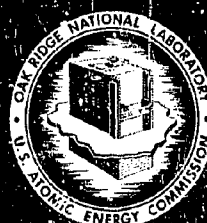


RELATIVISTIC HARTREE-FOCK-SLATER  
EIGENVALUES, RADIAL EXPECTATION VALUES,  
POTENTIALS AND ELECTRON DISTRIBUTION  
FUNCTIONS FOR ATOMS,  $56 \leq Z \leq 71$

C. W. Nestor

**MASTER**



**OAK RIDGE NATIONAL LABORATORY**

OPERATED BY UNION CARBIDE CORPORATION • FOR THE U.S. ATOMIC ENERGY COMMISSION

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COMPUTER SCIENCES DIVISION  
UNION CARBIDE CORPORATION, NUCLEAR DIVISION

RELATIVISTIC HARTREE-FOCK-SLATER EIGENVALUES,  
RADIAL EXPECTATION VALUES, POTENTIALS AND ELECTRON  
DISTRIBUTION FUNCTIONS FOR ATOMS,  $56 \leq Z \leq 71$

C. W. Nestor

SEPTEMBER 1973

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OAK RIDGE NATIONAL LABORATORY  
Oak Ridge, Tennessee 37830  
operated by  
UNION CARBIDE CORPORATION  
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U.S. ATOMIC ENERGY COMMISSION

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ACKNOWLEDGEMENT

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Physics Division

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RELATIVISTIC HARTREE-FOCK-SLATER EIGENVALUES,  
RADIAL EXPECTATION VALUES, POTENTIALS AND ELECTRON  
DISTRIBUTION FUNCTIONS FOR ATOMS,  $56 \leq Z \leq 71$

ABSTRACT

We have recalculated relativistic Hartree-Fock-Slater wavefunctions for the elements with  $Z=56$  to  $Z=71$ . From these wavefunctions we have obtained, and present in tables and graphs, the eigenvalues, the expectation values of  $r$ ,  $1/r$ ,  $1/r^2$ ,  $r^2$  and  $r^4$  and  $r_{\max}$ , the location of the principal maximum in the electron distribution function, for each orbital. We have also tabulated an equivalent point charge which would produce the computed total potential and estimates of the energies of the  $K\alpha_1$ ,  $K\alpha_2$ ,  $L\alpha_1$  and  $L\alpha_2$  X rays, and plotted a total electron distribution function for each atom.

---

INTRODUCTION

In a recent publication<sup>1</sup> Mann and Waber observed that the results for certain elements in our previous publication<sup>2</sup> were in error. On checking these results we found that the computations for some of the rare-earth elements were done using a multiplier for the exchange potential of 1.4, rather than 1.5 as required in the full Slater potential and which we used for all other atoms listed in reference 2. Since we have also made some minor changes in our computer programs we have repeated the calculations for the elements with  $Z=56$  to  $Z=71$ , using the configurations specified for the rare earths by Mann and Waber<sup>1</sup> and the full Slater exchange potential.

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## COMPUTATIONAL DETAILS

A complete discussion of the theoretical basis and numerical methods used in these calculations has appeared elsewhere.<sup>3</sup> Certain minor changes have been made in the computer programs to insure that the numerical solution of the radial differential equations and the numerical integrations used to calculate potentials are carried out with the same order of accuracy. We have also replaced the abrupt transition to the limiting value of the exchange potential in the original Latter prescription with a somewhat smoother transition.

The radial mesh for these calculations is logarithmic with a uniform step size of  $1/16$ . The mesh is adjusted so that 1 Bohr unit is a mesh point; the first mesh point is usually at about one-tenth the nuclear half-density radius, and the last mesh point is at a large enough distance to make the effects of further increase negligible.

In our programs we check the energy eigenvalues, the total potential, the exchange potential and the contribution of each orbital to the total potential for self-consistency. In this set of calculations we used self-consistency criteria of  $10^{-5}$  (relative error) for the potentials and  $5 \times 10^{-6}$  for the energy eigenvalues. We have made a few test calculations with these values replaced by  $10^{-8}$  and  $5 \times 10^{-9}$  and have found that the changes in eigenvalues and potentials are smaller than the original criteria.

## RESULTS

The energy eigenvalues, radial expectation values, total energies and equivalent point charge results are tabulated (Table 1) in the same format as in our previous paper.<sup>2</sup> We have also tabulated  $r_{\max}$ , the location of the principal maximum in the electron distribution function<sup>4</sup>

$$\varphi_i(r) = F_i^2(r) + G_i^2(r)$$

where  $F_i(r)$  and  $G_i(r)$  are  $r$  times the "small" and "large" components of the radial wavefunction for the  $i$ -th orbital.

We show in Fig. 1 a sample graph of the total electron distribution function

$$\Phi(r) = \sum_i q_i [F_i^2(r) + G_i^2(r)]$$

where  $q_i$  is the number of electrons in each orbital and the sum is taken over all occupied orbitals. Similar plots of the  $\varphi_i(r)$  for the 4f, 5d and 6s orbitals and of  $\Phi(r)$  are available on request.

We have plotted the eigenvalues for the 6s orbital as a function of  $Z$  in Fig. 2 together with the two sets of values reported by Mann and Waber<sup>1</sup> and experimental values<sup>5</sup> for the ionization potentials. It is interesting to note that the peak at gadolinium ( $Z=64$ ) is well followed by all three calculations, but that the computed values for cerium ( $Z=58$ ) all fall above the computed values for lanthanum, rather than below. We have used the nomenclature of Ref. 1 in labelling our graphs and tables.

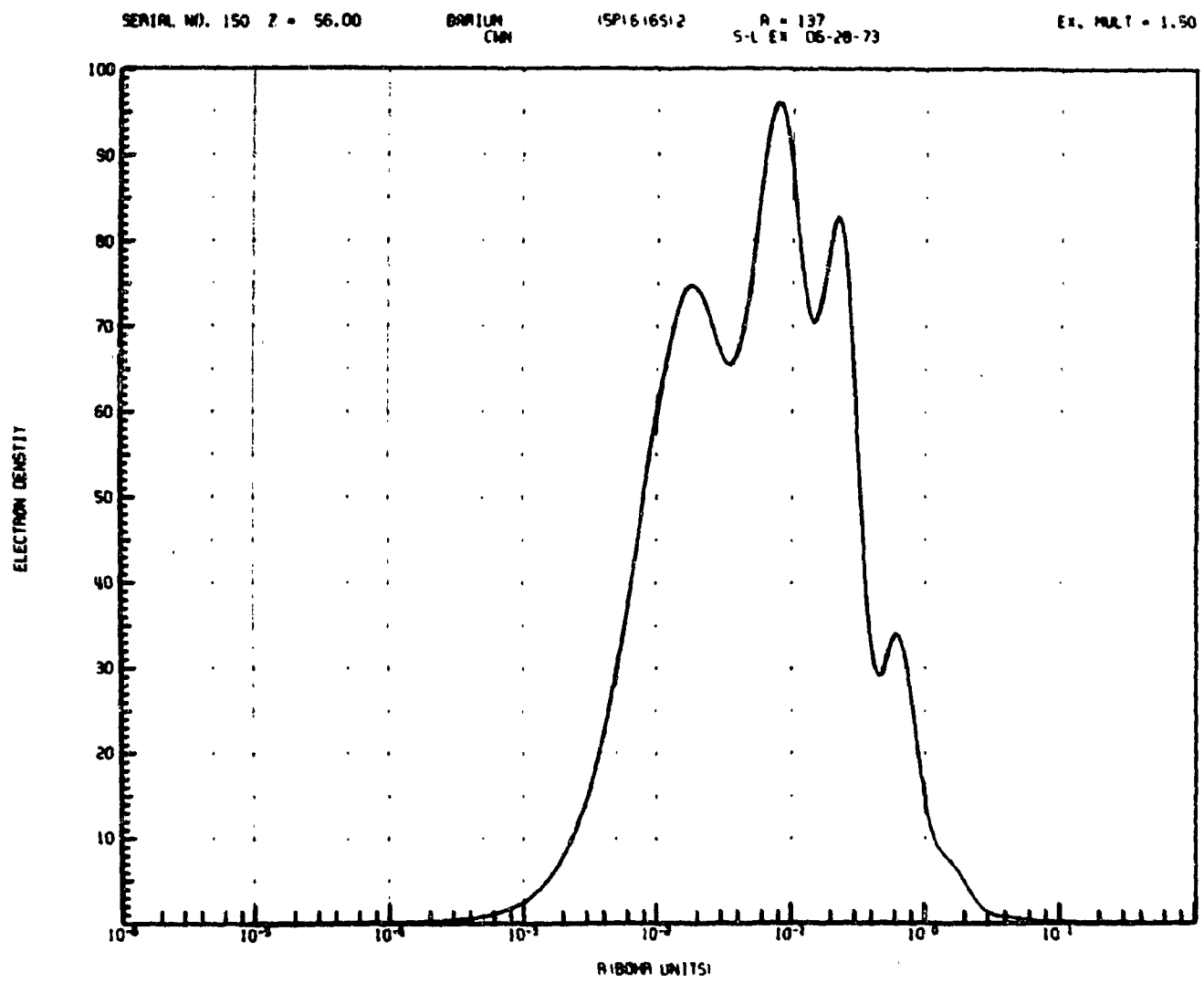


Fig. 1. Total Electron Distribution Function for Barium ( $Z=56$ ).

TABLE 1  
Energy Eigenvalues, Radial Expectation Values,  
Total Energies and Equivalent Point Charge

ORNL-DWG 73-8396

BAPTIUM (SP)6(S)2 A = 137 CWN S-L FX 07-24-73  
NUCLEAR CHARGE= 56.0 RADIUS= 5.6067 FERMI =.0001060 BOHR SURFACE THICKNESS=0.5666 FERMI =.000107 BOHR  
SLATER-LATTER EXCHANGE APPROXIMATION WITH MULTIPLIER 1.50

| SHELL   |    | ENERGY EIGENVALUES |                | RADIAL EXPECTATION VALUES (BOHR UNITS) |          | PMAK     |
|---------|----|--------------------|----------------|----------------------------------------|----------|----------|
|         |    | RYDBERGS           | ELECTRON VOLTS | 1/(R*R*R)                              | 1/R      |          |
| (1S1/2) | 2  | 2.752474490 03     | 3.744824110 04 | 0.0                                    | 60.77887 | 0.025539 |
| (2S1/2) | 2  | 4.381363170 02     | 5.960976040 03 | 0.0                                    | 14.30652 | 0.108905 |
| (2P1/2) | 2  | 4.138666770 02     | 5.630508200 03 | 0.0                                    | 14.30427 | 0.091474 |
| (2P3/2) | 4  | 3.853723000 02     | 5.243105760 03 | 6.373880 03                            | 13.04800 | 0.097463 |
| (3S1/2) | 2  | 9.361578380 01     | 1.273670820 03 | 0.0                                    | 5.15926  | 0.289711 |
| (3P1/2) | 2  | 8.323815570 01     | 1.132480080 03 | 0.0                                    | 5.07844  | 0.279143 |
| (3P3/2) | 4  | 7.768399990 01     | 1.056914120 03 | 1.274650 03                            | 4.76564  | 0.290563 |
| (3D3/2) | 4  | 5.928330760 01     | 8.065671850 02 | 2.085930 02                            | 4.63364  | 0.261384 |
| (3D5/2) | 6  | 5.806583910 01     | 7.902752670 02 | 1.908800 02                            | 4.55342  | 0.265106 |
| (4S1/2) | 2  | 1.885065140 01     | 2.564687670 02 | 0.0                                    | 2.12931  | 0.666414 |
| (4P1/2) | 2  | 1.501820580 01     | 2.043271950 02 | 0.0                                    | 2.02832  | 0.687021 |
| (4P3/2) | 4  | 1.384322100 01     | 1.883411740 02 | 2.704760 02                            | 1.92613  | 0.713736 |
| (4D3/2) | 4  | 7.508221300 00     | 1.021516030 02 | 3.633610 01                            | 1.70901  | 0.776215 |
| (4D5/2) | 6  | 7.303760890 00     | 9.936985800 01 | 3.295720 01                            | 1.68367  | 0.795814 |
| (5S1/2) | 2  | 2.823880240 00     | 3.841973790 01 | 0.0                                    | 0.83476  | 1.591436 |
| (5P1/2) | 2  | 1.787694250 00     | 2.432211650 01 | 0.0                                    | 0.73595  | 1.787851 |
| (5P3/2) | 4  | 1.616831810 00     | 2.199748190 01 | 3.902470 01                            | 0.69988  | 1.867169 |
| (6S1/2) | 2  | 3.411579670-01     | 4.641556490 00 | 0.0                                    | 0.26996  | 4.716357 |
| TOTAL   | 56 | 1.625369670 04     | 2.211364200 05 |                                        |          |          |

| R          | POT#R       | R          | POT#R       | R          | POT#R       | R          | POT#R       | R          | POT#R      |
|------------|-------------|------------|-------------|------------|-------------|------------|-------------|------------|------------|
| 0.00000894 | 6.63732685  | 0.00020347 | 55.94682911 | 0.00463092 | 54.70066815 | 0.10539922 | 35.96922150 | 2.39887529 | 2.20565579 |
| 0.00000952 | 7.06323223  | 0.00021659 | 55.94360265 | 0.00492559 | 54.61543798 | 0.11219689 | 35.13823822 | 2.55350946 | 2.02060205 |
| 0.00001013 | 7.51615960  | 0.00023056 | 55.93997397 | 0.00524752 | 54.52479750 | 0.11943297 | 34.29000839 | 2.71828183 | 1.85126725 |
| 0.00001078 | 7.99775961  | 0.00024543 | 55.93604220 | 0.00558595 | 54.42843723 | 0.12713573 | 33.42651587 | 2.89359594 | 1.69932420 |
| 0.00001148 | 8.50977042  | 0.00026126 | 55.93183066 | 0.00594622 | 54.32663511 | 0.13533528 | 32.55005551 | 3.08021685 | 1.56608607 |
| 0.00001222 | 9.05401936  | 0.00027811 | 55.92733458 | 0.00632572 | 54.21725669 | 0.14406366 | 31.66293959 | 3.27887377 | 1.45170894 |
| 0.00001301 | 9.63242401  | 0.00029604 | 55.92253909 | 0.00673795 | 54.10175523 | 0.15335497 | 30.76714834 | 3.49034296 | 1.35467314 |
| 0.00001385 | 10.24699226 | 0.00031514 | 55.91742540 | 0.00717251 | 53.97917191 | 0.16324551 | 29.86412793 | 3.71545074 | 1.27196129 |
| 0.00001474 | 10.89982133 | 0.00033546 | 55.91197265 | 0.00763509 | 53.84913609 | 0.17377394 | 28.95484013 | 3.95507672 | 1.19987523 |
| 0.00001569 | 11.59309521 | 0.00035710 | 55.90615839 | 0.00812152 | 53.71126550 | 0.18498140 | 28.04011340 | 4.21015726 | 1.13492086 |
| 0.00001670 | 12.32908024 | 0.00038013 | 55.89995865 | 0.00865170 | 53.56516651 | 0.19691168 | 27.12099517 | 4.48168907 | 1.07439736 |
| 0.00001778 | 13.11011841 | 0.00040465 | 55.89334783 | 0.00922568 | 53.41043432 | 0.20961139 | 26.19901587 | 4.77073318 | 1.02124056 |
| 0.00001893 | 13.93861768 | 0.00043074 | 55.88629860 | 0.00980366 | 53.24665305 | 0.22315016 | 25.27614444 | 5.07841904 | 1.00009964 |
| 0.00002015 | 14.81703867 | 0.00045852 | 55.87878184 | 0.01043594 | 53.07339588 | 0.23752082 | 24.35454708 | 5.40594893 | 1.00000000 |
| 0.00002145 | 15.74787696 | 0.00048810 | 55.87076646 | 0.01110900 | 52.89022499 | 0.25283960 | 23.43622450 | 5.72108200 | 1.00000000 |
| 0.00002283 | 16.73363981 | 0.00051957 | 55.86221930 | 0.01182547 | 52.69669146 | 0.26914635 | 22.52263222 |            |            |
| 0.00002430 | 17.77681615 | 0.00055308 | 55.85310498 | 0.01258814 | 52.49233511 | 0.28650480 | 21.61455472 |            |            |
| 0.00002587 | 18.87983838 | 0.00058876 | 55.84338575 | 0.01340001 | 52.27668438 | 0.30498277 | 20.71216426 |            |            |
| 0.00002754 | 20.04503394 | 0.00062673 | 55.83302135 | 0.01426423 | 52.04925627 | 0.32465247 | 19.81558925 |            |            |
| 0.00002931 | 21.27456481 | 0.00066715 | 55.82196881 | 0.01518420 | 51.80955655 | 0.34559075 | 18.92569700 |            |            |
| 0.00003120 | 22.57035173 | 0.00071017 | 55.81018231 | 0.01616349 | 51.55708050 | 0.36787944 | 18.04503798 |            |            |
| 0.00003322 | 23.93398063 | 0.00075598 | 55.79761258 | 0.01720555 | 51.29131444 | 0.39160563 | 17.17819740 |            |            |
| 0.00003536 | 25.36658682 | 0.00080473 | 55.78420866 | 0.01831564 | 51.01173836 | 0.41686202 | 16.33069254 |            |            |
| 0.00003764 | 26.86871269 | 0.00085663 | 55.76991374 | 0.01946690 | 50.71783023 | 0.44374731 | 15.50649474 |            |            |
| 0.00004007 | 28.44013333 | 0.00091198 | 55.75466892 | 0.02075434 | 50.40907214 | 0.47236655 | 14.70566645 |            |            |
| 0.00004265 | 30.07964377 | 0.00097069 | 55.73841094 | 0.02209288 | 50.08495872 | 0.50283158 | 13.92484361 |            |            |
| 0.00004540 | 31.78480021 | 0.00103330 | 55.72107238 | 0.02351775 | 49.74500776 | 0.53526143 | 13.15988211 |            |            |
| 0.00004833 | 33.55160690 | 0.00109994 | 55.70258134 | 0.02503451 | 49.38877226 | 0.56978282 | 12.40849080 |            |            |
| 0.00005144 | 35.37413940 | 0.00117088 | 55.68286119 | 0.02664910 | 49.01585282 | 0.60653066 | 11.67111677 |            |            |
| 0.00005476 | 37.24409509 | 0.00124639 | 55.66183029 | 0.02836782 | 48.62590731 | 0.64564853 | 10.95033046 |            |            |
| 0.00005829 | 39.15026341 | 0.00132678 | 55.63940162 | 0.03019738 | 48.21865567 | 0.68728928 | 10.24797591 |            |            |
| 0.00006205 | 41.07791421 | 0.00141235 | 55.61548254 | 0.03214495 | 47.79387034 | 0.73161563 | 9.57308486  |            |            |
| 0.00006606 | 43.00811635 | 0.00150344 | 55.58997435 | 0.03421812 | 47.35136345 | 0.77880078 | 8.92312933  |            |            |
| 0.00007032 | 44.91702909 | 0.00160040 | 55.56277205 | 0.03642500 | 46.89094759 | 0.82902912 | 8.30195481  |            |            |
| 0.00007485 | 46.77527308 | 0.00170362 | 55.53376387 | 0.03877421 | 46.41239802 | 0.88249690 | 7.71097237  |            |            |
| 0.00007968 | 48.5761467  | 0.00181349 | 55.50283098 | 0.04127493 | 45.91541208 | 0.93941306 | 7.15148495  |            |            |
| 0.00008482 | 50.19343200 | 0.00193045 | 55.46984701 | 0.04393693 | 45.39958437 | 1.00000000 | 6.62505528  |            |            |
| 0.00009029 | 51.66880029 | 0.00205496 | 55.43467775 | 0.04677062 | 44.86440662 | 1.06449446 | 6.13360122  |            |            |
| 0.00009611 | 52.93140591 | 0.00218749 | 55.39718065 | 0.04978707 | 44.30929544 | 1.13314845 | 5.67865295  |            |            |
| 0.00010231 | 53.94922259 | 0.00232857 | 55.35720448 | 0.05299806 | 43.73354337 | 1.20623025 | 5.26037913  |            |            |
| 0.00010891 | 54.71159054 | 0.00247875 | 55.31458889 | 0.05641614 | 43.13687735 | 1.28402542 | 4.87679331  |            |            |
| 0.00011593 | 55.23678836 | 0.00263862 | 55.26916396 | 0.06005467 | 42.51851613 | 1.36683794 | 4.52404339  |            |            |
| 0.00012341 | 55.56849390 | 0.00280879 | 55.22074987 | 0.06392786 | 41.87820793 | 1.45499141 | 4.19752906  |            |            |
| 0.00013137 | 55.76123272 | 0.00298995 | 55.16915643 | 0.06805085 | 41.21575235 | 1.54883030 | 3.89301382  |            |            |
| 0.00013984 | 55.86480313 | 0.00318278 | 55.11418275 | 0.07243976 | 40.53109630 | 1.64872127 | 3.60728553  |            |            |
| 0.00014886 | 55.91625377 | 0.00338805 | 55.05561683 | 0.07711172 | 39.82432018 | 1.75505466 | 3.33812382  |            |            |
| 0.00015846 | 55.93948775 | 0.00360656 | 54.99323526 | 0.08208500 | 39.09561544 | 1.86824596 | 3.08409960  |            |            |
| 0.00016868 | 55.94840804 | 0.00383917 | 54.92680288 | 0.08737903 | 38.34527150 | 1.98873747 | 2.84425794  |            |            |
| 0.00017956 | 55.95046288 | 0.00408677 | 54.85607256 | 0.09301449 | 37.57364721 | 2.11700002 | 2.61799298  |            |            |
| 0.00019114 | 55.94936269 | 0.00435035 | 54.78078491 | 0.09901341 | 36.78140951 | 2.25353479 | 2.40505687  |            |            |

LANTHANUM (5D) A = 139 CWN S-L FX 07-24-73  
 NUCLEAR CHARGE= 57.0 RADIUS= 5.6356 FERMI =.0001065 BOHR SURFACE THICKNESS=0.5666 FERMI =.0000107 BOMP  
 SLATER-LATTER EXCHANGE APPROXIMATION WITH MULTIPLIER 1.50

| ENERGY EIGENVALUES |    | RADIAL EXPECTATION VALUES |                | [BOMP UNITS] |          |
|--------------------|----|---------------------------|----------------|--------------|----------|
| SMFLI              | 0  | RYDBERGS                  | ELECTRON VOLTS | 1/(R*R*R)    | 1/R      |
| 11S1/2             | 2  | 2.862321160 03            | 3.894273810 04 | 0.0          | 62.09416 |
| 12S1/2             | 2  | 4.587902750 02            | 6.241979320 03 | 0.0          | 14.64469 |
| 12P1/2             | 2  | 4.338481730 02            | 5.902634540 03 | 0.0          | 14.64250 |
| 12P3/2             | 4  | 4.030404040 02            | 5.483485600 03 | 6.164420 03  | 13.30731 |
| 13S1/2             | 2  | 9.927202220 01            | 1.350625640 03 | 0.0          | 3.29249  |
| 13P1/2             | 2  | 8.856510660 01            | 1.205009270 03 | 0.0          | 5.21209  |
| 13P3/2             | 4  | 8.251134240 01            | 1.122591570 03 | 1.365010 03  | 4.87894  |
| 13D3/2             | 4  | 6.356448840 01            | 8.648139340 02 | 2.243470 02  | 4.74875  |
| 13D5/2             | 6  | 6.225415330 01            | 8.469864320 02 | 2.045510 02  | 4.66355  |
| 14S1/2             | 2  | 2.052110600 01            | 2.791558030 02 | 0.0          | 2.19826  |
| 14P1/2             | 2  | 1.652177000 01            | 2.247836370 02 | 0.0          | 2.09878  |
| 14P3/2             | 4  | 1.521453920 01            | 2.069983700 02 | 2.956260 02  | 1.58980  |
| 14D3/2             | 4  | 8.581760600 00            | 1.167574280 02 | 4.045410 01  | 1.77946  |
| 14D5/2             | 6  | 8.349845290 00            | 1.136021500 02 | 3.660700 01  | 1.75255  |
| 15S1/2             | 2  | 3.206904820 00            | 4.363090220 01 | 0.0          | 0.87938  |
| 15P1/2             | 2  | 2.080863090 00            | 2.831076660 01 | 0.0          | 0.78240  |
| 15P3/2             | 4  | 1.877174570 00            | 2.553952320 01 | 4.571850 01  | 0.74323  |
| 15D3/2             | 1  | 4.074864460 -01           | 5.543975350 00 | 3.218630 00  | 0.49632  |
| 16S1/2             | 2  | 3.770112200 -01           | 5.129350750 00 | 0.0          | 0.29239  |
| TOTAL              | 57 | 1.696943830 04            | 2.308742990 05 |              |          |

| R          | POT#R       | R          | POT#R       | R          | POT#R       | R          | POT#R       | R           | POT#R      |
|------------|-------------|------------|-------------|------------|-------------|------------|-------------|-------------|------------|
| 0.00001148 | 8.62279439  | 0.00026126 | 56.93007928 | 0.00594622 | 55.28096702 | 0.13533528 | 33.07207323 | 3.08021685  | 1.58490925 |
| 0.00001222 | 9.17431801  | 0.00077811 | 56.92546420 | 0.00632572 | 55.16936030 | 0.14406366 | 32.17242951 | 3.27887377  | 1.47072940 |
| 0.00001301 | 9.76046345  | 0.00029604 | 56.92054149 | 0.00673795 | 55.05087441 | 0.15335497 | 31.26431020 | 3.49034296  | 1.37038569 |
| 0.00001385 | 10.38326808 | 0.00031514 | 56.91529186 | 0.00717251 | 54.92514442 | 0.16326551 | 30.34896737 | 3.71545074  | 1.26222771 |
| 0.00001474 | 11.04486029 | 0.00033546 | 56.90969388 | 0.00763509 | 54.79179352 | 0.17377394 | 29.42726736 | 3.95507672  | 1.20180023 |
| 0.00001569 | 11.74745714 | 0.00035710 | 56.90372447 | 0.00812752 | 54.65043323 | 0.18498140 | 28.50008828 | 4.21015726  | 1.12722802 |
| 0.00001670 | 12.49335958 | 0.00038013 | 56.89735899 | 0.00865170 | 54.50066358 | 0.19691168 | 27.56863086 | 4.48168907  | 1.05689340 |
| 0.00001778 | 13.28494787 | 0.00040465 | 56.89057111 | 0.00920568 | 54.34207332 | 0.20961139 | 26.63458792 | 4.77073318  | 1.00843420 |
| 0.00001893 | 14.12466776 | 0.00043074 | 56.88333276 | 0.00980366 | 54.17424000 | 0.22313016 | 25.70000825 | 5.07841904  | 1.00000000 |
| 0.00002015 | 15.01502177 | 0.00045852 | 56.87561399 | 0.01043594 | 53.99673001 | 0.23752082 | 24.76698913 | 4.252108200 | 1.00000000 |
| 0.00002145 | 15.95854902 | 0.00048810 | 56.86738284 | 0.01110900 | 53.80909847 | 0.25283960 | 23.83731726 |             |            |
| 0.00002283 | 16.95780270 | 0.00051957 | 56.85860522 | 0.01182547 | 53.61088918 | 0.26914635 | 22.91213774 |             |            |
| 0.00002430 | 18.01532004 | 0.00055308 | 56.84924475 | 0.01258814 | 53.40163438 | 0.28650480 | 21.99195288 |             |            |
| 0.00002587 | 19.13358412 | 0.00058876 | 56.83926264 | 0.01340001 | 53.18085466 | 0.30498277 | 21.07683959 |             |            |
| 0.00002754 | 20.31497553 | 0.00062673 | 56.82861748 | 0.01426423 | 52.94805852 | 0.32465247 | 20.16718911 |             |            |
| 0.00002931 | 21.56171167 | 0.00066715 | 56.81726512 | 0.01518420 | 52.70274481 | 0.34559075 | 19.26458990 |             |            |
| 0.00003120 | 22.87577114 | 0.00071017 | 56.80515845 | 0.01616349 | 52.44439959 | 0.36787944 | 18.37261283 |             |            |
| 0.00003322 | 24.25879984 | 0.00075598 | 56.79224721 | 0.01720595 | 52.17250207 | 0.39160563 | 17.49662053 |             |            |
| 0.00003536 | 25.71199502 | 0.00080473 | 56.77847762 | 0.01831564 | 51.88652567 | 0.41686202 | 16.64183582 |             |            |
| 0.00003764 | 27.23596272 | 0.00085663 | 56.76379311 | 0.01949690 | 51.58594335 | 0.44374731 | 15.81064574 |             |            |
| 0.00004007 | 28.83054296 | 0.00091188 | 56.74813212 | 0.02075434 | 51.27023442 | 0.47236655 | 15.00125294 |             |            |
| 0.00004265 | 30.49459630 | 0.00097069 | 56.73142985 | 0.02209288 | 50.93889370 | 0.50283158 | 14.20952744 |             |            |
| 0.00004540 | 32.22574432 | 0.00103330 | 56.71361699 | 0.02351775 | 50.59144265 | 0.53526143 | 13.43194754 |             |            |
| 0.00004833 | 34.02005520 | 0.00109994 | 56.69461968 | 0.02503451 | 50.22744158 | 0.56978282 | 12.66749065 |             |            |
| 0.00005144 | 35.87166531 | 0.00117088 | 56.67435918 | 0.02664910 | 49.84650151 | 0.60653066 | 11.91775276 |             |            |
| 0.00005476 | 37.77232704 | 0.00124639 | 56.65275160 | 0.02836782 | 49.44829205 | 0.64564853 | 11.18590834 |             |            |
| 0.00005829 | 39.71087510 | 0.00132678 | 56.62970757 | 0.03019738 | 49.03254269 | 0.68728928 | 10.47565980 |             |            |
| 0.00006205 | 41.67260861 | 0.00141235 | 56.60513191 | 0.03214495 | 48.59903199 | 0.73161563 | 9.79021040  |             |            |
| 0.00006606 | 43.63859930 | 0.00150344 | 56.57892328 | 0.03421812 | 48.14756417 | 0.77880078 | 9.13197705  |             |            |
| 0.00007032 | 45.58496540 | 0.00160040 | 56.55097385 | 0.03642500 | 47.67793255 | 0.82902912 | 8.50261712  |             |            |
| 0.00007485 | 47.46821218 | 0.00170362 | 56.52116889 | 0.03877421 | 47.18987830 | 0.88249690 | 7.90350382  |             |            |
| 0.00007968 | 49.29486327 | 0.00181349 | 56.48938642 | 0.04127493 | 46.68305435 | 0.93941306 | 7.33630375  |             |            |
| 0.00008482 | 50.98183727 | 0.00193045 | 56.45549677 | 0.04393693 | 46.15700831 | 1.00000000 | 6.80310377  |             |            |
| 0.00009029 | 52.49839514 | 0.00205496 | 56.41936223 | 0.04677062 | 45.61119209 | 1.06449446 | 6.30605201  |             |            |
| 0.00009611 | 53.80088801 | 0.00218749 | 56.38083661 | 0.04978707 | 45.04499783 | 1.13314845 | 5.84613514  |             |            |
| 0.00010231 | 54.85535985 | 0.00232857 | 56.33976484 | 0.05299806 | 44.45781363 | 1.20623025 | 5.42218764  |             |            |
| 0.00010891 | 55.64891439 | 0.00247875 | 56.29598252 | 0.05641614 | 43.84908144 | 1.28402542 | 5.03075271  |             |            |
| 0.00011593 | 56.19810863 | 0.00263862 | 56.24931556 | 0.06005467 | 43.21935026 | 1.36683794 | 4.66714358  |             |            |
| 0.00012341 | 56.54630339 | 0.00280879 | 56.19957974 | 0.06392786 | 42.56530688 | 1.45499141 | 4.32687240  |             |            |
| 0.00013137 | 56.74918842 | 0.00298995 | 56.14658032 | 0.06805085 | 41.88979079 | 1.54883030 | 4.00647530  |             |            |
| 0.00013984 | 56.85841907 | 0.00318278 | 56.09011164 | 0.07243576 | 41.19178477 | 1.64872127 | 3.70375803  |             |            |
| 0.00014886 | 56.91276599 | 0.00338805 | 56.02995682 | 0.07711172 | 40.47139848 | 1.75505466 | 3.41747181  |             |            |
| 0.00015846 | 56.93736143 | 0.00360656 | 55.96588736 | 0.08208500 | 39.72884847 | 1.86824596 | 3.14702064  |             |            |
| 0.00016868 | 56.94685731 | 0.00383917 | 55.89766290 | 0.08737903 | 38.96445134 | 1.98873747 | 2.89218826  |             |            |
| 0.00017956 | 56.94911153 | 0.00408677 | 55.82503092 | 0.09301449 | 38.17864738 | 2.11700002 | 2.65305564  |             |            |
| 0.00019114 | 56.94804056 | 0.00435035 | 55.74772653 | 0.09901341 | 37.37205186 | 2.25353479 | 2.43003955  |             |            |
| 0.00020347 | 56.94546215 | 0.00463092 | 55.66547235 | 0.10539922 | 36.54555482 | 2.39887529 | 2.22388430  |             |            |
| 0.00021659 | 56.94215843 | 0.00492959 | 55.57797835 | 0.11219689 | 35.70341571 | 2.55358946 | 2.03561542  |             |            |
| 0.00023056 | 56.93843666 | 0.00524752 | 55.48494181 | 0.11943297 | 34.83834369 | 2.71828183 | 1.86621236  |             |            |
| 0.00024543 | 56.93440192 | 0.00558593 | 55.38604737 | 0.12713573 | 33.96145220 | 2.89359594 | 1.71615327  |             |            |

