Resonance and intercombination lines in Mg-like ions of atomic numbers Z=13–92

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Resonance and intercombination lines in Mg-like ions of atomic numbers Z=13-92

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While prominent lines of various Na-like ions have been measured with an accuracy of better than 100 ppm and corroborate equally accurate calculations, there have been remarkably large discrepancies between calculations for Mg-like ions of high atomic number. We present *ab initio* calculations using the Multi-Reference Møller-Plesset (MR-MP) approach for Mg-like ions of atomic numbers Z=13-92 and compare the results with other calculations of this isoelectronic sequence as well as with experimental data. Our results come very close to experiment (typically 100 ppm) over a wide range. Data at high values of Z are sparse, which calls for further accurate measurements in this range where relativistic and QED effects are large.

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I. INTRODUCTION

Ions with a single electron outside a core of closed electronic shells, such as in the ions of the Li, Na and Cu isoelectronic sequences, can be calculated very well [1–3] and also be measured rather accurately (see [4–12] and references therein), helped by the often bright appearance of the resonance lines. In many observations of hot plasmas and other light sources the resonance lines of alkaline earth-like ions are also seen brightly and at wavelengths close to their alkali-like ion counterparts. Hence those lines should be measurable with high precision, with the same information content as in single-valence electron ions as far as quantum electrodynamical (QED) contributions to the atomic structure are concerned. However, while there are measurements of the $3s^2$-3s3p $^{1,3}P^o_1$ transitions of Mg-like ions (in LS coupling notation) of practically all elements up to Z=55 (see the NIST on-line data base [13] and [7, 14–21]), there are very few such measurements of Mg-like ions in the Z range beyond [9, 10, 12, 22, 23]. Moreover, older measurements in this range have operated at the limit of what laser-produced plasmas could achieve at the time. A comparison of laser-produced plasma data on Na-like ions with the results of accurate measurements using electron beam ion traps (see the data and discussion in [12]) and with the results of high-quality *ab initio* calculations [2, 3, 11] suggests the presence of underestimated systematic errors in some of those experiments. It would be surprising if similar problems were not present also in the measurement of Mg-like ion spectra.

The most recent study of europium (Eu, Z=63) [12] has yielded high precision wavelength data (with an uncertainty below 100 ppm) on 3s-$3p_{3/2}$ transitions in, both, Na-like Eu^{52+} and Mg-like Eu^{51+}, ions. Quite a number of calculations have addressed Mg-like ions (see discussion below), and a number of them have produced results close to measurement at much lower values of Z. However, as we demonstrate, none so far combines meaningful accuracy and wide and continuous coverage of the table of elements (as are available for Na-like ions). We therefore have employed the Multi-Reference Møller-Plesset approach and computed *ab initio* energies of the $nsnp$ and np^2 n=3 levels of all elements up to Z=118 [24]. Out of these calculations we present here energies for the two lowest J=1 levels of Mg-like ions up to uranium (Z=92). In low-Z ions, the decays of these levels are called the resonance and intercombination transitions, both of which are prominent in the spectra of many light sources.

We compare our results with earlier computational work and with measurements. The new calculations reduce the difference between measurement and calculation by more than an order of magnitude for rare-earth elements such as Eu and thus come close to the accuracy of the best calculations on Na-like ions. Only in the comparison between such accurate calculations and the recent experimental findings one can recognize details in the isoelectronic trend that point at difficulties with some experimental data, as have recently been demonstrated with other isoelectronic sequences with one (mentioned above) or two valence shell electrons, such as the Zn sequence [25–28].

II. EXPERIMENTAL DATA

For ions of moderate charge state, measurements of Mg-like spectra have begun in the 1930s, employing various types of vacuum sparks. Since the 1970s, plasma discharges such as the tokamak and laser-produced plas-

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mas have given access to higher charge states [14–18], reaching Z=55 in the work of Ekberg et al. [16, 18]. Beyond Z=55, very few elements have been studied for the resonance and intercombination transitions in Mg-like ions, employing a foil-excited fast ion beam [22, 23] (with the Doppler effect playing a major role for measurement uncertainty) or electron beam ion traps [9–12, 20, 21, 23, 25]. The best of the measurements have reached uncertainties of less than 100 ppm. For a detailed comparison with theory, it is best to subtract the gross isoelectronic trend expected for such data. However, while the low-Z trend of the Δn=0 transition energy should be linear in Z (electrostatic interaction), relativity plays a major role for moderate and higher Z [30], and for high-Z elements QED corrections become sizable. Therefore we present the experimental data points by their deviation from a computation that includes these contributions. This brings up a key problem: Prior to this work there existed no published computation of these entities for Mg-like ions of all elements. Curtis had developed isoelectronic smoothing techniques to cope with such incomplete data sets (for Mg-like ions see [31]), but we are aiming at assessing accuracy and thus want to avoid secondary data. We therefore have opted to perform our own calculations in an isoelectronically consistent manner (described below) and then use the results as a reference for the graphical representation of the experimental data and the results of other computations in figures 1 and 2.

