Gaussian Basis Sets for the Fifth Row Elements, Mo-Cd, and the Sixth Row Elements W-RN.

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Gaussian basis sets, consisting of 17 s-type, 12 p-type, and 8 d-type functions, for the fifth row elements, Mo–Cd, and 19 s-type, 14 p-type (16 p-type), 10 d-type and 5 f-type functions for the sixth row elements, W–Rn, are presented. The basis sets are of double zeta quality, and are optimized to .002 a.u. in the energy. The energies are compared with D.Z. STO basis sets.

INTRODUCTION

Since the first publication of atomic optimized gaussian-type orbital (GTO) basis sets for the first row atoms by Huzinaga[1] in 1965, many basis sets of different quality have been reported for a large portion of the periodic table. The reported basis sets can be divided roughly into three groups consisting of small, medium, and large basis sets.

The large basis set group consists of basis sets larger than 9 s-type, 5 p-type for the first row atoms; 12 s-type, 9 p-type for the second row; 14–15 s-type, 8–11 p-type, 5 d-type for the third row; and 18 s-type, 14 p-type, 8 d-type for the fourth row.

Such basis sets have been published for the first row by Huzinaga[1] and van Duijeneveldt[2]; for the second row by Veillard[3]; for the third row (or parts thereof) by Huzinaga[4], Wachters[5], and Basch, Hornback, and Moskowitz[6]; and for the fourth row by Huzinaga.[7]

The medium basis set group can be defined as consisting of 7 or 8 s-type and 3 or 4 p-type GTOs for the first row; 10 s-type and 6 p-type GTOs for the second row; 12–13 s-type, 6p-type and 4 d-type GTOs for the third row; and 14–15 s-type, 8–9 p-type, and 6-7 d-type GTOs for the fourth row atoms.

Such basis sets have been presented for the first row atoms by Huzinaga[1], Whitman and Hornback[8], and Roos and Siegbahn[9]; for the transition elements of the third row by Roos, Veillard and Vinot[10]; for the main groups of the third row by Dunning[11]; and for the fourth row transition elements by Hyla-Kryspin, et al.[12] and Huzinaga[18], and for the fourth row main group elements by Stromberg, Gropen and Wahgren.[13]

The small basis set group, finally consists of the basis sets for the first–fourth row atoms suggested by Tatawaki, Huzinaga and Sakai.[14] These basis sets are, however, not small in terms of number of primitive Gaussians used, but specially designed for minimal basis set molecular calculations.

For the fourth row transition elements there exist two basis sets of medium size.[12,18] The basis sets presented by Hyla-Krypsin, et al.[12] give energies which are about .5 a.u. higher than the energies obtained with the STO-basis sets presented by Clementi and Roetti.[15] The other alternative are the sets presented by Huzinaga.[18] These sets give an energy very close to the STO-calculations.[15] The structure of these basis sets are, however, far from a double zeta type even if the energies are comparable. This makes both these basis sets inconvenient to use for ab initio molecular calculations because of either bad energy, or difficulties with the contractions, and for ECP-calculations[16] because of difficulties with truncation. In this work we present a 17 s-type, 12 p-type and 8 d-type basis set of the GTO type for the elements Mo–Cd.

There are, to our knowledge, no basis set presented for the sixth row elements of the

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GTO type. McLean and McLean[19] have, however, presented STO type basis sets for the elements with the atomic numbers Z = 55–92. These basis sets are of double Zeta quality. In this work we present a 19 s-type, 16 (14) p-type, 8 d-type and 5 f-type basis set of the GTO type for the elements W–Rn.

Both these basis sets may serve as a starting point for doing relativistic DHF-calculations, as well as non-relativistic and relativistic calculations using the ECP-method.[16] The size of the basis sets are comparable with the medium basis sets of the other groups. We have, however, emphasized the double zeta structure of the basis sets in order to make them suitable for a DZ-type contraction. This is a convenient structure both for doing all electron calculations as well as for the ECP-procedure.

COMPUTATIONAL PROCEDURE AND RESULTS

The calculations are carried out with a modified version of Huzinaga, et al's atomic program.[17] The exponents for the sets were obtained by energy optimization of each single exponent and scaling by the virial theorem. The convergency is almost complete for the outermost functions and to 0.002 a.u. in the energy for the inner functions. Care was taken to keep the double zeta structure. For basis sets of these size, there exists several minima on the energy surface which offer essentially equivalent descriptions of the electronic structure. We tried to find a balance between obtaining a energy minimum and to keep the double zeta structure of the basis sets.[19,20] In some cases, the outer exponents would drift into describing the inner shells because the improvement of the inner shells would gain more energy than an improvement of the valence shells. In these cases we had to constraint the optimization in order to keep the double zeta structure. The total energies obtained are presented in Tables 1 and 2, together with the STO basis set calculations from references 15 and 19.

The energies calculated for the fifth row elements are higher than obtained by the STO-calculations. The main reason for this is probably a poor description of the s-orbitals.

The energies calculated for the sixth row elements are lower than obtained by the STO-calculations. This is probably due to a better description of the 4f-orbital. As pointed out in ref. 19, the biggest deficiency in the STO basis is in the 4f-shell. This is probably improved in our set by using five GTO-functions. The orbital exponents and the expansion coefficients are presented in Tables 3 and 4.

The inclusion of diffuse functions for molecular calculations will probably improve the basis sets substantially. Experience in our laboratory indicates that one diffuse s-function and one diffuse d-function are important for a reasonable description of the valence electrons even on the atomic level.

Table I. Calculated total energies in a.u. compared with energies calculated in reference 15 where double Zeta STO basis are used.

Atom and State	Present Calc.	Reference 15
Mo ^{7}S	−3975.4931	−3975.5121
Tc ^{6}S	−4204.7354	−4204.7590
Ru ^{5}F	−4441.4642	−4441.5000
Rh ^{4}F	−4685.8016	−4685.8548
Pd ^{3}D	−4937.8005	−4937.8503
Ag ^{2}S	−5197.4193	−5197.4836
Cd ^{1}S	−5465.0379	−5465.0971

Table 2. Calculated total energies in a.u. compared with energies calculated in reference 15 where double Zeta STO basis are used.

Atom and State	Present Calc.	Reference 15
Wo ^{5}D	−15286.993538	−15286.876067
Re ^{6}S	−15784.095029	−15783.919344
Os ^{5}D	−16290.217241	−16290.050754
Ir ^{4}F	−16805.718162	−16805.543789
Pt ^{3}D	−17330.552566	−17330.513867
Au ^{2}S	−17864.895912	−17864.865797
Hg ^{1}S	−18408.535751	−18408.487050
Tl ^{2}P	−18961.396293	−18961.347975
Pb ^{3}P	−19523.619992	−19523.554686
Bi ^{4}S	−20095.221342	−20095.154591
Po ^{3}P	−20676.159552	−20676.088640
At ^{2}P	−21266.548777	−21266.487230
Rn ^{1}S	−21866.402620	−21866.394383

TABLE 3.

BASIS FOR MOLYBDENUM. D*5 S*1. HEPTET S.

TOTAL ENERGY=	-.397549313690401E+04					
ORBITAL SYMMETRY		1S	2S	3S	4S	5S
ENERGY		-721.1792	-102.8300	-18.5641	-2.7454	-.2147
	EXPONENT					
1S	.13994377E+07	.000118	.000038	.000016	-.000006	-.000002
1S	.20741559E+06	.000937	.000299	.000126	-.000049	-.000012
1S	.46322812E+05	.005061	.001621	.000684	-.000267	-.000067
1S	.12737284E+05	.021853	.007088	.002984	-.001168	-.000294
1S	.40254684E+04	.076821	.025744	.010946	-.004278	-.001075
1S	.14215613E+04	.208625	.076530	.032703	-.012851	-.003236
1S	.54970937E+03	.384236	.173208	.077045	-.030296	-.007619
1S	.22697959E+03	.360600	.242365	.112516	-.045163	-.011424
1S	.92850673E+02	.093505	-.020836	-.006351	.003466	.000978
1S	.43373793E+02	-.005942	-.587474	-.446131	.190952	.048507
1S	.20080156E+02	.003450	-.487460	-.479158	.230462	.060214
1S	.74634946E+01	-.001582	-.058387	.586543	-.379761	-.104361
1S	.35478167E+01	.000787	.008951	.709529	-.695005	-.201050
1S	.10927402E+01	-.000291	-.002594	.056198	.706076	.267313
1S	.47413495E+00	.000134	.001202	-.009853	.644693	.374337
1S	.82840386E-01	-.000035	-.000291	.002200	.021191	-.606869
1S	.32278163E-01	.000016	.000138	-.000986	-.010366	-.563797
ORBITAL SYMMETRY		2P	3P	4P		
ENERGY		-94.4239	-15.2660	-1.7059		
	EXPONENT					
2P	.12814278E+05	.000429	-.000188	-.000067		
2P	.97734671E+03	.021022	-.009344	-.003353		
2P	.30524815E+04	.003726	-.001609	-.000591		
2P	.36780059E+03	.080494	-.036046	-.013396		
2P	.16584593E+03	.170748	-.082976	-.029555		
2P	.89174683E+02	.268341	-.128938	-.050383		
2P	.45674792E+02	.386629	-.212584	-.075126		
2P	.21707005E+02	.225241	.029048	.014997		
2P	.90776430E+01	.027791	.552957	.300294		
2P	.39442996E+01	-.000986	.487333	.211397		
2P	.12465268E+01	.000363	.047174	-.643832		
2P	.44043815E+00	-.000137	-.005402	-.526367		
ORBITAL SYMMETRY		3D	4D			
ENERGY		-9.2627	-.3438			
	EXPONENT					
3D	.30880032E+03	.007176	-.001926			
3D	.91144846E+02	.054930	-.014582			
3D	.33443864E+02	.207721	-.057151			
3D	.13482412E+02	.417752	-.109454			
3D	.55363751E+01	.427832	-.100151			
3D	.21754915E+01	.137335	.180011			
3D	.72715031E+00	.001828	.557831			
3D	.20717186E+00	.000806	.491550			

