

Oscillator strengths for transitions in C-like ions between K XIV and Mn XX[★]

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Abstract. Energy levels and oscillator strengths (transition probabilities) have been calculated for transitions among 46 fine-structure levels of the $(1s^2) 2s^2 2p^2$, $2s 2p^3$, $2p^4$, $2s^2 2p 3s$, $2s^2 2p 3p$ and $2s^2 2p 3d$ configurations of C-like K XIV, Sc XVI, Ti XVII, V XVIII, Cr XIX and Mn XX using the GRASP code. Configuration interaction and relativistic effects have been included while generating the wavefunctions. Calculated values of energy levels agree within 3% with the experimentally compiled results, and the length and velocity forms of oscillator strengths agree within 20% for a majority of allowed transitions.

Key words. atomic data – atomic processes

1. Introduction

This is a continuation of our efforts to generate atomic data (energy levels, oscillator strengths, radiative rates, collision strengths, and excitation rates) for C-like ions. Several papers have been published over the past two decades reporting such data, particularly for energy levels and radiative rates. To summarise, these papers are by Aggarwal et al. (1997a) for O III, Aggarwal et al. (1997b) for Ca XV and Fe XXI, Aggarwal (1998) for Ne V, Mg VII, Si IX and S XI, and Aggarwal et al. (2001) for F IV, Na VI, Al VIII, P X, Cl XII and Ar XIII. In the present paper we report similar data for six other C-like ions, namely K XIV, Sc XVI, Ti XVII, V XVIII, Cr XIX and Mn XX. This work completes the sequence for ions with nuclear charges $8 \leq Z \leq 26$.

Emission lines of C-like ions are highly useful as diagnostics of solar, astrophysical and fusion plasmas, the interpretation of which requires the knowledge of atomic parameters. Emission lines of the ions for which we present data in this paper have already been observed (Kelly 1987). Therefore, a few researchers in the past have reported atomic data for C-like ions. However, most of the calculations have been confined to the lowest 20 levels of the $(1s^2) 2s^2 2p^2$, $2s 2p^3$ and $2p^4$ configurations. Similar data for transitions among the levels of the $2s^2 2p 3s$, $2s^2 2p 3p$ and $2s^2 2p 3d$ configurations, which mostly lie in the X-ray and EUV regions, are equally important, especially for the modeling of astrophysical and laboratory plasmas, and therefore have become increasingly in demand. Fawcett (1987)

has included levels of the $2s^2 2p 3s$ and $2s^2 2p 3d$ configurations in his calculations, whereas Zhang & Sampson (1996, 1997) have also included levels of the $2s^2 2p 3p$ configuration. Both Fawcett and Zhang & Sampson have included configuration interaction (CI) and relativistic effects (RE) in their calculations, as these are equally important particularly for the ions under discussion here. However, atomic data have been reported for a few transitions only, and therefore, our aim is to report results of oscillator strengths and radiative rates for *all* allowed transitions among 46 fine-structure levels of the $(1s^2) 2s^2 2p^2$, $2s 2p^3$, $2p^4$, $2s^2 2p 3s$, $2s^2 2p 3p$ and $2s^2 2p 3d$ configurations. Additionally, we find that there is scope for improvement over the earlier results, because the inclusion of CI in these calculations is rather restricted.

2. Calculations

In almost all our previous work referred to above, we have adopted the CIV3 program of Hibbert (1975) to perform our calculations for energy levels and radiative rates. However, in the cases of Ca XV and Fe XXI we also performed an additional set of calculations employing the GRASP code of Dyllal et al. (1989), as relativistic effects are very important for these and other ions with similar or higher Z . The inclusion of CI in our GRASP calculations was restricted to that within the basic (above listed six) configurations only. On the other hand, the CIV3 calculations considered more elaborate CI including *external* orbitals, but included only one-body relativistic operators in a Breit-Pauli approximation, namely spin-orbit, spin-other-orbit, spin-spin, Darwin and mass correction terms. In the present work we find this approach of LSJ coupling scheme to be inadequate, as both CI and RE are equally important

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[★] Tables 4 to 9 are only available in electronic form at <http://www.edpsciences.org>

for the ions under consideration here, and therefore we have adopted the fully relativistic GRASP code (which is based on the jj coupling scheme), but with inclusion of larger CI. To be specific, CI has been included among the $1s^2 2s^2 2p^2$, $2s 2p^3$, $2p^4$, $2s^2 2p 3\ell$, $2s 2p^2 3\ell$, $2p^3 3\ell$ and $2s^2 3\ell^2$ configurations. These 15 configurations give rise to 251 fine-structure levels, but results for energy levels and radiative rates are reported for those among the lowest 46 levels of the first six configurations only. The Breit and QED corrections have been included in the calculations, and the option of EAL (extended average level) has been adopted, as in all our earlier works. In this type of calculation, a weighted trace of the Hamiltonian matrix is minimized, which yields a compromise set of orbitals describing closely lying states with moderate accuracy.

3. Results and discussion

In Tables 1–3 we list the energy levels arising from the $(1s^2) 2s^2 2p^2$, $2s 2p^3$, $2p^4$, $2s^2 2p 3s$, $2s^2 2p 3p$ and $2s^2 2p 3d$ configurations of C-like ions, and compare our threshold energies for K XIV, Sc XVI, Ti XVII, V XVIII, Cr XIX and Mn XX with the experimental values compiled by NIST (National Institute for Standards and Technology: www.physics.nist.gov/PhysRefData). Since the ordering of the energy levels is *not* the same for all C-like ions, the levels are listed in Tables 1–3 for each ion. The first column of each table provides an index for the corresponding level. However, it may be noted that the experimental values are not available for all levels, and the accuracy for some of these, especially those among the $2s^2 2p 3s$, $2s^2 2p 3p$ and $2s^2 2p 3d$ configurations, is not very high. The theoretical values available in the literature are mostly confined to the lowest 20 levels, but corresponding results involving some of the higher excited levels have been reported by Fawcett (1987) and Zhang & Sampson (1997) in the form of transition wavelengths.

