1
$3d^3(^4F)4p$	$^5G^o_2$	262596	255796	254803	0.3375	0.3380	0.333
$3d^3(^4F)4p$	$^5G^o_3$	263260	256459	255399	0.9183	0.9187	0.917

TABLE II. (*Continued*.)

Level		Energy (cm^{-1})			g factor		
		CI	CI + Σ	Expt. [25]	CI	CI + Σ	*LS*
$3d^3(^4F)4p$	$^5G^o_4$	264129	257322	256178	1.1507	1.1510	1.15
$3d^3(^4F)4p$	$^5G^o_5$	265195	258401	257138	1.2668	1.2670	1.267
$3d^3(^4F)4p$	$^3D^o_1$	265667	258647	257742	0.6126	0.5627	0.5
$3d^3(^4F)4p$	$^5D^o_2$	266043	259035	258129	1.3169	1.2966	1.5
$3d^3(^4F)4p$	$^5G^o_6$	266462	259704	258297	1.3329	1.3329	1.333
$3d^3(^2D1)4s$	$^3D_3$	276666	263247	258434	1.3333	1.3333	1.333
$3d^3(^4F)4p$	$^5D^o_0$	266262	259350	258620			
$3d^3(^4F)4p$	$^3D^o_2$	267212	260268	258629	1.1958	1.2216	1.167
$3d^3(^2D1)4s$	$^3D_2$	276886	263430	258629	1.1661	1.1662	1.167
$3d^3(^4F)4p$	$^5D^o_3$	266638	259642	258680	1.4526	1.4456	1.5
$3d^3(^2D1)4s$	$^3D_1$	277045	263542	258770	0.5001	0.5001	0.5
$3d^3(^4F)4p$	$^5D^o_1$	266622	259702	258892	1.0781	1.1389	1.5
$3d^3(^4F)4p$	$^5D^o_4$	267420	260407	259345	1.4909	1.4889	1.5
$3d^3(^4F)4p$	$^5F^o_2$	268035	261065	259376	1.1482	1.1431	1
$3d^3(^4F)4p$	$^5F^o_3$	269624	262552	259955	1.3364	1.3368	1.25
$3d^3(^4F)4p$	$^5F^o_1$	268035	261065	259995	0.3115	0.3010	0
$3d^3(^4F)4p$	$^5F^o_4$	268609	261574	260521	1.3473	1.3504	1.35
$3d^3(^4F)4p$	$^5F^o_5$	269274	262279	261052	1.3863	1.3878	1.4
$3d^3(^4F)4p$	$^3D^o_3$	267884	260923	261180	1.2838	1.292	1.333
$3d^3(^2D1)4s$	$^1D_2$	280958	267772	262509	1.0003	1.0001	1
$3d^3(^4F)4p$	$^3G^o_3$	271508	265130	263899	0.7581	0.7567	0.75
$3d^3(^4F)4p$	$^3G^o_4$	272191	265776	264434	1.0600	1.0585	1.05
$3d^3(^4F)4p$	$^3G^o_5$	273082	266621	265113	1.2121	1.2103	1.2
$3d^3(^4F)4p$	$^3F^o_2$	274327	267991	266613	0.6699	0.6694	0.667
$3d^3(^4F)4p$	$^3F^o_3$	275101	268724	267240	1.0836	1.0834	1.083
$3d^3(^4F)4p$	$^3F^o_4$	275962	269561	267929	1.2491	1.2490	1.25
$3d^3(^4P)4p$	$^5P^o_1$	284981	275215	273643	2.4792	2.4772	2.5
$3d^3(^4P)4p$	$^5P^o_2$	285545	275753	274136	1.8216	1.8182	1.833
$3d^3(^4P)4p$	$^5D^o_0$	286600	276674	274753			
$3d^3(^4P)4p$	$^5P^o_3$	286333	276590	274930	1.6632	1.6631	1.667
$3d^3(^4P)4p$	$^5D^o_1$	286960	277063	275147	1.4913	1.4945	1.5
$3d^3(^4P)4p$	$^3P^o_2$	287234	277349	275374	1.4966	1.5017	1.5
$3d^3(^4P)4p$	$^3H^o_4$	286744	278504	276430	0.8136	0.8131	0.8
$3d^3(^4P)4p$	$^3P^o_0$	288302	278440	276435			
$3d^3(^4P)4p$	$^5D^o_2$	288604	278741	276759	1.5052	1.5081	1.5
$3d^3(^4P)4p$	$^3P^o_1$	288640	278794	276766	1.5087	1.5115	1.5
$3d^3(^4P)4p$	$^5D^o_3$	288842	279031	277069	1.4370	1.4982	1.5
$3d^3(^2G)4p$	$^3H^o_5$	287631	279446	277293	1.0456	1.0447	1.033
$3d^3(^4P)4p$	$^5D^o_4$	289939	280123	278076	1.4988	1.4993	1.5
$3d^3(^2G)4p$	$^3H^o_6$	289105	280926	278651	1.1651	1.1654	1.167
$3d^3(^2G)4p$	$^3G^o_3$	288901	280744	278794	0.8412	0.7940	0.75
$3d^3(^2G)4p$	$^3G^o_4$	289693	281543	279503	1.0457	1.0579	1.05
$3d^3(^2G)4p$	$^3G^o_5$	290205	282123	280040	1.1731	1.1773	1.2
$3d^3(^2G)4p$	$^3F^o_4$	290783	282411	280367	1.1014	1.1056	1.25
$3d^3(^2P)4p$	$^1S^o_0$	292453	282626	—[a]			
$3d^3(^2G)4p$	$^3F^o_2$	291494	282867	280540	0.6773	0.6896	0.667
$3d^3(^2G)4p$	$^3F^o_3$	291442	283023	280832	1.0486	1.0369	1.083
$3d^3(^2P)4p$	$^3P^o_1$	293803	284774	281945	1.4790	1.4507	1.5
$3d^3(^2G)4p$	$^1G^o_4$	292432	284178	282038	1.0956	1.0957	1
$3d^3(^2P)4p$	$^3P^o_0$	294016	285106	282235			
$3d^3(^4P)4p$	$^5S^o_2$	294802	284659	282424	1.6071	1.9561	2
$3d^3(^2G)4p$	$^1F^o_3$	293527	284950	282572	1.0041	1.0055	1
$3d^3(^2P)4p$	$^1D^o_2$	294577	285404	282605[b]	1.3162	1.0385	1
$3d^3(^2G)4p$	$^1H^o_5$	292926	285112	282872	1.0027	1.0020	1
$3d^3(^2P)4p$	$^3P^o_2$	295742	286616	283686	1.5446	1.4403	1.5
$3d^3(^2P)4p$	$^3D^o_1$	295327	286584	283754	0.5275	0.5457	0.5
$3d^3(^2H)4p$	$^3H^o_4$	294535	286730	284690	0.8471	0.8324	0.8

TABLE II. (*Continued*.)

Level		Energy (cm^{-1})			g factor		
		CI	CI + Σ	Expt. [25]	CI	CI + Σ	LS
$3d^3(^2H)4p$	$^3H^o_5$	294522	286832	284791	1.0347	1.0340	1.033
$3d^3(^2P)4p$	$^3D^o_2$	296908	287861	284911	1.1360	1.1232	1.167
$3d^3(^2H)4p$	$^3H^o_6$	294976	287304	285196	1.1634	1.1633	1.167
$3d^3(^2P)4p$	$^3D^o_3$	297195	288233	285474	1.3051	1.2826	1.333
$3d^3(^2D2)4p$	$^1P^o_1$	297957	288775	285962	0.9834	1.0092	1
$3d^3(^2D2)4p$	$^3F^o_2$	298947	288727	286155	0.8283	0.9229	0.667
$3d^3(^2P)4p$	$^3S^o_1$	298298	289076	286188	1.6914	1.6573	2
$3d^3(^4P)4p$	$^3D^o_3$	298134	288944	286431	1.3082	1.2502	1.333
$3d^3(^4P)4p$	$^3D^o_1$	298847	289484	286855	0.8332	0.8470	0.5
$3d^3(^4P)4p$	$^3D^o_2$	298118	289527	286863	1.0689	1.0060	1.167
$3d^3(^2D2)4p$	$^3F^o_3$	299436	289941	287110	1.1315	1.2089	1.083
$3d^3(^2H)4p$	$^3I^o_5$	297227	289714	287441	0.8476	0.8463	0.833
$3d^3(^2D2)4p$	$^3F^o_4$	300288	290528	287620	1.1417	1.2475	1.25
$3d^3(^2H)4p$	$^3I^o_6$	297970	290488	288167	1.0258	1.0259	1.024
$3d^3(^2D2)4p$	$^3D^o_1$	301168	291403	288670	0.5479	0.5373	0.5
$3d^3(^2H)4p$	$^3I^o_7$	299024	291599	289172	1.1429	1.1429	1.143
$3d^3(^2D2)4p$	$^3D^o_2$	302090	292210	289390	1.1780	1.1699	1.167
$3d^3(^2H)4p$	$^1G^o_4$	300530	291971	289546	1.1124	1.0034	1
$3d^3(^2D2)4p$	$^3D^o_3$	302829	292881	289913	1.2305	1.2901	1.333
$3d^3(^2H)4p$	$^1I^o_5$	299333	292356	290099	1.0065	1.0153	1
$3d^3(^2P)4p$	$^3P^o_2$	303091	293332	290408	1.4759	1.4836	1.5
$3d^3(^2D2)4p$	$^3P^o_1$	303347	293504	290584	1.4947	1.4846	1.5
$3d^3(^2D2)4p$	$^3P^o_0$	303732	293893	290903			
$3d^3(^2D2)4p$	$^1F^o_3$	303917	294076	291231	1.0519	0.9554	1
$3d^3(^2H)4p$	$^3G^o_5$	302388	294610	292288	1.1912	1.1822	1.2
$3d^3(^2H)4p$	$^1I^o_6$	301895	294661	292366	1.0033	1.0030	1
$3d^3(^2H)4p$	$^3G^o_4$	302649	294722	292431	1.0458	1.0475	1.05
$3d^3(^2H)4p$	$^3G^o_3$	302312	294871	292513	0.8122	0.8484	0.75
$3d^3(^4P)4p$	$^3S^o_1$	306062	297477	294644	1.9057	1.915	2
$3d^3(^2D2)4p$	$^1D^o_2$	307979	298897	295716	1.0088	1.0059	1
$3d^3(^2P)4p$	$^1P^o_1$	308019	299292	295973	1.0547	1.0665	1
$3d^3(^2F)4p$	$^3F^o_2$	316699	305486	302293	0.6779	0.6767	0.667
$3d^3(^2F)4p$	$^3F^o_3$	316778	305579	302377	1.0755	1.0779	1.083
$3d^3(^2F)4p$	$^3F^o_4$	317000	305844	302603	1.2392	1.2417	1.25
$3d^3(^2F)4p$	$^3G^o_3$	320036	309427	306194	0.7711	0.7686	0.75
$3d^3(^2F)4p$	$^3G^o_4$	320456	309892	306623	1.0589	1.0569	1.05
$3d^3(^2F)4p$	$^3G^o_5$	320929	310372	307064	1.1999	1.1999	1.2
$3d^3(^2F)4p$	$^3D^o_3$	321434	310780	307289	1.3155	1.3166	1.333
$3d^3(^2F)4p$	$^1D^o_2$	322198	311524	307644	1.0634	1.0641	1
$3d^3(^2F)4p$	$^3D^o_2$	322387	311756	308165	1.0933	1.0939	1.167
$3d^3(^2F)4p$	$^3D^o_1$	322827	312170	308672	0.5012	0.5011	0.5
$3d^3(^2F)4p$	$^1G^o_4$	324406	314671	311181	1.0020	1.0014	1
$3d^3(^2F)4p$	$^1F^o_3$	325128	315098	311539	1.0054	1.0042	1
$3d^3(^2D1)4p$	$^3D^o_1$	345129	333204	327534	0.5081	0.5092	0.5
$3d^3(^2D1)4p$	$^3D^o_2$	345197	333282	327605	1.1655	1.1652	1.167
$3d^3(^2D1)4p$	$^3D^o_3$	345512	333663	327924	1.3255	1.3238	1.333
$3d^3(^2D1)4p$	$^1D^o_2$	347377	335425	329849	0.9668	0.9472	1
$3d^3(^2D1)4p$	$^3F^o_2$	349286	337092	331334	0.7072	0.7285	0.667
$3d^3(^2D1)4p$	$^3F^o_3$	349341	337177	331367	1.0863	1.0887	1.083
$3d^3(^2D1)4p$	$^3F^o_4$	349982	337859	332017	1.2498	1.2497	1.25
$3d^3(^2D1)4p$	$^3P^o_2$	352735	340334	334509	1.4933	1.4918	1.5
$3d^3(^2D1)4p$	$^3P^o_1$	353518	341107	335268	1.4918	1.4907	1.5
$3d^3(^2D1)4p$	$^3P^o_0$	353898	341462	335643			
$3d^3(^2D1)4p$	$^1F^o_3$	353558	341962	335947	1.0043	1.0035	1
$3d^3(^2D1)4p$	$^1P^o_1$	360184	348790	342462	1.0000	1.0000	1

