TaN molecule as a candidate for the search for a *T,P*-violating nuclear magnetic quadrupole moment

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It is demonstrated that the TaN molecule is the best candidate to search for a *T,P*-violating nuclear magnetic quadrupole moment (MQM), and it looks promising for the search for other *T,P*-odd effects. We report results of coupled-cluster calculations of *T,P*-odd effects in TaN produced by the Ta nucleus MQM, electron electric dipole moment (EDM), and scalar-pseudoscalar nucleus-electron interactions, as well as of the molecule-axis hyperfine structure constant and dipole moment. Nuclear calculations of ^{181}Ta MQM are performed to express the *T,P*-odd effect in terms of the strength constants of *T,P*-odd nuclear forces, proton and neutron EDM, QCD parameter θ, and quark chromo-EDM.

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I. INTRODUCTION

During the last few years low-energy experiments on heavy atoms and diatomic molecules containing heavy atoms have proved to be very important for the search for new physics beyond the standard model [1–3]. The best limit on the electron electric dipole moment (*e*EDM) was obtained on the ThO molecular beam in Ref. [3]. The experiment was also sensitive to another effect that violates time-reversal (T) and parity symmetries (P): scalar-pseudoscalar nucleus-electron neutral current interactions [4]. If a heavy atom has nuclear spin $I > 1/2$ one can expect that the molecule will also be sensitive to another *T,P*-odd effect, the *T,P*-odd interaction of the nuclear magnetic quadrupole moment (MQM) with electrons [5–7]. Important ideas on the subject were suggested in Refs. [5–11].

There are a number of systems on which experiments to search for *T,P*-odd effects have already been conducted or suggested and that have been investigated theoretically and experimentally: HfF^+ [12–18], YbF [2,19–25], ThO [3,26–31], ThF^+ [13,32], WC [33,34], PbF [35–38], RaO [39,40], RaF [41,42], PtH^+ [16,43], etc.

Recently, the TaN molecule was suggested as a new system to search for the *T,P*-odd MQM of the tantalum nucleus [44], where the molecule was marked as a quite promising candidate to search for *T,P* violation in the nuclear sector using molecules. Indeed, the ^{181}Ta nucleus is stable and its MQM is strongly enhanced due to the collective effect [7]; the large nuclear charge Z of Ta leads to a higher than Z^2 electron enhancement of the *T,P*-odd effects [5,6,9,11], and TaN in the $^3\Delta_1$ state has Ω doublets which allow full polarization in a small electric field and cancellation of many systematic errors due to opposite signs of the effects on the doublet components [11,45], a very small magnetic moment due to cancellation of the orbital and spin contributions [16], and a long lifetime of the $^3\Delta_1$ electron state [44].

The TaN molecule has the triple bond order, i.e., higher than in some other recently experimentally considered systems used to search for *T,P*-violation effects, e.g., the ThO molecule [3]. This suggests a rather complicated electronic structure in terms of electron correlation effects. Up to now the molecule was rather poorly investigated both experimentally and theoretically [44,46]. There are no experimental data about the molecule-frame dipole moment, hyperfine structure, etc. Therefore, the aim of the present paper is to perform the first reliable *ab initio* treatment of the TaN electronic structure in the $^3\Delta_1$ state including different *T,P*-violating effects. Also we provide the values of the molecule-frame dipole moment and molecule-axis hyperfine structure constant, which can be important for experimental planning and determination of the quantities and acceleration of further experimental treatment of the system. To solve the problem we have developed a pure *ab initio* scheme of the calculation where electron correlation effects were considered within the most accurate all-order coupled-cluster method, in which we took account of up to quadruple cluster amplitudes.

A spin-dependent *T,P*-odd Hamitonian can be expressed in the following form [47,48]:

$$H^{T,P} = H^{\mathrm{SP}} + H^{d} + H^{\mathrm{MQM}}. \tag{1}$$

The *T,P*-odd scalar-pseudoscalar nucleus-electron Hamiltonian H^{SP} with a characteristic dimensionless constant k_{SP} is given by [49]

$$H^{\mathrm{SP}} = i\frac{G_F}{\sqrt{2}} Z k_{\mathrm{SP}} \gamma_0 \gamma_5 \rho_N(\mathbf{r}), \tag{2}$$

where Z is the heavy nucleus charge, G_F is the Fermi-coupling constant, γ_0 and γ_5 are the Dirac matrices, and $\rho_N(\mathbf{r})$ is the nuclear density normalized to unity. For the interaction of *e*EDM with inner molecular electric field $\boldsymbol{E}$, one has

$$H^{d} = 2d_e \begin{pmatrix} 0 & 0 \\ 0 & \boldsymbol{\sigma E} \end{pmatrix}, \tag{3}$$

where d_e is the value of *e*EDM and $\boldsymbol{\sigma}$ are the Pauli matrices. The Hamiltonian of the interaction of MQM with electrons is

