Calculations of atomic structures and electron impact excitation cross-sections of B-like Xe^{49+}

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INTRODUCTION

- Chemical inertness of Xe makes them befitting candidates for use in tokamaks, fusion plasma research and diagnosis.
- In the high temperature of the fusion reactor like ITER, all possible ionization stages of Xe up to helium-like Xe^{52+} can exist.
- Xenon ions are a potential extreme ultraviolet (EUV) laser sources for next generation lithography and their spectra are also observed in planetary nebula.
- Spectroscopic data on highly charged ions of Xe is essential to interpret the spectra correctly and to model the conditions in plasma containing these species.
- Previous results of the lowest 125 levels of Xe^{49+} are available.
- Multiconfiguration Dirac-Hartree-Fock (MCDHF) method is used to calculate the energies, electric dipole (E1) and quadrupole (E2), magnetic dipole (M1) and quadrupole (M2) transition parameters for the lowest 255 levels of B-like Xe^{49+}.
- The Relativistic Distorted Wave theory is implemented to obtain the electron impact excitation cross sections with our obtained atomic wave functions.
- The excitation rate coefficients are obtained in the temperature range of 5 – 100 eV considering the electron energy distribution to be Maxwellian in nature.

COMPUTATIONAL PROCEDURE

The Dirac – Coulomb Hamiltonian

$$H_{DC} = \sum_{i=1}^{N}\left(c\,\boldsymbol{\alpha}_i.\boldsymbol{p}_i + V_{nuc}(r_i) + c^2(\beta_i - 1)\right) + \sum_{j>i=1}^{N}\frac{1}{r_{ij}}$$

The atomic state function in MCDHF

$$\Psi(\mathrm{PJM}) = \sum_{i=1}^{n} a_i \Phi_i(PJM)$$

Transition matrix from electron impact excitation from state a to state b

$$T_{a\to b} = <\Psi_b(\mathbf{1},\mathbf{2},\ldots,\boldsymbol{n})F_b^{DW-}(\boldsymbol{k_b},\boldsymbol{n}+\mathbf{1}) \mid V_{in} - U_d(n+1) \mid \boldsymbol{A}\,\Psi_a(\mathbf{1},\mathbf{2},\ldots,\boldsymbol{n})F_a^{DW+}(\boldsymbol{k_a},\boldsymbol{n}+\mathbf{1})>$$

Integrated Excitation cross sections

$$\sigma_{a\to b} = (2\pi)^4 \frac{k_b}{k_a}\frac{1}{2(2J_a+1)}\sum_{M_a\mu_a M_b\mu_b}\int \left|T_{a\to b}^{RDW}\right|^2 d\omega$$

Rational polynomial fitting and Logarithmic fitting for cross-sections

$$\sigma_{a\to b} = \frac{\sum_i^n x_i E^i}{1 + y_1 E + y_2 E^2}\;, \qquad \sigma_{a\to b} = \frac{1}{E}\left(\mathrm{d}_0 + \mathrm{d}_1 \ln \mathrm{E}\right)$$

Excitation rate coefficients in Maxwellian electron energy distribution function

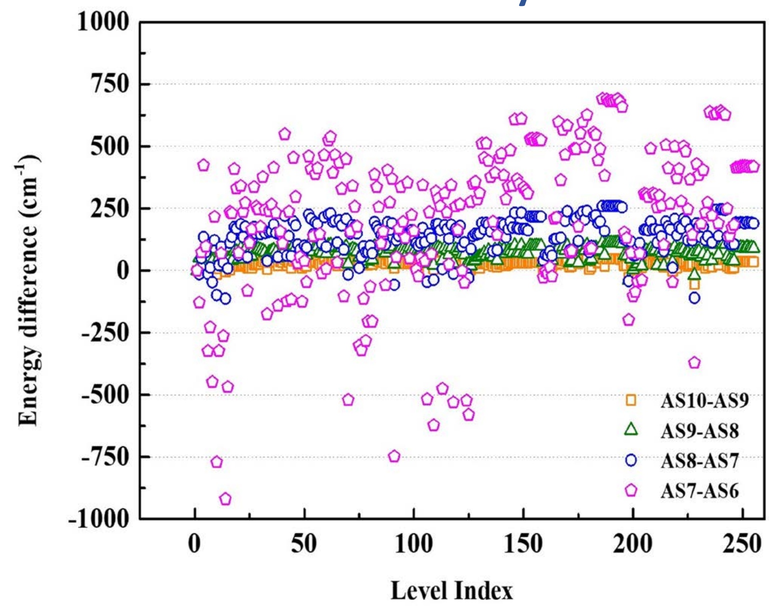
$$\gamma_{a\to b} = 2\left(\frac{2}{\pi m_e}\right)^{\frac{1}{2}}(k_B T)^{-3/2}\int_{E_{ab}}^{\infty}\sigma_{a\to b}\exp\left(-\frac{E_b}{k_B T}\right)d(E)$$

