All-electron scalar relativistic basis sets for the actinides

Dimitrios. A. Pantazis and Frank Neese*

Lehrstuhl für Theoretische Chemie, Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, D-53115 Bonn, Germany, and Max-Planck-Institut für Bioanorganische Chemie, Stiftstrasse 34-36, 45470 Mülheim an der Ruhr, Germany.

SUPPORTING INFORMATION

Complete listings of SARC basis sets in standard ORCA input format.

SARC-DKH2 basis sets

	sis set for element	: Ac
NewG S 9	TO 89	
1	55109808.74124400	0.0312766245
2	25049913.06420200 11386324.12009200	-0.0204119520 0.0582795151
4	5175601.872769000	0.0047558262
5	2352546.305804000	0.0899377462
6	1069339.229911000	0.0775555648
7	486063.2863230000	0.1904178134
8	220937.8574200000	0.2641478696
9 S 1	100426.2988270000	0.4915549572
1	45648.3176490000	1.0000000000
S 1 1	20749.2352950000	1.0000000000
S 1 1	9431.4705890000	1.0000000000
S 1 1	4287.0320860000	1.0000000000
S 1 1	1948.6509480000	1.0000000000
S 1 1	885.7504310000	1.0000000000
S 1 1	402.6138320000	1.0000000000
S 1		
1 S 1	183.0062870000	1.0000000000
1 5 1	83.1846760000	1.0000000000
1 S 1	37.8112160000	1.0000000000
1 S 1	17.1869170000	1.0000000000
1 S 1	7.8122350000	1.0000000000
1 S 1	3.5510160000	1.0000000000
1	1.6140980000	1.0000000000
S 1	0.7336810000	1.0000000000
S 1 1	0.3334910000	1.0000000000
S 1 1	0.1515870000	1.0000000000
S 1 1	0.0689030000	1.0000000000
S 1 1	0.0313200000	1.0000000000
S 1 1	0.0142360000	1.0000000000
P 8	782789.9000960001	0.0031757524
2	326162.4583730000	0.0008406366
3	135901.0243220000	0.0083656049
4	56625.4268010000	0.0126957020
5	23593.9278340000	0.0370008398
6	9830.8032640000	0.0908384712
7	4096.1680270000	0.2586186730
8 P 1	1706.7366780000	0.7139694175
1	711.1402820000	1.0000000000
P 1 1	296.3084510000	1.0000000000

P 1		
1	123.4618550000	1.0000000000
P 1		
1	51.4424390000	1.0000000000
P 1		
1	21.4343500000	1.0000000000
P 1		
1	8.9309790000	1.0000000000
P 1		
1	3.7212410000	1.0000000000
P 1	3.7212410000	1.000000000
	1 5505170000	1 000000000
1	1.5505170000	1.0000000000
P 1		
1	0.6460490000	1.0000000000
P 1		
1	0.2691870000	1.0000000000
P 1		
1	0.1121610000	1.0000000000
P 1	0.1121010000	1.000000000
	0.0467340000	1 000000000
1	0.0467340000	1.0000000000
D 7		
1	37896.8365590000	0.0001482612
2	15158.7346230000	0.0003702219
3	6063.4938490000	0.0020736881
4	2425.3975400000	0.0096748493
5	970.1590160000	0.0520379811
6	388.0636060000	0.2362709965
7	155.2254430000	0.7964725694
D 1		
1	62.0901770000	1.0000000000
D 1		
1	24.8360710000	1.0000000000
D 1		
1	9.9344280000	1.0000000000
D 1	2,221.1200000	2.0000000000
1	3.9737710000	1.0000000000
	3.9737710000	1.000000000
	1 500500000	4 000000000
1	1.5895090000	1.0000000000
D 1		
1	0.6358030000	1.0000000000
D 1		
1	0.2543210000	1.0000000000
D 1		
1	0.1017290000	1.0000000000
D 1	0.101/230000	1.000000000
	0.0406010000	1 000000000
1	0.0406910000	1.0000000000
F 6		
1	3860.7881580000	0.0000676369
2	1484.9185220000	0.0004993795
3	571.1225090000	0.0048810577
4	219.6625030000	0.0404316252
5	84.4855780000	0.2453229456
6	32.4944530000	0.8182721188
F 1	32113113333333	0.0101,11100
1	12.4978670000	1.0000000000
	12.4378070000	1.000000000
	4 0060730000	1 000000000
1	4.8068720000	1.0000000000
F 1		
1	1.8487970000	1.0000000000
F 1		
1	0.7110760000	1.0000000000
F 1		
1	0.2734910000	1.0000000000
F 1		
1	0.1051890000	1.0000000000
	0.1071070000	1.000000000
end		

Basis set for element : Th

		TO 90	
S	9		
	1	56363088.88971600	0.0318759066
	2	25619585.85896200	-0.0208607830
	3	11645266.29952800	0.0593104871
	4	5293302.863422000	0.0045173834
	5	2406046.756101000	0.0910942228
	6	1093657.616409000	0.0776539218
	7	497117.0983680000	0.1914375494
	8	225962.3174400000	0.2636687905
	9	102710.1442910000	0.4900758514
_		102/10.1442910000	0.4300736314
S	1		
	1	46686.4292230000	1.0000000000
S	1		
	1	21221.1041920000	1.0000000000
S	1		
	1	9645.9564510000	1.0000000000
S	1	20.37230.32000	
٦		4384 535660000	1 000000000
_	1	4384.5256600000	1.0000000000
S	1		
	1	1992.9662090000	1.0000000000
S	1		
	1	905.8937310000	1.0000000000
S	1		
,	1	411.7698780000	1.0000000000
_		411.7656760000	1.000000000
S	1		
	1	187.1681260000	1.0000000000
S	1		
	1	85.0764210000	1.0000000000
S	1		
_	1	38.6711000000	1.0000000000
S		30.0711000000	1.0000000000
2	1		
	1	17.5777730000	1.0000000000
S	1		
	1	7.9898970000	1.0000000000
S	1		
	1	3.6317710000	1.0000000000
S	1	3,031,,10000	
٦	1	1 6500050000	1 000000000
_		1.6508050000	1.0000000000
S	1		
	1	0.7503660000	1.0000000000
S	1		
	1	0.3410750000	1.0000000000
S	1		
	1	0.1550340000	1.0000000000
S	1	0.13303.0000	1.000000000
3		0.070470000	1 000000000
	1	0.0704700000	1.0000000000
S	1		
	1	0.0320320000	1.0000000000
S	1		
	1	0.0145600000	1.0000000000
Р	8		
•	1	801557.4232150000	0.0032622731
	2	333982.2596730000	0.0008569025
	3	139159.2748640000	0.0085578818
	4	57983.0311930000	0.0129143706
	5	24159.5963310000	0.0375326683
	6	10066.4984710000	0.0916129238
	7	4194.3743630000	0.2594858133
	8	1747.6559850000	0.7123765928
_		1/ 1 /.0000000	0./123/03320
Р	1	720 4000040000	1 00000000
	1	728.1899940000	1.0000000000
Р	1		
	1	303.4124970000	1.0000000000
Ρ	1		
	1	126.4218740000	1.0000000000
Р	1		
•	1	52.6757810000	1.0000000000
_		22.0/3/010000	1.00000000000
Р	1		

```
1
         21.9482420000
                             1.0000000000
P 1
  1
          9.1451010000
                             1.0000000000
P 1
  1
          3.8104590000
                             1.0000000000
P 1
  1
          1.5876910000
                             1.0000000000
P 1
          0.6615380000
                             1.0000000000
  1
P 1
  1
          0.2756410000
                             1.0000000000
P 1
  1
          0.1148500000
                             1.0000000000
P 1
          0.0478540000
                             1.0000000000
  1
D 7
      38933.2915440000
                             0.0001513887
  1
      15573.3166180000
                             0.0003759661
                             0.0020977831
  3
       6229.3266470000
  4
       2491.7306590000
                             0.0097347616
  5
                             0.0521624557
        996.6922640000
        398.6769050000
  6
                             0.2362677556
        159.4707620000
  7
                             0.7964070682
D 1
  1
         63.7883050000
                             1.0000000000
D 1
         25.5153220000
                             1.0000000000
D 1
         10.2061290000
                             1.0000000000
  1
D 1
          4.0824520000
                             1.0000000000
  1
D 1
  1
          1.6329810000
                             1.0000000000
D 1
          0.6531920000
                             1.0000000000
  1
D 1
                             1.0000000000
          0.2612770000
  1
D 1
                             1.0000000000
          0.1045110000
  1
D 1
          0.0418040000
                             1.0000000000
  1
F 6
  1
       4035.8413290000
                             0.0000665503
  2
       1552.2466650000
                             0.0004925640
  3
        597.0179480000
                             0.0047782956
  4
        229.6222880000
                             0.0397489860
  5
         88.3162650000
                             0.2429834827
         33.9677940000
  6
                             0.8203559595
F 1
  1
         13.0645360000
                             1.0000000000
F
 1
  1
          5.0248220000
                             1.0000000000
F 1
                             1.0000000000
  1
          1.9326240000
F 1
                             1.0000000000
  1
          0.7433170000
F 1
  1
          0.2858910000
                             1.0000000000
F 1
 1
          0.1099580000
                             1.0000000000
 end
# Basis set for element : Pa
NewGTO 91
S 9
  1
    57631858.17253400
                             0.0324936320
  2 26196299.16933400
                            -0.0213243242
  3 11907408.71333400
                             0.0603713014
```

	4	5412458.506061000	0.0042675023
	5	2460208.411846000	0.0922786745
	6	1118276.550839000	0.0777436539
	7	508307.5231090000	0.1924734529
	8	231048.8741400000	0.2631671960
	9	105022.2155180000	0.4885848292
S	1	103022.2133180000	0.4003040232
,	1	47737.3706900000	1.0000000000
S	1	47737.3700300000	1.000000000
٦	1	21698.8048590000	1.0000000000
S	1	21070.0040770000	1.000000000
٦	1	9863.0931180000	1.0000000000
S	1	3803.0331180000	1.000000000
3	1	4483.2241440000	1.0000000000
S	1	4403.2241440000	1.000000000
,	1	2037.8291570000	1.0000000000
S	1	2037.0231370000	1.000000000
,	1	926.2859800000	1.0000000000
S	1	720.2033000000	1.000000000
,	1	421.0390820000	1.0000000000
S	1	421.0330020000	1.000000000
,	1	191.3814010000	1.0000000000
S	1	171.701-010000	1.000000000
,	1	86.9915460000	1.0000000000
S	1	00.7713400000	1.000000000
٦	1	39.5416120000	1.0000000000
S	1	33.3410120000	1.000000000
٦	1	17.9734600000	1.0000000000
S	1	17.5754000000	1.000000000
٦	1	8.1697540000	1.0000000000
S	1	0.1057540000	1.000000000
٦	1	3.7135250000	1.0000000000
S	1	3.7133230000	1.000000000
٦	1	1.6879660000	1.0000000000
S	1	1.00/3000000	1.000000000
3	1	0.7672570000	1.0000000000
S	1	0.7072370000	1.000000000
٦	1	0.3487530000	1.0000000000
S	1	0.5407550000	1.000000000
_	1	0.1585240000	1.0000000000
S	1	0.13032.10000	1.000000000
_	1	0.0720560000	1.0000000000
S	1	0.07.20300000	
_	1	0.0327530000	1.0000000000
S	1	0.032,330000	
_	1	0.0148880000	1.0000000000
Р	8		
	1	820588.6600690000	0.0033507411
	2	341911.9416950000	0.0008734200
	3	142463.3090400000	0.0087537475
	4	59359.7121000000	0.0131359375
	5	24733.2133750000	0.0380705333
	6	10305.5055730000	0.0923923439
	7	4293.9606550000	0.2603540937
	8	1789.1502730000	0.7107726266
Р	1	1703.1302730000	0.7107720200
•	1	745.4792800000	1.0000000000
Р	1	743.4732000000	1.000000000
•	1	310.6163670000	1.0000000000
Р	1	310.0103070000	1.000000000
•	1	129.4234860000	1.0000000000
Р	1	127.4254000000	1.000000000
•	1	53.9264530000	1.0000000000
Р	1	JJ.J20 4 JJ0000	1.000000000
'	1	22.4693550000	1.0000000000
Р	1	22.7073330000	1.000000000
•	1	9.3622310000	1.0000000000
Р	1	3.3322310000	1.000000000
•	1	3.9009300000	1.0000000000
	-	3.200300000	1.000000000

```
P 1
          1.6253870000
                            1.0000000000
  1
P 1
  1
          0.6772450000
                            1.00000000000
P 1
          0.2821850000
                            1.0000000000
  1
P 1
  1
          0.1175770000
                            1.0000000000
P 1
                            1.0000000000
  1
          0.0489910000
D 7
  1
      39984.8312080000
                            0.0001545696
  2
     15993.9324830000
                            0.0003818697
  3
       6397.5729930000
                            0.0021222331
  4
       2559.0291970000
                            0.0097968379
  5
       1023.6116790000
                            0.0522921295
        409.4446720000
                            0.2362850042
  6
        163.7778690000
  7
                            0.7963212840
D 1
         65.5111470000
                            1.0000000000
  1
D 1
  1
         26.2044590000
                            1.0000000000
D 1
         10.4817840000
                            1.0000000000
  1
D 1
          4.1927130000
                            1.0000000000
  1
D 1
          1.6770850000
                            1.0000000000
  1
D 1
          0.6708340000
  1
                            1.0000000000
D 1
  1
          0.2683340000
                            1.0000000000
D 1
  1
          0.1073330000
                            1.0000000000
D 1
          0.0429330000
                            1.0000000000
F 6
       4212.3892570000
                             0.0000656512
  1
  2
       1620.1497140000
                            0.0004867345
  3
        623.1345050000
                            0.0046875705
        239.6671170000
                            0.0391377282
  4
         92.1796610000
                            0.2408751552
  5
  6
         35.4537160000
                            0.8222271707
F 1
  1
         13.6360440000
                            1.0000000000
F 1
          5.2446320000
                             1.0000000000
F 1
          2.0171660000
                            1.0000000000
  1
F 1
                             1.0000000000
  1
          0.7758330000
F 1
          0.2983970000
                            1.0000000000
  1
F 1
                            1.0000000000
 1
          0.1147680000
 end
# Basis set for element : U
NewGTO 92
S 9
 1 58915269.20406200
                            0.0331306134
  2 26779667.82002800
                           -0.0218032405
     12172576.28183100
                            0.0614632410
  4
     5532989.219014000
                            0.0040056242
  5 2514995.099552000
                            0.0934922512
  6 1143179.590705000
                            0.0778243085
     519627.0866840000
                            0.1935262084
  8 236194.1303110000
                            0.2626421889
```