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given by [47,50]

$$H^{\rm MQM} = -\frac{M}{2I(2I-1)} T_{i,k} \frac{3}{2} \frac{[\boldsymbol{\alpha}\times\boldsymbol{r}]_i r_k}{r^5}, \quad (4)$$

where Einstein's summation convention is implied, $\boldsymbol{\alpha}$ are the 4×4 Dirac matrices, $\boldsymbol{\alpha} = \left(\begin{smallmatrix} 0 & \sigma \\ \sigma & 0 \end{smallmatrix}\right)$, $\boldsymbol{r}$ is the displacement of the electron from the Ta nucleus, $\boldsymbol{I}$ is the nuclear spin, and M is the nuclear MQM,

$$M_{i,k} = \frac{3M}{2I(2I-1)} T_{i,k}, \quad (5)$$

$$T_{i,k} = I_i I_k + I_k I_i - \frac{2}{3}\delta_{i,k} I(I+1). \quad (6)$$

In the subspace of $\pm\Omega$ states ($\Omega = \langle\Psi|\boldsymbol{J}\cdot\boldsymbol{n}|\Psi\rangle$, $\boldsymbol{J}$ is the total electronic momentum, Ψ is the *electronic* wave function for the considered $^3\Delta_1$ state of TaN) the expressions (2)–(4) are reduced to the following effective molecular Hamiltonians, correspondingly [5]:

$$H^{\rm SP}_{\rm eff} = W_{\rm SP} k_{\rm SP} \mathbf{S}'\cdot\mathbf{n}, \quad (7)$$

$$H^{d}_{\rm eff} = W_d d_e \mathbf{S}'\cdot\mathbf{n}, \quad (8)$$

$$H^{\rm MQM}_{\rm eff} = -\frac{W_M M}{2I(2I-1)} \boldsymbol{S}'\hat{\boldsymbol{T}}\mathbf{n}, \quad (9)$$

where $\mathbf{n}$ is the unit vector along the molecular axis ζ directed from Ta to N, and $\boldsymbol{S}'$ is the effective electron spin [51] defined by the following equations: $\mathbf{S}'_\zeta|\Omega\rangle = \Omega|\Omega\rangle$, $\mathbf{S}'_\pm|\Omega=\pm 1\rangle = 0$ [47,48], $S{=}|\Omega|{=}1$.

To extract the fundamental parameters $k_{\rm SP}$, d_e, and M from an experiment one needs to know the factors $W_{\rm SP}$, W_d, and W_M, correspondingly, which are determined by the electronic structure of a studied molecular state on a given nucleus (discussed in Refs. [44,47,51,52]):

$$W_{\rm SP} = \frac{1}{\Omega}\langle\Psi|\sum_i \frac{H^{\rm SP}(i)}{k_{\rm SP}}|\Psi\rangle, \quad (10)$$

$$W_d = \frac{1}{\Omega}\langle\Psi|\sum_i \frac{H^{d}(i)}{d_e}|\Psi\rangle, \quad (11)$$

$$W_M = \frac{3}{2\Omega}\langle\Psi|\sum_i \left(\frac{\boldsymbol{\alpha}_i\times\boldsymbol{r}_i}{r_i^5}\right)_\zeta r_\zeta|\Psi\rangle. \quad (12)$$

Note that a parameter known as the effective electric field acting of unpaired electrons, $E_{\rm eff} = W_d|\Omega|$, is often used.