[a]This level was not observed in the experimental data.

[b]This level was identified in the experimental data as $3d^3(^4P)4p^5S^o_2$.

TABLE III. Calculated sensitivities to α variation q, specific mass shift constant $k_{\rm SMS}$, and field shift constant F (all relative to the ground state) of $4s$ and $4p$ energy levels in Fe^{4+}. CI: quantities obtained using the configuration interaction. CI + Σ: quantities obtained using the configuration interaction plus many-body perturbation theory.

		q (cm^{-1})		$k_{\rm SMS}$ (GHz amu)		F (MHz fm^{-2})	
Level		CI	CI + Σ	CI	CI + Σ	CI	CI + Σ
$3d^4$	$^5D_0$	0	0	0	0	−4298	−3685
$3d^4$	$^5D_1$	172	179	8	7	−4297	−3684
$3d^4$	$^5D_2$	496	517	22	20	−4296	−3683
$3d^4$	$^5D_3$	941	978	42	39	−4294	−3681
$3d^4$	$^5D_4$	1479	1533	66	65	−4292	−3679
$3d^4$	$^3P2_0$	−940	−977	335	−131	−4272	−3669
$3d^4$	$^3H_4$	283	180	346	1451	−4268	−3645
$3d^4$	$^3P2_1$	67	129	380	−80	−4268	−3665
$3d^4$	$^3H_5$	681	623	363	1474	−4267	−3643
$3d^4$	$^3H_6$	1082	1067	380	1505	−4265	−3641
$3d^4$	$^3P2_2$	1628	1734	452	−8	−4262	−3659
$3d^4$	$^3F2_2$	516	586	413	499	−4264	−3659
$3d^4$	$^3F2_3$	490	518	413	530	−4264	−3659
$3d^4$	$^3F2_4$	638	679	419	545	−4264	−3659
$3d^4$	$^3G_3$	675	751	459	958	−4260	−3654
$3d^4$	$^3G_4$	1077	1146	477	982	−4258	−3652
$3d^4$	$^3G_5$	1307	1410	488	1022	−4257	−3651
$3d^4$	$^1G2_4$	1097	1276	582	971	−4248	−3656
$3d^4$	$^3D_3$	662	788	597	288	−4250	−3669
$3d^4$	$^3D_2$	754	929	601	293	−4249	−3668
$3d^4$	$^3D_1$	953	1102	610	300	−4249	−3668
$3d^4$	$^1I_6$	875	853	535	2211	−4252	−3625
$3d^4$	$^1S2_0$	948	1255	678	−140	−4240	−3688
$3d^4$	$^1D2_2$	913	982	712	384	−4244	−3636
$3d^4$	$^1F_3$	669	781	819	747	−4233	−3643
$3d^4$	$^3P1_2$	187	324	973	174	−4219	−3629
$3d^4$	$^3F1_4$	652	774	984	698	−4215	−3612
$3d^4$	$^3F1_2$	711	799	989	701	−4215	−3611
$3d^4$	$^3F1_3$	828	933	993	704	−4215	−3611
$3d^4$	$^3P1_1$	1228	1395	1021	219	−4215	−3624
$3d^4$	$^3P1_0$	1767	1948	1046	244	−4213	−3623
$3d^4$	$^1G1_4$	691	779	1097	1208	−4208	−3601
$3d^4$	$^1D1_2$	531	721	1492	628	−4176	−3598
$3d^4$	$^1S1_0$	382	611	1932	302	−4135	−3548
$3d^3(^4F)4s$	$^5F_1$	−6896	−6690	11109	11489	−1666	−1024
$3d^3(^4F)4s$	$^5F_2$	−6549	−6344	11123	11503	−1664	−1023
$3d^3(^4F)4s$	$^5F_3$	−6030	−5829	11144	11523	−1662	−1021
$3d^3(^4F)4s$	$^5F_4$	−5353	−5161	11172	11550	−1659	−1018
$3d^3(^4F)4s$	$^5F_5$	−4546	−4370	11206	11583	−1656	−1015
$3d^3(^4F)4s$	$^3F_2$	−6360	−6151	10978	11294	−1825	−1186
$3d^3(^4F)4s$	$^3F_3$	−5461	−5264	11014	11329	−1822	−1183
$3d^3(^4F)4s$	$^3F_4$	−4406	−4230	11057	11369	−1817	−1179
$3d^3(^4P)4s$	$^5P_1$	−6220	−5930	11423	11099	−1641	−1022
$3d^3(^4P)4s$	$^5P_2$	−6039	−5733	11431	11106	−1641	−1021
$3d^3(^4P)4s$	$^5P_3$	−5243	−4975	11463	11135	−1637	−1018
$3d^3(^2G)4s$	$^3G_3$	−5963	−5750	11379	12046	−1679	−1046
$3d^3(^2G)4s$	$^3G_4$	−5737	−5510	11389	12062	−1678	−1046
$3d^3(^2G)4s$	$^3G_5$	−5294	−5060	11408	12090	−1676	−1043
$3d^3(^4P)4s$	$^3P_0$	−6456	−6095	11292	10915	−1784	−1168
$3d^3(^4P)4s$	$^3P_1$	−6282	−5961	11287	10907	−1792	−1174
$3d^3(^2G)4s$	$^1G_4$	−5783	−5496	11326	12007	−1750	−1118
$3d^3(^4P)4s$	$^3P_2$	−5215	−4886	11321	10930	−1792	−1178
$3d^3(^2P)4s$	$^3P_2$	−5872	−6026	11473	11169	−1681	−1053
$3d^3(^2P)4s$	$^3P_1$	−5745	−5776	11471	11151	−1683	−1058
$3d^34s$	$_0$	−5292	−5120	11470	11133	−1693	−1061

TABLE III. (*Continued*.)

