

Multipole transition amplitudes and radiative decay rates in neutral cadmium

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We present a comprehensive study of the electronic transitions in neutral cadmium (Cd I) with a focus on forbidden transitions, motivated by recent advances in laser technology and the growing relevance of cadmium in quantum gas research, precision metrology, and atom trapping. General analytic expressions are derived for transition matrix elements of all multipolar orders, formulated to be applicable for experimental use. Using configuration interaction combined with many-body perturbation theory, we calculate not only the previously reported contributions from electric dipole (E1) transitions, but also the electric quadrupole (E2), electric octupole (E3), magnetic dipole (M1), and magnetic quadrupole transitions (M2) that have not yet been investigated for cadmium. These matrix elements are then employed to determine the lifetimes of key excited states, particularly those pertinent to laser cooling and optical frequency standards, and to evaluate the long-range dispersion coefficient C_6 . The linewidths of the strongest transitions, along with the atomic energy levels, are compared with available experimental data to validate the accuracy of the simulations. Overall, the results are in good agreement, with the calculated energy levels exhibiting an average relative deviation of 0.3% from experiments. These values serve as benchmarks for both bosonic and fermionic isotopes, providing a foundation for future experimental and theoretical work in cadmium-based precision spectroscopy and cold-collision studies.

I. INTRODUCTION

The production of cold, dense, and large atomic samples is a cornerstone of modern atomic, molecular, and optical physics [1], underpinning a wide range of fundamental and applied experiments, including frequency metrology [2], searches for exotic forces [3, 4], and atom interferometry [5]. State-of-the-art optical atomic clocks have reached fractional accuracies and stabilities on the order of 10^{-18} [6–11], motivating a potential optical redefinition of the second [12] and enabling applications such as chronometric leveling and searches for variations of fundamental constants [3, 13, 14]. At this level of precision, blackbody radiation (BBR) shifts remain a significant source of systematic uncertainty [7, 8, 10]. While cryogenic interrogation has mitigated this effect in several systems, alternative atomic species with intrinsically low BBR sensitivity, including Hg, Mg, Tm, and Cd, offer the possibility of simpler experimental implementations with improved accuracy [15–17].

Alkaline-earth-like atoms, such as cadmium, are particularly attractive for precision metrology due to their electronic structure, which features narrow intercombination transitions suitable for high-accuracy measurements of fundamental physics [18–20], alongside broad, dipole-allowed transitions that enable rapid laser cooling. Advances in laser technology have produced ultra-narrow linewidth lasers [21], making it possible to probe these forbidden transitions and to implement schemes based on magnetic-dipole couplings [22–25].

Cadmium exhibits a particularly advantageous set of properties for atomic and optical applications. It pos-

sesses eight stable isotopes, most of which occur with relatively comparable natural abundances. Furthermore, the majority of its strong transitions lie in the ultraviolet domain, which makes cadmium vapor an attractive medium for ultraviolet generation via four-wave mixing [26]. This feature is of particular relevance to emerging deep-UV nuclear clock schemes [27].

These characteristics make it an excellent candidate for probing physics beyond the Standard Model through the measurement of isotope shifts using techniques such as King’s plots [28, 29]. The bosonic isotopes allow access to ultranarrow clock transitions, while the fermionic isotopes possess nuclear spin, providing hyperfine-induced clock transitions with natural linewidths of $\Gamma/2\pi = 7.0$ and 7.6 mHz [30]. Figure 1 presents the most common transitions of neutral cadmium employed in cold atom physics.

The spin-forbidden $(5s^2) ^1S_0 \rightarrow (5s5p) ^3P_1$ transition at 326 nm enables Doppler cooling to the μK level [31–33]. Its short wavelength also reduces radiation trapping and allows the preparation of dense, cold ensembles, which may enable rapid or even continuous production of quantum-degenerate gases [34–37].

Despite these attractive features, experimental realizations of cold Cd remain limited. Early demonstrations include magneto-optical traps (MOTs) on the broad $(5s^2) ^1S_0 \rightarrow (5s5p) ^1P_1$ transition at 229 nm [31] and, more recently, on the narrow 326 nm intercombination line [38, 39]. The development of robust, high-flux sources is hindered by challenges associated with ultraviolet light generation, vacuum compatibility, and photoionization [33, 40].

Most studies on cadmium have focused on a limited number of transitions, primarily restricted to low-lying states [17, 39, 41, 42]. While more recent works employing Configuration Interaction combined with Many-

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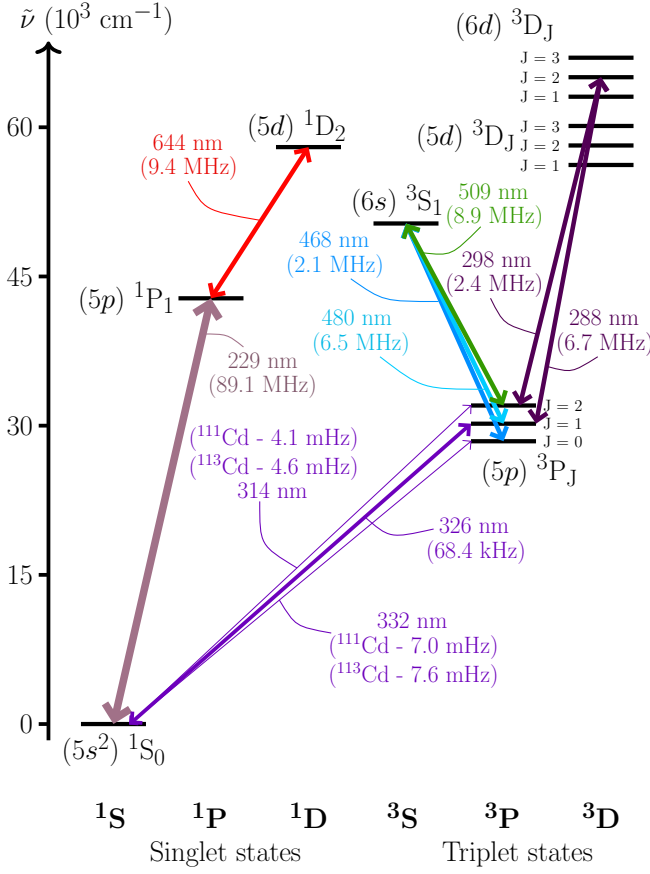


Figure 1. Simplified energy-level structure of neutral cadmium (Cd I) and its principal optical transitions relevant to laser-cooling and spectroscopic applications. Wavelengths and natural linewidths $\Gamma/2\pi$ of the transitions are also reported. The different 3D_J and 3P_J levels are not drawn to scale; they have been separated for readability.

Body Perturbation Theory (CI+MBPT) have extended the scope to larger sets of transitions, including higher-lying states [26, 43], these investigations have remained limited to the so-called ‘allowed’ electric-dipole transitions. Complementary studies based on Multiconfiguration Dirac-Hartree-Fock combined with Configuration Interaction have investigated cadmium isotope shifts and clock-transition frequencies, including detailed King-plot analyses for the extraction of nuclear parameters [44]. Nevertheless, systematic calculations of higher-order forbidden multipole transitions remain lacking.

In this work, we compute, using CI+MBPT, the previously unreported higher-order multipole matrix elements E2, E3, M1, and M2 of neutral cadmium. These matrix elements are subsequently employed to analyze the lifetimes of key transitions with particular emphasis on the previously unexplored bosonic clock transition and to determine the long-range van der Waals C_6 coefficient. Unless otherwise specified, all formulas and results are expressed in atomic units.

II. CI+MBPT FRAMEWORK

A. Theory

CI+MBPT is an ab initio approach that has shown high precision in calculating atomic properties [45–47]. This approach combines Configuration Interaction (CI) to account for valence–valence electron correlations, with Many-Body Perturbation Theory (MBPT) to treat core–valence interactions [48].

The procedure begins by solving the Dirac-Fock (DF) equations, the relativistic generalization of the Hartree-Fock equations, for both core and valence electrons. This is done within one of the standard approximations of the potential: V^N , V^{N-1} , or V^{N-M} , where N is the total number of electrons and M is the number of valence electrons. The DF Hamiltonian takes the form [49]

$$h_{\text{DF}} = c\boldsymbol{\alpha} \cdot \mathbf{p} + (\beta - 1)c^2 - \frac{Z}{r} + V^{N_{\text{DF}}} \quad (1)$$

where $\boldsymbol{\alpha}$ and β are the Dirac matrices and $V^{N_{\text{DF}}}$ is the self-consistent potential in the chosen approximation.

