

Extended calculations of level and transition properties in the nitrogen isoelectronic sequence: Cr XVIII, Fe XX, Ni XXII, and Zn XXIV[★]

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ABSTRACT

Extensive multiconfiguration Dirac-Hartree-Fock (MCDHF) calculations and relativistic configuration interaction (RCI) calculations are performed for 272 states of the $2s^22p^3$, $2s2p^4$, $2p^5$, $2s^22p^23l$, $2s2p^33l$, and $2p^43l$ ($l = 0, 1, 2$) configurations in the nitrogen-like ions Cr XVIII, Fe XX, Ni XXII, and Zn XXIV. Valence, core-valence, and core-core electron correlation effects are accounted for through large configuration state function expansions. Calculated energy levels are compared with data from other calculations and with experimental data from the NIST database. Landé g_J -factors; hyperfine structures; isotope shifts; and radiative electric dipole (E1), electric quadrupole (E2), and magnetic dipole (M1) transition rates are given for all ions. The accuracy of the calculated energy levels is high enough to facilitate identification of observed spectral lines involving the $2l^43l'$ configurations, for which experimental data are largely missing.

Key words. atomic data

1. Introduction

Spectroscopic data for the nitrogen isoelectronic sequence are of importance in astrophysics. Nitrogen-like ions provide several lines that are used for diagnosing the physical conditions of the solar chromosphere, transition region, and corona in the Solar Ultraviolet Measurement of Emitted Radiation (SUMER) spectrograph on the SOHO spacecraft (Wilhelm et al. 1997; Lemaire et al. 1997). Moreover, the X-ray telescopes on board the space observatories *Chandra* and *XMM-Newton* provide high-resolution spectra that are rich in emission and absorption lines from various iron ions, including Fe XX (Mewe et al. 2001, 2003; van der Heyden et al. 2003).

Data for nitrogen-like ions are also of importance in fusion science. The X-ray and Extreme Ultraviolet Spectrometer (XEUS) and Long-Wavelength and Extreme Ultraviolet Spectrometer (LoWEUS), which operate in the 5–400 Å region, were used to find impurities, both for intrinsic elements present in the plasma and for metal impurities resulting from damage to various components in the National Spherical Tokamak Experiment (NSTX). The most commonly seen metal impurity is iron followed by copper and nickel. Iron, nickel, and chromium are present in NSTX as the makeup of stainless steel found in the outer wall, in a number of hardware components, and in the shielding of magnetic sensors and cables. Identification of metal impurities can determine which components are affected and to what degree (Lepson et al. 2010). These spectrometers provide information about plasma conditions, but the identification of lines is problematic without experimental or theoretical data.

Because they provide important information, *N*-like ions have been studied using a number of different theoretical methods. Vilkas & Ishikawa (1998) did calculations in the framework of the relativistic multireference Møller-Plesset perturbation theory (MRMP) of energy levels and transition probabilities for a number of ions in the sequence. Merkelis et al. used the second-order many-body perturbation theory (MBPT) with relativistic corrections in the Breit-Pauli approximation to compute oscillator strengths between the levels of the $2s^22p^3$, $2s2p^4$, and $2p^5$ configurations (Merkelis et al. 1997) and between the levels of the $2s^22p^3$ configuration (Merkelis et al. 1999). Ions in the range $Z = 10, \dots, 30$ were covered. Kotochigova et al. (2010) evaluated the wavelengths and oscillator strengths for the $2s^22p^23s, 3d \rightarrow 2s^22p^3$, and $2s2p^33p \rightarrow 2s^22p^3$ transitions in Fe XX using a configuration interaction Dirac-Fock-Sturm (MDFS) method combined with the second-order Brillouin-Wigner perturbation theory. Bhatia et al. (1989) determined transition parameters between $n = 2$ and $n = 3$ levels of Ar XII, Ti XVI, Fe XX, Zn XXIV, and Kr XXX using the SUPERSTRUCTURE (SS) code. Within the Iron Project, Nahar (2004) used the Breit-Pauli R-matrix (BPRM) method and the SUPERSTRUCTURE code to derive an extensive set of oscillator strengths, line strengths, and radiative decay rates for transitions in Fe XX. Jonauskas et al. (2005) took a broad approach and performed multiconfiguration Dirac-Hartree-Fock (MCDHF) and configuration interaction calculations on the basis of transformed radial orbitals (CITRO) with variable parameters including relativistic effects in the Breit-Pauli approximation to derive the energies of the 700 lowest levels in Fe XX and the corresponding transition parameters. A combined configuration interaction and relativistic many-body perturbation theory (RMBPT) approach was used by Gu (2005) to obtain energies in iron and nickel ions with high accuracy. Rynkun et al. (2014) used relativistic configuration

[★] Tables 5–21 are only available at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via <http://cdsarc.u-strasbg.fr/viz-bin/qcat?J/A+A/582/A61>

interaction (RCI) to compute energies, transition rates, and lifetimes of $n = 2$ levels for all N -like ions with $Z = 9, \dots, 36$.