Atomic Structure Results

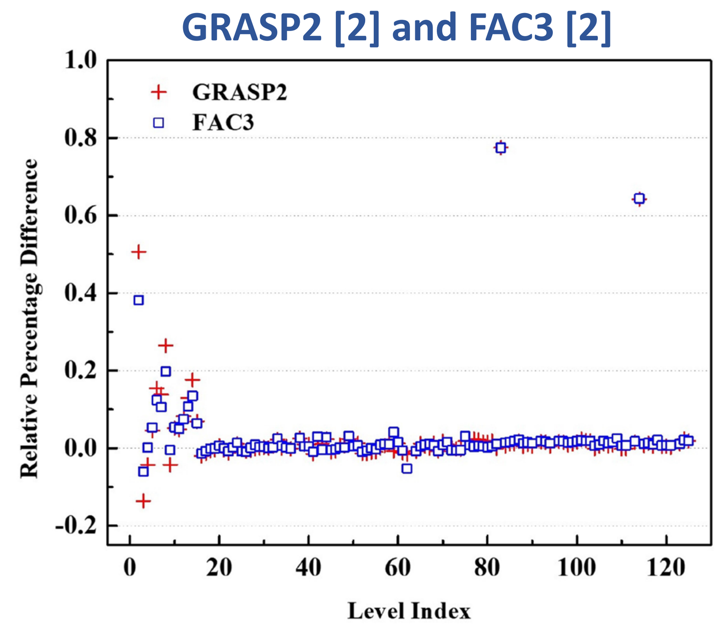
Number of CSFs generated in active layers

AS Layer	Number of CSFs odd	Number of CSFs even
AS5 = $5s,\ 5p,\ 5d,\ 5f$	7343	7322
AS6 = $6s,\ 6p,\ 6d,\ 6f$	16004	15998
AS7 = $7s,\ 7p,\ 7d,\ 7f$	28209	28179
AS8 = $8s,\ 8p,\ 8d,\ 8f$	43955	43808
AS9 = $9s,\ 9p,\ 9d,\ 9f$	63236	63071
AS10 = $10s,\ 10p,\ 10d,\ 10f$	86052	85788

Energy difference between consecutive active set layers



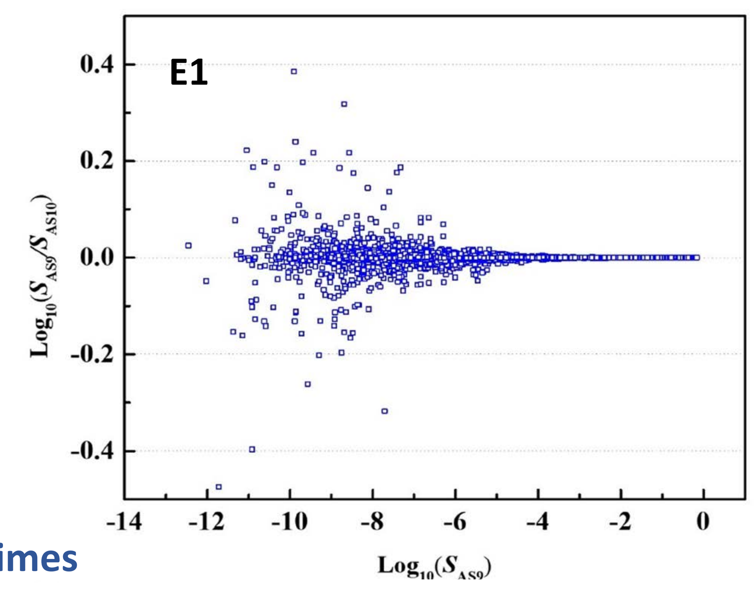
Relative percentage difference with GRASP2 [2] and FAC3 [2]