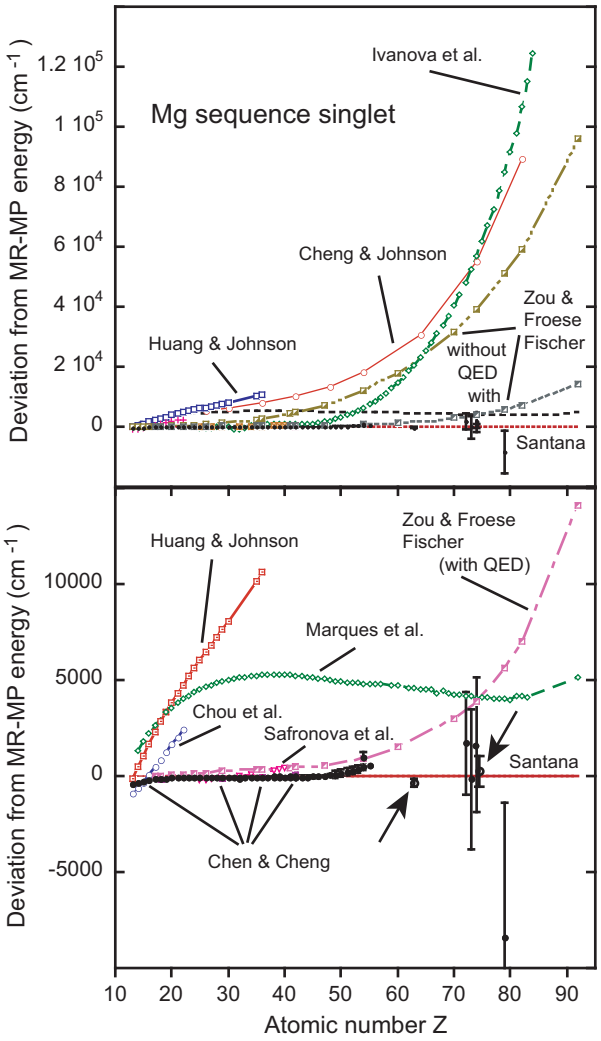

FIG. 1: (Color on-line only) Measured and calculated 3s3p $^1P_1^o$ level energies ($13 \leq Z \leq 92$) relative to the Multi-Reference Møller-Plesset calculated values from this work. Top: Full vertical range, bottom: Expanded view near the base line ("Santana": This work). The downward slope of the experimental data at low Z is an artifact of the reference to our calculation which at low Z overestimates the results. The high-Z experimental data [9, 10, 12] are all from electron beam ion traps. Arrows point to the two most precise of the high-Z data. Selected calculations in historical order: Cheng and Johnson [32], Huang and Johnson [33], Ivanova et al. [34], Chou, Chi, and Huang [35], Marques, Parente, and Indelicato [36], Chen and Cheng [37], Safronova et al. [38], Zou and Froese Fischer [39] (without QED in the upper figure, with QED in the lower figure). The four results obtained by Chen & Cheng almost coincide with the measured data.

For the low-Z third of the Mg isoelectronic sequence, the experimental error bars are so small in a practical plot of the data that any sensible symbol for a data point exceeds the size of the error bar. This roughly coincides with the range for which we adopt the experimental data listed in the NIST on-line data base [13]. In the range 30 $\leq Z \leq$ 55, many error bars are only a little larger than our chosen symbol size and thus hardly visible; we invite the reader to enjoy the (dominant) internal consistency of the experimental data, but also to recognize slight kinks in the data trend (most notably in the data near Z=50) as well as data subsets that do not perfectly agree with each other (triplet level data near Z=40, scatter of data for Z=54). In the high-Z range, most error bars are larger and thus easily depicted. We note the small uncertainty of the Eu (Z=63) singlet data point recently obtained by high-resolution spectroscopy at the Livermore electron beam ion trap [12] and the relatively small error bar of the singlet data point for W (Z=74) [10] from the same laboratory (these data have been marked with arrows in figure 1). There also are four high-Z singlet level data points from the NIST EBIT [9] and an early triplet level measurement on Au (Z=79) [23] also from the Livermore EBIT.

