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Nuclear-spin optical rotation in xenon

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The nuclear-spin optical rotation (NSOR) effect, which has potential applications in correlated nuclear-spin-resonance optical spectroscopy, has been explored earlier experimentally and theoretically in liquid Xe. Calculations of the Xe NSOR constant are very challenging because the result is sensitive to correlations, relativistic effects, and the choice of the basis, with strong cancellation between contributions from lowest and remaining states. The relativistic configuration-interaction many-body theory approach, presented here, is promising since this approach has been successful in predicting various properties of noble-gas atoms, such as energies, oscillator strengths (OSs), Verdet constants, and photoionization cross sections. However, correlations become stronger along the sequence of noble-gas atoms and theoretical accuracy in Xe is not as high as for example in neon and argon. To improve the accuracy of the Xe Verdet and NSOR constants, which are calculated as the explicit sums over the excited states, theoretical values for several lowest levels are replaced with empirical values of energies, OSs, and hyperfine structure constants. We found that Xe Verdet constant is in excellent agreement with accurate measurements. To take into account liquid effects, empirical data for energy shifts were also used to correct the NSOR constant. The resulting Xe NSOR constant is in a good agreement with experiment, although the liquid-state effect is treated quite approximately.

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I. INTRODUCTION

The optical detection of the nuclear magnetic resonance (NMR) signal based on the nuclear-spin optical rotation (NSOR) effect [1], as well as other optical-NMR phenomena [2], including frequency shift by circularly polarized light [3–10], is a promising method for realizing correlated optical-NMR spectroscopy and imaging. NSOR constants have been measured and calculated in various liquids [1, 11–15], including liquid Xe [1, 11]. It was found that results vary substantially depending on theoretical methods and that relativistic and correlation corrections are important [11] as well as the choice of the basis functions.

The Xe case is particularly interesting for theory. First, NSOR can be calculated using molecular and atomic structure computational methods for comparison, especially since atomic codes usually have more advanced treatment of relativistic and correlation effects for an atom. Second, experimental NSOR constants were measured for three substantially different wavelengths. This provides the basis for testing theoretical wavelength dependence. Third, the approximation of an isolated atom can be a good starting point, since van der Waals' interaction is fairly weak. In fact, as we will discuss later, the shift for the transitions that give large contributions to the NSOR effect measured in the visible range is quite small. Apart from this, NSOR experiments can be in future conducted with Xe gas to exclude liquid effects to enable precision test of theory. Fourth, relativistic effects and correlations within the atom are substantial and require careful treatment. Variation of results when relativistic and non-relativistic methods are compared is a clear indication of this [11]. Finally, experimental values of hyperfine constants and oscillator strengths of the lowest levels that give the dominant contributions to the NSOR effect have been measured, so not only theory can be tested but also *ab initio* results can be corrected with the empirical data, as we will demonstrate.

In this paper, the Xe NSOR constant is calculated with two particle-hole configuration-interaction many-body perturbation theory (CI-MBPT) methods: 1) full CI-MBPT and 2) CI-hole MBPT (CI-hMBPT), which is a truncated version of the first. Both methods are based on CI expansion of particle-hole states with inclusion of interactions of hole states with the core. Particle-hole excited states present additional difficulty to the theory because of poor convergence of MBPT for hole energies. MBPT needs to be modified from its standard form to include some large corrections that are present in single-double couple-cluster method and beyond [16]. The interaction of excited states with the core is included in full CI-MBPT, but not in CI-hMBPT. The CI-MBPT and CI-hMBPT have been successful in noble-gas atoms and gave energies and oscillator strengths (OSs) [17–19], g-factors [20], photo-ionization cross-sections [21], and Verdet constants [22] in agreement with experiment. From Ne to Xe accuracy deteriorates due to increase in correlation corrections. Because of this, in Xe CI-MBPT is no much more accurate than CI-hMBPT.

After explaining the theoretical methods in some detail, we will calculate Xe CI-MBPT and CI-hMBPT energies, OSs, hyperfine structure (HFS) constants, and NSOR constants. *Ab initio* NSOR constants will be corrected using empirical data for OSs and HFS constants. Finally, we will take into account liquid effects by modifying energies of two lowest states. The results will be compered with experiment and other theories.

