method of resonance distortion and its relation to other approximate methods of solving collision problems. First of all, the method of resonance distortion is restricted to problems involving near-resonance, since the limiting case of exact resonance is taken as the zeroth-order approximation. This method is most suitable for cases where the coupling between the initial and final states is strong. We can illustrate the nature of this method through a partial-wave analysis. The partial cross sections corresponding to large $l$ for the strong coupling case reduce to the Born partial cross sections, because partial waves of large $l$ are classically equivalent to distant impacts and at large distances, $U_{00}$, $U_{nn}$, and $U_{0n}$ are sufficiently small so that the Born approximation is applicable. At lower $l$ the "effective" coupling becomes so large that the use of the Born approximation and the method of distorted waves, which are valid for weak coupling, is not always justifiable. It is in this region of $l$ (called "low-$l$ region") that the method of resonance distortion is useful. For collision-induced transitions with a long-range inter-action potential, where the contribution from the partial cross sections in the "low-$l$ region" constitutes a substantial part of the total cross section (e.g., Table IV), we may expect the method of resonance distortion to yield more accurate results than the usual Born approximation.

For very weak coupling, the results of the method of resonance distortion approach those of the method of distorted waves. This can be seen from Eqs. (108) and (109). When $U_{0n}$ becomes very small, $F_0^{(0)}$ in Eq. (109) is nearly equal to the zeroth-order solution in the method of distorted waves, which is defined by

$$(\nabla^2 + k_0^2 - U_{00})(F_0^{(0)})_{DW} = 0.$$

The difference in $F_n$ as calculated by these two zeroth-order functions should be small compared to $F_n$ itself.

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# Analytical Self-Consistent Field Functions for Cr+, Cr and Its Excited States*

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Self-consistent field calculations by the expansion method were carried out for Cr+, Cr and some of its excited states. The results represent closely the absolute Hartree-Fock solutions. The wave functions were calculated with the requirement to satisfy exactly the cusp condition so that they can be considered to be particularly accurate in the immediate vicinity of the nucleus. The differences in calculated energy levels are compared with experiment.

## INTRODUCTION

THE self-consistent field (SCF) expansion method of Roothaan[1-3] was applied on a number of cases.[4-9] In this paper the application is carried out for Cr+, Cr and some of its excited states. Vector coupling coefficients $J_{\lambda\mu\nu}$ and $K_{\lambda\mu\nu}$ were taken from the tables calculated recently.[10]

The computation was done on an IBM 7090 computer with a modification of the previously established program.[8]

## RESULTS AND DISCUSSION

The notation and the units used are the usual ones and are identical with those employed in a recent work.[7]

Some of the important results are presented in

[1] C. C. J. Roothaan, Rev. Mod. Phys. **23**, 69 (1951).
[2] C. C. J. Roothaan, Rev. Mod. Phys. **32**, 179 (1960).
[3] C. C. J. Roothaan and P. S. Bagus, in *Methods in Computational Physics*, edited by B. Alder *et al.* (Pergamon Press, Inc., New York, 1963), Vol. 2.
[4] C. C. J. Roothaan, L. M. Sachs, and A. W. Weiss, Rev. Mod. Phys. **32**, 186 (1960).
[5] E. Clementi, C. C. J. Roothaan, and M. Yoshimine, Phys. Rev. **127**, 1618 (1962).
[6] C. C. J. Roothaan and P. S. Kelley, Phys. Rev. **131**, 1177 (1963).
[7] M. Synek, Phys. Rev. **131**, 1572 (1963); this article, with numerical tabulations and graphs of some wave functions included, is also printed in the Technical Report, Laboratory of Molecular Structure and Spectra, Dept. of Physics, University of Chicago, 1962-3, Pt. 1, p. 229.
[8] H. D. Cohen, Technical Report, Laboratory of Molecular Structure and Spectra, Dept. of Physics, University of Chicago, 1962-3, Pt. 1, p. 251.
[9] C. C. J. Roothaan and M. Synek (to be published).
[10] G. L. Malli and C. C. J. Roothaan (to be published).

Tables I–VI.[11] The values of cusps are not presented since the cusp conditions are exactly satisfied.