The one-electron solutions of the Dirac equation can be expressed as

$$\psi(r) = \frac{1}{r} \begin{pmatrix} iP_{n\kappa}(r)\Omega_{\kappa m}(\hat{r}) \\ Q_{n\kappa}(r)\Omega_{-\kappa m}(\hat{r}) \end{pmatrix} \quad (2)$$

where $\kappa = (-1)^{j+l+\frac{1}{2}}(j+\frac{1}{2})$, $P_{n\kappa}$ and $Q_{n\kappa}$ typically refer to the large and small radial components respectively and $\Omega_{\kappa m}$ are the spherical spinors.

The DF operator can be extended to include relativistic corrections such as the Breit interaction and QED effects [49], with the Breit operator given by

$$B_{ij} = -\frac{1}{2r_{ij}} \left(\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j + \frac{(\boldsymbol{\alpha}_i \cdot \mathbf{r}_{ij})(\boldsymbol{\alpha}_j \cdot \mathbf{r}_{ij})}{r_{ij}^2} \right) \quad (3)$$

The remaining valence orbitals and pseudostates are constructed as linear combinations of B-spline basis functions [50]. The resulting one-particle basis functions are then used to build anti-symmetrized many-electron basis states $|\text{proj}_n\rangle$, expressed as superpositions of Slater determinants [49].

Configuration state functions (CSFs) $|I\rangle$ are defined as eigenfunctions of $\hat{J}^2$ and $\hat{J}_z$, obtained as linear combinations of $|\text{proj}_n\rangle$:

$$|I\rangle = \sum_n c_n |\text{proj}_n\rangle \quad (4)$$

The atomic wavefunction is expressed as a CI expansion over the CSFs [50]:

$$\Psi = \sum_{I \in P} C_I |I\rangle \quad (5)$$

where P denotes the model space included in the CI calculation.

The dimension of the CI matrix grows rapidly with the number of orbitals included, making it computationally prohibitive to account for all core–valence correlations or core excitations directly within CI. These effects are instead incorporated perturbatively: MBPT is applied to second order to modify the CI matrix elements [47, 48]. The resulting CI+MBPT eigenvalue problem is

$$\sum_{J \in P} \left(H_{IJ} + \sum_{M \in Q} \frac{\langle I | \hat{H} | M \rangle \langle M | \hat{H} | J \rangle}{E - E_M} \right) C_J = E C_I \quad (6)$$

where Q is the complementary space containing states excluded from the CI model space P .

B. AMBiT

AMBiT is a software for fully relativistic atomic structure calculations, integrating CI+MBPT to enable determinations of energy levels, transition matrix elements, g-factors, and isotope shifts in complex systems. In AMBiT, the CI space is assembled from CSFs generated by permitting electron and/or hole excitations from a designated set [50]. The allowed excitations are restricted by upper bounds on the principal quantum number n and orbital angular momentum l . To further decrease the computational burden, AMBiT employs the *emu* CI strategy [51]. This approach partitions the CSFs into two groups: the *large-side* set, constructed with more generous limits on n and l , and the *small-side* set, produced with tighter restrictions. Frequently, the small-side space is supplemented by configurations obtained through single excitations to higher- n and higher- l orbitals than those defining its primary limits. Core–valence correlations are subsequently incorporated in a perturbative fashion via the MBPT operator, contributing second-order energy shifts.

The choice of parameters for the cadmium simulations with AMBiT is guided by the work of Penyazkov *et al.* [26], who employed AMBiT for the calculation of E1 matrix elements. However, whereas most studies using CI+MBPT have focused on specific states for targeted applications, such as four-wave mixing [26] or magic trapping conditions [43], our objective is to minimize the overall relative deviation between calculated and experimental energy levels [52–56] rather than optimize for a restricted set of states. Consequently, while our approach is inspired by these earlier works, some differences in computed values arise. The parameters were iteratively optimized until the mean relative deviation between the computed energy levels and those reported in the NIST database was reduced to below 0.5%, with a maximum relative deviation of 5%.

The final computational setup employed a V^{N-2} potential to solve the Dirac–Hartree–Fock (DHF) equa-

tions. The valence orbital basis is specified as $12spdf$, including all s -, p -, d -, and f -orbitals with $n < 12$. The $5s^2$ and $5s, 5p$ configurations serve as the reference set. Large-side CSFs are obtained by allowing all single and double excitations from these references into orbitals up to $12spdf$. The small-side CSFs are generated from the same references, with single and double excitations restricted to $6sp5d4f$, in addition to single excitations extending up to $20spdf$. In every calculation, single and double excitations from the $4d$ core are also included. MBPT corrections are computed by accounting for all one-, two-, and three-body diagrams within a $30spdfg$ basis. The present calculation does not include ionization effects.

III. REDUCED MATRIX ELEMENTS

A. Theory and selection rules

This section is largely based on the lecture notes of W. R. Johnson [49]. For more detailed discussions, particularly regarding selection rules, the reader can refer to Refs. [57–59].

Let $\psi(\mathbf{r})$ denote the Dirac wavefunction, $\hat{\epsilon}$ the polarization vector of the electromagnetic field, $\mathbf{k}$ its wave vector, and $|a\rangle$ and $|b\rangle$ the initial and final states, respectively. The transition amplitude for a one-electron transition can be expressed as

$$T_{ba} = \int \psi_b^\dagger(\mathbf{r}) \boldsymbol{\alpha} \cdot \hat{\epsilon} e^{i\mathbf{k} \cdot \mathbf{r}} \psi_a(\mathbf{r}) d^3r \quad (7)$$

The exponential factor $e^{i\mathbf{k} \cdot \mathbf{r}}$ is of central interest, as it generates the multipole operators. For neutral atoms or ions with small nuclear charge Z , the condition $|\mathbf{k} \cdot \mathbf{r}| \ll 1$ holds, allowing the exponential to be expanded in a Taylor series.

To zeroth order, the exponential term reduces to unity, and within the Pauli approximation, the nonrelativistic length-form transition amplitude is obtained

$$T_{ba}^{(0)} = i \frac{\omega_{ba}}{c} \langle b | \mathbf{r} | a \rangle \cdot \hat{\epsilon} \quad (8)$$

where $\hbar\omega_{ba}$ is the energy difference between $|a\rangle$ and $|b\rangle$.

Since this amplitude is proportional to the electric-dipole operator $\mathbf{d} = e\mathbf{r}$, it is referred to as the electric-dipole (E1) amplitude. In the spherical basis, the electric-dipole operator is an odd-parity irreducible tensor of rank one. Consequently, $|a\rangle$ and $|b\rangle$ must have opposite parity for the transition matrix element to be nonzero, representing a fundamental selection rule for E1 transitions.

The next-order term in the nonrelativistic expansion, $i\mathbf{k} \cdot \mathbf{r}$, gives rise to the transition amplitude

$$T_{ba}^{(1)} = i \frac{k}{c} \langle b | \mathbf{M} | a \rangle \cdot [\hat{\mathbf{k}} \times \hat{\epsilon}] - \frac{k\omega_{ba}}{6c} \sum_{i,j} \langle b | Q_{ij} | a \rangle \hat{k}_i \hat{\epsilon}_j \quad (9)$$

where $\mathbf{M} = \frac{1}{2m}(\mathbf{L} + 2\mathbf{S})$ is the magnetic-dipole operator, and $Q_{ij} = 3x_i x_j - r^2 \delta_{ij}$ is the electric quadrupole operator. The first term corresponds to the magnetic-dipole (M1) amplitude, while the second term represents the electric quadrupole (E2) amplitude.

In general, under the long-wavelength approximation and the Pauli approximation, the one-electron electric multipole reduced matrix elements of order η in the *length gauge* can be written as

$$\begin{aligned} \langle \kappa_a | \mathbf{O}^{(E\eta)} | \kappa_b \rangle &= \langle \kappa_a | C_\eta | \kappa_b \rangle \\ &\times \int_0^\infty r^\eta [P_a(r) P_b(r) + Q_a(r) Q_b(r)] dr \end{aligned} \quad (10)$$

while the magnetic multipole reduced matrix elements of order η in the *transverse gauge* are given by

$$\begin{aligned} \langle \kappa_a | \mathbf{O}^{(M\eta)} | \kappa_b \rangle &= \langle -\kappa_a | C_\eta | \kappa_b \rangle \frac{\kappa_a + \kappa_b}{\eta + 1} \\ &\times \int_0^\infty r^\eta [P_a(r) Q_b(r) + Q_a(r) P_b(r)] dr \end{aligned} \quad (11)$$

where C_λ denotes the normalized spherical harmonic tensor, and the approximation $j_n(z) \sim z^n/(2n+1)!!$ has been used for the spherical Bessel functions of order n [60, 61]. While Eqs. 8–11 are written in the nonrelativistic form, AMBiT instead performs its simulations using the full Dirac equation and therefore evaluates relativistic matrix elements. The general matrix element is then obtained via the Wigner-Eckart Theorem.