II. METHOD

A. Particle-hole CI-MBPT

The particle-hole CI-MBPT method has been described and applied to calculations of properties of noble-gas atoms in previous work [16–20]. An orthogonal set of orbitals is introduced

$$\Phi_{JM}(av) = \sqrt{2J+1} \sum_{m_a,m_v} (-1)^{j_v - m_v} \times \begin{pmatrix} j_v & J & j_a \\ -m_v & M & m_a \end{pmatrix} a^\dagger_{vm_v} a_{am_a} \tag{1}$$

and the effective Hamiltonian for particle-hole states $H^{eft}_{v'a',va} = H^{(1)}_{v'a',va} + H^{(2)}_{v'a',va}$, where

$$H^{(1)} = \delta_{vv'}\delta_{aa'}(\epsilon_v - \epsilon_a) + \frac{1}{2J+1}(-1)^{j_v+j_a+J+1} Z_J(av'va'), \tag{2}$$

and $H^{(2)}$ is given in [16], is used to calculate eigenstates. Here v denotes a particle state and a denotes a hole state; for complete explanation of the method and notations the reader is referred to [16]. The second-order correction to the hole states is particularly important, and we provide separate calculations with CI-hMBPT. Beyond the Dirac-Hartree-Fock (DHF) approximation, relativistic effects are also included by adding Hartree-Fock hole Breit correction also defined in [16]. The states (i) are formed as linear combinations of the particle-hole orbitals,

$$\Psi_i = \sum_{av} C_i(av)\Phi_{JM}(av) \tag{3}$$

and reduced matrix elements are calculated between these states. For example, the reduced matrix element of r is

$$r_i = \sum_{av} C_i(av)\langle a||r||v\rangle(-1)^{j_a - j_v} \tag{4}$$

B. B-spline basis

To obtain the basis, first the DHF equation is solved for the Xe ground state to obtain the DHF potential. Then B-spline expansion of the ground and excited states is obtained by solving the DHF equation for an atom in a cavity, with the size chosen to minimize distortion of the lowest atomic states and to achieve completeness of the basis with relatively small number of splines, 40. It has been shown that such bases are accurately complete and MBPT implementations that involve summation over basis function states provide high precision. In order to test the convergence of the results with the basis, we compared NSOR calculations using the cavity radii of 60 atomic units (a.u.) and 40 a.u. and the number of particle-hole states 28, 122, and 152. Configurations (the case of 122) were chosen as follows: $5p^{-1}_{1/2}ns$, $5p^{-1}_{3/2}ns$, $5p^{-1}_{1/2}nd_{3/2}$, $5p^{-1}_{3/2}nd_{3/2}$, $5p_{3/2}nd_{5/2}$ with n up to 26, and $5s^{-1}np_{1/2}$ $5s^{-1}np_{3/2}$ with n up to 12, included. After comparison of various cases, we found that the cavity $R = 40$ a.u. and 122 configurations were optimal.

C. NSOR formula with explicit summation

The Xe NSOR constant is calculated using third-order perturbation-theory expression with explicit summation over intermediate excited states:

$$\phi = -\frac{2\pi l\omega N}{nc}(\alpha^{(1)}_v + \alpha^{(1)}_v)I_z \tag{5}$$

$$\alpha^{(1)}_v I_z = \frac{2\omega r_e c^2}{\hbar} \sum_k \frac{f_k a_k}{(\omega_k^2 - \omega^2)^2} I_z, \tag{6}$$

$$\alpha^{(2)}_v I_z = \frac{2\omega r_e c^2}{3\hbar} \sum_{i\neq j} \frac{r_i r_j(\omega_i + \omega_j)a_{ij}}{(\omega_i^2 - \omega^2)(\omega_j^2 - \omega^2)} I_z, \tag{7}$$