For a completely polarized molecule the energy shifts due to eEDM, a scalar-pseudoscalar nucleus-electron neutral current, and MQM interactions are

$$\delta_d = d_e W_d \Omega, \quad (13)$$

$$\delta_{\rm SP} = k_{\rm SP} W_{\rm SP} \Omega, \quad (14)$$

$$\delta_M(J,F) = (-1)^{I+F} C(J,F) M W_M \Omega, \quad (15)$$

$$C(J,F) = \frac{(2J+1)}{2} \frac{\left(\begin{smallmatrix} J & 2 & J \\ -\Omega & 0 & \Omega \end{smallmatrix}\right)}{\left(\begin{smallmatrix} I & 2 & I \\ -I & 0 & I \end{smallmatrix}\right)} \left\{\begin{smallmatrix} J & I & F \\ I & J & 2 \end{smallmatrix}\right\}, \quad (16)$$

where $(\ldots)$ means elements with 3j symbols and $\{\ldots\}$ with 6j symbols [53], F is the total angular momentum, and J is the number of rotational level. Note that both δ_d and $\delta_{\rm SP}$ are independent of J and F quantum numbers, whereas δ_M depends on them. Also, as opposed to $H^{\rm SP}_{\rm eff}$ and $H^{d}_{\rm eff}$ Hamiltonian $H^{\rm MQM}_{\rm eff}$ has nonzero off-diagonal matrix elements on the J quantum number (between different rotational levels). This should be taken into account when mixing of different rotational levels becomes significant. In Eq. (15) this effect is neglected. For ^{181}TaN ($I{=}7/2$) and ground rotational level $J{=}1$ Eq. (15) gives the MQM energy shifts, $|\delta(J,F)|$, equal to $0.107\ W_M M$, $0.143\ W_M M$, $0.05\ W_M M$ for $F = 5/2, 7/2$, and $9/2$, correspondingly.

To compute the hyperfine structure constant $A_{||}$ on ^{181}Ta in the $^3\Delta_1$ electronic state of the ^{181}TaN molecule the following matrix element can be evaluated:

$$A_\parallel = \frac{\mu_{\rm Ta}}{I\Omega}\langle\Psi|\sum_i \left(\frac{\boldsymbol{\alpha}_i\times\boldsymbol{r}_i}{r_i^3}\right)_\zeta|\Psi\rangle, \quad (17)$$

where $\mu_{\rm Ta}$ is the nuclear magnetic moment of a Ta isotope with spin I.

II. NUCLEAR MAGNETIC QUADRUPOLE MOMENT

The main contribution to MQM is produced by the nucleon-nucleon T,P-odd interaction which exceeds the nucleon EDM contribution by 1–2 orders of magnitude [5]. In a spherical nucleus MQM is determined mainly by a valence nucleon which carries the nuclear angular momentum I [5]:

$$M = [d - 2\times 10^{-21}\eta(\mu - q)(e\times{\rm cm})]\lambda_p(2I-1)t_I, \quad (18)$$

where $t_I = 1$ for $I = l + 1/2$ and $t_I = -I/(I+1)$ for $I = l - 1/2$, I and l are the total and orbital angular momenta of a valence nucleon respectively, η is the dimensionless strength constant of the T,P-odd nuclear potential $\eta G/(2^{3/2}m_p)(\sigma\cdot\nabla\rho)$ acting on the valence nucleon, ρ is the total nucleon number density, and the nucleon magnetic moments are $\mu_p = 2.79$ for the valence proton and $\mu_n = -1.91$ for the valence neutron, $q_p = 1$ and $q_n = 0$, $\lambda_p = \hbar/m_p c = 2.10\times 10^{-14}$ cm; the contribution of the valence nucleon EDM d was calculated in Ref. [6].

In deformed nuclei MQM has a collective nature and is enhanced by an order of magnitude [7] (comparable to the enhancement of an ordinary collective electric quadrupole moment). An estimate of the collective MQM can be made as follows. In a deformed nucleus the strong field splits orbitals with different absolute values $|I_z|$ of the projections of the angular momentum on the nuclear symmetry axis. Summing over all I_z gives a zero contribution to MQM. However, due to the difference in energies for different $|I_z|$ some of the I_z orbitals are vacant, and the remaining contribution is not zero. As a result, the MQM of a deformed nucleus in the "frozen" frame (rotating together with a nucleus) may be estimated using the following formula [7]:

$$M^{\rm nucl}_{zz} = \sum M^{\rm single}_{zz}(I,I_z,l) n(I,I_z,l), \quad (19)$$

where the sum goes over occupied orbitals, $M^{\rm single}_{zz}(I,I_z,l)$ is given by Eqs. (18) and (5), and $T_{zz} = 2I_z^2 - \frac{2}{3}I(I+1)$, $n(I,I_z,l)$ are the orbital occupation numbers, which may be

found in Ref. [54]. The sum over a complete shell gives zero; therefore, for shells more than half-filled it is convenient to use hole numbers in place of particle numbers, using the relation $M_{zz}^{\rm single}({\rm hole}) = -M_{zz}^{\rm single}({\rm particle})$.