CEPTUM (4F) (5C) A = 140 CMN S-L EX OT-24-73  
 NUCLEAR CHARGE = 58.0 RADIUS = 5.6499 FPMI = .0001069 ROMR SURFACE THICKNESS = 0.5666 FERMI = .0000107 ROMR  
 SLATER-LATYER EXCHANGE APPROXIMATION WITH MULTIPLIER 1.50

| SHELL Q  |   | ENERGY FICENVALUES |                | RADIAL EXPECTATION VALUES (ROMP UNITS) |          | RMAX     |             |
|----------|---|--------------------|----------------|----------------------------------------|----------|----------|-------------|
|          |   | RYDRERGS           | ELECTFCN VOLTS | 1/(REROR)                              | 1/R      | R        | ROROR       |
| (1S1/2)  | 2 | 2.974047050 03     | 4.046280230 04 | 0.0                                    | 63.42403 | 0.024535 | 8.181860-04 |
| (2S1/2)  | 2 | 4.793280180 02     | 6.521401480 03 | 0.0                                    | 14.98844 | 0.104380 | 1.291190-02 |
| (2P1/2)  | 2 | 4.537405320 02     | 6.173276060 03 | 0.0                                    | 14.98609 | 0.097522 | 9.441140-03 |
| (2P3/2)  | 4 | 4.204445350 02     | 5.720274040 03 | 7.173120 03                            | 13.56814 | 0.093719 | 1.069450-02 |
| (3S1/2)  | 2 | 1.043169110 02     | 1.419262870 03 | 0.0                                    | 5.42784  | 0.276543 | 8.750850-02 |
| (3P1/2)  | 2 | 9.328909560 01     | 1.269226000 03 | 0.0                                    | 5.34802  | 0.265891 | 8.216960-02 |
| (3P3/2)  | 4 | 8.668981670 01     | 1.179440960 03 | 1.460470 03                            | 4.99326  | 0.277976 | 8.959070-02 |
| (3D3/2)  | 4 | 6.720356830 01     | 9.143247080 02 | 2.411300 02                            | 4.86535  | 0.248650 | 7.293270-02 |
| (3D5/2)  | 6 | 6.577115330 01     | 8.948362720 02 | 2.191190 02                            | 4.77489  | 0.252447 | 7.503600-02 |
| (4S1/2)  | 2 | 2.155856100 01     | 2.933106900 02 | 0.0                                    | 2.25933  | 0.630832 | 4.497260-01 |
| (4P1/2)  | 2 | 1.740150410 01     | 2.367526830 02 | 0.0                                    | 2.15962  | 0.647650 | 4.769630-01 |
| (4P3/2)  | 4 | 1.596643690 01     | 2.172281630 02 | 3.186530 02                            | 2.04280  | 0.674463 | 5.169920-01 |
| (4D3/2)  | 4 | 9.064486900 00     | 1.233250640 02 | 4.406030 01                            | 1.83284  | 0.723842 | 6.070050-01 |
| (4D5/2)  | 6 | 8.808020220 00     | 1.198357580 02 | 3.566380 01                            | 1.80395  | 0.733253 | 6.277340-01 |
| (5S1/2)  | 2 | 3.325647900 00     | 4.574643740 01 | 0.0                                    | 0.90083  | 1.481725 | 2.466680 00 |
| (5P1/2)  | 2 | 2.152879580 00     | 2.929057250 01 | 0.0                                    | 0.80160  | 1.648975 | 3.075600 00 |
| (5P3/2)  | 4 | 1.931494950 00     | 2.627856830 01 | 4.875190 01                            | 0.75952  | 1.726771 | 3.374030 00 |
| (4F5/2)  | 1 | 9.454628510-01     | 1.286330570 01 | 5.106440 00                            | 1.31213  | 0.984369 | 1.237730 00 |
| (5D3/2)  | 1 | 4.067077350-01     | 5.533380750 00 | 3.385420 00                            | 0.50436  | 2.619561 | 8.235880 00 |
| (6S1/2)  | 2 | 3.831759900-01     | 5.213224300 00 | 0.0                                    | 0.29685  | 4.302561 | 7.123210 01 |
| TOTAL 58 |   | 1.770412060 04     | 2.408658720 05 |                                        |          |          |             |

| R          | POT#R       | R          | POT#R       | R          | POT#R       | R          | POT#R       | R          | POT#R      |
|------------|-------------|------------|-------------|------------|-------------|------------|-------------|------------|------------|
| 0.00001222 | 9.31448916  | 0.00027811 | 57.92349295 | 0.00637572 | 56.11902401 | 0.14406366 | 32.62897077 | 3.27887377 | 1.44325532 |
| 0.00001301 | 9.90961785  | 0.00029604 | 57.91843615 | 0.00673795 | 55.99740470 | 0.15335497 | 31.70442797 | 3.49034296 | 1.34684535 |
| 0.00001385 | 10.54197332 | 0.00031514 | 57.91304326 | 0.00717251 | 55.86837056 | 0.16324551 | 30.77227059 | 3.71545074 | 1.26077641 |
| 0.00001474 | 11.21371818 | 0.00033546 | 57.90729223 | 0.00763509 | 55.73153813 | 0.17377394 | 29.83331573 | 3.95507672 | 1.18222639 |
| 0.00001569 | 11.92710535 | 0.00035710 | 57.90115934 | 0.00812752 | 55.58651213 | 0.18498140 | 28.88849211 | 4.21015726 | 1.10903199 |
| 0.00001670 | 12.68447378 | 0.00038013 | 57.89461921 | 0.00865170 | 55.43268569 | 0.19691168 | 27.93915605 | 4.48168907 | 1.04075505 |
| 0.00001778 | 13.48824179 | 0.00040465 | 57.88764479 | 0.00920968 | 55.27024047 | 0.20961139 | 26.98711233 | 4.77073318 | 1.00306066 |
| 0.00001893 | 14.34089742 | 0.00043074 | 57.88020718 | 0.00980366 | 55.09814671 | 0.22313016 | 26.03443357 | 5.07841904 | 1.00000000 |
| 0.00002015 | 15.24498517 | 0.00045852 | 57.87227558 | 0.01043594 | 54.91616322 | 0.23752082 | 25.08311755 | 5.35212151 | 1.00000000 |
| 0.00002145 | 16.20308821 | 0.00048810 | 57.86381712 | 0.01110900 | 54.72363728 | 0.25283960 | 24.13470482 |            |            |
| 0.00002283 | 17.21780501 | 0.00051957 | 57.85479673 | 0.01182547 | 54.52070446 | 0.26914635 | 23.19011341 |            |            |
| 0.00002430 | 18.29171917 | 0.00055308 | 57.84517698 | 0.01258814 | 54.30628846 | 0.28650420 | 22.24964297 |            |            |
| 0.00002587 | 19.42736086 | 0.00058876 | 57.83491798 | 0.01340001 | 54.08010056 | 0.30498277 | 21.31388466 |            |            |
| 0.00002754 | 20.62715809 | 0.00062673 | 57.82397713 | 0.01426423 | 53.84164175 | 0.32465247 | 20.38247704 |            |            |
| 0.00002931 | 21.89337548 | 0.00066715 | 57.81230901 | 0.01518420 | 53.59039922 | 0.34559075 | 19.45903366 |            |            |
| 0.00003120 | 23.22803794 | 0.00071017 | 57.79986516 | 0.01616439 | 53.32585155 | 0.36787944 | 18.54762493 |            |            |
| 0.00003322 | 24.63283589 | 0.00075598 | 57.78659352 | 0.01720555 | 53.04746857 | 0.39160563 | 17.65384401 |            |            |
| 0.00003536 | 26.10900825 | 0.00080473 | 57.77244013 | 0.01831564 | 52.75471732 | 0.41686202 | 16.78204865 |            |            |
| 0.00003764 | 27.65719845 | 0.00085663 | 57.75734503 | 0.01949690 | 52.44706357 | 0.44374731 | 15.93285913 |            |            |
| 0.00004007 | 29.27727788 | 0.00091108 | 57.74124591 | 0.02075434 | 52.12398337 | 0.47236655 | 15.10334367 |            |            |
| 0.00004265 | 30.96813037 | 0.00097069 | 57.72407554 | 0.02209288 | 51.78497083 | 0.50283158 | 14.28951291 |            |            |
| 0.00004540 | 32.72738994 | 0.00103330 | 57.70576386 | 0.02351775 | 51.42954998 | 0.53526143 | 13.48907624 |            |            |
| 0.00004833 | 34.55112307 | 0.00109994 | 57.68623371 | 0.02503451 | 51.05728716 | 0.56978282 | 12.70248652 |            |            |
| 0.00005144 | 36.43344613 | 0.00117088 | 57.66540454 | 0.02664910 | 50.66780155 | 0.60653066 | 11.93241280 |            |            |
| 0.00005476 | 38.36606806 | 0.00124639 | 57.64319014 | 0.02836782 | 50.26077158 | 0.64564853 | 11.18270626 |            |            |
| 0.00005829 | 40.33775005 | 0.00132678 | 57.61949862 | 0.03019738 | 49.83593205 | 0.68728926 | 10.45715843 |            |            |
| 0.00006205 | 42.33367920 | 0.00141235 | 57.59423219 | 0.03214495 | 49.39305952 | 0.73161563 | 9.75891727  |            |            |
| 0.00006606 | 44.33476569 | 0.00150344 | 57.56728672 | 0.03421812 | 48.93194568 | 0.77880078 | 9.09018185  |            |            |
| 0.00007032 | 46.31690180 | 0.00160040 | 57.53855143 | 0.03642500 | 48.45235513 | 0.82902912 | 8.45250560  |            |            |
| 0.00007485 | 48.25028125 | 0.00170362 | 57.50790847 | 0.03877421 | 47.95398827 | 0.88249690 | 7.84731681  |            |            |
| 0.00007968 | 50.09903445 | 0.00181349 | 57.47523256 | 0.04127493 | 47.43644895 | 0.93941306 | 7.27629545  |            |            |
| 0.00008482 | 51.82140820 | 0.00193045 | 57.44039060 | 0.04393693 | 46.89923599 | 1.00000000 | 6.74145404  |            |            |
| 0.00009029 | 53.37196731 | 0.00205496 | 57.40324121 | 0.04677762 | 46.34176166 | 1.06449446 | 6.24433166  |            |            |
| 0.00009611 | 54.70599522 | 0.00218749 | 57.36363437 | 0.04978707 | 45.76339586 | 1.13314845 | 5.78499889  |            |            |
| 0.00010231 | 55.78827756 | 0.00232857 | 57.32141099 | 0.05295806 | 45.16352237 | 1.20623025 | 5.36130769  |            |            |
| 0.00010891 | 56.60466843 | 0.00247875 | 57.27640248 | 0.05641614 | 44.54159827 | 1.28402542 | 4.96930244  |            |            |
| 0.00011593 | 57.17096326 | 0.00263862 | 57.22843034 | 0.06005467 | 43.89719736 | 1.36683794 | 4.60443059  |            |            |
| 0.00012341 | 57.53069279 | 0.00280879 | 57.17730576 | 0.06392786 | 43.23003920 | 1.45499141 | 4.26265725  |            |            |
| 0.00013137 | 57.74059138 | 0.00298995 | 57.12282922 | 0.06805085 | 42.53999190 | 1.54883030 | 3.94108450  |            |            |
| 0.00013984 | 57.85370184 | 0.00318278 | 57.06479011 | 0.07243976 | 41.82706329 | 1.64872127 | 3.63785351  |            |            |
| 0.00014886 | 57.91001642 | 0.00338805 | 57.00296639 | 0.07711172 | 41.09137969 | 1.75505466 | 3.35191082  |            |            |
| 0.00015846 | 57.93552198 | 0.00360656 | 56.93712427 | 0.08208500 | 40.33317062 | 1.86824536 | 3.08266802  |            |            |
| 0.00016868 | 57.94538678 | 0.00383917 | 56.86701790 | 0.08737903 | 39.55277227 | 1.98873747 | 2.82985675  |            |            |
| 0.00017956 | 57.94775012 | 0.00408677 | 56.79238913 | 0.09301449 | 38.75065618 | 2.11700002 | 2.59350937  |            |            |
| 0.00019114 | 57.94666969 | 0.00435035 | 56.71296729 | 0.09901341 | 37.92750527 | 2.25353479 | 2.37398102  |            |            |
| 0.00020347 | 57.94402904 | 0.00463092 | 56.62846910 | 0.10539922 | 37.08430469 | 2.39887529 | 2.17199930  |            |            |
| 0.00021659 | 57.94063868 | 0.00492959 | 56.53859849 | 0.11219689 | 36.22244762 | 2.55358946 | 1.98848897  |            |            |
| 0.00023056 | 57.93681712 | 0.00524752 | 56.44304663 | 0.11943297 | 35.34377008 | 2.71828183 | 1.82425390  |            |            |
| 0.00024543 | 57.93267335 | 0.00558595 | 56.34149189 | 0.12713573 | 34.45046728 | 2.89339594 | 1.67944860  |            |            |
| 0.00026126 | 57.92823349 | 0.00594622 | 56.23359998 | 0.13533228 | 33.54484386 | 3.08021685 | 1.55314750  |            |            |

PRASEODYMIUM (4F)3 A = 141 CMN  
 NUCLEAR CHARGE= 59.0 RADIUS= 3.6642 FERMI \*0.0001070 BOHR SURFACE THICKNESS=0.5666 FERMI \*0.000107 BOHR  
 SLATER-LATYER EXCHANGE APPROXIMATION WITH MULTIPLIER 1.50

| ENERGY EIGENVALUES |    |                |                | RADIAL EXPECTATION VALUES (BOHR UNITS) |          |          |             |
|--------------------|----|----------------|----------------|----------------------------------------|----------|----------|-------------|
| SHELL              | Q  | RYDMERGS       | ELECTRON VOLTS | 1/(R*R*R)                              | 1/R      | R        | R*R         |
| (1S1/2)            | 2  | 3.087703900 03 | 4.200913790 04 | 0.0                                    | 64.76895 | 0.024057 | 7.870800-04 |
| (2S1/2)            | 2  | 4.997894290 02 | 6.799789120 03 | 0.0                                    | 15.33773 | 0.102222 | 1.238720-02 |
| (2P1/2)            | 2  | 4.735620160 02 | 6.442953290 03 | 0.0                                    | 15.33508 | 0.085637 | 9.042680-03 |
| (2P3/2)            | 4  | 4.376155570 02 | 5.953890940 03 | 7.600430 03                            | 13.83037 | 0.091938 | 1.029100-02 |
| (3S1/2)            | 2  | 1.087974620 02 | 1.480222110 03 | 0.0                                    | 5.56520  | 0.270315 | 8.361830-02 |
| (3P1/2)            | 2  | 9.744482620 01 | 1.325766090 03 | 0.0                                    | 5.48607  | 0.259628 | 7.835360-02 |
| (3P3/2)            | 4  | 9.026437610 01 | 1.228073920 03 | 1.561120 03                            | 5.10844  | 0.271857 | 8.569190-02 |
| (3D3/2)            | 4  | 7.024417350 01 | 9.556930540 02 | 2.585600 02                            | 4.98320  | 0.242659 | 6.942940-02 |
| (3D5/2)            | 6  | 6.868017030 01 | 9.344143210 02 | 2.344650 02                            | 4.88717  | 0.246498 | 7.150360-02 |
| (4S1/2)            | 2  | 2.199727820 01 | 2.992795700 02 | 0.0                                    | 2.31405  | 0.616884 | 4.295580-01 |
| (4P1/2)            | 2  | 1.768889720 01 | 2.406627530 02 | 0.0                                    | 2.21279  | 0.632946 | 4.558040-01 |
| (4P3/2)            | 4  | 1.612968880 01 | 2.194492550 02 | 3.399120 02                            | 2.08708  | 0.660525 | 4.961270-01 |
| (4D3/2)            | 4  | 8.979495720 00 | 1.221687330 02 | 4.709370 01                            | 1.87260  | 0.708942 | 5.830530-01 |
| (4D5/2)            | 6  | 8.701222120 00 | 1.183827370 02 | 4.218420 01                            | 1.84132  | 0.718759 | 5.991800-01 |
| (5S1/2)            | 2  | 3.182667840 00 | 4.330115080 01 | 0.0                                    | 0.90134  | 1.477007 | 2.452120 00 |
| (5P1/2)            | 2  | 2.003619270 00 | 2.725584130 01 | 0.0                                    | 0.79580  | 1.656037 | 3.108940 00 |
| (5P3/2)            | 4  | 1.781343040 00 | 2.423570540 01 | 4.793010 01                            | 0.75090  | 1.741039 | 3.438310 00 |
| (4F5/2)            | 3  | 5.512459030-01 | 7.499865880 00 | 5.169110 00                            | 1.29535  | 1.026761 | 1.399170 00 |
| (6S1/2)            | 2  | 3.594593560-01 | 4.890552370 00 | 0.0                                    | 0.28383  | 4.484111 | 2.310450 01 |
| TOTAL              | 59 | 1.845823910 04 | 2.511298800 05 |                                        |          |          |             |

| R          | POTR        | R          | POTR        | R          | POTR        | R          | POTR        | R           | POTR       |
|------------|-------------|------------|-------------|------------|-------------|------------|-------------|-------------|------------|
| 0.00001148 | 8.88574161  | 0.00026126 | 58.92629593 | 0.00594622 | 57.18400139 | 0.13533528 | 33.97009088 | 3.08021685  | 1.47269438 |
| 0.00001222 | 9.45112999  | 0.00027811 | 58.92142372 | 0.00632972 | 57.06631983 | 0.14406366 | 33.03441404 | 3.27887377  | 1.37244672 |
| 0.00001301 | 10.05820854 | 0.00029404 | 58.91622619 | 0.00673795 | 56.94142305 | 0.15335497 | 32.08949628 | 3.49034296  | 1.28695685 |
| 0.00001385 | 10.70007949 | 0.00031514 | 58.91068294 | 0.00717251 | 56.80893255 | 0.16324551 | 31.13624245 | 3.71545074  | 1.21265190 |
| 0.00001474 | 11.38193954 | 0.00033546 | 58.90477129 | 0.00763509 | 56.66845771 | 0.17377394 | 30.17541654 | 3.95507672  | 1.14608284 |
| 0.00001569 | 12.10607740 | 0.00035710 | 58.89846681 | 0.00812752 | 56.51959595 | 0.18498140 | 29.20804345 | 4.21015726  | 1.08448841 |
| 0.00001670 | 12.87486954 | 0.00038013 | 58.89174340 | 0.00865170 | 56.36193243 | 0.19691168 | 28.23558999 | 4.48168907  | 1.02823329 |
| 0.00001778 | 13.69077348 | 0.00040465 | 58.88457321 | 0.00920468 | 56.19504256 | 0.20961139 | 27.25995084 | 4.77073318  | 1.00105189 |
| 0.00001893 | 14.55631813 | 0.00043074 | 58.87692650 | 0.00980366 | 56.01848711 | 0.22313016 | 26.28318404 | 5.07841904  | 1.00000000 |
| 0.00002015 | 15.47409047 | 0.00045852 | 58.86877157 | 0.01043594 | 55.83181706 | 0.23752082 | 25.30713944 | 42.52108200 | 1.00000000 |
| 0.00002145 | 16.44647175 | 0.00048810 | 58.86007459 | 0.01110900 | 55.63457099 | 0.25283960 | 24.33317718 |             |            |
| 0.00002283 | 17.47684322 | 0.00051957 | 58.85079946 | 0.01182547 | 55.42627542 | 0.26914635 | 23.36199195 |             |            |
| 0.00002430 | 18.56709730 | 0.00055308 | 58.84090768 | 0.01258814 | 55.20644452 | 0.28650480 | 22.39388061 |             |            |
| 0.00002587 | 19.72005712 | 0.00058876 | 58.83035816 | 0.01340001 | 54.97458013 | 0.30498277 | 21.42924802 |             |            |
| 0.00002754 | 20.93819816 | 0.00062673 | 58.81910709 | 0.01426423 | 54.73017187 | 0.32465247 | 20.46953239 |             |            |
| 0.00002931 | 22.22383238 | 0.00066715 | 58.80710771 | 0.01518420 | 54.47269788 | 0.34559075 | 19.51797164 |             |            |
| 0.00003120 | 23.57903116 | 0.00071017 | 58.79431017 | 0.01616349 | 54.20162620 | 0.36787944 | 18.57960009 |             |            |
| 0.00003322 | 25.00552970 | 0.00075598 | 58.78066127 | 0.01720595 | 53.91641750 | 0.39160563 | 17.65979629 |             |            |
| 0.00003536 | 26.50460894 | 0.00080473 | 58.76610430 | 0.01831364 | 53.61632911 | 0.41686202 | 16.76160125 |             |            |
| 0.00003764 | 28.07695013 | 0.00085663 | 58.75057873 | 0.01949690 | 53.30142119 | 0.44374731 | 15.88429563 |             |            |
| 0.00004007 | 29.72245669 | 0.00091188 | 58.73402016 | 0.02079434 | 52.97056488 | 0.47236655 | 15.02451598 |             |            |
| 0.00004265 | 31.44003651 | 0.00097069 | 58.71635972 | 0.02209288 | 52.62345266 | 0.50283158 | 14.17418732 |             |            |
| 0.00004540 | 33.22733704 | 0.00103330 | 58.69752413 | 0.02351775 | 52.25961023 | 0.53526143 | 13.34755297 |             |            |
| 0.00004833 | 35.08042440 | 0.00109994 | 58.67743528 | 0.02503451 | 51.87860825 | 0.56978282 | 12.53152072 |             |            |
| 0.00005144 | 36.99339659 | 0.00117088 | 58.65600991 | 0.02664910 | 51.48007215 | 0.60653066 | 11.73491521 |             |            |
| 0.00005476 | 38.95792113 | 0.00124639 | 58.63315932 | 0.02836782 | 51.06368538 | 0.64564853 | 10.96217219 |             |            |
| 0.00005829 | 40.96268824 | 0.00132678 | 58.60878908 | 0.03014738 | 50.62918369 | 0.68728928 | 10.21746134 |             |            |
| 0.00006205 | 42.99277620 | 0.00141235 | 58.58279861 | 0.03201449 | 50.17533564 | 0.73161563 | 9.50398888  |             |            |
| 0.00006606 | 45.02893755 | 0.00150344 | 58.55508088 | 0.03392182 | 49.70491115 | 0.77880078 | 8.82398511  |             |            |
| 0.00007032 | 47.04684346 | 0.00160040 | 58.52552203 | 0.03584250 | 49.21464085 | 0.82902912 | 8.17897704  |             |            |
| 0.00007485 | 49.01638325 | 0.00170362 | 58.49400047 | 0.03777421 | 48.70517785 | 0.88249690 | 7.57019839  |             |            |
| 0.00007968 | 50.90123766 | 0.00181349 | 58.46038898 | 0.04127493 | 48.17607321 | 0.93941306 | 6.99904613  |             |            |
| 0.00008482 | 52.65917361 | 0.00193045 | 58.42434934 | 0.04393693 | 47.62677575 | 1.00000000 | 6.46682419  |             |            |
| 0.00009020 | 54.24388707 | 0.00205496 | 58.38633688 | 0.04677062 | 47.05605986 | 1.06449446 | 5.97428286  |             |            |
| 0.00009611 | 55.60965951 | 0.00218749 | 58.34559759 | 0.04970707 | 46.46507361 | 1.13314845 | 5.52071896  |             |            |
| 0.00010231 | 56.72001435 | 0.00232857 | 58.30216818 | 0.05295806 | 45.85139877 | 1.20623025 | 5.10558319  |             |            |
| 0.00010891 | 57.55953330 | 0.00247875 | 58.25587567 | 0.05641614 | 45.21510343 | 1.28402542 | 4.7194583   |             |            |
| 0.00011593 | 58.14320830 | 0.00263862 | 58.20653658 | 0.06005467 | 44.55578416 | 1.36683794 | 4.36372197  |             |            |
| 0.00012341 | 58.51469804 | 0.00280879 | 58.15395852 | 0.06392786 | 43.87318273 | 1.45499141 | 4.03295384  |             |            |
| 0.00013137 | 58.73176365 | 0.00298895 | 58.09793577 | 0.06805085 | 43.16718843 | 1.54883030 | 3.72421814  |             |            |
| 0.00013984 | 58.84884404 | 0.00318278 | 58.03825298 | 0.07243976 | 42.43782089 | 1.64872127 | 3.43543802  |             |            |
| 0.00014886 | 58.90717280 | 0.00338805 | 57.97468273 | 0.07711172 | 41.68521218 | 1.75505466 | 3.16505713  |             |            |
| 0.00015846 | 58.93360942 | 0.00360656 | 57.90698569 | 0.08208500 | 40.90959584 | 1.86824596 | 2.91186468  |             |            |
| 0.00016868 | 58.94385058 | 0.00383917 | 57.83491028 | 0.08737503 | 40.11131579 | 1.98873747 | 2.67486640  |             |            |
| 0.00017956 | 58.94632385 | 0.00408677 | 57.75819247 | 0.09301449 | 39.29087559 | 2.11700002 | 2.45348199  |             |            |
| 0.00019114 | 58.94523166 | 0.00435035 | 57.67655558 | 0.09901341 | 38.44901199 | 2.25353479 | 2.24740729  |             |            |
| 0.00020347 | 58.94252499 | 0.00463092 | 57.58971010 | 0.10539422 | 37.58680723 | 2.39887529 | 2.05701843  |             |            |
| 0.00021659 | 58.93904346 | 0.00492959 | 57.49733366 | 0.11219689 | 36.70576323 | 2.55358946 | 1.88326453  |             |            |
| 0.00023056 | 58.93511708 | 0.00524752 | 57.39917098 | 0.11943297 | 35.80781561 | 2.71828183 | 1.72742112  |             |            |
| 0.00024543 | 58.93085885 | 0.00558595 | 57.29483388 | 0.12713573 | 34.89518572 | 2.89359594 | 1.59054040  |             |            |