where ϕ is the light polarization rotation angle in rad, I_z average nuclear spin along the quantization axis, α_v is the vector polarizability, with the superscripts denoting either single or double sum parts, ω is the light frequency, f_k are oscillator strengths between the ground and excited states k, n is the refractive index, a_k is the hyperfine coupling coefficient defined with $H_k^{hf} = a_k J \cdot I$, a_{ij} are the corresponding off-diagonal matrix elements. This expression can be derived using formalism developed in [23], where instead of three photon absorption, we use the absorption of one photon with frequency ω, then absorption of one hyper-fine "photon" with zero frequency, and emission of photon with frequency ω and the reverse process where the photon is first emitted and then absorbed. The Verdet constant, as well as the NSOR constant, is also proportional to the difference between the refractive index of positive and negative circularly polarized photons, so there will be corresponding diagrams of these types. Note that the third-order term with double summation $\alpha_v^{(2)}$ was neglected in [1]. Although this term is expected to be small, owing to strong cancellation between low- and high-energy contributions, it is still important to evaluate it. In case of the Verdet constant, the equation contains the off-diagonal magnetic-dipole moment matrix elements. In non-relativistic approximation, many off-diagonal hyperfine matrix elements disappear due to the fact that the summation is carried out over the singlet states and the hyperfine operator can be reduced to L/r^3, where L is the angular momentum operator. In the case of the Verdet constant, all non-diagonal matrix elements vanish and the Verdet constant becomes proportional to the frequency derivative of the refractive index. With this approach of explicit summation and separation of the diagonal contribution, it is possible not only to analyze contributions from various states and estimate the accuracy of the theory from comparison with the available data for f_k, a_k, and ω_k, but also to make corrections using the experimental data. Furthermore, effects of interatomic interactions can be included from external data: changes in OSs from gas to liquid, changes in transition energies and broadening. Below we will demonstrate how the results can be corrected using experimentally available transition energies [24].

D. Results

We used CI-MBPT and CI-hMBPT methods to calculate Xe energies, OSs, HFS and Verdet constants, and finally NSOR constants from Eq.5. Table I shows the compilation of energies, OSs, HFS constants calculated with CI-hMBPT and CI-MBPT methods for four lowest J=1 odd states. Since hole energies are the main contributor to the particle-hole energy of states and are strongly correlated with core states, they are calculated beyond regular second-order MBPT, with modified MBPT [16], as we discussed above. It can be observed that energies calculated with both CI-hMBPT and CI-MBPT agree well with experiment, with the average deviation of a few percent, with energies being slightly overestimated by CI-hMBPT and underestimated by CI-MBPT. In the case of OSs, there are many measurements (a compilation is given in Ref.[25]) that substantially disagree, so for comparison we averaged the measured values listed in Ref.[25]. Theoretical values show agreement with experiment for strong transitions, but the agreement is of qualitative nature for weaker transitions. This is quite expected taking into account limited precision of theory to which weak transitions are more sensitive and does not affect much the accuracy of the NSOR calculations because their contributions are small. Calculations of HFS constants also show agreement with experiment, especially taking into account their strong sensitivity to correlations. To further improve accuracy, it can be important to use all-order methods, such as coupled-cluster single-double method with energy adjusted pseudo potential and perturbatively added triple excitations[26] (note that some technical difficulties might exist with this method in calculations of hyper-fine matrix elements). Although semi-empirical methods were quite successful in Xe [27], they were applied to lowest states without giving a complete basis set required in NSOR calculations with Eq.5.

The Verdet constant is calculated similarly as the NSOR constant, with the third order expression that involves summation over excited states, including continuum. Effectively, HFS matrix elements are replaced with g-factors or magnetic-dipole matrix elements. In non-relativistic case the summation is over singlet states due to the fact that singlet-triplet transitions are forbidden. In addition it is possible to calculate the refractive index for a given frequency and from its derivative obtain the Verdet constant [28]:

$$V = 1.024 \times 10^6 \omega \frac{dn}{d\omega}. \tag{8}$$

Here the Verdet constant has units of μmin Oe^{-1} cm^{-1} at STP. In Table II we listed the relativistic results. In addition to purely *ab initio* values we replaced OSs and energies for four first excited levels to improve accuracy using experimental values. This replacement procedure led to more consistent agreement between CI-MBPT and CI-hMBPT Verdet constants. Also after the addition of off-diagonal contributions, the agreement of both CI-MBPT and CI-hMBPT calculations with experiment became very close, especially at 1064 nm, at which precise measurements were recently reported [29]. Previously, the Verdet constant calculated with the CI-hMBPT method for He,Ne, Ar, Kr, and Xe [28] using only the diagonal contribution (single sum) showed very good agreement for lighter atoms, which is expected from the smallness of correlations and relativistic effects.

After investigating Verdet constants, we calculated NSOR constants using both CI-MBPT and CI-hMBPT methods. In addition, similarly as in the case of the Verdet constant, we replaced energies and OSs and HFS constants for the lowest excited states that give dominant contribution. The results are presented in Table III. We also show the contribution from the lowest four excited states to give an idea of strong cancellation between this part and the rest. Due to the cancellation the results are quite different between CI-MBPT and CI-hMBPT even after additional empirical corrections and adding off-diagonal contributions. This is quite unlike the case of the Verdet constant. This is not surprising because even larger variation was observed between theoretical methods in [11] (Table IV).