III. PREVIOUS CALCULATIONS

Calculations of Mg-like ions have applied a variety of computational approaches (for example, [32–45]), but not many have treated ions of $Z \geq 42$ (Mo). Figures 1 and 2 show the isoelectronic trends of some of the calculations

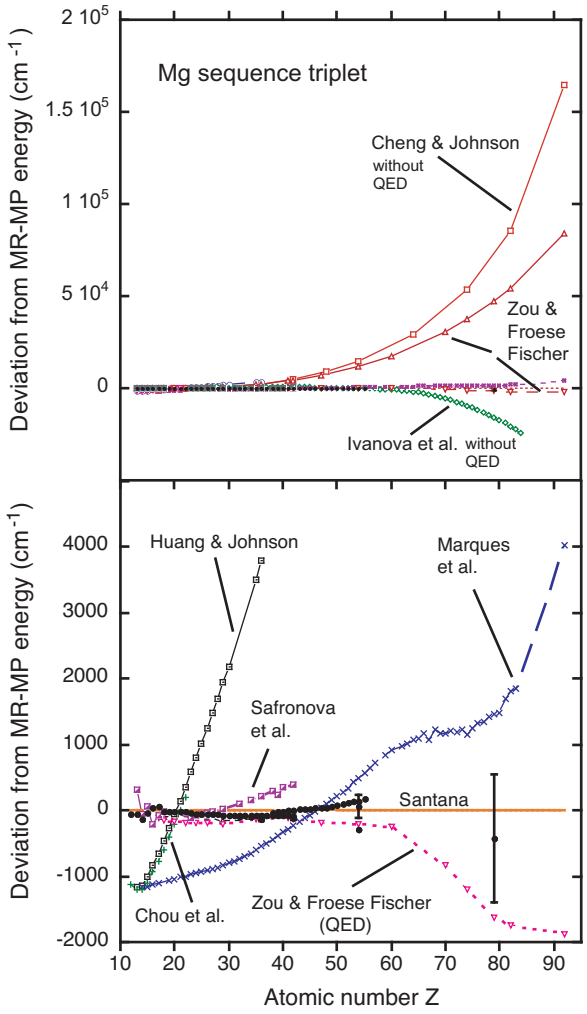

FIG. 2: (Color on-line only) Measured and calculated 3s3p $^3P^o_1$ level energies ($13 \leq Z \leq 92$) relative to the Multi-Reference Møller-Plesset calculated values from this work. Top: Full vertical range, bottom: Expanded view near the base line ("Santana": This work). Only one of the data points at Z=54 is given a representative error bar. The high-Z experimental data [10, 12, 23] are all from electron beam ion traps. Selected calculations in historical order: Cheng and Johnson [32], Huang and Johnson [33], Ivanova et al. [34], Chou, Chi, and Huang [35], Marques, Parente, and Indelicato [36], Chen and Cheng [37], Safronova et al. [38], Zou and Froese Fischer [39] (without and with QED corrections).

in comparison to our own Multi-Reference Møller-Plesset approach (which is explained in the next section). Evidently some of the predictions deviate widely from the range of the experimental data. Almost a quarter of a century has elapsed between the early attempt by Cheng and Johnson [32], a calculation by Ivanova et al [34], and the computation by Zou and Froese Fischer [39]. For the singlet level in question and high atomic numbers Z, the result has improved only by about a factor of two and thus has remained grossly inadequate as long as the computations did not include QED. However, Zou and Froese Fischer provide results also for computations with QED contributions, and then the agreement with experiment is much better (although still not very good at high Z). The wide gap between the predictions for high-Z ions with and without QED contributions illustrates that in this range QED is not merely a small correction to atomic structure, and this observation underlines the high sensitivity of accurate measurements in testing the calculation of radiative corrections.