S	9 1	107360.9683230000	0.4870813929
	1	48800.4401470000	1.0000000000
S	1 1	22182.0182490000	1.0000000000
S	1 1	10082.7355680000	1.0000000000
S	1 1	4583.0616220000	1.0000000000
S	1 1	2083.2098280000	1.0000000000
S	1	946.9135580000	1.0000000000
S	1		
S	1 1	430.4152540000	1.0000000000
S	1 1	195.6432970000	1.0000000000
S	1 1	88.9287710000	1.0000000000
S	1 1	40.4221690000	1.0000000000
	1	18.3737130000	1.0000000000
S	1	8.3516880000	1.0000000000
S	1 1	3.7962220000	1.0000000000
S	1 1	1.7255550000	1.0000000000
S	1 1	0.7843430000	1.0000000000
S	1 1	0.3565200000	1.0000000000
S	1		
S	1 1	0.1620540000	1.0000000000
S	1 1	0.0736610000	1.0000000000
S	1 1	0.0334820000	1.0000000000
Р	1 8	0.0152190000	1.0000000000
	1	839813.6669700000	0.0034411220
	2	349922.3612380000	0.0008901889
	3	145800.9838490000	0.0089531291
	4	60750.4099370000	0.0133603309
	5	25312.6708070000	0.0386144089
	6	10546.9461700000	0.0931768584
	7	4394.5609040000	0.2612253423
	8	1831.0670430000	0.7091556378
Ρ	1		
Р	1 1	762.9446010000	1.0000000000
•	1	317.8935840000	1.0000000000
Ρ	1		
Р	1 1	132.4556600000	1.0000000000
Р	1	55.1898580000	1.0000000000
	1	22.9957740000	1.0000000000
Р	1 1	9.5815730000	1.0000000000
Р	1 1	3.9923220000	1.0000000000
Р	1 1	1.6634670000	1.0000000000
Р	1		
Р	1 1	0.6931110000	1.0000000000

```
1
          0.2887960000
                             1.0000000000
P 1
  1
          0.1203320000
                             1.0000000000
P 1
  1
          0.0501380000
                             1.0000000000
D 7
  1
      41049.8202270000
                             0.0001578167
  2
      16419.9280910000
                            0.0003878999
  3
       6567.9712360000
                             0.0021472035
  4
       2627.1884950000
                             0.0098608714
  5
       1050.8753980000
                             0.0524286051
  6
        420.3501590000
                             0.2363168740
  7
        168.1400640000
                             0.7962195195
D 1
         67.2560250000
                            1.0000000000
  1
D 1
         26.9024100000
                             1.0000000000
  1
D 1
         10.7609640000
                             1.0000000000
  1
D 1
          4.3043860000
                             1.0000000000
  1
D 1
  1
          1.7217540000
                             1.0000000000
D 1
  1
          0.6887020000
                             1.0000000000
D 1
          0.2754810000
                             1.0000000000
D 1
          0.1101920000
                             1.0000000000
  1
D 1
          0.0440770000
                             1.0000000000
  1
F 6
  1
       4391.9602590000
                             0.0000648280
  2
       1689.2154840000
                             0.0004816285
  3
        649.6982630000
                            0.0046032038
  4
        249.8839470000
                             0.0385657246
  5
         96.1092110000
                             0.2388464606
  6
         36.9650810000
                             0.8240173974
F 1
         14.2173390000
                             1.0000000000
  1
F 1
  1
          5.4682070000
                             1.0000000000
F 1
          2.1031570000
                             1.0000000000
  1
F 1
          0.8089060000
                             1.0000000000
  1
F 1
                             1.0000000000
  1
          0.3111180000
F 1
  1
          0.1196610000
                             1.0000000000
 end
# Basis set for element : Np
NewGTO 93
S 9
     60212393.78258100
                            0.0337877053
  1
  2
    27369269.90117300
                            -0.0222982323
    12440577.22780600
                            0.0625876540
  3
  4
     5654807.830821000
                             0.0037311573
     2570367.195828000
                            0.0947361564
    1168348.725376000
                            0.0778954004
  7
     531067.6024440000
                            0.1945965254
  8
     241394.3647470000
                             0.2620928230
  9
     109724.7112490000
                             0.4855650387
S 1
  1
      49874.8687490000
                             1.0000000000
S 1
  1
      22670.3948860000
                             1.0000000000
```

_	1		
S	1 1	10304.7249480000	1.0000000000
S	1 1	4683.9658860000	1.0000000000
S	1 1	2129.0754030000	1.0000000000
S	1	2129.0754050000	
S	1 1	967.7615470000	1.0000000000
S	1 1	439.8916120000	1.0000000000
	1	199.9507330000	1.0000000000
S	1 1	90.8866970000	1.0000000000
S	1 1	41.3121350000	1.0000000000
S	1 1	18.7782430000	1.0000000000
S	1 1	8.5355650000	1.0000000000
S	1 1	3.8798020000	1.0000000000
S	1 1	1.7635460000	1.0000000000
S	1 1	0.8016120000	1.0000000000
S	1 1	0.3643690000	1.0000000000
S	1	0.1656220000	1.0000000000
S	1	0.0752830000	1.0000000000
S	1	0.0342190000	1.000000000
S	1		
Р	8	0.0155540000	1.0000000000
	1	859302.8310040000	0.0035335599
	2	358042.8462520000	0.0009072179
	3	149184.5192720000	0.0091562829
	4	62160.2163630000	0.0135877381
	5	25900.0901510000	0.0391645831
	6	10791.7042300000	0.0939664749
	7	4496.5434290000	0.2620978347
	8	1873.5597620000	0.7075269947
Р	1	780.6499010000	1.0000000000
Р	1		
Р	1	325.2707920000	1.0000000000
Р	1 1	135.5294970000	1.0000000000
Р	1 1	56.4706240000	1.0000000000
Р	1 1	23.5294270000	1.0000000000
Р	1	9.8039280000	1.0000000000
Р	1 1	4.0849700000	1.0000000000
Р	1	1.7020710000	1.0000000000
' Р	1	0.7091960000	1.0000000000
r P	1	0.2954980000	1.0000000000
	1	0.1231240000	1.0000000000
Р	1 1	0.0513020000	1.0000000000

```
D 7
  1
      42129.4422870000
                             0.0001611265
  2
      16851.7769150000
                             0.0003940653
  3
       6740.7107660000
                             0.0021726234
  4
       2696.2843060000
                             0.0099267939
  5
       1078.5137230000
                             0.0525706620
  6
        431.4054890000
                             0.2363631910
  7
        172.5621960000
                             0.7961024818
D 1
  1
         69.0248780000
                             1.0000000000
D 1
  1
         27.6099510000
                             1.0000000000
D 1
  1
         11.0439810000
                             1.0000000000
D 1
  1
          4.4175920000
                             1.0000000000
D 1
          1.7670370000
                             1.0000000000
D 1
          0.7068150000
                             1.0000000000
  1
D 1
  1
          0.2827260000
                             1.0000000000
D 1
          0.1130900000
                             1.0000000000
  1
D 1
  1
          0.0452360000
                             1.0000000000
F 6
       4574.1842730000
                             0.0000640986
  1
  2
       1759.3016440000
                             0.0004772097
  3
        676.6544780000
                             0.0045257498
  4
        260.2517220000
                             0.0380362075
  5
        100.0968160000
                             0.2369289742
  6
         38.4987760000
                             0.8257014451
  1
  1
         14.8072210000
                             1.0000000000
F
 1
          5.6950850000
                             1.0000000000
  1
F
 1
                             1.0000000000
          2.1904170000
  1
F 1
          0.8424680000
                             1.0000000000
  1
F 1
  1
          0.3240260000
                             1.0000000000
F 1
  1
          0.1246250000
                             1.0000000000
 end
# Basis set for element : Pu
NewGTO 94
S 9
  1
     61522220.62252900
                             0.0344658099
  2 27964645.73751300
                            -0.0228100400
  3 12711202.60796100
                             0.0637459626
  4
     5777819.367255000
                             0.0034434745
  5
     2626281.530570000
                             0.0960116578
    1193764.332077000
                             0.0779564129
  6
  7
     542620.1509440000
                             0.1956851492
  8
     246645.5231560000
                             0.2615180971
  9
     112111.6014350000
                             0.4840352422
S 1
  1
      50959.8188340000
                             1.0000000000
S 1
                             1.0000000000
  1
      23163.5540150000
S 1
      10528.8881890000
                             1.0000000000
  1
S 1
                             1.0000000000
       4785.8582680000
  1
S 1
```