Liquid Xe posses further complications for theory. Not only energies, OSs and HFS constants are expected to be significantly different but also the error in the NSOR constant calculations due to overall uncertainty in them is amplified by strong cancellation, as in an isolated Xe atom. Because the NSOR constant depends on energies of the excited states very sharply, we attempted to take into account liquid effects by replacing identifiable energy shifts in the solid Xe at 53 K given in [24]. We chose to use the data at the highest available temperature, 53 K, because the solid state approaches the liquid state when temperature is raised. To some extent, using empirical data for solid Xe is a better approximation for liquid Xe than using a dimer [11], which takes into account only the interaction with one atom. Ideally it is desirable to replace not only energies, but also OSs and HFS constants, but these data are not available. Nevertheless, it seems that the empirical corrections for liquid effects attempted here bring the results in closer agreement with the experiment (Table V). Further reduction in the NSOR constant about 1.4 times is also included due to the refractive index n according to Eq.5. Since we did not find the value of n for different wavelengths in liquid Xe in the literature, we estimated it in the long wavelength limit from a known dielectric constant and then used theoretical calculations to extrapolate n to different wavelengths. With energy shift and refractive index corrections, we find that the average value of CI-MBPT and CI-hMBPT NSOR constants agrees well with the experimental measurements for all measured wavelength. Although such agreement could be coincidental, the refractive index reduction is estimated quite accurately, and the factors due to other liquid-state effects, such as changes in OSs, hyperfine matrix elements, and energies of higher excited states, can be considered to have uncertainty of 100%. The variation between CI-MBPT and CI-hMBPT results gives the estimate of accuracy of our result as being 50%, which is not much influenced by uncertainty arising from liquid effects. Because the trend is well reproduced, it becomes possible to extrapolate experimental values to different wavelength with better accuracy then theoretical uncertainty for absolute values. For example, at 405 nm, we predict that the NSOR constant is -2.2$\pm$0.5$\times 10^{-5}$ rad/M/cm. It is also interesting to note that the absorption peak shifts in the solid Xe depend on temperature and hence some variation of results is expected for liquid itself. This is a clear indication of sensitivity of the NSOR effect to the structure properties of liquid, and this sensitivity can be used to study the liquid structure. Apart from our empirical analysis based on energy shifts, in Ref.[11] a theoretical estimate based on dimers was made that liquid effects reduce the NSOR constant by 35-45%, which is consistent with the calculations we presented here.

In general, one conclusion can be made that in order to have more stringent test of theory, it is important to conduct measurements of the NSOR constant in gas. This should be quite possible, since liquid experiment was done with only 1 cc of 3%-polarized Xe, while much longer path length and higher polarization can be used with hyper polarized Xe gas. On the other hand, liquid Xe can be further experimentally studied to obtain energies and OSs; however, the hyperfine constant is hard to extract due to broadening. Most likely path is to elaborate theory for Xe liquid and test it against the absorption spectrum. Then the theoretical values can be substituted for example in our calculations to take into account liquid effects.

III. CONCLUSION

In this paper we calculated the Xe Verdet and NSOR constants (both for gas and liquid) using relativistic mixed configuration-interaction many-body perturbation theory. The theory was tested by comparison of energies, OSs, and HFS constants with experiment. Energies are in good agreement, while OSs and HFS constants have substantial deviations. Nevertheless, we refined our Verdet and NSOR constant calculations in vacuo by replacing energies and OSs of four and HFSs of three lowest odd excited states of J=1 with experimental values. The replacement of energies and OSs leads to an excellent agreement for the Verdet constant of Xe gas calculated with both CI-MBPT and CI-hMBPT methods. Furthermore, using the NSOR explicit summation formula, we replaced energies of two lowest $J = 1$ odd states with those in solid Xe at 53K and divided results by the refractive index to estimate the NSOR constant in liquid Xe. The result was found in good agreement with experiment, although the theoretical error is about 50%. One conclusion can be made that the approach of using explicit summation and experimental values works and can be further refined by using experimental and theoretical data: measured absorption peaks in liquid Xe, absolute measurements of absorption coefficients or OSs, HFS constant calculations. Finally, to verify theoretical methods at higher level of precision, it would be important to conduct measurements using hyperpolarized Xe gas.