NEODYMIUM (4F14) A = 144 CWN  
 NUCLEAR CHARGE = 60.0 RADIUS = 5.7067 FERMI = 0.0001078 R<sub>NHR</sub> SURFACE THICKNESS = 0.5666 FERMI = 0.0000107 BOMP  
 SLATER-LATTER EXCHANGE APPROXIMATION WITH MULTIPLIER 1.50

| SHELL Q |    | ENERGY EIGENVALUES |                | RADIAL EXPECTATION VALUES (BOMP UNITS) |          | R <sub>MAX</sub> |
|---------|----|--------------------|----------------|----------------------------------------|----------|------------------|
|         |    | RYDBERGS           | FLCTFCN VOLTS  | 1/(R <sub>NHR</sub> <sup>2</sup> )     | 1/R      |                  |
| (1S1/2) | 2  | 3.204384170 03     | 4.359660790 04 | 0.0                                    | 66.12899 | 0.023594         |
| (2S1/2) | 2  | 5.213597420 02     | 7.093255700 03 | 0.0                                    | 15.69094 | 0.100141         |
| (2P1/2) | 2  | 4.944735620 02     | 6.727461150 03 | 0.0                                    | 15.68804 | 0.083820         |
| (2P3/2) | 4  | 4.557158440 02     | 6.200150770 03 | 8.044960 03                            | 14.09249 | 0.090226         |
| (3S1/2) | 2  | 1.140628400 02     | 1.551859160 03 | 0.0                                    | 5.70328  | 0.264351         |
| (3P1/2) | 2  | 1.023778040 02     | 1.392880730 03 | 0.0                                    | 5.62465  | 0.253650         |
| (3P3/2) | 4  | 9.477332830 01     | 1.286780140 03 | 1.666180 03                            | 5.22317  | 0.266224         |
| (3D3/2) | 4  | 7.401768450 01     | 1.006564780 03 | 2.775300 02                            | 5.10007  | 0.236996         |
| (3D5/2) | 6  | 7.230954670 01     | 9.837930750 02 | 2.503510 02                            | 4.99830  | 0.240876         |
| (4S1/2) | 2  | 2.304840140 01     | 7.135804150 02 | 0.0                                    | 4.602118 | 0.092800         |
| (4P1/2) | 2  | 1.857756240 01     | 2.527533090 02 | 0.0                                    | 2.37528  | 0.616973         |
| (4P3/2) | 4  | 1.687333170 01     | 2.255667400 02 | 3.650390 02                            | 2.13932  | 0.644507         |
| (4D3/2) | 4  | 9.447600330 00     | 1.285374370 02 | 5.099900 01                            | 1.92504  | 0.688800         |
| (4D5/2) | 6  | 9.141641830 00     | 1.243747800 02 | 4.548140 01                            | 1.89158  | 0.699730         |
| (5S1/2) | 2  | 3.292558380 00     | 4.479624450 01 | 0.0                                    | 0.92203  | 1.444555         |
| (5P1/2) | 2  | 2.066929930 00     | 2.812120180 01 | 0.0                                    | 0.81406  | 1.619409         |
| (5P3/2) | 4  | 1.826491040 00     | 2.484995850 01 | 5.085500 01                            | 0.76597  | 1.706431         |
| (4F5/2) | 4  | 5.980863030 -01    | 8.137143580 00 | 5.794410 00                            | 1.34970  | 0.982640         |
| (6S1/2) | 2  | 3.646741690 -01    | 4.961501470 00 | 0.0                                    | 0.28784  | 4.421140         |
| TOTAL   | 60 | 1.923206790 04     | 2.616580530 05 |                                        |          |                  |

| R          | POT-R       | R          | POT-R       | R          | POT-R       | R           | POT-R       | R           | POT-R      |
|------------|-------------|------------|-------------|------------|-------------|-------------|-------------|-------------|------------|
| 0.00001148 | 8.97731705  | 0.00026126 | 59.92440241 | 0.00594622 | 58.13528184 | 0.13533528  | 34.43076669 | 3.08021685  | 1.44604463 |
| 0.00001222 | 9.55163140  | 0.00027811 | 59.91940120 | 0.00632572 | 58.01455999 | 0.14406366  | 33.47305855 | 3.27887377  | 1.34967488 |
| 0.00001301 | 10.16202219 | 0.00029604 | 59.91406572 | 0.00673795 | 57.88645646 | 0.15335497  | 32.51570762 | 3.49034296  | 1.26756184 |
| 0.00001385 | 10.81061743 | 0.00031514 | 59.90837502 | 0.00717251 | 57.75058616 | 0.16324551  | 31.54451232 | 3.71545074  | 1.19551844 |
| 0.00001474 | 11.49964139 | 0.00033546 | 59.90230581 | 0.00763509 | 57.60655177 | 0.17373794  | 30.56526099 | 3.95505172  | 1.13045786 |
| 0.00001569 | 12.23141238 | 0.00035710 | 59.89583299 | 0.00812752 | 57.45394389 | 0.18498140  | 29.57909711 | 4.21015726  | 1.06985649 |
| 0.00001670 | 13.00833860 | 0.00038013 | 59.88892977 | 0.00865170 | 57.29244214 | 0.19691148  | 28.58761956 | 4.48168907  | 1.01626537 |
| 0.00001778 | 13.83291165 | 0.00040465 | 59.88156736 | 0.00920568 | 57.12131024 | 0.20961139  | 27.59278273 | 4.77073318  | 1.00000000 |
| 0.00001893 | 14.70769710 | 0.00043074 | 59.87371536 | 0.00980366 | 56.94040596 | 0.22313016  | 26.59659111 | 42.52108200 |            |
| 0.00002015 | 15.63532138 | 0.00045852 | 59.86534112 | 0.01043594 | 56.74917101 | 0.23752082  | 25.60072418 |             |            |
| 0.00002145 | 16.61845414 | 0.00048810 | 59.85640986 | 0.01110900 | 56.54713587 | 0.252783960 | 24.60632337 |             |            |
| 0.00002283 | 17.65978500 | 0.00051957 | 59.84688449 | 0.01182547 | 56.33381856 | 0.26914635  | 23.61392051 |             |            |
| 0.00002430 | 18.76199355 | 0.00055308 | 59.83672540 | 0.01258814 | 56.10872446 | 0.28650480  | 22.62385081 |             |            |
| 0.00002587 | 19.92771025 | 0.00058876 | 59.82589039 | 0.01340001 | 55.87134626 | 0.30498277  | 21.63688813 |             |            |
| 0.00002754 | 21.15947073 | 0.00062673 | 59.81433440 | 0.01426423 | 55.62116429 | 0.32465247  | 20.65518155 |             |            |
| 0.00002931 | 22.45964856 | 0.00066715 | 59.80200937 | 0.01518420 | 55.35764737 | 0.34559075  | 19.68280041 |             |            |
| 0.00003120 | 23.83038485 | 0.00071017 | 59.78886466 | 0.01616349 | 55.08025463 | 0.36787944  | 18.72515448 |             |            |
| 0.00003322 | 25.27349026 | 0.00075598 | 59.77484381 | 0.01720595 | 54.78343849 | 0.39160563  | 17.78699579 |             |            |
| 0.00003536 | 26.79032830 | 0.00080473 | 59.75989030 | 0.01831564 | 54.48164943 | 0.41686202  | 16.86991287 |             |            |
| 0.00003764 | 28.38167080 | 0.00085663 | 59.74394137 | 0.01949490 | 54.15934262 | 0.44374731  | 15.97201082 |             |            |
| 0.00004007 | 30.04752073 | 0.00091188 | 59.72693075 | 0.02075434 | 53.82098686 | 0.47273665  | 15.08994389 |             |            |
| 0.00004265 | 31.78689553 | 0.00097069 | 59.70874775 | 0.02209288 | 53.46607531 | 0.50283158  | 14.22170640 |             |            |
| 0.00004540 | 33.59756342 | 0.00103330 | 59.68943707 | 0.02351775 | 53.09413758 | 0.53526143  | 13.36796525 |             |            |
| 0.00004833 | 35.47572357 | 0.00109944 | 59.66879843 | 0.02503451 | 52.70475087 | 0.56978282  | 12.53179352 |             |            |
| 0.00005144 | 37.41562036 | 0.00117088 | 59.64678630 | 0.02664910 | 52.29754814 | 0.60653066  | 11.71770369 |             |            |
| 0.00005476 | 39.40908138 | 0.00124639 | 59.62330961 | 0.02836782 | 51.87221861 | 0.64564853  | 10.93034606 |             |            |
| 0.00005829 | 41.44497308 | 0.00132678 | 59.59827132 | 0.03015738 | 51.42849808 | 0.68728928  | 10.17377480 |             |            |
| 0.00006205 | 43.50854798 | 0.00141235 | 59.57156819 | 0.03214495 | 50.96614523 | 0.73181563  | 9.45093891  |             |            |
| 0.00006606 | 45.58075305 | 0.00150344 | 59.54309032 | 0.03421812 | 50.48490656 | 0.77880078  | 8.76381460  |             |            |
| 0.00007032 | 47.67374267 | 0.00160040 | 59.51272082 | 0.03642500 | 49.98447734 | 0.82907912  | 8.11377266  |             |            |
| 0.00007485 | 49.64685780 | 0.00170362 | 59.48033542 | 0.03877421 | 49.46446257 | 0.88249690  | 7.50197792  |             |            |
| 0.00007968 | 51.57788627 | 0.00181349 | 59.44580204 | 0.04127493 | 48.92436562 | 0.93941306  | 6.92967871  |             |            |
| 0.00008482 | 53.38287027 | 0.00193045 | 59.40898042 | 0.04393693 | 48.36359088 | 1.00000000  | 6.39784611  |             |            |
| 0.00009029 | 55.01651069 | 0.00205496 | 59.36972168 | 0.04677062 | 47.78148379 | 1.06449446  | 5.90660441  |             |            |
| 0.00009611 | 56.43160363 | 0.00218745 | 59.32786790 | 0.04978707 | 47.17738100 | 1.13314845  | 5.45452904  |             |            |
| 0.00010231 | 57.58071702 | 0.00232957 | 59.28325170 | 0.05295806 | 46.55067070 | 1.20623025  | 5.03863079  |             |            |
| 0.00010891 | 58.47047447 | 0.00247875 | 59.23569584 | 0.05641614 | 45.90084092 | 1.28402542  | 4.65499587  |             |            |
| 0.00011593 | 59.08745357 | 0.00263862 | 59.18501276 | 0.06005467 | 45.22751548 | 1.36683794  | 4.29665037  |             |            |
| 0.00012341 | 59.48248001 | 0.00280879 | 59.13100423 | 0.06392786 | 44.53046407 | 1.45499141  | 3.96924737  |             |            |
| 0.00013137 | 59.71431777 | 0.00298895 | 59.07346091 | 0.06805085 | 43.80959926 | 1.54883030  | 3.66118892  |             |            |
| 0.00013984 | 59.83974590 | 0.00318278 | 59.01216203 | 0.07243576 | 43.06495731 | 1.64872127  | 3.37355230  |             |            |
| 0.00014886 | 59.90238560 | 0.00338805 | 58.94687458 | 0.07711172 | 42.29668153 | 1.75505466  | 3.10481724  |             |            |
| 0.00015846 | 59.93086968 | 0.00360656 | 58.87735510 | 0.08208500 | 41.50501813 | 1.86824596  | 2.85373438  |             |            |
| 0.00016868 | 59.94199478 | 0.00383917 | 58.80334530 | 0.08737903 | 40.69033493 | 1.98873747  | 2.61929331  |             |            |
| 0.00017956 | 59.94479492 | 0.00408677 | 58.72457589 | 0.09301449 | 39.85318334 | 2.11700002  | 2.40080647  |             |            |
| 0.00019114 | 59.94377858 | 0.00435035 | 58.64076441 | 0.09901341 | 38.99438099 | 2.25333479  | 2.19808881  |             |            |
| 0.00020347 | 59.94103982 | 0.00463092 | 58.55161545 | 0.10539527 | 38.11512342 | 2.39887529  | 2.01154613  |             |            |
| 0.00021659 | 59.93748030 | 0.00492959 | 58.45682061 | 0.11219489 | 37.21703745 | 2.55358946  | 1.84214973  |             |            |
| 0.00023056 | 59.93345488 | 0.00524752 | 58.35605847 | 0.11943297 | 36.30215131 | 2.71828183  | 1.69109291  |             |            |
| 0.00024543 | 59.92908560 | 0.00558595 | 58.24999464 | 0.12713573 | 35.37269223 | 2.89359594  | 1.55916953  |             |            |

PROMETHIUM (4F15) A = 145 CHN S-L FX 07-24-73  
 NUCLEAR CHARGE = 61.0 RADIUS = 5.7207 FERMI = 0.0001081 RCHN SURFACE THICKNESS = 0.5666 FERMI = 0.000107 RCHN  
 SLATER-LATTER EXCHANGE APPROXIMATION WITH MULTIPLIER 1.50

| ENERGY LEVEL VALUES |    |            |                | RADIAL EXPECTATION VALUES (BOHR UNITS) |          |          |                    |
|---------------------|----|------------|----------------|----------------------------------------|----------|----------|--------------------|
| SHELL               | Q  | RYDBERGS   | ELECTRON VOLTS | 1/(R <sup>3</sup> CHN)                 | 1/R      | R        | R <sup>2</sup> CHN |
| (1S1/2)             | 2  | 3.32359358 | 4.52194878     | 0.0                                    | 67.50513 | 0.023145 | 7.294350-04        |
| (2S1/2)             | 2  | 5.43463449 | 7.39398326     | 0.0                                    | 16.04918 | 0.098126 | 1.142170-02        |
| (2P1/2)             | 2  | 5.15910985 | 7.01912373     | 0.0                                    | 16.04594 | 0.082062 | 8.310990-03        |
| (2P3/2)             | 4  | 4.74163735 | 6.45120789     | 0.0                                    | 14.35527 | 0.088573 | 9.550270-03        |
| (3S1/2)             | 2  | 1.19445475 | 1.62509152     | 0.0                                    | 5.84283  | 0.258614 | 7.654900-02        |
| (3P1/2)             | 2  | 1.07424160 | 1.46153792     | 0.0                                    | 5.76465  | 0.247909 | 7.145620-02        |
| (3P3/2)             | 4  | 9.89664372 | 1.34646807     | 0.0                                    | 5.33814  | 0.260431 | 7.864100-02        |
| (3D3/2)             | 4  | 7.78497168 | 1.05916875     | 0.0                                    | 5.21711  | 0.231590 | 6.318510-02        |
| (3D5/2)             | 6  | 7.59984023 | 1.03398104     | 0.0                                    | 5.10937  | 0.235512 | 6.520550-02        |
| (4S1/2)             | 2  | 2.41108276 | 1.28035043     | 0.0                                    | 2.43658  | 0.588063 | 3.904370-01        |
| (4P1/2)             | 2  | 1.94751727 | 1.64456556     | 0.0                                    | 2.33468  | 0.601820 | 4.121840-01        |
| (4P3/2)             | 4  | 1.76164950 | 2.79677704     | 0.0                                    | 2.19113  | 0.630131 | 4.516130-01        |
| (4D3/2)             | 4  | 9.91217297 | 1.34860808     | 0.0                                    | 1.97686  | 0.671885 | 5.237790-01        |
| (4D5/2)             | 6  | 9.57700459 | 1.30298021     | 0.0                                    | 1.94112  | 0.681939 | 5.394420-01        |
| (5S1/2)             | 2  | 3.40079731 | 4.62688677     | 0.0                                    | 0.94236  | 1.414011 | 2.248540           |
| (5P1/2)             | 2  | 2.12843148 | 2.89579488     | 0.0                                    | 0.83190  | 1.585125 | 2.850920           |
| (5P3/2)             | 4  | 1.86909487 | 2.54295964     | 0.0                                    | 0.78050  | 1.674663 | 3.184390           |
| (4F5/2)             | 5  | 6.37136286 | 8.66911058     | 0.0                                    | 1.40145  | 0.944673 | 1.180320           |
| (6S1/2)             | 2  | 3.69695170 | 5.02981370     | 0.0                                    | 0.29172  | 4.361960 | 2.189610           |
| TOTAL               | 61 | 2.00254654 | 2.74579670     | 05                                     |          |          |                    |

| R          | POT <sup>CHN</sup> | R          | POT <sup>CHN</sup> | R          | POT <sup>CHN</sup> | R          | POT <sup>CHN</sup> | R           | POT <sup>CHN</sup> |
|------------|--------------------|------------|--------------------|------------|--------------------|------------|--------------------|-------------|--------------------|
| 0.00001148 | 9.10726423         | 0.00026126 | 60.92248666        | 0.00594622 | 59.08588841        | 0.13533528 | 34.88555171        | 3.08021685  | 1.42145671         |
| 0.00001222 | 9.69991858         | 0.00027811 | 60.91735494        | 0.00632572 | 58.96209138        | 0.14406366 | 33.91538356        | 3.27887377  | 1.32902491         |
| 0.00001301 | 10.30917369        | 0.00029604 | 60.91147908        | 0.00675755 | 58.83074511        | 0.15335497 | 32.93509130        | 3.49034296  | 1.24956090         |
| 0.00001395 | 10.96719372        | 0.00031514 | 60.90603878        | 0.00717251 | 58.69145753        | 0.16324551 | 31.94541033        | 3.71545074  | 1.17951395         |
| 0.00001474 | 11.66623676        | 0.00033546 | 60.89980970        | 0.00763509 | 58.54382579        | 0.17377394 | 30.94718955        | 3.95507672  | 1.11577929         |
| 0.00001569 | 12.40865670        | 0.00035710 | 60.89316605        | 0.00812752 | 58.38743243        | 0.18498140 | 29.94170089        | 4.21015726  | 1.05606387         |
| 0.00001670 | 13.19689855        | 0.00038013 | 60.88608025        | 0.00865170 | 58.22184940        | 0.19691168 | 28.93065752        | 4.48168907  | 1.01057827         |
| 0.00001778 | 14.03349488        | 0.00040465 | 60.87852286        | 0.00920568 | 58.04663613        | 0.20961139 | 27.91803823        | 4.77073318  | 1.00000000         |
| 0.00001893 | 14.92104870        | 0.00043076 | 60.87046249        | 0.00980366 | 57.86133982        | 0.22313016 | 26.89975990        | 4.252108200 | 1.03030000         |
| 0.00002015 | 15.86223024        | 0.00045822 | 60.86186565        | 0.01043594 | 57.66549952        | 0.23752082 | 25.88331818        |             |                    |
| 0.00002145 | 16.85975340        | 0.00048810 | 60.85269657        | 0.01110900 | 57.45862486        | 0.25283960 | 24.86766049        |             |                    |
| 0.00002283 | 17.91635240        | 0.00051957 | 60.84291715        | 0.01182547 | 57.24023787        | 0.26914635 | 23.85323135        |             |                    |
| 0.00002430 | 19.03675308        | 0.00055308 | 60.83248670        | 0.01258814 | 57.00963077        | 0.28650480 | 22.84052565        |             |                    |
| 0.00002587 | 20.21763358        | 0.00058876 | 60.82136182        | 0.01340001 | 56.76688705        | 0.30498277 | 21.83082171        |             |                    |
| 0.00002754 | 21.46757523        | 0.00062673 | 60.80949623        | 0.01426423 | 56.51087766        | 0.32465247 | 20.82704247        |             |                    |
| 0.00002931 | 22.78700087        | 0.00066715 | 60.79684055        | 0.01518420 | 56.24126217        | 0.34559075 | 19.83395556        |             |                    |
| 0.00003120 | 24.17809775        | 0.00071017 | 60.78334211        | 0.01616349 | 55.95749084        | 0.36787944 | 18.85697402        |             |                    |
| 0.00003322 | 25.64272177        | 0.00075598 | 60.76894475        | 0.01720555 | 55.65910818        | 0.39160563 | 17.89985193        |             |                    |
| 0.00003536 | 27.18227906        | 0.00080473 | 60.75359856        | 0.01831564 | 55.34525816        | 0.41686202 | 16.96276945        |             |                    |
| 0.00003764 | 28.79758024        | 0.00085863 | 60.73720968        | 0.01949490 | 55.01569158        | 0.44374731 | 16.04314808        |             |                    |
| 0.00004007 | 30.48866144        | 0.00091888 | 60.71974000        | 0.02075434 | 54.66977523        | 0.47236655 | 15.13817579        |             |                    |
| 0.00004265 | 32.25456554        | 0.00097669 | 60.70110495        | 0.02209288 | 54.30700454        | 0.50283158 | 14.24712879        |             |                    |
| 0.00004540 | 34.09307743        | 0.00103330 | 60.68123315        | 0.02351775 | 53.92691264        | 0.53526143 | 13.37202542        |             |                    |
| 0.00004833 | 36.00039746        | 0.00109594 | 60.66003617        | 0.02503451 | 53.52908353        | 0.56978282 | 12.51690234        |             |                    |
| 0.00005144 | 37.97075541        | 0.00117088 | 60.63742817        | 0.02664510 | 53.11315655        | 0.60653066 | 11.68674650        |             |                    |
| 0.00005476 | 39.99594257        | 0.00124639 | 60.61331543        | 0.02836782 | 52.67882588        | 0.64564853 | 10.88626242        |             |                    |
| 0.00005829 | 42.06475656        | 0.00132678 | 60.58759885        | 0.03015738 | 52.22582793        | 0.68728928 | 10.11929302        |             |                    |
| 0.00006205 | 44.16235760        | 0.00141235 | 60.56017213        | 0.03214495 | 51.75169263        | 0.73161563 | 9.38850230         |             |                    |
| 0.00006606 | 46.26953546        | 0.00150344 | 60.53092238        | 0.03427182 | 51.26275431        | 0.77880078 | 8.69560901         |             |                    |
| 0.00007032 | 48.36192265        | 0.00160040 | 60.49972576        | 0.03644250 | 50.75206194        | 0.82902912 | 8.04183270         |             |                    |
| 0.00007485 | 50.44023953        | 0.00170362 | 60.46646678        | 0.03877421 | 50.22137415        | 0.88249690 | 7.42621706         |             |                    |
| 0.00007968 | 52.57476784        | 0.00181349 | 60.43095756        | 0.04127493 | 49.67014472        | 0.93941306 | 6.85579732         |             |                    |
| 0.00008482 | 54.71548229        | 0.00193045 | 60.39317946        | 0.04393693 | 49.09773986        | 1.00000000 | 6.32511463         |             |                    |
| 0.00009029 | 56.88361845        | 0.00205496 | 60.35285867        | 0.04677627 | 48.50348057        | 1.06449446 | 5.83565701         |             |                    |
| 0.00009611 | 57.33097504        | 0.00218749 | 60.30987371        | 0.04978707 | 47.88669736        | 1.13314845 | 5.38537535         |             |                    |
| 0.00010231 | 58.51732278        | 0.00232857 | 60.26405310        | 0.05295806 | 47.24679874        | 1.20623025 | 4.97090773         |             |                    |
| 0.00010891 | 59.42260466        | 0.00247875 | 60.21521528        | 0.05641614 | 46.58326442        | 1.28402542 | 4.58832680         |             |                    |
| 0.00011593 | 60.05783057        | 0.00263862 | 60.16316682        | 0.06005467 | 45.89577493        | 1.36683794 | 4.23388518         |             |                    |
| 0.00012341 | 60.46535041        | 0.00280879 | 60.10770899        | 0.06392786 | 45.18411538        | 1.45499141 | 3.90451911         |             |                    |
| 0.00013137 | 60.70487344        | 0.00298995 | 60.04862341        | 0.06805085 | 44.44821813        | 1.54883030 | 3.59783689         |             |                    |
| 0.00013984 | 60.83458558        | 0.00318278 | 59.98568567        | 0.07243976 | 43.68813278        | 1.64872127 | 3.31199876         |             |                    |
| 0.00014886 | 60.89940973        | 0.00339803 | 59.91865758        | 0.07711172 | 42.90401213        | 1.75505466 | 3.04547704         |             |                    |
| 0.00015846 | 60.92890884        | 0.00360656 | 59.84729030        | 0.08208500 | 42.09611632        | 1.86824596 | 2.79696965         |             |                    |
| 0.00016868 | 60.94044931        | 0.00383917 | 59.77132004        | 0.08737903 | 41.26484155        | 1.98873747 | 2.5542613          |             |                    |
| 0.00017956 | 60.94337599        | 0.00409477 | 59.69047186        | 0.09307449 | 40.41079511        | 2.11700002 | 2.35015805         |             |                    |
| 0.00019114 | 60.94235507        | 0.00435035 | 59.60445750        | 0.09901341 | 39.53484362        | 2.25333479 | 2.15102523         |             |                    |
| 0.00020347 | 60.93955347        | 0.00463092 | 59.51297563        | 0.10534922 | 38.63941779        | 2.39887529 | 1.96848965         |             |                    |
| 0.00021659 | 60.93590429        | 0.00492959 | 59.41571186        | 0.11219689 | 37.72314781        | 2.55358946 | 1.80353568         |             |                    |
| 0.00023056 | 60.93177506        | 0.00524752 | 59.31233863        | 0.11943297 | 36.79114923        | 2.71828183 | 1.65724377         |             |                    |
| 0.00024543 | 60.92729214        | 0.00558595 | 59.20251535        | 0.12713573 | 35.84443254        | 2.89359594 | 1.53012660         |             |                    |