_	1	2175.3901220000	1.0000000000
S	1 1	988.8136920000	1.0000000000
S	1	449.4607690000	1.0000000000
S	1 1	204.3003500000	1.0000000000
S	1		
S	1 1	92.8637950000	1.0000000000
S	1	42.2108160000	1.0000000000
S	1 1	19.1867350000	1.0000000000
S	1	8.7212430000	1.0000000000
	1	3.9642010000	1.0000000000
S	1 1	1.8019100000	1.0000000000
S	1	0.8190500000	1.0000000000
S	1 1	0.3722950000	1.0000000000
S	1		
S	1 1	0.1692250000	1.0000000000
S	1	0.0769210000	1.0000000000
S	1 1	0.0349640000	1.0000000000
P	1	0.0158930000	1.0000000000
г	1	879013.3813660000	0.0036280441
	2	366255.5755690000	0.0009245055
	3	152606.4898210000	0.0093631710
	4	63586.0374250000	0.0138180947
	5	26494.1822610000	0.0397209745
	6	11039.2426090000	0.0947610975
	7	4599.6844200000	0.2629722435
	8	1916.5351750000	0.7058860729
Р	1		
	1	798.5563230000	1.0000000000
Р	1	332.7318010000	1.0000000000
Р	1 1	138.6382510000	1.0000000000
Р	1		
Р	1	57.7659380000	1.0000000000
Р	1 1	24.0691410000	1.0000000000
Р	1 1	10.0288090000	1.0000000000
	1	4.1786700000	1.0000000000
Р	1 1	1.7411130000	1.0000000000
Р	1 1	0.7254640000	1.0000000000
Р	1 1	0.3022760000	1.0000000000
Р	1	0.1259490000	1.0000000000
Р	1		
D	1 7	0.0524790000	1.0000000000
	1	43223.8765000000	0.0001644977
	2	17289.5506000000	0.0004003774
	3	6915.8202400000	0.0021984643
	4	2766.3280960000	0.0099946905
	+	2700.3200300000	0.0055540505

```
5
       1106.5312380000
                            0.0527180463
  6
        442.6124950000
                             0.2364259417
  7
        177.0449980000
                             0.7959685659
D 1
                             1.0000000000
  1
         70.8179990000
D 1
  1
         28.3272000000
                             1.0000000000
D 1
         11.3308800000
                             1.0000000000
  1
D 1
  1
          4.5323520000
                             1.0000000000
D 1
  1
          1.8129410000
                             1.0000000000
D 1
          0.7251760000
                             1.0000000000
  1
D 1
          0.2900710000
                             1.0000000000
  1
D 1
          0.1160280000
                             1.0000000000
  1
D 1
                             1.0000000000
          0.0464110000
  1
F 6
                             0.0000634702
  1
       4758.8680260000
  2
       1830.3338560000
                             0.0004734278
  3
        703.9745600000
                             0.0044552586
  4
        270.7594460000
                            0.0375494378
  5
        104.1382490000
                             0.2351391900
         40.0531730000
  6
                             0.8272671140
F
 1
  1
         15.4050660000
                             1.0000000000
F 1
  1
          5.9250260000
                             1.0000000000
F 1
  1
          2.2788560000
                             1.0000000000
F 1
          0.8764830000
                             1.0000000000
F 1
          0.3371090000
                             1.0000000000
F 1
          0.1296570000
                             1.0000000000
 1
 end
# Basis set for element : Am
NewGTO 95
S 9
  1
     62843653.32610500
                             0.0351658825
     28565296.96641200
                            -0.0233394478
  2
  3 12984225.89382300
                            0.0649396714
  4 5901920.860829000
                            0.0031419101
     2682691.300377000
                            0.0973200958
  6
     1219405.136535000
                            0.0780067978
  7
     554275.0620610000
                            0.1967928683
     251943.2100280000
  8
                            0.2609169513
  9
                             0.4824914468
    114519.6409220000
S 1
      52054.3822370000
                             1.0000000000
  1
S 1
 1
      23661.0828350000
                             1.0000000000
S 1
  1
      10755.0376520000
                             1.0000000000
S 1
       4888.6534780000
                             1.0000000000
  1
S 1
                             1.0000000000
  1
       2222.1152170000
S 1
  1
       1010.0523720000
                             1.0000000000
S 1
  1
        459.1147140000
                             1.0000000000
```

_	_		
S	1	208.6885070000	1.0000000000
S	1	94.8584120000	1.0000000000
S	1		
S	1 1	43.1174600000	1.0000000000
S	1	19.5988450000	1.0000000000
S	1	8.9085660000	1.0000000000
	1	4.0493480000	1.0000000000
S	1 1	1.8406130000	1.0000000000
S	1 1	0.8366420000	1.0000000000
S	1 1	0.3802920000	1.0000000000
S	1		
S	1 1	0.1728600000	1.0000000000
S	1	0.0785730000	1.0000000000
S	1 1	0.0357150000	1.0000000000
	1	0.0162340000	1.0000000000
Р	8	000000 0004060000	0.0027246164
	1	898929.0904960000	0.0037246164
	2	374553.7877070000	0.0009420557
	3	156064.0782110000	0.0095738607
	4	65026.6992550000	0.0140514412
	5	27094.4580230000	0.0402836985
	6	11289.3575090000	0.0955608348
	7	4703.8989620000	0.2638489693
	8	1959.9579010000	0.7042322614
Ρ	1		
	1	816.6491250000	1.0000000000
_		010.0431230000	1.000000000
Р	1 1	340.2704690000	1.0000000000
Р	1 1	141.7793620000	1.0000000000
Р	1	59.0747340000	1.0000000000
Р	1		
Р	1 1	24.6144730000	1.0000000000
Р	1 1	10.2560300000	1.0000000000
Р	1	4.2733460000	1.0000000000
Р	1 1	1.7805610000	1.0000000000
	1	0.7419000000	1.0000000000
Р	1 1	0.3091250000	1.0000000000
Р	1 1	0.1288020000	1.0000000000
Р	1	0.0536680000	1.0000000000
D	7		
	1	44331.4203980000	0.0001679383
	2	17732.5681590000	0.0004068217
	3	7093.0272640000	0.0022248332
	4	2837.2109050000	0.0100645341
	5	1134.8843620000	0.0528720089
	6	453.9537450000	0.2365032043
	7	181.5814980000	0.7958188325
ь		101.7014700000	0.770100323
D	1 1	72.6325990000	1.0000000000

```
D 1
         29.0530400000
                             1.0000000000
  1
D 1
         11.6212160000
                             1.0000000000
  1
D 1
          4.6484860000
                             1.0000000000
  1
D 1
  1
          1.8593950000
                             1.0000000000
D 1
  1
          0.7437580000
                             1.0000000000
D 1
  1
          0.2975030000
                             1.0000000000
D 1
  1
          0.1190010000
                             1.0000000000
D 1
  1
          0.0476010000
                             1.0000000000
F 6
  1
       4946.8424820000
                             0.0000628938
       1902.6317240000
                             0.0004701484
  2
  3
        731.7814320000
                             0.0043891511
        281.4543970000
                             0.0370904453
  4
        108.2516910000
  5
                             0.2334062650
         41.6352660000
  6
                             0.8287755370
F
 1
  1
         16.0135640000
                             1.0000000000
F 1
          6.1590630000
                             1.0000000000
F 1
          2.3688700000
                             1.0000000000
  1
F 1
          0.9111040000
                             1.0000000000
  1
F 1
  1
          0.3504250000
                             1.0000000000
F 1
          0.1347790000
                             1.0000000000
  1
 end
# Basis set for element : Cm
NewGTO 96
S 9
     64183659.71228800
                            0.0358890046
 1
  2 29174390.77831300
                            -0.0238873385
  3 13261086.71741500
                            0.0661705007
  4 6027766.689734000
                             0.0028257430
                            0.0986630440
  5
    2739893.949879000
     1245406.340854000
                             0.0780460170
  7
     566093.7912970000
                            0.1979206486
     257315.3596810000
                             0.2602882009
  9
     116961.5271280000
                             0.4809328290
S 1
  1
      53164.3305130000
                             1.0000000000
S 1
                             1.0000000000
  1
      24165.6047780000
S 1
                             1.0000000000
  1
      10984.3658080000
S 1
  1
       4992.8935490000
                             1.0000000000
S 1
  1
       2269.4970680000
                             1.0000000000
S 1
       1031.5895760000
                             1.0000000000
  1
S 1
        468.9043530000
                             1.0000000000
  1
S 1
        213.1383420000
                             1.0000000000
  1
S 1
                             1.0000000000
         96.8810650000
  1
S 1
```

1	44.0368480000	1.0000000000
S 1 1	20.0167490000	1.0000000000
S 1	0.0005330000	1 000000000
1 5 1	9.0985220000	1.0000000000
1 5 1	4.1356920000	1.0000000000
1	1.8798600000	1.0000000000
S 1 1	0.8544820000	1.0000000000
5 1 1	0.3884010000	1.0000000000
S 1 1	0.1765460000	1.0000000000
S 1 1	0.0802480000	1.0000000000
S 1 1		
S 1	0.0364760000	1.0000000000
1 P 8	0.0165800000	1.0000000000
1	919065.4160050000	0.0038233559
2	382943.9233360000	0.0009598734
3	159559.9680560000	0.0097884845
4	66483.3200240000	0.0142878620
5	27701.3833430000	0.0408529100
6	11542.2430600000	0.0963657199
7	4809.2679420000	0.2647275734
		0.7025657657
8 P 1	2003.8616420000	0./02565/65/
1 P 1	834.9423510000	1.0000000000
1	347.8926460000	1.0000000000
P 1	347.8320400000	1.000000000
1 P 1	144.9552690000	1.0000000000
1 P 1	60.3980290000	1.0000000000
1 P 1	25.1658450000	1.0000000000
1	10.4857690000	1.0000000000
P 1	4.3690700000	1.0000000000
P 1	1.8204460000	1.0000000000
P 1	0.7585190000	1.0000000000
P 1		
1 P 1	0.3160500000	1.0000000000
	0 1316070000	1 000000000
1 P 1	0.1316870000	1.0000000000
1 D 7	0.0548700000	1.0000000000
1	45453.5554980000	0.0001714478
2	18181.4221990000	0.0004133915
3	7272.5688800000	0.0022516908
4		
	2909.0275520000	0.0101360687
5	1163.6110210000	0.0530312799
6	465.4444080000	0.2365910587
7	186.1777630000	0.7956572424
D 1	74 4744050000	1 0000000
1 D 1	74.4711050000	1.0000000000
1	29.7884420000	1.0000000000
D 1	44 0455======	4 00000000
1	11.9153770000	1.0000000000
D 1		

```
1
          4.7661510000
                            1.0000000000
D 1
  1
          1.9064600000
                             1.0000000000
D 1
  1
          0.7625840000
                            1.0000000000
D 1
  1
          0.3050340000
                             1.0000000000
D 1
          0.1220130000
                             1.0000000000
  1
D 1
  1
          0.0488050000
                            1.0000000000
F 6
  1
       5137.9626210000
                            0.0000623692
                            0.0004673406
  2
       1976.1394700000
  3
        760.0536420000
                            0.0043272570
  4
        292.3283240000
                            0.0366582974
  5
        112.4339710000
                            0.2317312383
                            0.8302266034
  6
         43.2438350000
F 1
         16.6322440000
                            1.0000000000
  1
F 1
          6.3970170000
  1
                            1.0000000000
F 1
          2.4603910000
                            1.0000000000
  1
F 1
          0.9463040000
                            1.0000000000
  1
F 1
          0.3639630000
                            1.0000000000
  1
F 1
  1
          0.1399860000
                            1.0000000000
 end
# Basis set for element : Bk
NewGTO 97
S 9
    65541743.54207900
                            0.0366362262
 1
     29791701.61003600
                            -0.0244545791
                            0.0674400979
  3 13541682.55001600
  4 6155310.250007000
                            0.0024942219
  5 2797868.295458000
                            0.1000419508
                            0.0780734218
    1271758.316117000
  7
     578071.9618710000
                            0.1990693119
  8
     262759.9826690000
                            0.2596306533
  9
    119436.3557590000
                            0.4793588927
S 1
  1
      54289.2526180000
                            1.0000000000
S 1
      24676.9330080000
                            1.0000000000
 1
S 1
                             1.0000000000
  1
      11216.7877310000
S 1
  1
       5098.5398780000
                            1.0000000000
S 1
  1
       2317.5181260000
                            1.0000000000
S 1
       1053.4173300000
                            1.0000000000
  1
S 1
        478.8260590000
                            1.0000000000
  1
S 1
        217.6482090000
                            1.0000000000
  1
S 1
         98.9310040000
                            1.0000000000
  1
S 1
                             1.0000000000
  1
         44.9686380000
S 1
  1
         20.4402900000
                             1.0000000000
S 1
  1
          9.2910410000
                            1.0000000000
```