The agreement of our level energies with the experimental ones is excellent (within 3%) for all levels and for all ions. It may be noted that the energy order of the theoretical and experimental energy levels is slightly different in a few instances; see, for example, the highest two levels of K XIV and Sc XVI. However, the energy differences for such levels are very small (≤ 0.03 Ryd). This problem of energy order is frequently encountered in all theoretical work, especially when the energy separation of the levels is very small. Furthermore, in the absence of definitive experimental level energies in most of the cases, a correct energy order cannot be confirmed. In any event, it does not affect the computed values of the oscillator strengths and collision strengths.

In Tables 4–9 we present our oscillator strengths and radiative rates (in length form only) for allowed transitions in K XIV, Sc XVI, Ti XVII, V XVIII, Cr XIX and Mn XX. The indices used to represent the levels of a transition are already given in Tables 1–3. Since the indices of the various levels are *not* the same for all the ions, we have included in these tables the *shorter* forms of the lower and upper levels of a transition. This should facilitate their identification.

The other values available in the literature for oscillator strengths (f -values) and radiative rates (A -values), apart from

those of Fawcett (1987), are of Zhang & Sampson (1996) for a few transitions among the lowest 20 levels. Their results are not only the most recent for the present ions, but are also similar and comparable to our present calculations, as they too have adopted the GRASP code, but have restricted the inclusion of CI among the first three configurations only, i.e. $2s^2 2p^2$, $2s 2p^3$ and $2p^4$. Zhang & Sampson (1997) have performed a larger calculation including the levels of the $2s^2 2p 3s$, $2s^2 2p 3p$ and $2s^2 2p 3d$ configurations, but have not reported any data for the ions under discussion here. However, a comparison between our present and their earlier results for oscillator strengths shows agreement within 20% for the available common transitions for all ions. This is an expected result considering the limited amount of CI included by them.

Among the higher excited levels, the only results available in the literature are by Fawcett (1987), who has adopted the Hartree-Fock relativistic (HFR) code of Cowan (1981). In Table 10 we compare our values of oscillator strengths for a few representative transitions with his HFR results. The indices used to represent a transition correspond to those of K XIV, but a shorter form of the transitions has been included in Col. 3 in order to facilitate an easy identification of the same transition in different ions. Generally, our GRASP and earlier HFR f -values agree within 10%, but for a few transitions (such as 2-40 and 5-45) the differences are up to 30%, and for the 2-45 ($2s^2 2p^2 \ ^3P_1 - 2s^2 2p 3d \ ^1P_1^\circ$) and 4-37 ($2s^2 2p^2 \ ^1D_2 - 2s^2 2p 3d \ ^1D_2^\circ$) transitions, the two sets of results differ by a factor of two. However, the transitions for which differences between the two sets of calculations are significant are weaker transitions, whose f -values are comparatively small. These differences arise due to different amount of CI included in the calculations.

In general, inclusion of larger CI improves the wavefunctions, and hence leads to a more accurate determination of energy levels and radiative rates for a majority of transitions. However, occasionally it may also result in comparatively reduced accuracy for a few transitions, as has specifically been discussed by Aggarwal (1998) for transitions in Fe XXI. A further example of this is provided by the 2-45 ($2s^2 2p^2 \ ^3P_1 - 2s^2 2p 3d \ ^1P_1^\circ$) transition in Sc XVI, whose f -value of 7.545×10^{-4} is incongruous with the corresponding f -values of other ions as shown in Table 10. Our calculations with 6, 12, 15, 16, 19 and 20 configurations yield the f -values 3.807×10^{-3} , 1.535×10^{-4} , 7.545×10^{-4} , 5.168×10^{-3} , 5.184×10^{-3} and 5.130×10^{-3} , respectively. Clearly, the f -value for this transition should be $\sim 10^{-3}$, and the presently reported result of 7.545×10^{-4} is underestimated by a factor of seven. There could be some other similar examples, but a majority of transitions are unaffected by such inconsistencies.

The accuracy of the calculated f - or A -values is generally (but not conclusively) determined by the agreement between their length and velocity forms. In any large calculation involving a large number of transitions, as in the present work, the agreement between the two forms for *all* the transitions is never satisfactory. Weak transitions ($f < 0.10$) being sensitive to mixing often show large variations, which can be over an order of magnitude. However, these transitions are not very important, in general. For transitions whose f -values are

Table 1. Target levels of K XIV and Sc XVI, and their threshold energies (in Ryd).