The nucleus ^{181}Ta has the following occupation numbers: 10 neutron holes in orbitals $[\bar{I}_I, I_z] = [\bar{p}_{3/2}, \pm 3/2]$, $[\bar{i}_{13/2}, \pm 13/2, \pm 11/2]$, $[\bar{h}_{9/2}, \pm 9/2, \pm 7/2]$, and 9 proton holes $[\bar{d}_{5/2}, \pm 5/2]$, $[\bar{h}_{11/2}, \pm 11/2, \pm 9/2]$, $[\bar{d}_{3/2}, \pm 3/2]$, $[\bar{g}_{7/2}, 7/2]$.

The MQM in the laboratory frame $M \equiv M_{\rm lab}$ can be expressed via MQM in the rotating frame (19):

$$\begin{aligned} M^{\rm lab} &= \frac{I(2I-1)}{(I+1)(2I+3)} M_{zz}^{\rm nucl} \\ &= (1.1\eta_p - 0.9\eta_n) \times 10^{-33} (e \times {\rm cm}^2) \\ &\quad - (3.0 d_p + 2.3 d_n) \times 10^{-13}\ {\rm cm}, \end{aligned} \tag{20}$$

where $I = 7/2$ is the nuclear spin of ^{181}Ta.

The *T,P*-odd nuclear forces are dominated by the π_0 meson exchange [5]. Therefore, we may express the strength constants via the strong πNN coupling constant $g = 13.6$ and *T,P*-odd πNN coupling constants corresponding to the isospin channels $T = 0,1,2$: $\eta_n = -\eta_p = 5 \times 10^6 g(\bar{g}_1 + 0.4\bar{g}_2 - 0.2\bar{g}_0)$ (see details in Ref. [29]). As a result, we obtain

$$M(g) = -[g(\bar{g}_1 + 0.4\bar{g}_2 - 0.2\bar{g}_0) \times 8 \times 10^{-27} e \times {\rm cm}^2. \tag{21}$$

Possible CP violation in the strong interaction sector is described by the CP violation parameter $\tilde{\theta}$. According to Ref. [55] $g\bar{g}_0 = -0.37\tilde{\theta}$. This gives the following value of MQM for ^{181}Ta:

$$M(\theta) = -5 \times 10^{-28} \tilde{\theta} \times e \times {\rm cm}^2. \tag{22}$$

Almost the same final results for $M(\theta)$ can be obtained by using recently calculated relations of g_0 and g_1 constants by using chiral perturbation theory [56] and lattice data for the strong part of the proton-neutron mass difference [57], which gives updated value of gg_0.

Finally, we can express MQM in terms of the quark chromo-EDM $\tilde{d}_u$ and $\tilde{d}_d$ using the relations $g\bar{g}_1 = 4 \times 10^{15}(\tilde{d}_u - \tilde{d}_d)/{\rm cm}$, $g\bar{g}_0 = 0.8 \times 10^{15}(\tilde{d}_u + \tilde{d}_n)/{\rm cm}$ [58]:

$$M(\tilde{d}) = -3 \times 10^{-11}(\tilde{d}_u - \tilde{d}_d) \times e \times {\rm cm}. \tag{23}$$

The contributions of d_p and d_n to MQM in Eqs. (21)–(23) are from one to two orders of magnitude smaller than the contributions of the nucleon CP-odd interactions.

III. ELECTRONIC STRUCTURE CALCULATION DETAILS

To obtain the electronic state-specific parameters $W_{\rm SP}$, $E_{\rm eff}$, W_M, and $A_{||}$ described by Eqs. (10–12) and (17) we have performed a series of calculations using the two-step procedure to study the relativistic four-component electronic structure in the vicinity of the Ta nucleus [32,52,59]. For this the space around the given heavy atom, Ta, is divided into the valence and core regions. In the first step inactive core electrons are excluded from molecular calculations using the generalized relativistic effective core potential (GRECP) method [60,61]. The approach allows one also to take into account the contribution from Breit interaction and finite nuclear size [62,63]. After this stage we obtain a wave function that is very accurate in the valence region but has incorrect behavior in the core region. The correct four-component behavior of the wave function in the core region is restored at the second step using the procedure [32,52] based on a proportionality of valence and virtual (unoccupied in the reference Slater determinant) spinors [64] in the inner-core regions of the heavy atom. The splitting of the solution of the four-component relativistic full-electron problem into two consequent steps allows one to consider high-order correlation effects (see below) that are important for reliable and accurate calculation of the properties that cannot be measured experimentally.