The results computed represent the Hartree-Fock values to about six significant figures for total energies, and to about three decimal places for the radial functions $P_{i\lambda}(r)$. The condition for the required number of nodes of $P_{i\lambda}(r)$ is usually satisfied to four decimal places; as a rule,[12] the occasional deviation did not exceed nine units at the fifth decimal place (in the original computer tabulation). While keeping the same numbers of basis functions, the values of total energies

TABLE I. Comparison with other calculations for total energy $E$(au).

| State \ Source | Other calculations | This work |
|---|---|---|
| $Cr^+$, $3d^5$, $^6S$ | $-1043.1346$[a] | $-1043.1379$ |
| $Cr$, $3d^44s^2$, $^5D$ | $-1043.3036$[b] | $-1043.3084$ |
| $Cr$, $3d^6$, $^5D$ | $-1043.0909$[a] | $-1043.0957$ |

[a] See Ref. 14.
[b] See Ref. 15.

TABLE II. Optimized exponents[a] $\zeta$ of the basis functions for $Cr^+$, $Cr$ and its excited states.

| Basis function \ Atom and state | $Cr^+$ $3d^5$ $^6S$ | $Cr$ $3d^44s4p$ $^7F$ | $Cr$ $3d^44s^2$ $^5D$ | $Cr$ $3d^54s$ $^5S$ | $Cr$ $3d^54s$ $^5P$ | $Cr$ $3d^54s$ $^5G$ | $Cr$ $3d^54s$ $^7S$ | $Cr$ $3d^54p$ $^7P$ | $Cr$ $3d^6$ $^5D$ |
|---|---|---|---|---|---|---|---|---|---|
| $1s$ | 24.000 | 24.000 | 24.000 | 24.000 | 24.000 | 24.000 | 24.000 | 24.000 | 24.000 |
| $3s$ | 25.696 | 25.763 | 25.671 | 25.763 | 25.763 | 25.763 | 25.763 | 25.782 | 25.518 |
| $3s$ | 19.410 | 21.115 | 21.668 | 21.115 | 21.115 | 21.115 | 21.115 | 20.785 | 21.037 |
| $3s$ | 13.643 | 13.769 | 13.874 | 13.769 | 13.769 | 13.769 | 13.769 | 13.760 | 13.859 |
| $3s$ | 9.696 | 9.822 | 9.726 | 9.756 | 9.756 | 9.756 | 9.756 | 9.744 | 9.860 |
| $3s$ | 5.233 | 4.891 | 5.082 | 5.104 | 4.799 | 4.865 | 5.129 | 5.044 | 4.958 |
| $3s$ | 3.375 | 3.335 | 3.442 | 3.372 | 3.187 | 3.237 | 3.360 | 3.357 | 3.239 |
| $4s$ | | 1.646 | 1.745 | 1.592 | 1.613 | 1.601 | 1.602 | | |
| $4s$ | | 0.936 | 1.014 | 0.881 | 0.911 | 0.912 | 0.880 | | |
| $2p$ | 12.000 | 12.000 | 12.000 | 12.000 | 12.000 | 12.000 | 12.000 | 12.000 | 12.000 |
| $4p$ | 27.700 | 27.178 | 27.178 | 27.178 | 27.178 | 27.178 | 27.178 | 27.178 | 27.454 |
| $4p$ | 12.950 | 13.033 | 12.967 | 12.909 | 12.909 | 12.909 | 12.909 | 12.909 | 12.963 |
| $4p$ | 8.885 | 9.073 | 9.006 | 8.958 | 8.958 | 8.958 | 8.958 | 8.977 | 9.133 |
| $4p$ | 5.602 | 5.830 | 5.506 | 5.572 | 5.571 | 5.588 | 5.606 | 5.606 | 5.694 |
| $4p$ | 3.344 | 3.582 | 3.318 | 3.310 | 3.314 | 3.317 | 3.336 | 3.286 | 3.314 |
| $4p$ | | 1.688 | | | | | | 1.279 | |
| $4p$ | | 0.954 | | | | | | 0.684 | |
| $3d$ | 8.000 | 8.000 | 8.000 | 8.000 | 8.000 | 8.000 | 8.000 | 8.000 | 8.000 |
| $5d$ | 10.829 | 10.243 | 10.243 | 10.547 | 10.547 | 10.547 | 10.547 | 10.322 | 7.893 |
| $5d$ | 7.038 | 6.393 | 6.393 | 6.393 | 6.393 | 6.393 | 6.393 | 6.393 | 6.950 |
| $5d$ | 4.433 | 3.771 | 3.653 | 3.662 | 3.783 | 3.715 | 3.653 | 3.603 | 4.505 |
| $5d$ | 2.944 | 3.059 | 3.021 | 3.025 | 2.972 | 3.004 | 3.021 | 2.971 | 2.446 |
| $5d$ | 1.924 | 2.008 | 1.950 | 1.843 | 1.749 | 1.759 | 1.800 | 1.875 | 1.255 |

[a] Calculated to five decimal places. Values in the table are to be followed by two zeros beyond the third decimal place.