K XIV					Sc XVI			
Index	Configuration	Level	Expt. ^a	GRASP	Configuration	Level	Expt. ^a	GRASP
1.....	1s ² 2s ² 2p ²	³ P ₀	0.0000	0.0000	1s ² 2s ² 2p ²	³ P ₀	0.0000	0.0000
2.....	1s ² 2s ² 2p ²	³ P ₁	0.1206	0.1196	1s ² 2s ² 2p ²	³ P ₁	0.2092	0.2076
3.....	1s ² 2s ² 2p ²	³ P ₂	0.2572	0.2564	1s ² 2s ² 2p ²	³ P ₂	0.4103	0.4099
4.....	1s ² 2s ² 2p ²	¹ D ₂	0.8740	0.9017	1s ² 2s ² 2p ²	¹ D ₂	1.1241	1.1495
5.....	1s ² 2s ² 2p ²	¹ S ₀	1.6304	1.6390	1s ² 2s ² 2p ²	¹ S ₀	1.9931	1.9996
6.....	1s ² 2s2p ³	⁵ S ^o ₂	2.2840	2.2160	1s ² 2s2p ³	⁵ S ^o ₂	2.7460	2.6986
7.....	1s ² 2s2p ³	³ D ^o ₂	4.1805	4.2224	1s ² 2s2p ³	³ D ^o ₂	4.8899	4.9325
8.....	1s ² 2s2p ³	³ D ^o ₁	4.1873	4.2293	1s ² 2s2p ³	³ D ^o ₁	4.9000	4.9433
9.....	1s ² 2s2p ³	³ D ^o ₃	4.2010	4.2413	1s ² 2s2p ³	³ D ^o ₃	4.9393	4.9800
10.....	1s ² 2s2p ³	³ P ^o ₀	4.8972	4.9500	1s ² 2s2p ³	³ P ^o ₀	5.7280	5.7816
11.....	1s ² 2s2p ³	³ P ^o ₁	4.9029	4.9556	1s ² 2s2p ³	³ P ^o ₁	5.7432	5.7965
12.....	1s ² 2s2p ³	³ P ^o ₂	4.9203	4.9722	1s ² 2s2p ³	³ P ^o ₂	5.7813	5.8332
13.....	1s ² 2s2p ³	³ S ^o ₁	6.1757	6.2936	1s ² 2s2p ³	³ S ^o ₁	7.1293	7.2478
14.....	1s ² 2s2p ³	¹ D ^o ₂	6.1643	6.2994	1s ² 2s2p ³	¹ D ^o ₂	7.1601	7.2941
15.....	1s ² 2s2p ³	¹ P ^o ₁	6.8805	7.0246	1s ² 2s2p ³	¹ P ^o ₁	7.9900	8.1345
16.....	1s ² 2p ⁴	³ P ₂	9.3869	9.5251	1s ² 2p ⁴	³ P ₂	10.824	10.9652
17.....	1s ² 2p ⁴	³ P ₁	9.5740	9.7092	1s ² 2p ⁴	³ P ₁	11.129	11.2655
18.....	1s ² 2p ⁴	³ P ₀	9.6248	9.7608	1s ² 2p ⁴	³ P ₀	11.188	11.3278
19.....	1s ² 2p ⁴	¹ D ₂	10.104	10.2920	1s ² 2p ⁴	¹ D ₂	11.714	11.9019
20.....	1s ² 2p ⁴	¹ S ₀	11.435	11.6672	1s ² 2p ⁴	¹ S ₀	13.226	13.4574
21.....	1s ² 2s ² 2p3s	³ P ^o ₀	32.6831	1s ² 2s ² 2p3s	³ P ^o ₀	41.8443
22.....	1s ² 2s ² 2p3s	³ P ^o ₁	32.7250	1s ² 2s ² 2p3s	³ P ^o ₁	41.970	41.8981
23.....	1s ² 2s ² 2p3s	³ P ^o ₂	32.9437	1s ² 2s ² 2p3s	³ P ^o ₂	42.330	42.2547
24.....	1s ² 2s ² 2p3s	¹ P ^o ₁	33.1109	1s ² 2s ² 2p3s	¹ P ^o ₁	42.490	42.4381
25.....	1s ² 2s ² 2p3p	¹ P ₁	33.7630	1s ² 2s ² 2p3p	³ D ₁	43.0839
26.....	1s ² 2s ² 2p3p	³ D ₁	33.9296	1s ² 2s ² 2p3p	¹ P ₁	43.3261
27.....	1s ² 2s ² 2p3p	³ D ₂	33.9419	1s ² 2s ² 2p3p	³ D ₂	43.3370
28.....	1s ² 2s ² 2p3p	³ P ₀	34.1207	1s ² 2s ² 2p3p	³ P ₀	43.5175
29.....	1s ² 2s ² 2p3p	³ D ₃	34.1253	1s ² 2s ² 2p3p	³ P ₁	43.6380
30.....	1s ² 2s ² 2p3p	³ S ₁	34.1557	1s ² 2s ² 2p3p	³ D ₃	43.6360
31.....	1s ² 2s ² 2p3p	³ P ₁	34.2616	1s ² 2s ² 2p3p	³ S ₁	43.7675
32.....	1s ² 2s ² 2p3p	³ P ₂	34.3046	1s ² 2s ² 2p3p	³ P ₂	43.8172
33.....	1s ² 2s ² 2p3p	¹ D ₂	34.6637	1s ² 2s ² 2p3p	¹ D ₂	44.2242
34.....	1s ² 2s ² 2p3p	¹ S ₀	35.0815	1s ² 2s ² 2p3d	³ F ^o ₂	44.000	44.6449
35.....	1s ² 2s ² 2p3d	³ F ^o ₂	35.1118	1s ² 2s ² 2p3p	¹ S ₀	44.6965
36.....	1s ² 2s ² 2p3d	³ F ^o ₃	35.281	35.2249	1s ² 2s ² 2p3d	³ F ^o ₃	44.8108
37.....	1s ² 2s ² 2p3d	¹ D ^o ₂	35.2784	1s ² 2s ² 2p3d	¹ D ^o ₂	44.8758
38.....	1s ² 2s ² 2p3d	³ F ^o ₄	35.3805	1s ² 2s ² 2p3d	³ D ^o ₁	45.070	45.0389
39.....	1s ² 2s ² 2p3d	³ D ^o ₁	35.4403	1s ² 2s ² 2p3d	³ F ^o ₄	45.0710
40.....	1s ² 2s ² 2p3d	³ D ^o ₂	35.540	35.5013	1s ² 2s ² 2p3d	³ D ^o ₂	45.100	45.1766
41.....	1s ² 2s ² 2p3d	³ D ^o ₃	35.646	35.5992	1s ² 2s ² 2p3d	³ D ^o ₃	45.330	45.3115
42.....	1s ² 2s ² 2p3d	³ P ^o ₂	35.715	35.6591	1s ² 2s ² 2p3d	³ P ^o ₂	45.400	45.3875
43.....	1s ² 2s ² 2p3d	³ P ^o ₁	35.6754	1s ² 2s ² 2p3d	³ P ^o ₁	45.430	45.4037
44.....	1s ² 2s ² 2p3d	³ P ^o ₀	35.6872	1s ² 2s ² 2p3d	³ P ^o ₀	45.4177
45.....	1s ² 2s ² 2p3d	¹ P ^o ₁	36.075	36.0297	1s ² 2s ² 2p3d	¹ P ^o ₁	45.820	45.8118
46.....	1s ² 2s ² 2p3d	¹ F ^o ₃	36.046	36.0519	1s ² 2s ² 2p3d	¹ F ^o ₃	45.810	45.8299