The applied computation scheme includes the following steps: (1) Consideration of leading correlation and relativistic effects within the relativistic two-component coupled-cluster with single, double, and perturbative triple cluster amplitudes. The correlation calculations include valence and outer-core electrons of Ta ($5s^25p^66s^25d^3$) and N ($1s^22s^22p^3$), i.e., 20 electrons. For Ta we used the basis set consisting of 15 *s*-, 10 *p*-, 10 *d*-, 5 *f*-, and 2 *g*-type uncontracted Gaussians.[1] For N we used the aug-ccpVQZ basis set [65] with removed two g-type basis functions. Below this basis set will be called MBas. (2) Consideration of correction on basis set enlargement. It was calculated as a difference between results of the 20-electron scalar-relativistic calculation within the CCSD(T) method in an enlarged basis[2] and basis used in step (1). (3) Consideration of high-order correlation effects. They were calculated as a difference between results of 20-electron two-component calculations within the couple cluster with single, double, triple, and perturbative quadruple cluster amplitudes, the CCSDT(Q), and the CCSD(T) calculation using a compact basis set [30,66]. (4) Consideration of contribution of the sub-outer-core $4s^24p^64d^{10}4f^{14}$ electrons of Ta. Their contribution was obtained as a difference between the results of 52-electron and 20-electron two-component CCSD(T) calculations.[3] Core electrons of Ta ($1s$–$4f$) in the first three steps were excluded from correlation treatment by the 60-electron GRECP. For step 4 we constructed the GRECP version for 45 explicitly treated electrons of the Ta atom and a very small 28-electron inner core.

The coupled-cluster calculations were performed using the MRCC [67,68] code interfaced with DIRAC code [69]. Scalar-relativistic calculations were performed using the CFOUR program package [70]. Restoration of the four-component electronic structure was performed using the code developed in Refs. [32,71,72] and interfaced to the above-mentioned packages.

Equilibrium Ta-N distance and other spectroscopic parameters were obtained by approximation of potential energy curve

[1]The basis sets used are available at http://qchem.pnpi.spb.ru.

[2]The basis for Ta was increased up to 18 *s*-, 18 *p*-, 15 *d*-, 15 *f*-, 10 *g*-, 7 *h*- and 7 *i*- type Gaussian basis functions.

[3]In the 20-electron calculations $4s^24p^64d^{10}4f^{14}$ electrons were frozen from atomic calculation, i.e., in the spherical form rather than the relaxed molecular form. For Ta we used basis set consisting of 18 *s*-, 18 *p*-, 10 *d*-, 7 *f*-, and 4 *g*-type Gaussian basis functions.

TABLE I. Equilibrium internuclear distance R_e, harmonic vibrational wave number ω_e, and vibrational anharmonicity $\omega_e x_e$ for the $^3\Delta_1$ state of TaN.

Method	R_e (a.u.)	ω_e (cm^{-1})	$\omega_e x_e$ (cm^{-1})
20e-2c-CCSD(T), this work	3.19	1028	3.5
Experiment, [46]	3.20	—	—

calculated within the 20-electron two-component CCSD(T) method in the MBas basis set.

IV. RESULTS AND DISCUSSIONS

The equilibrium internuclear distance calculated for the $^3\Delta_1$ state of TaN is 3.19 a.u., which agrees well with the experimental data [46]; see Table I. In calculations of the parameters under consideration we have set R(Ta–N) to 3.20 a.u.

TaN has triple bond order (one σ bond and two π bonds) provided mainly by d electrons of Ta and p electrons of N [73–76]. Unpaired electrons in the $^3\Delta_1$ state are nonbonding electrons localized on Ta. They determine the $\sigma^1\delta^1$ configuration, where σ is mainly the 6s atomic orbital of Ta and δ is mainly 5d atomic orbital of Ta.