TABLE III. Eigenvectors of coefficients $C_{i\lambda p}$ for $Cr^+$, $Cr$ and its excited states.

| Basis function \ Atom and state | $Cr^+$ $3d^5$, $^6S$ | $Cr$ $3d^44s4p$, $^7F$ | $Cr$ $3d^44s^2$, $^5D$ | $Cr$ $3d^54s$, $^5S$ | $Cr$ $3d^54s$, $^5P$ | $Cr$ $3d^54s$, $^5G$ | $Cr$ $3d^54s$, $^7S$ | $Cr$ $3d^54p$, $^7P$ | $Cr$ $3d^6$, $^5D$ |
|---|---|---|---|---|---|---|---|---|---|
| | $1s$ | $1s$ | $1s$ | $1s$ | $1s$ | $1s$ | $1s$ | $1s$ | $1s$ |
| $1s$ | 0.97998 | 0.97996 | 0.97996 | 0.97997 | 0.97997 | 0.97997 | 0.97997 | 0.97997 | 0.97999 |
| $3s$ | 0.02557 | 0.02470 | 0.02523 | 0.02473 | 0.02466 | 0.02468 | 0.02473 | 0.02467 | 0.02648 |
| $3s$ | 0.00332 | 0.00364 | 0.00273 | 0.00356 | 0.00369 | 0.00366 | 0.00356 | 0.00382 | 0.00141 |
| $3s$ | 0.00355 | 0.00441 | 0.00490 | 0.00444 | 0.00428 | 0.00431 | 0.00444 | 0.00406 | 0.00491 |
| $3s$ | $-0.00150$ | $-0.00179$ | $-0.00200$ | $-0.00183$ | $-0.00167$ | $-0.00171$ | $-0.00183$ | $-0.00160$ | $-0.00189$ |
| $3s$ | 0.00036 | 0.00049 | 0.00063 | 0.00051 | 0.00043 | 0.00045 | 0.00050 | 0.00038 | 0.00041 |
| $3s$ | $-0.00016$ | $-0.00028$ | $-0.00034$ | $-0.00026$ | $-0.00025$ | $-0.00025$ | $-0.00026$ | $-0.00018$ | $-0.00019$ |
| $4s$ | | 0.00005 | 0.00007 | 0.00005 | 0.00005 | 0.00005 | 0.00005 | | |
| $4s$ | | 0.00002 | $-0.00003$ | $-0.00002$ | $-0.00002$ | $-0.00002$ | $-0.00002$ | | |

[11] The numerical tabulations are presented in Tables VII–XV. As a rule (see Ref. 12) the tabulated values are rounded to four decimal places. The tables are deposited as Document number 7766 with the ADI Auxiliary Publications Project, Photoduplication Service, Library of Congress, Washington, D. C. A copy may be secured by citing the Document number and by remitting $1.25 for photoprints, or $1.25 for 35-mm microfilm. Advance payment is required. Make checks or money orders payable to: Chief, Photoduplication Service, Library of Congress.

[12] The only exception occurs for the state $3d^44s4p$, $^7F$.

TABLE III (continued).