^a NIST.

Table 2. Target levels of Ti XVII and V XVIII, and their threshold energies (in Ryd).

Ti XVII					V XVIII			
Index	Configuration	Level	Expt. ^a	GRASP	Configuration	Level	Expt. ^a	GRASP
1.....	1s ² 2s ² 2p ²	³ P ₀	0.0000	0.0000	1s ² 2s ² 2p ²	³ P ₀	0.0000	0.0000
2.....	1s ² 2s ² 2p ²	³ P ₁	0.2703	0.2683	1s ² 2s ² 2p ²	³ P ₁	0.3450	0.3427
3.....	1s ² 2s ² 2p ²	³ P ₂	0.5070	0.5078	1s ² 2s ² 2p ²	³ P ₂	0.6210	0.6216
4.....	1s ² 2s ² 2p ²	¹ D ₂	1.2817	1.3057	1s ² 2s ² 2p ²	¹ D ₂	1.4663	1.4888
5.....	1s ² 2s ² 2p ²	¹ S ₀	2.2069	2.2141	1s ² 2s ² 2p ²	¹ S ₀	2.4500	2.4565
6.....	1s ² 2s2p ³	⁵ S ^o ₂	3.0405	2.9745	1s ² 2s2p ³	⁵ S ^o ₂	3.3439	3.2770
7.....	1s ² 2s2p ³	³ D ^o ₂	5.2752	5.3180	1s ² 2s2p ³	³ D ^o ₂	5.6850	5.7271
8.....	1s ² 2s2p ³	³ D ^o ₁	5.2863	5.3304	1s ² 2s2p ³	³ D ^o ₁	5.6957	5.7402
9.....	1s ² 2s2p ³	³ D ^o ₃	5.3469	5.3878	1s ² 2s2p ³	³ D ^o ₃	5.7860	5.8260
10.....	1s ² 2s2p ³	³ P ^o ₀	6.1824	6.2364	1s ² 2s2p ³	³ P ^o ₀	6.6692	6.7221
11.....	1s ² 2s2p ³	³ P ^o ₁	6.2049	6.2588	1s ² 2s2p ³	³ P ^o ₁	6.7016	6.7542
12.....	1s ² 2s2p ³	³ P ^o ₂	6.2584	6.3107	1s ² 2s2p ³	³ P ^o ₂	6.7739	6.8256
13.....	1s ² 2s2p ³	³ S ^o ₁	7.6395	7.7588	1s ² 2s2p ³	³ S ^o ₁	8.1770	8.2966
14.....	1s ² 2s2p ³	¹ D ^o ₂	7.7014	7.8347	1s ² 2s2p ³	¹ D ^o ₂	8.2781	8.4102
15.....	1s ² 2s2p ³	¹ P ^o ₁	8.5970	8.7398	1s ² 2s2p ³	¹ P ^o ₁	9.2441	9.3859
16.....	1s ² 2p ⁴	³ P ₂	11.586	11.7279	1s ² 2p ⁴	³ P ₂	12.381	12.5239
17.....	1s ² 2p ⁴	³ P ₁	11.967	12.1049	1s ² 2p ⁴	³ P ₁	12.856	12.9921
18.....	1s ² 2p ⁴	³ P ₀	12.026	12.1671	1s ² 2p ⁴	³ P ₀	12.905	13.0481
19.....	1s ² 2p ⁴	¹ D ₂	12.578	12.7659	1s ² 2p ⁴	¹ D ₂	13.490	13.6767
20.....	1s ² 2p ⁴	¹ S ₀	14.187	14.4184	1s ² 2p ⁴	¹ S ₀	15.202	15.4332
21.....	1s ² 2s ² 2p3s	³ P ^o ₀	46.8526	1s ² 2s ² 2p3s	³ P ^o ₀	52.1481
22.....	1s ² 2s ² 2p3s	³ P ^o ₁	46.870	46.9122	1s ² 2s ² 2p3s	³ P ^o ₁	52.170	52.2135