Focusing on matrix elements up to E3 and M2, the corresponding selection rules are summarized in Table I.

Table I. Selection rules for electric (E1–E3) and magnetic (M1–M2) multipole transitions, showing allowed changes in total angular momentum J , parity, and the corresponding restrictions in LS coupling.

Type	ΔJ	Parity Change	In LS coupling
E1	$0, \pm 1$ ($0 \not\rightarrow 0$)	Yes	$\Delta S = 0$ $\Delta L = 0, \pm 1$ ($0 \not\rightarrow 0$)
E2	$0, \pm 1, \pm 2$ ($0 \not\rightarrow 0, 1$) ($\frac{1}{2} \not\rightarrow \frac{1}{2}$)	No	$\Delta S = 0$ $\Delta L = 0, \pm 1, \pm 2$ ($0 \not\rightarrow 0, 1$)
E3	$0, \pm 1, \pm 2, \pm 3$ ($0 \not\rightarrow 0, 1, 2$) ($\frac{1}{2} \not\rightarrow \frac{1}{2}, \frac{3}{2}$) ($1 \not\rightarrow 1$)	Yes	$\Delta S = 0$ $\Delta L = 0, \pm 1, \pm 2, \pm 3$ ($0 \not\rightarrow 0, 1, 2$) ($1 \not\rightarrow 1$)
M1	$0, \pm 1$ ($0 \not\rightarrow 0$)	No	$\Delta S = 0$ $\Delta L = 0$
M2	$0, \pm 1, \pm 2$ ($0 \not\rightarrow 0, 1$) ($\frac{1}{2} \not\rightarrow \frac{1}{2}$)	Yes	$\Delta S = 0$ $\Delta L = 0, \pm 1, \pm 2$ ($0 \not\rightarrow 0, 1$)

B. Level Structure

The calculated energy levels for states up to the ground state of the 9th shell are presented in Table II. Each level was cross-checked accounting for the relativistic g -factor, and the corresponding magnetic moment amplitude, $|\mu| = |g \mu_B \mathbf{J}/\hbar| = g \mu_B \sqrt{J(J+1)}$, is reported in units of the Bohr magneton with $\mathbf{J}$ the total angular momentum operator and J its associated quantum number [62].

The AMBiT parameters were optimized to reproduce the experimental energy levels reported in the NIST database [52–56], with an overall relative deviation below 0.5% and a maximum relative deviation below 5%. In the final configuration (Table II), the obtained average relative deviation is 0.3%, with the largest relative deviation of 1.4% occurring for the highest calculated state, (5s9s) 1S_0 . The computation time was on the order of 10 hours using a standard workstation with 48 GB of RAM. This comparison with experimental data serves to ensure the highest accuracy of the subsequent reduced matrix elements.

C. Multipole Matrix Elements

Table III presents the E1-E3 and M1-M2 transition matrix elements expressed in atomic units (a.u.), calculated using CI+MBPT. Empty entries indicate either that the transition is forbidden by selection rules or that the corresponding matrix element is smaller than 10^{-3} a.u. Coupling to the nuclear spin, as well as mixed multipole contributions (e.g., E1M1), are not included; consequently, the clock transitions of fermionic isotopes are absent in this table.

The code generates on the order of 10^4 transitions. In the following, we focus on transitions most relevant to quantum gases, metrology, and atom trapping, as outlined in the Introduction. We highlight (i) transitions involving the ground state (5s²) 1S_0 , (ii) the ten strongest transitions of each multipole type, and (iii) we make sure all the transitions available on the NIST database are present. Transitions for which all five multipole matrix elements vanish are omitted. AMBiT requires the simulation parameters to be compiled in an `.input` file, which is provided as Supplementary Material. This file enables readers to reproduce the calculations and examine additional transitions not reported in the main text. To facilitate the identification of individual transitions, their corresponding wavelengths, expressed in ångströms, are provided. These wavelength values are taken from the NIST database [52–56].

In general, when a matrix element exists, its magnitude tends to increase for transitions involving higher shells. Similarly, when the interaction is expressed in atomic units, whether electric or magnetic, higher multipole orders correspond to larger matrix elements.

Table II. Energy levels (in cm^{-1}), g -factors, and magnetic moment amplitudes (in μ_B) for neutral cadmium states from $(5s^2) {}^1S_0$ to $(5s9s) {}^1S_0$. CI+MBPT results are compared with the NIST database. The atomic states are represented by symbols of the form $2S+1L_J^{\text{parity}}$.

State	g -factor	$ \mu $ (μ_B)	CI+MBPT (cm^{-1})	NIST (cm^{-1})
$(5s^2) {}^1S_0$	/	0	0.000	0.000 (0.007)
$(5s5p) {}^3P_0^o$	/	0	30 440	30 113.990 (0.002)
$(5s5p) {}^3P_1^o$	1.4987	2.1195	30 998	30 656.087 (0.002)
$(5s5p) {}^3P_2^o$	1.5000	3.6742	32 200	31 826.952 (0.002)
$(5s5p) {}^1P_1^o$	1.0012	1.4159	44 076	43 692.384 (0.002)
$(5s6s) {}^3S_1$	2.0000	2.8284	51 477	51 483.980 (0.002)
$(5s6s) {}^1S_0$	/	0	53 461	53 310.101 (0.010)
$(5s6p) {}^3P_0^o$	/	0	58 300	58 390.9 (2.5)
$(5s6p) {}^3P_1^o$	1.4974	2.1176	58 373	58 461.6 (2.5)
$(5s6p) {}^3P_2^o$	1.5000	3.6742	58 548	58 635.7 (2.5)
$(5s5d) {}^1D_2$	1.0001	2.4500	59 205	59 219.734 (0.002)
$(5s5d) {}^3D_1$	0.5000	0.7071	59 396	59 485.768 (0.002)
$(5s5d) {}^3D_2$	1.1666	2.8576	59 409	59 497.868 (0.002)
$(5s5d) {}^3D_3$	1.3333	4.6187	59 430	59 515.990 (0.020)
$(5s6p) {}^1P_1^o$	1.0026	1.4179	60 099	59 907.28 (0.18)
$(5s7s) {}^3S_1$	2.0000	2.8284	62 415	62 563.435 (0.002)
$(5s7s) {}^1S_0$	/	0	62 984	63 086.896 (0.002)
$(5s7p) {}^3P_0^o$	/	0	64 870	64 995.9 (2.5)
$(5s7p) {}^3P_1^o$	1.4957	2.1152	64 902	65 025.5 (0.3)
$(5s7p) {}^3P_2^o$	1.5000	3.6742	64 971	65 093.702 (0.016)
$(5s6d) {}^1D_2$	1.0001	2.4497	65 068	65 134.783 (0.002)
$(5s6d) {}^3D_1$	0.5000	0.7071	65 234	65 353.372 (0.002)
$(5s6d) {}^3D_2$	1.1667	2.8578	65 240	65 358.881 (0.002)
$(5s6d) {}^3D_3$	1.3333	4.6187	65 250	65 367.227 (0.020)
$(5s7p) {}^1P_1^o$	1.0043	1.4202	65 447	65 501.412 (0.016)
$(5s4f) {}^3F_2^o$	0.6667	1.6330	65 448	65 586.0 (0.3)
$(5s4f) {}^3F_3^o$	1.0668	3.6955	65 448	65 586.0 (0.3)
$(5s4f) {}^3F_4^o$	1.2500	5.5902	65 450	65 586.0 (0.3)
$(5s8s) {}^3S_1$	2.0000	2.8284	66 576	66 682.029 (0.002)
$(5s8s) {}^1S_0$	/	0	66 849	66 905.641 (0.010)
$(5s8p) {}^3P_0^o$	/	0	67 940	67 829.656 (0.020)
$(5s8p) {}^3P_1^o$	1.4949	2.1141	67 960	67 842.06 (0.05)
$(5s8p) {}^3P_2^o$	1.5000	3.6742	68 008	67 875.191 (0.016)
$(5s7d) {}^1D_2$	1.0001	2.4497	67 910	67 838.401 (0.002)
$(5s7d) {}^3D_1$	0.5000	0.7071	68 073	67 989.814 (0.002)
$(5s7d) {}^3D_2$	1.1667	2.8578	68 077	67 992.708 (0.002)
$(5s7d) {}^3D_3$	1.3333	4.6186	68 080	67 997.101 (0.020)
$(5s8p) {}^1P_1^o$	1.0051	1.4214	68 323	68 059.393 (0.016)
$(5s5f) {}^3F_2^o$	0.6667	1.6330	68 088	68 093.7 (2.5)
$(5s5f) {}^3F_3^o$	1.0441	3.6169	68 088	68 093.7 (2.5)
$(5s5f) {}^3F_4^o$	1.2500	5.5902	68 090	68 093.7 (2.5)
$(5s9s) {}^3S_1$	2.0000	2.8284	69 488	68 682.325 (0.002)
$(5s9s) {}^1S_0$	/	0	69 788	68 798.760 (0.010)