VIRIAL THEOREM: -.19999747E+01

*BASIS FOR TECHNETIUM. D*6 S*2. SEXTET S.*

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TOTAL ENERGY=      -.420473540231477E+04
ORBITAL SYMMETRY        1S          2S          3S          4S          5S
ENERGY                -758.0297   -109.0593    -20.1215     -3.1438     -.2280
                EXPONENT
    1S  .15731666E+07   .000109     .000035     .000015    -.000006    -.000001
    1S  .23289764E+06   .000861     .000276     .000117    -.000047    -.000012
    1S  .51835668E+05   .004683     .001502     .000638    -.000255    -.000064
    1S  .14174690E+05   .020434     .006637     .002812    -.001125    -.000284
    1S  .44470834E+04   .072902     .024406     .010445    -.004169    -.001051
    1S  .15578361E+04   .201748     .073791     .031715    -.012732    -.003217
    1S  .59784772E+03   .380735     .169802     .075952    -.030490    -.007688
    1S  .24554507E+03   .368512     .245310     .114342    -.046913    -.011913
    1S  .10131417E+03   .100584    -.004837     .002438    -.000022     .000130
    1S  .46493236E+02  -.004572    -.583098    -.443506     .193659     .049275
    1S  .21434534E+02   .003128    -.499704    -.493286     .243830     .064165
    1S  .79092461E+01  -.001477    -.061586     .585263    -.395319    -.110112
    1S  .38034466E+01   .000751     .010223     .710755    -.708926    -.205134
    1S  .11850711E+01  -.000279    -.002953     .058385     .728725     .277709
    1S  .52311456E+00   .000128     .001354    -.010334     .633618     .367773
    1S  .87916720E-01  -.000031    -.000310     .002143     .019392    -.651998
    1S  .33520096E-01   .000014     .000140    -.000945    -.006192    -.518181
ORBITAL SYMMETRY        2P          3P          4P
ENERGY                -100.3959   -16.6889    -2.0321
                EXPONENT
    2P  .13538999E+05   .000423    -.000187    -.000069
    2P  .10987462E+04   .018120    -.008152    -.003008
    2P  .32869923E+04   .003478    -.001507    -.000571
    2P  .41791019E+03   .074155    -.033268    -.012713
    2P  .17743542E+03   .186940    -.092048    -.033923
    2P  .94234405E+02   .233164    -.109104    -.044635
    2P  .52630900E+02   .363210    -.208730    -.075804
    2P  .25314813E+02   .266542    -.014824    -.003052
    2P  .10174657E+02   .039323     .537511     .301222
    2P  .43919374E+01  -.002724     .517980     .239654
    2P  .13838060E+01   .000896     .053748    -.646450
    2P  .50081377E+00  -.000321    -.006524    -.527267
ORBITAL SYMMETRY        3D          4D
ENERGY                 -10.4330     -.5368
                EXPONENT
    3D  .33908626E+03   .006689    -.001998
    3D  .10070527E+03   .051286    -.015288
    3D  .37089871E+02   .199865    -.061185
    3D  .14843255E+02   .421221    -.125211
    3D  .60191678E+01   .438144    -.108671
    3D  .23214327E+01   .133886     .206877
    3D  .82615014E+00  -.000468     .576001
    3D  .26044969E+00   .001474     .426276

     VIRIAL THEOREM:   -.19999822E+01
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*BASIS FOR RUTHENIUM . D*7 S*1. QUINTET F.*

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TOTAL ENERGY=     -.444146429515842E+04
ORBITAL SYMMETRY       1S          2S          3S          4S          5S
ENERGY              -795.4865 -115.1343  -21.3901   -3.2369     -.2141
                EXPONENT
    1S .17762998E+07   .000099    .000032    .000014   -.000005   -.000001
    1S .26241432E+06   .000788    .000253    .000108   -.000043   -.000010
    1S .58160992E+05   .004316    .001386    .000593   -.000238   -.000056
    1S .15803900E+05   .019042    .006194    .002640   -.001065   -.000248
    1S .49207114E+04   .068961    .023061    .009927   -.003995   -.000930
    1S .17090379E+04   .194723    .070999    .030676   -.012421   -.002898
    1S .65027786E+03   .376999    .166339    .074754   -.030257   -.007046
    1S .26551075E+03   .376162    .247777    .115923   -.047978   -.011252
    1S .11045011E+03   .108115    .010318    .010575   -.003417   -.000676
    1S .49678437E+02  -.002961   -.579251   -.440915    .194097    .045604
    1S .22788409E+02   .002717   -.510726   -.506956    .253774    .061686
    1S .83548995E+01  -.001319   -.063770    .590099   -.409155   -.105471
    1S .40435407E+01   .000678    .011084    .708695   -.711687   -.189740
    1S .12802130E+01  -.000244   -.003071    .056876    .748689    .262936
    1S .54822423E+00   .000107    .001331   -.008898    .624729    .327952
    1S .86042842E-01  -.000025   -.000297    .001881    .018572   -.587593
    1S .32594322E-01   .000012    .000140   -.000847   -.007450   -.562567
ORBITAL SYMMETRY       2P          3P          4P
ENERGY              -106.2150   -17.8243    -2.0806
                EXPONENT
    2P .13522324E+05   .000443   -.000198   -.000074
    2P .12853649E+04   .015113   -.006873   -.002558
    2P .36094964E+04   .002938   -.001273   -.000489
    2P .47199567E+03   .070896   -.031914   -.012291
    2P .18760231E+03   .203246   -.101296   -.037832
    2P .98704283E+02   .188894   -.082947   -.035565
    2P .60774834E+02   .351715   -.210350   -.076838
    2P .28708834E+02   .304537   -.048056   -.016865
    2P .11120195E+02   .048396    .529715    .301355
    2P .47808765E+01  -.004282    .534627    .251720
    2P .15007803E+01   .001347    .056004   -.650900
    2P .53274440E+00  -.000476   -.006530   -.527585
ORBITAL SYMMETRY       3D          4D
ENERGY              -11.3181     -.3955
                EXPONENT
    3D .37965324E+03   .006002   -.001771
    3D .11199223E+03   .047775   -.014060
    3D .41037036E+02   .192118   -.058108
    3D .16401644E+02   .417754   -.123079
    3D .66367535E+01   .448119   -.110502
    3D .25348109E+01   .136869    .210348
    3D .88078549E+00  -.000835    .565578
    3D .25515802E+00   .001749    .454345

     VIRIAL THEOREM:   -.19999611E+01
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*BASIS FOR RHODIUM . D*8 S*1. QUARTET F.*

TOTAL ENERGY= -.468580164122818E+04

ORBITAL SYMMETRY		1S	2S	3S	4S	5S
ENERGY		-834.0100	-121.5367	-22.8535	-3.4817	-.2130
	EXPONENT					
1S	.20192245E+07	.000089	.000029	.000012	-.000005	-.000001
1S	.29740701E+06	.000715	.000230	.000098	-.000040	-.000009
1S	.65520721E+05	.003958	.001272	.000547	-.000223	-.000050
1S	.17663478E+05	.017684	.005760	.002468	-.001008	-.000225
1S	.54540361E+04	.065024	.021717	.009402	-.003829	-.000853
1S	.18776569E+04	.187394	.068112	.029574	-.012122	-.002707
1S	.70798545E+03	.372815	.162663	.073437	-.030077	-.006698
1S	.28703175E+03	.384139	.250235	.117450	-.049209	-.011047
1S	.11997225E+03	.116091	.023670	.017828	-.006514	-.001323
1S	.52777524E+02	-.001436	-.577298	-.440993	.196500	.044124
1S	.24106461E+02	.002333	-.518483	-.516386	.262923	.061303
1S	.87681195E+01	-.001176	-.065371	.601288	-.430393	-.106893
1S	.42766989E+01	.000615	.012136	.699934	-.711812	-.180630
1S	.13791556E+01	-.000220	-.003320	.055894	.768019	.256212
1S	.58562612E+00	.000093	.001386	-.008046	.616811	.308530
1S	.86662238E-01	-.000021	-.000299	.001670	.017366	-.578069
1S	.32566892E-01	.000010	.000142	-.000761	-.006525	-.562663

ORBITAL SYMMETRY		2P	3P	4P
ENERGY		-112.3596	-19.1531	-2.2687
	EXPONENT			
2P	.14624408E+05	.000442	-.000199	.000075
2P	.10946812E+04	.021722	-.009998	.003771
2P	.34213898E+04	.003980	-.001749	.000680
2P	.44935425E+03	.054458	-.023703	.009710
2P	.29561964E+03	.067284	-.034856	.012417
2P	.14505149E+03	.277775	-.133969	.053878
2P	.63389245E+02	.439843	-.244771	.094349
2P	.28339691E+02	.279930	-.030520	.007777
2P	.11452496E+02	.038804	.547412	-.318680
2P	.49802699E+01	-.002290	.513123	-.239701
2P	.16121201E+01	.000706	.051842	.663668
2P	.57282901E+00	-.000264	-.005345	.517544

ORBITAL SYMMETRY		3D	4D
ENERGY		-12.3937	-.4309
	EXPONENT		
3D	.42776314E+03	.005298	-.001624
3D	.12521726E+03	.043879	-.013422
3D	.45589600E+02	.183415	-.057637
3D	.18144297E+02	.413796	-.127300
3D	.73275618E+01	.456968	-.117950
3D	.28016571E+01	.142478	.212465
3D	.98418167E+00	-.000756	.568104
3D	.28675251E+00	.001986	.448121

VIRIAL THEOREM: -.19999575E+01

*BASIS FOR PALADIUM . D*9 S*1. TRIPLET D*

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TOTAL ENERGY=     -.4937800514941O6E+04
ORBITAL SYMMETRY       1S          2S          3S          4S          5S
ENERGY              -873.4474   -128.1068    -24.3518     -3.7274     -.2119
                EXPONENT
    1S  .22793016E+07   .000081     .000026     .000011    -.000005    -.000001
    1S  .33720433E+06   .000644     .000208     .000089    -.000037    -.000008
    1S  .74226048E+05   .003596     .001157     .000500    -.000206    -.000044
    1S  .19823488E+05   .016357     .005336     .002299    -.000949    -.000202
    1S  .60538445E+04   .061206     .020409     .008883    -.003657    -.000776
    1S  .20648846E+04   .179796     .065168     .028422    -.011776    -.002508
    1S  .77180532E+03   .367766     .158517     .071876    -.029746    -.006316
    1S  .31056919E+03   .392163     .252700     .118902    -.050352    -.010782
    1S  .13030006E+03   .124842     .035257     .024143    -.009288    -.001848
    1S  .55612160E+02   .000347    -.580290    -.446309     .201192     .043072
    1S  .25280193E+02   .001820    -.520764    -.519700     .269072     .059948
    1S  .91129412E+01  -.000965    -.065068     .627416    -.464036    -.110517
    1S  .44708590E+01   .000512     .012949     .678411    -.700296    -.168672
    1S  .14778940E+01  -.000182    -.003530     .052844     .792627     .250358
    1S  .62057754E+00   .000074     .001412    -.006721     .605265     .288478
    1S  .86030333E-01  -.000016    -.000295     .001390     .015629    -.574446
    1S  .32431645E-01   .000008     .000142    -.000649    -.005660    -.556675
ORBITAL SYMMETRY       2P          3P          4P
ENERGY              -118.6706    -20.5154     -2.4580
                EXPONENT
    2P  .16006171E+05   .000402    -.000183     .000070
    2P  .12529862E+04   .019085    -.008856     .003392
    2P  .38726491E+04   .003400    -.001497     .000591
    2P  .47870615E+03   .067624    -.029896     .012192
    2P  .29733321E+03   .043406    -.024874     .008576
    2P  .16490561E+03   .255642    -.121395     .049759
    2P  .71536904E+02   .440067    -.247600     .097026
    2P  .31643287E+02   .308204    -.059070     .020160
    2P  .12452625E+02   .047173     .538870    -.319423
    2P  .53988806E+01  -.003757     .529044    -.253874
    2P  .17457600E+01   .001151     .054805     .666545
    2P  .62047777E+00  -.000415    -.005627     .517997
ORBITAL SYMMETRY       3D          4D
ENERGY              -13.5023     -.4675
                EXPONENT
    3D  .49340496E+03   .004455    -.001413
    3D  .14199436E+03   .039477    -.012480
    3D  .50898298E+02   .174383    -.056684
    3D  .20087953E+02   .409057    -.130578
    3D  .80977120E+01   .465245    -.126250
    3D  .31150208E+01   .150120     .209090
    3D  .11035083E+01   .000031     .569900
    3D  .32310687E+00   .002211     .447450 1