23.....	1s ² 2s ² 2p3s	³ P ^o ₂	47.320	47.3586	1s ² 2s ² 2p3s	³ P ^o ₂	52.720	52.7656
24.....	1s ² 2s ² 2p3s	¹ P ^o ₁	47.000	47.5500	1s ² 2s ² 2p3s	¹ P ^o ₁	52.890	52.9651
25.....	1s ² 2s ² 2p3p	³ D ₁	48.1722	1s ² 2s ² 2p3p	³ D ₁	53.5478
26.....	1s ² 2s ² 2p3p	¹ P ₁	48.4584	1s ² 2s ² 2p3p	¹ P ₁	53.8823
27.....	1s ² 2s ² 2p3p	³ D ₂	48.4708	1s ² 2s ² 2p3p	³ D ₂	53.8979
28.....	1s ² 2s ² 2p3p	³ P ₀	48.6474	1s ² 2s ² 2p3p	³ P ₀	54.0667
29.....	1s ² 2s ² 2p3p	³ P ₁	48.8317	1s ² 2s ² 2p3p	³ P ₁	54.3316
30.....	1s ² 2s ² 2p3p	³ D ₃	48.8459	1s ² 2s ² 2p3p	³ D ₃	54.3637
31.....	1s ² 2s ² 2p3p	³ S ₁	48.9724	1s ² 2s ² 2p3p	³ S ₁	54.4834
32.....	1s ² 2s ² 2p3p	³ P ₂	49.0232	1s ² 2s ² 2p3p	³ P ₂	54.5329
33.....	1s ² 2s ² 2p3p	¹ D ₂	49.4567	1s ² 2s ² 2p3p	¹ D ₂	54.9960
34.....	1s ² 2s ² 2p3d	³ F ^o ₂	49.860	49.8455	1s ² 2s ² 2p3d	³ F ^o ₂	55.3380
35.....	1s ² 2s ² 2p3p	¹ S ₀	49.9541	1s ² 2s ² 2p3p	¹ S ₀	55.5161
36.....	1s ² 2s ² 2p3d	³ F ^o ₃	50.0419	1s ² 2s ² 2p3d	³ F ^o ₃	55.5678
37.....	1s ² 2s ² 2p3d	¹ D ^o ₂	50.130	50.1092	1s ² 2s ² 2p3d	¹ D ^o ₂	55.6347
38.....	1s ² 2s ² 2p3d	³ D ^o ₁	50.290	50.2727	1s ² 2s ² 2p3d	³ D ^o ₁	55.7988
39.....	1s ² 2s ² 2p3d	³ F ^o ₄	50.3724	1s ² 2s ² 2p3d	³ F ^o ₄	55.9829
40.....	1s ² 2s ² 2p3d	³ D ^o ₂	50.500	50.4702	1s ² 2s ² 2p3d	³ D ^o ₂	56.100	56.0732
41.....	1s ² 2s ² 2p3d	³ D ^o ₃	50.630	50.6220	1s ² 2s ² 2p3d	³ D ^o ₃	56.260	56.2403
42.....	1s ² 2s ² 2p3d	³ P ^o ₂	50.730	50.7071	1s ² 2s ² 2p3d	³ P ^o ₂	56.380	56.3353
43.....	1s ² 2s ² 2p3d	³ P ^o ₁	50.7224	1s ² 2s ² 2p3d	³ P ^o ₁	56.450	56.3488
44.....	1s ² 2s ² 2p3d	³ P ^o ₀	50.7374	1s ² 2s ² 2p3d	³ P ^o ₀	56.3646
45.....	1s ² 2s ² 2p3d	¹ P ^o ₁	51.140	51.1544	1s ² 2s ² 2p3d	¹ P ^o ₁	56.8048
46.....	1s ² 2s ² 2p3d	¹ F ^o ₃	51.150	51.1723	1s ² 2s ² 2p3d	¹ F ^o ₃	56.800	56.8221