The calculated values of $E_{\rm eff}$, $W_{\rm SP}$, W_M, and $A_{||}$ are given in Table II. The effective electric field is rather strong (1.5 times more than that in HfF^+ [14,15] and similar to other considered transition elements compounds $E_{\rm eff}$ (PbF) [36] and WC [33]) but about two times smaller than $E_{\rm eff}$ in ThO [28,30,31]. The value of the W_M parameter estimated in Ref. [44] ($\approx$1) agrees with the value obtained in this paper. Thus the calculated large value of the W_M parameter confirms that the ^{181}TaN molecule with a stable ^{181}Ta isotope having nucleus spin $I > 1/2$ is probably the most promising candidate to date among considered heavy-atom diatomic molecules to search for nuclear MQM. According to the results listed in Table II and our previous error analysis from Ref. [30] for a comparable situation (ThO in the $^3\Delta_1$ state) we expect that the theoretical uncertainty of the calculated characteristics is less than 7%. Direct experimental check of $E_{\rm eff}$, $W_{\rm SP}$, and W_M parameters is impossible; however, one can in principle seize here the opportunity of measurement of the hyperfine structure constant in the $^3\Delta_1$ state of TaN, which can be performed later. As was argued earlier [52,64,77] the "equal-footing calculation" of the the hyperfine structure constants can provide a very important (though indirect) test for the $E_{\rm eff}$, $W_{\rm SP}$, and W_M parameters. The calculated value of the molecule-axis hyperfine structure constant is given in Table II.

One can express the MQM energy shift, $(-1)^{I+F}C(J,F)MW_M\Omega$ in terms of the fundamental CP-violating physical quantities d_p, d_n, $\tilde{\theta}$, and $\tilde{d}_{u,d}$ using Eqs. (20), (22), and (23). For the lowest rotational level, for which the coefficient $|C(J{=}1,F{=}7/2)| = 0.143$ reaches a maximum value, we have

$$0.143W_M M = -\frac{10^{25}(4.5d_p + 3.5d_n)}{e \times \text{cm}} \times \mu\text{Hz} \quad (24)$$

$$0.143W_M M = -7.7 \times 10^{10}\tilde{\theta} \times \mu\text{Hz}, \quad (25)$$

$$0.143W_M M = -4.6 \times \frac{10^{27}(\tilde{d}_u - \tilde{d}_d)}{\text{cm}} \times \mu\text{Hz}. \quad (26)$$

The current limits on d_p, $|\tilde{\theta}|$ and $|\tilde{d}_u - \tilde{d}_d|$ ($|d_p| < 8.6 \times 10^{-25} e\times$cm, $|\tilde{\theta}| < 2.4 \times 10^{-10}$, $|\tilde{d}_u - \tilde{d}_d| < 6 \times 10^{-27}$ cm [80] correspond to the shifts $|0.143\ W_M M| < 40\ \mu$Hz, 18 μHz, and 28 μHz, respectively. Currently the best limit on the energy shift produced by the T,P-odd effects (electron EDM and scalar-pseudoscalar nucleus-electron interactions) in the $^3\Delta_1$ state of ^{232}ThO is 700 μHz [3] and is expected to be improved by an order of magnitude over the next five years [81,82] due to experimental developments. Such progress with the ^{181}TaN experiment on the $^3\Delta_1$ state can result in comparable improvement with limitations on the T,P-odd effects in the nuclear sector as well.

TABLE II. The calculated values of the molecule-frame dipole moment (d), effective electric field ($E_{\rm eff}$), parameter of the T,P-odd scalar-pseudoscalar nucleus-electron interaction ($W_{\rm SP}$), parameter of T,P-odd MQM interaction (W_M), and hyperfine structure constant ($A_{||}$) of the $^3\Delta_1$ state of TaN using the coupled-cluster methods.

Method	d (Debye)	$E_{\rm eff}$ (GV/cm)	$W_{\rm SP}$ (kHz)	W_M ($\frac{10^{33}\text{Hz}}{e\text{cm}^2}$)	$A_{||}$[a] (MHz)
20e-2c-CCSD	4.70	37.5	34	1.15	−3082
20e-2c-CCSD(T)	4.81	35.6	32	1.10	−3015
Correlation correction	−0.04	0.2	0	−0.01	−32
Basis set correction	−0.03	−0.4	0	0.00	−33
Core correction	0.00	−0.5	−1	−0.01	−51
Final	4.74	34.9	31	1.08	−3132

[a]Magnetic moment of Ta ($\mu_{^{181}Ta}$) was set to $2.371\mu_{\rm N}$ [78,79].

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