SAMARIUM (4F)6 A = 150 CWA S-L EX 07-24-73  
 NUCLEAR CHARGE= 62.0 RADIUS= 5.7897 FERMI =.0001094 BOHR SURFACE THICKNESS=0.5666 FERMI =.0000107 BOHR  
 SLATER-LATTER EXCHANGE APPROXIMATION WITH MULTIPLIER 1.50

|       |    | ENERGY EIGENVALUES |                | RADIAL EXPECTATION VALUES (BOHR UNITS) |          |          |             |
|-------|----|--------------------|----------------|----------------------------------------|----------|----------|-------------|
| SHFL  | Q  | RYDBERGS           | ELFCTPON VOLTS | 1/(ROROR)                              | 1/R      | R        | ROROR       |
| 151/2 | 2  | 3.445354630 03     | 4.687508330 04 | 0.0                                    | 68.89750 | 0.022709 | 7.026960-04 |
| 251/2 | 2  | 5.661109030 02     | 7.702108660 03 | 0.0                                    | 16.41254 | 0.096174 | 1.097570-02 |
| 2P1/2 | 2  | 5.378856990 02     | 7.318096300 03 | 0.0                                    | 16.40896 | 0.080359 | 7.973590-03 |
| 2P3/2 | 4  | 4.929773660 02     | 6.707104960 03 | 8.990230 03                            | 14.61871 | 0.086577 | 9.208600-03 |
| 351/2 | 2  | 1.249509930 02     | 1.699995740 03 | 0.0                                    | 5.98388  | 0.253089 | 7.332070-02 |
| 3P1/2 | 2  | 1.125895820 02     | 1.531815040 03 | 0.0                                    | 5.90613  | 0.242388 | 6.851890-02 |
| 3P3/2 | 4  | 1.034293320 02     | 1.407187090 03 | 1.891580 03                            | 5.45336  | 0.255062 | 7.543420-02 |
| 451/2 | 4  | 8.175875620 01     | 1.112352410 03 | 3.175330 02                            | 5.33434  | 0.226421 | 6.037370-02 |
| 4D5/2 | 6  | 7.974978890 01     | 1.085019800 03 | 2.842470 02                            | 5.22038  | 0.230387 | 6.236990-02 |
| 4S1/2 | 2  | 2.518781850 01     | 3.426878270 02 | 0.0                                    | 2.49804  | 0.574654 | 3.728750-01 |
| 4P1/2 | 2  | 2.038489870 01     | 2.773426630 02 | 0.0                                    | 2.39574  | 0.587405 | 3.927310-01 |
| 4P3/2 | 4  | 1.836178870 01     | 2.498176440 02 | 4.186570 02                            | 2.24259  | 0.616110 | 4.317890-01 |
| 4D3/2 | 4  | 1.037609390 01     | 1.411658700 02 | 5.936890 01                            | 2.02819  | 0.655043 | 4.979090-01 |
| 4D5/2 | 6  | 1.000949530 01     | 1.361821870 02 | 5.246420 01                            | 1.99006  | 0.665231 | 5.133880-01 |
| 551/2 | 2  | 3.508263210 00     | 4.773097340 01 | 0.0                                    | 0.96243  | 1.385080 | 2.158020 00 |
| 5P1/2 | 2  | 2.188817340 00     | 2.977951660 01 | 0.0                                    | 0.84944  | 1.552786 | 2.737020 00 |
| 5P3/2 | 4  | 1.909763760 00     | 2.908290890 01 | 5.692360 01                            | 0.79459  | 1.644718 | 3.073130 00 |
| 4F5/2 | 6  | 6.697242150-01     | 9.111798860 00 | 7.116110 00                            | 1.45120  | 0.911287 | 1.098030 00 |
| 651/2 | 2  | 3.745866270-01     | 5.096366150 00 | 0.0                                    | 0.29552  | 4.305811 | 2.135180 01 |
| TOTAL | 62 | 2.083988970 04     | 2.835329520 05 |                                        |          |          |             |

| R          | POTOR       | R          | POTOR       | R          | POTOR       | R          | POTOR       | R           | POTOR      |
|------------|-------------|------------|-------------|------------|-------------|------------|-------------|-------------|------------|
| 0.00001148 | 9.15925257  | 0.00026126 | 61.92054579 | 0.00594622 | 60.03582417 | 0.13533528 | 35.33451959 | 3.08021685  | 1.39870353 |
| 0.00001222 | 9.74533808  | 0.00027811 | 61.91528116 | 0.00632972 | 59.90891754 | 0.14406366 | 34.36645280 | 3.27887377  | 1.30968440 |
| 0.00001301 | 10.36826650 | 0.00029404 | 61.90986387 | 0.00673795 | 59.77429307 | 0.15335497 | 33.34771831 | 3.49034296  | 1.23276419 |
| 0.00001385 | 11.03021808 | 0.00031514 | 61.90367154 | 0.00717251 | 59.63155248 | 0.16324551 | 32.33903083 | 3.71545074  | 1.16447299 |
| 0.00001474 | 11.73347056 | 0.00033546 | 61.89728079 | 0.00763509 | 59.48028499 | 0.17377394 | 31.32132814 | 3.95507672  | 1.10189952 |
| 0.00001569 | 12.48040122 | 0.00035710 | 61.89046392 | 0.00812752 | 59.32006741 | 0.18498140 | 30.29601135 | 4.21015726  | 1.04303813 |
| 0.00001670 | 13.27348110 | 0.00038013 | 61.88319301 | 0.00865170 | 59.15046419 | 0.19691168 | 29.26488468 | 4.48168907  | 1.00527212 |
| 0.00001778 | 14.11526926 | 0.00040465 | 61.87543782 | 0.00920968 | 58.97102739 | 0.20961139 | 28.22991696 | 4.77073318  | 1.00030000 |
| 0.00001893 | 15.00840375 | 0.00043074 | 61.86716609 | 0.00980366 | 58.78129656 | 0.22313016 | 27.19291070 | 42.32108200 | 1.00030000 |
| 0.00002015 | 15.95558902 | 0.00045852 | 61.85834341 | 0.01043594 | 58.58079855 | 0.23732082 | 26.15517729 |             |            |
| 0.00002145 | 16.95957872 | 0.00048810 | 61.84893306 | 0.01110900 | 58.36904725 | 0.25283960 | 25.11751089 |             |            |
| 0.00002283 | 18.02315315 | 0.00051957 | 61.83889586 | 0.01182547 | 58.14554337 | 0.26914435 | 24.08035845 |             |            |
| 0.00002430 | 19.14908922 | 0.00055308 | 61.82819003 | 0.01258814 | 57.90977427 | 0.28650480 | 23.04449864 |             |            |
| 0.00002587 | 20.34012578 | 0.00058876 | 61.81677099 | 0.01340001 | 57.66121414 | 0.30498277 | 22.01182500 |             |            |
| 0.00002754 | 21.59890978 | 0.00062673 | 61.80459118 | 0.01426423 | 57.39932452 | 0.32465247 | 20.98603008 |             |            |
| 0.00002931 | 22.92794203 | 0.00066715 | 61.79159988 | 0.01518420 | 57.12355577 | 0.34559075 | 19.97235603 |             |            |
| 0.00003120 | 24.32949889 | 0.00071017 | 61.77774300 | 0.01616349 | 56.83334949 | 0.36787944 | 18.97583035 |             |            |
| 0.00003322 | 25.80553924 | 0.00075598 | 61.76296283 | 0.01720595 | 56.52814252 | 0.39160563 | 17.99898820 |             |            |
| 0.00003536 | 27.35758863 | 0.00080473 | 61.74719786 | 0.01831564 | 56.20737280 | 0.41686202 | 17.04084814 |             |            |
| 0.00003764 | 28.98659639 | 0.00085663 | 61.73038249 | 0.01945690 | 55.87048731 | 0.44374731 | 16.09867342 |             |            |
| 0.00004007 | 30.69276038 | 0.00091188 | 61.71246678 | 0.02072434 | 55.51695213 | 0.47236655 | 15.17056975 |             |            |
| 0.00004265 | 32.47531240 | 0.00097069 | 61.69331620 | 0.02209288 | 55.14626380 | 0.50283158 | 14.25716864 |             |            |
| 0.00004540 | 34.33225669 | 0.00103330 | 61.67291130 | 0.02351775 | 54.75796106 | 0.53526143 | 13.36169961 |             |            |
| 0.00004833 | 36.26705242 | 0.00109694 | 61.65114745 | 0.02503451 | 54.35163358 | 0.56978282 | 12.48895324 |             |            |
| 0.00005144 | 38.25322993 | 0.00117088 | 61.62793449 | 0.02664610 | 53.92692789 | 0.60653066 | 11.64419813 |             |            |
| 0.00005476 | 40.30392999 | 0.00124639 | 61.60317640 | 0.02836782 | 53.48353727 | 0.64564853 | 10.83206100 |             |            |
| 0.00005829 | 42.40135549 | 0.00132678 | 61.57677099 | 0.03019738 | 53.02118802 | 0.68728928 | 10.05610527 |             |            |
| 0.00006205 | 44.53112986 | 0.00141235 | 61.54880947 | 0.03214495 | 52.53960618 | 0.73161563 | 9.31868965  |             |            |
| 0.00006606 | 46.67456030 | 0.00150344 | 61.51857614 | 0.03421812 | 52.03847932 | 0.77880078 | 8.62128245  |             |            |
| 0.00007032 | 48.80783691 | 0.00160040 | 61.48654797 | 0.03642500 | 51.51741940 | 0.82902912 | 7.96494275  |             |            |
| 0.00007485 | 50.90123347 | 0.00170362 | 61.45239419 | 0.03877421 | 50.97593347 | 0.88249690 | 7.35055182  |             |            |
| 0.00007968 | 52.91848806 | 0.00181249 | 61.41597592 | 0.04127493 | 50.41343249 | 0.93941306 | 6.77885812  |             |            |
| 0.00008482 | 54.81673676 | 0.00193045 | 61.37714570 | 0.04393693 | 49.82924662 | 1.00000000 | 6.24991921  |             |            |
| 0.00009029 | 56.54773543 | 0.00205496 | 61.33574713 | 0.04677062 | 49.22267867 | 1.06449446 | 5.76261138  |             |            |
| 0.00009611 | 58.06161677 | 0.00218749 | 61.29161438 | 0.04978707 | 48.59305603 | 1.13314845 | 5.31437591  |             |            |
| 0.00010231 | 59.31471783 | 0.00232857 | 61.24657180 | 0.05295806 | 47.93979249 | 1.20623025 | 4.90161852  |             |            |
| 0.00010891 | 60.28176433 | 0.00247875 | 61.19443351 | 0.05641614 | 47.26241587 | 1.28402542 | 4.52048226  |             |            |
| 0.00011593 | 60.96821312 | 0.00263862 | 61.14100254 | 0.06005467 | 46.56361415 | 1.36683794 | 4.16744843  |             |            |
| 0.00012341 | 61.41310589 | 0.00280879 | 61.08407249 | 0.06392786 | 45.83419311 | 1.45499141 | 3.83968226  |             |            |
| 0.00013137 | 61.67662754 | 0.00298995 | 61.02342310 | 0.06805085 | 45.08310540 | 1.54883030 | 3.53493155  |             |            |
| 0.00013984 | 61.82010654 | 0.00318278 | 60.95882389 | 0.07243976 | 44.30741114 | 1.64872127 | 3.25138801  |             |            |
| 0.00014886 | 61.89211421 | 0.00338805 | 60.89003188 | 0.07711172 | 43.50727175 | 1.75505466 | 2.98749065  |             |            |
| 0.00015846 | 61.92506291 | 0.00360656 | 60.81679165 | 0.08208500 | 42.68296345 | 1.86824596 | 2.74188259  |             |            |
| 0.00016868 | 61.93812376 | 0.00383917 | 60.73883509 | 0.08737503 | 41.83491665 | 1.98873747 | 2.51348548  |             |            |
| 0.00017956 | 61.94164743 | 0.00408677 | 60.65588121 | 0.09301449 | 40.96380245 | 2.11700002 | 2.30162685  |             |            |
| 0.00019114 | 61.94080849 | 0.00435035 | 60.56763594 | 0.09901341 | 40.07062345 | 2.25353479 | 2.10622118  |             |            |
| 0.00020347 | 61.93801266 | 0.00463092 | 60.47379207 | 0.10535522 | 39.15680713 | 2.39887529 | 1.92778745  |             |            |
| 0.00021659 | 61.93429688 | 0.00492959 | 60.37402919 | 0.11215689 | 38.22419645 | 2.55358946 | 1.76730170  |             |            |
| 0.00023056 | 61.93007025 | 0.00524752 | 60.26801363 | 0.11943297 | 37.27491977 | 2.71828183 | 1.62570304  |             |            |
| 0.00024543 | 61.92547452 | 0.00558595 | 60.15539858 | 0.12713573 | 36.31109896 | 2.89359594 | 1.50320521  |             |            |

EUROPIUM (4F17) A = 152 CNM  
 NUCLEAR CHARGE= 63.0 RADIUS= 5.8169 FERMI =.0001099 EOMR SURFACE THICKNESS=0.5666 FERMI =.0000107 BOMP  
 SLATER-LATTER EXCHANGE APPROXIMATION WITH MULTIPLIER 1.5C

| ENERGY EIGENVALUES |    |             |               | RACIAL EXPECTATION VALUES (RMP UNITS) |     |          |          |
|--------------------|----|-------------|---------------|---------------------------------------|-----|----------|----------|
| SHFL               | Q  | RYOBERGS    | FLCTPCN VOLTS | 1/(ROROR)                             | 1/R | R        | ROROR    |
| (151/2)            | 2  | 3.569723800 | 03            | 4.856716320                           | 04  | 0.0      | 70.30721 |
| (251/2)            | 2  | 5.893269530 | 07            | 8.017569990                           | 03  | 0.0      | 16.78128 |
| (2P1/2)            | 2  | 5.604203510 | 02            | 7.624686990                           | 03  | 0.0      | 16.77728 |
| (2P3/2)            | 4  | 5.121558240 | 02            | 6.968033630                           | 03  | 9.492820 | 14.88281 |
| (351/2)            | 2  | 1.305965230 | 02            | 1.776804870                           | 03  | 0.0      | 6.12655  |
| (3P1/2)            | 2  | 1.178907960 | 02            | 1.603939650                           | 03  | 0.0      | 6.04919  |
| (3P3/2)            | 4  | 1.079824520 | 02            | 1.469133660                           | 03  | 2.012300 | 5.56887  |
| (3D3/2)            | 4  | 8.575436710 | 01            | 1.166713890                           | 03  | 3.390120 | 5.45180  |
| (3D5/2)            | 6  | 8.357786290 | 01            | 1.137101900                           | 03  | 3.022530 | 5.23137  |
| (451/2)            | 2  | 2.628886130 | 01            | 3.576678450                           | 02  | 0.0      | 2.55992  |
| (4P1/2)            | 2  | 2.131584800 | 01            | 2.900085060                           | 02  | 0.0      | 2.45720  |
| (4P3/2)            | 4  | 1.911736260 | 01            | 2.600574530                           | 02  | 4.473380 | 2.29397  |
| (4D3/2)            | 4  | 1.086630520 | 01            | 1.475672360                           | 02  | 6.387260 | 2.07940  |
| (4D5/2)            | 6  | 1.044644960 | 01            | 1.421270800                           | 02  | 5.617840 | 2.03876  |
| (551/2)            | 2  | 3.617042280 | 00            | 4.921099980                           | 01  | 0.0      | 0.89252  |
| (5P1/2)            | 2  | 2.249661690 | 00            | 3.060732220                           | 01  | 0.0      | 0.86697  |
| (5P3/2)            | 4  | 1.949839790 | 00            | 2.652815530                           | 01  | 6.006300 | 1.80850  |
| (4F5/2)            | 1  | 7.009712270 | -01           | 9.536923840                           | 00  | 7.828190 | 0.55041  |
| (4F7/2)            | 1  | 6.490624100 | -01           | 8.870688800                           | 00  | 7.543750 | 0.48191  |
| (651/2)            | 2  | 3.794692280 | -01           | 5.162792680                           | 00  | 0.0      | 0.29932  |
| TOTAL              | 63 | 2.167441290 | 04            | 2.942268900                           | 05  |          |          |

| R          | POTR        | R          | POTR        | R          | POTR        | R           | POTR        | R           | POTR       |
|------------|-------------|------------|-------------|------------|-------------|-------------|-------------|-------------|------------|
| 0.00001148 | 9.26857529  | 0.00026126 | 62.91858483 | 0.00594622 | 60.98511785 | 0.13533528  | 35.77852877 | 3.08021685  | 1.37747515 |
| 0.00001222 | 9.86169871  | 0.00027811 | 62.91318578 | 0.00632572 | 60.85506941 | 0.14406366  | 34.77217762 | 3.27867377  | 1.29155845 |
| 0.00001301 | 10.49211670 | 0.00029604 | 62.90742469 | 0.00673795 | 60.71713365 | 0.15335497  | 33.75457317 | 3.49034296  | 1.21490026 |
| 0.00001385 | 11.16203687 | 0.00031514 | 62.90127902 | 0.00717251 | 60.57090567 | 0.16324551  | 32.72644818 | 3.71545074  | 1.15014551 |
| 0.00001474 | 11.87376845 | 0.00033546 | 62.89472355 | 0.00763509 | 60.41546793 | 0.17377394  | 31.68884890 | 3.95507672  | 1.03858370 |
| 0.00001569 | 12.62972041 | 0.00035710 | 62.88773165 | 0.00812752 | 60.25189031 | 0.18498140  | 30.64329806 | 4.21015726  | 0.93167969 |
| 0.00001670 | 13.43239746 | 0.00038013 | 62.88027243 | 0.00865170 | 60.07823008 | 0.19691165  | 29.59166362 | 4.48168907  | 1.00185656 |
| 0.00001778 | 14.28439578 | 0.00040465 | 62.87231665 | 0.00920968 | 59.89453150 | 0.20961139  | 28.53587195 | 4.77073318  | 1.00000000 |
| 0.00001893 | 15.18839038 | 0.00043074 | 62.86383058 | 0.00980366 | 59.70032755 | 0.22313016  | 27.47759174 | 42.52108200 | 1.00000000 |
| 0.00002015 | 16.14712633 | 0.00045852 | 62.85477885 | 0.01043594 | 59.49513583 | 0.23752082  | 26.41796147 |             |            |
| 0.00002145 | 17.16339981 | 0.00048810 | 62.84512377 | 0.01110900 | 59.27846216 | 0.25283960  | 25.35767570 |             |            |
| 0.00002283 | 18.24003593 | 0.00051957 | 62.83482510 | 0.01182547 | 59.04979844 | 0.26914635  | 24.29728205 |             |            |
| 0.00002430 | 19.37985941 | 0.00055308 | 62.82383993 | 0.01258814 | 58.80862288 | 0.28630460  | 23.23764034 |             |            |
| 0.00002587 | 20.58565666 | 0.00058876 | 62.81212247 | 0.01340001 | 58.55440031 | 0.30498277  | 22.18229248 |             |            |
| 0.00002754 | 21.86012930 | 0.00062673 | 62.79962388 | 0.01426423 | 58.28658291 | 0.32465247  | 21.13466241 |             |            |
| 0.00002931 | 23.20583146 | 0.00066715 | 62.78629208 | 0.01518420 | 58.00461150 | 0.34539075  | 20.10049689 |             |            |
| 0.00003120 | 24.62509452 | 0.00071017 | 62.77207153 | 0.01616349 | 57.70792043 | 0.36787944  | 19.08409533 |             |            |
| 0.00003322 | 26.11994277 | 0.00075598 | 62.75690256 | 0.01720595 | 57.39593864 | 0.39160563  | 18.08673207 |             |            |
| 0.00003536 | 27.69195726 | 0.00080473 | 62.74072322 | 0.01831564 | 57.06809715 | 0.416886202 | 17.10664396 |             |            |
| 0.00003764 | 29.34215284 | 0.00085663 | 62.72346456 | 0.01945690 | 56.72386157 | 0.44374731  | 16.14141138 |             |            |
| 0.00004007 | 31.07079254 | 0.00091188 | 62.70505637 | 0.02075434 | 56.36237001 | 0.47236655  | 15.19029915 |             |            |
| 0.00004265 | 32.87717455 | 0.00097069 | 62.68542095 | 0.02209288 | 55.98398260 | 0.50283158  | 14.25526312 |             |            |
| 0.00004540 | 34.75937004 | 0.00103330 | 62.66447715 | 0.02351775 | 55.58742208 | 0.53526143  | 13.34056689 |             |            |
| 0.00004833 | 36.71390473 | 0.00109994 | 62.64213811 | 0.02503451 | 55.17255141 | 0.56978282  | 12.45155220 |             |            |
| 0.00005144 | 38.73537375 | 0.00117088 | 62.61831130 | 0.02664910 | 54.73902018 | 0.60653066  | 11.59360144 |             |            |
| 0.00005476 | 40.81597901 | 0.00124639 | 62.59289821 | 0.02836782 | 54.28652178 | 0.64564853  | 10.77115897 |             |            |
| 0.00005829 | 42.94497757 | 0.00132678 | 62.56579399 | 0.03015738 | 53.81477172 | 0.68728928  | 9.98746248  |             |            |
| 0.00006205 | 45.10803647 | 0.00141235 | 62.53688870 | 0.03214495 | 53.32347332 | 0.73161563  | 9.24456082  |             |            |
| 0.00006606 | 47.28648624 | 0.00150344 | 62.50605877 | 0.03421812 | 52.81227864 | 0.77880078  | 8.54368070  |             |            |
| 0.00007032 | 49.45650903 | 0.00160040 | 62.47318294 | 0.03642500 | 52.28075349 | 0.82902912  | 7.88571123  |             |            |
| 0.00007485 | 51.58831570 | 0.00170362 | 62.43812533 | 0.03877421 | 51.72835967 | 0.88249690  | 7.27133111  |             |            |
| 0.00007968 | 53.64549621 | 0.00181349 | 62.40074420 | 0.04127493 | 51.15446222 | 0.93941306  | 6.70094493  |             |            |
| 0.00008482 | 55.58483201 | 0.00193045 | 62.36088786 | 0.04393693 | 50.55836189 | 1.00000000  | 6.17410227  |             |            |
| 0.00009029 | 57.35749786 | 0.00205496 | 62.31839628 | 0.04677662 | 49.93934733 | 1.06449446  | 5.68911882  |             |            |
| 0.00009611 | 58.91254395 | 0.00218749 | 62.27309963 | 0.04978707 | 49.29675074 | 1.13314845  | 5.24303938  |             |            |
| 0.00010231 | 60.20460332 | 0.00232857 | 62.22481811 | 0.05295806 | 48.63000013 | 1.20623025  | 4.83214805  |             |            |
| 0.00010891 | 61.20612634 | 0.00247875 | 62.17336146 | 0.05641414 | 47.93865058 | 1.28402542  | 4.45270869  |             |            |
| 0.00011593 | 61.92031871 | 0.00263862 | 62.11852858 | 0.06005467 | 47.22240314 | 1.36683794  | 4.10141724  |             |            |
| 0.00012341 | 62.38511461 | 0.00280879 | 62.06010714 | 0.06392786 | 46.48109415 | 1.45499141  | 3.77561783  |             |            |
| 0.00013137 | 62.66130174 | 0.00298995 | 61.99787320 | 0.06805685 | 45.71468582 | 1.54883030  | 3.47314625  |             |            |
| 0.00013984 | 62.81200550 | 0.00318278 | 61.93159082 | 0.07243976 | 44.92324663 | 1.64872127  | 3.19219121  |             |            |
| 0.00014886 | 62.88776060 | 0.00338805 | 61.86101179 | 0.07711172 | 44.10694679 | 1.75505466  | 2.93114569  |             |            |
| 0.00015846 | 62.92248909 | 0.00360656 | 61.78587532 | 0.08202900 | 43.26608200 | 1.86824596  | 2.68860365  |             |            |
| 0.00016868 | 62.93631081 | 0.00383917 | 61.70590778 | 0.08737903 | 42.40112353 | 1.98873747  | 2.46347352  |             |            |
| 0.00017956 | 62.94010747 | 0.00408677 | 61.62082251 | 0.09301449 | 41.51281443 | 2.11760002  | 2.25511480  |             |            |
| 0.00019114 | 62.93932084 | 0.00435033 | 61.53031970 | 0.09901341 | 40.60225868 | 2.25353479  | 2.06350424  |             |            |
| 0.00020347 | 62.93648178 | 0.00463392 | 61.43408623 | 0.10539522 | 39.67099562 | 2.39887529  | 1.88921056  |             |            |
| 0.00021659 | 62.93268143 | 0.00492959 | 61.33179567 | 0.11219689 | 38.72095042 | 2.55358946  | 1.73317718  |             |            |
| 0.00023056 | 62.92835062 | 0.00524752 | 61.22310829 | 0.11943297 | 37.75425134 | 2.71828183  | 1.59617103  |             |            |
| 0.00024543 | 62.92363993 | 0.00558595 | 61.10767107 | 0.12713573 | 36.77291308 | 2.89359594  | 1.47809096  |             |            |

GADOLINIUM (4F7/5C) A = 157 CMW S-L FX 07-24-73  
 NUCLEAR CHARGE = 64.0 RADIUS = 5.9838 FERMI = 0.0001112 BOHR SURFACE THICKNESS = 0.5666 FERMI = 0.0000107 BOHR  
 SLATER-LATTER EXCHANGE APPROXIMATION WITH MULTIPLIER 1.50

| ENERGY EIGENVALUES |    |                | RADIAL EXPECTATION VALUES (BOHR UNITS) |             |          |          |             |             |          |
|--------------------|----|----------------|----------------------------------------|-------------|----------|----------|-------------|-------------|----------|
| SHELL              | Q  | RYDBERGS       | ELFTREN VOLTS                          | 1/(R+R0)    | 1/R      | R        | R0          | R0+R        | RMAX     |
| (1S1/2)            | 2  | 3.697252480 03 | 5.030222920 04                         | 0.0         | 71.73426 | 0.071876 | 6.529490-04 | 1.133890-06 | 0.013910 |
| (2S1/2)            | 2  | 6.136979480 02 | 8.349544700 03                         | 0.0         | 17.15482 | 0.092453 | 1.015010-02 | 1.784340-04 | 0.079039 |
| (2P1/2)            | 2  | 5.840921340 02 | 7.946748710 03                         | 0.0         | 17.15046 | 0.077112 | 7.350160-03 | 1.098280-04 | 0.059636 |
| (2P3/2)            | 4  | 5.322771180 02 | 7.241789870 03                         | 1.001440 04 | 15.14697 | 0.093946 | 8.577260-03 | 1.443370-04 | 0.065438 |
| (3S1/2)            | 2  | 1.370369910 02 | 1.864421210 03                         | 0.0         | 6.27024  | 0.242447 | 6.740770-02 | 6.871230-03 | 0.223917 |
| (3P1/2)            | 2  | 1.239787440 02 | 1.686768010 03                         | 0.0         | 6.19312  | 0.231979 | 6.259580-02 | 6.298680-03 | 0.210802 |
| (3P3/2)            | 4  | 1.132773050 02 | 1.541171720 03                         | 2.138660 03 | 5.68406  | 0.244963 | 6.958320-02 | 7.615540-03 | 0.223117 |
| (3D3/2)            | 4  | 9.047938920 01 | 1.730999730 03                         | 3.613680 02 | 5.56854  | 0.216766 | 5.529710-02 | 5.459120-03 | 0.176711 |
| (3D5/2)            | 6  | 8.812640090 01 | 1.198986120 03                         | 3.709420 02 | 5.44144  | 0.220820 | 5.724890-02 | 5.816880-03 | 0.180090 |
| (4S1/2)            | 2  | 2.802313830 01 | 3.812632040 02                         | 0.0         | 2.62680  | 0.548621 | 3.398590-01 | 1.678380-01 | 0.513426 |
| (4P1/2)            | 2  | 2.287138630 01 | 3.111720720 02                         | 0.0         | 2.52453  | 0.559288 | 3.560270-01 | 1.893290-01 | 0.516511 |
| (4P3/2)            | 4  | 2.047409840 01 | 2.785562510 02                         | 4.800030 02 | 2.35138  | 0.588487 | 3.938920-01 | 2.317050-01 | 0.543114 |
| (4D3/2)            | 4  | 1.189712810 01 | 1.618667180 02                         | 6.922660 01 | 2.13998  | 0.620905 | 4.470510-01 | 3.238620-01 | 0.548471 |
| (4D5/2)            | 6  | 1.145773270 01 | 1.558858910 02                         | 6.065870 01 | 2.09709  | 0.631138 | 4.617630-01 | 3.456320-01 | 0.556990 |
| (5S1/2)            | 2  | 0.011653100 00 | 5.457574390 01                         | 0.0         | 1.02195  | 1.309797 | 1.925640 00 | 5.474690 00 | 1.181720 |
| (5P1/2)            | 2  | 2.554551050 00 | 3.475543330 01                         | 0.0         | 0.90827  | 1.456800 | 2.406370 00 | 8.923770 00 | 1.281287 |
| (5P3/2)            | 4  | 2.210396040 00 | 3.007310130 01                         | 6.792380 01 | 0.84608  | 1.547919 | 2.718840 00 | 1.145690 01 | 1.355484 |
| (4F5/2)            | 6  | 1.226163820 00 | 1.668232670 01                         | 9.142570 00 | 1.60304  | 0.805003 | 8.307220-01 | 1.782550 00 | 0.550844 |
| (4F7/2)            | 1  | 1.163647320 00 | 1.583170290 01                         | 8.824280 00 | 1.58525  | 0.815053 | 8.532920-01 | 1.898130 00 | 0.555613 |
| (6S1/2)            | 2  | 4.184133930-01 | 5.692639730 00                         | 0.0         | 0.32222  | 3.960713 | 1.806120 01 | 5.428830 02 | 3.245762 |
| (5D3/2)            | 1  | 3.773116430-01 | 5.133438100 00                         | 4.204490 00 | 0.53533  | 2.492779 | 7.638180 00 | 1.294000 02 | 1.815138 |
| TOTAL              | 64 | 2.252956600 04 | 3.065215040 05                         |             |          |          |             |             |          |