^a NIST.

Table 3. Target levels of Cr XIX and Mn XX, and their threshold energies (in Ryd).

Cr XIX					Mn XX			
Index	Configuration	Level	Expt. ^a	GRASP	Configuration	Level	Expt. ^a	GRASP
1.....	1s ² 2s ² 2p ²	³ P ₀	0.0000	0.0000	1s ² 2s ² 2p ²	³ P ₀	0.0000	0.0000
2.....	1s ² 2s ² 2p ²	³ P ₁	0.4357	0.4329	1s ² 2s ² 2p ²	³ P ₁	0.5420	0.5410
3.....	1s ² 2s ² 2p ²	³ P ₂	0.7514	0.7525	1s ² 2s ² 2p ²	³ P ₂	0.8980	0.9020
4.....	1s ² 2s ² 2p ²	¹ D ₂	1.6822	1.7034	1s ² 2s ² 2p ²	¹ D ₂	1.9342	1.9540
5.....	1s ² 2s ² 2p ²	¹ S ₀	2.7220	2.7311	1s ² 2s ² 2p ²	¹ S ₀	3.0352	3.0422
6.....	1s ² 2s2p ³	⁵ S ^o ₂	3.6748	3.6090	1s ² 2s2p ³	⁵ S ^o ₂	4.0374	3.9730
7.....	1s ² 2s2p ³	³ D ^o ₂	6.1203	6.1628	1s ² 2s2p ³	³ D ^o ₂	6.5858	6.6282
8.....	1s ² 2s2p ³	³ D ^o ₁	6.1307	6.1747	1s ² 2s2p ³	³ D ^o ₁	6.5892	6.6358
9.....	1s ² 2s2p ³	³ D ^o ₃	6.2588	6.2985	1s ² 2s2p ³	³ D ^o ₃	6.7701	6.8092
10.....	1s ² 2s2p ³	³ P ^o ₀	7.1913	7.2424	1s ² 2s2p ³	³ P ^o ₀	7.7488	7.8016
11.....	1s ² 2s2p ³	³ P ^o ₁	7.2366	7.2871	1s ² 2s2p ³	³ P ^o ₁	7.8080	7.8617
12.....	1s ² 2s2p ³	³ P ^o ₂	7.3334	7.3826	1s ² 2s2p ³	³ P ^o ₂	7.9333	7.9863
13.....	1s ² 2s2p ³	³ S ^o ₁	8.7470	8.8644	1s ² 2s2p ³	³ S ^o ₁	9.3451	9.4660
14.....	1s ² 2s2p ³	¹ D ^o ₂	8.8959	9.0259	1s ² 2s2p ³	¹ D ^o ₂	9.5581	9.6872
15.....	1s ² 2s2p ³	¹ P ^o ₁	9.9388	10.0787	1s ² 2s2p ³	¹ P ^o ₁	10.685	10.8245
16.....	1s ² 2p ⁴	³ P ₂	13.215	13.3569	1s ² 2p ⁴	³ P ₂	14.086	14.2310
17.....	1s ² 2p ⁴	³ P ₁	13.800	13.9329	1s ² 2p ⁴	³ P ₁	14.796	14.9331
18.....	1s ² 2p ⁴	³ P ₀	13.833	13.9737	1s ² 2p ⁴	³ P ₀	14.798	14.9467
19.....	1s ² 2p ⁴	¹ D ₂	14.455	14.6399	1s ² 2p ⁴	¹ D ₂	15.476	15.6618
20.....	1s ² 2p ⁴	¹ S ₀	16.286	16.5100	1s ² 2p ⁴	¹ S ₀	17.432	17.6580
21.....	1s ² 2s ² 2p3s	³ P ^o ₀	57.7323	1s ² 2s ² 2p3s	³ P ^o ₀	63.6071
22.....	1s ² 2s ² 2p3s	³ P ^o ₁	57.8035	1s ² 2s ² 2p3s	³ P ^o ₁	63.6839
23.....	1s ² 2s ² 2p3s	³ P ^o ₂	58.4790	1s ² 2s ² 2p3s	³ P ^o ₂	64.5025
24.....	1s ² 2s ² 2p3s	¹ P ^o ₁	58.6867	1s ² 2s ² 2p3s	¹ P ^o ₁	64.7184
25.....	1s ² 2s ² 2p3p	³ D ₁	59.2125	1s ² 2s ² 2p3p	³ D ₁	65.1680
26.....	1s ² 2s ² 2p3p	¹ P ₁	59.5998	1s ² 2s ² 2p3p	¹ P ₁	65.6133
27.....	1s ² 2s ² 2p3p	³ D ₂	59.6202	1s ² 2s ² 2p3p	³ D ₂	65.6400
28.....	1s ² 2s ² 2p3p	³ P ₀	59.7770	1s ² 2s ² 2p3p	³ P ₀	65.7798
29.....	1s ² 2s ² 2p3p	³ P ₁	60.1408	1s ² 2s ² 2p3p	³ P ₁	66.2625
30.....	1s ² 2s ² 2p3p	³ D ₃	60.1932	1s ² 2s ² 2p3p	³ D ₃	66.3386
31.....	1s ² 2s ² 2p3p	³ S ₁	60.3047	1s ² 2s ² 2p3p	³ S ₁	66.4407
32.....	1s ² 2s ² 2p3p	³ P ₂	60.3497	1s ² 2s ² 2p3p	³ P ₂	66.4770
33.....	1s ² 2s ² 2p3p	¹ D ₂	60.8463	1s ² 2s ² 2p3p	¹ D ₂	67.0120
34.....	1s ² 2s ² 2p3d	³ F ^o ₂	61.1247	1s ² 2s ² 2p3d	³ F ^o ₂	67.2078
35.....	1s ² 2s ² 2p3p	¹ S ₀	61.3854	1s ² 2s ² 2p3d	³ F ^o ₃	67.5120
36.....	1s ² 2s ² 2p3d	³ F ^o ₃	61.3904	1s ² 2s ² 2p3p	¹ S ₀	67.5645
37.....	1s ² 2s ² 2p3d	¹ D ^o ₂	61.4547	1s ² 2s ² 2p3d	¹ D ^o ₂	67.5718
38.....	1s ² 2s ² 2p3d	³ D ^o ₁	61.6191	1s ² 2s ² 2p3d	³ D ^o ₁	67.7359
39.....	1s ² 2s ² 2p3d	³ F ^o ₄	61.9066	1s ² 2s ² 2p3d	³ F ^o ₄	68.1478
40.....	1s ² 2s ² 2p3d	³ D ^o ₂	61.9896	1s ² 2s ² 2p3d	³ D ^o ₂	68.2234
41.....	1s ² 2s ² 2p3d	³ D ^o ₃	62.1706	1s ² 2s ² 2p3d	³ D ^o ₃	68.4171
42.....	1s ² 2s ² 2p3d	³ P ^o ₂	62.2760	1s ² 2s ² 2p3d	³ P ^o ₂	68.5336
43.....	1s ² 2s ² 2p3d	³ P ^o ₁	62.2865	1s ² 2s ² 2p3d	³ P ^o ₁	68.5390
44.....	1s ² 2s ² 2p3d	³ P ^o ₀	62.3028	1s ² 2s ² 2p3d	³ P ^o ₀	68.5544
45.....	1s ² 2s ² 2p3d	¹ P ^o ₁	62.7629	1s ² 2s ² 2p3d	¹ P ^o ₁	69.0318
46.....	1s ² 2s ² 2p3d	¹ F ^o ₃	62.7836	1s ² 2s ² 2p3d	¹ F ^o ₃	69.0611

^a NIST.