The aim of the present work is to provide highly accurate spectroscopic data for four ions in the N -like isoelectronic sequence that are important for plasma diagnostics. It is a continuation of our previous paper for the C -like sequence (Ekman et al. 2014a), where uncertainties in energies around 0.03% were reported. Compared with the recent work by Rynkun et al. (2014), the calculations are extended to include additional 257 levels of the $2s^2 2p^2 3l$, $2s 2p^3 3l$, and $2p^4 3l$ ($l = 0, 1, 2$) configurations. The calculations also extend the work by Gu (2005) to include levels of the Cr XVIII and Zn XXIV ions.

2. Theory

2.1. MCDHF theory

We used the MCDHF approach to generate numerical representations of atomic state functions (ASFs), which are approximations to the exact wave functions of the states. The atomic state functions $\Psi(\gamma P J M)$ are obtained as expansions of configuration state functions (CSFs) $\Phi(\gamma_i P J M)$

$$\Psi(\gamma P J M) = \sum_{i=1}^{N_{\text{CSFs}}} c_i \Phi(\gamma_i P J M). \quad (1)$$

The CSFs are anti-symmetrized and coupled products of one-electron Dirac orbitals and are eigenfunctions of the parity operator P and the total angular momentum operator J^2 and its projection J_z .

In the present work the extended optimal level (EOL) computational scheme (Dyall et al. 1989) was used. In this scheme the radial parts of the one-electron orbitals and the expansion coefficients $\{c_i\}$ of the CSFs are obtained by iteratively solving the self-consistent field equations that result from the stationary condition of a weighted energy functional of all the studied states with respect to small variations of the radial orbitals and the expansion coefficients. In fully relativistic calculations the energy functional is based on the Dirac-Coulomb Hamiltonian (in a.u.)

$$H_{DC} = \sum_{j=1}^N \left(c \alpha_j \cdot \mathbf{p}_j + (\beta_j - 1) c^2 + V(r_j) \right) + \sum_{j < k}^N \frac{1}{r_{jk}}, \quad (2)$$

where α and β are the Dirac matrices, \mathbf{p} is the momentum operator, $V(r_j)$ is the monopole part of the electron-nucleus Coulomb interaction, and r_{jk} is the distance between electrons j and k . The sums run over the number of electrons N . The angular integrations needed for the construction of the energy functional are based on second quantization in the coupled tensorial form (Gaigalas et al. 1997, 2001).

The Breit interaction

$$H_{\text{Breit}} = - \sum_{j < k}^N \left[\alpha_j \cdot \alpha_k \frac{\cos(\omega_{jk} r_{jk}/c)}{r_{jk}} + (\alpha_j \cdot \nabla_j) (\alpha_k \cdot \nabla_k) \frac{\cos(\omega_{jk} r_{jk}/c) - 1}{\omega_{jk}^2 r_{jk}/c^2} \right] \quad (3)$$

and leading QED corrections (vacuum polarization and self-energy) are included in subsequent RCI calculations (McKenzie et al. 1980). In relativistic calculations, the states are given in jj -coupling. To adhere to the labeling conventions used

by the experimentalists, the ASFs are transformed from the jj -coupling to the LS -coupling scheme using the methods developed by Gaigalas et al. (2003, 2004). All calculations were performed with the GRASP2K code (Jönsson et al. 2013).

2.2. Computation of transition parameters

Transition parameters (transition probabilities A and oscillator strengths gf) for a transition between two states $\gamma' P' J' M'$ and $\gamma P J M$ can be expressed in terms reduced matrix elements

$$\left\langle \Psi(\gamma P J) \parallel \mathbf{T} \parallel \Psi(\gamma' P' J') \right\rangle = \sum_{j,k} c_j c'_k \left\langle \Phi(\gamma_j P J) \parallel \mathbf{T} \parallel \Phi(\gamma'_k P' J') \right\rangle, \quad (4)$$

where \mathbf{T} is the transition operator. In cases where the initial and final state wave functions result from separate EOL calculations the wave functions are transformed in such a way that the orbital sets became biorthonormal (Olsen et al. 1995) in which case standard methods can be used to evaluate the matrix elements between the CSFs.