The $(5s^2) {}^1S_0 \leftrightarrow (5s5p) {}^1P_1^o$ transition exhibits a relatively large E1 matrix element; this is the broad cooling transition of neutral cadmium at 229 nm. However, the transition linewidth must account not only for the intrinsic width but also for the wavelength, as discussed in the following section. The second cooling transition is also present, albeit with a smaller amplitude. Among the

clock transitions, the 3P_0 state has vanishing matrix elements for all multipolar orders, whereas the $(5s5p) {}^3P_2^o$ state exhibits a nonzero M2 matrix element, as detailed in the next section.

IV. RADIATIVE DECAY RATES

A. Theory

The total decay rate is the sum of all multipole contributions. The type and number of multipoles that contribute to the sum is limited by selection rules. Therefore, for a transition from an initial state $|a\rangle$ of higher energy to a final state $|b\rangle$ of lower energy, the Einstein A -coefficient A_{ba} is the sum of each multipole element [49]

$$A_{ab} = 8\pi\alpha\omega \sum_{\eta,\xi} \left| \int \psi_b^\dagger \boldsymbol{\alpha} \cdot \mathbf{a}_\eta^{(\xi)} \psi_a d^3r \right|^2 \quad (12)$$

with α the fine structure constant, ω the light field frequency, ψ_a and ψ_b the Dirac wavefunctions of respectively the states a and b , $\xi = E$ to designate the electric multipole potentials of order η of the vector potential $\mathbf{a}_\eta^{(E)}$ and $\xi = M$ to designate the magnetic multipole potential of order η of the vector potential $\mathbf{a}_\eta^{(M)}$.

The lifetime τ in a state a is then the sum over all the possible transitions from this state

$$\tau = \sum_{b \leq a} \frac{1}{A_{ba}} \quad (13)$$

Using equations 10 and 11, the decay rates of each multipole channel $A_{ba}^{(\xi\eta)}$ can be expressed either in SI units, or in customary units, where the multipole matrix elements are expressed in a.u. and the wavelength in ångström [49, 63]

In table IV, $[J] = 2J+1$ denotes the statistical weights with J being the total angular momentum of the upper level. e is the unit of electric charge, a_0 the Bohr radius, h the Planck constant and ϵ_0 the vacuum permittivity. μ_0 and μ_B are respectively the vacuum permeability and the Bohr magneton.

The line strength of the transition $a \leftrightarrow b$ is $S^{(\xi\eta)} = |\langle b | \mathbf{O}^{(\xi\eta)} | a \rangle|^2$. $\mathcal{C}_\eta$ and $\mathcal{N}_\eta^{(\xi)}$, the two constants of order η used to adapt the decay rates from one unit system to the other, are shown in table V.

B. Results

Table VI presents the decay rates (in s^{-1}) corresponding to each multipole contribution. These rates are obtained by applying the equations in Tables IV and V to the matrix elements listed in Table III, and are compared with the strongest available transition rates reported in the NIST database. An empty entry indi-

Table III. Matrix elements in atomic units for electric dipole, electric quadrupole, electric octupole, magnetic dipole, and magnetic quadrupole transitions. The corresponding wavelengths in ångström are taken from the NIST database.

States	λ (Å)	E1	E2	E3	M1	M2
$(5s^2)^1S_0 \leftrightarrow (5s5p)^3P_1^o$	3262	1.784×10^{-1}				
$(5s^2)^1S_0 \leftrightarrow (5s5p)^3P_2^o$	3142					1.497×10^1
$(5s^2)^1S_0 \leftrightarrow (5s5p)^1P_1^o$	2289	3.788				
$(5s^2)^1S_0 \leftrightarrow (5s5d)^1D_2$	1689		1.201×10^1			
$(5s^2)^1S_0 \leftrightarrow (5s5d)^3D_2$	1681		2.601×10^{-1}			
$(5s^2)^1S_0 \leftrightarrow (5s6p)^1P_1^o$	1669	9.096×10^{-1}				
$(5s^2)^1S_0 \leftrightarrow (5s6d)^1D_2$	1535		6.203			
$(5s^2)^1S_0 \leftrightarrow (5s6d)^3D_2$	1530		5.204×10^{-2}			
$(5s^2)^1S_0 \leftrightarrow (5s7p)^1P_1^o$	1527	4.643×10^{-1}				
$(5s^2)^1S_0 \leftrightarrow (5s8p)^1P_1^o$	1469	3.563×10^{-1}				
$(5s5p)^3P_0^o \leftrightarrow (5s5p)^3P_1^o$	1.845×10^5				1.412	
$(5s5p)^3P_0^o \leftrightarrow (5s5p)^3P_2^o$	5.838×10^4		1.205×10^1			
$(5s5p)^3P_0^o \leftrightarrow (5s5p)^1P_1^o$	7365				6.155×10^{-2}	
$(5s5p)^3P_0^o \leftrightarrow (5s6s)^3S_1$	4679	1.479				
$(5s5p)^3P_0^o \leftrightarrow (5s5d)^1D_2$	3436					7.581
$(5s5p)^3P_0^o \leftrightarrow (5s5d)^3D_1$	3405	2.377				
$(5s5p)^3P_0^o \leftrightarrow (5s5d)^3D_2$	3403					2.426
$(5s5p)^3P_0^o \leftrightarrow (5s5d)^3D_3$	3401			1.041×10^2		
$(5s5p)^3P_0^o \leftrightarrow (5s6d)^3D_1$	2838	1.108				
$(5s5p)^3P_0^o \leftrightarrow (5s6d)^3D_2$	2837					1.088
$(5s5p)^3P_0^o \leftrightarrow (5s6d)^3D_3$	2837			2.490×10^1		
$(5s5p)^3P_1^o \leftrightarrow (5s5p)^3P_2^o$	8.540×10^4		1.828×10^1		1.578	
$(5s5p)^3P_1^o \leftrightarrow (5s5p)^1P_1^o$	7671		1.476		5.368×10^{-2}	
$(5s5p)^3P_1^o \leftrightarrow (5s6s)^3S_1$	4801	2.621				5.588
$(5s5p)^3P_1^o \leftrightarrow (5s5d)^1D_2$	3501	1.816×10^{-1}		4.494		1.097×10^1
$(5s5p)^3P_1^o \leftrightarrow (5s5d)^3D_1$	3469	2.098				2.077
$(5s5p)^3P_1^o \leftrightarrow (5s5d)^3D_2$	3467	3.623		1.075×10^2		9.772
$(5s5p)^3P_1^o \leftrightarrow (5s5d)^3D_3$	3465			1.518×10^2		3.198
$(5s5p)^3P_1^o \leftrightarrow (5s6d)^3D_1$	2882	9.627×10^{-1}				9.636×10^{-1}
$(5s5p)^3P_1^o \leftrightarrow (5s6d)^3D_2$	2882	1.677		2.462×10^1		4.461
$(5s5p)^3P_1^o \leftrightarrow (5s6d)^3D_3$	2881			3.509×10^1		1.474
$(5s5p)^3P_2^o \leftrightarrow (5s6s)^3S_1$	5087	3.572				1.075×10^1
$(5s5p)^3P_2^o \leftrightarrow (5s5d)^1D_2$	3651	9.339×10^{-2}		3.778		1.030×10^1
$(5s5p)^3P_2^o \leftrightarrow (5s5d)^3D_1$	3615	5.617×10^{-1}		1.547×10^2		1.033×10^{-1}
$(5s5p)^3P_2^o \leftrightarrow (5s5d)^3D_2$	3614	2.176		1.630×10^2		7.103
$(5s5p)^3P_2^o \leftrightarrow (5s5d)^3D_3$	3611	5.160		1.263×10^2		2.133×10^1
$(5s5p)^3P_2^o \leftrightarrow (5s6d)^3D_1$	2983	2.514×10^{-1}		3.246×10^1		5.619×10^{-2}
$(5s5p)^3P_2^o \leftrightarrow (5s6d)^3D_2$	2982	9.796×10^{-1}		3.443×10^1		1.049×10^1
$(5s5p)^3P_2^o \leftrightarrow (5s6d)^3D_3$	2981	2.339		2.693×10^1		9.695
$(5s5p)^1P_1^o \leftrightarrow (5s5d)^1D_2$	6440	5.754		4.081×10^2		1.458×10^1
$(5s5p)^1P_1^o \leftrightarrow (5s6d)^1D_2$	4662	9.915×10^{-1}		5.644×10^1		4.100
$(5s5p)^1P_1^o \leftrightarrow (5s7d)^1D_2$	4140	1.815×10^{-1}		4.067×10^1		2.206
$(5s5d)^3D_1 \leftrightarrow (5s5d)^3D_2$	8.333×10^6		7.690×10^1		2.121	
$(5s5d)^3D_2 \leftrightarrow (5s5d)^3D_3$	5.556×10^6		8.251×10^1		2.159	
$(5s7p)^3P_2^o \leftrightarrow (5s6d)^3D_3$	3.663×10^5	3.364×10^1		8.777×10^3		1.376×10^2
$(5s7p)^3P_2^o \leftrightarrow (5s5f)^3F_4^o$	3.333×10^4		7.251×10^2			
$(5s6d)^3D_1 \leftrightarrow (5s6d)^3D_2$	1.667×10^7		3.248×10^2		2.121	
$(5s6d)^3D_2 \leftrightarrow (5s6d)^3D_3$	1.250×10^7		3.480×10^2		2.160	
$(5s6d)^3D_2 \leftrightarrow (5s4f)^3F_3^o$	4.405×10^5	2.349×10^1		3.263×10^3		1.114×10^2
$(5s6d)^3D_3 \leftrightarrow (5s4f)^3F_4^o$	4.566×10^5	3.140×10^1		9.041×10^3		1.639×10^2
$(5s6d)^3D_3 \leftrightarrow (5s5f)^3F_4^o$	3.667×10^4	2.550×10^1		1.314×10^4		1.33×10^2
$(5s4f)^3F_2^o \leftrightarrow (5s4f)^3F_3^o$	$> 10^8$		1.968×10^2		2.311	
$(5s4f)^3F_3^o \leftrightarrow (5s4f)^3F_4^o$	$> 10^8$		2.009×10^2		2.323	
$(5s8s)^3S_1 \leftrightarrow (5s8p)^3P_2^o$	8.382×10^4	3.003×10^1		9.787×10^{-1}		9.009×10^1
$(5s8s)^3S_1 \leftrightarrow (5s7d)^3D_2$	7.628×10^4		8.190×10^2			
$(5s8s)^3S_1 \leftrightarrow (5s7d)^3D_3$	7.605×10^4		9.685×10^2			
$(5s8s)^3S_1 \leftrightarrow (5s5f)^3F_4^o$	7.082×10^4			3.117×10^4		
$(5s8s)^1S_0 \leftrightarrow (5s7d)^1D_2$	1.072×10^5		8.735×10^2			
$(5s8p)^3P_1^o \leftrightarrow (5s8p)^3P_2^o$	3.030×10^6		9.506×10^2		1.572	