The singlet J=1 level ($3p_{3/2}$ wave function) is somewhat more affected by relativistic effects than the triplet J=1 level ($3p_{1/2}$ wave function). Even apart from the missing QED contributions, the three calculations mentioned last fare rather differently with the determination of the two levels. The high-Z deviations from our reference calculation are rather similar for singlet and triplet levels calculated by Cheng and Johnson and also (at half the total deviation) for the level energies computed by Zou and Froese Fischer. The computations by Ivanova et al. point to an even larger high-Z discrepancy than that obtained by Cheng and Johnson for the singlet level, but predict a much smaller one of opposite sign for the triplet level. For the further discussion we disregard these three wide-range calculations that do not take QED into account.

The other computations produce results that spread less than these non-QED calculations by a factor of twenty and better; the results are shown on expanded scales in the lower parts of Figures 1 and 2, respectively. Unfortunately, most of those other calculations address only a very limited range of atomic numbers. For example, the early computations by Huang and Johnson [33] feature a Z dependence that steers clearly away from experiment, and the later computation by Chou, Chi, and Huang [35] covers an ever shorter part of the isoelectronic sequence, but at a similarly wrong slope. The computation by Safronova et al. [38] comes out promisingly close to experiment at low to moderate values of Z, but begins to diverge from experiment for $Z \geq 30$, before the list of their results ends at Mo (Z=42). Marques, Parente, and Indelicato [36] did not set out for a general atomic structure investigation, but for a calculation of hyperfine effects. Nevertheless, their level energy values have been particularly useful for isoelectronic estimates, because they cover almost all elements and because their singlet level data are at a sizable, but almost constant offset from experiment, which is helpful for practical interpolations. Chen and Cheng [37] give results of their Relativistic Configuration Interaction (RCI) computations for only four elements, where they agree within 100 cm^{-1} with experiment. Zou and Froese Fischer, in their computations with QED effects, are similarly close to experiment as Safronova et al. [38, 42, 45] in the low-Z third of the isoelectronic sequence. However, their results progressively deviate from the experimental trend at mid Z, and at high Z, their mismatch exceeds that of the computations by Marques et al. Various other computations (not depicted in our figures) scatter in the same wide

range as the ones selected for display in our figures. For example, Wang *et al.* [43, 44] apply MCDF calculations to six Mg-like ion species with Z in the range from 53 to 62. Their 3s3p triplet level results (given for three ion species only) are less than 900 cm^{-1} away from experiment and thus among the better ones, but their singlet level results deviate from experiment by more than 5000 cm^{-1} and thus are poorer than, for example, the results obtained by Marques et al. some 13 years earlier. Judging from our figures at face value, the often touted 'predictive value of theory' is much in the eye of the beholder. It certainly varies as a function of time, and one can only hope that it improves with the increasing availability of computing resources.

In conclusion, some people have been able to compute atomic structure accurately even several decades ago. However, even with greatly expanded computer resources, not all computational recipes have been equally successful since. Relativistic multiconfiguration Dirac-Fock (MCDF) and configuration interaction (CI) calculations have become the standard methods to generate atomic data. A central problem with these methods is that a large expansion is required to describe all electron dynamics, resulting in computationally expensive and impractical calculations for many-electron systems. The computational cost is normally reduced by including only the dominant configurations in the expansion. Such truncated expansions can effectively account for valence-valence correlation, but they often fail to accurately describe core-valence and core-core electron correlations. The missing electron correlations can be incorporated into CI calculations by means of many-body perturbation methods. This is the route we have chosen for our computations that are described below.

IV. NEW CALCULATIONS

We apply our accurate computational methods in order to close the wide gaps between the good ones among the early computed results and to extend the coverage to all elements, all by one common set of computations, so that isoelectronic trends can be established that are free from technical changes in the computation.

The relativistic Multi-Reference Many-Body Perturbation Theory method employed in the present work originates in an ansatz by Møller and Plesset [46]. Their relativistic perturbative approach allows one to simultaneously take into account both relativistic and electron correlation effects with a relatively small computational effort. The method yields term energies and decay probabilities of spectroscopic quality for multi-valence-electron ions. Theoretical details of the method have been presented elsewhere [47–49]. Therefore, we include here only a brief sketch of the process without a detailed description of the theory.