For electric dipole (E1) and electric quadrupole (E2) transitions there are two forms of the transition operator, the length (Babushkin) form and the velocity (Coulomb) form. The length form is more sensitive to the outer parts of the wave functions and it is the preferred form. For RCI calculations the differences between the transition parameters evaluated with the two forms can be used as an indicator of the uncertainty (Ekman et al. 2014b). The quantity dT , characterizing the uncertainty of the computed transition rates, is defined as

$$dT = \frac{|A_l - A_v|}{\max(A_l, A_v)}, \quad (5)$$

where A_l and A_v are transitions rates in length and velocity form.

2.3. Hyperfine structure

In atoms with nuclear spin I the fine-structure levels J are split into closely spaced hyperfine levels. The splittings of the fine-structure levels are to the first order given by the magnetic dipole A_J and electric quadrupole B_J hyperfine interaction constants (Jönsson et al. 1996)

$$A_J = \frac{\mu_I}{I} \frac{1}{\sqrt{J(J+1)}} \times \left\langle \Psi(\gamma P J) \parallel \sum_{j=1}^N -i \sqrt{2} \alpha r_j^{-2} (\alpha_j \mathbf{C}^{(1)}(j))^{(1)} \parallel \Psi(\gamma P J) \right\rangle, \quad (6)$$

$$B_J = 2Q \sqrt{\frac{J(2J-1)}{(J+1)(2J+3)}} \times \left\langle \Psi(\gamma P J) \parallel \sum_{j=1}^N -r_j^{-3} \mathbf{C}^{(2)}(j) \parallel \Psi(\gamma P J) \right\rangle. \quad (7)$$

The hyperfine levels of closely spaced fine-structure levels are also affected by the off-diagonal hyperfine interaction (Andersson et al. 2006). This effect is small, however, and is neglected in the present study. The calculations are done with the nuclear parameters I , μ_I , and Q all set to 1. To obtain the A_J and B_J values for a specific isotope, the given values should be scaled with the tabulated values of I , μ_I , and Q (Stone 2005).

Table 1. Energy levels in cm⁻¹ for the 15 lowest states in Fe XX as a function of increasing active sets of orbitals.

Pos	Conf.	<i>LSJ</i>	MR	<i>n</i> = 3	<i>n</i> = 4	<i>n</i> = 5	<i>n</i> = 6	<i>n</i> = 7	<i>n</i> = 8	<i>n</i> = 9	<i>E</i> _{obs}
1	2s ² 2p ³	⁴ S _{3/2} ^o	0	0	0	0	0	0	0	0	0
2		² D _{3/2} ^o	142 564	142 464	140 512	139 411	138 985	138 854	138 814	138 787	138 620
3		² D _{5/2} ^o	180 433	180 363	177 886	176 901	176 496	176 367	176 332	176 308	176 130
4		² P _{1/2} ^o	263 718	263 044	263 293	261 487	260 828	260 630	260 573	260 533	260 270
5		² P _{3/2} ^o	326 426	326 053	325 739	324 303	323 759	323 592	323 549	323 520	323 340
6	2s2p ⁴	⁴ P _{5/2}	756 552	755 964	754 312	752 983	752 667	753 346	752 844	752 725	752 730
7		⁴ P _{3/2}	824 202	823 604	822 144	820 861	820 557	821 237	820 743	820 628	820 630
8		⁴ P _{1/2}	846 426	845 775	844 215	842 795	842 436	843 111	842 610	842 492	842 480
9		² D _{3/2}	1 056 030	1 055 207	1 047 209	1 044 066	1 043 019	1 043 621	1 042 999	1 042 839	1 042 570
10		² D _{5/2}	1 071 189	1 070 330	1 062 812	1 059 765	1 058 759	1 059 363	1 058 748	1 058 590	1 058 360
11		² S _{1/2}	1 210 845	1 209 054	1 201 978	1 197 566	1 196 045	1 196 601	1 195 901	1 195 713	1 195 260
12		² P _{3/2}	1 261 249	1 259 748	1 248 317	1 244 514	1 243 178	1 243 757	1 243 106	1 242 934	1 242 430
13		⁴ P _{1/2}	1 357 678	1 356 013	1 346 103	1 342 158	1 340 774	1 341 346	1 340 689	1 340 516	1 340 040
14	2p ⁵	² P _{3/2}	1 983 635	1 981 308	1 963 292	1 956 866	1 954 974	1 954 738	1 954 735	1 954 623	1 954 310
15		² P _{1/2}	2 090 757	2 088 025	2 070 782	2 064 485	2 062 626	2 062 396	2 062 402	2 062 298	2 061 990

Notes. Orbital sets are labeled with the highest principal quantum number *n*. Observed energies *E*_{obs} are the NIST recommended values (NIST Atomic Spectra Database 2013, [Kramida et al. 2013](#)).