| Basis function | Cr+ $3d^5$, $^6S$ | Cr $3d^44s4p$, $^7F$ | Cr $3d^44s^2$, $^5D$ | Cr $3d^54s$, $^5S$ | Cr $3d^54s$, $^5P$ | Cr $3d^54s$, $^5G$ | Cr $3d^54s$, $^7S$ | Cr $3d^54p$, $^7P$ | Cr $3d^6$, $^5D$ |
|---|---|---|---|---|---|---|---|---|---|
| | $2s$ | $2s$ | $2s$ | $2s$ | $2s$ | $2s$ | $2s$ | $2s$ | $2s$ |
| $1s$ | −0.29373 | −0.29358 | −0.29364 | −0.29362 | −0.29363 | −0.29363 | −0.29364 | −0.29364 | −0.29364 |
| $3s$ | −0.00091 | −0.01743 | −0.01942 | −0.01565 | −0.01588 | −0.01582 | −0.01560 | −0.01177 | −0.01639 |
| $3s$ | 0.10826 | 0.10399 | 0.09324 | 0.09967 | 0.10019 | 0.10005 | 0.09957 | 0.09869 | 0.10115 |
| $3s$ | 0.52078 | 0.52396 | 0.54316 | 0.53563 | 0.53470 | 0.53494 | 0.53580 | 0.53325 | 0.51317 |
| $3s$ | 0.44741 | 0.46139 | 0.45820 | 0.45364 | 0.45500 | 0.45469 | 0.45354 | 0.45391 | 0.47416 |
| $3s$ | 0.00625 | 0.01308 | 0.00694 | 0.00983 | 0.00989 | 0.00986 | 0.00969 | 0.00882 | 0.01185 |
| $3s$ | 0.00132 | −0.00252 | 0.00078 | −0.00026 | −0.00121 | −0.00101 | −0.00021 | 0.00002 | −0.00115 |
| $4s$ | | 0.00060 | −0.00013 | 0.00003 | 0.00031 | 0.00027 | 0.00021 | | |
| $4s$ | | 0.00011 | 0.00006 | −0.00019 | −0.00004 | −0.00003 | 0.00006 | | |
| | $3s$ | $3s$ | $3s$ | $3s$ | $3s$ | $3s$ | $3s$ | $3s$ | $3s$ |
| $1s$ | 0.10596 | 0.10713 | 0.10714 | 0.10604 | 0.10646 | 0.10642 | 0.10622 | 0.10610 | 0.10596 |
| $3s$ | 0.00448 | 0.00626 | 0.01008 | 0.00874 | 0.00430 | 0.00548 | 0.01039 | 0.00501 | 0.00866 |
| $3s$ | −0.05851 | −0.04054 | −0.04250 | −0.04600 | −0.03559 | −0.03833 | −0.04986 | −0.04069 | −0.04572 |
| $3s$ | −0.16396 | −0.20250 | −0.20042 | −0.19068 | −0.21303 | −0.20749 | −0.18393 | −0.19912 | −0.18312 |
| $3s$ | −0.35633 | −0.31096 | −0.32959 | −0.32993 | −0.29655 | −0.30482 | −0.34067 | −0.31717 | −0.32907 |
| $3s$ | 0.61141 | 0.69610 | 0.62296 | 0.62120 | 0.75169 | 0.72111 | 0.63050 | 0.63162 | 0.69135 |
| $3s$ | 0.59404 | 0.47469 | 0.56120 | 0.56523 | 0.41863 | 0.45307 | 0.56279 | 0.54992 | 0.49067 |
| $4s$ | | 0.00142 | 0.00274 | 0.00405 | −0.00029 | 0.00059 | 0.00124 | | |
| $4s$ | | 0.00036 | −0.00045 | −0.00024 | 0.00030 | 0.00009 | 0.00004 | | |
| | | $4s$ | $4s$ | $4s$ | $4s$ | $4s$ | $4s$ | | |
| $1s$ | | −0.02630 | −0.02372 | −0.01648 | −0.02179 | −0.02169 | −0.02220 | | |
| $3s$ | | −0.00538 | −0.00519 | −0.00284 | −0.00372 | −0.00458 | −0.00592 | | |
| $3s$ | | 0.01895 | 0.01548 | 0.01063 | 0.01387 | 0.01583 | 0.01919 | | |
| $3s$ | | 0.03314 | 0.03437 | 0.02322 | 0.03188 | 0.02801 | 0.02217 | | |
| $3s$ | | 0.10485 | 0.09337 | 0.06389 | 0.08126 | 0.08607 | 0.09916 | | |
| $3s$ | | −0.25596 | −0.19616 | −0.13275 | −0.22081 | −0.21732 | −0.19912 | | |
| $3s$ | | −0.05693 | −0.09634 | −0.06549 | −0.03300 | −0.03684 | −0.07238 | | |