     VIRIAL THEOREM:   -.19999467E+01
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*BASIS FOR SILVER, D*9 S*2, DOUBLET D*

```
TOTAL ENERGY=     -.5197419374883 46E+04
ORBITAL SYMMETRY        1S          2S          3S          4S          5S
ENERGY                -914.0261  -135.0790   -26.1160    -4.1801     -.2559
              EXPONENT
    1S  .24664478E+07   .000077     .000025   -.000011    -.000005    -.000001
    1S  .36512837E+06   .000616     .000199   -.000086    -.000036    -.000009
    1S  .80073473E+05   .003465     .001114   -.000485    -.000203    -.000048
    1S  .21268394E+05   .015911     .005211   -.002253    -.000946    -.000226
    1S  .64341100E+04   .060595     .020159   -.008837    -.003691    -.000881
    1S  .21663029E+04   .181244     .066065   -.028899    -.012189    -.002911
    1S  .80083475E+03   .372256     .159857   -.073184    -.030697    -.007339
    1S  .32188857E+03   .387164     .256316   -.120469    -.052169    -.012495
    1S  .13916735E+03   .122296     .015836   -.015563    -.004959    -.001194
    1S  .54807387E+02   .004813    -.630683    .509000     .233128     .056693
    1S  .24693249E+02  -.000549    -.470188    .451248     .248017     .061503
    1S  .87455636E+01   .000246    -.049068   -.768089    -.629623    -.166971
    1S  .43406869E+01  -.000195     .011207   -.545291    -.541479    -.152793
    1S  .14361951E+01   .000081    -.003175   -.044497     .912737     .355349
    1S  .62039870E+00  -.000033     .001354    .008282     .476313     .257340
    1S  .10009996E+00   .000008    -.000296   -.001866     .011110    -.731501
    1S  .36414185E-01  -.000003     .000131    .000820    -.003720    -.423225
ORBITAL SYMMETRY        2P          3P          4P
ENERGY                -125.3816   -22.1413    -2.8372
              EXPONENT
    2P  .15926060E+05   .000441    -.000204    .000079
    2P  .13487612E+04   .016542    -.007854    .003036
    2P  .38771796E+04   .003563    -.001561    .000633
    2P  .54691358E+03   .061054    -.026871    .011191
    2P  .28257251E+03   .070404    -.040702    .014567
    2P  .17615632E+03   .214416    -.096776    .041846
    2P  .78878744E+02   .440345    -.253885    .100622
    2P  .34122269E+02   .330516    -.066380    .024824
    2P  .12737152E+02   .048323     .575387   -.357178
    2P  .54645251E+01  -.004929     .500301   -.213207
    2P  .17446082E+01   .001437     .043437    .727249
    2P  .63233187E+00  -.000518    -.004439    .445005
ORBITAL SYMMETRY        3D          4D
ENERGY                 -14.8723     -.6970
              EXPONENT
    3D  .51326732E+03   .004488    -.001515
    3D  .15189997E+03   .037912    -.012773
    3D  .54850920E+02   .172013    -.059537
    3D  .21319618E+02   .420746    -.143517
    3D  .84550623E+01   .466916    -.131032
    3D  .32668348E+01   .138006     .240073
    3D  .11758928E+01   .000659     .587705
    3D  .36162557E+00   .001861     .391317  1

     VIRIAL THEOREM:   -.20000171E+01
```

*BASIS FOR CADMIUM. D*10 S*2. SINGLET S*

```
TOTAL ENERGY=     -.5465037989415 29E+04
ORBITAL SYMMETRY       1S          2S          3S          4S          5S
ENERGY              -955.2903   -141.9846    -27.6876     -4.4335     -.2593
              EXPONENT
    1S  .26966473E+07   .000073     .000024     .000010   -.000004     .000001
    1S  .39716818E+06   .000586     .000190     .000082   -.000035     .000008
    1S  .87165314E+05   .003275     .001056     .000461   -.000195     .000046
    1S  .23333882E+05   .014841     .004857     .002114   -.000894     .000209
    1S  .71327509E+04   .055939     .018638     .008193   -.003457     .000808
    1S  .24263210E+04   .167182     .060398     .026589   -.011288     .002646
    1S  .90602687E+03   .351326     .148517     .067858   -.028775     .006727
    1S  .36744488E+03   .396089     .247376     .116938   -.050689     .011944
    1S  .15964308E+03   .151260     .074508     .044261   -.018539     .004242
    1S  .64314338E+02   .007702    -.545882    -.414862    .191597    -.045231
    1S  .29090498E+02  -.000331    -.560877    -.566118    .299138    -.073291
    1S  .10383109E+02   .000045    -.077787     .579772   -.444924     .117428
    1S  .51857168E+01  -.000066     .016679     .718369   -.749912     .200532
    1S  .17235995E+01   .000026    -.004594     .062974    .775526    -.275036
    1S  .74367228E+00  -.000009     .001890    -.008852    .630289    -.333147
    1S  .11726346E+00   .000002    -.000401     .001802    .017191     .604863
    1S  .42439518E-01  -.000001     .000179    -.000783   -.005463     .551198
ORBITAL SYMMETRY       2P          3P          4P
ENERGY              -132.0252   -23.5754     -3.0355
              EXPONENT
    2P  .18879856E+05   .000352    -.000163     .000064
    2P  .14846041E+04   .016740    -.007875     .003112
    2P  .45781388E+04   .002968    -.001321     .000538
    2P  .56323368E+03   .062663    -.027978     .011736
    2P  .34065261E+03   .038181    -.022694     .008042
    2P  .19501957E+03   .235741    -.112164     .047468
    2P  .84455826E+02   .434542    -.246877     .100141
    2P  .37130829E+02   .336302    -.091726     .035287
    2P  .14452454E+02   .057984     .517709    -.319717
    2P  .62890997E+01  -.005302     .554735    -.282919
    2P  .20519356E+01   .001648     .061931     .666459
    2P  .74386972E+00  -.000592    -.006421     .523965
ORBITAL SYMMETRY       3D          4D
ENERGY              -16.0491     -.7478
              EXPONENT
    3D  .57877186E+03   .003960    -.001357
    3D  .16731679E+03   .035656    -.012246
    3D  .59938384E+02   .164659    -.057860
    3D  .23520380E+02   .406110    -.141846
    3D  .94516036E+01   .475445    -.137866
    3D  .36296557E+01   .153321     .224393
    3D  .13373112E+01  -.001826     .579209
    3D  .41853493E+00   .002047     .408811

     VIRIAL THEOREM:   -.19999530E+01
```

TABLE 4.

BASIS FOR TUNGSTEN, D*4, QUINTET D.

TOTAL ENERGY=	-.152869935382614E+05						
ORBITAL SYMMETRY	1S	2S	3S	4S	5S	6S	
ENERGY	-2362.6906	-393.3003	-91.7559	-19.4679	-2.8749	-.2190	
EXPONENT							
1S .60852057E+07	.000079	.000026	.000012	.000006	-.000002	.000001	
1S .90890775E+06	.000598	.000201	.000094	.000046	-.000018	.000005	
1S .20811144E+06	.003218	.001057	.000498	.000243	-.000096	.000025	
1S .57003673E+05	.013946	.004759	.002238	.001091	-.000430	.000112	
1S .18464107E+05	.047832	.016070	.007623	.003718	-.001468	.000381	
1S .66224047E+04	.141171	.053010	.025228	.012337	-.004868	.001264	
1S .25060364E+04	.320546	.131245	.064487	.031707	-.012539	.003257	
1S .10054513E+04	.416153	.264214	.135727	.067667	-.026806	.006967	
1S .42543920E+03	.194509	.085903	.051131	.026120	-.010467	.002720	
1S .14296992E+03	.010503	-.669139	-.601341	-.340289	.139008	-.036260	
1S .66373961E+02	-.001974	-.433058	-.483207	-.313503	.131621	-.034539	
1S .27531745E+02	.000819	-.083710	.666601	.696533	-.323679	.086244	
1S .16232591E+02	-.000498	.034770	.641324	.757295	-.372162	.099521	
1S .61112354E+01	.000176	-.013307	.140378	-.741380	.532961	-.149979	
1S .30893488E+01	-.000089	.007356	-.040964	-.726147	.748671	-.230390	
1S .99779247E+00	.000030	-.002532	.012553	-.027553	-.848978	.339165	
1S .42693012E+00	-.000014	.001095	-.005425	.000871	-.574412	.370200	
1S .80834364E-01	.000004	-.000283	.001381	.000075	-.007471	-.708398	
1S .29729150E-01	-.000002	.000120	-.000585	-.000057	.001214	-.486812	
ORBITAL SYMMETRY	2P	3P	4P	5P			
ENERGY	-376.4200	-83.8973	-16.1262	-1.8058			
EXPONENT							
2P .11457796E+05	.002936	.001465	.000709	.000254			
2P .48782941E+05	.000328	.000164	.000079	.000029			
2P .36559435E+04	.016920	.008599	.004133	.001504			
2P .13605025E+04	.071049	.036950	.018053	.006484			
2P .56312982E+03	.208432	.115523	.056592	.020708			
2P .25153958E+03	.389491	.232026	.117884	.042373			
2P .11794034E+03	.366038	.202071	.095165	.036055			
2P .56683851E+02	.114348	-.274222	-.199183	-.082736			
2P .27215283E+02	.005124	-.632796	-.539031	-.206663			
2P .13460768E+02	.000254	-.241362	.111642	.056931			
2P .59275072E+01	-.000206	-.020292	.756716	.480875			
2P .27725557E+01	.000038	.001934	.312240	.028698			
2P .93128499E+00	-.000011	-.000670	.016848	-.772935			
2P .34792891E+00	.000004	.000234	-.002238	-.356148			
ORBITAL SYMMETRY	3D	4D	5D				
ENERGY	-69.4281	-10.0577	-.4209				
EXPONENT							
3D .30172831E+04	.000965	.000495	.000124				
3D .89107070E+03	.010363	.005022	.001308				
3D .31031861E+03	.070764	.036445	.009294				
3D .11844351E+03	.274059	.139601	.036467				
3D .48572138E+02	.498357	.258671	.065169				
3D .20916549E+02	.320310	-.053802	-.020872				
3D .81792389E+01	.039688	-.615630	-.206851				
3D .32793553E+01	-.001265	-.418553	-.034076				
3D .90551736E+00	.000517	-.038065	.544300				
3D .26710639E+00	-.000164	.005582	.599636				
ORBITAL SYMMETRY	4F						
ENERGY	-2.0727						
EXPONENT							
4F .13593927E+03	.018888						
4F .44699368E+02	.116273						
4F .17078576E+02	.333584						
4F .65692527E+01	.480982						
4F .23025627E+01	.375678						