2.4. Landé *g_J*-factors

The Landé *g_J*-factors are given by

$$g_J = \frac{2}{\sqrt{J(J+1)}} \times \left\langle \Psi(\gamma PJ) \left\| \sum_{j=1}^N \left[-i \frac{\sqrt{2}}{2\alpha^2} r_j (\alpha_j \mathbf{C}^{(1)}(j))^{(1)} + \frac{g_s - 2}{2} \beta_j \Sigma_j \right] \right\| \Psi(\gamma PJ) \right\rangle, \quad (8)$$

and determine the splitting of magnetic sublevels in external magnetic fields. Here *g_s* is the electron *g*-factor and Σ the relativistic spin-matrix. The Landé *g_J*-factors were calculated using the Zeeman module of GRASP2K ([Andersson & Jönsson 2008](#)).

2.5. Isotope shift

Isotope shift calculations using the MCDHF and RCI methods have recently been reviewed by [Nazé et al. \(2014\)](#), and we refer to this paper for details. There are two contributions to the isotope shift: the mass shift and the field shift. For an atomic state γPJM the mass shift is expressed in terms of the normal \tilde{K}_{NMS} and specific \tilde{K}_{SMS} mass shift parameters (in GHz u.):

$$\tilde{K}_{\text{NMS}} = \frac{M}{h} \langle \Psi(\gamma PJ) | H_{\text{NMS}} | \Psi(\gamma PJ) \rangle, \quad (9)$$

$$\tilde{K}_{\text{SMS}} = \frac{M}{h} \langle \Psi(\gamma PJ) | H_{\text{SMS}} | \Psi(\gamma PJ) \rangle. \quad (10)$$

The field shift is the energy shift arising from the difference in nuclear charge distributions between two isotopes. The level field shift is given in terms of the $\tilde{\mathcal{F}}$ parameter (in GHz/fm²), which is proportional to electron density at the origin

$$\tilde{\mathcal{F}} = \frac{2\pi}{3h} Z \left(\frac{e^2}{4\pi\epsilon_0} \right) |\Psi(0)|^2. \quad (11)$$

The isotope shift parameters were calculated in the first-order perturbation approach using the RCI atomic state functions as zero-order wave functions. All calculations were done with the isotope shift module of GRASP2K ([Nazé et al. 2013](#)).

3. Generation of configuration expansions

Separate calculations were performed in the EOL scheme for the 132 states of even parity and the 140 states of odd parity belonging to the 2s²2p³, 2s2p⁴, 2p⁵, 2s²2p²3l, 2s2p³3l, and 2p⁴3l (*l* = 0, 1, 2) configurations. The CSF expansions were obtained using the active set method ([Olsen et al. 1988](#); [Sturesson et al. 2007](#)). Defining the multireference (MR) as the CSFs that can be formed from, respectively, the even and odd parity configurations, the CSF expansions were generated from configurations obtained by single and double (SD) substitutions of the orbitals in the MR with orbitals in an active set with principal quantum numbers *n* = 3, ..., 8 (for Fe XX *n* = 3, ..., 9) and angular symmetries s, p, d, f, g, and h. Of the generated CSFs only those interacting with the CSFs of the MR were kept.

To monitor the convergence of the calculated energies and transition parameters, the active sets were increased in a systematic way by adding layers of orbitals. To reduce the number of CSFs in the self-consistent field calculations, the 1s² core was closed from *n* = 6, but opened again in the subsequent RCI calculations. For the *n* = 8 expansion this resulted in 1 076 078 (6 206 696) CSFs with odd parity and 916 973 (5 255 680) CSFs with even parity with the 1s² core closed (open). The self-consistent field calculations for each layer of orbitals were followed by RCI calculations, including the Breit interaction and the leading QED effects (vacuum polarization and self-energy).

4. Results

4.1. Fe XX

Computed energies of the 15 lowest states are given in Table 1 as functions of the increasing active orbital set. The mean relative difference between theory and experimental data from NIST is 1.32%, 1.21%, 0.58%, 0.21%, 0.08%, 0.09%, 0.05%, 0.04% for calculations based on the MR expansion and expansions obtained from SD substitutions to orbital sets with the highest principal quantum numbers *n* = 3, 4, 5, 6, 7, 8, 9. The calculations are well converged with respect to the increasing orbital set. A general observation is that the quartets states are energetically lower than the doublet states because electron correlation effects are smaller and converge faster with respect to the orbital set for high spin states than for low spin states ([Froese Fischer et al. 1997](#); [Galvez et al. 2005](#)). The calculations

Table 2. Energy levels in cm⁻¹ and the difference (Diff) between theoretical energies and observed E_{obs} .