States	λ (Å)	E1	E2	E3	M1	M2
$(5s8p) {}^3P_1^o \leftrightarrow (5s7d) {}^3D_2$	6.622×10^5	3.523×10^1		2.246×10^4		8.941×10^1
$(5s8p) {}^3P_1^o \leftrightarrow (5s7d) {}^3D_3$	6.452×10^5			3.177×10^4		3.973×10^1
$(5s8p) {}^3P_2^o \leftrightarrow (5s7d) {}^3D_1$	8.696×10^5	5.260		3.031×10^4		4.645×10^{-2}
$(5s8p) {}^3P_2^o \leftrightarrow (5s7d) {}^3D_2$	8.475×10^5	2.039×10^1		3.197×10^4		6.282×10^1
$(5s8p) {}^3P_2^o \leftrightarrow (5s7d) {}^3D_3$	8.197×10^5	4.830×10^1		2.479×10^4		1.973×10^2
$(5s8p) {}^3P_2^o \leftrightarrow (5s5f) {}^3F_4^o$	4.566×10^5		1.305×10^3			
$(5s7d) {}^1D_2 \leftrightarrow (5s8p) {}^1P_1^o$	4.525×10^5	3.696×10^1		3.712×10^4		8.151×10^1
$(5s7d) {}^1D_2 \leftrightarrow (5s5f) {}^3F_3^o$	3.906×10^5	3.121×10^1		2.381×10^4		1.487×10^2
$(5s7d) {}^1D_2 \leftrightarrow (5s5f) {}^3F_4^o$	3.906×10^5			1.296×10^2		1.274×10^2
$(5s7d) {}^3D_1 \leftrightarrow (5s7d) {}^3D_2$	3.333×10^7		6.784×10^2		2.121	
$(5s7d) {}^3D_1 \leftrightarrow (5s5f) {}^3F_2^o$	9.615×10^5	3.495×10^1		1.462×10^4		5.829×10^1
$(5s7d) {}^3D_2 \leftrightarrow (5s7d) {}^3D_3$	2.500×10^7		7.257×10^2		2.160	
$(5s7d) {}^3D_2 \leftrightarrow (5s5f) {}^3F_3^o$	9.901×10^5	3.110×10^1		9.216×10^3		1.764×10^2
$(5s7d) {}^3D_2 \leftrightarrow (5s9s) {}^3S_1$	1.451×10^5		7.316×10^2			
$(5s7d) {}^3D_3 \leftrightarrow (5s8p) {}^1P_1^o$	1.613×10^6			3.248×10^3		1.103×10^2
$(5s7d) {}^3D_3 \leftrightarrow (5s5f) {}^3F_4^o$	1.031×10^6	5.110×10^1		3.132×10^4		2.666×10^2
$(5s7d) {}^3D_3 \leftrightarrow (5s9s) {}^3S_1$	1.460×10^5		8.682×10^2			
$(5s8p) {}^1P_1^o \leftrightarrow (5s5f) {}^3F_3^o$	2.857×10^6		8.095×10^2			
$(5s5f) {}^3F_2^o \leftrightarrow (5s5f) {}^3F_3^o$	$> 10^8$		4.029×10^2		1.878	
$(5s5f) {}^3F_3^o \leftrightarrow (5s5f) {}^3F_4^o$	$> 10^8$		4.112×10^2		1.890	
$(5s5f) {}^3F_4^o \leftrightarrow (5s9s) {}^3S_1$	1.701×10^5			2.633×10^4		

Table IV. Comparison of the general formulas for multipole transition probabilities $A_{ba}^{(E\eta)}$ and $A_{ba}^{(M\eta)}$ expressed in SI units and customary atomic units.

	SI units	Customary units
Electric Multipole	$A_{ba}^{(E\eta)} = \mathcal{E}_\eta \frac{S^{(E\eta)}}{2h\epsilon_0\lambda^{2\eta+1}[J]}$	$A_{ba}^{(E\eta)} = \mathcal{N}_\eta^{(E)} \frac{S^{(E\eta)}}{\lambda^{2\eta+1}[J]}$
Magnetic Multipole	$A_{ba}^{(M\eta)} = \mathcal{E}_\eta \frac{\mu_0 S^{(M\eta)}}{2h\lambda^{2\eta+1}[J]}$	$A_{ba}^{(M\eta)} = \mathcal{N}_\eta^{(M)} \frac{S^{(M\eta)}}{\lambda^{2\eta+1}[J]}$

Table V. Constants of order η involved in the calculations of the multipole channels.