Level		q (cm^{-1})		k_{SMS} (GHz amu)		F (MHz fm^{-2})	
		CI	CI + Σ	CI	CI + Σ	CI	CI + Σ
$3d^3(^2D2)4s$	$^3D_1$	−6198	−5455	11479	11230	−1684	−1056
$3d^3(^2D2)4s$	$^3D_3$	−5043	−4792	11549	11316	−1664	−1051
$3d^3(^2D2)4s$	$^3D_2$	−4752	−4162	11554	11288	−1665	−1047
$3d^3(^2H)4s$	$^3H_4$	−5172	−5102	11484	12628	−1678	−1031
$3d^3(^2H)4s$	$^3H_5$	−5394	−5254	11491	12676	−1670	−1025
$3d^3(^2H)4s$	$^3H_6$	−5163	−5008	11502	12696	−1669	−1023
$3d^3(^2P)4s$	$^1P_1$	−4227	−4171	11485	11107	−1736	−1117
$3d^3(^2D2)4s$	$^1D_2$	−5030	−4735	11472	11208	−1745	−1130
$3d^3(^2H)4s$	$^1H_5$	−5216	−5063	11423	12579	−1750	−1106
$3d^3(^2F)4s$	$^3F_4$	−5711	−5450	11768	11821	−1650	−1031
$3d^3(^2F)4s$	$^3F_3$	−5545	−5286	11775	11823	−1650	−1031
$3d^3(^2F)4s$	$^3F_2$	−5392	−5133	11782	11827	−1649	−1030
$3d^3(^2F)4s$	$^1F_3$	−5426	−5168	11703	11722	−1731	−1113
$3d^3(^4F)4p$	$^5G^o_2$	−5411	−5156	9556	10018	−3673	−3086
$3d^3(^4F)4p$	$^5G^o_3$	−4710	−4451	9594	10090	−3672	−3086
$3d^3(^4F)4p$	$^5G^o_4$	−3812	−3552	9643	10162	−3671	−3085
$3d^3(^4F)4p$	$^5G^o_5$	−2728	−2458	9704	10236	−3669	−3084
$3d^3(^4F)4p$	$^3D^o_1$	−5473	−5249	10207	10255	−3672	−3085
$3d^3(^4F)4p$	$^5D^o_2$	−4706	−4490	10389	10440	−3671	−3084
$3d^3(^4F)4p$	$^5G^o_6$	−1431	−1123	9778	10283	−3669	−3084
$3d^3(^2D1)4s$	$^3D_3$	−5751	−5410	12144	11467	−1620	−1002
$3d^3(^4F)4p$	$^5D^o_0$	−3825	−3480	10707	10573	−3678	−3091
$3d^3(^4F)4p$	$^3D^o_2$	−3720	−3321	10293	10545	−3675	−3091
$3d^3(^2D1)4s$	$^3D_2$	−5566	−5267	12153	11474	−1620	−1001
$3d^3(^4F)4p$	$^5D^o_3$	−3810	−3576	10542	10606	−3669	−3082
$3d^3(^2D1)4s$	$^3D_1$	−5420	−5159	12160	11479	−1619	−1001
$3d^3(^4F)4p$	$^5D^o_1$	−3872	−3478	10512	10571	−3676	−3091
$3d^3(^4F)4p$	$^5D^o_4$	−2854	−2616	10663	10688	−3666	−3080
$3d^3(^4F)4p$	$^5F^o_2$	−3370	−3046	10331	10398	−3670	−3085
$3d^3(^4F)4p$	$^5F^o_3$	−1847	−1568	10427	10536	−3665	−3079
$3d^3(^4F)4p$	$^5F^o_1$	−3370	−3046	10231	10465	−3673	−3089
$3d^3(^4F)4p$	$^5F^o_4$	−2795	−2501	10087	10312	−3672	−3089
$3d^3(^4F)4p$	$^5F^o_5$	−2421	−2095	10078	10398	−3668	−3086
$3d^3(^4F)4p$	$^3D^o_3$	−3375	−2997	10141	10425	−3674	−3091
$3d^3(^2D1)4s$	$^1D_2$	−5464	−5160	12079	11366	−1702	−1084
$3d^3(^4F)4p$	$^3G^o_3$	−3737	−3424	10482	10672	−3673	−3088
$3d^3(^4F)4p$	$^3G^o_4$	−2984	−2688	10505	10687	−3670	−3085
$3d^3(^4F)4p$	$^3G^o_5$	−1993	−1752	10531	10710	−3665	−3081
$3d^3(^4F)4p$	$^3F^o_2$	−3673	−3368	10457	10481	−3670	−3085
$3d^3(^4F)4p$	$^3F^o_3$	−2860	−2593	10492	10587	−3667	−3082
$3d^3(^4F)4p$	$^3F^o_4$	−2111	−1878	10529	10662	−3664	−3079
$3d^3(^4P)4p$	$^5P^o_1$	−4269	−3906	10678	10219	−3651	−3084
$3d^3(^4P)4p$	$^5P^o_2$	−3630	−3296	10708	10100	−3650	−3083
$3d^3(^4P)4p$	$^5D^o_0$	−5187	−4829	10079	9661	−3649	−3087
$3d^3(^4P)4p$	$^5P^o_3$	−2798	−2410	10767	10258	−3651	−3085
$3d^3(^4P)4p$	$^5D^o_1$	−4829	−4435	10088	9713	−3648	−3086
$3d^3(^4P)4p$	$^3P^o_2$	−4498	−4042	10195	9814	−3648	−3084
$3d^3(^4P)4p$	$^3H^o_4$	−4650	−4377	10022	10790	−3647	−3066
$3d^3(^4P)4p$	$^3P^o_0$	−3587	−3166	10265	9901	−3652	−3091
$3d^3(^4P)4p$	$^5D^o_2$	−3157	−2773	10196	9852	−3650	−3089
$3d^3(^4P)4p$	$^3P^o_1$	−2874	−2458	10362	9968	−3650	−3089
$3d^3(^4P)4p$	$^5D^o_3$	−3443	−2903	10087	9796	−3650	−3090
$3d^3(^2G)4p$	$^3H^o_5$	−3914	−3575	10109	11011	−3647	−3066
$3d^3(^4P)4p$	$^5D^o_4$	−2140	−1729	10088	9800	−3650	−3090
$3d^3(^2G)4p$	$^3H^o_6$	−2252	−1912	10141	11070	−3647	−3066
$3d^3(^2G)4p$	$^3G^o_3$	−4149	−4046	10703	11206	−3649	−3070
$3d^3(^2G)4p$	$^3G^o_4$	−3153	−3003	10788	11208	−3649	−3070

TABLE III. (*Continued*.)

Level		q (cm^{-1})		k_{SMS} (GHz amu)		F (MHz fm^{-2})	
		CI	CI + Σ	CI	CI + Σ	CI	CI + Σ
$3d^3(^2G)4p$	$^3G^o_5$	−2653	−2316	10773	11297	−3649	−3071
$3d^3(^2G)4p$	$^3F^o_4$	−4260	−3764	10744	11161	−3649	−3071
$3d^3(^2P)4p$	$^1S^o_0$	−3329	−2668	10230	9718	−3642	−3076
$3d^3(^2G)4p$	$^3F^o_2$	−3363	−3322	10757	10777	−3650	−3074
$3d^3(^2G)4p$	$^3F^o_3$	−3258	−2825	10789	11177	−3650	−3071
$3d^3(^2P)4p$	$^3P^o_1$	−4531	−4428	10691	10219	−3645	−3067
$3d^3(^2G)4p$	$^1G^o_4$	−2774	−2235	10826	11231	−3649	−3071
$3d^3(^2P)4p$	$^3P^o_0$	−3280	−3186	10639	10111	−3646	−3066
$3d^3(^4P)4p$	$^5S^o_2$	−3665	−2679	10177	9678	−3648	−3094
$3d^3(^2G)4p$	$^1F^o_3$	−2437	−2172	10615	10880	−3644	−3066
$3d^3(^2P)4p$	$^1D^o_2$	−3840	−3584	10378	10159	−3644	−3068
$3d^3(^2G)4p$	$^1H^o_5$	−3195	−2888	10262	11117	−3643	−3062
$3d^3(^2P)4p$	$^3P^o_2$	−2610	−2461	10618	10284	−3644	−3066
$3d^3(^2P)4p$	$^3D^o_1$	−4422	−4077	10457	10195	−3647	−3075
$3d^3(^2H)4p$	$^3H^o_4$	−2742	−2730	10782	11654	−3643	−3054
$3d^3(^2H)4p$	$^3H^o_5$	−3231	−3002	10745	11715	−3643	−3052
$3d^3(^2P)4p$	$^3D^o_2$	−2437	−2395	10474	10178	−3643	−3073
$3d^3(^2H)4p$	$^3H^o_6$	−2872	−2607	10758	11649	−3643	−3053
$3d^3(^2P)4p$	$^3D^o_3$	−2726	−2598	10682	10363	−3647	−3079
$3d^3(^2D2)4p$	$^1P^o_1$	−3314	−2768	11029	10329	−3646	−3079
$3d^3(^2D2)4p$	$^3F^o_2$	−3090	−3117	10699	10391	−3638	−3080
$3d^3(^2P)4p$	$^3S^o_1$	−2574	−2125	10995	10499	−3648	−3079
$3d^3(^4P)4p$	$^3D^o_3$	−3231	−2970	10960	10410	−3648	−3082
$3d^3(^4P)4p$	$^3D^o_1$	−2595	−2278	11074	10394	−3643	−3080
$3d^3(^4P)4p$	$^3D^o_2$	−3374	−2531	10902	10424	−3646	−3077
$3d^3(^2D2)4p$	$^3F^o_3$	−3047	−2456	10719	10501	−3638	−3075
$3d^3(^2H)4p$	$^3I^o_5$	−3570	−3381	10134	11549	−3639	−3050
$3d^3(^2D2)4p$	$^3F^o_4$	−2748	−1822	10658	10511	−3641	−3079
$3d^3(^2H)4p$	$^3I^o_6$	−3085	−2829	10141	11442	−3640	−3051
$3d^3(^2D2)4p$	$^3D^o_1$	−4196	−3628	10679	10331	−3642	−3077
$3d^3(^2H)4p$	$^3I^o_7$	−2114	−1822	10203	11539	−3641	−3052
$3d^3(^2D2)4p$	$^3D^o_2$	−3023	−2522	10714	10413	−3640	−3076
$3d^3(^2H)4p$	$^1G^o_4$	−2648	−2859	10698	11441	−3638	−3052
$3d^3(^2D2)4p$	$^3D^o_3$	−2248	−1844	10678	10308	−3638	−3075
$3d^3(^2H)4p$	$^1I^o_5$	−3126	−3000	10603	12229	−3642	−3049
$3d^3(^2P)4p$	$^3P^o_2$	−2923	−2469	10944	10394	−3641	−3084
$3d^3(^2D2)4p$	$^3P^o_1$	−2868	−2493	10982	10487	−3642	−3085
$3d^3(^2D2)4p$	$^3P^o_0$	−2294	−1941	10999	10342	−3641	−3084
$3d^3(^2D2)4p$	$^1F^o_3$	−2144	−2450	11207	11099	−3639	−3072
$3d^3(^2H)4p$	$^3G^o_5$	−2762	−2381	10984	11838	−3638	−3050
$3d^3(^2H)4p$	$^1I^o_6$	−2744	−2475	10676	11824	−3640	−3052
$3d^3(^2H)4p$	$^3G^o_4$	−2425	−2283	10995	11801	−3640	−3052
$3d^3(^2H)4p$	$^3G^o_3$	−2951	−1918	10984	11559	−3639	−3061
$3d^3(^4P)4p$	$^3S^o_1$	−2637	−2403	11122	10389	−3642	−3079
$3d^3(^2D2)4p$	$^1D^o_2$	−2697	−2374	11423	10799	−3639	−3076
$3d^3(^2P)4p$	$^1P^o_1$	−1886	−1598	10887	10410	−3639	−3070
$3d^3(^2F)4p$	$^3F^o_2$	−3690	−3323	10744	10673	−3621	−3060
$3d^3(^2F)4p$	$^3F^o_3$	−3663	−3279	10736	10661	−3622	−3060
$3d^3(^2F)4p$	$^3F^o_4$	−3386	−2941	10748	10729	−3622	−3061
$3d^3(^2F)4p$	$^3G^o_3$	−3645	−3315	10564	10815	−3619	−3055
$3d^3(^2F)4p$	$^3G^o_4$	−3120	−2732	10607	10700	−3622	−3057
$3d^3(^2F)4p$	$^3G^o_5$	−2697	−2311	10634	10755	−3623	−3060
$3d^3(^2F)4p$	$^3D^o_3$	−3605	−3233	11094	10842	−3620	−3053
$3d^3(^2F)4p$	$^1D^o_2$	−2933	−2595	11047	10629	−3617	−3048
$3d^3(^2F)4p$	$^3D^o_2$	−2793	−2413	11100	10793	−3620	−3051
$3d^3(^2F)4p$	$^3D^o_1$	−2292	−1918	11190	11012	−3620	−3053
$3d^3(^2F)4p$	$^1G^o_4$	−2844	−2538	10878	11015	−3622	−3053

TABLE III. (*Continued*.)