Pos	Conf.	LSJ	E^a_{obs}	E^b_{cal}	Diff ^c _{cal}	Diff ^c _{RCI}	Diff ^d _{MRMP}	Diff ^e _{SS}	Diff ^f _{BPRM}	Diff ^g _{CITRO}	Diff ^g _{MCDF}	Diff ^h _{MBPT}	Diff ⁱ _{CI+MBPT}	Diff ^j _{MDFS}
Fe XX Z = 26														
1	2s ² 2p ³	4S ^o _{3/2}	0	0	0	0	0	0	0	0	0	0	0	0
2		2D ^o _{3/2}	138 620	138 787	167	198	5	1978	2283	236	3095	432	53	262
3		2D ^o _{5/2}	176 130	176 308	178	212	5	2859	5485	-178	3407	-213	6	258
4		2P ^o _{1/2}	260 270	260 533	263	307	1052	-2697	4307	201	2939	-1323	366	627
5		2P ^o _{3/2}	323 340	323 520	180	226	2703	-3463	5214	-972	2622	-3299	241	567
6	2s2p ⁴	4P _{5/2}	752 730	752 725	-5	-60	-224	-5629	4677	-2344	919	-2767	420	
7		4P _{3/2}	820 630	820 628	-2	-46	-222	-7932	3497	-2927	779	-4303	483	
8		4P _{1/2}	842 480	842 492	12	-27	-164	-8037	3704	-3057	1056	-4538	466	
9		2D _{3/2}	1 042 570	1 042 839	269	267	-104	1707	8055	-3326	8354	-4795	32	
10		2D _{5/2}	1 058 360	1 058 590	230	227	-188	2856	9713	-2893	7862	-5396	36	
11		2S _{1/2}	1 195 260	1 195 713	453	476	3191	24	9985	-3135	10 229	-7329	314	
12		2P _{3/2}	1 242 430	1 242 934	504	522	6112	8974	10 880	-3222	13 338	-8014	-9	
13		2P _{1/2}	1 340 040	1 340 516	476	509	-133	5272	11 265	-3781	12 356	-10 430	2	
14	2p ⁵	2P ^o _{3/2}	1 954 310	1 954 623	313	611	1419		12 380	-5869	17 474	-10 477	-536	
15		2P ^o _{1/2}	2 061 990	2 062 298	308	619	1476		14 086	-6348	17 189	-13 195	-426	

References. ^(a) Kramida et al. (2013); ^(b) present calculations; ^(c) Rynkun et al. (2014); ^(d) Vilkas & Ishikawa (1998); ^(e) Bhatia et al. (1989); ^(f) Nahar (2004); ^(g) Jonauskas et al. (2005); ^(h) Merkeliš et al. (1997); ⁽ⁱ⁾ Gu (2005); ^(j) Kotochigova et al. (2010).

do not quite manage to balance this. In Table 2 the current results are compared with results from other calculations. The current results and the results from Rynkun et al. (2014) and Gu (2005) stand out in a positive sense, with mean uncertainties of, respectively, 0.04%, 0.05%, and 0.04%. With the exception of the calculation by Vilkas & Ishikawa (1998), the other calculations are associated with uncertainties that are larger by a factor of 10 or more. In Table 5 in the on-line material, calculated energies for all 272 states are compared with energies from Gu (2005). There is perfect agreement; the two methods agree at the 0.025% level. There are a few experimental energies of 2s²2p²3d levels from NIST. Of these only half of them are validated by the calculations. Table 6 in the on-line material gives the energies, the A_J and B_J hyperfine constants, the Landé g_J factors, and the level mass- and field-shift parameters. Eigenvector compositions of the states in LSJ -coupling, which are used as labels, can be found on line in Table 7. LSJ -coupling is ideal for labeling and many of the states are heavily mixed.

Selected transition rates A are compared with rates from other calculations in Table 3. There is a detailed agreement with rates from Rynkun et al. (2014), which is expected since the calculations are very similar. There is a good overall agreement between all calculated values. Table 14 in the on-line material contains transition energies, wavelengths, transition rates, weighted oscillator strengths, and uncertainty estimators dT for transitions between all 272 states. The uncertainty of the transition rates, as estimated by dT in Eq. (5), is around 1% for strong allowed transitions. For weak intercombination transitions the uncertainties are often larger. There are a number of weak two-electron one-photon transitions. These transitions are zero in the single configuration approximation and are allowed only through electron correlation effects. The two-electron one-photon transitions are known to be very difficult to compute and are associated with large uncertainties. From the transition rates the lifetimes of the states have been computed. The lifetimes in length and velocity form are given in Table 18. There is excellent agreement between the lifetimes in the two forms. There are, to the knowledge of the authors, no experimental lifetime data to compare with.