VIRIAL THEOREM: -.19998915E+01

BASIS FOR RHENIUM. D*5. SEXTET S.

```
TOTAL ENERGY=     -.15784095029664E+05
ORBITAL SYMMETRY        1S          2S          3S          4S          5S          6S
ENERGY              -2429.6841  -405.7485   -95.1956   -20.4674    -3.0964     -.2266
              EXPONENT
    1S .59574938E+07   .000082   -.000027    .000013   -.000006   -.000003    .000001
    1S .92311920E+06   .000608   -.000204    .000096   -.000047   -.000019    .000005
    1S .20677388E+06   .003406   -.001124    .000531   -.000259   -.000104    .000027
    1S .56878059E+05   .014146   -.004815    .002267   -.001111   -.000446    .000115
    1S .18607131E+05   .049576   -.016779    .007978   -.003902   -.001570    .000406
    1S .66033710E+04   .144737   -.054198    .025820   -.012704   -.005103    .001321
    1S .25188993E+04   .326654   -.135870    .067015   -.033011   -.013320    .003447
    1S .99672900E+03   .420449   -.268134    .138122   -.069477   -.027997    .007252
    1S .42600373E+03   .177092   -.075565    .046374   -.023132   -.009601    .002484
    1S .14926384E+03   .013409    .645943   -.582116    .327899    .137071   -.035633
    1S .69417818E+02  -.004679    .462223   -.508794    .337150    .142788   -.037359
    1S .27120619E+02   .003018    .068580    .849168   -.921508   -.433473    .115243
    1S .13950235E+02  -.002274   -.025641    .524055   -.595364   -.319352    .085567
    1S .58412793E+01   .001276    .012627    .055589    .987861    .773517   -.219398
    1S .28911472E+01  -.000681   -.006755   -.011131    .535384    .569737   -.180301
    1S .10012995E+01   .000253    .002510    .003793    .024358   -.934325    .389680
    1S .43950785E+00  -.000106   -.001050   -.001658   -.003179   -.494336    .315610
    1S .83149854E-01   .000026    .000256    .000397    .000769   -.010975   -.726542
    1S .30854805E-01  -.000011   -.000108   -.000168   -.000317    .003112    -.4606
ORBITAL SYMMETRY        2P          3P          4P          5P
ENERGY              -388.5863   -87.1810   -17.0378    -1.9793
              EXPONENT
    2P .11478492E+05   .003071    .001543    .000748   -.000275
    2P .48871491E+05   .000343    .000171    .000083   -.000031
    2P .36567095E+04   .017731    .008990    .004357   -.001625
    2P .13615728E+04   .073790    .038703    .018954   -.006978
    2P .56428271E+03   .214832    .118853    .058784   -.022054
    2P .25224467E+03   .393396    .238181    .121062   -.044610
    2P .11840648E+03   .362231    .186591    .088606   -.034440
    2P .55405819E+02   .108040   -.299550   -.228166    .097191
    2P .27188163E+02  -.000238   -.632711   -.518628    .202422
    2P .12797341E+02   .002291   -.224763    .138794   -.071818
    2P .60750185E+01  -.001286   -.002260    .745600   -.492213
    2P .28556970E+01   .000492   -.003906    .305043   -.019560
    2P .99091449E+00  -.000150    .001064    .013760    .791411
    2P .36487415E+00   .000047   -.000305   -.001187    .340068
ORBITAL SYMMETRY        3D          4D          5D
ENERGY              -72.4262   -10.8000     -.4952
              EXPONENT
    3D .30689345E+04   .000979   -.000500    .000132
    3D .89771214E+03   .011126   -.005496    .001512
    3D .30802084E+03   .075737   -.039129    .010516
    3D .11811218E+03   .283869   -.147052    .040626
    3D .48537097E+02   .504424   -.258538    .068250
    3D .20753554E+02   .304437    .071109   -.027167
    3D .83588104E+01   .031989    .622983   -.223415
    3D .33426642E+01   .000534    .404737   -.020078
    3D .93864691E+00  -.000010    .030762    .589012
    3D .27793945E+00   .000008   -.004044    .551245
ORBITAL SYMMETRY        4F
ENERGY              -2.5448
              EXPONENT
    4F .13515114E+03   .020699
    4F .44688561E+02   .126681
    4F .17034683E+02   .346990
    4F .65914094E+01   .491031
    4F .22367939E+01   .345338

     VIRIAL THEOREM:   -.19999490E+01
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BASIS FOR OSMIUM, D*6, QUINTET D.

```
TOTAL ENERGY=     -.162902172412274E+05
ORBITAL SYMMETRY        1S          2S          3S          4S          5S          6S
ENERGY             -2497.6066  -418.3557   -98.6602    -21.4557     -3.3133     -.2339
                EXPONENT
    1S  .67613397E+07   .000074     .000024     .000012     .000006     .000002     .000001
    1S  .10098975E+07   .000561     .000188     .000089     .000044     .000018     .000005
    1S  .23123493E+06   .003017     .000993     .000470     .000231     .000094     .000024
    1S  .63337414E+05   .013086     .004464     .002102     .001033     .000421     .000109
    1S  .20515674E+05   .045003     .015144     .007221     .003549     .001450     .000375
    1S  .73582274E+04   .133722     .049937     .023757     .011714     .004779     .001237
    1S  .27844849E+04   .308928     .125637     .062049     .030720     .012577     .003257
    1S  .11171681E+04   .417503     .257012     .131192     .065928     .026985     .006992
    1S  .47271022E+03   .213070     .113651     .068843     .035296     .014692     .003808
    1S  .15885547E+03   .014410    -.621981    -.557265    -.315846    -.133767    -.034802
    1S  .73748846E+02  -.003152    -.491042    -.530675    -.345155    -.149008    -.038991
    1S  .27590828E+02   .001508    -.080546     .831900     .906063     .436888     .116353
    1S  .15036212E+02  -.001096     .034138     .506229     .588159     .314196     .084355
    1S  .61902616E+01   .000551    -.015717     .092356    -.907492    -.713499    -.203266
    1S  .31326098E+01  -.000292     .008558    -.027327    -.598743    -.663038    -.208777
    1S  .11086583E+01   .000102    -.003043     .009126    -.024199     .927119     .385659
    1S  .47436680E+00  -.000040     .001213    -.003715     .000968     .534808     .331806
    1S  .89815960E-01   .000010    -.000300     .000911    -.000177     .006840    -.709706
    1S  .33032389E-01  -.000004     .000126    -.000384     .000061    -.001233    -.479065
ORBITAL SYMMETRY        2P          3P          4P          5P
ENERGY             -400.9216   -90.4929    -17.9385     -2.1510
                EXPONENT
    2P  .12730885E+05   .002693     .001349     .000659     .000246
    2P  .54203268E+05   .000300     .000151     .000073     .000028
    2P  .40621594E+04   .015577     .007943     .003854     .001467
    2P  .15116695E+04   .065972     .034374     .016958     .006353
    2P  .62569980E+03   .196871     .109163     .053948     .020654
    2P  .27948842E+03   .379729     .226170     .115965     .043459
    2P  .13104482E+03   .377416     .216544     .104632     .041585
    2P  .62982057E+02   .129135    -.237459    -.176249    -.077920
    2P  .30239203E+02   .006541    -.636421    -.546470    -.218425
    2P  .14956409E+02   .000437    -.268526     .061869     .033597
    2P  .65861191E+01  -.000314    -.023171     .765744     .521092
    2P  .30806174E+01   .000088     .001944     .330462     .026579
    2P  .10347611E+01  -.000026    -.000619     .016472    -.808799
    2P  .38658768E+00   .000010     .000224    -.001905    -.319603
ORBITAL SYMMETRY        3D          4D          5D
ENERGY             -75.4526    -11.5301     -.5154
                EXPONENT
    3D  .33525368E+04   .000873     .000455     .000125
    3D  .99007856E+03   .009448     .004650     .001333
    3D  .34479846E+03   .065539     .034283     .009560
    3D  .13160390E+03   .261156     .135266     .038855
    3D  .53969042E+02   .494566     .262441     .072343
    3D  .23240610E+02   .337077    -.031200    -.015784
    3D  .90880432E+01   .045187    -.618326    -.234034
    3D  .36437281E+01  -.001771    -.427431    -.028172
    3D  .10061304E+01   .000650    -.034886     .605510
    3D  .29678488E+00  -.000208     .004815     .536442
ORBITAL SYMMETRY        4F
ENERGY             -3.0089
                EXPONENT
    4F  .13593927E+03   .022744
    4F  .44699368E+02   .135834
    4F  .17078576E+02   .365152
    4F  .65692527E+01   .489931
    4F  .23025627E+01   .313150 1

     VIRIAL THEOREM:   -.19999925E+01
```

BASIS FOR IRIDIUM, D*7, QUARTET F.