Level		q (cm^{-1})		k_{SMS} (GHz amu)		F (MHz fm^{-2})	
		CI	CI + Σ	CI	CI + Σ	CI	CI + Σ
$3d^3(^2F)4p$	$^1F_3^o$	−2854	−2512	11650	11315	−3620	−3054
$3d^3(^2D1)4p$	$^3D_1^o$	−3654	−3315	11374	10694	−3588	−3019
$3d^3(^2D1)4p$	$^3D_2^o$	−3663	−3298	11364	10477	−3588	−3019
$3d^3(^2D1)4p$	$^3D_3^o$	−3278	−2868	11386	10595	−3589	−3019
$3d^3(^2D1)4p$	$^1D_2^o$	−3618	−3364	11521	10639	−3591	−3028
$3d^3(^2D1)4p$	$^3F_2^o$	−3275	−2776	11077	10440	−3587	−3026
$3d^3(^2D1)4p$	$^3F_3^o$	−3514	−3036	11027	10470	−3588	−3026
$3d^3(^2D1)4p$	$^3F_4^o$	−2778	−2295	11065	10380	−3591	−3029
$3d^3(^2D1)4p$	$^3P_2^o$	−3371	−2910	11068	10257	−3586	−3026
$3d^3(^2D1)4p$	$^3P_1^o$	−2685	−2266	11114	10393	−3587	−3027
$3d^3(^2D1)4p$	$^3P_0^o$	−2358	−1949	11134	10182	−3587	−3027
$3d^3(^2D1)4p$	$^1F_3^o$	−2787	−2418	11345	10596	−3585	−3019
$3d^3(^2D1)4p$	$^1P_1^o$	−3084	−2675	11878	10818	−3585	−3021

The operator $\tilde{Q}$ has the same symmetry and structure as the ordinary Coulomb operator [26]. Our results were obtained by performing a five-point fit using values of $\lambda = -0.002$, -0.001, 0.0, 0.001, and 0.002.

The field shift constant F can be calculated using one of two methods. The first approach is to vary the nuclear radius R in the finite nuclear potential directly, which in turn varies the mean squared charge radius $\langle r^2 \rangle$. We perform the full CI + MBPT calculation for each value of R and extract F using

$$F = \frac{d\omega}{d\langle r^2 \rangle}. \tag{8}$$

We used five values of $\langle r^2 \rangle$ in order to ensure linearity of F with respect to $\langle r^2 \rangle$.

The second approach used is similar to the finite-field method described for calculating k_{SMS}. A finite perturbation δU is added to the nuclear potential,

$$\delta U(r) = \lambda[U(R + \delta R, r) - U(R, r)], \tag{9}$$

where R is the nuclear radius and $U(R,r)$ is the nuclear potential (e.g., a Fermi distribution with a finite thickness parameter). The change in nuclear potential corresponds to a change in mean nuclear charge radius $\delta\langle r^2 \rangle_U$, and we can extract the field shift constant by calculating ω for several values of λ:

$$F = \frac{1}{\delta\langle r^2 \rangle_U} \frac{d\omega}{d\lambda}\bigg|_{\lambda=0}.$$

Our calculations using the two methods were consistent within 1%.

B. B-spline basis set

The calculation of the field shift constant, F, is sensitive to the behavior of the wave function at the origin. The B-spline basis of the Notre Dame (ND) group [23] was compared with B splines generated using the dual-kinetic-balance (DKB) finite basis set method [29,30]. In our calculations, we found that the ND B splines were unstable when used to calculate F, leading to inconsistencies when the size of the set of valence states used in the CI calculation was varied. The DKB B splines, on the other hand, produced consistent values of F regardless of the parameters used in the calculation. The ND calculation agreed with the DKB calculation only after the inclusion of a larger number of B splines and a readjustment of the grid used.

This result reinforces the findings in [29], where the DKB B splines were found to have a behavior at the origin that is closer to the physical reality. The original authors found that they required fewer B splines when the DKB method was used compared to the ND method, a result our calculations also agree with.

C. Error estimate

The error in the total isotope shift, $\Delta\delta\nu_{A,A'}$, is largely given by the uncertainty in the SMS constant. We estimate this uncertainty by using the difference between the CI and the CI + MBPT calculations as an upper bound, which can be obtained using Table III. The nuclear radii of the various isotopes and their errors are listed in Table I.

IV. DISCUSSION

Using our calculations for the relativistic shifts q and isotopic shifts $\delta\nu_{A,A'}$ in Table III (for energy levels), we present a summary table containing these shifts for transitions observed in white-dwarf stars using the Hubble STIS in Table IV. For these observed lines, the extent of α variation is found to be $\Delta\alpha/\alpha = (4.2 \pm 1.6) \times 10^{-5}$ for Fe^{4+}. Furthermore, a limit on the deviation of isotopic abundances in white-dwarf stars from their terrestrial values can be placed using the differences between their observed and their terrestrial wavelengths in conjunction with the information in Table IV. In both the astronomical data and our reference laboratory wavelengths, the spectra of individual isotopes are not resolved. Thus, the available wavelength values are averages weighted by the isotopic abundances. For a particular white-dwarf line with wavelength λ_{obsv} observed from Earth containing isotopes with

TABLE IV. Calculated sensitivities to α variation q and isotope shifts $\delta\nu_{A,A'}$ of selected transitions in Fe^{4+}. Asterisks indicate transitions that may have underestimated errors due to differences in state mixing between CI and CI + Σ calculations.