4.2. Cr XVIII, Ni XXII, and Zn XXIV

To reduce the computational effort the orbital sets were restricted to include orbitals with the highest principal quantum

Table 3. Comparison of transition rates: E1 transition rates between states of the upper (U) configuration 2s2p⁴ and the lower (L) configuration 2s²2p³, E2 transition rates between states of the upper (U) configuration 2p⁵ and the lower (L) configuration 2s²2p³, and M1 transition rates between states of 2s²2p³ in Fe XX.

U	L	A^a_{obs}	A^b_{cal}	A^c_{RCI}	A^d_{MCDF}	A^e_{BPRM}	A^f_{MBPT}
E1							
2P _{3/2}	2P ^o _{3/2}	9.40[09] ^C	9.042[09]	9.038[09]	9.36[09]		9.187[09]
2P _{3/2}	2P ^o _{1/2}	9.1[09] ^C	8.380[09]	8.380[09]	8.64[09]		8.315[09]
2P _{3/2}	2D ^o _{5/2}	1.0[11] ^C	9.323[10]	9.321[10]	9.74[10]		9.247[10]
2P _{3/2}	2D ^o _{3/2}	1.47[10] ^C	1.362[10]	1.362[10]	1.47[10]		1.372[10]
2P _{1/2}	2P ^o _{3/2}	9.6[10] ^C	8.837[10]	8.835[10]	9.20[10]	8.26[10]	8.769[10]
2P _{1/2}	2P ^o _{1/2}	4.4[09] ^D	3.676[09]	3.677[09]	4.14[09]		3.720[09]
2P _{1/2}	2D ^o _{5/2}	2.91[10] ^C	2.648[10]	2.648[10]	2.85[10]		2.614[10]
2D _{3/2}	2P ^o _{1/2}	2.98[09] ^C	2.670[09]	2.668[09]	2.81[09]		2.661[09]
2D _{3/2}	2D ^o _{5/2}	4.3[07] ^E	3.056[07]	3.036[07]	4.95[07]		2.539[07]
2D _{3/2}	2D ^o _{3/2}	4.3[10] ^C	3.850[10]	3.849[10]	3.97[10]		3.825[10]
2D _{5/2}	2P ^o _{3/2}	6.0[09] ^C	5.419[09]	5.416[09]	5.61[09]		5.500[09]
2D _{5/2}	2D ^o _{3/2}	2.7[07] ^E	1.448[07]	1.446[07]	1.39[07]	1.09[07]	1.096[07]
2D _{5/2}	2D ^o _{5/2}	3.3[10] ^C	2.932[10]	2.930[10]	3.04[10]		2.916[10]
4P _{1/2}	4S ^o _{3/2}	2.09[10] ^C	1.877[10]	1.875[10]	1.92[10]	1.28[10]	1.852[10]
4P _{3/2}	4S ^o _{3/2}	1.86[10] ^C	1.677[10]	1.676[10]	1.72[10]	1.37[10]	1.667[10]
4P _{5/2}	4S ^o _{3/2}	1.3[10] ^C	1.187[10]	1.186[10]	1.22[10]	1.19[10]	1.194[10]
2D _{5/2}	4S ^o _{3/2}		1.590[07]	1.583[07]	1.40[07]		1.602[07]
2D _{3/2}	4S ^o _{3/2}	1.9[09] ^E	1.554[09]	1.555[09]	1.52[09]	2.87[09]	1.428[09]
2S _{1/2}	4S ^o _{3/2}	1.9[09] ^E	1.662[09]	1.663[09]	1.69[09]	1.48[10]	1.539[09]
2P _{3/2}	4S ^o _{3/2}	4.6[09] ^E	4.079[09]	4.082[09]	4.16[09]	8.75[09]	3.811[09]
2P _{1/2}	4S ^o _{3/2}		1.211[08]	1.212[08]	1.32[08]		1.226[08]
E2							
2P ^o _{1/2}	2D ^o _{3/2}	5.2 ^E	5.212	5.297		5.40	4.99
2P ^o _{3/2}	2D ^o _{5/2}	1.5[01] ^E	1.459[01]	1.497[01]		1.54[01]	1.39[01]
2P ^o _{1/2}	2P ^o _{3/2}	2.2 ^E	2.066	2.072		2.15	1.87
M1							
2P ^o _{1/2}	4S ^o _{3/2}	3.3[04] ^D	3.135[04]	3.136[04]	3.13[04]	2.97[04]	2.98[04]
2P ^o _{3/2}	4S ^o _{3/2}	2.91[04] ^C	2.921[04]	2.921[04]	2.98[04]	2.91[04]	2.85[04]
2P ^o _{1/2}	2D ^o _{3/2}	6.100[03] ^D	5.801[03]	5.801[03]	5.87[03]	6.06[03]	5.62[03]
2P ^o _{3/2}	2D ^o _{5/2}	4.49[04] ^D	4.339[04]	4.341[04]	4.28[04]	4.34[04]	4.06[04]

Notes. Transition rates A are given in s⁻¹. Numbers in the brackets are powers of ten.