```
TOTAL ENERGY=     -.168057181622308E+05
ORBITAL SYMMETRY        1S          2S          3S          4S          5S          6S
ENERGY              -2566.4475  -431.1527  -102.1788   -22.4503    -3.5197     -.2377
                EXPONENT
    1S  .80290909E+07   .000062     .000020    -.000010    -.000005     .000002     .000001
    1S  .11992533E+07   .000468     .000156    -.000074    -.000036     .000015     .000004
    1S  .27459148E+06   .002517     .000833    -.000395    -.000194     .000080     .000021
    1S  .75213179E+05   .010938     .003707    -.001749    -.000865     .000358     .000091
    1S  .24362363E+05   .037896     .012807    -.006107    -.003004     .001242     .000317
    1S  .87378950E+04   .114453     .041852    -.019926    -.009888     .004093     .001046
    1S  .33065758E+04   .276559     .110648    -.054368    -.026878     .011128     .002843
    1S  .13266371E+04   .413380     .232405    -.117773    -.059576     .024765     .006333
    1S  .56134339E+03   .266025     .180984    -.104533    -.052808     .022008     .005625
    1S  .18864087E+03   .030980    -.478243     .400947     .220834    -.093878    -.024073
    1S  .87576754E+02  -.008826    -.619012     .687723     .446188    -.196405    -.050712
    1S  .32764108E+02   .005041    -.112094    -.545541    -.608023     .299061     .078643
    1S  .17855502E+02  -.003416     .030493    -.772997    -.864614     .445625     .117788
    1S  .61159357E+01   .001725    -.011329    -.112188     .962302    -.763249    -.216003
    1S  .31499741E+01  -.001227     .007814     .040636     .512119    -.663332    -.209954
    1S  .13165318E+01   .000512    -.003194    -.014142     .032549     .831200     .334709
    1S  .56331057E+00  -.000169     .001040     .004524    -.002230     .682468     .379206
    1S  .87656452E-01   .000034    -.000207    -.000873     .000644     .016136    -.752110
    1S  .31625962E-01  -.000015     .000092     .000385    -.000282    -.004991    -.4203
ORBITAL SYMMETRY        2P          3P          4P          5P
ENERGY              -413.4332   -93.8538    -18.8447     -2.3149
                EXPONENT
    2P  .15117926E+05   .002098     .001052     .000517     .000197
    2P  .64366381E+05   .000233     .000117     .000057     .000022
    2P  .48238142E+04   .012255     .006247     .003041     .001176
    2P  .17951076E+04   .052996     .027511     .013626     .005201
    2P  .74301851E+03   .165259     .090743     .044910     .017447
    2P  .33189250E+03   .346345     .203732     .104541     .040006
    2P  .15561573E+03   .401825     .244693     .122030     .048560
    2P  .74791192E+02   .178371    -.118697    -.096204    -.044503
    2P  .35909054E+02   .014507    -.616704    -.521000    -.215010
    2P  .17760735E+02   .000769    -.367868    -.121903    -.048699
    2P  .78210165E+01  -.000521    -.039962     .720667     .478985
    2P  .36582332E+01   .000180     .002207     .448972     .175190
    2P  .12287788E+01  -.000059    -.000660     .027877    -.776859
    2P  .45907287E+00   .000021     .000235    -.002861    -.404202
ORBITAL SYMMETRY        3D          4D          5D
ENERGY              -78.5260    -12.2657     -.5483
                EXPONENT
    3D  .39811374E+04   .000637     .000336     .000096
    3D  .11757183E+04   .007044     .003486     .001041
    3D  .40944817E+03   .050757     .026678     .007748
    3D  .15627964E+03   .218715     .113944     .034034
    3D  .64088238E+02   .468841     .254136     .073643
    3D  .27598224E+02   .395705     .056320     .011380
    3D  .10792051E+02   .073110    -.563560    -.223006
    3D  .43269271E+01  -.003795    -.510271    -.089071
    3D  .11947799E+01   .001391    -.053303     .577754
    3D  .35243204E+00  -.000448     .007407     .578023 ORBITAL  SYMMETRY      4F  ENER
               -3.4746
                EXPONENT
    4F  .13593927E+03   .024871
    4F  .44699368E+02   .146052
    4F  .17078576E+02   .380563
    4F  .65692527E+01   .491054
    4F  .23025627E+01   .283633 1

     VIRIAL THEOREM:   -.19999768E+01
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BASIS FOR PLATINUM. D*9 S*1. TRIPLET D.

```
TOTAL ENERGY=     -.173305525663101E+05
ORBITAL SYMMETRY        1S          2S          3S          4S          5S          6S
ENERGY              -2636.0390  -443.9333  -105.5565   -23.2693    -3.5599     -.2075
              EXPONENT
    1S  .91300140E+07   .000054   -.000018   -.000008   -.000004    .000002    .000000
    1S  .13580639E+07   .000423   -.000142   -.000067   -.000033    .000014    .000003
    1S  .30373397E+06   .002285   -.000755   -.000358   -.000177    .000074    .000016
    1S  .84109073E+05   .009828   -.003338   -.001579   -.000783    .000325    .000073
    1S  .26951215E+05   .035158   -.011832   -.005642   -.002784    .001160    .000260
    1S  .96066990E+04   .105634   -.038595   -.018415   -.009174    .003812    .000854
    1S  .36777407E+04   .255827   -.100394   -.049199   -.024387    .010177    .002279
    1S  .14750260E+04   .414408   -.225967   -.114393   -.057996    .024159    .005414
    1S  .60753748E+03   .295203   -.202120   -.114909   -.058309    .024626    .005522
    1S  .19962257E+03   .034750    .436738    .362263    .199561   -.086053   -.019354
    1S  .93973887E+02  -.008692    .649949    .709555    .456238   -.199496   -.045083
    1S  .31685057E+02   .004294    .139241   -.663598   -.746326    .362717    .083467
    1S  .16361737E+02  -.003402   -.058878   -.681593   -.789704    .439077    .102410
    1S  .67583203E+01   .002045    .029890   -.032896    .922723   -.767993   -.190207
    1S  .36036514E+01  -.001117   -.015926   -.007353    .610789   -.616930   -.165255
    1S  .11429253E+01   .000348    .004891    .003270    .058909    .923164    .343599
    1S  .52176034E+00  -.000147   -.002052   -.001370   -.015440    .487946    .232136
    1S  .72085695E-01   .000029    .000402    .000288    .002940    .016256   -.714856
    1S  .27356546E-01  -.000014   -.000191   -.000137   -.001402   -.006855   -.417253
ORBITAL SYMMETRY        2P          3P          4P          5P
ENERGY              -425.9412   -97.0760   -19.5777    -2.3285
              EXPONENT
    2P  .16818821E+05   .001832    .000919    .000453    .000174
    2P  .71696656E+05   .000202    .000102    .000050    .000019
    2P  .53590053E+04   .010749    .005489    .002684    .001046
    2P  .19941195E+04   .047061    .024377    .012116    .004651
    2P  .82255038E+03   .151225    .082848    .041147    .016103
    2P  .36596725E+03   .329631    .192432    .098904    .038058
    2P  .17195961E+03   .404851    .252105    .127416    .051098
    2P  .83736123E+02   .204807   -.060460   -.058221   -.029096
    2P  .39832673E+02   .024337   -.592160   -.497198   -.206181
    2P  .19688815E+02  -.000588   -.421289   -.208148   -.090845
    2P  .86049659E+01   .000090   -.053355    .690458    .463336
    2P  .39991649E+01  -.000086    .003158    .504095    .221178
    2P  .13126846E+01   .000023   -.000904    .032195   -.773242
    2P  .48329870E+00  -.000005    .000322   -.003198   -.418228
ORBITAL SYMMETRY        3D          4D          5D
ENERGY              -81.4588   -12.8277    -.4309
              EXPONENT
    3D  .45376197E+04   .000527    .000280    .000079
    3D  .13057359E+04   .006012    .002995    .000894
    3D  .45842919E+03   .043066    .022759    .006579
    3D  .17636922E+03   .192797    .101024    .030099
    3D  .72102443E+02   .454035    .248604    .072007
    3D  .30551202E+02   .430652    .099010    .024960
    3D  .11836229E+02   .087573   -.543302   -.216051
    3D  .46983347E+01  -.004255   -.542263   -.105202
    3D  .12802324E+01   .001553   -.057268    .570102
    3D  .36019201E+00  -.000494    .007238    .596799
ORBITAL SYMMETRY        4F
ENERGY              -3.7672
              EXPONENT
    4F  .16136418E+03   .018914
    4F  .53029396E+02   .122022
    4F  .20141209E+02   .356544
    4F  .77059678E+01   .506728
    4F  .26867557E+01   .313062

     VIRIAL THEOREM:   -.19999234E+01
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BASIS FOR GOLD, S*1, DOUBLET S

```
TOTAL ENERGY=     -.178648959125274E+05
ORBITAL SYMMETRY        1S          2S          3S          4S          5S          6S
ENERGY              -2706.7650  -457.1115  -109.1884   -24.2921    -3.7640     -.2062
              EXPONENT
    1S  .94240863E+07   .000054     .000018     .000008   -.000004     .000002     .000000
    1S  .13754422E+07   .000432     .000145     .000068   -.000034     .000014     .000003
    1S  .30669080E+06   .002330     .000772     .000367   -.000182     .000077     .000017
    1S  .84491492E+05   .010200     .003457     .001636   -.000813     .000342     .000074
    1S  .26543620E+05   .037664     .012753     .006095   -.003024     .001273     .000275
    1S  .93046797E+04   .113411     .041451     .019794   -.009876     .004150     .000896
    1S  .35641327E+04   .265762     .106053     .052232   -.026060     .010997     .002377
    1S  .14459715E+04   .412190     .227998     .115662   -.058715     .024738     .005345
    1S  .60364506E+03   .279305     .194621     .112189   -.057617     .024621     .005335
    1S  .20491458E+03   .030844   -.453044    -.376998    .210405    -.091727    -.019940
    1S  .94866768E+02  -.007146   -.639726    -.709951    .456920    -.202420    -.044066
    1S  .35234607E+02   .003815   -.124000     .499195   -.546406     .265929     .058664
    1S  .19540386E+02  -.002661    .036135     .795789   -.945417     .514986     .116270
    1S  .72801752E+01   .001284   -.013110     .126908    .747765    -.631625    -.153081
    1S  .38905484E+01  -.000735    .007277    -.032503    .736467    -.761046    -.192156
    1S  .12522517E+01   .000230   -.002213     .008089    .046837     .927479     .321990
    1S  .55311110E+00  -.000093    .000888    -.003255   -.007686     .517437     .243690
    1S  .75507140E-01   .000019   -.000180     .000638    .001384     .013920    -.661631
    1S  .28534686E-01  -.000009    .000086    -.000304   -.000652    -.005222    -.468528
ORBITAL SYMMETRY        2P          3P          4P          5P
ENERGY              -438.8397  -100.5518   -20.5097    -2.4916
              EXPONENT
    2P  .16873054E+05   .001916     .000964     .000477     .000186
    2P  .72158456E+05   .000210     .000106     .000052     .000020
    2P  .53365550E+04   .011393     .005823     .002863     .001131
    2P  .19709859E+04   .050309     .026183     .013062     .005090
    2P  .80633572E+03   .162199     .089196     .044591     .017694
    2P  .35552526E+03   .347578     .205112     .105934     .041401
    2P  .16579167E+03   .403082     .246965     .125035     .050908
    2P  .80216366E+02   .180453    -.108912    -.092132    -.044175
    2P  .38790536E+02   .016819    -.606838    -.514786    -.216758
    2P  .19337199E+02   .000236    -.381025    -.154651    -.067198
    2P  .86522832E+01  -.000258    -.044962     .706282     .486031
    2P  .40697338E+01   .000060     .002311     .477393     .201278
    2P  .13807124E+01  -.000019    -.000658     .029673    -.780146
    2P  .50972635E+00   .000009     .000246    -.002503    -.412726
ORBITAL SYMMETRY        3D          4D          5D
ENERGY              -84.6452    -13.5882     -.4758
              EXPONENT
    3D  .47268080E+04   .000523     .000278     .000081
    3D  .13290893E+04   .006228     .003134     .000961
    3D  .46465094E+03   .044157     .023495     .006977
    3D  .18003014E+03   .193618     .102325     .031369
    3D  .74171925E+02   .451732     .249039     .074068
    3D  .31616362E+02   .429056     .100655     .026178
    3D  .12357104E+02   .088740    -.539731    -.222699
    3D  .49448522E+01  -.004127    -.545014    -.108996
    3D  .13681377E+01   .001556    -.057498     .579251
    3D  .38991085E+00  -.000480     .007809     .586922
ORBITAL SYMMETRY        4F
ENERGY              -4.2570
              EXPONENT
    4F  .16457891E+03   .019678
    4F  .54510867E+02   .124473
    4F  .20887159E+02   .358766
    4F  .80698463E+01   .505569
    4F  .28511552E+01   .304567