$\mathcal{E}_\eta$	$\mathcal{N}_\eta^{(E)}$	$\mathcal{N}_\eta^{(M)}$
$\frac{(2\eta+2)(2\eta+1)(2\pi)^{2\eta+1}}{\eta!(2\eta+1)!!^2}$	$\mathcal{E}_\eta \frac{e^2 a_0^{2\eta}}{2h\epsilon_0} (10^{20\eta+10})$	$\mathcal{E}_\eta \frac{\mu_0 \mu_B^2 a_0^{2\eta-2}}{2h} (10^{20\eta+10})$

cates that the corresponding matrix element is negligible. For some cases—particularly transitions within the $(5s4f) {}^3F_3^o$ manifold—the energy separation between the levels is below 1 cm^{-1} . Consequently, the corresponding wavelength is effectively infinite, yielding a negligible decay rate; this situation is denoted by “0” in Table VI.

The decay rate is often denoted by Γ , although for experimental purposes the more relevant quantity is typically $A_{ba}^{(\xi\eta)}/2\pi$. Some strong transitions are absent from the NIST database, such as $(5s^2) {}^1S_0 \leftrightarrow (5s7p) {}^1P_1$ or $(5s^2) {}^1S_0 \leftrightarrow (5s8p) {}^1P_1$. This omission occurs because NIST does not report transitions below 200 nm for cadmium, while this atom exhibits a substantial number of deep-UV transitions.

In most cases, a single multipole contribution dominates the decay, with contributions of the same order of

magnitude being rare. However, exceptions do exist—for example, in the transition $(5s5p) {}^3P_1^o \leftrightarrow (5s6d) {}^3D_3$, the E3 and M2 decay rates are of comparable strength.

It is noteworthy that some of the largest matrix elements correspond to decay rates well below the hertz level, highlighting the crucial role of the transition wavelength in determining the overall rate.

A comparison with the NIST database yields an average relative deviation of 18 % and a maximum relative deviation of 53 %. Only one case differs by an order of magnitude: the $(5s5p) {}^1P_1^o \leftrightarrow (5s7d) {}^1D_2$ transition. This discrepancy may stem from a misassignment in the spectroscopic interpretation of the AMBiT output. Because the computed states are strongly mixed, the identification relies on comparison of both the energy levels and the g -factors with the NIST reference. An alternative candidate assignment exists, located 2823 cm^{-1} from the reference (rather than 71 cm^{-1} as in our initial identification). For this second candidate, the calculated decay rate agrees with the NIST value. Both assignments are reported in Table VI, with the alternative shown in brackets.

The experimental uncertainties reported in the ‘NIST’ column are taken from [52]. Accounting for a more precise determination of the line wavelength, for instance, using the NIST database, does not lead to results more accurate than those reported in Table VI.

For physicists working with cadmium near the ground state $(5s^2) {}^1S_0$, most relevant transitions are already well known. Nevertheless, we draw attention to the transition at 298.3 nm with $\Gamma = 2\pi \times 256 \text{ kHz}$, which could prove useful for cooling or repumping schemes. Researchers from other fields may likewise find valuable reference data in this table for their applications.

Table VI. Spontaneous decay rate A_{ba} in s^{-1} expressed as the sum of the first five multipole decay rates $A_{ba}^{(\xi\eta)}$ and compared to the NIST database for the strongest lines.

States	$A_{ba}^{(E1)}$	$A_{ba}^{(E2)}$	$A_{ba}^{(E3)}$	$A_{ba}^{(M1)}$	$A_{ba}^{(M2)}$	A_{ba}	NIST
$(5s^2) {}^1S_0 \leftrightarrow (5s5p) {}^3P_0^o$	6.192×10^5					6.192×10^5	$4.06(102) \times 10^5$
$(5s^2) {}^1S_0 \leftrightarrow (5s5p) {}^3P_2^o$					2.183×10^{-3}	2.183×10^{-3}	
$(5s^2) {}^1S_0 \leftrightarrow (5s5p) {}^1P_1^o$	8.079×10^8					8.079×10^8	$5.3(13) \times 10^8$
$(5s^2) {}^1S_0 \leftrightarrow (5s5d) {}^1D_2$		2.350×10^3				2.350×10^3	
$(5s^2) {}^1S_0 \leftrightarrow (5s5d) {}^3D_2$		1.129				1.129	
$(5s^2) {}^1S_0 \leftrightarrow (5s6p) {}^1P_1^o$	1.202×10^8					1.202×10^8	
$(5s^2) {}^1S_0 \leftrightarrow (5s6d) {}^1D_2$		1.011×10^3				1.011×10^3	
$(5s^2) {}^1S_0 \leftrightarrow (5s6d) {}^3D_2$		7.235×10^{-2}				7.235×10^{-2}	
$(5s^2) {}^1S_0 \leftrightarrow (5s7p) {}^1P_1^o$	4.089×10^7					4.089×10^7	
$(5s^2) {}^1S_0 \leftrightarrow (5s8p) {}^1P_1^o$	2.704×10^7					2.704×10^7	
$(5s5p) {}^3P_0^o \leftrightarrow (5s5p) {}^3P_1^o$				2.854×10^{-3}		2.854×10^{-3}	
$(5s5p) {}^3P_0^o \leftrightarrow (5s5p) {}^3P_2^o$		4.796×10^{-5}				4.796×10^{-5}	
$(5s5p) {}^3P_0^o \leftrightarrow (5s5p) {}^1P_1^o$				8.526×10^{-2}		8.526×10^{-2}	
$(5s5p) {}^3P_0^o \leftrightarrow (5s6s) {}^3S_1$	1.442×10^7					1.442×10^7	$1.3(3) \times 10^7$
$(5s5p) {}^3P_0^o \leftrightarrow (5s5d) {}^1D_2$					3.579×10^{-4}	3.579×10^{-4}	
$(5s5p) {}^3P_0^o \leftrightarrow (5s5d) {}^3D_1$	9.665×10^7					9.665×10^7	$7.7(19) \times 10^7$
$(5s5p) {}^3P_0^o \leftrightarrow (5s5d) {}^3D_2$					3.846×10^{-5}	3.846×10^{-5}	
$(5s5p) {}^3P_0^o \leftrightarrow (5s5d) {}^3D_3$			9.250×10^{-13}			9.250×10^{-13}	
$(5s5p) {}^3P_0^o \leftrightarrow (5s6d) {}^3D_1$	3.627×10^7					3.627×10^7	$2.8(14) \times 10^7$
$(5s5p) {}^3P_0^o \leftrightarrow (5s6d) {}^3D_2$					1.921×10^{-5}	1.921×10^{-5}	
$(5s5p) {}^3P_0^o \leftrightarrow (5s6d) {}^3D_3$			1.883×10^{-5}			1.883×10^{-5}	
$(5s5p) {}^3P_1^o \leftrightarrow (5s5p) {}^3P_2^o$		1.648×10^{-5}		2.157×10^{-2}		2.159×10^{-2}	
$(5s5p) {}^3P_1^o \leftrightarrow (5s5p) {}^1P_1^o$		3.062×10^{-2}		5.740×10^{-2}		8.802×10^{-2}	
$(5s5p) {}^3P_1^o \leftrightarrow (5s6s) {}^3S_1$	4.193×10^7				6.085×10^{-5}	4.192×10^7	$4.1(10) \times 10^7$
$(5s5p) {}^3P_1^o \leftrightarrow (5s5d) {}^1D_2$	3.114×10^5		1.970×10^{-7}		6.823×10^{-4}	3.114×10^5	
$(5s5p) {}^3P_1^o \leftrightarrow (5s5d) {}^3D_1$	7.120×10^7				4.268×10^{-5}	7.120×10^7	$6.7(34) \times 10^7$
$(5s5p) {}^3P_1^o \leftrightarrow (5s5d) {}^3D_2$	1.276×10^8		1.207×10^{-4}		5.685×10^{-4}	1.276×10^8	$1.2(6) \times 10^8$
$(5s5p) {}^3P_1^o \leftrightarrow (5s5d) {}^3D_3$			1.719×10^{-4}		4.362×10^{-5}	2.156×10^{-4}	
$(5s5p) {}^3P_1^o \leftrightarrow (5s6d) {}^3D_1$	2.615×10^7				2.321×10^{-5}	2.615×10^7	$2.4(12) \times 10^7$
$(5s5p) {}^3P_1^o \leftrightarrow (5s6d) {}^3D_2$	4.760×10^7		2.308×10^{-5}		2.985×10^{-4}	4.760×10^7	$4.2(21) \times 10^7$
$(5s5p) {}^3P_1^o \leftrightarrow (5s6d) {}^3D_3$			3.358×10^{-5}		2.332×10^{-5}	5.690×10^{-5}	
$(5s5p) {}^3P_2^o \leftrightarrow (5s6s) {}^3S_1$	6.545×10^7				1.686×10^{-4}	6.545×10^7	$5.6(14) \times 10^7$
$(5s5p) {}^3P_2^o \leftrightarrow (5s5d) {}^1D_2$	7.261×10^4		1.038×10^{-7}		4.877×10^{-4}	7.261×10^4	
$(5s5p) {}^3P_2^o \leftrightarrow (5s5d) {}^3D_1$	4.510×10^6		3.109×10^{-4}		8.591×10^{-8}	4.510×10^6	
$(5s5p) {}^3P_2^o \leftrightarrow (5s5d) {}^3D_2$	4.064×10^7		2.075×10^{-4}		2.441×10^{-4}	4.064×10^7	$3.5(18) \times 10^7$
$(5s5p) {}^3P_2^o \leftrightarrow (5s5d) {}^3D_3$	1.637×10^8		8.951×10^{-5}		1.579×10^{-3}	1.637×10^8	$1.3(7) \times 10^8$
$(5s5p) {}^3P_2^o \leftrightarrow (5s6d) {}^3D_1$	1.608×10^6		5.255×10^{-5}		6.644×10^{-8}	1.608×10^6	
$(5s5p) {}^3P_2^o \leftrightarrow (5s6d) {}^3D_2$	1.466×10^7		3.556×10^{-5}		1.392×10^{-3}	1.466×10^7	$1.5(8) \times 10^7$
$(5s5p) {}^3P_2^o \leftrightarrow (5s6d) {}^3D_3$	5.977×10^7		1.557×10^{-5}		8.506×10^{-4}	5.977×10^7	$5.9(29) \times 10^7$
$(5s5p) {}^1P_1^o \leftrightarrow (5s5d) {}^1D_2$	5.023×10^7		2.280×10^{-5}		5.723×10^{-5}	5.023×10^7	$5.9(29) \times 10^7$
$(5s5p) {}^1P_1^o \leftrightarrow (5s6d) {}^1D_2$	3.931×10^6		4.186×10^{-6}		2.276×10^{-5}	3.932×10^6	$5.5(14) \times 10^6$
$(5s5p) {}^1P_1^o \leftrightarrow (5s7d) {}^1D_2$	1.881×10^5		4.991×10^{-6}		1.193×10^{-5}	1.885×10^5	$4.7(24) \times 10^6$
$((5s5p) {}^1P_1^o \leftrightarrow (5s7d) {}^1D_2)$	(1.035×10^6)		(4.991×10^{-6})		(1.193×10^{-5})	(1.035×10^6)	$4.7(24) \times 10^6$
$(5s5d) {}^3D_1 \leftrightarrow (5s5d) {}^3D_2$		3.300×10^{-14}		4.194×10^{-8}		4.194×10^{-8}	
$(5s5d) {}^3D_2 \leftrightarrow (5s5d) {}^3D_3$		2.057×10^{-13}		1.047×10^{-7}		1.047×10^{-7}	
$(5s7p) {}^3P_2^o \leftrightarrow (5s6d) {}^3D_3$	6.664×10^3		3.911×10^{-15}		6.116×10^{-12}	6.664×10^3	
$(5s7p) {}^3P_2^o \leftrightarrow (5s5f) {}^3F_4^o$		1.591				1.591	
$(5s6d) {}^3D_1 \leftrightarrow (5s6d) {}^3D_2$		1.836×10^{-14}		5.239×10^{-9}		5.239×10^{-9}	
$(5s6d) {}^3D_2 \leftrightarrow (5s6d) {}^3D_3$		6.349×10^{-14}		9.205×10^{-9}		9.205×10^{-9}	
$(5s6d) {}^3D_2 \leftrightarrow (5s4f) {}^3F_3^o$	1.868×10^3		1.486×10^{-16}		1.594×10^{-12}	1.868×10^3	
$(5s6d) {}^3D_3 \leftrightarrow (5s4f) {}^3F_4^o$	2.331×10^3		6.903×10^{-16}		2.243×10^{-12}	2.331×10^3	
$(5s6d) {}^3D_3 \leftrightarrow (5s5f) {}^3F_4^o$	2.968×10^6		6.766×10^{-8}		4.420×10^{-7}	2.968×10^6	
$(5s4f) {}^3F_2^o \leftrightarrow (5s4f) {}^3F_3^o$		0		0		0	
$(5s4f) {}^3F_3^o \leftrightarrow (5s4f) {}^3F_4^o$		0		0		0	
$(5s8s) {}^3S_1 \leftrightarrow (5s8p) {}^3P_2^o$	6.205×10^5		2.072×10^{-18}		5.850×10^{-9}	6.205×10^5	
$(5s8s) {}^3S_1 \leftrightarrow (5s7d) {}^3D_2$		5.817×10^{-2}				5.817×10^{-2}	
$(5s8s) {}^3S_1 \leftrightarrow (5s7d) {}^3D_3$		5.899×10^{-2}				5.899×10^{-2}	
$(5s8s) {}^3S_1 \leftrightarrow (5s5f) {}^3F_4^o$			3.799×10^{-9}			3.799×10^{-9}	
$(5s8s) {}^1S_0 \leftrightarrow (5s7d) {}^1D_2$		1.207×10^{-2}				1.207×10^{-2}	
$(5s8p) {}^3P_1^o \leftrightarrow (5s8p) {}^3P_2^o$		7.925×10^{-10}		4.792×10^{-7}		4.800×10^{-7}	