| $4s$ | | 0.74737 | 0.53841 | 0.38375 | 0.56579 | 0.56795 | 0.61536 | | |
| $4s$ | | 0.34613 | 0.56328 | 0.70890 | 0.53342 | 0.52825 | 0.49368 | | |
| | $2p$ | $2p$ | $2p$ | $2p$ | $2p$ | $2p$ | $2p$ | $2p$ | $2p$ |
| $2p$ | 0.72387 | 0.72388 | 0.72377 | 0.72384 | 0.72383 | 0.72383 | 0.72383 | 0.72386 | 0.72396 |
| $4p$ | 0.00434 | 0.00432 | 0.00452 | 0.00480 | 0.00479 | 0.00480 | 0.00480 | 0.00484 | 0.00470 |
| $4p$ | 0.22953 | 0.21977 | 0.22570 | 0.22971 | 0.22980 | 0.22978 | 0.22972 | 0.22918 | 0.22288 |
| $4p$ | 0.12813 | 0.13712 | 0.12980 | 0.12525 | 0.12520 | 0.12525 | 0.12534 | 0.12552 | 0.12979 |
| $4p$ | −0.00728 | −0.00702 | −0.00478 | −0.00435 | −0.00444 | −0.00446 | −0.00448 | −0.00416 | −0.00161 |
| $4p$ | 0.00273 | 0.00336 | 0.00210 | 0.00200 | 0.00200 | 0.00200 | 0.00199 | 0.00211 | 0.00144 |
| $4p$ | | −0.00078 | | | | | | −0.00033 | |
| $4p$ | | 0.00037 | | | | | | 0.00018 | |
| | $3p$ | $3p$ | $3p$ | $3p$ | $3p$ | $3p$ | $3p$ | $3p$ | $3p$ |
| $2p$ | −0.25297 | −0.25653 | −0.25633 | −0.25302 | −0.25400 | −0.25389 | −0.25343 | −0.25313 | −0.25254 |
| $4p$ | −0.00077 | −0.00000 | −0.00051 | −0.00078 | −0.00079 | −0.00087 | −0.00083 | −0.00114 | −0.00109 |
| $4p$ | −0.07296 | −0.06931 | −0.07651 | −0.07445 | −0.07460 | −0.07377 | −0.07394 | −0.07061 | −0.06911 |
| $4p$ | 0.07096 | 0.04597 | 0.07977 | 0.07309 | 0.07301 | 0.06994 | 0.06983 | 0.06023 | 0.04923 |
| $4p$ | 0.60242 | 0.56620 | 0.63795 | 0.61394 | 0.61913 | 0.61800 | 0.60855 | 0.62698 | 0.61382 |
| $4p$ | 0.44463 | 0.48389 | 0.40061 | 0.43358 | 0.42785 | 0.43145 | 0.44089 | 0.43017 | 0.45461 |
| $4p$ | | 0.01969 | | | | | | 0.00315 | |
| $4p$ | | −0.00309 | | | | | | 0.00034 | |
| | | $4p$ | | | | | | $4p$ | |
| $2p$ | | 0.05196 | | | | | | 0.03446 | |
| $4p$ | | 0.00013 | | | | | | 0.00032 | |
| $4p$ | | 0.01427 | | | | | | 0.00770 | |
| $4p$ | | −0.01201 | | | | | | −0.00425 | |
| $4p$ | | −0.12820 | | | | | | −0.10582 | |
| $4p$ | | −0.09909 | | | | | | −0.02989 | |
| $4p$ | | 0.34420 | | | | | | 0.41273 | |
| $4p$ | | 0.74890 | | | | | | 0.68564 | |
| | $3d$ | $3d$ | $3d$ | $3d$ | $3d$ | $3d$ | $3d$ | $3d$ | $3d$ |
| $3d$ | 0.15360 | 0.16224 | 0.16364 | 0.15064 | 0.14777 | 0.14821 | 0.14912 | 0.15174 | 0.14436 |
| $5d$ | 0.03178 | 0.06190 | 0.05956 | 0.05238 | 0.05278 | 0.05192 | 0.05167 | 0.05397 | 0.16649 |
| $5d$ | 0.28184 | 0.38530 | 0.39558 | 0.37786 | 0.36559 | 0.36973 | 0.37485 | 0.37286 | 0.06577 |
| $5d$ | 0.36364 | 0.39340 | 0.43949 | 0.37656 | 0.31463 | 0.33393 | 0.37440 | 0.44134 | 0.41303 |
| $5d$ | 0.26447 | 0.08687 | 0.04863 | 0.12272 | 0.19863 | 0.17093 | 0.12070 | 0.04231 | 0.38617 |
| $5d$ | 0.20465 | 0.19501 | 0.17622 | 0.22957 | 0.24785 | 0.25151 | 0.24914 | 0.24809 | 0.20894 |