λ (nm)	Lower state		Upper state		q (cm^{-1})	$\delta\nu_{54,56}$ (ms^{-1})	$\delta\nu_{57,56}$ (ms^{-1})	$\delta\nu_{58,56}$ (ms^{-1})
119.6202	$3d^3(^4F)4s$	$^3F_2$	$3d^3(^2G)4p$	$^3G^o_3$	2105 (106)	41.8 (15.2)	−27.3 (7.9)	−43.8 (14.2)
119.6607	$3d^3(^4F)4s$	$^3F_3$	$3d^3(^2G)4p$	$^3G^o_4$	2261 (46)	44.3 (9.1)	−28.5 (5.4)	−46.1 (8.4)
120.1909	$3d^3(^4F)4s$	$^3F_4$	$3d^3(^2G)4p$	$^3G^o_5$	1914 (161)	39.9 (17.3)	−26.5 (8.8)	−42 (16.1)
123.4648	$3d^3(^4P)4s$	$^3P_2$	$3d^3(^4P)4p$	$^3S^o_1$	2482 (96)	75.9 (28.1)	−43.8 (13.8)	−75.8 (26.2)
125.8791	$3d^3(^4F)4s$	$^3F_3$	$3d^3(^4P)4p$	$^3P^o_2$	1223 (260)	156.3 (58.0)	−82.2 (27.8)	−150.9 (54.1)
128.0471	$3d^3(^2G)4s$	$^3G_5$	$3d^3(^2D2)4p$	$^3F^o_4$	3238 (691)	156.9 (70.2)	−83.2 (33.6)	−151.9 (65.5)
128.4109	$3d^3(^4P)4s$	$^5P_1$	$3d^3(^4P)4p$	$^5S^o_2$*	3251 (696)	142.1 (15.5)	−76.4 (8.3)	−138.3 (14.4)
128.5918	$3d^3(^4P)4s$	$^3P_1$	$3d^3(^2D2)4p$	$^3P^o_1$	3468 (53)	63.8 (10.6)	−38.5 (6.2)	−64.7 (9.8)
128.7046	$3d^3(^2G)4s$	$^1G_4$	$3d^3(^2D2)4p$	$^1F^o_3$*	3046 (593)	103.6 (67.3)	−57.5 (32.1)	−102 (62.7)
128.8169	$3d^3(^4P)4s$	$^5P_2$	$3d^3(^4P)4p$	$^5S^o_2$*	3054 (680)	142.8 (15.5)	−76.7 (8.3)	−138.9 (14.4)
129.1187	$3d^3(^4P)4s$	$^5P_2$						
129.3377	$3d^3(^2G)4s$	$^3G_3$	$3d^3(^2D2)4p$	$^3F^o_2$	2634 (239)	164 (83.5)	−86.7 (39.8)	−158.6 (77.8)
129.7547	$3d^3(^4P)4s$	$^5P_3$	$3d^3(^4P)4p$	$^5S^o_2$*	2296 (718)	145.4 (15.3)	−78 (8.3)	−141.3 (14.2)
130.0608	$3d^3(^4P)4s$	$^5P_3$	$3d^3(^2P)4p$	$^1D^o_2$	1391 (11)	105.2 (10.4)	−58.8 (6.3)	−103.9 (9.6)
130.2787	$3d^3(^4P)4s$	$^3P_2$	$3d^3(^2P)4p$	$^3P^o_2$	2425 (179)	83.7 (6.5)	−47.9 (4.7)	−83.3 (5.9)
131.1828	$3d^3(^2P)4s$	$^1P_1$	$3d^3(^2D2)4p$	$^1D^o_2$	1797 (267)	51.2 (21.8)	−32.9 (11.0)	−53.3 (20.3)
131.4492	$3d^3(^2D1)4s$	$^3D_3$	$3d^3(^2D1)4p$	$^3P^o_2$	2500 (119)	126.6 (12.4)	−69 (7.1)	−123.8 (11.5)
132.0410	$3d^3(^2H)4s$	$^3H_4$	$3d^3(^2H)4p$	$^3G^o_3$*	3183 (962)	114.2 (49.9)	−63.2 (24)	−112.3 (46.5)
132.1341	$3d^3(^2G)4s$	$^3G_4$	$3d^3(^2H)4p$	$^3H^o_5$	2508 (2)	52.2 (26.2)	−33.6 (13.0)	−54.3 (24.4)
132.1490	$3d^3(^2G)4s$	$^3G_5$	$3d^3(^2H)4p$	$^3H^o_6$	2453 (31)	60.1 (18.8)	−37.4 (9.7)	−61.8 (17.5)
132.1850	$3d^3(^2H)4s$	$^3H_4$	$3d^3(^2H)4p$	$^3G^o_4$	2819 (72)	93.4 (29.9)	−53.3 (14.7)	−92.9 (27.8)
132.3269	$3d^3(^2H)4s$	$^3H_5$	$3d^3(^2H)4p$	$^3G^o_4$	2971 (1)	97.4 (33.5)	−55.2 (16.4)	−96.6 (31.2)
132.5781	$3d^3(^2H)4s$	$^3H_5$	$3d^3(^2H)4p$	$^3G^o_5$	2874 (241)	94.2 (29.4)	−53.7 (14.5)	−93.6 (27.4)
132.7101	$3d^3(^2D2)4s$	$^1D_2$	$3d^3(^2P)4p$	$^1P^o_1$	3137 (7)	94.4 (19.2)	−53.4 (9.9)	−93.5 (17.9)
133.0401	$3d^3(^2H)4s$	$^3H_6$	$3d^3(^2H)4p$	$^3G^o_5$	2627 (226)	95.8 (30.3)	−54.5 (14.9)	−95.2 (28.2)
133.1185	$3d^3(^2D2)4s$	$^3D_1$	$3d^3(^2D2)4p$	$^3P^o_0$	3514 (389)	98.4 (36.2)	−55.7 (17.6)	−97.6 (33.7)
133.1640	$3d^3(^2D2)4s$	$^1D_2$	$3d^3(^2D2)4p$	$^1D^o_2$	2361 (28)	59.8 (32.0)	−37 (15.7)	−61.3 (29.8)
135.0535	$3d^3(^4P)4s$	$^3P_1$	$3d^3(^4P)4p$	$^3D^o_2$*	3430 (522)	67.5 (9.7)	−40.6 (6.0)	−68.5 (9.0)
135.1755	$3d^3(^4F)4s$	$^5F_1$	$3d^3(^4F)4p$	$^3D^o_2$	3369 (192)	101.4 (12.3)	−57.5 (7.1)	−100.6 (11.4)
135.3737	$3d^3(^2D2)4s$	$^3D_3$	$3d^3(^2P)4p$	$^3P^o_2$	2332 (100)	111.6 (10.1)	−62.1 (6.3)	−110 (9.3)
135.4847	$3d^3(^2F)4s$	$^1F_3$	$3d^3(^2F)4p$	$^1F^o_3$	2656 (83)	59 (32.0)	−36.8 (15.7)	−60.6 (29.8)
135.7675	$3d^3(^2F)4s$	$^3F_4$	$3d^3(^2F)4p$	$^3D^o_3$	2216 (110)	106.7 (27.8)	−59.8 (13.8)	−105.4 (25.9)
135.8567	$3d^3(^2D2)4s$	$^3D_1$	$3d^3(^2D2)4p$	$^3D^o_2$	2933 (241)	92.2 (6.7)	−52.9 (5.1)	−91.9 (6.1)
135.9006	$3d^3(^2D1)4s$	$^3D_3$	$3d^3(^2D1)4p$	$^3F^o_4$	3115 (142)	116.1 (4.8)	−64.3 (4.6)	−114.1 (4.2)
136.1447	$3d^3(^2F)4s$	$^1F_3$	$3d^3(^2F)4p$	$^1G^o_4$	2630 (47)	85.8 (11.5)	−49.5 (6.7)	−85.6 (10.7)
136.1825	$3d^3(^2F)4s$	$^3F_4$	$3d^3(^2F)4p$	$^3G^o_5$	3138 (124)	114.2 (7.7)	−63.4 (5.5)	−112.4 (7.1)
136.2864	$3d^3(^2D2)4s$	$^3D_3$	$3d^3(^2D2)4p$	$^3D^o_3$	2948 (153)	109.1 (13.1)	−61 (7.4)	−107.7 (12.2)
136.3077	$3d^3(^4F)4s$	$^5F_3$	$3d^3(^4F)4p$	$^5F^o_4$	3279 (157)	125.5 (14.7)	−69 (8.1)	−123.1 (13.6)
136.3642	$3d^3(^4F)4s$	$^5F_4$	$3d^3(^4F)4p$	$^5F^o_5$	3066 (133)	120.3 (7.2)	−66.5 (5.4)	−118.2 (6.6)
136.4824	$3d^3(^4F)4s$	$^5F_2$	$3d^3(^4F)4p$	$^3D^o_1$	1095 (18)	129.1 (30.3)	−70.7 (15.0)	−126.4 (28.2)
136.4984	$3d^3(^2F)4s$	$^3F_2$	$3d^3(^2F)4p$	$^3D^o_3$	1900 (112)	107.2 (27.3)	−60.1 (13.6)	−105.9 (25.4)
136.5115	$3d^3(^4F)4s$	$^5F_3$	$3d^3(^4F)4p$	$^3D^o_2$	2508 (197)	104.4 (12.4)	−59 (7.2)	−103.4 (11.5)
136.5571	$3d^3(^4F)4s$	$^5F_2$	$3d^3(^4F)4p$	$^5F^o_3$	4776 (74)	104 (24.9)	−58.7 (12.5)	−103 (23.2)
137.0303	$3d^3(^2H)4s$	$^3H_6$	$3d^3(^2H)4p$	$^1H^o_5$	2008 (28)	60 (39.4)	−37.7 (19.1)	−61.9 (36.7)
137.0947	$3d^3(^4F)4s$	$^5F_1$	$3d^3(^4F)4p$	$^5F^o_2$	4189 (87)	114.9 (28.7)	−64 (14.2)	−113.3 (26.7)
137.1987	$3d^3(^2D2)4s$	$^3D_1$	$3d^3(^2D2)4p$	$^3D^o_1$	1827 (175)	99.4 (10.2)	−56.4 (6.3)	−98.7 (9.4)
137.3587	$3d^3(^4F)4s$	$^5F_4$	$3d^3(^4F)4p$	$^5F^o_4$	2611 (166)	127.9 (14.7)	−70.2 (8.1)	−125.4 (13.6)
137.3967	$3d^3(^4P)4s$	$^3P_2$	$3d^3(^4P)4p$	$^3D^o_3$	1916 (68)	70.2 (15.1)	−42 (8.1)	−71 (14.0)
137.4116	$3d^3(^2F)4s$	$^3F_3$	$3d^3(^2F)4p$	$^3G^o_4$	2554 (128)	119.5 (6.3)	−66 (5.1)	−117.4 (5.7)
137.4789	$3d^3(^2D1)4s$	$^3D_2$	$3d^3(^2D1)4p$	$^3F^o_3$	2231 (179)	108.8 (12.0)	−60.9 (7.0)	−107.4 (11.1)
137.6337	$3d^3(^4F)4s$	$^5F_5$	$3d^3(^4F)4p$	$^5F^o_5$	2275 (149)	123.2 (7.2)	−68 (5.4)	−121 (6.6)
137.6455	$3d^3(^4F)4s$	$^5F_2$	$3d^3(^4F)4p$	$^5F^o_2$	3843 (88)	116.2 (28.8)	−64.6 (14.3)	−114.4 (26.8)
137.8560	$3d^3(^4P)4s$	$^5P_3$	$3d^3(^4P)4p$	$^5D^o_4$	3246 (143)	136.8 (6.1)	−74.5 (5.1)	−133.7 (5.5)
137.9040	$3d^3(^2G)4s$	$^3G_5$	$3d^3(^2G)4p$	$^1G^o_4$	2825 (304)	95.4 (25.6)	−54.6 (12.8)	−94.9 (23.9)
138.0112	$3d^3(^4F)4s$	$^5F_1$	$3d^3(^4F)4p$	$^5D^o_1$	3212 (187)	99 (29.6)	−56.5 (14.7)	−98.4 (27.6)
138.4055	$3d^3(^2P)4s$	$^3P_1$	$3d^3(^4P)4p$	$^3D^o_2$*	3245 (874)	83.7 (15.2)	−49 (8.3)	−84 (14.1)
138.5313	$3d^3(^4F)4s$	$^5F_1$	$3d^3(^4F)4p$	$^5D^o_0$	3209 (138)	98.7 (47.2)	−56.4 (22.8)	−98.2 (44.0)

TABLE IV. (*Continued.*)