The method consists of three steps. The process begins with a state-averaged Multi-Configuration Dirac-Fock-Breit Self-Consistent Field (MCDFB-SCF) calculation [49] for the ground and low-lying excited states of the ions, to obtain a single set of core and valence spinors in the V^N potential. In this relativistic method, the large and small radial components of the bound Dirac spinors are expanded in sets of even-tempered Gaussian-type functions (GTF) that satisfy the boundary conditions associated with a finite nucleus and that are automatically kinetically balanced [50]. We employed the so-called universal Gaussian basis set [51] to avoid the process of fine-tuning the basis exponents. For all systems, we used basis sets of $34s32p30d28f$ Gaussian (G) spinors for angular momentum values up to L=3, 26 G spinors for L=4-5, and 15 G spinors for L=6-11. (Larger basis sets are expected to improve the convergence and the results for low-Z atomic systems, at the cost of computing power and time. However, we wanted to provide an internally consistent data set without discontinuities introduced by external parameter changes, and still afford to do calculations for all elements.) The parameter α defining the basis exponents, $\{\zeta_i = \alpha\beta^{i-1};\ i = 1, 2, ..., N_\kappa\}$, of the even-tempered basis set is chosen such that the maximum exponent of the $34s$ set equals $\frac{9.89\times10^{10}}{118^{-4}}$ Z^4 for β = 2.1. The parameter α defining the basis exponents, $\{\zeta_i = \alpha\beta^{i-1};\ i = 1, 2, ..., N_\kappa\}$, of the even-tempered basis set is chosen such that the maximum exponent of the $34s$ set equals $a\times Z^4$ with a = 510 for β = 2.1. The ground and low-lying excited states in Mg-like ions were optimized by averaging the energies of even- and odd-parity states with J=0-4 arising from the nonrelativistic configurations $3s^{n_1}3p^{n_2}3d^{n_3}$ where $\sum_{i=1}^{3} n_i = 2$. Intermediate coupling is built in through the MCDFB-SCF process.

Subsequently, relativistic Multi-Reference Configuration Interaction (MR-CI) calculations were performed including all relativistic excited states arising from the nonrelativistic configurations $3s^{n_1}3p^{n_2}3d^{n_3}$ where $\sum_{i=1}^{3} n_i$ = 2, in order to account for near-degeneracy effects or strong configuration mixing among the excited states. The relativistic MR-CI, however, fails to account for the bulk of dynamic correlation among all levels unless a very large number of configurations, on the order of 1×10^6, are included in the CI calculations. The residual dynamic correlation corrections, however, can be accounted for by state-specific MR-MP calculations based on the CI wave functions. Therefore, in a final step, each of the states was subjected to additional many-body refinement to account for the residual dynamic correlation. All electrons have been included in the MR-MP calculations to determine accurately the effects of relativity and electron correlations. Radiative corrections and the Lamb shift for each state were estimated evaluating the electron self-energy and vacuum polarization by following the recipe in [52].

The $3s3p\ ^{1,3}P^o_1$ (in LS coupling notation) level energies of Mg-like ions of elements up to uranium (Z=92) are given in table I. Results for a wider range of Z and including other n=3 levels will be presented elsewhere [24].

A. Estimate of computational uncertainty

It is difficult to establish an objective measure of computational uncertainty, because the challenging uncertainties lie not so much in the computation *per se*, but in the approximation to theoretical concepts that is being coded into a large suite of computer programs. The uncertainty of the computational results thus depends on numerical as well as intellectual problems. There are established means of guessing computational reliability by convergence studies or by employing ever increasing sets of wave functions. The code used here has undergone extensive testing and consecutive improvements. We present results of computations that on purpose are not done with the highest computational effort affordable for a single or a few atomic systems, but with the same basis set for all ions of a given isoelectronic sequence, in order to provide guidance for future work in ranges of (high) Z that have not been covered appropriately yet. Hence we know (see discussion above) that at low Z the calculational accuracy can be improved by an expansion of the basis set, but in that range, experimental data are far superior in accuracy anyway. At high Z, where the experimental data are sparse, the calculations converge easily. Nevertheless it would cost an overly large effort to establish an explicit measure of uncertainty based on computation alone. Therefore we apply a pragmatic measure, the comparison with accurate experiments.

For the Mg isoelectronic sequence and the high-Z range, this means largely uncharted territory, so we first check how our type of computation has fared on a related problem, the computation of Zn-like ions. Recent calculations and intercomparisons [26–29] have shown our comptutations to be competitive with the best such computations (that employ various approximations), and the results of MR-MP computations as we perform here are seen to agree with the most accurate measurements up to Z=92 within about 100 ppm.