Table 10. Comparison between our present GRASP (first rows) oscillator strengths with the HFR (second rows) results of Fawcett (1987) for a few transitions of C-like ions. ($a \pm b \equiv a \times 10^{\pm b}$).

<i>i</i>	<i>j</i>	Transition	K XIV	Sc XVI	Ti XVII	V XVIII	Cr XIX	Mn XX
1	22	$^3P_0-^3P^o_1$	5.995-2	5.813-2	5.748-2	5.697-2	5.655-2	5.619-2
			6.600-2	6.400-2	6.400-2	6.300-2	6.300-2	6.300-2
1	24	$^3P_0-^1P^o_1$	2.042-3	2.044-3	1.941-3	1.789-3	1.605-3	1.404-3
			2.000-3	2.000-3	2.000-3	2.000-3	2.000-3	2.000-2
1	39	$^3P_0-^3D^o_1$	1.235-0	1.262-0	1.274-0	1.285-0	1.295-0	1.305-0
			1.320-0	1.340-0	1.349-0	1.359-0	1.368-0	1.377-0
2	37	$^3P_1-^1D^o_2$	1.507-1	2.593-1	3.113-1	3.567-1	3.944-1	4.250-1
			1.600-1	2.720-1	3.253-1	3.713-1	3.790-1	3.487-1
2	39	$^3P_1-^3D^o_1$	1.039-1	9.406-2	9.002-2	8.645-2	8.327-2	8.045-2
			1.077-1	9.500-2	9.100-2	8.730-2	8.430-2	8.130-2
2	40	$^3P_1-^3D^o_2$	6.162-1	5.015-1	4.480-1	4.019-1	3.643-1	3.347-1
			6.400-1	5.200-1	4.647-1	4.177-1	4.090-1	4.397-1
2	42	$^3P_1-^3P^o_2$	6.010-2	7.564-2	8.093-2	8.484-2	8.756-2	8.927-2
			7.700-2	8.970-2	9.400-2	9.700-2	9.900-2	1.000-1
2	43	$^3P_1-^3P^o_1$	2.081-1	2.226-1	2.290-1	2.352-1	2.414-1	2.482-1
			2.280-1	2.400-1	2.457-1	2.510-1	2.563-1	2.617-1
2	44	$^3P_1-^3P^o_0$	1.035-1	1.051-1	1.059-1	1.066-1	1.072-1	1.072-1
			1.100-1	1.110-1	1.120-1	1.130-1	1.133-1	1.140-1
2	45	$^3P_1-^1P^o_1$	5.607-3	7.545-4	6.570-3	1.004-2	1.421-2	2.039-2
			7.700-3	6.700-3	9.000-3	8.000-3	8.700-3	1.070-2
3	22	$^3P_2-^3P^o_1$	1.695-2	1.760-2	1.808-2	1.863-2	1.921-2	1.979-2
			1.840-2	1.960-2	1.960-2	2.020-2	2.080-2	2.140-2
3	23	$^3P_2-^3P^o_2$	4.530-2	4.247-2	4.088-2	3.918-2	3.737-2	3.550-2
			4.940-2	4.600-2	4.420-2	4.220-2	4.020-2	3.820-2
3	35	$^3P_2-^3F^o_2$	1.136-2	1.751-2	2.107-2	2.482-2	2.866-2	3.244-2
			1.060-2	1.700-2	2.080-2	2.480-2	2.880-2	3.260-2
3	36	$^3P_2-^3F^o_3$	5.376-2	8.743-2	1.078-1	1.300-1	1.536-1	1.781-1
			5.120-2	8.540-2	1.062-1	1.292-1	1.536-1	1.788-1
3	37	$^3P_2-^1D^o_2$	1.190-2	1.988-2	2.387-2	2.757-2	3.086-2	3.367-2
			1.720-2	2.600-2	3.020-2	3.400-2	2.300-2	3.120-2
3	41	$^3P_2-^3D^o_3$	7.378-1	7.170-1	7.020-1	6.845-1	6.650-1	6.443-1
			7.902-1	7.642-1	7.466-1	7.264-1	7.040-1	6.808-1
3	42	$^3P_2-^3P^o_2$	3.398-1	3.213-1	3.082-1	2.927-1	2.753-1	2.565-1
			3.564-1	3.328-1	3.174-1	2.998-1	2.804-1	2.600-1
3	43	$^3P_2-^3P^o_1$	8.213-2	7.940-2	7.726-2	7.453-2	7.114-2	6.678-2
			8.580-2	8.440-2	7.980-2	7.680-2	7.370-2	6.920-2
3	46	$^3P_2-^1F^o_3$	4.921-3	1.299-2	1.943-2	2.760-2	3.730-2	4.809-2
			6.400-3	1.600-2	2.360-2	3.320-2	4.420-2	5.640-2
4	24	$^1D_2-^1P^o_1$	4.696-2	4.428-2	4.305-2	4.185-2	4.066-2	3.947-2
			5.440-2	5.040-2	4.860-2	4.700-2	4.520-2	4.360-2
4	35	$^1D_2-^3F^o_2$	3.957-2	3.449-2	3.153-2	2.839-2	2.517-2	2.198-2
			5.280-2	3.060-2	2.860-2	2.600-2	2.320-2	2.040-2
4	37	$^1D_2-^1D^o_2$	1.170-1	8.670-2	7.182-2	5.856-2	4.729-2	3.798-2
			1.356-1	9.600-2	7.840-2	6.300-2	5.020-2	7.540-2
4	42	$^1D_2-^3P^o_2$	2.728-2	4.809-2	6.188-2	7.782-2	9.554-2	1.145-1
			3.120-2	5.480-2	7.020-2	8.740-2	1.064-1	1.262-1
4	45	$^1D_2-^1P^o_1$	1.263-2	9.475-3	1.235-2	1.292-2	1.332-2	1.330-2
			7.400-3	8.200-3	8.600-3	7.400-3	8.800-3	9.400-3