λ (nm)	Lower state		Upper state		q (cm^{-1})	$\delta\nu_{54,56}$ (ms^{-1})	$\delta\nu_{57,56}$ (ms^{-1})	$\delta\nu_{58,56}$ (ms^{-1})
138.7938	$3d^3(^2H)4s$	$^3H_6$	$3d^3(^2H)4p$	$^3I_7^o$	3186 (136)	122.6 (13.9)	−67.6 (7.8)	−120.4 (12.9)
138.8195	$3d^3(^4P)4s$	$^5P_1$	$3d^3(^4P)4p$	$^3P_1^o$	3472 (126)	118.5 (8.1)	−65.8 (5.7)	−116.7 (7.4)
138.8328	$3d^3(^4P)4s$	$^5P_1$	$3d^3(^4P)4p$	$^5D_2^o$	3157 (94)	129.2 (5.3)	−70.9 (4.9)	−126.7 (4.7)
139.3073	$3d^3(^4P)4s$	$^5P_2$	$3d^3(^4P)4p$	$^5D_2^o$	2960 (78)	129.9 (5.3)	−71.3 (4.9)	−127.3 (4.7)
139.4272	$3d^3(^2G)4s$	$^3G_4$	$3d^3(^2G)4p$	$^3F_3^o$	2685 (205)	97.8 (26.8)	−55.8 (13.4)	−97.3 (24.9)
139.4665	$3d^3(^2G)4s$	$^3G_3$	$3d^3(^2G)4p$	$^3F_2^o$	2428 (171)	133.1 (59.8)	−72.6 (28.7)	−130.2 (55.8)
139.7106	$3d^3(^2P)4s$	$^3P_1$	$3d^3(^2P)4p$	$^3S_1^o$	3650 (479)	76.4 (13.8)	−45.7 (6.8)	−77.4 (13.0)
139.7972	$3d^3(^4P)4s$	$^5P_3$	$3d^3(^4P)4p$	$^5D_3^o$	2072 (272)	137.5 (6.1)	−74.9 (5.1)	−134.4 (5.5)
140.0243	$3d^3(^4F)4s$	$^3F_2$	$3d^3(^4F)4p$	$^3F_2^o$	2782 (95)	96.8 (27.4)	−54.8 (13.6)	−96 (25.5)
140.3370[a]	$3d^3(^2G)4s$	$^3G_4$	$3d^3(^2G)4p$	$^3F_4^o$	1745 (268)	99.2 (21.3)	−56.6 (10.4)	−98.7 (20.1)
140.4260	$3d^3(^4P)4s$	$^3P_0$	$3d^3(^2P)4p$	$^3D_1^o$	2018 (16)	87.8 (11.6)	−50.6 (6.8)	−87.6 (10.7)
140.6669	$3d^3(^4F)4s$	$^3F_4$	$3d^3(^4F)4p$	$^3F_4^o$	2352 (57)	86.9 (17.2)	−50.2 (9.1)	−86.8 (16)
140.7248	$3d^3(^2H)4s$	$^1H_5$	$3d^3(^2H)4p$	$^1I_6^o$	2587 (115)	89.2 (4.8)	−51.5 (4.6)	−89.1 (4.2)
140.8117	$3d^3(^4F)4s$	$^5F_1$	$3d^3(^4F)4p$	$^5F_2^o$	3299 (120)	110 (14.4)	−61.9 (8.1)	−108.8 (13.4)
140.9026	$3d^3(^4F)4s$	$^5F_3$	$3d^3(^4F)4p$	$^5D_2^o$	1339 (15)	114.4 (31.0)	−64 (15.3)	−112.9 (28.8)
140.9220	$3d^3(^4F)4s$	$^5F_4$	$3d^3(^4F)4p$	$^5D_3^o$	1585 (42)	101.4 (29.7)	−57.8 (14.7)	−100.8 (27.6)
141.6219	$3d^3(^2D2)4s$	$^1D_2$	$3d^3(^2D2)4p$	$^1F_3^o$*	2285 (601)	28.8 (15.3)	−22.8 (8.3)	−32.8 (14.2)
142.0602	$3d^3(^2G)4s$	$^3G_4$	$3d^3(^2G)4p$	$^3G_4^o$	2506 (77)	94.7 (24.3)	−54.6 (12.3)	−94.5 (22.7)
142.2481	$3d^3(^2P)4s$	$^3P_1$	$3d^3(^2P)4p$	$^3D_2^o$	3381 (73)	106.4 (5.4)	−60 (4.9)	−105.3 (4.8)
142.9004	$3d^3(^2G)4s$	$^3G_5$	$3d^3(^2G)4p$	$^3G_4^o$	2057 (83)	97.1 (25.2)	−55.8 (12.7)	−96.8 (23.5)
143.0309	$3d^3(^2F)4s$	$^1F_3$	$3d^3(^2F)4p$	$^1D_2^o$	2573 (79)	121.4 (41.6)	−66.9 (20.2)	−119.2 (38.8)
143.0573	$3d^3(^4F)4s$	$^5F_5$	$3d^3(^4F)4p$	$^5G_6^o$	3247 (131)	134.7 (13.0)	−73.8 (7.6)	−132 (12.1)
143.0751	$3d^3(^2D2)4s$	$^3D_3$	$3d^3(^4P)4p$	$^3D_3^o$	1823 (10)	99.2 (30.4)	−56.8 (15.0)	−98.7 (28.3)
144.0528	$3d^3(^4F)4s$	$^5F_4$	$3d^3(^4F)4p$	$^5G_5^o$	2704 (78)	136.4 (15.5)	−74.7 (8.5)	−133.6 (14.3)
144.0792	$3d^3(^4P)4s$	$^5P_1$	$3d^3(^4P)4p$	$^5P_2^o$	2635 (45)	106.6 (27.5)	−60.5 (13.8)	−105.8 (25.6)
144.1049	$3d^3(^4P)4s$	$^5P_3$	$3d^3(^4P)4p$	$^5P_3^o$	2565 (120)	94.7 (18.0)	−54.9 (9.6)	−94.7 (16.7)
144.2221	$3d^3(^2G)4s$	$^1G_4$	$3d^3(^2G)4p$	$^1H_5^o$	2608 (20)	101.7 (17.2)	−57.6 (9.2)	−100.9 (16.0)
144.6618[a]	$3d^3(^2G)4s$	$^3G_5$	$3d^3(^2G)4p$	$^3H_6^o$	3148 (106)	110.4 (24.2)	−62.1 (12.3)	−109.2 (22.5)
144.8494	$3d^3(^2G)4s$	$^1G_4$	$3d^3(^2G)4p$	$^1F_3^o$	3324 (21)	124.1 (40.1)	−68.3 (19.5)	−121.8 (37.3)
144.8846	$3d^3(^4F)4s$	$^5F_3$	$3d^3(^4F)4p$	$^5G_4^o$	2277 (59)	141.2 (14.3)	−77 (8.1)	−138.1 (13.3)
144.9928	$3d^3(^2F)4s$	$^3F_4$	$3d^3(^2F)4p$	$^3F_4^o$	2508 (183)	117 (8.5)	−65.4 (5.9)	−115.4 (7.8)
145.3618	$3d^3(^2H)4s$	$^1H_5$	$3d^3(^2H)4p$	$^1H_5^o$	2063 (26)	49.8 (45.4)	−33 (21.9)	−52.5 (42.3)
145.6161	$3d^3(^4F)4s$	$^5F_2$	$3d^3(^4F)4p$	$^5G_3^o$	1893 (54)	146.3 (12.3)	−79.5 (7.3)	−142.9 (11.4)
145.6285	$3d^3(^4P)4s$	$^5P_2$	$3d^3(^4P)4p$	$^5P_1^o$	1828 (58)	95.7 (13.9)	−55.4 (7.9)	−95.7 (12.9)
145.7727	$3d^3(^4P)4s$	$^5P_3$	$3d^3(^4P)4p$	$^5P_2^o$	1679 (66)	109.8 (27.5)	−62.2 (13.8)	−108.9 (25.6)
146.0726	$3d^3(^4F)4s$	$^5F_4$	$3d^3(^4F)4p$	$^5G_4^o$	1609 (68)	144 (14.5)	−78.4 (8.2)	−140.7 (13.4)
146.2631	$3d^3(^4F)4s$	$^5F_1$	$3d^3(^4F)4p$	$^5G_2^o$	1534 (48)	152 (9.5)	−82.2 (6.3)	−148.3 (8.7)
146.4876	$3d^3(^2F)4s$	$^3F_2$	$3d^3(^2F)4p$	$^3F_2^o$	1810 (108)	123.2 (12.4)	−68.4 (7.3)	−121.2 (11.5)
146.6649	$3d^3(^2G)4s$	$^3G_4$	$3d^3(^2G)4p$	$^3H_5^o$	1935 (112)	113.6 (22.7)	−63.8 (11.6)	−112.3 (21.1)
146.8911	$3d^3(^4F)4s$	$^5F_2$	$3d^3(^4F)4p$	$^5G_2^o$	1188 (49)	153.5 (9.6)	−83 (6.4)	−149.7 (8.8)
146.9000	$3d^3(^2H)4s$	$^3H_6$	$3d^3(^2H)4p$	$^3H_6^o$	2401 (110)	112.7 (29.8)	−63.4 (14.8)	−111.5 (27.8)
147.2098	$3d^3(^2H)4s$	$^3H_5$	$3d^3(^2H)4p$	$^3H_5^o$	2252 (89)	104.5 (21.6)	−59.6 (11.1)	−103.9 (20.1)
147.2512	$3d^3(^2H)4s$	$^3H_4$	$3d^3(^2H)4p$	$^3H_4^o$	2372 (57)	106 (27.0)	−60.2 (13.5)	−105.2 (25.1)
147.5604	$3d^3(^2G)4s$	$^3G_5$	$3d^3(^2G)4p$	$^3H_5^o$	1485 (105)	116.1 (22.1)	−65.1 (11.4)	−114.7 (20.6)
147.9471	$3d^3(^2G)4s$	$^3G_4$	$3d^3(^2G)4p$	$^3H_4^o$	1132 (44)	135.2 (10.5)	−74.2 (6.7)	−132.5 (9.7)
149.6266	$3d^3(^2G)4s$	$^1G_4$	$3d^3(^2G)4p$	$^3F_4^o$	1732 (209)	96.7 (26.6)	−55.6 (13.3)	−96.4 (24.7)
153.0439	$3d^3(^2D2)4s$	$^1D_2$	$3d^3(^2D2)4p$	$^1P_1^o$	1967 (251)	100 (44.4)	−57.4 (21.5)	−99.6 (41.4)
154.3234	$3d^3(^4F)4s$	$^3F_2$	$3d^3(^4F)4p$	$^3D_1^o$	901 (13)	118.7 (27.9)	−66.1 (13.9)	−117 (25.9)
155.4219	$3d^3(^4F)4s$	$^3F_4$	$3d^3(^4F)4p$	$^3D_3^o$	1234 (202)	108.3 (5.8)	−61.3 (5.2)	−107.4 (5.2)

[a]In [31], these lines are unresolved and could be misidentified.

mass numbers A and A', we can write

$$\lambda_{\rm obsv} = (1+z)\left[(1-P_{A'})\lambda_A + P_{A'}\lambda_{A'}\right], \qquad (10)$$

where z is the red shift, $P_{A'}$ is the isotopic abundance of isotope A', and λ_A and $\lambda_{A'}$ are the transition wavelengths assuming 100% abundance of isotopes A and A', respectively. Using Eq. (4), we may write this as

$$\frac{\Delta\lambda}{\lambda_A} = \frac{\lambda_{\rm obsv}-\lambda_A}{\lambda_A} = z - P_{A'}\frac{\delta\omega_{A',A}}{\omega_A}(1+z). \qquad (11)$$

Plotting $\Delta\lambda/\lambda_A$ versus $\delta\omega_{A',A}/\omega_A \equiv Q_{\rm IS}$ allows us to extract the abundance of isotope A' immediately. The range of $Q_{\rm IS}$

TABLE V. Calculated energies and q values (relative to the ground state $3d^6\ {}^5D_4$) and Landé g factors of $4s$ and $4p$ energy levels in Ni^{4+}.