     VIRIAL THEOREM:   -.19999352E+01
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BASIS FOR MERCURY. SINGLET S

```
TOTAL ENERGY=     -.184085357515647E+05
ORBITAL SYMMETRY        1S          2S          3S          4S          5S          6S
ENERGY             -2778.6348  -470.6871  -113.0878   -25.5310    -4.1516     -.2514
                EXPONENT
    1S .94998897E+07   .000054     .000018     .000009    -.000004     .000002     .000000
    1S .14085815E+07   .000432     .000145     .000069    -.000034     .000015     .000004
    1S .31224217E+06   .002376     .000788     .000375    -.000187     .000080     .000020
    1S .84765340E+05   .010582     .003588     .001701    -.000849     .000362     .000090
    1S .26389035E+05   .039366     .013352     .006388    -.003182     .001362     .000339
    1S .91661112E+04   .119645     .043893     .021016    -.010523     .004492     .001118
    1S .34817789E+04   .277613     .111908     .055242    -.027688     .011880     .002959
    1S .14165063E+04   .410424     .232370     .118550    -.060444     .025866     .006443
    1S .60008268E+03   .262990     .180582     .104842    -.054141     .023587     .005887
    1S .20737130E+03   .028226    -.462404    -.387786     .218143    -.096906    -.024268
    1S .96896340E+02  -.006444    -.631416    -.700840     .452291    -.203382    -.051111
    1S .34782672E+02   .003453    -.128594     .594130    -.648900     .321813     .082301
    1S .18868997E+02  -.002706     .048045     .720428    -.898647     .512277     .133693
    1S .80205980E+01   .001466    -.021034     .089582     .713650    -.607520    -.168971
    1S .42275907E+01  -.000744     .010352    -.009533     .812759    -.836684    -.247287
    1S .13057630E+01   .000232    -.003151     .001909     .062021     .926578     .389163
    1S .60473886E+00  -.000105     .001407    -.000889    -.014045     .512604     .278065
    1S .10090940E+00   .000022    -.000299     .000170     .002650     .016607    -.702062
    1S .36877299E-01  -.000010     .000130    -.000074    -.001137    -.005807    -.462065
ORBITAL SYMMETRY        2P          3P          4P          5P
ENERGY             -452.1373  -104.2931   -21.6573    -2.8219
                EXPONENT
    2P .17078800E+05   .001972     .000995     .000495    -.000196
    2P .73262682E+05   .000214     .000108     .000053    -.000021
    2P .53541727E+04   .011945     .006113     .003020    -.001217
    2P .19588228E+04   .053328     .027865     .013960    -.005560
    2P .79590756E+03   .171561     .094713     .047617    -.019283
    2P .34912051E+03   .361077     .214952     .111629    -.044613
    2P .16187452E+03   .400525     .240912     .121840    -.050602
    2P .77508827E+02   .161760    -.155144    -.125462     .059706
    2P .37749779E+02   .010938    -.620042    -.532578     .229806
    2P .18864161E+02   .000945    -.340415    -.088730     .035152
    2P .85572345E+01  -.000579    -.036146     .729152    -.519199
    2P .40781769E+01   .000201     .001826     .434419    -.164989
    2P .14423865E+01  -.000061    -.000512     .026370     .794405
    2P .54457330E+00   .000022     .000201    -.001994     .394580
ORBITAL SYMMETRY        3D          4D          5D
ENERGY              -88.0950    -14.5620     -.6808
                EXPONENT
    3D .47966911E+04   .000533     .000286     .000088
    3D .13591414E+04   .006303     .003193     .001036
    3D .47328686E+03   .045277     .024259     .007643
    3D .18246073E+03   .198704     .105815     .034340
    3D .75149950E+02   .455403     .252731     .079725
    3D .32185264E+02   .421460     .092394     .024252
    3D .12670732E+02   .085826    -.544318    -.238746
    3D .51390016E+01  -.004066    -.535561    -.112723
    3D .14813481E+01   .001579    -.057617     .594549
    3D .44523871E+00  -.000499     .007594     .564423
ORBITAL SYMMETRY        4F
ENERGY              -4.9606
                EXPONENT
    4F .16505605E+03   .021286
    4F .54797342E+02   .131612
    4F .21145438E+02   .366968
    4F .82595480E+01   .501236
    4F .29666792E+01   .288729

     VIRIAL THEOREM:   -.19999594E+01
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BASIS FOR THALLIUM . DOUBLET P

```
TOTAL ENERGY=     -.1896139629377 68E+05
ORBITAL SYMMETRY       1S          2S          3S          4S          5S          6S
ENERGY              -2851.4887  -484.5016  -117.0933   -26.8330    -4.5846     -.3513
              EXPONENT
    1S .10412005E+08   .000050   -.000017   -.000008   -.000004    .000002    .000000
    1S .15422508E+07   .000398   -.000133   -.000063   -.000032    .000014    .000004
    1S .34213756E+06   .002179   -.000725   -.000346   -.000173    .000075    .000021
    1S .93746789E+05   .009540   -.003227   -.001530   -.000766    .000332    .000094
    1S .29520329E+05   .035201   -.011957   -.005735   -.002870    .001246    .000352
    1S .10322653E+05   .107556   -.039036   -.018662   -.009362    .004057    .001144
    1S .39321581E+04   .256530   -.102204   -.050484   -.025423    .011067    .003126
    1S .16008010E+04   .402589   -.216384   -.109440   -.055757    .024219    .006834
    1S .67784839E+03   .297621   -.212767   -.122301   -.063648    .028041    .007942
    1S .23356123E+03   .043050    .364051    .300224    .169056   -.076052   -.021625
    1S .10817799E+03  -.010513    .708922    .753446    .475868   -.217121   -.061761
    1S .34731466E+02   .006711    .178188   -.532678   -.600499    .306159    .088516
    1S .20025449E+02  -.005752   -.084839   -.735629   -.912862    .521398    .155555
    1S .80817193E+01   .002991    .034597   -.107363    .785321   -.672433   -.216311
    1S .40941789E+01  -.001760   -.019425    .019466    .751370   -.859813   -.290224
    1S .15419007E+01   .000722    .007772   -.005881    .028036    .854295    .388015
    1S .72547769E+00  -.000300   -.003200    .002377    .002541    .655810    .422379
    1S .13884241E+00   .000065    .000688   -.000477   -.000631    .029264   -.684033
    1S .52500756E-01  -.000027   -.000289    .000199    .000283   -.009300   -.521073
ORBITAL SYMMETRY       2P          3P          4P          5P          6P
ENERGY              -465.6724  -108.1406   -22.8679    -3.2002     -.1863
              EXPONENT
    2P .18807773E+05   .001736    .000877    .000438    .000178   -.000037
    2P .80462178E+05   .000190    .000096    .000047    .000019   -.000004
    2P .59380019E+04   .010420    .005337    .002645    .001085   -.000224
    2P .21870575E+04   .046509    .024268    .012208    .004972   -.001029
    2P .89394009E+03   .152074    .083551    .042099    .017331   -.003583
    2P .39413457E+03   .335173    .197846    .102953    .042142   -.008731
    2P .18327376E+03   .411347    .254066    .130360    .054521   -.011266
    2P .87775530E+02   .197376   -.077487   -.072935   -.035970    .007507
    2P .42670520E+02   .018134   -.594843   -.506556   -.226753    .047746
    2P .21310751E+02   .001302   -.406632   -.201437   -.085795    .017310
    2P .96569177E+01  -.000803   -.052928    .672336    .470655   -.103632
    2P .46563983E+01   .000328    .002732    .515660    .289306   -.063461
    2P .17264800E+01  -.000122   -.000905    .044291   -.711201    .207538
    2P .69886614E+00   .000051    .000389   -.004343   -.502268    .132077
    2P .15177337E+00  -.000013   -.000087    .000995   -.024274   -.475372
    2P .46958149E-01   .000005    .000032   -.000373    .004722   -.653194
ORBITAL SYMMETRY       3D          4D          5D
ENERGY              -91.6494    -15.5976     -.9336
              EXPONENT
    3D .52766386E+04   .000457   -.000247    .000081
    3D .14940667E+04   .005502   -.002804    .000956
    3D .51894180E+03   .040227   -.021678    .007236
    3D .19982636E+03   .182568   -.097762    .033401
    3D .82507943E+02   .435431   -.244153    .081871
    3D .35615962E+02   .442197   -.127750    .037831
    3D .14128155E+02   .107541    .492637   -.228373
    3D .58207067E+01  -.005509    .579585   -.164670
    3D .17464820E+01   .002357    .079164    .561224
    3D .55078308E+00  -.000762   -.010381    .599242
ORBITAL SYMMETRY       4F
ENERGY              -5.7255
              EXPONENT
    4F .16356065E+03   .023593
    4F .54324579E+02   .141985
    4F .21085377E+02   .378735
    4F .83282789E+01   .494317
    4F .30449131E+01   .268568