could be made more accurate, mainly, if the cusp condition were sacrificed.

The results are compared with other calculations wherever available.

A numerical SCF calculation for the state $3d^6$, $^5D$ of Cr was published by Porter.[13] However, his calculation was done without exchange and, furthermore, it was done only for the purpose of an approximate orientation. Hence, his numerical wave functions (after normalization) cannot be compared with ours.

Analytical (i.e., expansion method) SCF calculations on the ground state of Cr+, $3d^5$, $^6S$, and on the two states of Cr, $3d^6$, $^5D$ and $3d^44s^2$, $^5D$, were carried out by Watson.[14,15] The comparison of the results for the total energies is given in Table I.

TABLE IV. Calculated energies and experimental energies.[a]

| Atom or ion | State | Calculated total energy | Energies relative to ground state | | Estimate of correlation energy difference |
|---|---|---|---|---|---|
| | | | Calculated | Experimental | |
| Cr+ | $3d^5$, $^6S$ | −1043.1379 | 0.2160 | 0.2486 | −0.0326 |
| Cr | $3d^44s4p$, $^7F$ | −1043.2744 | 0.0795 | 0.1152 | −0.0357 |
| | $3d^44s^2$, $^5D$ | −1043.3084 | 0.0455 | 0.0364 | 0.0091 |
| | $3d^54s$, $^5S$ | −1043.3154 | 0.0385 | 0.0346 | 0.0039 |
| | $3d^54s$, $^5P$ | −1043.2132 | 0.1407 | 0.0996 | 0.0411 |
| | $3d^54s$, $^5G$ | −1043.2305 | 0.1234 | 0.0935 | 0.0299 |
| | $3d^54s$, $^7S$ | −1043.3539 | 0 | 0 | 0 |
| | $3d^54p$, $^7P$ | −1043.2583 | 0.0956 | 0.1066 | −0.0110 |
| | $3d^6$, $^5D$ | −1043.0957 | 0.2582 | 0.1620 | 0.0962 |

[a] See Ref. 16.

TABLE V. Orbital energies $\epsilon$.

| Atom and state / Orbital | Cr+ $3d^5$ $^6S$ | Cr $3d^44s4p$ $^7F$ | Cr $3d^44s^2$ $^5D$ | Cr $3d^54s$ $^5S$ | Cr $3d^54s$ $^5P$ | Cr $3d^54s$ $^5G$ | Cr $3d^54s$ $^7S$ | Cr $3d^54p$ $^7P$ | Cr $3d^6$ $^5D$ |
|---|---|---|---|---|---|---|---|---|---|
| 1s | −220.65076 | −220.62782 | −220.59149 | −220.39096 | −220.42135 | −220.41613 | −220.38375 | −220.44881 | −220.30459 |
| 2s | −26.46663 | −26.47595 | −26.43855 | −26.20988 | −26.24773 | −26.24204 | −26.20758 | −26.26771 | −26.11747 |
| 3s | −3.54816 | −3.53224 | −3.49864 | −3.29183 | −3.31511 | −3.31077 | −3.28394 | −3.34649 | −3.18330 |
| 4s | | −0.33145 | −0.23933 | −0.17818 | −0.21751 | −0.21679 | −0.22079 | | |
| 2p | −22.39883 | −22.40307 | −22.36467 | −22.14117 | −22.17770 | −22.17209 | −22.13781 | −22.19968 | −22.05020 |
| 3p | −2.31925 | −2.28422 | −2.24831 | −2.06079 | −2.07916 | −2.07514 | −2.04994 | −2.11635 | −1.95714 |
| 4p | | −0.18370 | | | | | | −0.12148 | |
| 3d | −0.64713 | −0.60656 | −0.56849 | −0.38500 | −0.33606 | −0.34070 | −0.37265 | −0.44176 | −0.20060 |

TABLE VI. Virial theorem. (Values of $E_p/E_k$.)

| Atom or ion | State | $E_p/E_k$ |
|---|---|---|
| Cr+ | $3d^5$, $^6S$ | −1.9999691 |
| Cr | $3d^44s4p$, $^7F$ | −2.0000015 |
| | $3d^44s^2$, $^5D$ | −2.0000009 |
| | $3d^54s$, $^5S$ | −1.9999815 |
| | $3d^54s$, $^5P$ | −1.9999836 |
| | $3d^54s$, $^5G$ | −1.9999807 |
| | $3d^54s$, $^7S$ | −1.9999770 |
| | $3d^54p$, $^7P$ | −1.9999872 |
| | $3d^6$, $^5D$ | −1.9999509 |

Since total experimental energies are not available, the energy differences between the excited states and the ground states are used for the comparison with

experiment in Table IV. Since the spin-orbit interaction is neglected in the calculation, the experimental energies[16] are averaged over the multiplet components. An estimate of the correlation energy differences between the excited states and the ground state is given by the last column in Table IV. It shows that the correlation energy depends significantly on the state, not only on the configuration.

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