Level		Energy		g factor		q (cm^{-1})
		CI + Σ	Expt. [25]	CI + Σ	LS	
$3d^5(^6S)4s$	$^7S_3$	161376	164526	1.9991	2	−6960
$3d^5(^6S)4s$	$^5S_2$	175638	178020	1.9985	2	−6447
$3d^5(^4G)4s$	$^5G_6$	206960	208046	1.3329	1.333	−7062
$3d^5(^4G)4s$	$^5G_5$	206965	208131	1.2665	1.2666	−7031
$3d^5(^4G)4s$	$^5G_2$	206820	208152	0.3360	0.3333	−7299
$3d^5(^4G)4s$	$^5G_4$	206930	208164	1.1503	1.15	−7091
$3d^5(^4G)4s$	$^5G_3$	206873	208165	0.9178	0.9166	−7195
$3d^5(^4P)4s$	$^5P_3$	212267	212096	1.6411	1.6667	−8160
$3d^5(^4P)4s$	$^5P_2$	212451	212253	1.7889	1.8333	−7860
$3d^5(^4P)4s$	$^5P_1$	212727	212456	2.4308	2.5	−7393
$3d^5(^4D)4s$	$^5D_4$	215975	216190	1.4871	1.5	−7159
$3d^5(^4D)4s$	$^5D_1$	216201	216435	1.5650	1.5	−6679
$3d^5(^4D)4s$	$^5D_2$	216469	216591	1.5398	1.5	−6265
$3d^5(^4D)4s$	$^5D_3$	216518	216596	1.5098	1.5	−6221
$3d^5(^4G)4s$	$^3G_5$	216442	217049	1.1994	1.2	−6723
$3d^5(^4G)4s$	$^3G_3$	216298	217101	0.7626	0.75	−6962
$3d^5(^4G)4s$	$^3G_4$	216431	217129	1.0621	1.05	−6709
$3d^5(^4P)4s$	$^3P_2$	221778	221088	1.4475	1.5	−7849
$3d^5(^4P)4s$	$^3P_1$	222149	222429	1.4014	1.5	−7136
$3d^5(^4D)4s$	$^3D_3$	225486	225201	1.3314	1.3333	−6770
$3d^5(^4D)4s$	$^3D_1$	225865	225545	0.5927	0.5	−6044
$3d^5(^4D)4s$	$^3D_2$	226048	225617	1.2088	1.1667	−5846
$3d^5(^2I)4s$	$^3I_6$	228688	229409	1.0252	1.0238	−7225
$3d^5(^2I)4s$	$^3I_5$	228624	229413	0.8357	0.8333	−7340
$3d^5(^2I)4s$	$^3I_7$	228804	229441	1.1429	1.1428	−6984
$3d^5(^2D3)4s$	$^3D_3$	233464	232546	1.2718	1.333	−8403
$3d^5(^2D3)4s$	$^3D_2$	233636	232656	1.0541	1.1667	−8239
$3d^5(^2D3)4s$	$^3D_1$	233948	232911	0.3490	0.5	−7838
$3d^5(^2I)4s$	$^1I_6$	233405	233839	1.0027	1	−7078
$3d^5(^4F)4s$	$^5F_5$	235539	234082	1.3931	1.4	−7340
$3d^5(^4F)4s$	$^5F_4$	235474	234125	1.3328	1.35	−7495
$3d^5(^4F)4s$	$^5F_3$	235590	234275	1.2302	1.25	−7232
$3d^5(^4F)4s$	$^5F_2$	235649	234413	0.9136	1	−7353
$3d^5(^2F1)4s$	$^3F_4$	236638	235421	1.2612	1.25	−6580
$3d^5(^2F1)4s$	$^3F_2$	236988	235737	0.9453	1	−6269
$3d^5(^4F)4s$	$^5F_1$	236450	236117	0.1604	0	−5828
$3d^5(^2F1)4s$	$^3F_3$	237751	236454	1.1382	1.08333	−5420
$3d^5(^2D3)4s$	$^1D_2$	240573	239108	0.9180	0.6667	−4743
$3d^5(^2F1)4s$	$^1F_3$	241603	240193	0.9904	1	−6201
$3d^5(^2H)4s$	$^3H_4$	241859	240960	0.8957	0.8	−7936
$3d^5(^2H)4s$	$^3H_5$	242009	241082	1.0978	1.0333	−7590
$3d^5(^2H)4s$	$^3H_6$	242951	241774	1.1631	1.16667	−6291
$3d^5(^2G2)4s$	$^3G_3$	243251	242290	0.8036	0.75	−6434
$3d^5(^2G2)4s$	$^3G_4$	243603	242504	0.9836	1.05	−6387
$3d^5(^6S)4p$	$^7P^o_2$	240905	242837	2.3276	2.3333	−5019
$3d^5(^2G2)4s$	$^3G_5$	243904	242863	1.1335	1.2	−5864
$3d^5(^4F)4s$	$^3F_2$	245147	243266	0.6806	0.6667	−6547
$3d^5(^4F)4s$	$^3F_4$	245028	243332	1.2041	1.25	−6892
$3d^5(^4F)4s$	$^3F_3$	245219	243371	1.0676	1.0833	−6517
$3d^5(^6S)4p$	$^7P^o_3$	241735	243609	1.9116	1.9166	−4272
$3d^5(^6S)4p$	$^7P^o_4$	243090	244901	1.7493	1.75	−2726
$3d^5(^2H)4s$	$^1H_5$	247646	246241	1.0072	1	−6190
$3d^5(^2G2)4s$	$^1G_4$	248295	247049	1.0600	1	−6125
$3d^5(^2F2)4s$	$^3F_3$	248495	247105	1.0845	1.08333	−6791
$3d^5(^2F2)4s$	$^3F_2$	248504	247165	0.6704	0.6667	−6690
$3d^5(^2F2)4s$	$^3F_4$	248806	247282	1.2127	1.25	−6167
$3d^5(^2F2)4s$	$^1F_3$	253353	251655	1.0033	1	−6483

TABLE V. (*Continued*.)

Level		Energy		g factor		
		CI + Σ	Expt. [25]	CI + Σ	LS	q (cm^{-1})
$3d^5(^6S)4p$	$^5P^o_3$	252631	253863	1.6699	1.666	−3726
$3d^5(^2S)4s$	$^3S_1$	256093	253905	1.9994	2	−6879
$3d^5(^6S)4p$	$^5P^o_2$	253294	254496	1.8365	1.833	−3143
$3d^5(^6S)4p$	$^5P^o_1$	253703	254885	2.4978	2.5	−2796
$3d^5(^2D2)4s$	$^3D_1$	266973	263701	0.5006	0.5	−6959
$3d^5(^2D2)4s$	$^3D_2$	267037	263736	1.1657	1.1667	−6841
$3d^5(^2D2)4s$	$^3D_3$	267155	263806	1.3310	1.333	−6614
$3d^5(^2D2)4s$	$^1D_2$	271824	268274	0.9996	1	−6622
$3d^5(^2G1)4s$	$^3G_5$	278280	274695	1.2000	1.2	−6976
$3d^5(^2G1)4s$	$^3G_4$	278290	274739	1.0500	1.05	−6928
$3d^5(^2G1)4s$	$^3G_3$	278290	274774	0.7507	0.75	−6890
$3d^5(^2G1)4s$	$^1G_4$	282992	279200	1.0002	1	−6774
$3d^5(^4G)4p$	$^5G^o_2$	284138	284216	0.3529	0.333	−4971
$3d^5(^4G)4p$	$^5G^o_3$	284206	284249	0.8936	0.9166	−4935
$3d^5(^4G)4p$	$^5G^o_4$	284319	284309	1.1246	1.15	−4835
$3d^5(^4G)4p$	$^5G^o_5$	284484	284403	1.2461	1.266	−4689
$3d^5(^4G)4p$	$^5G^o_6$	284749	284580	1.3171	1.333	−4397
$3d^5(^4G)4p$	$^5H^o_3$	286124	286294	0.5405	0.5	−5074
$3d^5(^4G)4p$	$^5H^o_4$	286614	286707	0.9385	0.9	−4480
$3d^5(^4G)4p$	$^5H^o_5$	287133	287127	1.1395	1.1	−4004
$3d^5(^4G)4p$	$^5H^o_6$	287727	287646	1.2262	1.214	−3160
$3d^5(^4P)4p$	$^5D^o_1$	289613	287756	0.7500	1.5	−4060
$3d^5(^4G)4p$	$^5F^o_5$	288106	287907	1.3754	1.4	−4216
$3d^5(^4G)4p$	$^5F^o_3$	288522	287960	1.2793	1.25	−4599
$3d^5(^4G)4p$	$^5H^o_7$	288175	288022	1.2853	1.285	−2911
$3d^5(^4G)4p$	$^5F^o_4$	288413	288162	1.3388	1.35	−4131
$3d^5(^4P)4p$	$^5S^o_2$	290418	288878	1.8675	2	−5098
$3d^5(^4G)4p$	$^5F^o_1$	288825	289163	0.7410	0	−5028
$3d^5(^4G)4p$	$^5F^o_2$	288627	289247	1.1612	1	−4974
$3d^5(^4P)4p$	$^5D^o_0$	289135	290262			−5601
$3d^5(^4P)4p$	$^5P^o_3$	292068	290757	1.5931	1.6667	−4083
$3d^5(^4G)4p$	$^3F^o_3$	291701	291329	1.1180	1.0833	−3713
$3d^5(^4P)4p$	$^5P^o_2$	292791	291390	1.7914	1.8333	−3576
$3d^5(^4P)4p$	$^5P^o_1$	293024	291542	2.3610	2.5	−3852
$3d^5(^4G)4p$	$^3F^o_4$	292101	291555	1.2688	1.25	−3273
$3d^5(^4G)4p$	$^3H^o_6$	292235	291891	1.1699	1.1667	−3681
$3d^5(^4G)4p$	$^3H^o_5$	292626	292353	1.0366	1.0333	−3403
$3d^5(^4G)4p$	$^3H^o_4$	292818	292631	0.8046	0.8	−3367
$3d^5(^4D)4p$	$^5F^o_2$	294870	294086	1.0694	1	−4169
$3d^5(^4D)4p$	$^5F^o_3$	295332	294443	1.2708	1.25	−3806
$3d^5(^4D)4p$	$^5F^o_4$	295953	294940	1.3604	1.35	−3147
$3d^5(^4D)4p$	$^5F^o_5$	296412	295444	1.3983	1.4	−2890
$3d^5(^4D)4p$	$^5D^o_3$	297672	296574	1.4912	1.5	−4770
$3d^5(^4G)4p$	$^3G^o_3$	297427	296847	0.7556	0.75	−3760
$3d^5(^4G)4p$	$^3G^o_4$	297564	296897	1.0547	1.05	−3532
$3d^5(^4D)4p$	$^5D^o_4$	297899	296919	1.4841	1.5	−4379
$3d^5(^4G)4p$	$^3G^o_5$	297689	296933	1.2018	1.2	−3399
$3d^5(^4D)4p$	$^5D^o_2$	298147	297014	1.5342	1.5	−4084
$3d^5(^4D)4p$	$^5D^o_1$	299204	297418	1.7653	1.5	−3511
$3d^5(^4D)4p$	$^5P^o_1$	298499	297983	1.9948	2.5	−3858
$3d^5(^4P)4p$	$^3D^o_1$	300187	298601	0.7187	0.5	−3362
$3d^5(^4D)4p$	$^3D^o_3$	301604	298972	1.4074	1.333	−2865
$3d^5(^4D)4p$	$^3D^o_2$	301654	300225	1.1698	1.1667	−2944
$3d^5(^4D)4p$	$^3D^o_1$	302123	300563	0.5256	0.5	−2333
$3d^5(^4D)4p$	$^3F^o_4$	302325	300918	1.2623	1.25	−3443
$3d^5(^4D)4p$	$^3F^o_3$	303003	301470	1.1439	1.0833	−2496
$3d^5(^4D)4p$	$^3F^o_2$	303042	301553	0.7569	0.6667	−2556