TABLE I: Comparison of theoretical and experimental energies (atomic units), OSs (dimensionless), and HFS constants (HFSC)(MHz) of relevant odd $J = 1$ states that enter Eq.5.

Levels	$6s[3/2]$	$6s'[1/2]$	$5d[1/2]$	$5d[3/2]$
CI-hMBPT energy	0.3253	0.3617	0.3790	0.3957
CI-MBPT energy	0.2957	0.3356	0.3511	0.3802
NIST energy	0.3100	0.3517	0.3644	0.3822
NIST-CI-MBPT Diff.	0.0144	0.0161	0.0134	0.0020
OS CI+hMBPT	0.241	0.214	0.059	0.266
OS CI-MBPT	0.318	0.266	0.044	0.752
OS expt. Avr.	0.253	0.200	0.012	0.385
HFSC CI-hMBPT	-901	-2940	-4376	415
HFSC CI-MBPT	-560	-3950	-3989	437
HFSC expt	-963	-5793	-2421	

TABLE II: Comparison of CI-MBPT and CI-hMBPT (only hole states contain MBPT corrections) theoretical Verdet constants (micromin/Oe/cm) with experiment: Σ_{122} is obtained with the summation over 122 particle-hole states, $+\Sigma_4^{E-T}$ with energies and OSs replaced with experimental for four lowest states; $+\Sigma_{i\neq j}$ with the double summation non-diagonal contribution. Experimental Verdet constants are obtained using the empirical formula given in Ref. [30]; in addition, for 1064 nm two accurate measurements are also listed, [a] [31] and [b] [29].

$\lambda(nm)$	CI-MBPT			CI-hMBPT			Expt.
	Σ_{122}	$+\Sigma_4^{E-T}$	$+\Sigma_{i\neq j}$	Σ_{122}	$+\Sigma_4^{E-T}$	$+\Sigma_{i\neq j}$	
300	337	247	208	209	233	195	247
350	221	164	138	140	155	130	151
405	153	115	97	99	109	92	100
488.8	98	75	63	65	71	60	63
505	91	70	59	60	66	55	58
514.5	87	67	57	58	63	53	55
532.0	81	62	52	54	59	50	51
589	65	50	42	43	47	39	41
694.3	45	35	30	30	33	28	28
770	37	28	24	25	27	23	22
1064	18.6	14.1	12.1	12.6	13.7	11.5	11
							11.9 ± 0.1^a
							12.2 ± 0.3^b

IV. ACKNOWLEDGEMENT

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TABLE III: Theoretical in vacuo CI-MBPT and CI-hMBPT NSOR constants (rad/M/cm): Σ_4 obtained with the summation over 4 lowest states; Σ_{122} - with summation over 122 states, $+\Sigma_4^{E-T}$ with energies, OSs, and hyperfine constants replaced with experimental for four (three, in case of HFS constants) lowest states; $+\Sigma_{i\neq j}$ with the double summation non-diagonal contribution

	CI-MBPT				CI-hMBPT		
$\lambda(nm)$	Σ_4	Σ_{122}	$+\Sigma_4^{E-T}$	$+\Sigma_{i\neq j}$	Σ_{122}	$+\Sigma_4^{E-T}$	$+\Sigma_{i\neq j}$
300	4.59[-4]	-3.52[-5]	-8.28[-5]	-1.05[-4]	-1.26[-4]	2.25[-5]	4.11[-6]
350	2.91[-4]	-5.58[-5]	-8.18[-5]	-8.60[-5]	-1.06[-4]	-1.26[-5]	-3.15[-6]
405	1.97[-4]	-5.38[-5]	-6.96[-5]	-6.76[-5]	-8.49[-5]	-2.18[-5]	-6.11[-6]
488.8	1.24[-4]	-4.32[-5]	-5.28[-5]	-4.86[-5]	-6.12[-5]	-2.16[-5]	-6.52[-6]
505	1.15[-4]	-4.12[-5]	-4.95[-5]	-4.52[-5]	-5.78[-5]	-2.11[-5]	-6.42[-6]
514.5	1.10[-4]	-4.01[-5]	-4.79[-5]	-4.36[-5]	-5.58[-5]	-2.07[-5]	-6.33[-6]
532.0	1.02[-4]	-3.81[-5]	-4.53[-5]	-4.10[-5]	-5.25[-5]	-2.00[-5]	-6.16[-6]
589	8.07[-5]	-3.23[-5]	-3.78[-5]	-3.37[-5]	-4.34[-5]	-1.77[-5]	-5.55[-6]
694.3	5.62[-5]	-2.43[-5]	-2.79[-5]	-2.45[-5]	-3.17[-5]	-1.38[-5]	-4.41[-6]
770	4.49[-5]	-2.01[-5	-2.29[-5]	-1.99[-5]	-2.60[-5]	-1.17[-5]	-3.78[-6]
1064	2.28[-5]	-1.09[-5]	-1.23[-5]	-1.06[-5]	-1.34[-5]	-6.55[-6]	-2.15[-6]