States	$A_{ba}^{(E1)}$	$A_{ba}^{(E2)}$	$A_{ba}^{(E3)}$	$A_{ba}^{(M1)}$	$A_{ba}^{(M2)}$	A_{ba}	NIST
$(5s8p) {}^3P_1^o \leftrightarrow (5s7d) {}^3D_2$	1.732×10^3		5.682×10^{-16}		1.872×10^{-13}	1.732×10^3	
$(5s8p) {}^3P_1^o \leftrightarrow (5s7d) {}^3D_3$			9.742×10^{-16}		3.007×10^{-14}	3.105×10^{-14}	
$(5s8p) {}^3P_2^o \leftrightarrow (5s7d) {}^3D_1$	2.841×10^1		2.561×10^{-16}		2.157×10^{-20}	2.841×10^1	
$(5s8p) {}^3P_2^o \leftrightarrow (5s7d) {}^3D_2$	2.767×10^2		2.047×10^{-16}		2.692×10^{-14}	2.767×10^2	
$(5s8p) {}^3P_2^o \leftrightarrow (5s7d) {}^3D_3$	1.226×10^3		1.110×10^{-16}		2.241×10^{-13}	1.226×10^3	
$(5s8p) {}^3P_2^o \leftrightarrow (5s5f) {}^3F_4^o$		1.068×10^{-5}				1.068×10^{-5}	
$(5s7d) {}^1D_2 \leftrightarrow (5s8p) {}^1P_1^o$	9.957×10^3		3.718×10^{-14}		1.741×10^{-12}	9.957×10^3	
$(5s7d) {}^1D_2 \leftrightarrow (5s5f) {}^3F_3^o$	4.731×10^3		1.836×10^{-14}		5.181×10^{-12}	4.731×10^3	
$(5s7d) {}^1D_2 \leftrightarrow (5s5f) {}^3F_4^o$			4.231×10^{-19}		2.958×10^{-12}	2.958×10^{-12}	
$(5s7d) {}^3D_1 \leftrightarrow (5s7d) {}^3D_2$		2.506×10^{-15}		6.555×10^{-10}		6.555×10^{-10}	
$(5s7d) {}^3D_1 \leftrightarrow (5s5f) {}^3F_2^o$	5.568×10^2		1.769×10^{-17}		1.233×10^{-14}	5.568×10^2	
$(5s7d) {}^3D_2 \leftrightarrow (5s7d) {}^3D_3$		8.628×10^{-15}		1.151×10^{-9}		1.151×10^{-9}	
$(5s7d) {}^3D_2 \leftrightarrow (5s5f) {}^3F_3^o$	2.884×10^2		4.091×10^{-18}		6.967×10^{-14}	2.884×10^2	
$(5s7d) {}^3D_2 \leftrightarrow (5s9s) {}^3S_1$		3.107×10^{-3}				3.107×10^{-3}	
$(5s7d) {}^3D_3 \leftrightarrow (5s8p) {}^1P_1^o$			3.893×10^{-20}		5.538×10^{-15}	5.538×10^{-15}	
$(5s7d) {}^3D_3 \leftrightarrow (5s5f) {}^3F_4^o$	5.363×10^2		2.768×10^{-17}		1.011×10^{-13}	5.363×10^2	
$(5s7d) {}^3D_3 \leftrightarrow (5s9s) {}^3S_1$		4.242×10^{-3}				4.242×10^{-3}	
$(5s8p) {}^1P_1^o \leftrightarrow (5s5f) {}^3F_3^o$		5.508×10^{-10}				5.508×10^{-10}	
$(5s5f) {}^3F_2^o \leftrightarrow (5s5f) {}^3F_3^o$		0		0		0	
$(5s5f) {}^3F_3^o \leftrightarrow (5s5f) {}^3F_4^o$		0		0		0	
$(5s5f) {}^3F_4^o \leftrightarrow (5s9s) {}^3S_1$			1.764×10^{-11}			1.764×10^{-11}	