| R          | POT-R       | R           | POT-R        | R           | POT-R       | R          | POT-R       | R           | POT-R      |
|------------|-------------|-------------|--------------|-------------|-------------|------------|-------------|-------------|------------|
| 0.00001148 | 9.32097646  | 0.000026126 | 63.91666841  | 0.00594622  | 61.93531660 | 0.13533528 | 36.25879485 | 3.08021685  | 1.41199471 |
| 0.00001222 | 9.91755603  | 0.00027811  | 63.91113777  | 0.00632972  | 61.80219466 | 0.14406366 | 35.23688532 | 3.27887377  | 1.32085755 |
| 0.00001301 | 10.55166886 | 0.00029604  | 63.90523574  | 0.00673795  | 61.66102158 | 0.15335497 | 34.20335023 | 3.49034296  | 1.23857505 |
| 0.00001385 | 11.22554121 | 0.00031514  | 63.89893932  | 0.00717251  | 61.51138628 | 0.16324551 | 33.15898974 | 3.71545074  | 1.16268221 |
| 0.00001474 | 11.94150284 | 0.00033566  | 63.89272266  | 0.00763509  | 61.35286451 | 0.17377394 | 32.10498469 | 3.95507672  | 1.09140258 |
| 0.00001569 | 12.70198538 | 0.00035710  | 63.88505783  | 0.00812752  | 61.18502066 | 0.18498140 | 31.04297658 | 4.21015726  | 1.02776412 |
| 0.00001670 | 13.50951896 | 0.00038013  | 63.87741499  | 0.00865170  | 61.00740474 | 0.19691168 | 29.97487351 | 4.48168907  | 1.00042534 |
| 0.00001778 | 14.36672656 | 0.00040465  | 63.86926229  | 0.00920568  | 60.81955476 | 0.20961139 | 28.90252873 | 4.77073318  | 1.00030000 |
| 0.00001893 | 15.27631542 | 0.00043074  | 63.86051572  | 0.00980166  | 60.62099401 | 0.22313016 | 27.82745794 | 42.52108200 | 1.02000000 |
| 0.00002015 | 16.24106564 | 0.00045852  | 63.85128903  | 0.01043594  | 60.41123523 | 0.23752082 | 26.75063716 |             |            |
| 0.00002145 | 17.26381077 | 0.00048810  | 63.84139352  | 0.01110900  | 60.18977551 | 0.25283960 | 25.67271583 |             |            |
| 0.00002283 | 18.34742172 | 0.00051957  | 63.83083792  | 0.01182547  | 59.95609857 | 0.26914635 | 24.59444477 |             |            |
| 0.00002430 | 19.49477273 | 0.00055308  | 63.81957820  | 0.01258814  | 59.70967422 | 0.28650480 | 23.51752886 |             |            |
| 0.00002587 | 20.70870723 | 0.00058876  | 63.80756738  | 0.01340001  | 59.44995875 | 0.30498277 | 22.44531142 |             |            |
| 0.00002754 | 21.99199088 | 0.00062673  | 63.79475536  | 0.01424423  | 59.17639551 | 0.32465247 | 21.38277822 |             |            |
| 0.00002931 | 23.34725265 | 0.00066715  | 63.78109872  | 0.01518420  | 58.88941866 | 0.34559075 | 20.33325695 |             |            |
| 0.00003120 | 24.77691116 | 0.00071017  | 63.76651047  | 0.01616349  | 58.58545389 | 0.36787944 | 19.30604445 |             |            |
| 0.00003322 | 26.28708299 | 0.00075598  | 63.75099583  | 0.01720595  | 58.26692452 | 0.39160563 | 18.29518843 |             |            |
| 0.00003536 | 27.86746856 | 0.00080473  | 63.73437267  | 0.01831564  | 57.93225954 | 0.41686202 | 17.30046778 |             |            |
| 0.00003764 | 29.53121394 | 0.00085663  | 63.71667795  | 0.01945690  | 57.58090158 | 0.44374731 | 16.32006515 |             |            |
| 0.00004007 | 31.27473453 | 0.00091188  | 63.69780400  | 0.02075434  | 57.21231813 | 0.47236655 | 15.35443770 |             |            |
| 0.00004265 | 33.09750781 | 0.00097069  | 63.67767171  | 0.02220928  | 56.82601297 | 0.50283158 | 14.40666220 |             |            |
| 0.00004540 | 34.99781394 | 0.00103320  | 63.65615746  | 0.02351775  | 56.42153660 | 0.53526143 | 13.48169752 |             |            |
| 0.00004833 | 36.97242259 | 0.00109594  | 63.63329220  | 0.02503451  | 55.99849206 | 0.56578282 | 12.58504495 |             |            |
| 0.00005144 | 39.01621384 | 0.00117088  | 63.60886109  | 0.02664510  | 55.55653343 | 0.60853066 | 11.72181146 |             |            |
| 0.00005476 | 41.12172150 | 0.00124639  | 63.58280314  | 0.02836782  | 55.09535217 | 0.64564853 | 10.89591691 |             |            |
| 0.00005829 | 43.27858782 | 0.00132674  | 63.55501091  | 0.03015738  | 54.61465176 | 0.68728928 | 10.11001585 |             |            |
| 0.00006205 | 45.47292045 | 0.00141235  | 63.52537006  | 0.03214495  | 54.11411104 | 0.73161563 | 9.36570570  |             |            |
| 0.00006606 | 47.86654964 | 0.00150344  | 63.49375904  | 0.03421812  | 53.59334569 | 0.77880078 | 8.66395561  |             |            |
| 0.00007032 | 49.85620172 | 0.00160040  | 63.46004862  | 0.03642500  | 53.05187758 | 0.82902912 | 8.00557181  |             |            |
| 0.00007485 | 52.07264560 | 0.00170362  | 63.42410155  | 0.03877421  | 52.48912426 | 0.88249690 | 7.39115387  |             |            |
| 0.00007968 | 54.17995599 | 0.00181349  | 63.38577207  | 0.04127493  | 51.90441446 | 0.93441306 | 6.82083728  |             |            |
| 0.00008482 | 56.17521529 | 0.00193045  | 63.34490557  | 0.04393493  | 51.29702689 | 1.00000000 | 6.29363186  |             |            |
| 0.00009029 | 58.00931024 | 0.00205496  | 63.30133807  | 0.04677667  | 50.66524540 | 1.06449446 | 5.80716812  |             |            |
| 0.00009611 | 59.61000919 | 0.00218749  | 63.25489988  | 0.04977670  | 50.01141326 | 1.13314845 | 5.35795209  |             |            |
| 0.00010231 | 60.98998977 | 0.00232857  | 63.20539509  | 0.05295406  | 49.33198105 | 1.20623025 | 4.94205914  |             |            |
| 0.00010891 | 62.05381244 | 0.00247875  | 63.15264123  | 0.05641014  | 48.62753720 | 1.28402542 | 4.55588845  |             |            |
| 0.00011593 | 62.82189259 | 0.00263862  | 63.09642878  | 0.060005467 | 47.89779359 | 1.36683794 | 4.19647358  |             |            |
| 0.00012341 | 63.32704486 | 0.00280879  | 63.03654085  | 0.06392786  | 47.14262682 | 1.45499141 | 3.86156662  |             |            |
| 0.00013137 | 63.62969735 | 0.00298595  | 62.97274876  | 0.068005085 | 46.36200949 | 1.54883030 | 3.54941799  |             |            |
| 0.00013984 | 63.79579923 | 0.00318278  | 62.90481169  | 0.07243576  | 45.55602484 | 1.64872127 | 3.25863776  |             |            |
| 0.00014886 | 63.87965847 | 0.00338805  | 62.83247641  | 0.07711172  | 44.72486124 | 1.75505466 | 2.98809656  |             |            |
| 0.00015846 | 63.91929873 | 0.00360656  | 62.75547655  | 0.08208500  | 43.86884771 | 1.86824596 | 2.73694304  |             |            |
| 0.00016868 | 63.93385586 | 0.00383917  | 62.67353440  | 0.08737903  | 42.99851431 | 1.98873747 | 2.50471087  |             |            |
| 0.00017956 | 63.93834144 | 0.00408677  | 62.58635670  | 0.09301449  | 42.08469527 | 2.11700002 | 2.29135197  |             |            |
| 0.00019114 | 63.93777410 | 0.00435035  | 62.49363850  | 0.09901341  | 41.15861364 | 2.25353479 | 2.09721529  |             |            |
| 0.00020347 | 63.93495523 | 0.00463092  | 62.399536109 | 0.10551522  | 40.21192542 | 2.39887529 | 1.92276891  |             |            |
| 0.00021659 | 63.93109379 | 0.00492459  | 62.29029237  | 0.11219689  | 39.24662865 | 2.55358946 | 1.76817649  |             |            |
| 0.00023056 | 63.92666756 | 0.00524752  | 62.17898681  | 0.11942297  | 38.26463002 | 2.71828183 | 1.63280432  |             |            |
| 0.00024543 | 63.92184477 | 0.00559595  | 62.06078558  | 0.12713573  | 37.26941721 | 2.89359594 | 1.51495102  |             |            |

TERMIUM (4519) A = 159 CWN S-L EX 07-24-73  
 NUCLEAR CHARGE = 65.0 RADIUS = 5.9102 FERMI = 0.000117 BOHR SURFACE THICKNESS = 0.5666 FERMI = 0.000107 BOHR  
 SLATER-LATYER EXCHANGE APPROXIMATION WITH MULTIPLIER 1.50

| SHELL Q |    | ENERGY EIGENVALUES |     | RACIAL EXPECTATION VALUES (BOHR UNITS) |    | RMAX      |          |
|---------|----|--------------------|-----|----------------------------------------|----|-----------|----------|
|         |    | RYDBERGS           |     | ELECTRON VOLTS                         |    | 1/(RERRR) |          |
|         |    |                    |     |                                        |    |           |          |
| (151/2) | 2  | 3.826372650        | 03  | 5.205894780                            | C4 | 0.0       | 73.18024 |
| (251/2) | 2  | 6.374747510        | 02  | 8.673035240                            | 03 | 0.0       | 17.53557 |
| (2P1/2) | 2  | 6.071828730        | 02  | 8.260905140                            | C3 | 0.0       | 17.53062 |
| (2P3/2) | 4  | 5.515991530        | 02  | 7.504671960                            | 03 | 1.055E7D  | 04       |
| (351/2) | 2  | 1.422931650        | 02  | 1.935941200                            | 03 | 0.0       | 6.41686  |
| (3P1/2) | 2  | 1.288864400        | 02  | 1.753538680                            | 03 | 0.0       | 6.34019  |
| (3P3/2) | 4  | 1.173361280        | 02  | 1.596393220                            | 03 | 2.27063D  | 03       |
| (3D3/2) | 4  | 9.398115740        | 01  | 1.278641840                            | C3 | 3.85146E  | 02       |
| (3D5/2) | 6  | 9.143832780        | 01  | 1.244045880                            | C3 | 3.40E57D  | C2       |
| (451/2) | 2  | 2.855205180        | 01  | 3.884552300                            | 02 | 0.0       | 2.68467  |
| (4P1/2) | 2  | 2.323057230        | 01  | 3.160589050                            | 02 | 0.0       | 2.58105  |
| (4P3/2) | 4  | 2.064714060        | 01  | 2.809105420                            | 02 | 5.08575D  | C2       |
| (4D3/2) | 4  | 1.179432490        | 01  | 1.604653290                            | 02 | 7.35381E  | 01       |
| (4D5/2) | 6  | 1.132177040        | 01  | 1.540360820                            | 02 | 6.40530D  | 01       |
| (551/2) | 2  | 3.836149940        | 00  | 5.219197080                            | 01 | 0.0       | 1.02245  |
| (5P1/2) | 2  | 3.225627000        | 00  | 3.225627000                            | C1 | 0.0       | 0.90170  |
| (5P3/2) | 4  | 2.026497940        | 00  | 2.757111240                            | 01 | 6.65653C  | 01       |
| (4F5/2) | 6  | 7.497676040        | -01 | 1.020081320                            | 01 | 9.34717D  | 00       |
| (4F7/2) | 3  | 6.847172970        | -01 | 9.515764240                            | 00 | 8.57572D  | 00       |
| (651/2) | 2  | 3.891197410        | -01 | 5.294090810                            | 00 | 0.0       | 0.30681  |
| TOTAL   | 65 | 2.340616490        | 04  | 3.184478950                            | C5 |           |          |

| R          |             | POT#R      |             | R          |             | POT#R      |             | R           |            | POT#R |  | R |  | POT#R |  |
|------------|-------------|------------|-------------|------------|-------------|------------|-------------|-------------|------------|-------|--|---|--|-------|--|
| 0.00001148 | 9.42919912  | 0.00026126 | 64.91459243 | 0.00594622 | 62.88169079 | 0.13533528 | 36.64939534 | 3.00021685  | 1.33905305 |       |  |   |  |       |  |
| 0.00001222 | 10.03274541 | 0.00027811 | 64.90891922 | 0.00632972 | 62.74525771 | 0.14406366 | 35.60514085 | 3.27887377  | 1.25848859 |       |  |   |  |       |  |
| 0.00001301 | 10.67427158 | 0.00029604 | 64.90286466 | 0.00673795 | 62.60059538 | 0.15335497 | 34.54838435 | 3.49034296  | 1.18763414 |       |  |   |  |       |  |
| 0.00001385 | 11.35603216 | 0.00031514 | 64.89640516 | 0.00717251 | 62.44728567 | 0.16324551 | 33.47998831 | 3.71545074  | 1.12342849 |       |  |   |  |       |  |
| 0.00001474 | 12.08038691 | 0.00033546 | 64.88951415 | 0.00763509 | 62.28489743 | 0.17377394 | 32.40124203 | 3.95507672  | 1.06356060 |       |  |   |  |       |  |
| 0.00001569 | 12.84798999 | 0.00035710 | 64.88216297 | 0.00812152 | 62.11298652 | 0.18498140 | 31.31386548 | 4.21015726  | 1.01475831 |       |  |   |  |       |  |
| 0.00001670 | 13.66683247 | 0.00038013 | 64.87412097 | 0.00865170 | 61.93109571 | 0.19691168 | 30.21976996 | 4.48168907  | 1.00000000 |       |  |   |  |       |  |
| 0.00001778 | 14.53414566 | 0.00040465 | 64.86595540 | 0.00920968 | 61.73875457 | 0.20961139 | 29.12072124 | 4.752108200 | 1.03030000 |       |  |   |  |       |  |
| 0.00001893 | 15.45448363 | 0.00043074 | 64.85703135 | 0.00980366 | 61.53547915 | 0.22313016 | 28.01810569 |             |            |       |  |   |  |       |  |
| 0.00002015 | 16.43066561 | 0.00045852 | 64.84751158 | 0.01043594 | 61.32077113 | 0.23752082 | 26.91280729 |             |            |       |  |   |  |       |  |
| 0.00002145 | 17.46556890 | 0.00048810 | 64.83735633 | 0.01110500 | 61.09412051 | 0.25283960 | 25.80553654 |             |            |       |  |   |  |       |  |
| 0.00002283 | 18.56210702 | 0.00051957 | 64.82652321 | 0.01182547 | 60.85499942 | 0.26914635 | 24.69735732 |             |            |       |  |   |  |       |  |
| 0.00002430 | 19.72320130 | 0.00055308 | 64.81496699 | 0.01258814 | 60.60286815 | 0.28650480 | 23.59053814 |             |            |       |  |   |  |       |  |
| 0.00002587 | 20.95174428 | 0.00058876 | 64.80263942 | 0.01340001 | 60.33717269 | 0.30498277 | 22.48905376 |             |            |       |  |   |  |       |  |
| 0.00002754 | 22.25055278 | 0.00062671 | 64.78948905 | 0.01424423 | 60.05734653 | 0.32485247 | 21.39814765 |             |            |       |  |   |  |       |  |
| 0.00002931 | 23.62230981 | 0.00066715 | 64.77546100 | 0.01518420 | 59.76281304 | 0.34559075 | 20.32265770 |             |            |       |  |   |  |       |  |
| 0.00003120 | 25.06449009 | 0.00071017 | 64.76045674 | 0.01616349 | 59.45298914 | 0.36787944 | 19.26482793 |             |            |       |  |   |  |       |  |
| 0.00003322 | 26.59426861 | 0.00075598 | 64.74453387 | 0.01720595 | 59.12729097 | 0.39160563 | 18.22394593 |             |            |       |  |   |  |       |  |
| 0.00003536 | 28.19840677 | 0.00080473 | 64.72750584 | 0.01831564 | 58.78514144 | 0.41686202 | 17.19301199 |             |            |       |  |   |  |       |  |
| 0.00003764 | 29.88311154 | 0.00085663 | 64.70934173 | 0.01945690 | 58.42597983 | 0.44374731 | 16.18628896 |             |            |       |  |   |  |       |  |
| 0.00004007 | 31.64886474 | 0.00091188 | 64.68996594 | 0.02075434 | 58.04927299 | 0.47236655 | 15.19061969 |             |            |       |  |   |  |       |  |
| 0.00004265 | 33.44520754 | 0.00097069 | 64.66929793 | 0.02209288 | 57.65452642 | 0.50283158 | 14.21526694 |             |            |       |  |   |  |       |  |
| 0.00004540 | 35.42048614 | 0.00103320 | 64.64725186 | 0.02351775 | 57.24129377 | 0.53526143 | 13.26598609 |             |            |       |  |   |  |       |  |
| 0.00004833 | 37.42153557 | 0.00109994 | 64.62373632 | 0.02503451 | 56.80918045 | 0.56978282 | 12.34867748 |             |            |       |  |   |  |       |  |
| 0.00005144 | 39.49329956 | 0.00117088 | 64.59865358 | 0.02664910 | 56.35783900 | 0.60653066 | 11.46854790 |             |            |       |  |   |  |       |  |
| 0.00005476 | 41.62837208 | 0.00124639 | 64.57190123 | 0.02836782 | 55.88695168 | 0.64564853 | 10.62945655 |             |            |       |  |   |  |       |  |
| 0.00005829 | 43.81644937 | 0.00132678 | 64.54336782 | 0.03015738 | 55.39620162 | 0.68728928 | 9.83391566  |             |            |       |  |   |  |       |  |
| 0.00006205 | 46.04368271 | 0.00141235 | 64.51293649 | 0.03214495 | 54.88523468 | 0.73161563 | 9.08336268  |             |            |       |  |   |  |       |  |
| 0.00006606 | 48.29192893 | 0.00150344 | 64.48048754 | 0.03421812 | 54.35362249 | 0.77880078 | 8.37855339  |             |            |       |  |   |  |       |  |
| 0.00007032 | 50.53791280 | 0.00160040 | 64.44587349 | 0.03642500 | 53.80083699 | 0.82902912 | 7.71997840  |             |            |       |  |   |  |       |  |
| 0.00007485 | 52.75235410 | 0.00170362 | 64.40898862 | 0.03877421 | 53.22624745 | 0.88249690 | 7.10778744  |             |            |       |  |   |  |       |  |
| 0.00007968 | 54.89919651 | 0.00181349 | 64.36961856 | 0.04127493 | 52.62914365 | 0.93941306 | 6.54158047  |             |            |       |  |   |  |       |  |
| 0.00008482 | 56.93524789 | 0.00193045 | 64.32766485 | 0.04393493 | 52.00877986 | 1.00000000 | 6.01991851  |             |            |       |  |   |  |       |  |
| 0.00009029 | 58.81087042 | 0.00205496 | 64.28273956 | 0.04677662 | 51.36443165 | 1.06449446 | 5.54021444  |             |            |       |  |   |  |       |  |
| 0.00009611 | 60.47289341 | 0.00218749 | 64.23526478 | 0.04978707 | 50.69544759 | 1.13314845 | 5.09902676  |             |            |       |  |   |  |       |  |
| 0.00010231 | 61.87144781 | 0.00232857 | 64.18445225 | 0.05295806 | 50.00129227 | 1.20623025 | 4.69262209  |             |            |       |  |   |  |       |  |
| 0.00010891 | 62.97190230 | 0.00247875 | 64.13030293 | 0.05641614 | 49.28136561 | 1.28402542 | 4.31755434  |             |            |       |  |   |  |       |  |
| 0.00011593 | 63.76929949 | 0.00263862 | 64.07260658 | 0.06005467 | 48.53600842 | 1.36683794 | 3.97086055  |             |            |       |  |   |  |       |  |
| 0.00012341 | 64.29596557 | 0.00280879 | 64.01114137 | 0.06392786 | 47.76449844 | 1.45499141 | 3.65010142  |             |            |       |  |   |  |       |  |
| 0.00013137 | 64.61257279 | 0.00298995 | 63.94567351 | 0.06805085 | 46.96698510 | 1.54883030 | 3.35316961  |             |            |       |  |   |  |       |  |
| 0.00013984 | 64.78674107 | 0.00318278 | 63.87595693 | 0.07243576 | 46.14357954 | 1.64872127 | 3.07818425  |             |            |       |  |   |  |       |  |
| 0.00014886 | 64.87481877 | 0.00338805 | 63.80173254 | 0.07711172 | 45.29446317 | 1.75505466 | 2.82343755  |             |            |       |  |   |  |       |  |
| 0.00015846 | 64.91547125 | 0.00360656 | 63.72272998 | 0.08200500 | 44.41998407 | 1.86824596 | 2.58745676  |             |            |       |  |   |  |       |  |
| 0.00016868 | 64.93189513 | 0.00383917 | 63.63866338 | 0.08717503 | 43.52071650 | 1.98873747 | 2.36916892  |             |            |       |  |   |  |       |  |
| 0.00017956 | 64.93669589 | 0.00408677 | 63.54923518 | 0.09301449 | 42.59756845 | 2.11700002 | 2.16803476  |             |            |       |  |   |  |       |  |
| 0.00019114 | 64.93619478 | 0.00435035 | 63.45613403 | 0.09901341 | 41.65185272 | 2.25353479 | 1.98416197  |             |            |       |  |   |  |       |  |
| 0.00020347 | 64.93333337 | 0.00463092 | 63.35303505 | 0.10535522 | 40.68530356 | 2.39887529 | 1.81818232  |             |            |       |  |   |  |       |  |
| 0.00021659 | 64.92938360 | 0.00492939 | 63.24559485 | 0.11219689 | 39.69993589 | 2.55358946 | 1.67090040  |             |            |       |  |   |  |       |  |
| 0.00023056 | 64.92484773 | 0.00524752 | 63.13147653 | 0.11943297 | 38.69777382 | 2.71728183 | 1.54266626  |             |            |       |  |   |  |       |  |
| 0.00024543 | 64.91990171 | 0.00558595 | 63.01029975 | 0.12713573 | 37.68052900 | 2.89359594 | 1.43274330  |             |            |       |  |   |  |       |  |

MOLYBDEUM (4F111) A = 165 CWA  
 NUCLEAR CHARGE = 67.0 RADIUS = 5.6879 FERMI = 0.0001132 BOHR  
 SLATEP-LATTER EXCHANGE APPROXIMATION WITH MULTIPLIER 1.50 SURFACE THICKNESS = 0.5666 FERMI = 0.0009107 BOHR

| ENERGY EIGENVALUES |    |                |                | RADIAL EXPECTATION VALUES (BOHR UNITS) |          |          |             |             |
|--------------------|----|----------------|----------------|----------------------------------------|----------|----------|-------------|-------------|
| SHELL              | 0  | HYDROGENS      | ELECTRON VOLTS | 1/(R*P*P)                              | R        | P*P      | P*P*P       | PNAX        |
| (1S1/2)            | 2  | 4.09381973D 03 | 5.56976320D C4 | 0.0                                    | 76.12963 | 0.020711 | 5.86540D-04 | 9.19962D-07 |
| (2S1/2)            | 2  | 6.87982589 02  | 9.36030026D C3 | 0.0                                    | 18.31373 | 0.087264 | 7.05341D-03 | 0.074645    |
| (2P1/2)            | 2  | 6.56278597D 02 | 4.92866719D C3 | 0.0                                    | 18.39766 | 0.072586 | 6.52398D-03 | 0.056087    |
| (2P3/2)            | 4  | 5.92502396D 02 | 8.06117785D C3 | 1.171C6D 04                            | 15.54952 | 0.097475 | 7.73975D-03 | 1.17456D-04 |
| (3S1/2)            | 2  | 1.54559524D 02 | 2.10282869D C3 | 0.0                                    | 6.71624  | 0.228241 | 5.96689D-02 | 5.38230D-03 |
| (3P1/2)            | 2  | 1.40434304D 01 | 1.91065088D C3 | 0.0                                    | 6.63313  | 0.217665 | 5.51409D-02 | 4.81669D-03 |
| (3P3/2)            | 4  | 1.27031363D 02 | 1.72429380D C3 | 7.55279C 01                            | 6.03365  | 0.231141 | 6.19643D-02 | 6.03254D-03 |
| (4S3/2)            | 4  | 1.02533099D 02 | 1.39499537D C3 | 4.35726D 02                            | 5.52293  | 0.203626 | 4.87537D-02 | 4.23220D-03 |
| (3D5/2)            | 6  | 9.65794333D 01 | 1.35480806D 03 | 3.82161E 02                            | 5.77501  | 0.207820 | 5.06541D-02 | 4.59379D-03 |
| (4S1/2)            | 2  | 3.09087504D 01 | 4.20522822D 02 | 0.0                                    | 2.81116  | 0.155394 | 3.00111D-01 | 1.31115D-01 |
| (4P1/2)            | 2  | 2.52269703D 01 | 3.43220499D 02 | 0.0                                    | 2.70655  | 0.524115 | 3.12894D-01 | 1.46602D-01 |
| (4P3/2)            | 4  | 2.20880200D 01 | 1.07157414D 02 | 5.75334D 02                            | 2.49784  | 0.564940 | 3.05017D-01 | 1.88403D-01 |
| (4D3/2)            | 4  | 1.27585476D 01 | 1.73583868D 02 | 8.41479D 01                            | 2.28183  | 0.582967 | 3.94639E-01 | 2.54023E-01 |
| (4D5/2)            | 6  | 1.20244411D 01 | 1.66045082D 02 | 7.25552C 01                            | 3.23012  | 0.593884 | 4.09439D-01 | 2.73631D-01 |
| (5S1/2)            | 2  | 4.05979819D 00 | 5.52347723D 01 | 0.0                                    | 1.06240  | 1.257396 | 1.78073D 03 | 4.73595D 00 |
| (5P1/2)            | 2  | 2.49327563D 00 | 3.39217656D 01 | 0.0                                    | 0.97632  | 1.410709 | 2.26413D 00 | 1.84971D 00 |
| (5P3/2)            | 4  | 2.09969684D 00 | 2.85657265D 01 | 7.34272C 01                            | 0.86174  | 1.515398 | 2.61581D 00 | 1.09336D 00 |
| (4F5/2)            | 6  | 7.83451731D-01 | 1.06590998D 01 | 1.1003D 01                             | 1.18686  | 0.782839 | 6.12704D-01 | 2.01312D 00 |
| (4F7/2)            | 5  | 7.03354205D-01 | 9.6934496D 00  | 1.05295D 01                            | 1.66156  | 0.797726 | 4.84911D-01 | 2.26295D 00 |
| (6S1/2)            | 2  | 3.98652847D-01 | 5.27392763D 00 | 0.0                                    | 0.31626  | 4.950188 | 1.84960D 01 | 6.06544D 02 |
| TOTAL              | 67 | 2.52235339D 04 | 3.43173746D C5 |                                        |          |          |             |             |