Table 10. continued.

i	j	Transition	K XIV	Sc XVI	Ti XVII	V XVIII	Cr XIX	Mn XX
4	46	$^1D_2-^1F_3$	1.032-0	1.033-0	1.028-0	1.020-0	1.009-0	9.956-1
			1.072-0	1.068-0	1.060-0	1.050-0	1.036-0	1.020-0
5	22	$^1S_0-^3P_1$	3.358-3	3.595-3	3.560-3	3.443-3	3.263-3	3.041-3
			4.000-3	4.000-3	4.000-3	4.000-3	4.000-3	4.000-3
5	24	$^1S_0-^1P_1$	7.402-2	7.097-2	6.978-2	6.876-2	6.788-2	6.712-2
			7.800-2	7.500-2	7.300-2	7.200-2	7.100-2	7.000-2
5	39	$^1S_0-^3D_1$	1.092-2	1.320-2	1.384-2	1.410-2	1.402-2	1.362-2
			1.300-2	1.500-2	1.500-2	1.500-2	1.500-2	1.500-2
5	43	$^1S_0-^3P_1$	2.246-3	3.195-3	3.803-3	4.507-3	5.294-3	6.115-3
			2.000-3	3.000-3	3.000-3	4.000-3	4.000-3	5.000-3
5	45	$^1S_0-^1P_1$	1.337-0	1.174-0	1.314-0	1.281-0	1.198-0	1.004-0
			1.394-0	1.387-0	1.368-0	1.334-0	1.365-0	1.344-0

significantly larger (≥ 0.10), the agreement between the two forms is within 20%, and the only exception is the 33-46 ($2p3p\ ^1D_2-2p3d\ ^1F_3$) transition in K XIV, for which the length form is higher by a factor of two. For transitions with f -values ≥ 0.01 , the two forms agree within a factor of two for all transitions in all ions. In fact, for a majority of weak transitions the two forms agree to better than 40%. This is highly satisfactory.

The measurements of A -values, in the form of lifetimes, can provide a good check on the theoretical results, and hence can help to improve the accuracy. However, to the best of our knowledge there are no experimental values available in the literature for the ions considered here. Some experiments have reported the lifetimes for the $2s^22p^2\ ^1S_0$, 1D_2 and $2s2p^3\ ^5S_2$ levels in other C-like ions, (see, for example, Trabert 2002 and references therein). We hope experiments in the future will be performed for other C-like ions also, which will help us in improving upon the accuracy of the calculated atomic data.

4. Conclusions

In this paper we have reported values of oscillator strengths and radiative rates for transitions among the $(1s^2)\ 2s^22p^2$, $2s2p^3$, $2p^4$, $2s^22p3s$, $2s^22p3p$ and $2s^22p3d$ configurations of C-like K XIV, Sc XVI, Ti XVII, V XVIII, Cr XIX and Mn XX. Relativistic effects as well as elaborate CI have been included in the calculations. The results have been compared with the earlier available values obtained by Fawcett (1987) from the HFR code of Cowan (1981).

The energy levels agree to better than 3% with the experimental compilations, but the levels ordering are slightly different in a few instances. Furthermore, experimental energies for all the levels are not available, and the deficiency is greater for the higher levels, in particular. This may result in an incorrect order of some of the levels, leaving scope for future amendments.

The oscillator strengths for transitions among the $[1s^2]\ 2s^22p^2$, $2s^3$ and $2p^4$ configurations have been calculated by many workers, and have been compared and discussed in

detail in the literature. However, similar calculations including the levels of the $2s^22p3\ell$ configurations are rather limited, and radiative rates are available for a few transitions only. Therefore, the present calculations have reported values of oscillator strengths and radiative rates for *all* allowed transitions among 46 levels of the above six configurations, as well as improving the accuracy of the earlier work. The differences with the earlier calculations are generally within 30%, and the accuracy of our present calculations may not be better than 20%, especially for those transitions whose f -values are large (≥ 0.1). For weaker transitions having smaller f -values, the corresponding accuracy estimate may be much lower.

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References

- Aggarwal, K. M. 1998, ApJS, 118, 589
- Aggarwal, K. M., Hibbert, A., & Keenan, F. P. 1997a, ApJS, 108, 393
- Aggarwal, K. M., Hibbert, A., Keenan, F. P., & Norrington, P. H. 1997b, ApJS, 108, 575
- Aggarwal, K. M., Keenan, F. P., & Msezane, A. Z. 2001, ApJS, 136, 763
- Cowan, R. D. 1981, The Theory of Atomic Structure and Spectra (Berkeley: Univ. of California Press)
- Dyall, K. G., Grant, I. P., Johnson, C. T., Parpia, F. A., & Plummer, E. P. 1989, Comput. Phys. Commun., 55, 425
- Fawcett, B. C. 1987, At. Data Nucl. Data Tables, 37, 367
- Hibbert, A. 1975, Comput. Phys. Commun., 9, 141
- Kelly, R. L. 1987, J. Phys. Chem. Ref. Data Suppl., 16, 1
- Trabert, E. 2002, Phys. Scr., T100, 88
- Zhang, H. L., & Sampson, D. H. 1996, At. Data Nucl. Data Tables, 63, 275
- Zhang, H. L., & Sampson, D. H. 1997, At. Data Nucl. Data Tables, 65, 183