Mg-like ions feature a less complex electronic core than Zn-like ions; however, that is not a guarantee that a given type of computation yields more accurate results for one or the other. For Mg-like ions of moderate nuclear charge Z, the trend of the experimental data is easily interpolated, and our *ab initio* calculations match that trend, revealing deviations of individual experimental data from the underlying smooth trend. The most accurate data point among the few that are available above Z=54 is the one for Eu (Z = 63). Our computation for this element was intentionally done without knowing this experimental datum [12], and the agreement of calculation and experiment is, again, within about 100 ppm (and thus rather similar to the measurement uncertainty).

From this combination of past performance on a related atomic system and the comparison with accurate experimental data in the isoelectronic sequence of present interest we derive the expectation that our new computations are reliable within about 100 ppm in the mid- to high-Z range.

TABLE I: Energies of the 3s3p ^{1,3}P^{o} J=1 levels in Mg-like ions (Z=13 to 92) calculated by the Multi-Reference Møller-Plesset method (this work) and data from measurements.

	$3s3p_{3/2}$ (Singlet)			$3s3p_{1/2}$ (Triplet)		
Z	Theory cm^{-1}	Experiment cm^{-1}	Unc. cm^{-1}	Theory cm^{-1}	Experiment cm^{-1}	Unc. cm^{-1}
12	36380	35051[a]		22024	21870[a]	
13	60298	59852[a]		37502	37454[a]	
14	83219	82884[a]		52887	52853[a]	
15	105487	105190[a]		68168	68146[a]	
16	127353	127151[a]		83392	83394[a]	
17	149104	148947[a]		98637	98621[a]	
18	170845	170722[a]		113918	113906[a]	
19	192648	192537[a]		129254	129209[a]	
20	214575	214482[a]		144663	144675[a]	
21	236692	236610[a]		160174	160141[a]	
22	259049	258972[a]		175797	175747[a]	
23	281699	281627[a]		191550	191509[a]	
24	304699	304629[a]		207446	207399[a]	
25	328105	328042[a]		223499	223438[a]	
26	351978	351911[a]		239718	239660[a]	
27	376379	376323[a]		256115	256060[a]	
28	401376	401302[a]		272695	272634[a]	
29	427039	426987[b]	9	289466	289401[b]	4
30	453442	453375[b]		306430	306361[b]	
31	480667	480591[b]		323592	323519[b]	
32	508795	508690[c]		340951	340862[c]	
32	508795	508719[b]		340951	340876[b]	
33	537919	537848[b]		358508	358433[b]	
34	568132	568090[c]		376263	376178[c]	
34	568132	568069[b]		376263	376189[b]	
35	599536	599480[b]		394214	394143[b]	
36	632235	632187[b]	20	412358	412290[b]	8
36	632235	632178[d]	47	412358	412233[d]	55
37	666340	666298[b]		430693	430626[b]	
38	701965	701948[c]		449217	449183[c]	
38	701965	701927[b]		449217	449152[b]	
39	739230	739206[c]		467925	467901[c]	
39	739230	739191[b]		467925	467858[b]	
40	778259	778227[c]		486815	486792[c]	
40	778259	778216[b]		486815	486744[b]	
41	819179	819150[e]		505884	505880[e]	
41	819179	819135[b]		505884	505802[b]	
42	862122	862076[b]	37	525128	525028[b]	14
42	862122	862110[d]	94	525128	525024[d]	48
42	862122	862090[e]		525128	525130[e]	
43	907224	907190[e]		544545	544560[e]	
44	954624	954590[e]		564134	564150[e]	
45	1004469	1004440[e]		583894	583920[e]	
46	1056906	1056890[e]		603822	603860[e]	
47	1112093	1112100[e]		623922	623970[e]	
48	1170182	1170220[e]		644189	644240[e]	
49	1231348	1231420[e]		664633	664700[e]	
50	1295755	1295880[e]		685250	685330[e]	
51	1363586	1363780[e]		706050	706150[e]	
52	1435016	1435290[e]		727028	727140[e]	
53	1510261	1510620[e]		748214	748350[e]	
54	1589490	1589960[e]		769585	769730[e]	
54	1589490	1590457[f]	303	769585	769650[g]	180
55	1672931	1673520[e]	560	791169	791340[e]	140
56	1760780			812957		
57	1853281			834977		

TABLE I: Continued.