_	_		
5	1 1	4.2232000000	1.0000000000
S	1 1	1.9196370000	1.0000000000
S	1		
S	1 1	0.8725620000	1.0000000000
S	1 1	0.3966190000	1.0000000000
	1	0.1802810000	1.0000000000
S	1 1	0.0819460000	1.0000000000
S	1 1	0.0372480000	1.0000000000
S	1 1	0.0169310000	1.0000000000
Р	8		
	1	939440.7605340000	0.0039243336
	2	391433.6502220000	0.0009779604
	3	163097.3542590000	0.0100071543
	4	67957.2309410000	0.0145274046
	5	28315.5128920000	0.0414286822
	6	11798.1303720000	0.0971756151
	7	4915.8876550000	0.2656073518
Р	8 1	2048.2865230000	0.7008871987
Р	1 1	853.4527180000	1.0000000000
Р	1	355.6052990000	1.0000000000
•	1	148.1688750000	1.0000000000
Ρ	1		
Р	1 1	61.7370310000	1.0000000000
Р	1	25.7237630000	1.0000000000
	1	10.7182350000	1.0000000000
P	1	4.4659310000	1.0000000000
P	1	1.8608050000	1.0000000000
P	1	0.7753350000	1.0000000000
P	1	0.3230560000	1.0000000000
Р	1 1	0.1346070000	1.0000000000
Р	1	0.0560860000	1.0000000000
D	7		
	1	46590.6458960000	0.0001750203
	2	18636.2583580000	0.0004201197
	3	7454.5033430000	0.0022789545
	4	2981.8013370000	0.0102096143
	5	1192.7205350000	0.0531954810
		477.0882140000	0.2366963299
	6	477.0882140000	
	7	190.8352860000	0.7954780716
D	1		1
	1	76.3341140000	1.0000000000
_		,0.5541140000	1.000000000
D	1		
	1	30.5336460000	1.0000000000
D	1	12 2124500000	1 0000000000
_	1	12.2134580000	1.0000000000
D	1		
D	1	4.8853830000	1.0000000000
U	1	1.9541530000	1.0000000000
D	1	1.234133666	1.000000000
U	1	0.7816610000	1.0000000000
	-	0.7.010010000	

```
D 1
          0.3126650000
                             1.0000000000
  1
D 1
          0.1250660000
                             1.0000000000
  1
D 1
          0.0500260000
                             1.0000000000
  1
F 6
  1
       5327.8457110000
                             0.0000619947
  2
       2049.1714270000
                             0.0004653579
  3
        788.1428570000
                             0.0042749941
  4
        303.1318680000
                             0.0362878121
  5
        116.5891800000
                             0.2302770619
         44.8419920000
  6
                             0.8314823055
F
 1
  1
         17.2469200000
                             1.0000000000
F
  1
          6.6334310000
                             1.0000000000
  1
F 1
                             1.0000000000
          2.5513200000
  1
F 1
                             1.0000000000
          0.9812770000
  1
F 1
                             1.0000000000
  1
          0.3774140000
F 1
  1
          0.1451590000
                             1.0000000000
 end
# Basis set for element : Cf
NewGTO 98
S 9
 1
     66908672.67153500
                            0.0374085968
  2
     30413033.03251600
                            -0.0250420417
  3
     13824105.92387100
                            0.0687500948
  4 6283684.510850000
                            0.0021465649
  5 2856220.232205000
                             0.1014582118
  6 1298281.923729000
                            0.0780882908
  7
     590128.1471500000
                             0.2002396174
  8
     268240.0668860000
                             0.2589431115
    121927.3031300000
                             0.4777692911
S 1
  1
      55421.5014230000
                             1.0000000000
S 1
      25191.5915560000
                             1.0000000000
  1
S 1
     11450.7234340000
  1
                             1.0000000000
S 1
       5204.8742880000
                             1.0000000000
  1
S 1
  1
       2365.8519490000
                             1.0000000000
S 1
  1
       1075.3872500000
                             1.0000000000
S 1
                             1.0000000000
  1
        488.8123860000
S 1
                             1.0000000000
  1
        222.1874480000
S 1
  1
        100.9942950000
                             1.0000000000
S 1
  1
         45.9064980000
                             1.0000000000
S 1
         20.8665900000
                             1.0000000000
  1
S 1
          9.4848140000
                             1.0000000000
  1
S 1
          4.3112790000
                             1.0000000000
  1
S 1
                             1.0000000000
          1.9596720000
  1
S 1
```

1	0.8907600000	1.0000000000
S 1 1	0.4048910000	1.0000000000
S 1	0.101032000	1.000000000
1 S 1	0.1840410000	1.0000000000
1 S 1	0.0836550000	1.0000000000
1 S 1	0.0380250000	1.0000000000
1 P 8	0.0172840000	1.0000000000
1	960041.3086390001	0.0040276045
2	400017.2119330000	0.0040270043
3	166673.8383050000	
		0.0102299597
4	69447.4326270000	0.0147701296
5	28936.4302610000	0.0420111673
6	12056.8459420000	0.0979906843
7	5023.6858090000	0.2664887009
8	2093.2024210000	0.6991958875
	2033:2024210000	0.0551550075
P 1		
1 P 1	872.1676750000	1.0000000000
1	363.4031980000	1.0000000000
	363.4631986666	1.000000000
P 1		
1	151.4179990000	1.0000000000
P 1		
1	63.0908330000	1.0000000000
	03.0300330000	1.000000000
P 1		
1	26.2878470000	1.0000000000
P 1		
1	10.9532700000	1.0000000000
P 1		
	4 5639639999	1 000000000
1	4.5638620000	1.0000000000
P 1		
1	1.9016090000	1.0000000000
P 1		
1	0.7923370000	1.0000000000
	0.7923370000	1.000000000
P 1		
1	0.3301410000	1.0000000000
P 1		
1	0.1375590000	1.0000000000
	0.1575556666	1.000000000
1	0.0573160000	1.0000000000
D 7		
1	47740.9667690000	0.0001786657
2	19096.3867080000	0.0004269828
3	7638.5546830000	0.0023067483
4	3055.4218730000	0.0102850279
5	1222.1687490000	0.0533657826
6	488.8675000000	0.2368148452
7	195.5470000000	0.7952843597
	193.3470000000	0.7332643337
D 1		
1	78.2188000000	1.0000000000
D 1		
1	31.2875200000	1.0000000000
D 1	321207320000	_,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
	42 545000000	4 000000000
1	12.5150080000	1.0000000000
D 1		
1	5.0060030000	1.0000000000
D 1		
	2 002404000	1 000000000
1	2.0024010000	1.0000000000
D 1		
1	0.8009610000	1.0000000000
D 1		
	0 2202040000	1 000000000
1	0.3203840000	1.0000000000
D 1		
1	0.1281540000	1.0000000000
D 1		

```
1
          0.0512610000
                             1.0000000000
F 6
  1
       5522.2215080000
                             0.0000616371
       2123.9313490000
                             0.0004636186
  2
  3
        816.8966730000
                             0.0042245181
  4
        314.1910280000
                             0.0359285881
  5
        120.8427030000
                             0.2288308799
  6
         46.4779630000
                             0.8327258043
  1
  1
         17.8761400000
                             1.0000000000
F
 1
  1
          6.8754380000
                             1.0000000000
F 1
  1
          2.6443990000
                             1.0000000000
F 1
  1
          1.0170770000
                             1.0000000000
F 1
          0.3911830000
                             1.0000000000
F 1
          0.1504550000
                             1.0000000000
 1
 end
# Basis set for element : Es
NewGTO 99
S 9
    68291966.01786400
                             0.0382073668
  2 31041802.73539300
                           -0.0256507539
     14109910.33426900
                             0.0701024687
  4
    6413595.606486000
                            0.0017819093
  5 2915270.730221000
                            0.1029136072
  6 1325123.059191000
                            0.0780899367
  7
     602328.6632690000
                            0.2014326209
  8
     273785.7560310000
                             0.2582241751
 9
     124448.0709230000
                             0.4761632255
S 1
     56567.3049650000
                             1.0000000000
  1
S 1
                             1.0000000000
      25712.4113480000
  1
S 1
      11687.4597040000
                             1.0000000000
  1
S 1
  1
       5312.4816830000
                             1.0000000000
S 1
  1
       2414.7644020000
                             1.0000000000
S 1
  1
       1097.6201830000
                             1.0000000000
S 1
        498.9182650000
                             1.0000000000
  1
S 1
        226.7810290000
                             1.0000000000
  1
S 1
        103.0822860000
                             1.0000000000
  1
S 1
  1
         46.8555850000
                             1.0000000000
S 1
         21.2979930000
                             1.0000000000
  1
S 1
          9.6809060000
                             1.0000000000
  1
S 1
          4.4004120000
                             1.0000000000
  1
S 1
          2.0001870000
                             1.0000000000
  1
S 1
                             1.0000000000
  1
          0.9091760000
S 1
  1
          0.4132620000
                             1.0000000000
S 1
          0.1878460000
                             1.0000000000
```

S 1 1	0.0853850000	1.0000000000
S 1 1	0.0200110000	1 000000000
5 1	0.0388110000	1.0000000000
1 P 8	0.0176410000	1.0000000000
1	980851.9776920000	0.0041332085
2	408688.3240390000	0.0010149594
3	170286.8016830000	0.0104569563
4	70952.8340340000	0.0150160479
5	29563.6808480000	0.0426004057
6	12318.2003530000	0.0988108855
7	5132.5834810000	0.2673716902
8	2138.5764500000	0.6974916631
P 1		0.007, 1520052
	001 0735310000	1 000000000
1	891.0735210000	1.0000000000
P 1		
1	371.2806340000	1.0000000000
P 1		
1	154.7002640000	1.0000000000
P 1	134.7002040000	1.0000000000
. –	64 4504430000	4 000000000
1	64.4584430000	1.0000000000
P 1		
1	26.8576850000	1.0000000000
P 1		
1	11 100702000	1 000000000
	11.1907020000	1.0000000000
P 1		
1	4.6627920000	1.0000000000
P 1		
1	1.9428300000	1.0000000000
P 1	1.5120300000	1.000000000
1	0.8095130000	1.0000000000
P 1		
1	0.3372970000	1.0000000000
P 1		
1	0.1405400000	1.0000000000
	0.1403400000	1.000000000
P 1		
1	0.0585580000	1.0000000000
D 7		
1	48905.6146030000	0.0001823817
2	19562.2458410000	0.0004339877
3	7824.8983360000	0.0023350216
4	3129.9593350000	0.0103622607
5	1251.9837340000	0.0535412927
6	500.7934940000	0.2369464545
7	200.3173970000	0.7950766376
	200.3173970000	0.7930700370
D 1		
1	80.1269590000	1.0000000000
D 1		
1	32.0507840000	1.0000000000
D 1		
1	12.8203130000	1.0000000000
	12.8203130000	1.000000000
D 1		
1	5.1281250000	1.0000000000
D 1		
1	2.0512500000	1.0000000000
D 1		
1	0.8205000000	1.0000000000
	0.0203000000	1.0000000000
D 1		
1	0.3282000000	1.0000000000
D 1		
1	0.1312800000	1.0000000000
D 1		
1	0 0525120000	1 0000000000
	0.0525120000	1.0000000000
F 6		
1	5719.1357660000	0.0000613354
2	2199.6676020000	0.0004622721
3	846.0260010000	0.0041780067
		2.00.2700007

```
5
        125.1517750000
                            0.2274579329
  6
         48.1352980000
                            0.8339018758
F
 1
                            1.0000000000
  1
         18.5135760000
F 1
  1
          7.1206060000
                            1.0000000000
F 1
          2.7386950000
                            1.0000000000
  1
F 1
  1
          1.0533440000
                             1.0000000000
F 1
  1
          0.4051320000
                            1.0000000000
F 1
          0.1558200000
                            1.0000000000
 1
 end
# Basis set for element : Fm
NewGTO 100
S 9
    69690927.07216800
                            0.0390337818
 1
  2 31677694.12371300
                           -0.0262817473
                            0.0714991707
  3 14398951.87441500
  4
    6544978.124734000
                            0.0013993543
  5 2974990.056697000
                            0.1044098445
  6 1352268.207590000
                            0.0780775752
  7
     614667.3670860000
                            0.2026492856
  8
     279394.2577660000
                            0.2574724267
  9
     126997.3898940000
                            0.4745401221
S 1
  1
      57726.0863150000
                            1.0000000000
S 1
  1
      26239.1301430000
                            1.0000000000
S 1
  1
      11926.8773380000
                            1.0000000000
S 1
  1
       5421.3078810000
                             1.0000000000
S 1
       2464.2308550000
                            1.0000000000
  1
S 1
  1
       1120.1049340000
                            1.0000000000
S 1
        509.1386060000
                            1.0000000000
  1
S 1
                            1.0000000000
  1
        231.4266390000
S 1
        105.1939270000
                            1.0000000000
  1
S 1
  1
         47.8154210000
                            1.0000000000
S 1
  1
         21.7342820000
                            1.0000000000
S 1
          9.8792190000
                            1.0000000000
  1
S 1
                            1.0000000000
  1
          4.4905540000
S 1
  1
          2.0411610000
                            1.0000000000
S 1
  1
          0.9278000000
                             1.0000000000
S 1
          0.4217270000
                             1.0000000000
  1
S 1
          0.1916940000
                             1.0000000000
  1
S 1
          0.0871340000
                            1.0000000000
  1
S 1
          0.0396060000
                            1.0000000000
  1
S 1
```