DYSPROSIUM 14F110 4 = 163 CWN S-L EX 07-24-73  
 NUCLEAR CHARGE= 66.0 44PIUS= 5.9827 FERMI =.0001127 ROMP SURFACE THICKNESS=0.5666 FERMI =.0000107 ROMP  
 SLATEP-LATTER EXCHANGE APPROXIMATION WITH MULTIPLIER 1.50

| ENERGY EICFNUVALUES |    |                |                | RADIAL EXPECTATION VALUES (ROHR UNITS) |          |          |             |             |          |
|---------------------|----|----------------|----------------|----------------------------------------|----------|----------|-------------|-------------|----------|
| SHELL               | 0  | RYDRFRGS       | ELECTRON VOLTS | 1/R(ROHR)                              | 1/R      | R        | ROR         | RMAX        |          |
| (151/21)            | 2  | 3.958725070 03 | 5.385964220 04 | 0.0                                    | 74.64494 | 0.021088 | 6.076680-04 | 9.855970-07 | 0.013377 |
| (1251/21)           | 2  | 6.624100220 02 | 9.017559180 03 | 0.0                                    | 17.92154 | 0.388942 | 9.401150-03 | 1.532570-04 | 0.076138 |
| (121/21)            | 2  | 6.314332730 02 | 8.590839110 03 | 0.0                                    | 17.91606 | 0.074050 | 6.785650-03 | 9.382600-05 | 0.057226 |
| (121/21)            | 4  | 5.718675360 02 | 7.780429390 03 | 1.112360 04                            | 15.67914 | 0.041059 | 8.004990-03 | 1.256650-04 | 0.063265 |
| (131/21)            | 2  | 1.483130127 02 | 2.018387240 03 | 0.0                                    | 6.56463  | 0.232874 | 6.210670-02 | 5.831590-03 | 0.219921 |
| (131/21)            | 2  | 1.345893110 02 | 1.831127950 03 | 0.0                                    | 6.48826  | 0.222262 | 5.748370-02 | 5.234900-03 | 0.202039 |
| (131/21)            | 4  | 1.221402900 02 | 1.661755290 03 | 2.408620 03                            | 5.91705  | 0.235572 | 6.435940-02 | 6.509990-03 | 0.214680 |
| (1301/21)           | 4  | 9.821577150 01 | 1.336255040 03 | 4.098620 02                            | 5.80553  | 0.207820 | 5.080010-02 | 4.598260-03 | 0.169592 |
| (1301/21)           | 6  | 9.547179890 01 | 1.298942770 03 | 3.610080 02                            | 5.66414  | 0.211967 | 5.271330-02 | 4.919890-03 | 0.173251 |
| (141/21)            | 2  | 2.571789540 01 | 4.043208820 02 | 0.0                                    | 2.74768  | 0.526320 | 3.129320-01 | 1.425340-01 | 0.492323 |
| (141/21)            | 2  | 2.421779540 01 | 3.294503640 02 | 0.0                                    | 2.64357  | 0.535734 | 3.268720-01 | 1.599580-01 | 0.494874 |
| (1401/21)           | 4  | 2.142354520 01 | 2.914737590 02 | 5.412380 02                            | 2.44704  | 0.566117 | 3.647330-01 | 1.992090-01 | 0.521289 |
| (1401/21)           | 4  | 1.227403590 01 | 1.669919410 02 | 7.872000 01                            | 2.23147  | 0.595570 | 4.123780-01 | 2.772520-01 | 0.525204 |
| (1401/21)           | 6  | 1.176166640 01 | 1.600237270 02 | 6.822320 01                            | 2.18770  | 0.606734 | 4.272780-01 | 2.978590-01 | 0.534296 |
| (151/21)            | 2  | 3.947244650 00 | 5.370344770 01 | 0.0                                    | 1.04240  | 1.280953 | 1.847510 00 | 5.091070 00 | 1.147510 |
| (151/21)            | 2  | 2.431805030 00 | 3.108543700 01 | 0.0                                    | 0.91900  | 1.436852 | 2.347780 00 | 8.635590 00 | 1.246450 |
| (151/21)            | 2  | 2.063525910 00 | 2.807488900 01 | 6.995100 01                            | 0.84671  | 1.533887 | 2.696080 00 | 1.147630 01 | 1.228081 |
| (141/21)            | 6  | 7.683065130-01 | 1.045304060 01 | 1.015730 01                            | 1.64144  | 0.874346 | 8.569770-01 | 2.220610 00 | 0.525731 |
| (141/21)            | 6  | 6.939818830-01 | 9.469042310 00 | 9.735350 00                            | 1.61800  | 0.818788 | 8.928190-01 | 2.476100 00 | 0.531065 |
| (141/21)            | 2  | 5.398946350-01 | 5.359454680 00 | 0.0                                    | 0.31054  | 4.098265 | 1.939900 01 | 6.330960 02 | 2.316104 |
| TOTAL               | 66 | 2.410384000 04 | 3.306630760 05 |                                        |          |          |             |             |          |

| R          |             | POTOP      |             | R          |             | POTOP      |             | R           |            | POTOP |  | R |  | POTOP |  |
|------------|-------------|------------|-------------|------------|-------------|------------|-------------|-------------|------------|-------|--|---|--|-------|--|
| 0.00001222 | 10.10826373 | 0.00027811 | 65.90674830 | 0.00532972 | 63.68928836 | 0.14406366 | 36.01232534 | 3.27837377  | 1.24328625 |       |  |   |  |       |  |
| 0.00001301 | 10.75470935 | 0.00029604 | 65.90054400 | 0.00673795 | 63.54121109 | 0.15335447 | 34.93531943 | 3.49034296  | 1.17461700 |       |  |   |  |       |  |
| 0.00001395 | 11.44172127 | 0.00031514 | 65.89392433 | 0.00717251 | 63.38430741 | 0.16224551 | 33.84617624 | 3.71545074  | 1.11066285 |       |  |   |  |       |  |
| 0.00001474 | 12.17167906 | 0.00033546 | 65.88686205 | 0.00763509 | 63.21813931 | 0.17377394 | 32.74616662 | 3.95507672  | 1.05169857 |       |  |   |  |       |  |
| 0.00001569 | 12.94707153 | 0.00035710 | 65.87932776 | 0.00812752 | 63.04225556 | 0.18498140 | 31.63722555 | 4.21015726  | 1.00870132 |       |  |   |  |       |  |
| 0.00001670 | 13.77049001 | 0.00038013 | 65.87123998 | 0.00865170 | 62.85619162 | 0.19691168 | 30.52118811 | 4.48168907  | 1.03000000 |       |  |   |  |       |  |
| 0.00001778 | 14.64462310 | 0.00040465 | 65.86271513 | 0.00920468 | 62.65946935 | 0.20961139 | 29.39973657 | 35.25121511 | 1.00000000 |       |  |   |  |       |  |
| 0.00001893 | 15.57224848 | 0.00043074 | 65.85356739 | 0.00980366 | 62.45159680 | 0.22313016 | 28.27409708 |             |            |       |  |   |  |       |  |
| 0.00002015 | 16.55627130 | 0.00045852 | 65.84380851 | 0.01043594 | 62.23206784 | 0.23752082 | 27.14513643 |             |            |       |  |   |  |       |  |
| 0.00002145 | 17.59945827 | 0.00048810 | 65.83339772 | 0.01110900 | 62.00036190 | 0.25283960 | 26.01365926 |             |            |       |  |   |  |       |  |
| 0.00002283 | 18.70491608 | 0.00051957 | 65.82229151 | 0.01182547 | 61.75544308 | 0.26914635 | 24.88116447 |             |            |       |  |   |  |       |  |
| 0.00002430 | 19.87556149 | 0.00055308 | 65.81044347 | 0.01258214 | 61.49826181 | 0.28650480 | 23.75053902 |             |            |       |  |   |  |       |  |
| 0.00002587 | 21.11434740 | 0.00058876 | 65.79780410 | 0.01340001 | 61.22675852 | 0.30498277 | 22.62632987 |             |            |       |  |   |  |       |  |
| 0.00002754 | 22.42414218 | 0.00062673 | 65.78432059 | 0.01426423 | 60.94062218 | 0.32465247 | 21.51388409 |             |            |       |  |   |  |       |  |
| 0.00002931 | 23.80769673 | 0.00066715 | 65.76993665 | 0.01518470 | 60.63995942 | 0.34559075 | 20.41727883 |             |            |       |  |   |  |       |  |
| 0.00003120 | 25.26755977 | 0.00071017 | 65.75459221 | 0.01616349 | 60.32348954 | 0.36787944 | 19.33777486 |             |            |       |  |   |  |       |  |
| 0.00003322 | 26.80598727 | 0.00075598 | 65.73822327 | 0.01720595 | 59.99085259 | 0.39160563 | 18.27409413 |             |            |       |  |   |  |       |  |
| 0.00003536 | 28.42483506 | 0.00080473 | 65.72076155 | 0.01831564 | 59.64146752 | 0.41686502 | 17.22475828 |             |            |       |  |   |  |       |  |
| 0.00003764 | 30.12541524 | 0.00085761 | 65.70213432 | 0.01945690 | 59.27477231 | 0.44374731 | 16.19016714 |             |            |       |  |   |  |       |  |
| 0.00004007 | 31.90837753 | 0.00091188 | 65.68226403 | 0.02075434 | 58.89023504 | 0.47236655 | 15.17338018 |             |            |       |  |   |  |       |  |
| 0.00004265 | 33.77325052 | 0.00097069 | 65.66106807 | 0.02223928 | 58.48736495 | 0.50281158 | 14.17963373 |             |            |       |  |   |  |       |  |
| 0.00004540 | 35.71868462 | 0.00103730 | 65.63845843 | 0.02381775 | 58.06572001 | 0.53526143 | 13.21507492 |             |            |       |  |   |  |       |  |
| 0.00004831 | 37.74164218 | 0.00110494 | 65.61434138 | 0.02543451 | 57.62490881 | 0.56978782 | 12.28572444 |             |            |       |  |   |  |       |  |
| 0.00005144 | 39.83726965 | 0.00117078 | 65.58861714 | 0.02664510 | 57.16458180 | 0.60653066 | 11.39649264 |             |            |       |  |   |  |       |  |
| 0.00005476 | 41.99839277 | 0.00124639 | 65.56117950 | 0.02836777 | 56.68441100 | 0.64564453 | 10.55090215 |             |            |       |  |   |  |       |  |
| 0.00005829 | 44.21497150 | 0.00132678 | 65.53191548 | 0.03015738 | 56.18405732 | 0.68728928 | 9.75109463  |             |            |       |  |   |  |       |  |
| 0.00006205 | 46.47145526 | 0.00141235 | 65.50070489 | 0.03214445 | 55.66313257 | 0.73161563 | 8.95818101  |             |            |       |  |   |  |       |  |
| 0.00006606 | 48.75503181 | 0.00150344 | 65.46742002 | 0.03421812 | 55.12116454 | 0.77880078 | 8.29273179  |             |            |       |  |   |  |       |  |
| 0.00007032 | 51.03978174 | 0.00159040 | 65.43192516 | 0.03642500 | 54.55757759 | 0.82902912 | 7.63495035  |             |            |       |  |   |  |       |  |
| 0.00007485 | 53.29578277 | 0.00167362 | 65.39407619 | 0.03877421 | 53.97169938 | 0.88249690 | 7.02472033  |             |            |       |  |   |  |       |  |
| 0.00007968 | 55.68828634 | 0.00175349 | 65.35372019 | 0.04127493 | 53.36278646 | 0.93941306 | 6.46118176  |             |            |       |  |   |  |       |  |
| 0.00008472 | 57.57424867 | 0.00183045 | 65.31069500 | 0.04393693 | 52.73307801 | 1.00000000 | 5.94246686  |             |            |       |  |   |  |       |  |
| 0.00009029 | 59.50380965 | 0.00205496 | 65.26482874 | 0.04677062 | 52.07264826 | 1.06449446 | 5.46565835  |             |            |       |  |   |  |       |  |
| 0.00009611 | 61.22786189 | 0.00218749 | 65.21593945 | 0.04978707 | 51.39045910 | 1.13314845 | 5.02717304  |             |            |       |  |   |  |       |  |
| 0.00010231 | 62.67929272 | 0.00232857 | 65.16383462 | 0.05255806 | 50.68239294 | 1.20623025 | 4.62336899  |             |            |       |  |   |  |       |  |
| 0.00010891 | 63.83479168 | 0.00247875 | 65.10831075 | 0.05641614 | 49.94827141 | 1.28402542 | 4.25090279  |             |            |       |  |   |  |       |  |
| 0.00011593 | 64.67966605 | 0.00263062 | 65.04915307 | 0.06005467 | 49.18785071 | 1.36683794 | 3.90696197  |             |            |       |  |   |  |       |  |
| 0.00012341 | 65.24249944 | 0.00280879 | 64.98613481 | 0.06392786 | 48.40160979 | 1.45499141 | 3.58913761  |             |            |       |  |   |  |       |  |
| 0.00013137 | 65.58320310 | 0.00298895 | 64.91901741 | 0.06805085 | 47.58773353 | 1.54883030 | 3.29532219  |             |            |       |  |   |  |       |  |
| 0.00013984 | 65.77154957 | 0.00318278 | 64.84754564 | 0.07243576 | 46.74810752 | 1.64872127 | 3.02358369  |             |            |       |  |   |  |       |  |
| 0.00014886 | 65.86713571 | 0.00338805 | 64.77146757 | 0.07711172 | 45.89234002 | 1.75505466 | 2.77216438  |             |            |       |  |   |  |       |  |
| 0.00015846 | 65.91147187 | 0.00360656 | 64.69049425 | 0.08208500 | 44.99080952 | 1.86824596 | 2.53958921  |             |            |       |  |   |  |       |  |
| 0.00016868 | 65.92945319 | 0.00383917 | 64.60433950 | 0.08737503 | 44.07615778 | 1.98873747 | 2.32480114  |             |            |       |  |   |  |       |  |
| 0.00017956 | 65.93488645 | 0.00408677 | 64.51269972 | 0.09301449 | 43.13337752 | 2.11700002 | 2.12733855  |             |            |       |  |   |  |       |  |
| 0.00019114 | 65.93457779 | 0.00435335 | 64.41525777 | 0.09901341 | 42.16988870 | 2.25353679 | 1.94735882  |             |            |       |  |   |  |       |  |
| 0.00020347 | 65.93172368 | 0.00463092 | 64.31168295 | 0.10535922 | 41.18549591 | 2.39887529 | 1.78550832  |             |            |       |  |   |  |       |  |
| 0.00021659 | 65.92770355 | 0.00492959 | 64.20163688 | 0.11219689 | 40.18221730 | 2.55358946 | 1.64248159  |             |            |       |  |   |  |       |  |
| 0.00023056 | 65.92306553 | 0.00524752 | 64.08474362 | 0.11943297 | 39.16197714 | 2.71828183 | 1.51839098  |             |            |       |  |   |  |       |  |
| 0.00024543 | 65.91800061 | 0.00558595 | 63.96064965 | 0.12713573 | 38.12629884 | 2.89359594 | 1.41219635  |             |            |       |  |   |  |       |  |
| 0.00026126 | 65.91256133 | 0.00594622 | 63.82896400 | 0.13533528 | 37.07620023 | 3.08021685 | 1.32156095  |             |            |       |  |   |  |       |  |

ERBIUM 14F112 A = 167 CWN S-L FX 07-24-73  
 NUCLEAR CHARGE= 68.0 RADIUS= 6.0133 FERMI =.0001136 BOHR SURFACE THICKNESS=0.5666 FERMI =.0000107 BOHR  
 SLATER-LATTER EXCHANGE APPROXIMATION WITH MULTIPLIER 1.50

| ENERGY EIGENVALUES |   |                |                | RADIAL EXPECTATION VALUES (BOHR UNITS) |          |          |             |
|--------------------|---|----------------|----------------|----------------------------------------|----------|----------|-------------|
| SHELL              | Q | RYDBERGS       | ELECTRON VOLTS | 1/(R*R*P)                              | 1/R      | R        | R*R         |
| (1S1/2)            | 2 | 4.231687390 03 | 5.757337650 04 | 0.0                                    | 77.63484 | 0.020343 | 5.663400-04 |
| (2S1/2)            | 2 | 7.141641220 02 | 9.716417130 03 | 0.0                                    | 18.71234 | 0.085633 | 8.721790-03 |
| (2P1/2)            | 2 | 6.817308267 07 | 9.275152410 03 | 0.0                                    | 18.70563 | 0.071163 | 6.274720-03 |
| (2P3/2)            | 4 | 6.135051580 02 | 8.346521720 03 | 1.23203E 04                            | 16.21349 | 0.078433 | 7.487000-03 |
| (3S1/2)            | 2 | 1.609167090 07 | 2.189320090 07 | 0.0                                    | 6.86576  | 0.223758 | 5.735710-02 |
| (3P1/2)            | 2 | 1.464254390 07 | 1.992162030 03 | 0.0                                    | 6.78989  | 0.213223 | 5.292410-02 |
| (3P3/2)            | 4 | 1.320106440 02 | 1.756044410 03 | 2.70323D 03                            | 6.15065  | 0.226867 | 5.969850-02 |
| (3D3/2)            | 4 | 1.069343810 02 | 1.454674370 03 | 4.62777E 02                            | 6.04259  | 0.199593 | 4.683590-02 |
| (3D5/2)            | 6 | 1.037575060 02 | 1.411652000 03 | 4.04139D 02                            | 5.88588  | 0.203834 | 4.871450-02 |
| (4S1/2)            | 2 | 3.212609430 01 | 4.370851510 02 | 0.0                                    | 2.87519  | 0.504867 | 2.880110-01 |
| (4P1/2)            | 2 | 2.625950020 01 | 3.572683780 02 | 0.0                                    | 2.77005  | 0.512938 | 2.997380-01 |
| (4P3/2)            | 4 | 2.300362600 01 | 3.129712330 02 | 6.105200 02                            | 2.54859  | 0.544214 | 3.371400-01 |
| (4D3/2)            | 4 | 1.324847700 01 | 1.802495040 02 | 8.98333D 01                            | 2.33209  | 0.570551 | 3.780650-01 |
| (4D5/2)            | 6 | 1.265002920 01 | 1.721074420 02 | 7.70534D 01                            | 2.27733  | 0.581624 | 3.927660-01 |
| (5S1/2)            | 2 | 4.174067130 00 | 5.678543560 01 | 0.0                                    | 1.82488  | 1.234443 | 1.717290 00 |
| (5P1/2)            | 2 | 2.555471020 00 | 3.476794980 01 | 0.0                                    | 0.95370  | 1.385469 | 2.184790 00 |
| (5P3/2)            | 4 | 2.135733860 00 | 2.905729990 01 | 7.70040D 01                            | 0.87463  | 1.492858 | 2.539930 00 |
| (4F5/2)            | 6 | 7.955191300-01 | 1.082327640 01 | 1.18861E 01                            | 1.73171  | 0.762828 | 7.727210-01 |
| (4F7/2)            | 6 | 7.071264430-01 | 0.620667400 00 | 1.13472D 01                            | 1.70443  | 0.778197 | 8.094200-01 |
| (6S1/2)            | 2 | 4.034510410-01 | 5.489072440 00 | 0.0                                    | 0.31799  | 4.003186 | 1.853550 01 |

TOTAL 68 2.61650942D 04 3.55983956D 05

| R          | POT*R       | R          | POT*R       | R          | POT*R       | R          | POT*R       | R           | POT*R      |
|------------|-------------|------------|-------------|------------|-------------|------------|-------------|-------------|------------|
| 0.00001222 | 10.33580936 | 0.00027811 | 67.90233362 | 0.00632972 | 65.57520135 | 0.14406366 | 36.80793820 | 3.27867377  | 1.21495928 |
| 0.00001301 | 10.99690333 | 0.00029404 | 67.89582352 | 0.00673795 | 65.42019140 | 0.15335497 | 35.68914639 | 3.49034296  | 1.14834994 |
| 0.00001385 | 11.69949820 | 0.00031514 | 67.88887673 | 0.00717251 | 65.25599411 | 0.16324551 | 34.55713783 | 3.71545074  | 1.08694912 |
| 0.00001474 | 12.44460360 | 0.00033546 | 67.88146461 | 0.00763509 | 65.08215769 | 0.17377394 | 33.41353720 | 3.95507672  | 1.03051191 |
| 0.00001569 | 13.23906914 | 0.00035710 | 67.87355622 | 0.00812752 | 64.89821659 | 0.18498140 | 32.26020402 | 4.21015726  | 1.00161009 |
| 0.00001670 | 14.08125453 | 0.00038013 | 67.86511845 | 0.00865170 | 64.70369134 | 0.19691168 | 31.09891643 | 4.48168907  | 1.00000000 |
| 0.00001778 | 14.97535142 | 0.00040465 | 67.85611556 | 0.00920568 | 64.49808821 | 0.20961139 | 29.93114758 | 35.25121511 | 1.00000000 |
| 0.00001893 | 15.92421189 | 0.00043074 | 67.84651104 | 0.00980366 | 64.28089853 | 0.22313016 | 28.75794538 |             |            |
| 0.00002015 | 16.93076973 | 0.00045852 | 67.83626346 | 0.01043594 | 64.05160025 | 0.23752082 | 27.58025337 |             |            |
| 0.00002145 | 17.99802460 | 0.00048810 | 67.82533032 | 0.01110900 | 63.80965373 | 0.25283960 | 26.39940747 |             |            |
| 0.00002283 | 19.12902087 | 0.00051957 | 67.81366563 | 0.01182547 | 63.55450568 | 0.26914635 | 25.21792956 |             |            |
| 0.00002430 | 20.32681982 | 0.00055308 | 67.80127117 | 0.01259814 | 63.28558758 | 0.28650480 | 24.03993761 |             |            |
| 0.00002587 | 21.59446376 | 0.00058876 | 67.78794425 | 0.01340001 | 63.00231712 | 0.30498277 | 22.87064522 |             |            |
| 0.00002754 | 22.93493021 | 0.00062673 | 67.77377554 | 0.01424623 | 62.70410038 | 0.32465247 | 21.71476800 |             |            |
| 0.00002931 | 24.35107358 | 0.00066715 | 67.75866780 | 0.01518420 | 62.39033524 | 0.34559075 | 20.57459634 |             |            |
| 0.00003120 | 25.84555440 | 0.00071017 | 67.74254589 | 0.01616349 | 62.06041670 | 0.36787944 | 19.44987135 |             |            |
| 0.00003322 | 27.42074459 | 0.00075598 | 67.72534647 | 0.01720595 | 61.71374405 | 0.39160563 | 18.33942945 |             |            |
| 0.00003536 | 29.07861881 | 0.00080473 | 67.70699778 | 0.01831564 | 61.34973002 | 0.41686202 | 17.24354704 |             |            |
| 0.00003764 | 30.82061335 | 0.00085663 | 67.68742334 | 0.01946590 | 60.96781152 | 0.44374731 | 16.16507436 |             |            |
| 0.00004007 | 32.64745517 | 0.00091188 | 67.66654164 | 0.02075434 | 60.56746052 | 0.47236655 | 15.10919158 |             |            |
| 0.00004265 | 34.55895186 | 0.00097049 | 67.64426588 | 0.02209288 | 60.14819342 | 0.50283158 | 14.08245975 |             |            |
| 0.00004540 | 36.55373479 | 0.00103330 | 67.62050359 | 0.02351775 | 59.70957512 | 0.53526143 | 13.09146113 |             |            |
| 0.00004833 | 38.62894635 | 0.00109554 | 67.59515637 | 0.02503451 | 59.25121538 | 0.56978282 | 12.14194721 |             |            |
| 0.00005144 | 40.77986030 | 0.00117088 | 67.56811930 | 0.02664910 | 58.77275290 | 0.60653066 | 11.23816093 |             |            |
| 0.00005476 | 42.99942354 | 0.00124639 | 67.53928105 | 0.02836782 | 58.27382426 | 0.64564453 | 10.38281100 |             |            |
| 0.00005829 | 45.27770639 | 0.00132678 | 67.50852299 | 0.03015738 | 57.75414724 | 0.68728928 | 9.57732304  |             |            |
| 0.00006205 | 47.60124997 | 0.00141235 | 67.47571908 | 0.03214495 | 57.21294427 | 0.73161563 | 8.82223027  |             |            |
| 0.00006606 | 49.95230374 | 0.00150344 | 67.44073538 | 0.03421817 | 56.64995557 | 0.77880078 | 8.11762811  |             |            |
| 0.00007032 | 52.30796986 | 0.00159640 | 67.40342966 | 0.03642500 | 56.06441553 | 0.82902912 | 7.46319383  |             |            |
| 0.00007485 | 54.69228881 | 0.00170362 | 67.36365054 | 0.03877421 | 55.45557272 | 0.88249690 | 6.85811487  |             |            |
| 0.00007968 | 56.91014703 | 0.00181349 | 67.32123912 | 0.04127493 | 54.82263476 | 0.93941306 | 6.30071955  |             |            |
| 0.00008482 | 59.07721102 | 0.00193045 | 67.27602448 | 0.04393693 | 54.16482121 | 1.00000000 | 5.78839026  |             |            |
| 0.00009029 | 61.08766255 | 0.00205496 | 67.22782726 | 0.04677062 | 53.48141526 | 1.06449446 | 5.31776777  |             |            |
| 0.00009611 | 62.89172960 | 0.00218749 | 67.17645725 | 0.04977077 | 52.77180774 | 1.13314845 | 4.88518581  |             |            |
| 0.00010231 | 64.42856468 | 0.00232857 | 67.12171337 | 0.05295806 | 52.03551834 | 1.20623025 | 4.48716411  |             |            |
| 0.00010891 | 65.65762485 | 0.00247875 | 67.06338320 | 0.05641614 | 51.27220346 | 1.28402542 | 4.12059394  |             |            |
| 0.00011593 | 66.56432347 | 0.00263862 | 67.00124244 | 0.06005467 | 50.48164411 | 1.36683794 | 3.78280686  |             |            |
| 0.00012341 | 67.17358487 | 0.00280879 | 66.93505549 | 0.06392786 | 49.66373187 | 1.45499141 | 3.47142131  |             |            |
| 0.00013137 | 67.54502244 | 0.00298995 | 66.86457313 | 0.06805085 | 48.81445846 | 1.54883030 | 3.18425808  |             |            |
| 0.00013984 | 67.75139776 | 0.00318278 | 66.78953416 | 0.07243976 | 47.94592281 | 1.64872127 | 2.91928983  |             |            |
| 0.00014886 | 67.85650134 | 0.00338805 | 66.70966417 | 0.07711172 | 47.04637399 | 1.75505466 | 2.67469622  |             |            |
| 0.00015846 | 67.90536050 | 0.00360655 | 66.62467542 | 0.08208500 | 46.12027737 | 1.86824596 | 2.44901643  |             |            |
| 0.00016868 | 67.92537877 | 0.00383917 | 66.53426671 | 0.08737903 | 45.16941957 | 1.98873747 | 2.24128753  |             |            |
| 0.00017956 | 67.93155170 | 0.00408677 | 66.43812318 | 0.09301449 | 44.19191126 | 2.11700002 | 2.05118345  |             |            |
| 0.00019114 | 67.93141744 | 0.00435035 | 66.33591622 | 0.09901341 | 43.19256175 | 2.25353479 | 1.87896249  |             |            |
| 0.00020347 | 67.92849557 | 0.00463092 | 66.22730341 | 0.10539572 | 42.17205191 | 2.39887529 | 1.72522329  |             |            |
| 0.00021659 | 67.92430474 | 0.00492959 | 66.11192851 | 0.11219689 | 41.13237729 | 2.55358946 | 1.59037947  |             |            |
| 0.00023056 | 67.91944799 | 0.00524752 | 65.98942147 | 0.11943297 | 40.07517934 | 2.71828183 | 1.47403724  |             |            |
| 0.00024543 | 67.91413769 | 0.00558595 | 65.85939852 | 0.12713573 | 39.00159803 | 2.89359594 | 1.37459292  |             |            |
| 0.00026126 | 67.90843231 | 0.00594622 | 65.72146217 | 0.13533528 | 37.91233994 | 3.08021685 | 1.28932360  |             |            |

YTTERRIUM 14F114 A = 173 CWN S-L EX 07-24-73  
 NUCLEAR CHARGE= 70.0 RADIUS= 6.0995 FERMI =.0001151 EFMH SURFACE THICKNESS=0.5666 FERMI =.0000107 BOHR  
 SLATER-LATYER EXCHANGE APPROXIMATION WITH MULTIPLIER 1.50

| ENERGY EIGENVALUES |                |                | RADIAL EXPECTATION VALUES |          |          | {BOMF UNITS} |             |          |
|--------------------|----------------|----------------|---------------------------|----------|----------|--------------|-------------|----------|
| SHELL Q            | RYDRERGS       | ELECTRON VOLTS | 1/(ROROR)                 | 1/R      | R        | ROR          | ROROROR     | RMAX     |
| 1S1/2) 2           | 4.515903590 03 | 6.144022310 04 | 0.0                       | 80.70962 | 0.019636 | 5.285130-04  | 7.513540-07 | 0.012368 |
| 2S1/2) 2           | 7.684104280 02 | 1.045445440 04 | 0.0                       | 15.52975 | 0.082503 | 8.103090-03  | 1.141840-04 | 0.070659 |
| 2P1/2) 2           | 7.345055130 02 | 9.993167850 03 | 0.0                       | 15.52177 | 0.068433 | 5.810280-03  | 6.916940-05 | 0.052819 |
| 2P3/2) 4           | 6.566196330 02 | 8.933507090 03 | 1.361030 04               | 16.75067 | 0.075926 | 7.015980-03  | 9.648010-05 | 0.059243 |
| 3S1/2) 2           | 1.740993570 02 | 2.369673990 03 | 0.0                       | 7.17481  | 0.215214 | 5.307790-02  | 4.258650-03 | 0.199223 |
| 3P1/2) 2           | 1.588622200 02 | 2.161368160 03 | 0.0                       | 7.09935  | 0.204769 | 4.883220-02  | 3.777920-03 | 0.186757 |
| 3P3/2) 4           | 1.422385390 02 | 1.935198000 03 | 3.024070 03               | 6.38553  | 0.218759 | 5.551640-02  | 4.838330-03 | 0.200015 |
| 3D3/2) 4           | 1.159932710 02 | 1.578123250 03 | 5.206030 02               | 6.28077  | 0.191471 | 4.331050-02  | 3.331400-03 | 0.157017 |
| 3D5/2) 6           | 1.123321020 02 | 1.528211950 03 | 4.506030 02               | 6.10760  | 0.196309 | 4.515800-02  | 3.595470-03 | 0.160799 |
| 4S1/2) 2           | 3.464587830 01 | 4.713678400 02 | 0.0                       | 3.00501  | 0.484907 | 2.657530-01  | 1.029700-01 | 0.453810 |
| 4P1/2) 2           | 2.839999960 01 | 3.863905140 02 | 0.0                       | 2.89881  | 0.491796 | 2.756240-01  | 1.138370-01 | 0.454362 |
| 4P3/2) 4           | 2.462445600 01 | 3.350231120 02 | 6.867830 02               | 2.65001  | 0.523594 | 3.126290-01  | 1.465280-01 | 0.482808 |
| 4D3/2) 4           | 1.424671600 01 | 1.938308450 02 | 1.020120 02               | 2.43245  | 0.567300 | 3.479870-01  | 1.977950-01 | 0.482292 |
| 4D5/2) 6           | 1.355155280 01 | 1.843783830 02 | 8.656670 01               | 2.37123  | 0.558694 | 3.625130-01  | 2.148530-01 | 0.491369 |
| 5S1/2) 2           | 4.408731180 00 | 5.998211840 01 | 0.0                       | 1.12298  | 1.191288 | 1.599570 00  | 3.837330 00 | 1.062971 |
| 5P1/2) 2           | 2.682759340 00 | 3.649574570 01 | 0.0                       | 0.98873  | 1.337370 | 2.037480 00  | 6.562490 00 | 1.154194 |
| 5P3/2) 4           | 2.206231210 00 | 3.001643750 01 | 8.448290 01               | 0.90009  | 1.450281 | 2.399680 00  | 9.193930 00 | 1.241991 |
| 4F5/2) 6           | 8.114910450-01 | 1.104057910 01 | 1.378640 01               | 1.81999  | 0.726564 | 7.031700-01  | 1.551020 00 | 0.473077 |
| 4F7/2) 8           | 7.048400720-01 | 9.589560630 00 | 1.308660 01               | 1.78842  | 0.743001 | 7.411850-01  | 1.795250 00 | 0.478355 |
| 6S1/2) 2           | 4.131283400-01 | 5.620735010 00 | 0.0                       | 0.32552  | 3.911907 | 1.772440 01  | 5.346250 02 | 3.140502 |
| TOTAL 70           | 2.811551210 04 | 3.825159760 05 |                           |          |          |              |             |          |