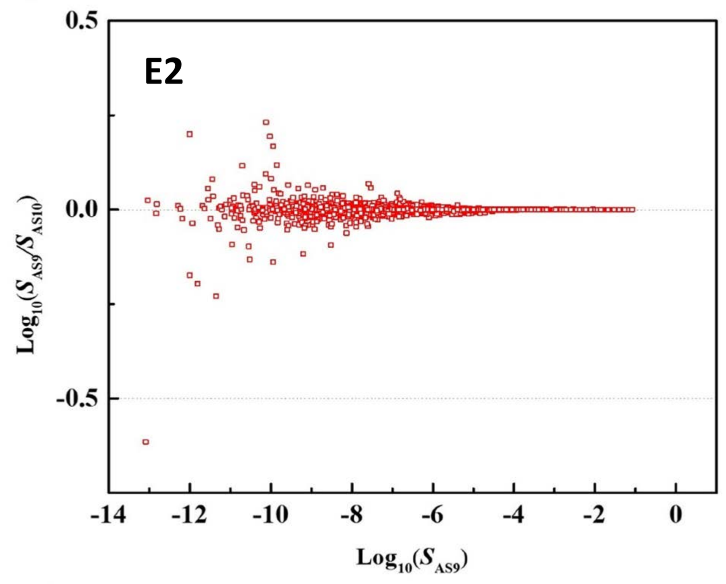


Percentage of S values lying in the NIST accuracy class

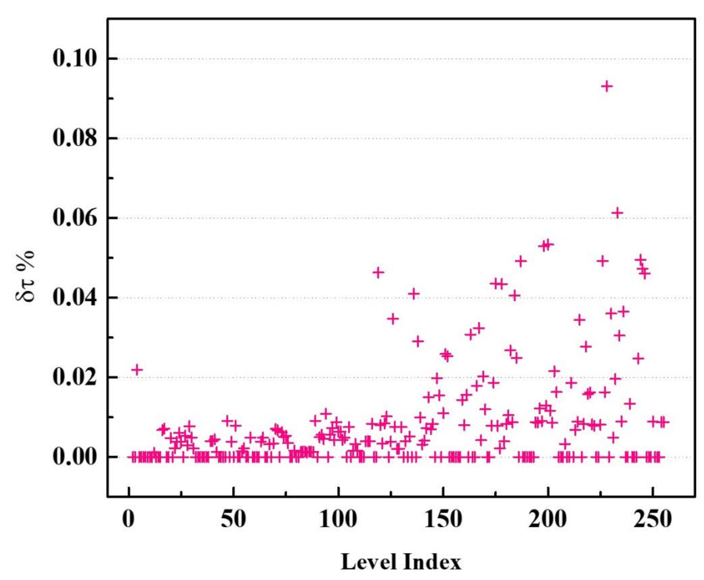
Accuracy class	E1	E2	M1	M2
	Percentage of Transitions			
$A+$ ($\leq 2\%$)	80	61	98.8	85.7
A ($\leq 3\%$)	4	6	0.5	6
$B+$ ($\leq 7\%$)	6	19	0.5	6
B ($\leq 10\%$)	2	14	0.1	1
$C+$ ($\leq 18\%$)	3	0	0.1	1
C ($\leq 25\%$)	1	0	0	0.1
$D+$ ($\leq 44\%$)	2	0	0	0.1
D ($\leq 54\%$)	0	0	0	0
E ($> 54\%$)	1	0	0	0