4

325.3946160000

0.0355948244

1	0 0190020000	1 000000000
1 P 8	0.0180030000	1.0000000000
1	1001894.089886000	0.0042412402
2	417455.8707860000	0.0010338777
3	173939.9461610000	0.0106883016
4	72474.9775670000	0.0152652560
5	30197.9073200000	0.0431965823
6	12582.4613830000	0.0996362565
7	5242.6922430000	0.2682558591
8	2184.4551010000	0.6957747230
P 1		
1	910.1896260000	1.0000000000
P 1		
1	379.2456770000	1.0000000000
P 1		
1	158.0190320000	1.0000000000
P 1		
1	65.8412630000	1.0000000000
P 1	27 4220600000	1 000000000
1 P 1	27.4338600000	1.0000000000
1	11.4307750000	1.0000000000
P 1	11.4307730000	1.000000000
1	4.7628230000	1.0000000000
P 1	11,7020230000	1.0000000000
1	1.9845100000	1.0000000000
P 1		
1	0.8268790000	1.0000000000
P 1		
1	0.3445330000	1.0000000000
P 1		
1	0.1435550000	1.0000000000
P 1		
1	0.0598150000	1.0000000000
D 7	F000F 12210F0000	0.0001061601
1 2	50085.1221850000 20034.0488740000	0.0001861691 0.0004411335
3	8013.6195500000	0.0023637654
4	3205.4478200000	0.0104412302
5	1282.1791280000	0.0537215840
6	512.8716510000	0.2370898560
7	205.1486600000	0.7948562136
D 1	203.140000000	0.7540502150
1	82.0594640000	1.0000000000
D 1		
1	32.8237860000	1.0000000000
D 1		
1	13.1295140000	1.0000000000
D 1		
1	5.2518060000	1.0000000000
D 1	1 1007030000	1 000000000
1 D 1	2.1007220000	1.0000000000
1	0.8402890000	1.0000000000
D 1	0.0402030000	1.0000000000
1	0.3361160000	1.0000000000
D 1		
1	0.1344460000	1.0000000000
D 1		
1	0.0537780000	1.0000000000
F 6	E040 =445::::::	0 0000
1	5918.7118140000	0.0000610840
2	2276.4276210000	0.0004612776
3	875.5490850000	0.0041350354
4	336.7496480000	0.0352838640
5 6	129.5190950000 49.8150370000	0.2261506375 0.8350176085
6 F 1	H9.012076H	0.0330170033
1	19.1596290000	1.0000000000
-		

```
F 1
          7.3690880000
                            1.0000000000
  1
F 1
  1
          2.8342650000
                            1.0000000000
F 1
          1.0901020000
                            1.0000000000
  1
F 1
  1
          0.4192700000
                            1.0000000000
F 1
  1
          0.1612580000
                            1.0000000000
 end
# Basis set for element : Md
NewGTO 101
S 9
  1 71095290.12593000
                            0.0398891130
  2 32316040.96633200
                           -0.0269360781
  3 14689109.53015100
                            0.0729421777
     6676867.968250000
                            0.0009979576
  5 3034939.985568000
                            0.1059486225
  6 1379518.175258000
                            0.0780503541
  7
     627053.7160270000
                            0.2038905511
  8
     285024.4163760000
                            0.2566864307
  9
     129556.5528980000
                            0.4728994876
S 1
  1
      58889.3422260000
                            1.0000000000
S 1
  1
      26767.8828300000
                             1.0000000000
S 1
     12167.2194680000
                            1.0000000000
  1
S 1
  1
       5530.5543040000
                            1.0000000000
S 1
       2513.8883200000
                            1.0000000000
  1
S 1
                            1.0000000000
       1142.6765090000
  1
S 1
        519.3984130000
                            1.0000000000
  1
S 1
        236.0901880000
                            1.0000000000
  1
S 1
  1
        107.3137220000
                            1.0000000000
S 1
  1
         48.7789640000
                            1.0000000000
S 1
         22.1722570000
                             1.0000000000
S 1
         10.0782980000
                             1.0000000000
  1
S 1
          4.5810450000
                             1.0000000000
  1
S 1
          2.0822930000
                            1.0000000000
  1
S 1
          0.9464970000
  1
                            1.0000000000
S 1
          0.4302260000
                            1.0000000000
  1
S 1
          0.1955570000
                            1.0000000000
  1
S 1
          0.0888900000
                            1.0000000000
  1
S 1
          0.0404040000
                            1.0000000000
  1
S 1
                             1.0000000000
  1
          0.0183660000
P 8
  1 1023192.458988000
                            0.0043518001
  2 426330.1912450000
                            0.0010530818
  3 177637.5796850000
                            0.0109241630
```

	4		
		74015.6582020000	0.0155178550
	5	30839.8575840000	0.0437998927
	6	12849.9406600000	0.1004668336
	7	5354.1419420000	0.2691407353
	8	2230.8924760000	0.6940452684
Р	1		
	1	929.5385320000	1.0000000000
_		323.3303320000	1.000000000
Р	1		
	1	387.3077210000	1.0000000000
Ρ	1		
	1	161.3782170000	1.0000000000
Р	1		
	1	67.2409240000	1.0000000000
Р	1	07.2103210000	1.000000000
•		28 017052000	1 000000000
_	1	28.0170520000	1.0000000000
Р	1		
	1	11.6737720000	1.0000000000
Ρ	1		
	1	4.8640710000	1.0000000000
Р	1		
•	1	2.0266960000	1.0000000000
_		2.0200300000	1.000000000
Р	1		
	1	0.8444570000	1.0000000000
Ρ	1		
	1	0.3518570000	1.0000000000
Р	1		
	1	0.1466070000	1.0000000000
Р	1	0.1400070000	1.000000000
-		0.0610060000	1 000000000
	1	0.0610860000	1.0000000000
D	7		
	1	51278.5205840000	0.0001900304
	2	20511.4082340000	0.0004484251
	3	8204.5632930000	0.0023930088
	4	3281.8253170000	0.0105220498
	5	1312.7301270000	0.0539072106
	6	525.0920510000	0.2372466561
	7	210.0368200000	0.7946214265
D	1		
	1	84.0147280000	1.0000000000
D	1		
	1	33.6058910000	1 000000000
D		33.0030310000	
υ			1.0000000000
_	1	12 4422570000	
		13.4423570000	1.0000000000
D	_		1.0000000000
υ	1	13.4423570000 5.3769430000	
D D	_		1.0000000000
_	1		1.0000000000
D	1 1 1	5.3769430000	1.0000000000
_	1 1 1	5.3769430000 2.1507770000	1.0000000000 1.0000000000 1.0000000000
D D	1 1 1 1	5.3769430000	1.0000000000
D D	1 1 1 1 1	5.3769430000 2.1507770000 0.8603110000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D	1 1 1 1 1 1	5.3769430000 2.1507770000	1.0000000000 1.0000000000 1.0000000000
D D	1 1 1 1 1 1 1	5.3769430000 2.1507770000 0.8603110000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D	1 1 1 1 1 1	5.3769430000 2.1507770000 0.8603110000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D D	1 1 1 1 1 1 1	5.3769430000 2.1507770000 0.8603110000 0.3441240000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D D	1 1 1 1 1 1 1 1	5.3769430000 2.1507770000 0.8603110000 0.3441240000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D D D	1 1 1 1 1 1 1 1 1 1	5.3769430000 2.1507770000 0.8603110000 0.3441240000 0.13765000000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D D	1 1 1 1 1 1 1 1 1 1 1 1 6	5.3769430000 2.1507770000 0.8603110000 0.3441240000 0.13765000000 0.05506000000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D D D	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	5.3769430000 2.15077700000 0.8603110000 0.3441240000 0.13765000000 0.05506000000 6120.85749600000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D D D	1 1 1 1 1 1 1 1 1 1 1 1 1 2 1 2 1 2 1 2	5.3769430000 2.15077700000 0.8603110000 0.3441240000 0.13765000000 0.05506000000 6120.85749600000 2354.17596000000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D D D	1 1 1 1 1 1 1 1 1 1 1 1 1 2 3	5.3769430000 2.15077700000 0.8603110000 0.3441240000 0.13765000000 0.05506000000 6120.85749600000 2354.17596000000 905.45229200000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D D D	1 1 1 1 1 1 1 1 1 1 1 1 1 2 1 2 1 2 1 2	5.3769430000 2.15077700000 0.8603110000 0.3441240000 0.13765000000 0.05506000000 6120.85749600000 2354.1759600000 905.45229200000 348.25088200000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D D D	1 1 1 1 1 1 1 1 1 1 1 1 1 2 3	5.3769430000 2.15077700000 0.8603110000 0.3441240000 0.13765000000 0.05506000000 6120.85749600000 2354.17596000000 905.45229200000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D D D	1 1 1 1 1 1 1 1 1 1 1 1 1 2 3 4	5.3769430000 2.15077700000 0.8603110000 0.3441240000 0.13765000000 0.05506000000 6120.85749600000 2354.1759600000 905.45229200000 348.25088200000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D D F	1 1 1 1 1 1 1 1 1 1 1 1 1 1 6 1 6 1 6 1	5.3769430000 2.15077700000 0.8603110000 0.3441240000 0.13765000000 0.05506000000 6120.85749600000 2354.17596000000 905.45229200000 348.25088200000 133.94264700000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D D D	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	5.3769430000 2.1507770000 0.8603110000 0.3441240000 0.1376500000 0.0550600000 6120.8574960000 2354.1759600000 905.4522920000 348.2508820000 133.94264700000 51.51640300000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D D F	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	5.3769430000 2.15077700000 0.8603110000 0.3441240000 0.13765000000 0.05506000000 6120.85749600000 2354.17596000000 905.45229200000 348.25088200000 133.94264700000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D D F	11111111116123456111	5.3769430000 2.1507770000 0.8603110000 0.3441240000 0.1376500000 0.05506000000 6120.85749600000 2354.1759600000 905.4522920000 348.2508820000 133.94264700000 51.51640300000 19.81400100000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D D F F F	111111111161234561111	5.3769430000 2.1507770000 0.8603110000 0.3441240000 0.1376500000 0.0550600000 6120.8574960000 2354.1759600000 905.4522920000 348.2508820000 133.94264700000 51.51640300000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D D F	1111111111612345611111	5.3769430000 2.1507770000 0.8603110000 0.3441240000 0.1376500000 0.0550600000 6120.8574960000 2354.1759600000 905.4522920000 348.2508820000 133.9426470000 51.5164030000 19.81400100000 7.62077000000	1.0000000000 1.0000000000 1.0000000000 1.00000000
D D D F F F	111111111161234561111	5.3769430000 2.1507770000 0.8603110000 0.3441240000 0.1376500000 0.05506000000 6120.85749600000 2354.1759600000 905.4522920000 348.2508820000 133.94264700000 51.51640300000 19.81400100000	1.0000000000 1.0000000000 1.0000000000 1.00000000

```
1
          1.1273330000
                            1.0000000000
F 1
          0.4335900000
                             1.0000000000
F 1
  1
          0.1667650000
                            1.0000000000
 end
# Basis set for element : No
NewGTO 102
S 9
  1
     72522948.25117100
                            0.0407748606
  2 32964976.47780500
                           -0.0276149861
  3 14984080.21718400
                            0.0744338617
  4
     6810945.553265000
                            0.0005766671
  5
     3095884.342393000
                            0.1075320682
    1407220.155633000
                            0.0780074140
  6
     639645.5252880000
  7
                            0.2051576486
    290747.9660400000
  8
                            0.2558644588
  9
     132158.1663820000
                            0.4712404642
S 1
      60071.8938100000
                            1.0000000000
  1
S 1
  1
      27305.4062770000
                            1.0000000000
S 1
      12411.5483080000
 1
                            1.0000000000
S 1
       5641.6128670000
                            1.0000000000
  1
S 1
  1
       2564.3694850000
                            1.0000000000
S 1
  1
       1165.6224930000
                            1.0000000000
S 1
  1
        529.8284060000
                            1.0000000000
S 1
        240.8310940000
                            1.0000000000
S 1
        109.4686790000
                             1.0000000000
  1
S 1
         49.7584900000
                            1.0000000000
  1
S 1
  1
         22.6174960000
                            1.0000000000
S 1
         10.2806800000
                            1.0000000000
  1
S 1
          4.6730360000
                            1.0000000000
  1
S 1
          2.1241070000
                            1.0000000000
  1
S 1
  1
          0.9655030000
                            1.0000000000
S 1
  1
          0.4388650000
                            1.0000000000
S 1
          0.1994840000
                            1.0000000000
  1
S 1
                            1.0000000000
  1
          0.0906750000
S 1
  1
          0.0412160000
                            1.0000000000
S 1
  1
          0.0187340000
                            1.0000000000
P 8
  1 1044695.317505000
                            0.0044648922
  2 435289.7156270000
                            0.0010725714
     181370.7148450000
                            0.0111645278
  3
  4
      75571.1311850000
                            0.0157738043
      31487.9713270000
                            0.0444103084
  5
      13119.9880530000
                            0.1013026162
       5466.6616890000
                            0.2700270522
  7
  8
       2277.7757040000
                            0.6923025030
```