| R          | POTR        | R           | POTR          | R          | POTR        | P          | POTR        | R           | POTR       |
|------------|-------------|-------------|---------------|------------|-------------|------------|-------------|-------------|------------|
| 0.00001148 | 9.88945357  | 0.00026126  | 69.90420818   | 0.00594622 | 67.61120183 | 0.13533528 | 38.72489043 | 3.08021685  | 1.26004190 |
| 0.00001222 | 10.52273053 | 0.00027811  | 69.85781623   | 0.00632572 | 67.45822308 | 0.14406366 | 37.57831064 | 3.27887377  | 1.18883057 |
| 0.00001301 | 11.19591448 | 0.00029604  | 69.80999198   | 0.00673795 | 67.29614410 | 0.15335497 | 36.41613155 | 3.49034296  | 1.12432789 |
| 0.00001385 | 11.91138622 | 0.00031514  | 69.76370902   | 0.00717251 | 67.12451316 | 0.16324551 | 35.23976889 | 3.71545074  | 1.06432383 |
| 0.00001474 | 12.67164028 | 0.00033546  | 69.71793729   | 0.00763509 | 66.94286447 | 0.17377394 | 34.05098546 | 3.95507672  | 1.01520463 |
| 0.00001569 | 13.47928406 | 0.00035710  | 69.66764426   | 0.00812752 | 66.75071794 | 0.18498140 | 32.85161844 | 4.21015726  | 1.00000000 |
| 0.00001670 | 14.33703523 | 0.00038013  | 69.61857913   | 0.00865170 | 66.54757886 | 0.19691168 | 31.64332015 | 4.252108200 | 1.00000000 |
| 0.00001778 | 15.24771689 | 0.00040465  | 69.56935274   | 0.00920968 | 66.33293759 | 0.20961139 | 30.42736291 |             |            |
| 0.00001893 | 16.21424956 | 0.00043074  | 69.52027745   | 0.00980366 | 66.10626909 | 0.22313016 | 29.20483217 |             |            |
| 0.00002015 | 17.23964214 | 0.00045852  | 69.47185268   | 0.01043594 | 65.86703262 | 0.23752082 | 27.97699610 |             |            |
| 0.00002145 | 18.32697253 | 0.00048810  | 69.4241705622 | 0.01110900 | 65.61467151 | 0.25283960 | 26.74605349 |             |            |
| 0.00002283 | 19.47937058 | 0.00051957  | 69.3770481705 | 0.01182547 | 65.34861135 | 0.26914635 | 25.51585159 |             |            |
| 0.00002430 | 20.69999090 | 0.00055308  | 69.330175814  | 0.01258814 | 65.06827066 | 0.28650480 | 24.29076007 |             |            |
| 0.00002587 | 21.99197401 | 0.00058876  | 69.28382477   | 0.01340001 | 64.77304255 | 0.30498277 | 23.07646539 |             |            |
| 0.00002754 | 23.35840528 | 0.00062673  | 69.238295257  | 0.01426423 | 64.46231746 | 0.32465247 | 21.87605946 |             |            |
| 0.00002931 | 24.80225580 | 0.00066715  | 69.194709730  | 0.01518420 | 64.13547761 | 0.34559075 | 20.69034270 |             |            |
| 0.00003120 | 26.32631105 | 0.00071017  | 69.153017461  | 0.01616349 | 63.79190524 | 0.36787944 | 19.51866665 |             |            |
| 0.00003322 | 27.93108121 | 0.00075598  | 69.11211978   | 0.01720595 | 63.43099082 | 0.39160563 | 18.36123489 |             |            |
| 0.00003536 | 29.62468979 | 0.00080473  | 69.07285744   | 0.01831564 | 63.05214304 | 0.41686202 | 17.22058322 |             |            |
| 0.00003764 | 31.40273597 | 0.00085663  | 69.034230728  | 0.01949690 | 62.65479957 | 0.44374731 | 16.10175023 |             |            |
| 0.00004007 | 33.26812464 | 0.00091188  | 68.99638369   | 0.02075434 | 62.23843717 | 0.47236655 | 15.01150464 |             |            |
| 0.00004265 | 35.22085583 | 0.00097069  | 68.95929959   | 0.02209288 | 61.80257808 | 0.50283158 | 13.95699979 |             |            |
| 0.00004540 | 37.25978346 | 0.00103330  | 68.92304555   | 0.02351775 | 61.34679003 | 0.53526143 | 12.94477731 |             |            |
| 0.00004833 | 39.38227690 | 0.00109994  | 68.887543148  | 0.02503451 | 60.87067548 | 0.56978282 | 11.97993665 |             |            |
| 0.00005144 | 41.58387156 | 0.00117088  | 68.852704230  | 0.02664910 | 60.37384969 | 0.60653066 | 11.06591164 |             |            |
| 0.00005476 | 43.85779867 | 0.00124639  | 68.818676152  | 0.02836782 | 59.85590749 | 0.64564853 | 10.20459348 |             |            |
| 0.00005829 | 46.19443928 | 0.00132678  | 68.784464687  | 0.03015738 | 59.31638644 | 0.68728928 | 9.39689506  |             |            |
| 0.00006205 | 48.58067149 | 0.00141235  | 68.75002031   | 0.03214495 | 58.75473501 | 0.73161563 | 8.64225516  |             |            |
| 0.00006606 | 50.99910276 | 0.00150344  | 68.715378758  | 0.03421812 | 58.17029784 | 0.77880078 | 7.94081073  |             |            |
| 0.00007032 | 53.42719149 | 0.00159940  | 68.680411780  | 0.03642500 | 57.56232463 | 0.82902912 | 7.29149752  |             |            |
| 0.00007485 | 55.83628684 | 0.00170262  | 68.645335302  | 0.03877421 | 56.93300236 | 0.88249690 | 6.69276227  |             |            |
| 0.00007968 | 58.19767929 | 0.00181349  | 68.610382582  | 0.04127493 | 56.27250538 | 0.93941306 | 6.14223724  |             |            |
| 0.00008482 | 60.44688850 | 0.00193045  | 68.575435883  | 0.04393693 | 55.58904788 | 1.00000000 | 5.63678153  |             |            |
| 0.00009029 | 62.55369289 | 0.00205496  | 68.54074631   | 0.04677052 | 54.87893275 | 1.06449446 | 5.17279755  |             |            |
| 0.00009611 | 64.45189806 | 0.00218749  | 68.50584373   | 0.04978707 | 54.14158059 | 1.13314445 | 4.74469031  |             |            |
| 0.00010231 | 66.08958527 | 0.00232857  | 68.470838731  | 0.05296806 | 53.37654521 | 1.20623025 | 4.35511829  |             |            |
| 0.00010891 | 67.41286140 | 0.00247875  | 68.435717366  | 0.05641614 | 52.58350709 | 1.28402512 | 3.99514410  |             |            |
| 0.00011593 | 68.40194804 | 0.00263762  | 68.400519635  | 0.06005467 | 51.76226163 | 1.36683794 | 3.66412852  |             |            |
| 0.00012341 | 69.07530509 | 0.00280879  | 68.365252655  | 0.06392786 | 50.91270477 | 1.45499141 | 3.35585707  |             |            |
| 0.00013137 | 69.49037077 | 0.00298545  | 68.330059267  | 0.06805085 | 50.03483211 | 1.54883030 | 3.07945680  |             |            |
| 0.00013984 | 69.72283752 | 0.00316278  | 68.29489013   | 0.07243976 | 49.12876749 | 1.64872127 | 2.82141941  |             |            |
| 0.00014886 | 69.84189356 | 0.00334805  | 68.259613557  | 0.07711172 | 48.19461630 | 1.75509466 | 2.58371730  |             |            |
| 0.00015846 | 69.89753144 | 0.00354056  | 68.22433172   | 0.08208500 | 47.23326207 | 1.86824596 | 2.36493856  |             |            |
| 0.00016868 | 69.92054630 | 0.00373917  | 68.189026517  | 0.08737903 | 46.24594953 | 1.98687347 | 2.16425710  |             |            |
| 0.00017956 | 69.92788612 | 0.00404877  | 68.1536151023 | 0.09301449 | 45.23334527 | 2.11700002 | 1.98146722  |             |            |
| 0.00019114 | 69.92809409 | 0.00435035  | 68.11846109   | 0.09901341 | 44.19746892 | 2.25353479 | 1.81688495  |             |            |
| 0.00020347 | 69.92516562 | 0.004641052 | 68.08344472   | 0.10535522 | 43.14019524 | 2.39887529 | 1.67097551  |             |            |
| 0.00021659 | 69.92082049 | 0.00492959  | 68.04984472   | 0.11219689 | 42.06324200 | 2.55358946 | 1.54379526  |             |            |
| 0.00023056 | 69.91576640 | 0.00524752  | 67.9151574    | 0.11943297 | 40.96749139 | 2.71828183 | 1.43444256  |             |            |
| 0.00024543 | 69.91018624 | 0.00558595  | 67.75591810   | 0.12713573 | 39.85494277 | 2.89359594 | 1.34084174  |             |            |

THULIUM (4F)13  $\Delta = 169$  CMN S-L EX 07-24-73  
NUCLEAR CHARGE = 69.0 RADIUS = 6.0386 FERMI = .0001141 BOHR SURFACE THICKNESS = 0.3666 FERMI = .0000107 BOHR  
SLAYER-LATTER EXCHANGE APPROXIMATION WITH MULTIPLIER 1.50

| SHELL   |   | Q              | ENERGY ETC VALUES |              | FLECTRN VOLTS |          | I/(R+ROR) |          | RADIAL EXPECTATION VALUES |             | (RORR UNITS) |          | RORROR   |          | P MAX |  |
|---------|---|----------------|-------------------|--------------|---------------|----------|-----------|----------|---------------------------|-------------|--------------|----------|----------|----------|-------|--|
| (151/2) | 2 | 4.37237102N    | 03                | 5.94974195N  | 04            | 0.0      | 79.16134  | 0.019985 | 5.470140-04               | 8.032560-07 | 0.012614     |          |          |          |       |  |
| (251/2) | 2 | 7.40967083D    | 02                | 1.008010794D | 03            | 0.0      | 19.11761  | 0.084047 | 8.405310-03               | 1.227650-04 | 0.070230     |          |          |          |       |  |
| (2P1/2) | 2 | 7.078021700    | 02                | 9.62986086D  | 04            | 0.0      | 19.11025  | 0.069780 | 6.037040-03               | 7.456490-05 | 0.053866     |          |          |          |       |  |
| (2P3/2) | 4 | 6.348771290    | 07                | 8.63769381D  | 03            | 1.29532D | 04        | 16.48177 | 0.077160                  | 7.245980-03 | 1.029200-04  | 0.060213 |          |          |       |  |
| (351/2) | 2 | 1.674287120    | 07                | 2.27791785D  | 03            | 0.0      | 7.01926   | 0.219419 | 5.516280-02               | 4.599720-03 | 0.202761     |          |          |          |       |  |
| (3P1/2) | 2 | 1.525667210    | 02                | 2.075716000  | 03            | 0.0      | 6.94360   | 0.208927 | 5.082390-02               | 4.092100-03 | 0.190231     |          |          |          |       |  |
| (3P3/2) | 4 | 1.370793150    | 02                | 1.865005200  | 03            | 2.86026C | 03        | 6.26792  | 0.227743                  | 5.755200-02 | 5.200970-03  | 0.203285 |          |          |       |  |
| (430/2) | 4 | 1.114207430    | 02                | 1.515912640  | 03            | 4.91056D | 02        | 6.16154  | 0.195711                  | 4.502260-02 | 3.602590-03  | 0.160370 |          |          |       |  |
| (3D5/2) | 6 | 1.080081880    | 02                | 1.469483800  | 03            | 4.26942C | 02        | 5.9674   | 0.200000                  | 4.688520-02 | 3.675500-03  | 0.163765 |          |          |       |  |
| (451/2) | 2 | 3.337134290    | 01                | 4.54027132D  | 02            | 0.0      | 2.39379   | 0.949712 | 2.765750-01               | 1.113970-01 | 0.463057     |          |          |          |       |  |
| (4P1/2) | 2 | 2.731671990    | 01                | 3.716521690  | 02            | 0.0      | 2.83413   | 0.502174 | 2.873350-01               | 1.236860-01 | 0.464128     |          |          |          |       |  |
| (4P3/2) | 4 | 2.380865840    | 01                | 3.739239400  | 07            | 6.48C48D | 07        | 7.59930  | 0.533900                  | 3.245320-01 | 1.578500-01  | 0.491958 |          |          |       |  |
| (4D3/2) | 4 | 1.374435710    | 01                | 1.865561020  | 02            | 9.57835D | 01        | 3.28229  | 0.558675                  | 3.625470-01 | 1.245880-01  | 0.492316 |          |          |       |  |
| (4D5/2) | 6 | 1.309906330    | 01                | 1.782166968  | 02            | 8.17223D | 01        | 2.32436  | 0.565908                  | 3.771570-01 | 2.324330-01  | 0.501797 |          |          |       |  |
| (551/2) | 2 | 4.290290740    | 00                | 5.937069250  | 01            | 0.0      | 1.0266    | 1.212626 | 1.656990                  | 00          | 4.112170     | 00       | 1.082433 |          |       |  |
| (5P1/2) | 2 | 2.618564110    | 00                | 3.562635070  | 01            | 0.0      | 0.97116   | 1.361047 | 2.109960                  | 00          | 7.018930     | 00       | 1.175605 |          |       |  |
| (5P3/2) | 4 | 2.171137160    | 00                | 2.953697240  | 01            | 8.06E72D | 01        | 0.87471  | 1.471178                  | 2.468010    | 00           | 9.698110 | 00       | 1.263822 |       |  |
| (4F5/2) | 6 | 8.047737640    | 01                | 1.094918850  | 01            | 1.28074D | 01        | 1.77660  | 0.744122                  | 7.363820-01 | 1.683610     | 00       | 0.484660 |          |       |  |
| (4F1/2) | 7 | 7.075392110-01 | 01                | 9.626283730  | 00            | 1.22C13C | 01        | 1.74670  | 0.760008                  | 7.736860-01 | 1.928070     | 00       | 0.489937 |          |       |  |
| (651/2) | 4 | 4.082580620-01 | 01                | 5.554473410  | 00            | 0.0      | 0.32175   | 3.957C76 | 1.812340                  | 01          | 5.574190     | 02       | 3.178602 |          |       |  |
| TOTAL   |   | 69             | 2.712898570       | 04           | 3.690579890   | 05       |           |          |                           |             |              |          |          |          |       |  |

| R          | POT#R         | R          | POT#R        | R          | POT#R        | R           | POT#R       | R | POT#R |
|------------|---------------|------------|--------------|------------|--------------|-------------|-------------|---|-------|
| 0.00001893 | 16.0738916 78 | 0.00043C74 | 68.84291702  | 0.00980366 | 65.19407700  | 0.22713016  | 28.98594629 |   |       |
| 0.00002015 | 17.11668650   | 0.00045852 | 68.83241978  | 0.01043594 | 64.95983037  | 0.23752082  | 27.78336603 |   |       |
| 0.00002145 | 18.19586514   | 0.00049810 | 68.80212975  | 0.0111C900 | 64.71269824  | 0.25283960  | 26.57749618 |   |       |
| 0.00002283 | 19.33954031   | 0.00051957 | 68.80976998  | 0.01102547 | 64.45211759  | 0.26914635  | 25.37152134 |   |       |
| 0.00002430 | 20.55081926   | 0.00055108 | 68.79652041  | 0.01258814 | 64.17751040  | 0.28450480  | 24.17001938 |   |       |
| 0.00002587 | 21.83279253   | 0.00058876 | 68.78291765  | 0.01340001 | 63.88824506  | 0.30498277  | 22.97826397 |   |       |
| 0.00002754 | 23.18848827   | 0.00062673 | 68.76840475  | 0.01426423 | 63.58383871  | 0.32463247  | 21.80028714 |   |       |
| 0.00002931 | 24.62081437   | 0.00068715 | 68.75292099  | 0.01518420 | 63.26356129  | 0.34559075  | 20.63758961 |   |       |
| 0.00003120 | 26.13248540   | 0.00071017 | 68.73640163  | 0.01612349 | 62.92684119  | 0.36787944  | 19.48992554 |   |       |
| 0.00003322 | 27.27593232   | 0.00075598 | 68.71877766  | 0.01720595 | 62.57307304  | 0.39160563  | 18.35551854 |   |       |
| 0.00003536 | 29.40318934   | 0.00080473 | 68.69997551  | 0.01831564 | 62.20166732  | 0.41686402  | 17.23694066 |   |       |
| 0.00003764 | 31.16575454   | 0.00085663 | 68.67991680  | 0.01949690 | 61.81206106  | 0.44374731  | 16.13777766 |   |       |
| 0.00004007 | 33.01441852   | 0.00091188 | 68.65851802  | 0.02075434 | 61.40372866  | 0.47236655  | 15.06410776 |   |       |
| 0.00004265 | 34.94905380   | 0.00097069 | 68.63569020  | 0.02209288 | 60.97619960  | 0.50283158  | 14.02282738 |   |       |
| 0.00004540 | 36.96835741   | 0.00103330 | 68.61133962  | 0.02351775 | 60.52901056  | 0.53526143  | 13.02060019 |   |       |
| 0.00004833 | 39.06537736   | 0.00109994 | 68.58536243  | 0.02503451 | 60.06179987  | 0.56978282  | 12.06284792 |   |       |
| 0.00005144 | 41.24793147   | 0.00117438 | 68.55976540  | 0.02664910 | 59.57618502  | 0.60653066  | 11.15344397 |   |       |
| 0.00005476 | 43.49654977   | 0.00124C39 | 68.52810008  | 0.02836787 | 59.06578574  | 0.64564853  | 10.29667770 |   |       |
| 0.00005829 | 45.80551420   | 0.00132678 | 68.49657835  | 0.03011578 | 58.53617527  | 0.68728928  | 9.44780592  |   |       |
| 0.00006205 | 48.16142807   | 0.00141235 | 68.46299609  | 0.03214495 | 57.98484500  | 0.73161563  | 8.73253260  |   |       |
| 0.00006606 | 50.56655776   | 0.00150344 | 68.42710821  | 0.03421882 | 57.41119774  | 0.77880078  | 8.02925022  |   |       |
| 0.00007032 | 52.93801754   | 0.00160040 | 68.38887717  | 0.03642500 | 56.81449137  | 0.82902912  | 7.37719645  |   |       |
| 0.00007485 | 55.30678554   | 0.00170762 | 68.34811254  | 0.03877421 | 56.19397300  | 0.88249990  | 6.77516842  |   |       |
| 0.00007968 | 57.61880721   | 0.00181349 | 68.30465050  | 0.04127493 | 55.54982167  | 0.93948306  | 6.22113625  |   |       |
| 0.00008482 | 59.82436747   | 0.00191045 | 68.258931764 | 0.04393693 | 54.87825214  | 0.00000000  | 5.71219262  |   |       |
| 0.00009029 | 61.87829963   | 0.00205496 | 68.20893013  | 0.04677022 | 54.18155714  | 1.06449446  | 5.24683277  |   |       |
| 0.00009611 | 63.72202601   | 0.00218749 | 68.15629364  | 0.04978707 | 53.45914169  | 1.13311945  | 4.81542649  |   |       |
| 0.00010231 | 65.29939054   | 0.00232857 | 68.10020273  | 0.05296004 | 52.70794404  | 1.20623025  | 4.42052156  |   |       |
| 0.00010891 | 66.56579732   | 0.00247875 | 68.04064053  | 0.05641614 | 51.92961324  | 1.28402542  | 4.05720950  |   |       |
| 0.00011593 | 67.50417013   | 0.00263862 | 67.97677826  | 0.06005467 | 51.12359930  | 1.36683796  | 3.72274556  |   |       |
| 0.00012141 | 68.13745910   | 0.00280879 | 67.90897493  | 0.06392786 | 50.28993288  | 1.45499161  | 3.41677504  |   |       |
| 0.00013137 | 68.52494501   | 0.00298995 | 67.83677653  | 0.06800585 | 49.422143855 | 1.548803030 | 3.13104974  |   |       |
| 0.00013984 | 68.74079750   | 0.00316278 | 67.759911775 | 0.07243976 | 48.53921581  | 1.64872127  | 2.86955686  |   |       |
| 0.00014888 | 68.85092514   | 0.00338825 | 67.67811776  | 0.07711172 | 47.62254125  | 1.75505466  | 2.62841181  |   |       |
| 0.00015846 | 68.90220494   | 0.00360656 | 67.59108379  | 0.08208700 | 46.67893853  | 1.86824596  | 2.40618666  |   |       |
| 0.00016888 | 68.92327791   | 0.00381917 | 67.49589316  | 0.08737403 | 45.70926978  | 1.99873747  | 2.20198716  |   |       |
| 0.00017956 | 68.92986644   | 0.00403677 | 67.400007340 | 0.09301449 | 44.71481099  | 2.11700002  | 2.01554870  |   |       |
| 0.00019114 | 68.92980793   | 0.00433033 | 67.29544217  | 0.09801241 | 42.49723068  | 2.25353479  | 1.84714795  |   |       |
| 0.00020347 | 68.92865417   | 0.00463092 | 67.19426722  | 0.10353522 | 42.65842606  | 2.398887529 | 1.69738506  |   |       |
| 0.00021659 | 68.92257717   | 0.00492959 | 67.08618640  | 0.11211689 | 41.48023245  | 2.55358966  | 1.56644324  |   |       |
| 0.00023056 | 68.91764078   | 0.00524752 | 66.94982363  | 0.11943297 | 40.52411439  | 2.71828183  | 1.45389390  |   |       |
| 0.00024543 | 68.912171393  | 0.00558595 | 66.80778901  | 0.12713573 | 39.43103917  | 2.89359594  | 1.35728107  |   |       |
| 0.00026126 | 68.90633254   | 0.00594622 | 66.686647881 | 0.13533528 | 38.32158376  | 3.08021685  | 1.27635288  |   |       |
| 0.00027811 | 68.90008841   | 0.00632977 | 66.51707556  | 0.14400366 | 37.19629617  | 3.27887377  | 1.20165049  |   |       |
| 0.00029604 | 68.89342226   | 0.00673795 | 66.35858067  | 0.15333497 | 36.05660076  | 3.49034296  | 1.13615631  |   |       |
| 0.00031514 | 68.88630851   | 0.00717251 | 66.19065161  | 0.16324551 | 34.90200186  | 3.71545674  | 1.07549119  |   |       |
| 0.00033546 | 68.878717740  | 0.00763509 | 66.0292678   | 0.17377394 | 33.73597893  | 3.95076732  | 1.02214498  |   |       |
| 0.00035710 | 68.87061841   | 0.00812752 | 65.82440141  | 0.18466160 | 32.55986743  | 4.218015726 | 1.0001778   |   |       |
| 0.00038013 | 68.86197634   | 0.00865170 | 65.62680824  | 0.19691188 | 31.37527405  | 4.48168907  | 1.0006000   |   |       |
| 0.00040465 | 68.85275547   | 0.00925068 | 65.43398564  | 0.20961139 | 30.18362618  | 4.723108200 | 1.00000000  |   |       |

LUTECIUM (4F114150) A = 175 CWN S-L FX 07-24-73  
 NUCLFAR CHARGE= 71.0 RADIUS= 6.1112 FERMI =.0001155 RDMR SURFACE THICKNESS=0.5666 FERMI =.0000107 RDMR  
 SLATER-LATTER EXCHANGE APPROXIMATION WITH MULTIPLIER 1.50

| SHELL Q   |                 | ENERGY FIT VALUES |               | RADIAL EXPECTATION VALUES (RDMR UNITS) |          | RMAX        |             |
|-----------|-----------------|-------------------|---------------|----------------------------------------|----------|-------------|-------------|
|           |                 | RYDRERG5          | FLCTPCN VOLTS | 1/(ROROR)                              | 1/R      | R           | ROROR       |
| (1S1/2) 2 | 4.662919170 03  | 6.344041410 04    | 0.0           | 82.79101                               | 0.019296 | 5.107910-04 | 7.032650-07 |
| (2S1/2) 2 | 7.971298530 02  | 1.084519080 04    | 0.0           | 19.94856                               | 0.081003 | 7.814680-03 | 1.062880-04 |
| (2P1/2) 2 | 7.624648690 02  | 1.037356330 04    | 0.0           | 19.93996                               | 0.067125 | 5.594140-03 | 6.421780-05 |
| (2P3/2) 4 | 6.793500080 02  | 9.242760670 03    | 1.429110 04   | 17.01988                               | 0.074730 | 6.796840-03 | 9.054170-05 |
| (3S1/2) 2 | 1.016185730 02  | 2.470975170 03    | 0.0           | 7.33196                                | 0.211150 | 5.110090-02 | 3.947380-03 |
| (3P1/2) 2 | 1.659976130 02  | 2.258447330 03    | 0.0           | 7.25656                                | 0.200758 | 4.694840-02 | 3.492340-03 |
| (3P3/2) 4 | 1.4481743890 02 | 2.015957010 03    | 3.194280 03   | 6.50295                                | 0.214524 | 5.359110-02 | 4.507380-03 |
| (3D3/2) 4 | 1.213298720 02  | 1.650729300 03    | 5.512750 02   | 6.39954                                | 0.188388 | 4.170170-02 | 3.086270-03 |
| (3D5/2) 6 | 1.174082100 02  | 1.507373920 03    | 4.745810 02   | 6.21774                                | 0.192774 | 4.353470-02 | 3.338390-03 |
| (4S1/2) 2 | 3.660782500 01  | 4.980604420 02    | 0.0           | 3.07426                                | 0.474966 | 2.549590-01 | 9.461070-02 |
| (4P1/2) 2 | 3.016331470 01  | 4.103809460 02    | 0.0           | 2.96811                                | 0.401171 | 2.638270-01 | 1.041850-01 |
| (4P3/2) 4 | 2.609151890 01  | 3.545829430 02    | 7.298170 02   | 2.70539                                | 0.513592 | 3.002940-01 | 1.350080-01 |
| (4D3/2) 4 | 1.538421160 01  | 2.093068140 02    | 1.091840 02   | 2.48975                                | 0.534677 | 3.319330-01 | 1.793320-01 |
| (4D5/2) 6 | 1.463247450 01  | 1.990792050 02    | 9.219260 01   | 2.42549                                | 0.546048 | 3.460720-01 | 1.950770-01 |
| (5S1/2) 2 | 4.870862140 00  | 6.626954070 01    | 0.0           | 1.16249                                | 1.153737 | 1.498780 00 | 3.348200 00 |
| (5P1/2) 2 | 3.045342180 00  | 4.141279400 01    | 0.0           | 1.03073                                | 1.285898 | 1.879970 00 | 5.527350 00 |
| (5P3/2) 4 | 2.505741830 00  | 3.409136930 01    | 9.448530 01   | 1.03761                                | 1.394538 | 2.213860 00 | 7.731960 00 |
| (4F5/2) 6 | 1.376986580 00  | 1.973431560 01    | 1.543010 01   | 1.90982                                | 0.679321 | 5.979530-01 | 9.782940-01 |
| (4F7/2) 8 | 1.254568560 00  | 1.706878160 01    | 1.469390 01   | 1.87957                                | 0.692124 | 6.233000-01 | 1.083920 00 |
| (6S1/2) 2 | 4.626336820-01  | 6.294270030 00    | 0.0           | 0.35269                                | 3.619522 | 1.514250 01 | 3.879920 02 |
| (5D3/2) 1 | 3.209108700-01  | 4.366088660 00    | 4.874160 00   | 0.54792                                | 2.492433 | 7.941130 00 | 1.608950 02 |
| TOTAL 71  | 2.912479740 04  | 3.962516060 05    |               |                                        |          |             |             |