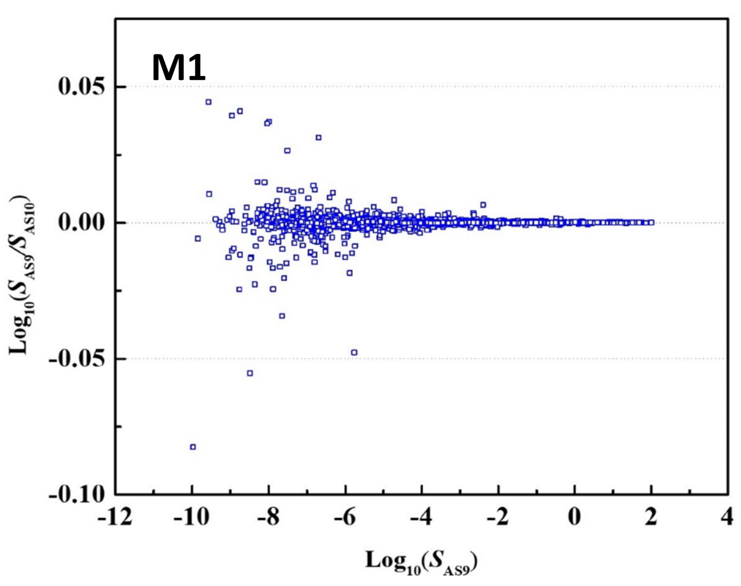
Agreement between the line strengths of AS10 and AS9 for E1, M1, E2 and M2 transitions

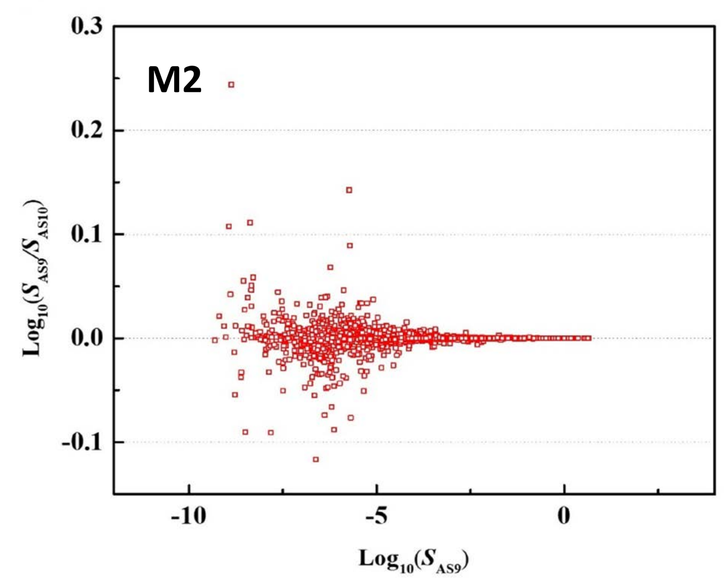




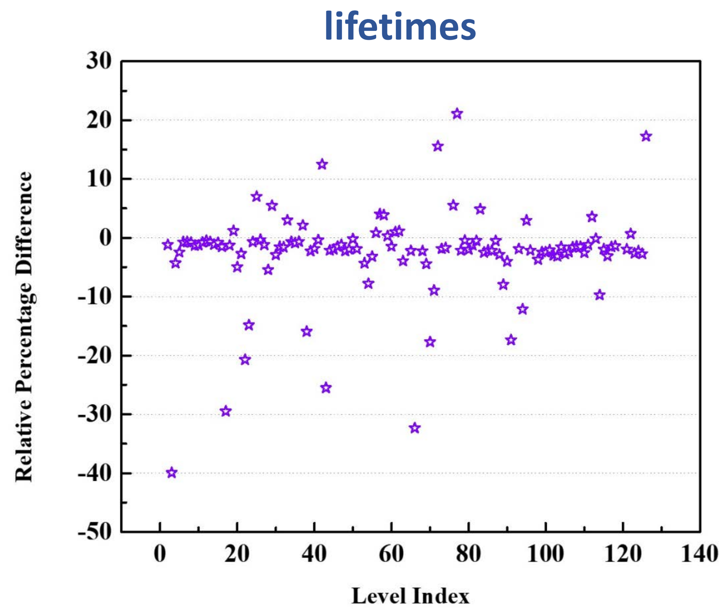
The uncertainty ($\delta\tau$ %) in the present lifetimes