_	_		
Р	1	949.0732100000	1.0000000000
Р	1 1	205 4471710000	1 0000000000
Р	1	395.4471710000	1.0000000000
Р	1 1	164.7696540000	1.0000000000
_	1	68.6540230000	1.0000000000
P	1	28.6058430000	1.0000000000
	1	11.9191010000	1.0000000000
P _	1	4.9662920000	1.0000000000
P _	1	2.0692880000	1.0000000000
P _	1	0.8622030000	1.0000000000
Р	1 1	0.3592510000	1.0000000000
Р	1 1	0.1496880000	1.0000000000
Р	1 1	0.0623700000	1.0000000000
D	7 1	52485.5878850000	0.0001939672
	2	20994.2351540000	0.0004558647
	3	8397.6940620000	0.0024227611
	4	3359.0776250000	0.0106047308
	5	1343.6310500000	0.0540982091
	6	537.4524200000	0.2374169324
	7	214.9809680000	0.7943721750
D	1		
	1	85.9923870000	1.0000000000
_		03.3323070000	1.000000000
D	1		
	1	34.3969550000	1.0000000000
D	1		
D	1 1	13.7587820000	1.0000000000
D	1	5.5035130000	1.0000000000
D	1 1	2.2014050000	1.0000000000
D	1 1	0.8805620000	1.0000000000
D	1 1	0.3522250000	1.0000000000
D	1 1	0.1408900000	1.0000000000
D		0.0563560000	
F	6		1.0000000000
	1	6334.4566490000	0.0000606051
	2	2436.3294800000	0.0004596386
	3	937.0498000000	0.0040517232
	4	360.4037690000	0.0346769906
	5	138.6168340000	0.2235293511
	6	53.3141670000	0.8372440483
F	1	20 5054400000	1 000000000
_	1	20.5054490000	1.0000000000
F	1 1	7.8867110000	1.0000000000
F	1		
F	1	3.0333500000	1.0000000000
F	1 1	1.1666730000	1.0000000000
F	1 1	0.4487200000	1.0000000000
	1	0.1725850000	1.0000000000

```
# Basis set for element : Lr
NewGTO 103
S 9
  1
     73963782.78320600
                             0.0416924538
  2
     33619901.26509300
                            -0.0283196623
  3 15281773.30231500
                            0.0759764420
  4 6946260.591961000
                            0.0001344127
     3157391.178164000
                             0.1091620804
  6
     1435177.808256000
                            0.0779477770
  7
     652353.5492070000
                            0.2064516167
  8
     296524.3405490000
                             0.2550048856
  9
    134783.7911590000
                             0.4695625357
S 1
      61265.3596180000
                             1.0000000000
  1
S 1
                             1.0000000000
  1
      27847.8907350000
S 1
      12658.1321520000
                             1.0000000000
  1
S 1
  1
       5753.6964330000
                             1.0000000000
S 1
  1
       2615.3165600000
                             1.0000000000
S 1
       1188.7802550000
                             1.0000000000
S 1
        540.3546610000
                             1.0000000000
  1
S 1
        245.6157550000
                             1.0000000000
  1
S 1
  1
        111.6435250000
                             1.0000000000
S 1
         50.7470570000
                             1.0000000000
  1
S 1
         23.0668440000
                             1.0000000000
  1
S 1
         10.4849290000
                             1.0000000000
  1
S 1
          4.7658770000
                             1.0000000000
  1
S 1
  1
          2.1663080000
                             1.0000000000
S 1
  1
          0.9846850000
                             1.0000000000
S 1
          0.4475840000
                             1.0000000000
S 1
          0.2034470000
                             1.0000000000
  1
S 1
                             1.0000000000
  1
          0.0924760000
S 1
          0.0420350000
                             1.0000000000
  1
S 1
                             1.0000000000
  1
          0.0191070000
P 8
     1066386.172543000
                             0.0045805752
  1
  2
     444327.5718930000
                             0.0010923505
                             0.0114094860
     185136.4882890000
  3
  4
      77140.2034540000
                             0.0160331521
      32141.7514390000
                             0.0450279439
  6
      13392.3964330000
                             0.1021436966
  7
       5580.1651800000
                             0.2709149807
  8
       2325.0688250000
                             0.6905460164
P 1
        968.7786770000
                             1.0000000000
  1
P 1
        403.6577820000
                             1.00000000000
  1
P 1
```

1	168.1907430000	1.0000000000
P 1 1	70.0794760000	1.0000000000
P 1	70.0754700000	1.000000000
1 P 1	29.1997820000	1.0000000000
1	12.1665760000	1.0000000000
P 1	F 0604070000	1 000000000
1 P 1	5.0694070000	1.0000000000
1 P 1	2.1122530000	1.0000000000
1	0.8801050000	1.0000000000
P 1 1	0.3667110000	1.0000000000
P 1	0.300/110000	1.0000000000
1 P 1	0.1527960000	1.0000000000
1	0.0636650000	1.0000000000
D 7		
1	53706.9942560000	0.0001979823
2	21482.7977020000	0.0004634382
3	8593.1190810000	0.0024530344
4	3437.2476320000	0.0106890240
5	1374.8990530000	0.0542940150
6	549.9596210000	0.2375962102
7	219.9838480000	0.7941125739
D 1		
1	87.9935390000	1.0000000000
D 1	0.11133310000	
1	35.1974160000	1.0000000000
	33.1974100000	1.000000000
D 1	14 0700660000	1 000000000
1	14.0789660000	1.0000000000
D 1		
1	5.6315870000	1.0000000000
D 1		
1	2.2526350000	1.0000000000
D 1		
1	0.9010540000	1.0000000000
D 1		
1	0.3604220000	1.0000000000
D 1		
1	0.1441690000	1.0000000000
D 1	371.12070000	
1	0.0576670000	1.0000000000
F 6	0.0370070000	1.000000000
	CE42 71120C0000	0.0000004635
1	6543.7113860000	0.0000604625
2	2516.8120/20000	0.00045945/2
3	968.0046430000	0.0040165681
4	372.3094780000	0.0344165711
5	143.1959530000	0.2223536006
6	55.0753670000	0.8382365256
F 1		
1	21.1828330000	1.0000000000
F 1		
1	8.1472440000	1.0000000000
F 1	5.1	
1	3.1335550000	1.0000000000
F 1	3.133335000	1.0000000000
	1 2052140000	1 000000000
1	1.2052140000	1.0000000000
F 1		
1	0.4635440000	1.0000000000
F 1		
1	0.1782860000	1.0000000000
end		

SARC-ZORA basis sets

	sis set for element	: Ac
NewG S 9	TO 89	
1	55109808.74124400	0.0178209759
2	25049913.06420200	-0.0048962533
3	11386324.12009200	0.0319255750
4	5175601.872769000	0.0167252354
5	2352546.305804000	0.0611584085
6	1069339.229911000	0.0785620392
7	486063.2863230000	0.1627798541
8	220937.8574200000	0.2738459149
9	100426.2988270000	0.5252374109
S 1		
1	45648.3176490000	1.0000000000
S 1	20740 2252050000	1 000000000
1	20749.2352950000	1.0000000000
S 1	0.434 470500000	4 000000000
1	9431.4705890000	1.0000000000
S 1	4207 0220060000	1 000000000
1	4287.0320860000	1.0000000000
S 1	1040 (50040000	1 000000000
1 S 1	1948.6509480000	1.0000000000
3 I 1	885.7504310000	1.0000000000
S 1	003.7304310000	1.0000000000
1	402.6138320000	1.0000000000
S 1	402.0130320000	1.0000000000
1	183.0062870000	1.0000000000
S 1	183.0002870000	1.0000000000
1	83.1846760000	1.0000000000
S 1	83.1846760000	1.0000000000
1	37.8112160000	1.0000000000
S 1	37.8112100000	1.0000000000
1	17.1869170000	1.0000000000
S 1	17.1809170000	1.0000000000
1	7.8122350000	1.0000000000
S 1	7.0122330000	1.000000000
1	3.5510160000	1.0000000000
S 1	3.3310100000	1.000000000
1	1.6140980000	1.0000000000
S 1	1101.000000	2.000000000
1	0.7336810000	1.0000000000
S 1		
1	0.3334910000	1.0000000000
S 1		
1	0.1515870000	1.0000000000
S 1		
1	0.0689030000	1.0000000000
S 1		
1	0.0313200000	1.0000000000
S 1		
1	0.0142360000	1.0000000000
P 8		
1	782789.9000960000	0.0009671587
2	326162.4583730000	0.0009821244
3	135901.0243220000	0.0040393628
4	56625.4268010000	0.0092656876
5	23593.9278340000	0.0271978860
6	9830.8032640000	0.0789132917
7	4096.1680270000	0.2465259563
8	1706.7366780000	0.7375427350
P 1		
1	711.1402820000	1.0000000000
P 1		
1	296.3084510000	1.0000000000

P 1	400 4640550000	1 000000000
1 P 1	123.4618550000	1.0000000000
1	51.4424390000	1.0000000000
P 1	31.1121330000	1.000000000
1	21.4343500000	1.0000000000
P 1		
1	8.9309790000	1.0000000000
P 1		
1	3.7212410000	1.0000000000
P 1		
1	1.5505170000	1.0000000000
P 1	0 6460400000	1.0000000000
1 P 1	0.6460490000	1.0000000000
1	0.2691870000	1.0000000000
P 1	0.2031070000	1.000000000
1	0.1121610000	1.0000000000
P 1		
1	0.0467340000	1.0000000000
D 7		
1	37896.8365590000	0.0001025871
2	15158.7346230000	0.0002818463
3	6063.4938490000	0.0017362414
4	2425.3975400000	0.0087081829
5	970.1590160000	0.0500634942
6	388.0636060000	0.2344308595
7	155.2254430000	0.7991184111
	133.2234436666	0.7331104111
D 1	62 0001770000	1 000000000
1	62.0901770000	1.0000000000
D 1 1	24.8360710000	1 000000000
D 1	24.8360710000	1.0000000000
1	9.9344280000	1.0000000000
D 1	9.9344280000	1.000000000
1	3.9737710000	1.0000000000
D 1	3.3737710000	1.000000000
1	1.5895090000	1.0000000000
D 1	2.505505000	1.000000000
1	0.6358030000	1.0000000000
D 1		
1	0.2543210000	1.00000000000
D 1		
1	0.1017290000	1.0000000000
D 1		
1	0.0406910000	1.0000000000
F 6		
1	3860.7881580000	0.0000567234
2	1484.9185220000	0.0004538133
3	571.1225090000	0.0046863670
4	219.6625030000	0.0399061529
5	84.4855780000	0.2448573163
- 6 - 1	32.4944530000	0.8188357754
F 1	12 107067000	1 000000000
1	12.4978670000	1.0000000000
F 1	4 0000730000	1 000000000
1 [1	4.8068720000	1.0000000000
F 1	1 0/07070000	1 0000000000
1 F 1	1.8487970000	1.0000000000
1	0 7110760000	1 0000000000
F 1	0.7110760000	1.0000000000
1	0.2734910000	1.0000000000
F 1	0.2/J45IUUUU	1.0000000000
1	0.1051890000	1.0000000000
end	3.103103000	1.000000000
Cita		