TABLE IV: Comparison of current and previous theoretical in vacuo NSOR constants ($10^5\times$rad/M/cm)

Method \ λ(nm)	1064	770	532
DFT/BLYP NR	2.39	4.85	11.71
DFT/BLYP R	1.79	3.67	9.03
DFT/B3LYP NR	1.76	3.57	8.59
DFT/B3LYP R	1.21	2.49	6.16
DFT/BHandHLYP NR	1.17	2.39	5.76
DFT/BHandHLYP R	0.68	1.42	3.59
HF NR	0.74	1.51	3.71
HF R	0.35	0.76	2.04
NR CCSD	1.29	2.60	6.17
CI-hMBPT $\Sigma_{122}+\Sigma_4^{E-T}$	0.66	1.17	2.00
CI-MBPT $\Sigma_{122}+\Sigma_4^{E-T}$	1.23	2.29	4.53
CI-hMBPT $\Sigma_{122}+\Sigma_4^{E-T}+\Sigma_{i\neq j}$	0.22	0.38	0.62
CI-MBPT $\Sigma_{122}+\Sigma_4^{E-T}+\Sigma_{i\neq j}$	1.06	1.99	4.53

TABLE V: Calculations of the NSOR constant for liquid Xe using corrections for energy shifts of the two lowest levels observed in solid Xe at 53K "E2 liq." and dividing the result by the refractive index, "E2 liq./n". The refractive index in the long wavelength limit is obtained from the experimental dielectric constant; the frequency dependence is obtained theoretically. As it can be seen, significant reduction of the NSOR constant is observed compared to in vacuo values. CI-MBPT and CI-hMPBT calculations are compared. The average of these is given as the final theoretical result with error bar computed from the difference for comparison with experiment. Agreement with experiment for average can be observed, and theory can be used to predict the NSOR constant at different wavelengths with uncertainty roughly equal to the experimental error bar at 532 nm, that is 20%. this agreement should be treated with caution because the energy shifts of solid Xe instead of liquid Xe were used and oscillator strength as well as hyperfine constants were assumed unchanged by van-der Waalse interactions. It might be also the case that the energy shifts themselves depend on the conditions of liquid Xe.

		CI-hMBPT			CI-MBPT				
λ (nm)	n	in vacuo	E2 liq.	E2 liq./n	in vacuo	E2 liq.	E2 liq./n	Th. Avr.	Expt.
300	1.46	0.41	-0.78	-0.54	-10.48	-8.44	-5.78	-3.2±1.9	
350	1.45	-0.31	-0.01	0.00	-8.60	-7.37	-5.08	-2.5±1.8	
405	1.43	-0.61	-0.38	-0.27	-6.76	-5.96	-4.17	-2.2±1.4	
488.8	1.42	-0.65	-0.50	-0.35	-4.86	-4.32	-3.05	-1.7±1.0	
505.0	1.42	-0.64	-0.50	-0.35	-4.52	-4.06	-2.86	-1.6±0.9	
514.5	1.42	-0.63	-0.50	-0.35	-4.36	-3.93	-2.77	-1.6±0.9	
532	1.42	-0.62	-0.49	-0.35	-4.10	-3.69	-2.60	-1.5±0.8	1.5±0.3
589	1.41	-0.55	-0.47	-0.33	-3.37	-3.05	-2.17	-1.3±0.7	
694.3	1.41	-0.44	-0.37	-0.27	-2.45	-2.23	-1.58	-0.9±0.5	
770	1.41	-0.38	-0.32	-0.23	-1.99	-1.83	-1.29	-0.8±0.4	0.6±0.2
1064	1.41	-0.22	-0.19	-0.13	-1.06	-0.97	-0.69	-0.4±0.2	0.4±0.2

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