References. ^(a) Kramida et al. (2013); ^(b) present calculations; ^(c) Rynkun et al. (2014); ^(d) Jonauskas et al. (2005); ^(e) Nahar (2004); ^(f) Merkeliš et al. (1997, 1999). ^C, ^D, and ^E are the estimated accuracies for transition probabilities. C : $\leq 25\%$, D : $\leq 50\%$, E : $\geq 50\%$.

Table 4. Energy levels in cm^{-1} and the difference (Diff) between theoretical energies and observed E_{obs} .

Pos	Conf.	LSJ	E^a_{obs}	E^b_{cal}	$\text{Diff}^b_{\text{cal}}$	$\text{Diff}^c_{\text{RCI}}$	$\text{Diff}^d_{\text{MRMP}}$	$\text{Diff}^e_{\text{SS}}$	$\text{Diff}^f_{\text{MBPT}}$	$\text{Diff}^i_{\text{CI+MBPT}}$
Cr XVIII $Z = 24$										
1	$2s^2 2p^3$	$4S^{\circ}_{3/2}$	0	0	0	0			0	
2		$2D^{\circ}_{3/2}$	126 060	126 328	268	266			587	
3		$2D^{\circ}_{5/2}$	150 810	151 075	265	269			149	
4		$2P^{\circ}_{1/2}$	226 180	226 546	366	364			765	
5		$2P^{\circ}_{3/2}$	264 540	264 860	320	330			-1829	
6	$2s 2p^4$	$4P_{5/2}$	667 080	667 344	264	279			-1 611	
7		$4P_{3/2}$	714 400	714 369	-31	-5			-2808	
8		$4P_{1/2}$	732 050	732 006	-44	-15			-3081	
9		$2D_{3/2}$	922 720	923 050	330	375			-3349	
10		$2D_{5/2}$	931 180	931 476	296	341			-3708	
11		$2S_{1/2}$	1 061 750	1 062 479	729	788			-5003	
12		$2P_{3/2}$	1 103 370	1 103 812	442	504			-5796	
13		$2P_{1/2}$	1 170 450	1 170 691	241	314			-7389	
14	$2p^5$	$2P^{\circ}_{3/2}$	1 738 700	1 738 860	160	298			-8144	
15		$2P^{\circ}_{1/2}$	1 813 560	1 813 685	125	280			-9937	
Ni XXII $Z = 28$										
1	$2s^2 2p^3$	$4S^{\circ}_{3/2}$	0	0	0	0			0	0
2		$2D^{\circ}_{3/2}$	157 536	157 732	196	211			-114	105
3		$2D^{\circ}_{5/2}$	209 380	209 602	222	243			-869	74
4		$2P^{\circ}_{1/2}$	302 600	302 989	389	407			-2391	485
5		$2P^{\circ}_{3/2}$	400 100	400 330	230	261			-4850	324
6	$2s 2p^4$	$4P_{5/2}$	847 940	847 906	-34	-63			4129	540
7		$4P_{3/2}$	942 827	942 686	-141	-152			-6673	523
8		$4P_{1/2}$	967 811	967 650	-161	-169			-6919	447
9		$2D_{3/2}$	1 176 022	1 176 331	309	340			-6842	265
10		$2D_{5/2}$	1 203 298	1 203 484	186	220			-7984	210
11		$2S_{1/2}$	1 344 300	1 344 953	653	687			-10 255	691
12		$2P_{3/2}$	1 398 800	1 399 316	516	581			-11 453	240
13		$2P_{1/2}$	1 536 500	1 536 685	185	265			-15 587	4
14	$2p^5$	$2P^{\circ}_{3/2}$	2 190 300	2 190 414	114	386			-14 593	-494
15		$2P^{\circ}_{1/2}$	2 340 900	2 340 835	-65	228			-18 982	-515
Zn XXIV $Z = 30$										
1	$2s^2 2p^3$	$4S^{\circ}_{3/2}$	0	0	0			0	0	
2		$2D^{\circ}_{3/2}$	188 130	187 907	-223	-204	-399	1 548	-2075	
3		$2D^{\circ}_{5/2}$	254 110	254 278	168	193	-10	5 355	-2394	
4		$2P^{\circ}_{1/2}$	357 130	357 220	90	111	-71	-140	-4548	
5		$2P^{\circ}_{3/2}$	501 140	500 593	-547	-507	-360	-2029	-10 138	
6	$2s 2p^4$	$4P_{5/2}$	956 600	956 373	-227	-170	-232	-2621	-6662	
7		$4P_{3/2}$	1 084 810	1 084 416	-394	-317	-369	-5263	-10 465	
8		$4P_{1/2}$	1 110 540	1 110 240	-300	-219	-280	-5592	-10 430	
9		$2D_{3/2}$	1 328 550	1 328 353	-197	-96	-306	3810	-11 027	
10		$2D_{5/2}$	1 371 750	1 371 841	91	193	-27	6956	-12 316	
11		$2S_{1/2}$	1 516 340	1 516 461	121	234	277	2625	-15 515	
12		$2P_{3/2}$	1 578 630	1 578 985	355	481	255	10 962	-16 618	
13		$2P_{1/2}$	1 767 650	1 766 778	-872	-727	-1101	5892	-23 667	
14	$2p^5$	$2P^{\circ}_{3/2}$	2 451 700	2 451 454	-246	70	920	19 335	-20 684	
15		$2P^{\circ}_{1/2}$	2 657 600	2 656 422	-1178	-835	117	20 374	-28 085	