     VIRIAL THEOREM:   -.19999307E+01
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BASIS FOR LEAD, TRIPLET P

```
TOTAL ENERGY=     -.195236199923144E+05
ORBITAL SYMMETRY        1S          2S          3S          4S          5S          6S
ENERGY              -2925.3321  -498.5573  -121.2006   -28.1848    -5.0314     -.4487
              EXPONENT
    1S  .10208720E+08   .000053    .000018    .000008   -.000004    .000002    .000001
    1S  .15269054E+07   .000414    .000139    .000066   -.000033    .000015    .000004
    1S  .34058461E+06   .002254    .000750    .000358   -.000180    .000079    .000024
    1S  .93707809E+05   .009797    .003316    .001574   -.000791    .000348    .000107
    1S  .29681270E+05   .035825    .012184    .005854   -.002936    .001294    .000397
    1S  .10426952E+05   .108954    .039603    .018956   -.009560    .004212    .001292
    1S  .39760750E+04   .259539    .103773    .051372   -.025912    .011437    .003514
    1S  .16187788E+04   .403197    .218069    .110497   -.056689    .025065    .007692
    1S  .68751568E+03   .292833    .209559    .121050   -.062846    .027992    .008626
    1S  .23673026E+03   .041742   -.379078   -.314517    .176533   -.080193   -.024816
    1S  .10940898E+03  -.010503   -.699172   -.749570    .481225   -.224590   -.069517
    1S  .36201095E+02   .006596   -.162716    .531008   -.618645    .327030    .102944
    1S  .20657198E+02  -.005391    .069221    .749464   -.882344    .499084    .162599
    1S  .77462394E+01   .003080   -.030101    .115705    .843482   -.733496   -.261661
    1S  .42299116E+01  -.002109    .019737   -.034261    .648569   -.813815   -.298930
    1S  .16749791E+01   .000844   -.007686    .010428    .054869    .852249    .419192
    1S  .77134800E+00  -.000348    .003137   -.004142   -.006932    .683061    .511033
    1S  .18549969E+00   .000088   -.000794    .001003    .001731    .019961   -.648366
    1S  .70961265E-01  -.000033    .000301   -.000378   -.000651   -.003682   -.609277
ORBITAL SYMMETRY        2P          3P          4P          5P          6P
ENERGY              -479.4481  -112.0899   -24.1278    -3.5884     -.2502
              EXPONENT
    2P  .18767709E+05   .001818    .000921    .000462    .000191   -.000047
    2P  .80209616E+05   .000199    .000101    .000050    .000021   -.000005
    2P  .59373450E+04   .010840    .005562    .002770    .001158   -.000282
    2P  .21957001E+04   .047836    .025030    .012646    .005255   -.001282
    2P  .90163193E+03   .154719    .085243    .043161    .018127   -.004411
    2P  .39872506E+03   .338120    .200405    .104776    .043775   -.010693
    2P  .18555823E+03   .410593    .253055    .130352    .055603   -.013507
    2P  .88685407E+02   .192404   -.089194   -.081909   -.040816    .009979
    2P  .43240355E+02   .016074   -.600736   -.515040   -.235871    .058761
    2P  .21610825E+02   .001637   -.395368   -.185725   -.078931    .018254
    2P  .98681563E+01  -.000991   -.049754    .682262    .490719   -.127386
    2P  .47934843E+01   .000429    .002437    .502780    .287145   -.075731
    2P  .18299713E+01  -.000164   -.000817    .043772   -.715979    .255022
    2P  .76161271E+00   .000069    .000367   -.004068   -.501425    .153980
    2P  .17869533E+00  -.000018   -.000086    .000977   -.025030   -.559314
    2P  .59339311E-01   .000007    .000032   -.000374    .004634   -.576441
ORBITAL SYMMETRY        3D          4D          5D
ENERGY              -95.3051    -16.6815     -1.1937
              EXPONENT
    3D  .52676211E+04   .000490    .000266   -.000091
    3D  .14796313E+04   .005982    .003071   -.001092
    3D  .51228876E+03   .043403    .023559   -.008212
    3D  .19765006E+03   .192373    .103802   -.037015
    3D  .81969436E+02   .442704    .249731   -.087363
    3D  .35648486E+02   .428531    .111588   -.032761
    3D  .14258977E+02   .099813   -.507307    .246440
    3D  .59519853E+01  -.005268   -.561625    .160580
    3D  .18458420E+01   .002261   -.075289   -.581088
    3D  .60512269E+00  -.000739    .009534   -.575018
ORBITAL SYMMETRY        4F
ENERGY              -6.5380
              EXPONENT
    4F  .16305935E+03   .025734
    4F  .54230856E+02   .151327
    4F  .21148600E+02   .389126
    4F  .84336050E+01   .487679
    4F  .31331156E+01   .250481

     VIRIAL THEOREM:   -.19999612E+01
```

BASIS FOR BISMUTH. QUARTET S

TOTAL ENERGY= -.200952213420771E+05

ORBITAL SYMMETRY		1S	2S	3S	4S	5S	6S
ENERGY		-3000.1312	-512.8206	-125.3822	-29.5642	-5.4810	-.5460
	EXPONENT						
1S	.10176927E+08	.000055	.000018	.000009	-.000004	.000002	.000001
1S	.15153220E+07	.000430	.000144	.000069	-.000035	.000015	.000005
1S	.33956667E+06	.002323	.000773	.000370	-.000186	.000083	.000027
1S	.93880328E+05	.010032	.003401	.001616	-.000815	.000364	.000119
1S	.29878560E+05	.036436	.012394	.005967	-.003006	.001344	.000439
1S	.10530252E+05	.110501	.040280	.019294	-.009755	.004359	.001420
1S	.40176218E+04	.262487	.105139	.052198	-.026462	.011857	.003872
1S	.16377872E+04	.403057	.219905	.111518	-.057322	.025697	.008368
1S	.69812863E+03	.288545	.205129	.119363	-.062490	.028298	.009284
1S	.24011366E+03	.040672	-.386757	-.324889	.184445	-.085261	-.028108
1S	.11150704E+03	-.010370	-.694483	-.740633	.475357	-.224881	-.073796
1S	.35736259E+02	.006816	-.167794	.611487	-.708026	.380099	.126462
1S	.20458210E+02	-.006138	.084363	.670804	-.819362	.480095	.169678
1S	.84921587E+01	.003727	-.040363	.106384	.738413	-.648851	-.252801
1S	.47032570E+01	-.002281	.023604	-.023456	.765061	-.912162	-.347845
1S	.17072317E+01	.000856	-.008593	.006611	.074199	.844708	.438751
1S	.82739050E+00	-.000409	.004068	-.003124	-.014847	.665304	.575607
1S	.22583838E+00	.000104	-.001033	.000761	.003309	.022783	-.705271
1S	.80547974E-01	-.000034	.000341	-.000248	-.001077	-.003224	-.608053
ORBITAL SYMMETRY		2P	3P	4P	5P	6P	
ENERGY		-493.4320	-116.1127	-25.4148	-3.9791	-.3160	
	EXPONENT						
2P	.18757914E+05	.001906	.000967	.000487	.000206	-.000056	
2P	.80110813E+04	.000208	.000105	.000053	.000022	-.000006	
2P	.59342456E+04	.011254	.005784	.002893	.001233	-.000333	
2P	.22085978E+04	.049019	.025720	.013050	.005527	-.001498	
2P	.90937420E+03	.157864	.087211	.044366	.018996	-.005135	
2P	.40247944E+03	.342047	.203618	.106966	.045557	-.012371	
2P	.18737659E+03	.409384	.251485	.129953	.056532	-.015244	
2P	.89390242E+02	.186616	-.102653	-.092124	-.046524	.012627	
2P	.43731648E+02	.013966	-.606419	-.523768	-.244856	.067969	
2P	.21867500E+02	.001957	-.383247	-.166996	-.070585	.017653	
2P	.10048275E+02	-.001175	-.046212	.694581	.514747	-.149042	
2P	.49120633E+01	.000530	.002132	.486940	.276915	-.081996	
2P	.19165877E+01	-.000209	-.000710	.042293	-.729439	.297169	
2P	.81766057E+00	.000090	.000337	-.003872	-.490194	.166616	
2P	.20717706E+00	-.000025	-.000082	.000966	-.024362	-.614675	
2P	.71514965E-01	.000009	.000030	-.000361	.004350	-.528751	
ORBITAL SYMMETRY		3D	4D	5D			
ENERGY		-99.0329	-17.7910	-1.4566			
	EXPONENT						
3D	.52223946E+04	.000531	-.000290	-.000103			
3D	.14618129E+04	.006503	-.003364	-.001241			
3D	.50630576E+03	.046572	-.025453	-.009215			
3D	.19599131E+03	.201558	-.109595	-.040579			
3D	.81647826E+02	.448912	-.254545	-.092383			
3D	.35745524E+02	.415597	-.096211	-.027335			
3D	.14420430E+02	.092948	.520347	.263563			
3D	.60895161E+01	-.004954	.545143	.155321			
3D	.19441886E+01	.002137	.071553	-.600578			
3D	.65797307E+00	-.000703	-.008746	-.551687			
ORBITAL SYMMETRY		4F					
ENERGY		-7.3757					
	EXPONENT						
4F	.16296888E+03	.027833					
4F	.54323144E+02	.160089					
4F	.21276302E+02	.398533					
4F	.85579530E+01	.480991					
4F	.32265185E+01	.233999					