C. Transitions to metastable ${}^3P_0^o$ and ${}^3P_2^o$ states

In atomic physics, a particular class of transitions, known as clock transitions, is of special interest for metrological applications. Such transitions must exhibit minimal sensitivity to external perturbations and involve two states with exceptionally long lifetimes. Cadmium, like other bosonic alkaline-earth-like elements, demonstrates extremely low sensitivity to stray electric and magnetic fields due to the absence of spin in its ground state [64]. Moreover, cadmium possesses two states with lifetimes sufficiently long to serve as clock transitions: $(5s5p) {}^3P_0^o$ and $(5s5p) {}^3P_2^o$.

For the fermionic isotope, the nonzero nuclear magnetic dipole moment induces hyperfine coupling, which mixes the $(5s5p) {}^3P_0^o$ and $(5s5p) {}^3P_2^o$ states with other states of the same parity, particularly the states $(5s5p) {}^3P_1^o$ and $(5s5p) {}^1P_1^o$. These mixed states can decay to the ground state via a standard electric dipole process, resulting in lifetimes on the order of 100 s [30].

In contrast, this hyperfine-mediated decay mechanism is absent for bosonic isotopes, so the decay rate is dominated by alternative channels. The $(5s5p) {}^3P_2^o$ state can decay to the $(5s^2) {}^1S_0$ ground state via a magnetic quadrupole transition, with a rate on the order of the millihertz. This behavior is comparable to that observed in Mg, Ca, and Sr, which have similar electronic structures [65]. Such a transition has been extensively studied in Sr [66]. Since the $(5s5p) {}^3P_1^o \leftrightarrow (5s5p) {}^3P_2^o$ transition is estimated to decay roughly an order of magnitude faster, the $(5s5p) {}^3P_2^o$ state may not be an ideal candidate for a clock transition.

On the other hand, the $(5s^2) {}^1S_0 \leftrightarrow (5s5p) {}^3P_0^o$ transition is strictly forbidden under all single-photon multi-

pole channels due to the $J = 0 \not\leftrightarrow J = 0$ selection rule. The only allowed decay channel is the two-photon E1M1 process, in which the $(5s5p) {}^3P_0^o$ state is coupled virtually to an intermediate state of the same parity via an M1 transition, followed by an E1 transition to the ground state [67].

$$A^{(E1M1)} = \frac{8}{27\pi} \alpha^6 \int_0^\Delta \omega^3 (\Delta - \omega)^3 |S(\omega, \Delta - \omega)|^2 d\omega \quad (14)$$

with Δ the energy difference between the initial state E_i : $(5s^5p) {}^3P_0$ denoted $|i\rangle$ and the final state E_f : $(5s^2) {}^1S_0$ denoted $|f\rangle$. This energy difference is equal to 30114 cm^{-1} and the two photons E1M1 line strength $S(\omega, \Delta - \omega)$ is defined in general by

$$S(\omega_1, \omega_2) = \sum_{n+} \frac{\langle f | \mathbf{O}^{(M1)} | n+ \rangle \langle n+ | \mathbf{O}^{(E1)} | i \rangle}{E_{n+} - E_i + \omega_1} + \sum_{n-} \frac{\langle f | \mathbf{O}^{(E1)} | n- \rangle \langle n- | \mathbf{O}^{(M1)} | i \rangle}{E_{n-} - E_i + \omega_2} \quad (15)$$

For bosonic cadmium, the lifetime of the upper $(5s5p) {}^3P_0$ state is consequently estimated to be on the order of 40 years. Table VII presents a comparison of neutral cadmium decay rates with those of other alkaline-earth-like atoms.

V. C6 LONG-RANGE DISPERSION COEFFICIENT

In the study of ultra-cold gases, atomic interactions play a central role and give rise to many of the most

Table VII. Comparison of decay rates (in s^{-1}) for the cadmium clock transition $(5s^2) ^1\text{S}_0 \leftrightarrow (5s5p) ^3\text{P}_0$ clock transition in bosonic and fermionic cadmium with those of other alkaline-earth-like species.

	Bosons	Fermions
Cd	8.8×10^{-10} (present work)	4.4×10^{-2} (^{111}Cd) [30] 4.8×10^{-2} (^{113}Cd) [30]
Sr [65, 68]	5.5×10^{-12}	9×10^{-3}
Ca [65, 68]	3.9×10^{-13}	3×10^{-3}
Mg [65, 68]	1.6×10^{-13}	9×10^{-4}

striking and useful phenomena [69, 70]. These interactions become important when atoms are cooled below the μK level, where even weak forces can strongly influence the behavior of the system. To describe these interactions accurately, it is essential to understand the interatomic potential, especially its behavior at large separations where long-range forces dominate. However, while the scattering length—a key quantity characterizing low-energy collisions—is highly sensitive to these long-range parameters, it cannot be reliably determined from them alone [71]. A meaningful prediction of the scattering length requires not only knowledge of the asymptotic form of the potential but also information about the short-range interactions, where atoms approach closely and exchange becomes significant. Thus, both regions of the potential must be considered together to provide a realistic description of cold collisions.

When considering two identical cadmium atoms in the electronic ground state $|f\rangle$ separated by a distance R , their long-range interaction is governed by the leading term of the van der Waals potential, $-C_6/R^6$. The dispersion coefficient C_6 plays a central role in the description of low-energy atomic collisions and can be expressed in terms of E1 transition matrix elements [72–74]:

$$C_6 = \frac{2}{3} \sum_{i,j} \frac{|\langle i | \mathbf{O}^{(E1)} | f \rangle|^2 |\langle j | \mathbf{O}^{(E1)} | f \rangle|^2}{E_i + E_j - 2E_f}, \quad (16)$$

where E_k is the energy of a state $|k\rangle$, and the zero of energy is taken at the ground state.

Table VIII. Comparison of C_6 coefficients in a.u. for neutral cadmium in the ground state from different sources.

[75]	[76]	[76]a	[76]b	[76]c	[41]a	[41]b	[77]	[78]	[39]	Present
466	372	509	611	417	511	840	686	401(8)	395	

Table VIII compares the different values of C_6 analytically [41, 76, 77], via dispersion of the refractive index [75], and via measurement of the magic wavelength [39]. The present calculation yields $C_6 = 395$ a.u.,

in agreement with the value 401 a.u. reported by Yamaguchi *et al.* This agreement is expected, as both approaches rely on the same fundamental formalism but differ in the determination of the underlying matrix elements. Including contributions from higher-lying states [26] modifies the result by less than 1 %, since the dominant term in the sum arises from the strong E1 coupling between the ground state and the $(5s5p) ^1\text{P}_1$ state.

VI. CONCLUSION

We have presented a comprehensive study of the atomic structure and long-range interactions of neutral cadmium using the CI+MBPT framework. General expressions for multipole matrix elements of arbitrary order were derived and applied to evaluate electric and magnetic transition amplitudes, including E1–E3 and M1–M2 processes.

These matrix elements were further employed to compute the lifetimes of the principal transitions relevant to laser cooling and atomic clock applications, including the bosonic clock transition, which has not previously been reported. In addition, they enabled the determination of the long-range van der Waals coefficient C_6 .

The computed energy levels and E1 matrix elements of the strongest transitions are in agreement with available experimental data, thereby validating the accuracy of the CI+MBPT approach for neutral cadmium. Remarkably, these results were obtained on a standard desktop workstation with 48 GB of RAM, with a total computation time on the order of ten hours.

The accurate characterization of the electronic level structure, together with the precise evaluation of the C_6 dispersion coefficient, provides essential groundwork for future investigations of the s -wave scattering length in neutral cadmium.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [79].

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