

Oscillator strengths for sextet transitions in Cr II

Oscillator strengths for transitions among low-lying sextet terms of singly ionized Chromium have been calculated using two different methods: the Multi-configuration Optimized Potential Model (MCOPM) and an R-matrix model based on target MCOPM wave functions. Estimates of numerical cancellation effects in the MCOPM calculation as well as direct comparison of the sets of independently calculated results, indicate an accuracy of 10% or better in the oscillator strengths reported. Exceptions, where relativistic effects not included in this work may be important, are noted. Comparison with available observations is given.

The transition or iron series elements are important in both terrestrial and astrophysical plasmas. However, even a nonrelativistic treatment of these elements is likely to encounter computational difficulties resulting in part from the occurrence of near degeneracies among terms of the same L and S coming from different configurations. A feature of the Cr II sextet system is that the low-lying terms are relatively widely spaced so we do not generally encounter such problems. Consequently, despite the substantial storage and speed demands caused by the importance of correlation effects, rather reliable calculations on present computers can be performed.

The Cr II sextet transitions considered in the present work are the following: $3d^4 4s - 3d^4 4p$, $3d^4 4d - 3d^4 4p$, $3d^4 5s - 3d^4 4p$, plus the one from the $3d^4 4p$ $^6P^o$ to the $3d^5$ 6S ground state. There are - to our knowledge - no other reliable calculations for the sextets, and there are few experimental data as well.

We have performed the calculations in two completely independent ways and present the results of both. A brief description of the two methods is given in the next paragraphs. Following that, we present comparison and discussion of the different sets of results.

The MCOPM approach proceeds basically in two stages (Aashamar *et al.*, 1981). In the first, with only a moderate set of configurations, we perform a variational calculation in which a weighted energy average over selected spectroscopic terms is minimized with

respect to variations in the potentials in which the orbitals are calculated. This gives a set of "best potentials" to be used in the second stage to calculate orbitals for a CI calculation involving an enlarged set of 41 configurations. This set includes configurations of the form $3d^5$, $3d^4 nl$, $3d^3 nln'$ ($l, l' \leq 4$).

In applications of the R-matrix method to bound state problems (Seaton, 1985, Berrington *et al.*, 1988) low-lying states of the atom or ion considered are treated as bound states in the collision of an electron with the corresponding ionized system. Wave functions for the Cr II states are thus taken to be properly symmetry-projected close coupling expansions over terms built from bound states of the N-1 electron core coupled to different "free channel" states of an electron bound to said core. Since the "free channel" functions are orthogonal to the orbitals used to construct the core, a sum over "bound channel" N electron functions is added for completeness. The expansion coefficients of the latter and the "free channel" wave functions are fully optimized for each state, being determined by the coupled integro-differential equations arising from the energy variational principle. Results are presented for two different sets of orbitals for the target ion core. The first set is a subset of the orbitals obtained in the MCOPM calculation for Cr II. The other set was obtained in a 6-configuration MCOPM calculation on Cr III using 50% weight on the ground state and 50% equally distributed on the 18 excited states. These sets are similar except for the 3d and 4d orbitals which are more compact in the Cr II optimization for reasons involving their dual spectroscopic/correlation roles. In the present R-matrix calculation we include free channels with s, p, and d waves associated with $3d^4$, $3d^3 4s$, 4p, 4d, and 5s target states, as well as bound channels needed for completeness.

Table 1 gives the three sets of oscillator strengths obtained for the transitions of present interest. They have been corrected for wavelengths differing from observation, the corrections being less than 10% in all cases. The three sets, being obtained using different combinations of methods and potentials, are seen to be very consistent, and the gf_i - gf_v differences are generally reasonable. The gf_i values are the more reliable. Estimates of cancellation effects in the MCOPM calculation suggest errors in the gf_v values of roughly twice the errors in the gf_i values from this source alone. The quite different MCOPM and R-matrix calculations give gf_i values with a spread of less than 10% except for the single transition involving the ground state.

There are few experimental results available, and we report these too in Table 1, as listed by Sugar and Corliss (1985) from the work of Musielok and Wujec (1979). The three values quoted have likely uncertainties of 50%, and do not serve to distinguish among the present calculations with a view to preferred method.

The $4p$ $^6D^o$, $4d$ 6D , and $4d$ 6F terms lie very close

in energy to certain other terms of different L and S. Admixtures of these through relativistic effects may alter corresponding oscillator strengths significantly. We have not attempted to estimate this mixing in the present work.

Table 1. Oscillator strengths for sextet transitions in Cr II in MCOPM and R-matrix calculations. (See text for descriptions.) Observed oscillator strengths are obtained from the observations of Musielok and Wujec (1979) assuming L-S coupling.

Transition (gf_{obs})	MCOPM		R-matrix			
	gf_i	gf_v	Cr II		Cr III	
	gf_i	gf_v	gf_i	gf_v	gf_i	gf_v
4d ${}^6G-4p$ ${}^6F^\circ$	31.9	28.2	33.4	-	33.0	31.1
4d ${}^6F-4p$ ${}^6F^\circ$	7.52	7.51	8.21	6.53	8.01	-
4d ${}^6F-4p$ ${}^6D^\circ$	16.4	14.9	17.1	15.1	16.7	15.5
4s ${}^6D-4p$ ${}^6F^\circ$ (10.4)	13.2	9.94	14.5	-	14.6	12.4
5s ${}^6D-4p$ ${}^6F^\circ$	6.76	6.05	6.64	6.03	6.33	6.24
4d ${}^6D-4p$ ${}^6F^\circ$	1.11	1.21	1.00	0.97	1.01	-
4s ${}^6D-4p$ ${}^6D^\circ$ (4.8-5.5)	9.04	8.58	10.0	8.04	9.89	7.47
5s ${}^6D-4p$ ${}^6D^\circ$	4.60	4.30	4.58	-	4.33	4.26
4d ${}^6D-4p$ ${}^6D^\circ$	10.5	10.3	11.2	9.08	10.9	9.28
4s ${}^6D-4p$ ${}^6P^\circ$ (6.4)	6.00	6.35	6.61	4.84	6.62	4.55
5s ${}^6D-4p$ ${}^6P^\circ$	3.26	3.23	3.21	-	3.07	3.00
4d ${}^6D-4p$ ${}^6P^\circ$	5.42	5.20	5.77	5.17	5.63	5.26
4d ${}^6P-4p$ ${}^6D^\circ$	2.83	2.94	2.81	2.44	2.76	2.50
4d ${}^6P-4p$ ${}^6P^\circ$	8.18	8.15	8.50	7.53	8.50	7.71
3d ⁵ ${}^6S-4p$ ${}^6P^\circ$	1.84	1.38	1.98	1.84	2.24	1.35
4d ${}^6S-4p$ ${}^6P^\circ$	2.65	2.51	2.79	2.22	2.64	-

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