Z	$3s3p_{3/2}$ (Singlet) Theory cm^{-1}	Experiment cm^{-1}	Unc. cm^{-1}	$3s3p_{1/2}$ (Triplet) Theory cm^{-1}	Experiment cm^{-1}	Unc. cm^{-1}
58	1950656			857231		
59	2053145			879727		
60	2160980			902458		
61	2274450			925463		
62	2393772			948702		
63	2519287	2518968[h]	200	972243		
64	2651220			996035		
65	2789941			1020151		
66	2935707			1044549		
67	3088877			1069268		
68	3249778			1094306		
69	3418772			1119681		
70	3596173			1145350		
71	3782443			1171397		
72	3977907	3979624[i]	2690	1197762		
73	4183037	4182875[i]	3670	1224505		
74	4398230			1251601		
74	4398230	4398504[j]	800			
74	4398230	4399859[i]	3480			
75	4623964			1279081		
76	4860642			1306889		
77	5108873			1335141		
78	5369075			1363754		
79	5641854	5633485[i]	6970	1392799	1392370[k]	970
80	5927652			1422172		
81	6227110			1451930		
82	6540902			1482132		
83	6869689			1512798		
84	7214207			1543989		
85	7574983			1575545		
86	7951873			1606668		
87	8347430			1638969		
88	8761402			1671482		
89	9195022			1704546		
90	9648485			1737525		
91	10123950			1771498		
92	10620502			1804756		

[a]NIST [13]
[b]Sugar *et al.* [15]
[c]Ekberg *et al.* [16]
[d]Jupén *et al.* [17]
[e]Ekberg *et al.* [18]
[f]Träbert *et al.* [7]
[g]Osin *et al.* [20]
[h]Träbert *et al.* [12]
[i]Gillaspy *et al.* [9]
[j]Clementson *et al.* [10]
[k]Träbert *et al.* [23]

V. COMPARISON WITH OTHER COMPUTATIONS

The present results form the reference for all other results and data in figures 1 and 2. The fact that at low Z (below Z=20) our calculation overestimates the level energies by more than 100 cm^{-1} (up to about 450 cm^{-1} for Z=13) results in a corresponding lowering of the energy values of other sources in our plots. Apart from that, our isoelectronic trends are expected to be smooth, because all calculations have been run at the very same degree of complexity. If then other calculations show changes of the slope of their isoelectronic trend - and several of them do - one has to suspect external parameter changes or the growing influence of a particular computational contribution. Such factors can possibly be identified by the authors of those other studies.

VI. DISCUSSION

The comparison of calculational results and measured data in the Mg isoelectronic sequence until recently was limited to the range up to about Z=55, and there was no close match for an extended range of Z values. Now details can be recognized that have remained inaccessible before. For example, the experimental data on both 3s3p J=1 levels undergo a slope change of the isoelectronic trend near Z=48; incidentally, this is largely the data sample collected by Ekberg et al. in 1991 [18] from experiments that employed laser-produced plasmas. Similar systematic effects have been seen in data on Na-like ions (see the discussion in [12]) and on Cu-like ions (see the discussions in [8, 27, 28]). However, the Livermore EBIT data point for the singlet level in Xe^{42+} [7] lies even farther away from the newly calculated expected isoelectronic trend, while for the triplet level in the same ion species two observations at the NIST EBIT lie closer to the new trend [20] or even on the other side [21]; unfortunately the uncertainties of these two measurements do not constrain the data range much. Near Z=40 there are several sets of experimental results which individually seem highly consistent along the isoelectronic sequence, but which differ from each other. At high Z, the very recent data point for the singlet transition energy in Eu^{51+} [12] constrains calculational treatments the most; the results of our new calculations differ from that measurement by only 100 ppm and lie just outside the 1-σ experimental error bar (and thus there is agreement within the mutual error bars). Next most significant is the corresponding measurement in W^{62+} [10] from the same Livermore electron beam ion trap and its high-resolution EUV spectrographs. Our calculation passes close to the center of the error bar of the tungsten measurement. The older triplet measurement on Au (Z=79) used a much smaller spectrograph of correspondingly poorer resolution [23]; short of nearby calibration lines for accurate wavelength reference, this measurement nevertheless turns out to agree with the presently computed theoretical prediction, and only with this one. The four measurements from the NIST EBIT (Z= 72,73,74,79) [9], however, with their scatter and larger error bars, do not rule out the calculations by Marques et al. [36] nor those by Zou and Froese Fischer [39]. Clearly, more of the accurate measurements are wanted in the high-Z range, where relativistic and

QED effects are so massive that most of the older calculations have failed. Which ever elements are being tried, there now is a set of predictions to test.

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