Basis set for element : Th

Nouc	TO 00	
S 9	TO 90	
1	56363088.88971600	0.0182637261
2	25619585.85896200	-0.0050406098
3	11645266.29952800	0.0326076658
4	5293302.863422000	0.0169207802
5	2406046.756101000	0.0620530411
6	1093657.616409000	0.0791967162
7	497117.0983680000	0.1637381891
8	225962.3174400000	0.2738796425
	102710.1442910000	0.5230263015
9 S 1	102/10.1442910000	0.5230203013
S 1 S 1	46686.4292230000	1.0000000000
1 5 1	21221.1041920000	1.0000000000
1	9645.9564510000	1.0000000000
1	4384.5256600000	1.0000000000
S 1 1	1992.9662090000	1.0000000000
S 1 1	905.8937310000	1.0000000000
S 1 1	411.7698780000	1.0000000000
S 1 1	187.1681260000	1.0000000000
S 1 1	85.0764210000	1.0000000000
S 1 1	38.6711000000	1.0000000000
S 1 1	17.5777730000	1.0000000000
S 1 1	7.9898970000	1.0000000000
S 1 1	3.6317710000	1.0000000000
S 1 1	1.6508050000	1.0000000000
S 1 1	0.7503660000	1.0000000000
S 1		
1 S 1	0.3410750000	1.0000000000
1 S 1	0.1550340000	1.0000000000
1 S 1	0.0704700000	1.0000000000
1 S 1	0.0320320000	1.0000000000
1 P 8	0.0145600000	1.0000000000
1	801557.4232150000	0.0009847016
2	333982.2596730000	0.0010011849
3	139159.2748640000	0.0041062120
4	57983.0311930000	0.0094027289
5	24159.5963310000	0.0275102389
6	10066.4984710000	0.0794834908
7	4194.3743630000	0.2472115083
8	1747.6559850000	0.7364057736
P 1	17-77-000000	0., Ju - 0J, / Ju
1 P 1	728.1899940000	1.0000000000
1 P 1	303.4124970000	1.0000000000
1	126.4218740000	1.0000000000
P 1	E) 67E7010000	1 000000000
1 P 1	52.6757810000	1.0000000000

```
1
         21.9482420000
                             1.0000000000
P 1
  1
          9.1451010000
                             1.0000000000
P 1
  1
          3.8104590000
                             1.0000000000
P 1
  1
          1.5876910000
                             1.0000000000
P 1
          0.6615380000
                             1.0000000000
  1
P 1
  1
          0.2756410000
                             1.0000000000
P 1
                             1.0000000000
  1
          0.1148500000
P 1
  1
          0.0478540000
                             1.0000000000
D 7
      38933.2915440000
                             0.0001043495
  1
                             0.0002856760
      15573.3166180000
                             0.0017526674
  3
       6229.3266470000
  4
       2491.7306590000
                             0.0087468045
  5
        996.6922640000
                             0.0501427023
        398.6769050000
                             0.2343835795
  6
        159.4707620000
  7
                             0.7991155197
D 1
  1
         63.7883050000
                             1.0000000000
D 1
         25.5153220000
                             1.0000000000
D 1
         10.2061290000
                             1.0000000000
  1
D 1
          4.0824520000
                             1.0000000000
  1
D 1
  1
          1.6329810000
                             1.0000000000
D 1
          0.6531920000
                             1.0000000000
  1
D 1
                             1.0000000000
          0.2612770000
  1
D 1
                             1.0000000000
          0.1045110000
  1
D 1
          0.0418040000
                             1.0000000000
  1
F 6
  1
       4035.8413290000
                             0.0000555544
  2
       1552.2466650000
                             0.0004464523
  3
        597.0179480000
                             0.0045802380
  4
        229.6222880000
                             0.0392090403
  5
         88.3162650000
                             0.2424968910
         33.9677940000
                             0.8209390710
  6
F 1
  1
         13.0645360000
                             1.0000000000
 1
  1
          5.0248220000
                             1.0000000000
F 1
                             1.0000000000
  1
          1.9326240000
F 1
                             1.0000000000
  1
          0.7433170000
F 1
  1
          0.2858910000
                             1.0000000000
F 1
  1
          0.1099580000
                             1.0000000000
 end
# Basis set for element : Pa
NewGTO 91
S 9
  1
    57631858.17253400
                             0.0187193263
  2 26196299.16933400
                            -0.0051902602
  3 11907408.71333400
                             0.0333074445
```

	4	5412458.506061000	0.0171165732
	5	2460208.411846000	
	6	1118276.550839000	
	7	508307.5231090000	0.1647021802
	8	231048.8741400000	
	9	105022.2155180000	
_		103022.2133180000	0.3207383403
S	1		
	1	47737.3706900000	1.0000000000
S	1		
	1	21698.8048590000	1.0000000000
S	1		2.000000000
ی		0063 003440000	1 000000000
	1	9863.0931180000	1.0000000000
S	1		
	1	4483.2241440000	1.0000000000
S	1		
_	1	2037.8291570000	1.0000000000
_		2037.8291370000	1.000000000
S	1		
	1	926.2859800000	1.0000000000
S	1		
	1	421.0390820000	1.0000000000
_		421.0330020000	1.000000000
S	1		
	1	191.3814010000	1.0000000000
S	1		
	1	86.9915460000	1.0000000000
S	1	0017723.00000	2.000000000
3		20 5446420000	4 000000000
	1	39.5416120000	1.0000000000
S	1		
	1	17.9734600000	1.0000000000
S	1		
,	1	9 1607540000	1.0000000000
_		8.1697540000	1.0000000000
S	1		
	1	3.7135250000	1.0000000000
S	1		
_	1	1.6879660000	1.0000000000
_		1.08/3000000	1.000000000
S	1		
	1	0.7672570000	1.0000000000
S	1		
	1	0.3487530000	1.0000000000
s	1	0.5 107 550000	1.000000000
3			
	1	0.1585240000	1.0000000000
S	1		
	1	0.0720560000	1.0000000000
S	1		
٦		0 0227520000	1 000000000
	1	0.0327530000	1.0000000000
S	1		
	1	0.0148880000	1.0000000000
Р	8		
•		920599 660060000	0 0010025701
	1	820588.6600690000	
	2	341911.9416950000	0.0010205136
	3	142463.3090400000	0.0041739348
	4	59359.7121000000	0.0095412197
	5	24733.2133750000	
	6	10305.5055730000	
	7	4293.9606550000	
	8	1789.1502730000	0.7352620311
Ρ	1		
	1	745.4792800000	1.0000000000
ь		, -,, -, , , , , , , , , , , , , , , ,	1.000000000
Р	1		
	1	310.6163670000	1.0000000000
Ρ	1		
	1	129.4234860000	1.0000000000
Р	1		
۲			4 000000
	1	53.9264530000	1.0000000000
Ρ	1		
	1	22.4693550000	1.0000000000
Р	1		
•		0 2622210000	1 000000000
_	1	9.3622310000	1.0000000000
Р	1		
	1	3.9009300000	1.0000000000

```
P 1
          1.6253870000
                            1.0000000000
  1
P 1
  1
          0.6772450000
                            1.0000000000
P 1
          0.2821850000
                            1.0000000000
  1
P 1
  1
          0.1175770000
                            1.0000000000
P 1
                            1.0000000000
  1
          0.0489910000
D 7
  1
      39984.8312080000
                            0.0001061301
  2
     15993.9324830000
                            0.0002896200
  3
       6397.5729930000
                            0.0017693155
  4
       2559.0291970000
                            0.0087871933
  5
       1023.6116790000
                            0.0502259708
        409.4446720000
                            0.2343540923
  6
        163.7778690000
                            0.7990953306
  7
D 1
         65.5111470000
                            1.0000000000
  1
D 1
  1
         26.2044590000
                            1.0000000000
D 1
         10.4817840000
                            1.0000000000
  1
D 1
          4.1927130000
                            1.0000000000
  1
D 1
          1.6770850000
                            1.0000000000
  1
D 1
  1
          0.6708340000
                            1.0000000000
D 1
  1
          0.2683340000
                            1.0000000000
D 1
  1
          0.1073330000
                            1.0000000000
D 1
          0.0429330000
                            1.0000000000
F 6
       4212.3892570000
                             0.0000545578
  1
  2
       1620.1497140000
                            0.0004400304
  3
        623.1345050000
                            0.0044858505
        239.6671170000
                            0.0385820377
  4
         92.1796610000
                            0.2403631201
  5
  6
         35.4537160000
                            0.8228337957
F 1
  1
         13.6360440000
                            1.0000000000
F 1
  1
          5.2446320000
                             1.0000000000
F 1
          2.0171660000
                            1.0000000000
  1
F 1
                             1.0000000000
  1
          0.7758330000
F 1
          0.2983970000
                            1.0000000000
  1
F 1
                            1.0000000000
 1
          0.1147680000
 end
# Basis set for element : U
NewGTO 92
S 9
 1 58915269.20406200
                            0.0191882768
  2 26779667.82002800
                           -0.0053454445
     12172576.28183100
                            0.0340255790
  4
     5532989.219014000
                            0.0173125062
  5 2514995.099552000
                            0.0638914339
  6 1143179.590705000
                            0.0804714997
     519627.0866840000
                            0.1656720091
  8 236194.1303110000
                            0.2739080595
```

9	107360.9683230000	0.5185531527
S 1	48800 4401470000	1 000000000
1 S 1	48800.4401470000	1.0000000000
1	22182.0182490000	1.0000000000
S 1		
1	10082.7355680000	1.0000000000
S 1 1	4583.0616220000	1.0000000000
S 1	4303.0010220000	1.000000000
1	2083.2098280000	1.0000000000
S 1	046 0435500000	4 000000000
1 S 1	946.9135580000	1.0000000000
1	430.4152540000	1.0000000000
S 1		
1	195.6432970000	1.0000000000
S 1 1	88.9287710000	1.0000000000
S 1	00.5207710000	1.000000000
1	40.4221690000	1.0000000000
S 1	40 2727420000	4 000000000
1 S 1	18.3737130000	1.0000000000
1	8.3516880000	1.0000000000
S 1		
1	3.7962220000	1.0000000000
S 1 1	1.7255550000	1.0000000000
S 1	1.7233330000	1.000000000
1	0.7843430000	1.0000000000
S 1	0.356530000	1 000000000
1 S 1	0.3565200000	1.0000000000
1	0.1620540000	1.0000000000
S 1		
1	0.0736610000	1.0000000000
S 1 1	0.0334820000	1.0000000000
S 1		
1	0.0152190000	1.0000000000
P 8	920912 6660700000	0 0010207624
2	839813.6669700000 349922.3612380000	0.0010207634 0.0010400968
3	145800.9838490000	0.0010400308
4	60750.4099370000	0.0096810982
5	25312.6708070000	0.0281429485
	10546.9461700000	0.0806360206
6		
7	4394.5609040000	0.2485904639
8 D 1	1831.0670430000	0.7341081564
P 1	762.9446010000	1.0000000000
P 1	702.9440010000	1.000000000
1	317.8935840000	1.0000000000
P 1		
1	132.4556600000	1.0000000000
P 1	55.1898580000	1.0000000000
P 1	33.1030300000	1.000000000
1	22.9957740000	1.0000000000
P 1	.	
1	9.5815730000	1.0000000000
P 1	3.9923220000	1.0000000000
P 1	3.3323220000	2.000000000
1	1.6634670000	1.0000000000
P 1	0.0034440000	1 000000000
1 P 1	0.6931110000	1.0000000000
, т		

```
1
          0.2887960000
                             1.0000000000
P 1
  1
          0.1203320000
                             1.0000000000
P 1
  1
          0.0501380000
                             1.0000000000
D 7
  1
      41049.8202270000
                             0.0001079397
  2
      16419.9280910000
                            0.0002936574
  3
       6567.9712360000
                             0.0017863611
  4
       2627.1884950000
                             0.0088293819
  5
       1050.8753980000
                             0.0503159404
  6
        420.3501590000
                             0.2343398683
  7
        168.1400640000
                             0.7990587936
D 1
         67.2560250000
                             1.0000000000
  1
D 1
         26.9024100000
                             1.0000000000
  1
D 1
         10.7609640000
                             1.0000000000
  1
D 1
          4.3043860000
                             1.0000000000
  1
D 1
  1
          1.7217540000
                             1.0000000000
D 1
  1
          0.6887020000
                             1.0000000000
D 1
          0.2754810000
                             1.0000000000
D 1
          0.1101920000
                             1.0000000000
  1
D 1
          0.0440770000
                             1.0000000000
  1
F 6
  1
       4391.9602590000
                             0.0000536296
  2
       1689.2154840000
                             0.0004343368
  3
        649.6982630000
                            0.0043978390
  4
        249.8839470000
                             0.0379947240
  5
         96.1092110000
                             0.2383103935
  6
         36.9650810000
                             0.8246462333
F 1
         14.2173390000
                             1.0000000000
  1
F 1
  1
          5.4682070000
                             1.0000000000
F 1
          2.1031570000
                             1.0000000000
  1
F 1
          0.8089060000
                             1.0000000000
  1
F 1
                             1.0000000000
  1
          0.3111180000
F 1
  1
          0.1196610000
                             1.0000000000
 end
# Basis set for element : Np
NewGTO 93
S 9
     60212393.78258100
                            0.0196711796
  1
  2
    27369269.90117300
                            -0.0055064269
    12440577.22780600
                            0.0347628812
  3
  4
     5654807.830821000
                             0.0175085406
     2570367.195828000
                            0.0648364627
    1168348.725376000
                            0.0811115338
  7
     531067.6024440000
                            0.1666480048
  8
     241394.3647470000
                             0.2739018403
  9
     109724.7112490000
                             0.5162898199
S 1
  1
      49874.8687490000
                             1.0000000000
S 1
  1
      22670.3948860000
                             1.0000000000
```