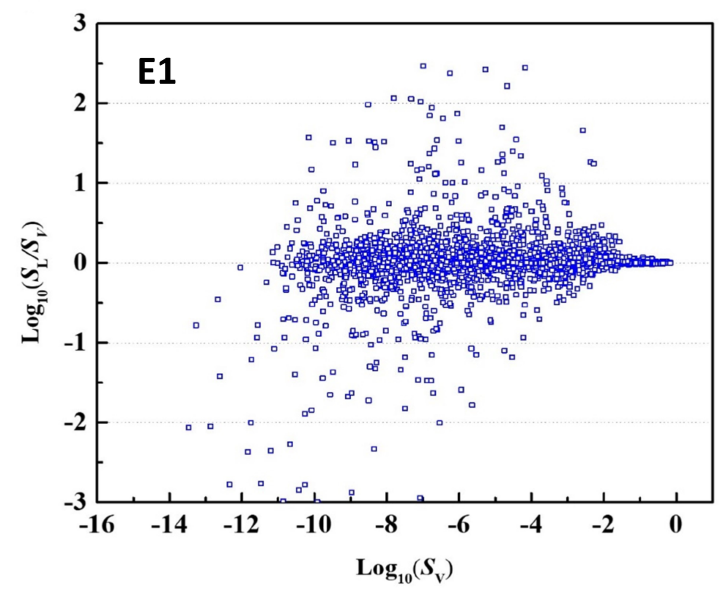


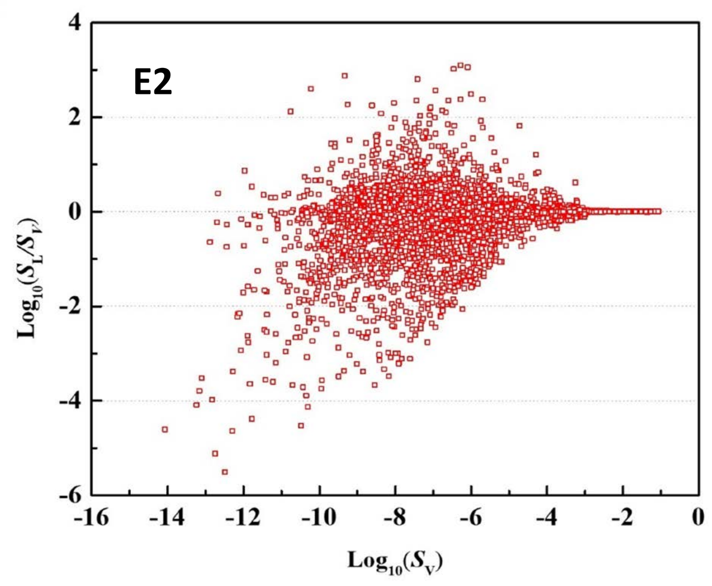


Relative percentage difference between the present and Aggarwal et al. [2] lifetimes