VIRIAL THEOREM: -.19999848E+01

BASIS FOR POLONIUM, TRIPLET P

```
TOTAL ENERGY=     -.206761595529536E+05
ORBITAL SYMMETRY        1S          2S          3S          4S          5S          6S
ENERGY              -3075.8947  -527.3028  -129.6467   -30.9808    -5.9459     -.6523
              EXPONENT
    1S  .10147462E+08   .000057     .000019     .000009     .000005    -.000002    -.000001
    1S  .15084181E+07   .000445     .000149     .000071     .000036    -.000016    -.000006
    1S  .33906481E+06   .002388     .000796     .000381     .000192    -.000087    -.000030
    1S  .94389636E+05   .010204     .003459     .001648     .000834    -.000378    -.000129
    1S  .30204647E+05   .036905     .012578     .006054     .003060    -.001387    -.000475
    1S  .10661010E+05   .111821     .040773     .019596     .009946    -.004507    -.001542
    1S  .40753468E+04   .263670     .106048     .052610     .026752    -.012151    -.004161
    1S  .16673611E+04   .402068     .219615     .111980     .057810    -.026289    -.008998
    1S  .71269345E+03   .286478     .205151     .118645     .062243    -.028561    -.009808
    1S  .24661525E+03   .040474    -.388928    -.322555    -.183370     .085891     .029624
    1S  .11451769E+03  -.010641    -.687619    -.749983    -.485152     .233175     .080632
    1S  .39773182E+02   .006979    -.159574     .469175     .538067    -.291375    -.102736
    1S  .22757103E+02  -.005731     .062492     .797973     .982746    -.576424    -.209274
    1S  .89256617E+01   .003310    -.026918     .136367    -.674154     .602128     .239503
    1S  .49559058E+01  -.002148     .016609    -.034443    -.810851     .985487     .412896
    1S  .18437346E+01   .000850    -.006354     .010091    -.074959    -.818244    -.477198
    1S  .90851021E+00  -.000404     .002986    -.004640     .012470    -.710692    -.597847
    1S  .23961861E+00   .000104    -.000766     .001139    -.002622    -.026828     .741147
    1S  .94819131E-01  -.000038     .000280    -.000411     .000950     .004740     .571862
ORBITAL SYMMETRY        2P          3P          4P          5P          6P
ENERGY              -507.6326  -120.2178   -26.7385    -4.3851     -.3367
              EXPONENT
    2P  .18704791E+05   .001982     .001008     .000509    -.000219    -.000064
    2P  .79719138E+05   .000220     .000112     .000056    -.000024    -.000007
    2P  .59637221E+04   .011593     .005968     .002999    -.001300    -.000378
    2P  .22256930E+04   .050109     .026361     .013428    -.005791    -.001687
    2P  .92088730E+03   .159515     .088335     .045152    -.019668    -.005716
    2P  .40894093E+03   .343568     .205236     .108265    -.046967    -.013711
    2P  .19063085E+03   .408437     .250487     .130028    -.057487    -.016666
    2P  .90886142E+02   .183704    -.109220    -.097925     .049989     .014616
    2P  .44638647E+02   .012835    -.607591    -.527115     .251790     .075228
    2P  .22370667E+02   .002226    -.377977    -.162772     .068332     .018200
    2P  .10382566E+02  -.001338    -.045321     .694607    -.524799    -.164290
    2P  .51125154E+01   .000626     .001902     .485828    -.290191    -.093039
    2P  .20571713E+01  -.000257    -.000653     .044035     .721217     .322453
    2P  .90034222E+00   .000112     .000324    -.003690     .504932     .190001
    2P  .24718975E+00  -.000031    -.000078     .000911     .027895    -.612665
    2P  .83494069E-01   .000011     .000026    -.000330    -.003706    -.546829
ORBITAL SYMMETRY        3D          4D          5D
ENERGY              -102.8421   -18.9365    -1.7355
              EXPONENT
    3D  .51075638E+04   .000595    -.000325    -.000120
    3D  .14236732E+04   .007260    -.003793    -.001445
    3D  .49524132E+03   .050621    -.027821    -.010432
    3D  .19341200E+03   .210891    -.115709    -.044321
    3D  .81366679E+02   .452003    -.256933    -.096476
    3D  .35996808E+02   .402067    -.084245    -.022647
    3D  .14780874E+02   .088147     .522781     .274319
    3D  .63216393E+01  -.004213     .537442     .160226
    3D  .20895515E+01   .001931     .071931    -.606045
    3D  .72669572E+00  -.000632    -.008242    -.545517
ORBITAL SYMMETRY        4F
ENERGY              -8.2487
              EXPONENT
    4F  .16322891E+03   .029854
    4F  .54719457E+02   .166927
    4F  .21619694E+02   .403180
    4F  .87952535E+01   .474850
    4F  .33628341E+01   .223378

     VIRIAL THEOREM:   -.19999928E+01
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BASIS FOR ASTETINE. DOUBLET P

TOTAL ENERGY= -.212665487772557E+05

ORBITAL SYMMETRY	1S	2S	3S	4S	5S	6S
ENERGY	-3152.6246	-542.0030	-133.9946	-32.4319	-6.4188	-.7604
EXPONENT						
1S .10091062E+08	.000059	.000020	-.000009	-.000005	-.000002	-.000001
1S .15026679E+07	.000460	.000154	-.000074	-.000037	-.000017	-.000006
1S .33995712E+06	.002439	.000813	-.000390	-.000198	-.000091	-.000032
1S .94893604E+05	.010456	.003549	-.001692	-.000859	-.000394	-.000140
1S .30337438E+05	.037678	.012850	-.006197	-.003142	-.001444	-.000514
1S .10744494E+05	.113530	.041497	-.019960	-.010167	-.004668	-.001661
1S .41096703E+04	.266874	.107642	-.053547	-.027320	-.012577	-.004480
1S .16840699E+04	.401979	.221361	-.112987	-.058567	-.026988	-.009611
1S .72186706E+03	.281844	.201166	-.117175	-.061673	-.028698	-.010248
1S .25038251E+03	.038780	-.398468	.333755	.190597	.090571	.032485
1S .11632881E+03	-.010026	-.682762	.743936	.484629	.236252	.085079
1S .39944751E+02	.006495	-.155626	-.518142	-.602598	-.331878	-.122266
1S .22833203E+02	-.005379	.063478	-.761247	-.931869	-.558737	-.211378
1S .88768669E+01	.003239	-.028700	-.130030	.758720	.703789	.292437
1S .49668397E+01	-.002221	.018753	.037876	.735809	.933440	.414380
1S .19445859E+01	.000931	-.007614	-.012028	.070991	-.844993	-.523049
1S .96935840E+00	-.000437	.003534	.005465	-.011272	-.710885	-.631060
1S .26999310E+00	.000112	-.000906	-.001352	.002433	-.027826	.773633
1S .10755789E+00	-.000039	.000319	.000470	-.000871	.004336	.568039

ORBITAL SYMMETRY	2P	3P	4P	5P	6P
ENERGY	-522.0518	-124.4061	-28.0964	-4.7983	-.3756
EXPONENT					
2P .18709470E+05	.002063	.001051	.000533	-.000233	-.000072
2P .79695936E+05	.000229	.000117	.000059	-.000026	-.000008
2P .59797809E+04	.011991	.006181	.003120	-.001376	-.000425
2P .22372501E+04	.051481	.027165	.013892	-.006089	-.001886
2P .92773469E+03	.162690	.090304	.046382	-.020554	-.006345
2P .41264004E+03	.347083	.208334	.110373	-.048663	-.015104
2P .19251291E+03	.406897	.248158	.129261	-.058203	-.017908
2P .91600505E+02	.178294	-.121116	-.107669	.055945	.017354
2P .45312523E+02	.010798	-.608440	-.530290	.257261	.081937
2P .22788781E+02	.002702	-.369422	-.154502	.066460	.018307
2P .10729663E+02	.001599	-.043706	.691245	-.538254	-.179358
2P .53312557E+01	.000752	.001379	.487855	-.292065	-.100876
2P .21471083E+01	-.000308	-.000466	.046066	.734947	.359950
2P .95791244E+00	.000137	.000261	-.004469	.492769	.189441
2P .27541427E+00	-.000039	-.000062	.001085	.027616	-.645142
2P .93213002E-01	.000013	.000019	-.000394	-.002741	-.522025

ORBITAL SYMMETRY	3D	4D	5D
ENERGY	-106.7331	-20.1146	-2.0215
EXPONENT			
3D .49997298E+04	.000660	-.000362	-.000138
3D .13978562E+04	.007933	-.004175	-.001639
3D .48910601E+03	.054024	-.029889	-.011547
3D .19225790E+03	.219105	-.121108	-.047812
3D .81338354E+02	.456102	-.260291	-.100568
3D .36195417E+02	.390522	-.070197	-.016780
3D .14985560E+02	.082585	.533405	.289785
3D .64715217E+01	-.003899	.523277	.153460
3D .21877427E+01	.001792	.068382	-.624831
3D .77863648E+00	-.000586	-.007594	-.523610

ORBITAL SYMMETRY	4F
ENERGY	-9.1545
EXPONENT	
4F .16462329E+03	.031571
4F .55288695E+02	.173947
4F .21906243E+02	.410650
4F .89715446E+01	.468875
4F .34730438E+01	.210258

VIRIAL THEOREM: -.20000090E+01

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TOTAL ENERGY=     -.2186640262000023E+05
ORBITAL SYMMETRY        1S          2S          3S          4S          5S          6S
ENERGY              -3230.3132  -556.9098  -138.4057   -33.9073    -6.8954     -.8694
              EXPONENT
    1S  .10129077E+08   .000060   -.000020   -.000010   -.000005    .000002    .000001
    1S  .15060856E+07   .000472   -.000158   -.000075   -.000038    .000018    .000007
    1S  .34100226E+06   .002503   -.000839   -.000404   -.000206    .000096    .000035
    1S  .95241961E+05   .010686   -.003608   -.001714   -.000873    .000406    .000149
    1S  .30525926E+05   .038432   -.013221   -.006421   -.003268    .001520    .000558
    1S  .10820874E+05   .115322   -.041838   -.020000   -.010216    .004752    .001746
    1S  .41459479E+04   .269923   -.110668   -.055671   -.028523    .013292    .004884
    1S  .17002808E+04   .401737   -.218535   -.110159   -.057254    .026740    .009837
    1S  .73240753E+03   .277032   -.207807   -.125051   -.066244    .031172    .011470
    1S  .25465598E+03   .037185    .452560    .388327    .223404   -.107339   -.039671
    1S  .10894726E+03  -.009834    .686218    .758721    .505842   -.251824   -.093976
    1S  .40687152E+02   .007308    .051537   -.685647   -.767824    .430862    .165131
    1S  .22566257E+02  -.005908    .011913   -.645335   -.791624    .480073    .186306
    1S  .86164571E+01   .004398   -.017827   -.183730    .743410   -.715873   -.304816
    1S  .54033839E+01  -.003211    .014054    .090602    .698425   -.887482   -.416525
    1S  .20141812E+01   .001092   -.005176   -.027556    .112796    .797655    .543701
    1S  .10354124E+01  -.000525    .002556    .013316   -.028565    .731064    .644205
    1S  .28426776E+00   .000127   -.000632   -.003242    .006058    .024418   -.855424
    1S  .11398046E+00  -.000045    .000225    .001147   -.002165   -.003042   -.500027
ORBITAL SYMMETRY        2P          3P          4P          5P          6P
ENERGY              -536.6834  -128.6686   -29.4809    -5.2160     -.4241
              EXPONENT
    2P  .18737546E+05   .002144    .001095    .000557   -.000248   -.000080
    2P  .79782044E+05   .000239    .000121    .000061   -.000027   -.000009
    2P  .59970870E+04   .012391    .006399    .003243   -.001454   -.000468
    2P  .22500440E+04   .052820    .027940    .014348   -.006393   -.002065
    2P  .93473708E+03   .165943    .092376    .047652   -.021467   -.006909
    2P  .41628646E+03   .350450    .211174    .112411   -.050390   -.016315
    2P  .19456000E+03   .404316    .245802    .128307   -.058737   -.018828
    2P  .92671724E+02   .173367   -.132336   -.116372    .061287    .019827
    2P  .45949512E+02   .009706   -.611640   -.537333    .265524    .088399
    2P  .23116982E+02   .002746   -.360518   -.137191    .057222    .015627
    2P  .10887373E+02  -.001641   -.040966    .707121   -.565317   -.197369
    2P  .54246018E+01   .000795    .001364    .468736   -.275621   -.100039
    2P  .22322063E+01  -.000338   -.000437    .042922    .753806    .394912
    2P  .10127940E+01   .000152    .000252   -.003906    .477327    .186103
    2P  .30585185E+00  -.000044   -.000060    .000967    .025691   -.668536
    2P  .10461085E+00   .000014    .000019   -.000323   -.003044   -.505408
ORBITAL SYMMETRY        3D          4D          5D
ENERGY              -110.6985   -21.3185    -2.3123
              EXPONENT
    3D  .48862576E+04   .000733   -.000404   -.000158
    3D  .13723612E+04   .008650   -.004587   -.001848
    3D  .48350323E+03   .057469   -.031992   -.012703
    3D  .19130103E+03   .227110   -.126481   -.051308
    3D  .81370736E+02   .459721   -.263104   -.104350
    3D  .36409605E+02   .379101   -.056591   -.010522
    3D  .15220747E+02   .077425    .542100    .303562
    3D  .66366908E+01  -.003493    .510339    .148197
    3D  .23000829E+01   .001630    .065585   -.639171
    3D  .83501182E+00  -.000529   -.006938   -.507141
ORBITAL SYMMETRY        4F
ENERGY              -10.0855
              EXPONENT
    4F  .16633742E+03   .033220
    4F  .55964801E+02   .180423
    4F  .22253964E+02   .416699
    4F  .91800629E+01   .462928
    4F  .35962920E+01   .199142

     VIRIAL THEOREM:   -.20000209E+01
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