TABLE V. (*Continued*.)

Level		Energy		g factor		q (cm^{-1})
		CI + Σ	Expt. [25]	CI + Σ	LS	
$3d^5(^4P)4p$	$^3S_1^o$	305408	303250	1.9338	2	−4071
$3d^5(^2I)4p$	$^3K_6^o$	305928	305591	0.9153	0.857	−5915
$3d^5(^4D)4p$	$^3P_1^o$	307575	305838	1.5480	1.5	−3562
$3d^5(^2I)4p$	$^3K_7^o$	306455	305996	1.0651	1.01785	−5335
$3d^5(^2I)4p$	$^3I_5^o$	306418	306049	0.8876	0.8333	−5775
$3d^5(^2D1)4s$	$^3D_3$	313819	306963	1.3333	1.333	−7015
$3d^5(^2D1)4s$	$^3D_2$	313867	307025	1.1680	1.167	−6897
$3d^5(^2D1)4s$	$^3D_1$	313924	307105	0.5090	0.5	−6754
$3d^5(^2I)4p$	$^3I_6^o$	307816	307400	0.9987	1.0238	−4316
$3d^5(^2I)4p$	$^3K_8^o$	308713	308139	1.1250	1.125	−2908
$3d^5(^2I)4p$	$^3I_7^o$	308828	308317	1.0918	1.1428	−2802
$3d^5(^2I)4p$	$^1H_5^o$	309509	308804	0.9593	1	−3337
$3d^5(^2I)4p$	$^3H_6^o$	309855	309264	1.1352	1.16	−3882
$3d^5(^2I)4p$	$^1K_7^o$	310317	309744	1.0063	1	−3595
$3d^5(^2I)4p$	$^3H_5^o$	310625	309920	1.0278	1.0333	−3261
$3d^5(^2I)4p$	$^3H_4^o$	310654	309953	0.8102	0.8	−3711
$3d^5(^2D_3)4p$	$^3F_4^o$	312537	310213	1.2088	1.25	−4007

values for Fe^{4+} available from our calculations spans an interval of $\sim 6 \times 10^{-7}$. However, the errors in the laboratory wavelengths limit the accuracy of $\Delta\lambda/\lambda$ to $\sim 1 \times 10^{-5}$, thus rendering it insufficient to determine the isotopic abundances in this case. On the other hand, a laboratory accuracy of $\sim 1 \times 10^{-7}$ would allow for a determination of $P_{A'}$ to a level of ∼20%.

The observation of $3d$-$4p$ transitions may be another option for determining the isotope abundance. Such transitions would have energy intervals in the range of (150 000, 350 000) cm^{-1}, corresponding to wavelengths in the range of (30, 65) nm. These wavelength ranges are not within the range of observable wavelengths of the STIS. Nevertheless, we calculate the NMSs to be in the range of (−4000, −2500) GHz amu, while the SMSs are in the range of (10 000, 11 000) GHz amu. The corresponding volume shifts are of the order of ∼600 MHz fm^{-2}, making them insignificant for these transitions. The total shift between ^{56}Fe and ^{58}Fe is then about $\delta\nu_{58,56} \sim -5$ GHz. Compared to the $4s$-$4p$ transitions, this means that $\delta\nu_{3d\text{-}4p} \sim -5\delta\nu_{4s\text{-}4p}$, while $\nu_{3d\text{-}4p} \sim 2\nu_{4s\text{-}4p}$. Thus $\frac{\delta\nu}{\nu}|_{3d\text{-}4p} \sim -2.5\frac{\delta\nu}{\nu}|_{4s\text{-}4p}$. Therefore, these transitions would allow for the accurate determination of isotopic abundances when combined with the $4s$-$4p$ transitions presented here.

V. CONCLUSION

In closing, we have used spectral data from a white-dwarf system to explore the possible coupling of the variation of fundamental constants to a strong gravitational potential. Furthermore, we have shown how the differences in isotopic abundances relative to terrestrial abundances may be extracted. This information can be used to constrain models of the chemical evolution of our galaxy. Finally, we note that our results are limited by the uncertainties in the known terrestrial wavelengths of the transitions in both Fe^{4+} and Ni^{4+}, with much tighter limits possible using accurate laboratory data. Our work therefore provides a strong motivation for new laboratory measurements.

[1] V. V. Flambaum and E. V. Shuryak, AIP Conf. Proc. **995**, 1 (2008).

[2] J. Magueijo, J. D. Barrow, and H. B. Sandvik, Phys. Lett. B **549**, 284 (2002).

[3] V. V. Flambaum, Int. J. Mod. Phys. A **22**, 4937 (2007).

[4] J. D. Bekenstein, Phys. Rev. D **25**, 1527 (1982).

[5] H. B. Sandvik, J. D. Barrow, and J. Magueijo, Phys. Rev. Lett. **88**, 031302 (2002).

[6] J. D. Barrow, H. B. Sandvik, and J. Magueijo, Phys. Rev. D **65**, 063504 (2002).

[7] J. D. Barrow and S. Z. W. Lip, Phys. Rev. D **85**, 023514 (2012).

[8] N. Leefer, C. T. M. Weber, A. Cingöz, J. R. Torgerson, and D. Budker, Phys. Rev. Lett. **111**, 060801 (2013).

[9] N. Reid and G. Wegner, Astrophys. J. **335**, 953 (1988).

[10] S. P. Preval, M. A. Barstow, J. B. Holberg, and N. J. Dickinson, Mon. Not. R. Astron. Soc. **436**, 659 (2013).

[11] J. K. Webb, V. V. Flambaum, C. W. Churchill, M. J. Drinkwater, and J. D. Barrow, Phys. Rev. Lett. **82**, 884 (1999).

[12] V. A. Dzuba, V. V. Flambaum, and J. K. Webb, Phys. Rev. Lett. **82**, 888 (1999).

[13] J. K. Webb, M. T. Murphy, V. V. Flambaum, V. A. Dzuba, J. D. Barrow, C. W. Churchill, J. X. Prochaska, and A. M. Wolfe, Phys. Rev. Lett. **87**, 091301 (2001).

[14] M. T. Murphy, J. K. Webb, and V. V. Flambaum, Mon. Not. R. Astron. Soc. **345**, 609 (2003).

[15] J. K. Webb, J. A. King, M. T. Murphy, V. V. Flambaum, R. F. Carswell, and M. B. Bainbridge, Phys. Rev. Lett. **107**, 191101 (2011).

[16] J. A. King, J. K. Webb, M. T. Murphy, V. V. Flambaum, R. F. Carswell, M. B. Bainbridge, M. R. Wilczynska, and F. E. Koch, Mon. Not. R. Astron. Soc. **422**, 3370 (2012).
[17] J. C. Berengut, V. V. Flambaum, A. Ong, J. K. Webb, J. D. Barrow, M. A. Barstow, S. P. Preval, and J. B. Holberg, Phys. Rev. Lett. **111**, 010801 (2013).
[18] V. A. Dzuba, V. V. Flambaum, and J. K. Webb, Phys. Rev. A **59**, 230 (1999).
[19] C. Kobayashi, A. I. Karakas, and H. Umeda, Mon. Not. R. Astron. Soc. **414**, 3231 (2011).
[20] V. A. Dzuba, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A **54**, 3948 (1996).
[21] J. C. Berengut, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A **73**, 012504 (2006).
[22] W. R. Johnson and J. Sapirstein, Phys. Rev. Lett. **57**, 1126 (1986).
[23] W. R. Johnson, S. A. Blundell, and J. Sapirstein, Phys. Rev. A **37**, 307 (1988).
[24] J. C. Berengut, Phys. Rev. A **84**, 052520 (2011).
[25] J. Sugar and C. Corliss, J. Phys. Chem. Ref. Data **14** (Suppl. 2), 1 (1985).
[26] J. C. Berengut, V. A. Dzuba, and V. V. Flambaum, Phys. Rev. A **68**, 022502 (2003).
[27] J. C. Berengut, V. V. Flambaum, and M. G. Kozlov, J. Phys. B: At. Mol. Opt. **41**, 235702 (2008).
[28] J. C. Berengut, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A **72**, 044501 (2005).
[29] V. M. Shabaev, I. I. Tupitsyn, V. A. Yerokhin, G. Plunien, and G. Soff, Phys. Rev. Lett. **93**, 130405 (2004).
[30] K. Beloy and A. Derevianko, Comput. Phys. Commun. **179**, 310 (2008).
[31] J. O. Ekberg, Phys. Scripta **12**, 42 (1975).