Agreement between the line strengths in velocity (S_V) and length (S_L) gauges





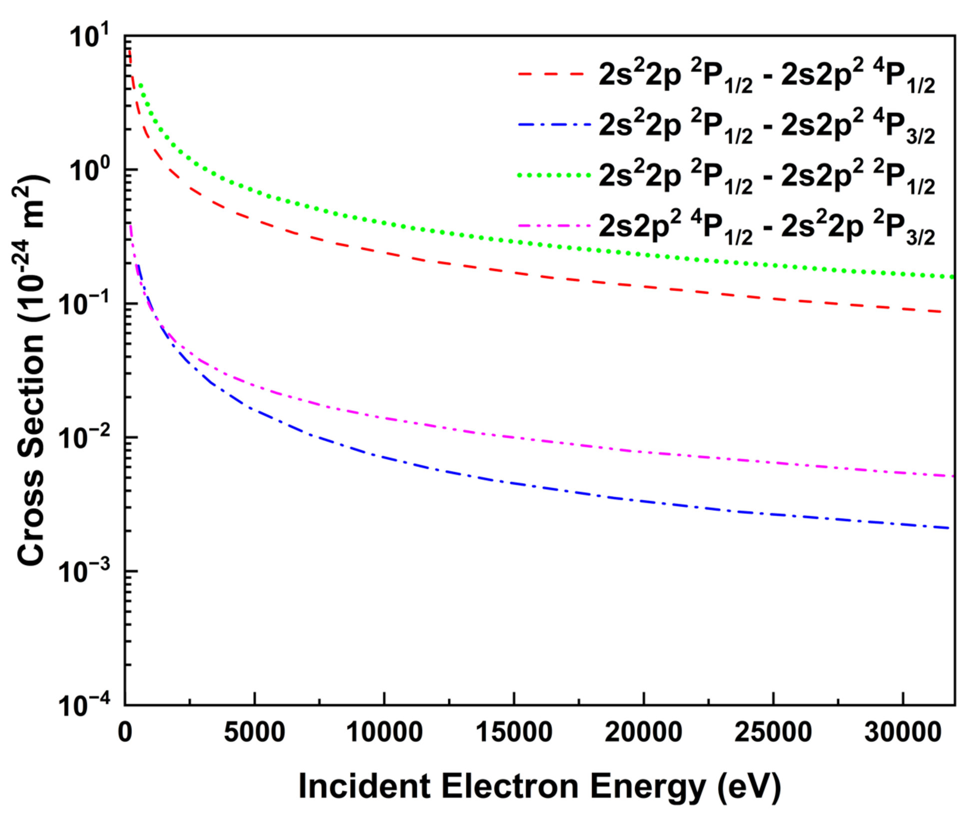
Contribution of Breit, self-energy and vacuum polarization and comparison with Aggarwal et al. [2]

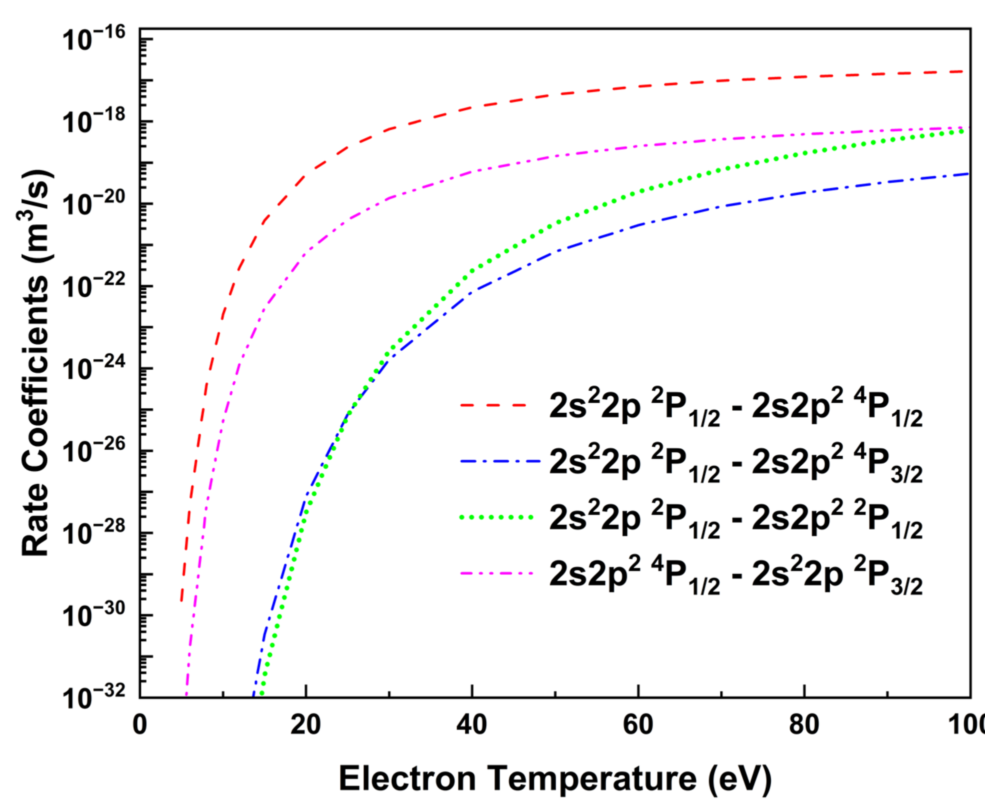
Level	MCDHF	Breit	SE	VP	Total	Other
$2s2p^2\ ^4P_{1/2}$	163.0	6.7	-7.1	0.9	163.5	164.3
$2s^22p\ ^2P_{3/2}$	363.9	-5.8	0.4	0.1	358.6	358.1
$2s2p^2\ ^4P_{3/2}$	477.5	0.8	- 6.5	0.9	472.6	472.4
$2s2p^2\ ^2D_{5/2}$	513.1	- 3.1	- 6.5	0.9	504.4	504.6
$2s2p^2\ ^2D_{3/2}$	561.5	-1.3	-6.5	0.9	554.6	555.5
$2s2p^2\ ^2P_{1/2}$	559.4	1.1	-6.5	0.9	554.9	555.7
$2p^3\ ^2D_{3/2}$	735.2	6.1	-13.5	1.8	729.6	731.6
$2s2p^2\ ^4P_{5/2}$	861.5	-7.0	-6.0	1.0	849.4	849.0
$2s2p^2\ ^2S_{1/2}$	931.4	-3.2	-6.0	1.0	923.2	923.6
$2s2p^2\ ^2P_{3/2}$	935.4	-6.0	- 6.0	1.0	924.4	924.9
$2p^3\ ^4S_{3/2}$	1067.0	0.7	-13.1	1.9	1056.5	1057.3
$2p^3\ ^2D_{5/2}$	1090.5	-3.1	-13.1	1.9	1076.1	1077.5
$2p^3\ ^2P_{1/2}$	1123.7	1.9	-13.1	1.9	1114.4	1116.4
$2p^3\ ^2P_{3/2}$	1463.4	- 5.1	-12.5	1.9	1447.6	1448.6