References. ^(a) Kramida et al. (2013); ^(b) Present calculations; ^(c) Rynkun et al. (2014); ^(d) Vilkas & Ishikawa (1998); ^(e) Bhatia et al. (1989); ^(h) Merkelis et al. (1997); ⁽ⁱ⁾ Gu (2005).

number $n = 8$. This will, based on the analysis of the convergence for Fe XX, only marginally affect the energies and transition rates. Energies of the 15 lowest states are given in Table 4. In the table, energies are compared with results from other calculations and with experimental energies from NIST. The mean

relative energy differences between the present calculations and experimental data from NIST are 0.07%, 0.04%, and 0.04% for the three ions. The relative energy differences are of similar size for the calculations by Rynkun et al. (2014) and, for Ni XXII, by Gu (2005). It is interesting to note that differences between the

calculated and experimental energies for Zn XXIV do not follow the trends of the other ions. This may be due to the experimental conditions. When comparing with experimental data one should bear in mind that there are also experimental uncertainties that cannot be neglected.

Tables 8, 10, 12 in the on-line material give energies, A_J and B_J hyperfine constants, Landé g_J factors, and the mass- and field-shift parameters for all levels of Cr XVIII, Ni XXII, and Zn XXIV. Eigenvector compositions of the states of these ions are found in Tables 9, 11, and 13. There are basically no experimental data above the first 15 levels. The CHIANTI database gives energies for some higher lying states in Zn XXIV. These energies are, however, calculated and associated with large uncertainties. In addition, the given LSJ -labels disagree with the labels obtained from the present calculation. Transition energies, wavelengths, transition rates, weighted oscillator strengths, and uncertainty estimators dT for transitions between all 272 states are available on line in Tables 15–17. Lifetimes in length and velocity form are given in Tables 19–21. The uncertainties estimated from dT are similar to the values for Fe XX. The mean relative difference between the lifetimes in the length and velocity form is around 2.5‰ for the three ions.

4.3. Summary and conclusions

Self-consistent MCDHF and subsequent RCI calculations were performed for the nitrogen-like ions Cr XVIII, Fe XX, Ni XXII, and Zn XXIV using GRASP2K. Energies, A_J and B_J hyperfine constants, Landé g_J -factors, mass- and field-shift parameters, and transition rates involving the $2s^22p^3$, $2s2p^4$, $2p^5$, $2s^22p^23l$, $2s2p^33l$, and $2p^43l$ ($l = 0, 1, 2$) configurations are given. Compositions of atomic state functions in LSJ -coupling are also reported. Previous theoretical and experimental data for Fe XX were used to validate computational methods. Energies from the RCI calculations are in excellent agreement with observations. For the 15 lowest states the mean relative energy differences are around 0.04% (NIST Atomic Spectra Database 2013) for the four ions. This translates to wavelengths that are accurate to within ± 10 mÅ and thus of spectroscopic accuracy. The high accuracy carries over also to the higher states.

Uncertainties in electric dipole transition rates between the lower states have been estimated from the expressions suggested by Ekman et al. (2014b) giving an average of only 1.9%. We thus argue that the transition rates are highly accurate and may serve as benchmarks for other calculations. To summarize, the present work has significantly increased the amount of accurate data for ions in the nitrogen-like sequence.

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