| R          | POTR        | R          | POTR        | R          | POTR        | P          | POTR        | R           | POTR       |
|------------|-------------|------------|-------------|------------|-------------|------------|-------------|-------------|------------|
| 0.00001148 | 9.99458031  | 0.00026126 | 70.90213554 | 0.00594422 | 68.55671235 | 0.13533528 | 39.16694029 | 3.08021685  | 1.30677889 |
| 0.00001222 | 10.63462513 | 0.00027811 | 70.69559865 | 0.00632972 | 68.40043443 | 0.14406366 | 38.00197453 | 3.27887377  | 1.22666224 |
| 0.00001301 | 11.31501050 | 0.00029604 | 70.88861913 | 0.00673795 | 68.23488656 | 0.15335497 | 36.82107709 | 3.49034296  | 1.15201701 |
| 0.00001385 | 12.03814590 | 0.00031514 | 70.88116996 | 0.00717251 | 68.05961069 | 0.16324551 | 35.62577663 | 3.71545074  | 1.08143506 |
| 0.00001474 | 12.80655377 | 0.00033546 | 70.87322037 | 0.00763509 | 67.87413447 | 0.17377394 | 34.41788739 | 3.95507672  | 1.02123184 |
| 0.00001569 | 13.62287282 | 0.00035710 | 70.86473704 | 0.00812752 | 67.67797095 | 0.18498140 | 33.19921479 | 4.21015726  | 1.00000000 |
| 0.00001670 | 14.48985341 | 0.00038013 | 70.85568433 | 0.00865170 | 67.47061831 | 0.19691168 | 31.97133594 | 42.52108200 | 1.00000000 |
| 0.00001778 | 15.41035329 | 0.00040465 | 70.84602417 | 0.00920968 | 67.25155939 | 0.20961139 | 30.73547314 |             |            |
| 0.00001893 | 16.38733003 | 0.00043074 | 70.83571598 | 0.00980366 | 67.02026132 | 0.22313016 | 29.49279371 |             |            |
| 0.00002015 | 17.42383005 | 0.00045852 | 70.82471642 | 0.01043594 | 66.77617518 | 0.23752082 | 28.24486745 |             |            |
| 0.00002145 | 18.52297325 | 0.00048810 | 70.81297931 | 0.01110900 | 66.51873583 | 0.25283960 | 26.99441094 |             |            |
| 0.00002283 | 19.68793291 | 0.00051957 | 70.80045535 | 0.01182547 | 66.24736226 | 0.26914635 | 25.74563849 |             |            |
| 0.00002430 | 20.92190758 | 0.00055308 | 70.78709199 | 0.01258814 | 65.96145842 | 0.28650480 | 24.50376147 |             |            |
| 0.00002587 | 22.22808625 | 0.00058876 | 70.77283318 | 0.01340001 | 65.66041521 | 0.30498277 | 23.27350091 |             |            |
| 0.00002754 | 23.60960583 | 0.00062673 | 70.75761913 | 0.01424423 | 65.34361358 | 0.32465247 | 22.05735511 |             |            |
| 0.00002931 | 25.06948818 | 0.00066715 | 70.74138613 | 0.01518420 | 65.01042949 | 0.34559075 | 20.85558741 |             |            |
| 0.00003120 | 26.61057423 | 0.00071017 | 70.72406624 | 0.01616349 | 64.66024061 | 0.36787944 | 19.66778676 |             |            |
| 0.00003322 | 28.23543135 | 0.00075598 | 70.70558737 | 0.01720595 | 64.29243535 | 0.39160563 | 18.49505566 |             |            |
| 0.00003536 | 29.94626239 | 0.00080475 | 70.68587134 | 0.01831564 | 63.90642162 | 0.41686202 | 17.34103085 |             |            |
| 0.00003764 | 31.74466781 | 0.00085663 | 70.66483701 | 0.01949690 | 63.50164078 | 0.44374731 | 16.21160218 |             |            |
| 0.00004007 | 33.63167568 | 0.00091188 | 70.64239639 | 0.02075434 | 63.07757208 | 0.47236655 | 15.11395093 |             |            |
| 0.00004265 | 35.60733305 | 0.00097069 | 70.61845624 | 0.02209288 | 62.63374269 | 0.50283158 | 14.05517241 |             |            |
| 0.00004540 | 37.67055061 | 0.00103330 | 70.59291728 | 0.02351775 | 62.16972085 | 0.53526143 | 13.04140675 |             |            |
| 0.00004833 | 39.81877130 | 0.00109594 | 70.56567383 | 0.02503451 | 61.68510375 | 0.56978282 | 12.07713537 |             |            |
| 0.00005144 | 42.04759188 | 0.00117088 | 70.53661350 | 0.02664910 | 61.17949208 | 0.60653066 | 11.16514643 |             |            |
| 0.00005476 | 44.35030518 | 0.00124639 | 70.50561672 | 0.02836782 | 60.65245452 | 0.64564853 | 10.30678455 |             |            |
| 0.00005829 | 46.71734945 | 0.00132678 | 70.47255642 | 0.03019738 | 60.10349380 | 0.68728928 | 9.50236138  |             |            |
| 0.00006205 | 49.13565190 | 0.00141235 | 70.43725759 | 0.03214495 | 59.53201497 | 0.73161563 | 8.75165157  |             |            |
| 0.00006606 | 51.58785652 | 0.00150344 | 70.39969688 | 0.03421812 | 58.93732054 | 0.77880078 | 8.05396940  |             |            |
| 0.00007032 | 54.05143742 | 0.00160040 | 70.35960212 | 0.03642500 | 58.31862664 | 0.82902912 | 7.40816758  |             |            |
| 0.00007485 | 56.49772476 | 0.00170362 | 70.31685157 | 0.03877421 | 57.67509687 | 0.88249690 | 6.81231421  |             |            |
| 0.00007968 | 58.89093084 | 0.00181349 | 70.27127541 | 0.04127493 | 57.00589871 | 0.93941306 | 6.26361675  |             |            |
| 0.00008482 | 61.18739315 | 0.00193045 | 70.22269133 | 0.04393693 | 56.31025253 | 1.00000000 | 5.75859294  |             |            |
| 0.00009029 | 63.33532395 | 0.00205496 | 70.17090810 | 0.04677062 | 55.58747651 | 1.06449446 | 5.29346297  |             |            |
| 0.00009611 | 65.27743754 | 0.00218749 | 70.11572312 | 0.04978707 | 54.83701220 | 1.13314845 | 4.86462248  |             |            |
| 0.00010231 | 66.95399937 | 0.00232857 | 70.05692241 | 0.05295806 | 54.05843089 | 1.20623025 | 4.46883431  |             |            |
| 0.00010891 | 68.31539167 | 0.00247875 | 69.99428021 | 0.05641614 | 53.25142774 | 1.28402542 | 4.10332623  |             |            |
| 0.00011593 | 69.33734008 | 0.00263862 | 69.92755857 | 0.06005467 | 52.41580700 | 1.36683794 | 3.76566626  |             |            |
| 0.00012341 | 70.03611047 | 0.00280879 | 69.85650702 | 0.06392786 | 51.55147137 | 1.45499141 | 3.45370318  |             |            |
| 0.00013137 | 70.46846129 | 0.00298895 | 69.78086219 | 0.06805085 | 50.65842713 | 1.54883030 | 3.16552756  |             |            |
| 0.00013984 | 70.71127647 | 0.00318278 | 69.70034756 | 0.07243976 | 49.73682281 | 1.64872127 | 2.89951866  |             |            |
| 0.00014886 | 70.83586781 | 0.00338805 | 69.61467317 | 0.07711172 | 48.78701142 | 1.75505466 | 2.65446389  |             |            |
| 0.00015846 | 70.89418892 | 0.00360656 | 69.52353540 | 0.08208100 | 47.80965241 | 1.86824596 | 2.42962372  |             |            |
| 0.00016868 | 70.91838134 | 0.00383917 | 69.42861680 | 0.08737903 | 46.80578703 | 1.98873747 | 2.22475750  |             |            |
| 0.00017956 | 70.92616926 | 0.00408677 | 69.32358557 | 0.09301449 | 45.77637342 | 2.11700002 | 2.03993264  |             |            |
| 0.00019114 | 70.92549754 | 0.00435035 | 69.21409746 | 0.09901341 | 44.72467702 | 2.25353479 | 1.87518226  |             |            |
| 0.00020347 | 70.92354388 | 0.00463692 | 69.09779171 | 0.10539522 | 43.65103215 | 2.39887529 | 1.73003018  |             |            |
| 0.00021659 | 70.91911602 | 0.00492959 | 68.97429508 | 0.11215689 | 42.55752654 | 2.55358946 | 1.60312759  |             |            |
| 0.00023056 | 70.91393258 | 0.00524752 | 68.84321985 | 0.11941297 | 41.44526781 | 2.71828183 | 1.49221250  |             |            |
| 0.00024543 | 70.90824844 | 0.00558595 | 68.70416421 | 0.12713573 | 40.31491981 | 2.89359594 | 1.39441742  |             |            |

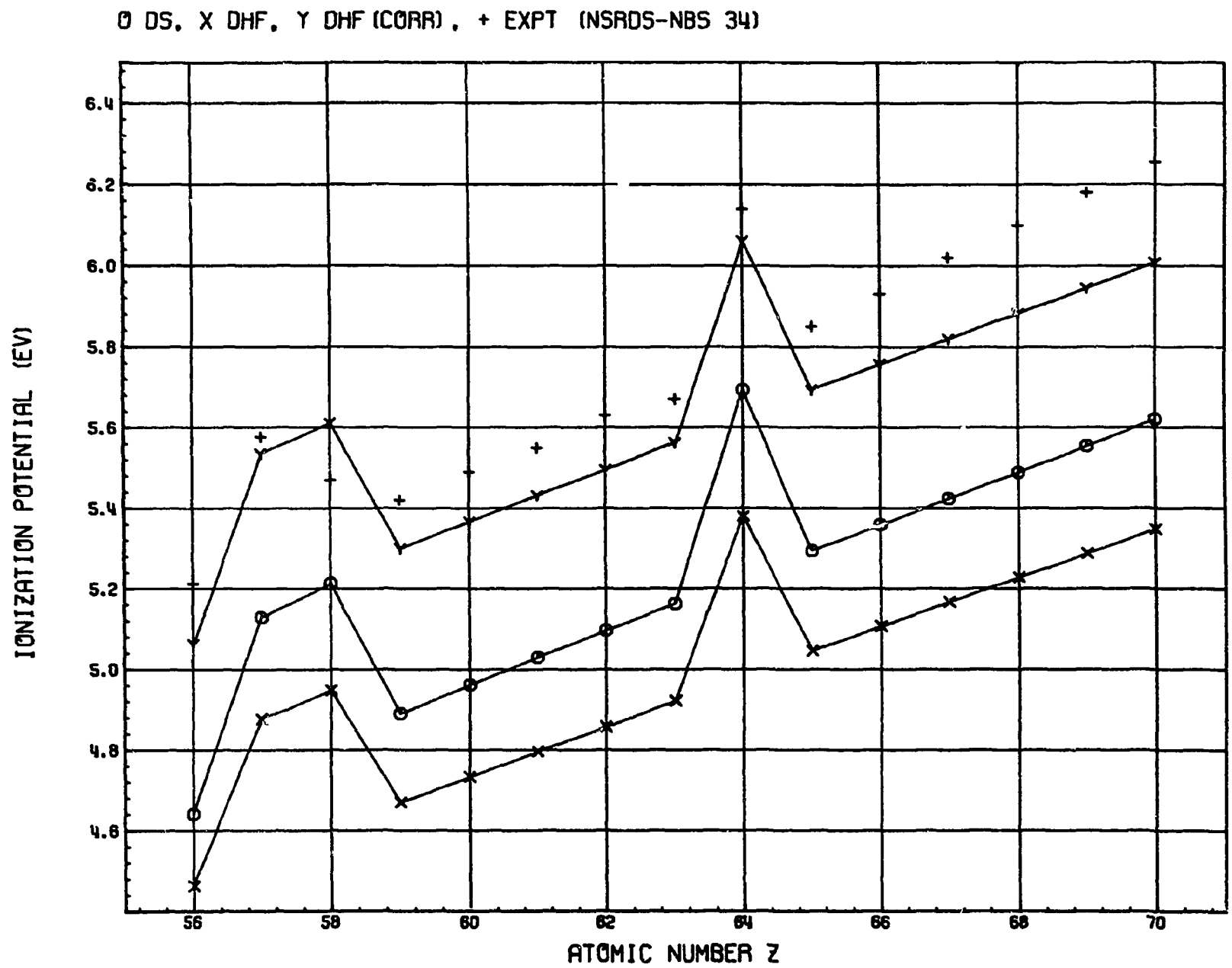


Fig. 2. Computed 6s Energy Eigenvalues and Experimental Ionization Potentials

We have tabulated (Table 2) estimates of the energies of the  $K\alpha_1$ ,  $K\alpha_2$ ,  $L\alpha_1$  and  $L\alpha_2$  X rays of the rare-earth elements obtained by subtraction of the appropriate eigenvalues from our calculations and from the corrected relativistic Hartree-Fock eigenvalues of Mann and Waber.<sup>1</sup> We also list the experimental values of these energies, computed from the wavelengths in Bearden's compilation<sup>6</sup> and the 1969 revision of the fundamental physical constants.<sup>7</sup> In Figs. 3a and 3b, we have plotted the differences of the computed  $K\alpha_1$ ,  $K\alpha_2$ ,  $L\alpha_1$  and  $L\alpha_2$  X ray energies and the experimental values. In Fig. 4 we have plotted the percentage relative errors in the form

$$\delta = \frac{E_{\text{obs}} - E_{\text{calc}}}{E_{\text{obs}}} \times 100$$

as functions of atomic number  $Z$ .

The plots in Figs. 2, 3 and 4 are intended to show trends with atomic number. The point-by-point comparison of theory with experiment should not be taken too seriously, because we have made no attempts to correct our computations for rearrangement effects, quantum electrodynamics effects, etc.

TABLE 2

X-Ray Energies (keV). Values in parentheses after experimental values are standard deviations in the last decimal place reported.

|             | Expt.       | DS      | RHF (Corr) |
|-------------|-------------|---------|------------|
| Z=57 La     |             |         |            |
| $K\alpha_1$ | 33.4423 (3) | 33.4592 | 33.5179    |
| $K\alpha_2$ | 33.0346 (3) | 33.0401 | 33.1091    |
| $L\alpha_1$ | 4.6510 (1)  | 4.6365  | 4.6705     |
| $L\alpha_2$ | 4.6343 (1)  | 4.6187  | 4.6535     |
| Z=58 Ce     |             |         |            |
| $K\alpha_1$ | 34.7202 (3) | 34.7425 | 43.7986    |
| $K\alpha_2$ | 34.2795 (3) | 34.2895 | 34.3567    |
| $L\alpha_1$ | 4.8402 (6)  | 4.8254  | 4.8596     |
| $L\alpha_2$ | 4.8231 (8)  | 4.8059  | 4.8406     |
| Z=59 Pr     |             |         |            |
| $K\alpha_1$ | 36.0269 (3) | 36.0552 | 36.1085    |
| $K\alpha_2$ | 35.5508 (3) | 35.5661 | 35.6313    |
| $L\alpha_1$ | 5.0338 (6)  | 5.0195  | 5.0537     |
| $L\alpha_2$ | 5.0137 (9)  | 4.9982  | 5.0323     |
| Z=60 Nd     |             |         |            |
| $K\alpha_1$ | 37.3616 (3) | 37.3964 | 37.4467    |
| $K\alpha_2$ | 36.8479 (3) | 36.8691 | 36.9321    |
| $L\alpha_1$ | 5.2305 (7)  | 5.2163  | 5.2507     |
| $L\alpha_2$ | 5.208 (1)   | 5.193   | 5.227      |

|             | Expt.       | DS      | RHF (Corr) |
|-------------|-------------|---------|------------|
| Z=61 Pm     |             |         |            |
| $K\alpha_1$ | 38.7253 (7) | 38.7672 | 38.8142    |
| $K\alpha_2$ | 38.1718 (7) | 38.1993 | 38.2599    |
| $L\alpha_1$ | 5.433 (1)   | 5.417   | 5.452      |
| $L\alpha_2$ | 5.408 (1)   | 5.392   | 5.425      |
| Z=62 Sm     |             |         |            |
| $K\alpha_1$ | 40.1188 (4) | 40.1679 | 40.2116    |
| $K\alpha_2$ | 39.5230 (4) | 39.5569 | 39.6151    |
| $L\alpha_1$ | 5.6361 (8)  | 5.6221  | 5.6566     |
| $L\alpha_2$ | 5.6085 (1)  | 5.5947  | 5.6277     |
| Z=63 Eu     |             |         |            |
| $K\alpha_1$ | 41.5429 (4) | 41.5991 | 41.6391    |
| $K\alpha_2$ | 40.9026 (4) | 40.9424 | 40.9979    |
| $L\alpha_1$ | 5.8458 (8)  | 5.8309  | 5.8651     |
| $L\alpha_2$ | 5.8167 (8)  | 5.8013  | 5.8342     |
| Z=64 Gd     |             |         |            |
| $K\alpha_1$ | 42.9970 (4) | 43.0604 | 43.0966    |
| $K\alpha_2$ | 42.3095 (4) | 42.3554 | 42.4080    |
| $L\alpha_1$ | 6.0574 (9)  | 6.0428  | 6.0770     |
| $L\alpha_2$ | 6.0250 (9)  | 6.0108  | 6.0434     |

|             | Expt.       | DS      | RHF (Corr) |
|-------------|-------------|---------|------------|
| Z=65 Tb     |             |         |            |
| $K\alpha_1$ | 44.4824 (5) | 44.5542 | 44.5864    |
| $K\alpha_2$ | 43.7449 (5) | 43.7980 | 43.8476    |
| $L\alpha_1$ | 6.2729 (9)  | 6.2606  | 6.2940     |
| $L\alpha_2$ | 6.2381 (9)  | 6.2260  | 6.2588     |
| Z=66 Dy     |             |         |            |
| $K\alpha_1$ | 45.9992(5)  | 46.0791 | 46.1070    |
| $K\alpha_2$ | 45.2085 (5) | 45.2687 | 45.3152    |
| $L\alpha_1$ | 6.4953 (2)  | 6.4815  | 6.5145     |
| $L\alpha_2$ | 6.4578 (1)  | 6.4442  | 6.4769     |
| Z=67 Ho     |             |         |            |
| $K\alpha_1$ | 47.5475 (5) | 47.6364 | 47.6597    |
| $K\alpha_2$ | 46.7004 (5) | 46.7687 | 46.8118    |
| $L\alpha_1$ | 6.720 (1)   | 6.706   | 6.739      |
| $L\alpha_2$ | 6.680 (1)   | 6.666   | 6.699      |
| Z=68 Er     |             |         |            |
| $K\alpha_1$ | 49.1284 (6) | 49.2264 | 49.2449    |
| $K\alpha_2$ | 48.2218 (6) | 48.2982 | 48.3377    |
| $L\alpha_1$ | 6.9487 (5)  | 6.9353  | 6.9671     |
| $L\alpha_2$ | 6.905 (1)   | 6.892   | 6.925      |
| Z=69 Tm     |             |         |            |
| $K\alpha_1$ | 50.7424 (6) | 50.8496 | 50.8632    |
| $K\alpha_2$ | 49.7734 (6) | 49.8575 | 49.8933    |
| $L\alpha_1$ | 7.180 (1)   | 7.168   | 7.199      |
| $L\alpha_2$ | 7.133 (1)   | 7.122   | 7.154      |

|             | Expt.       | DS      | RHF (Corr) |
|-------------|-------------|---------|------------|
| Z=70 Yb     |             |         |            |
| $K\alpha_1$ | 52.3898 (7) | 52.5066 | 52.5149    |
| $K\alpha_2$ | 51.3549 (6) | 51.4470 | 51.4789    |
| $L\alpha_1$ | 7.4157 (3)  | 7.4052  | 7.4357     |
| $L\alpha_2$ | 7.3674 (3)  | 7.3554  | 7.3878     |

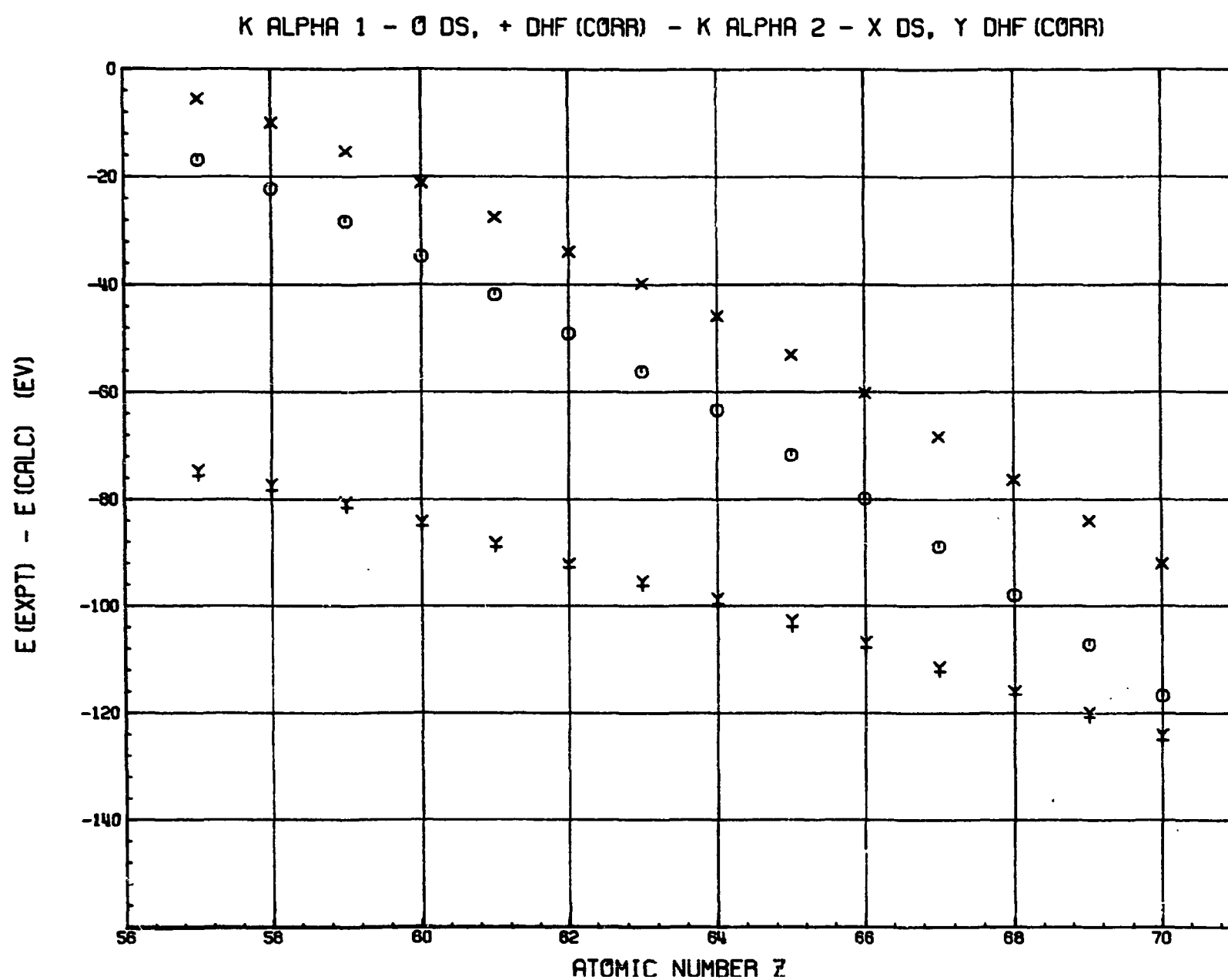


Fig. 3a. Difference of Experimental and Computed K $\alpha$  X-Ray Energies.

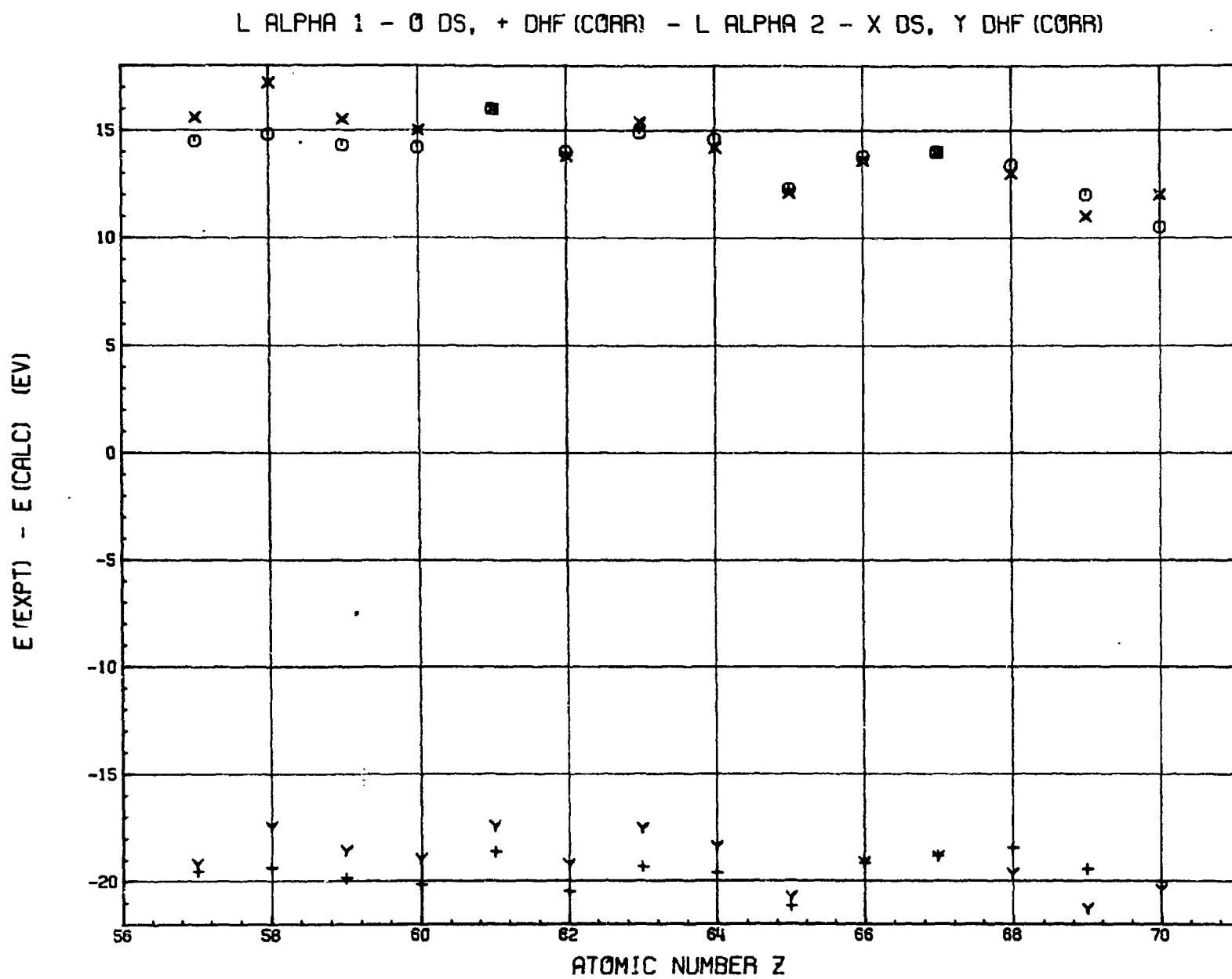


Fig. 3b. Differences of Experimental and Computed  $L\alpha$  X-Ray Energies.

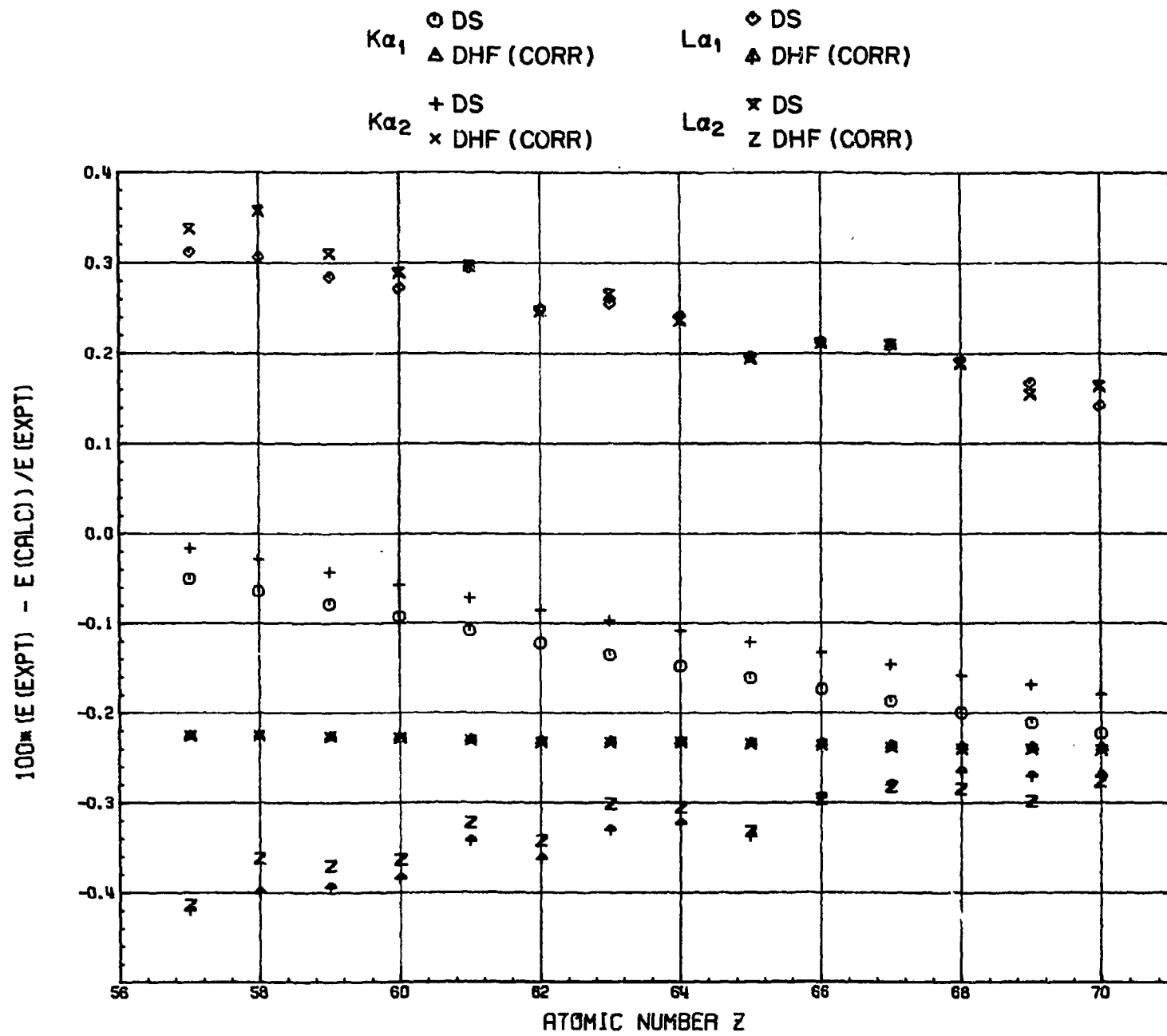


Fig. 4. Percentage Differences of Experimental and Computed and  $K\alpha$   $L\alpha$  X-Ray Energies.

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