Hyperfine Interaction constants, Landé g_J-factor and Isotope shift factors

Level	A_J (MHz/μ_I)	B_J (10^5 MHz/barn)	Lande′g_J factor	NMS (10^3 a.u.)	SMS (10^2 a.u.)	FS (10^4 GHz/fm^2)
$2s^2\,2p\ ^2P_{1/2}$	2.039E+06	0.000	0.64186	3.903	-1.846	6.866
$2s2p^2\ ^4P_{1/2}$	6.187E+06	0.000	2.17134	3.898	-3.655	6.479
$2s2p\ ^2P_{3/2}$	3.182E+05	5.921	1.31428	3.890	-1.982	6.847
$2s2p^2\ ^4P_{3/2}$	1.623E+06	4.679	1.65402	3.888	-3.759	6.469
$2s2p^2\ ^2D_{5/2}$	1.862E+06	3.972	1.35073	3.887	-3.765	6.478
$2s2p^2\ ^2D_{3/2}$	1.848E+04	3.736	0.96449	3.886	-3.749	6.466
$2s2p^2\ ^2P_{1/2}$	-2.034E+06	0.000	1.21692	3.886	-3.738	6.466
$2p^3\ ^2D_{3/2}$	2.934E+05	5.464	1.35723	3.882	-5.497	6.086
$2s2p^2\ ^4P_{5/2}$	1.548E+06	1.938	1.40759	3.875	-3.852	6.457
$2s2p^2\ ^2S_{1/2}$	6.373E+06	0.000	1.87987	3.873	-3.811	6.456
$2s2p^2\ ^2P_{3/2}$	-8.795E+05	-1.351	1.19049	3.874	-3.829	6.454
$2p^3\ ^4S_{3/2}$	-3.339E+04	0.727	1.43631	3.870	-5.641	6.066
$2p^3\ ^2D_{5/2}$	6.537E+05	-0.022	1.17983	3.869	-5.652	6.066
$2p^3\ ^2P_{1/2}$	2.038E+06	0.000	0.64193	3.868	-5.601	6.068
$2p^3\ ^2P_{3/2}$	3.172E+05	-6.176	1.28372	3.857	-5.707	6.056

Excitation Cross-sections and Rate Coefficients





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2. Aggarwal, K.M., Keenan, F.P. and Lawson, K.D. *Atomic Data and Nuclear Data Tables*, **2010**, *96*(2), 123-270.
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