_	_		
S	1 1	10304.7249480000	1.0000000000
S	1 1	4683.9658860000	1.0000000000
S	1 1	2129.0754030000	1.0000000000
S	1	2129.0734030000	1.000000000
S	1 1	967.7615470000	1.0000000000
S	1 1	439.8916120000	1.0000000000
	1	199.9507330000	1.0000000000
S	1	90.8866970000	1.0000000000
S	1 1	41.3121350000	1.0000000000
S	1 1	18.7782430000	1.0000000000
S	1	8.5355650000	1.0000000000
S	1	3.8798020000	1.0000000000
S	1	3.8798020000	1.000000000
S	1 1	1.7635460000	1.0000000000
S	1 1	0.8016120000	1.0000000000
S	1 1	0.3643690000	1.0000000000
S	1	0.1656220000	1.0000000000
	1	0.0752830000	1.0000000000
S	1 1	0.0342190000	1.0000000000
S	1	0.0155540000	1.0000000000
Р	8 1	859302.8310040000	
			0.0010393027
	2	358042.8462520000	0.0010599603
	3	149184.5192720000	0.0043120471
	4	62160.2163630000	0.0098224737
		25900.0901510000	0.0284634361
	5		
	6	10791.7042300000	0.0812184770
	7	4496.5434290000	0.2492844786
Р	8	1873.5597620000	0.7329467192
	1	780.6499010000	1.0000000000
Р	1 1	325.2707920000	1.0000000000
Р	1 1	135.5294970000	1.0000000000
Р	1 1	56.4706240000	1.0000000000
Р	1	23.5294270000	1.0000000000
Р	1		
Р	1 1	9.8039280000	1.0000000000
Р	1 1	4.0849700000	1.0000000000
Р	1 1	1.7020710000	1.0000000000
P	1	0.7091960000	1.0000000000
	1	0.2954980000	1.0000000000
P	1	0.1231240000	1.0000000000
Р	1 1	0.0513020000	1.0000000000

```
D 7
 1
      42129.4422870000
                             0.0001097745
  2
      16851.7769150000
                             0.0002977923
                             0.0018037274
  3
       6740.7107660000
  4
       2696.2843060000
                             0.0088732225
  5
       1078.5137230000
                             0.0504110447
  6
        431.4054890000
                             0.2343396171
  7
        172.5621960000
                             0.7990077350
D 1
  1
         69.0248780000
                             1.0000000000
D 1
  1
         27.6099510000
                             1.0000000000
D 1
  1
         11.0439810000
                             1.0000000000
D 1
  1
          4.4175920000
                             1.0000000000
D 1
          1.7670370000
  1
                             1.0000000000
D 1
          0.7068150000
                             1.0000000000
  1
D 1
  1
          0.2827260000
                             1.0000000000
D 1
          0.1130900000
                             1.0000000000
  1
D 1
  1
          0.0452360000
                             1.0000000000
F 6
                             0.0000527862
  1
       4574.1842730000
  2
       1759.3016440000
                             0.0004293200
        676.6544780000
  3
                             0.0043166642
  4
        260.2517220000
                             0.0374497757
  5
        100.0968160000
                             0.2363683935
  6
         38.4987760000
                             0.8263529071
  1
         14.8072210000
                             1.0000000000
  1
F 1
          5.6950850000
                             1.0000000000
  1
F
 1
                             1.0000000000
          2.1904170000
  1
F 1
          0.8424680000
                             1.0000000000
  1
F 1
  1
          0.3240260000
                             1.0000000000
F 1
  1
          0.1246250000
                             1.0000000000
 end
# Basis set for element : Pu
NewGTO 94
S 9
  1
     61522220.62252900
                            0.0201686722
  2 27964645.73751300
                            -0.0056734877
  3 12711202.60796100
                            0.0355202097
  4
     5777819.367255000
                            0.0177046354
  5
     2626281.530570000
                             0.0657997146
    1193764.332077000
                             0.0817534122
  6
  7
     542620.1509440000
                             0.1676305096
  8
     246645.5231560000
                             0.2738814262
  9
     112111.6014350000
                             0.5140073552
S 1
      50959.8188340000
                             1.0000000000
  1
S 1
                             1.0000000000
  1
      23163.5540150000
S 1
      10528.8881890000
                             1.0000000000
  1
S 1
                             1.0000000000
       4785.8582680000
  1
S 1
```

_	1	2175.3901220000	1.0000000000
S	1 1	988.8136920000	1.0000000000
S	1 1	449.4607690000	1.0000000000
S	1 1	204.3003500000	1.0000000000
S	1		
S	1 1	92.8637950000	1.0000000000
S	1 1	42.2108160000	1.0000000000
S	1 1	19.1867350000	1.0000000000
S	1	8.7212430000	1.0000000000
	1	3.9642010000	1.0000000000
S	1 1	1.8019100000	1.0000000000
S	1 1	0.8190500000	1.0000000000
S	1 1	0.3722950000	1.0000000000
S	1 1	0.1692250000	1.0000000000
S	1	0.0769210000	1.0000000000
S	1		
S	1 1	0.0349640000	1.0000000000
Р	1 8	0.0158930000	1.0000000000
	1	879013.3813660000	0.0010581923
	2	366255.5755690000	0.0010801019
	3	152606.4898210000	0.0043824941
	4	63586.0374250000	0.0099653234
	5	26494.1822610000	0.0287866938
	6	11039.2426090000	0.0818050183
	7	4599.6844200000	0.2499815412
	8	1916.5351750000	0.7317768089
Р	1 1	798.5563230000	1.0000000000
Р	1	332.7318010000	1.0000000000
Р	1 1	138.6382510000	1.0000000000
Р	1		1.000000000
Р	1	57.7659380000	1.0000000000
Р	1 1	24.0691410000	1.0000000000
Р	1 1	10.0288090000	1.0000000000
Р	1	4.1786700000	1.0000000000
	1	1.7411130000	1.0000000000
Р	1 1	0.7254640000	1.0000000000
Р	1 1	0.3022760000	1.0000000000
Р	1 1	0.1259490000	1.0000000000
Р	1 1	0.0524790000	1.0000000000
D	7		
-	1	43223.8765000000	0.0001116326
	2	17289.5506000000	
			0.0003020314
	3	6915.8202400000	0.0018213757
	4	2766.3280960000	0.0089187204

```
5
       1106.5312380000
                             0.0505106822
  6
        442.6124950000
                             0.2343542525
  7
        177.0449980000
                             0.7989416427
D 1
                             1.0000000000
  1
         70.8179990000
D 1
  1
         28.3272000000
                             1.0000000000
D 1
         11.3308800000
                             1.0000000000
  1
D 1
  1
          4.5323520000
                             1.0000000000
D 1
  1
          1.8129410000
                             1.0000000000
D 1
          0.7251760000
                             1.0000000000
  1
D 1
          0.2900710000
                             1.0000000000
  1
D 1
          0.1160280000
                             1.0000000000
  1
D 1
                             1.0000000000
          0.0464110000
  1
F 6
                             0.0000520342
  1
       4758.8680260000
  2
       1830.3338560000
                             0.0004249173
  3
        703.9745600000
                             0.0042422970
  4
        270.7594460000
                            0.0369469391
  5
        104.1382490000
                             0.2345517700
         40.0531730000
                             0.8279432543
  6
  1
  1
         15.4050660000
                             1.0000000000
F 1
  1
          5.9250260000
                             1.0000000000
F 1
  1
          2.2788560000
                             1.0000000000
F 1
          0.8764830000
                             1.0000000000
F 1
          0.3371090000
                             1.0000000000
F 1
          0.1296570000
                             1.0000000000
 1
 end
# Basis set for element : Am
NewGTO 95
S 9
  1
     62843653.32610500
                             0.0206813702
     28565296.96641200
                            -0.0058469133
  2
  3 12984225.89382300
                            0.0362983882
  4 5901920.860829000
                            0.0179006871
     2682691.300377000
                             0.0667818941
  6
     1219405.136535000
                            0.0823970363
  7
     554275.0620610000
                            0.1686198260
     251943.2100280000
  8
                             0.2738462218
  9
                             0.5117051466
    114519.6409220000
S 1
      52054.3822370000
                             1.0000000000
  1
S 1
 1
      23661.0828350000
                             1.0000000000
S 1
  1
      10755.0376520000
                             1.0000000000
S 1
       4888.6534780000
                             1.0000000000
  1
S 1
                             1.0000000000
  1
       2222.1152170000
S 1
  1
       1010.0523720000
                             1.0000000000
S 1
  1
        459.1147140000
                             1.0000000000
```

S 1 1	208.6885070000	1.0000000000
S 1		
1 S 1	94.8584120000	1.0000000000
1 5 1	43.1174600000	1.0000000000
1 S 1	19.5988450000	1.0000000000
1	8.9085660000	1.0000000000
S 1 1	4.0493480000	1.0000000000
S 1 1	1.8406130000	1.0000000000
5 1 1	0.8366420000	1.0000000000
S 1 1	0.3802920000	1.0000000000
S 1		
1 S 1	0.1728600000	1.0000000000
1 5 1	0.0785730000	1.0000000000
1 S 1	0.0357150000	1.0000000000
1	0.0162340000	1.0000000000
P 8	898929.0904960000	0.0010774408
2	374553.7877070000	0.0010774408
3	156064.0782110000	0.0044538914
4	65026.6992550000	0.0101096564
5	27094.4580230000	0.0291128237
6	11289.3575090000	0.0823958274
7	4703.8989620000	0.2506826608
8	1959.9579010000	0.7305972857
	1939.9379010000	0.7303372037
P 1	816.6491250000	1.0000000000
P 1	340.2704690000	1.0000000000
P 1	141.7793620000	1.0000000000
P 1	59.0747340000	1.0000000000
P 1 1	24.6144730000	1.0000000000
P 1 1	10.2560300000	1.0000000000
P 1 1	4.2733460000	1.0000000000
P 1		
1 P 1	1.7805610000	1.0000000000
1 P 1	0.7419000000	1.0000000000
1 P 1	0.3091250000	1.0000000000
1 P 1	0.1288020000	1.0000000000
1	0.0536680000	1.0000000000
D 7	44224 4222222	0.0004:5=5=
1	44331.4203980000	0.0001135209
2	17732.5681590000	0.0003063667
3	7093.0272640000	0.0018394225
4	2837.2109050000	0.0010334223
5	1134.8843620000	0.0506168335
6	453.9537450000	0.2343841307
7	181.5814980000	0.7988592880
D 1 1		
1	72.6325990000	1.0000000000

```
D 1
         29.0530400000
                             1.0000000000
  1
D 1
         11.6212160000
                             1.0000000000
  1
D 1
          4.6484860000
                             1.0000000000
  1
D 1
  1
          1.8593950000
                             1.0000000000
D 1
  1
          0.7437580000
                             1.0000000000
D 1
  1
          0.2975030000
                             1.0000000000
D 1
  1
          0.1190010000
                             1.0000000000
D 1
  1
          0.0476010000
                             1.0000000000
F 6
       4946.8424820000
                             0.0000513281
  1
                             0.0004210229
       1902.6317240000
  2
  3
        731.7814320000
                             0.0041723332
        281.4543970000
                             0.0364722578
  4
        108.2516910000
                             0.2327932976
  5
  6
         41.6352660000
                             0.8294751707
F
 1
  1
         16.0135640000
                             1.0000000000
F 1
          6.1590630000
                             1.0000000000
F 1
          2.3688700000
                             1.0000000000
  1
F 1
          0.9111040000
                             1.0000000000
  1
F 1
  1
          0.3504250000
                             1.0000000000
F 1
          0.1347790000
                             1.0000000000
  1
 end
# Basis set for element : Cm
NewGTO 96
S 9
     64183659.71228800
 1
                            0.0212102338
  2 29174390.77831300
                           -0.0060270545
  3 13261086.71741500
                            0.0370987287
  4 6027766.689734000
                             0.0180968760
  5
    2739893.949879000
                            0.0677843361
     1245406.340854000
                             0.0830429990
  7
     566093.7912970000
                             0.1696168268
     257315.3596810000
                             0.2737957782
  9
    116961.5271280000
                             0.5093806630
S 1
  1
      53164.3305130000
                             1.0000000000
S 1
                             1.0000000000
  1
      24165.6047780000
S 1
  1
      10984.3658080000
                             1.0000000000
S 1
  1
       4992.8935490000
                             1.0000000000
S 1
  1
       2269.4970680000
                             1.0000000000
S 1
       1031.5895760000
                             1.0000000000
  1
S 1
        468.9043530000
                             1.0000000000
  1
S 1
        213.1383420000
                             1.0000000000
  1
S 1
                             1.0000000000
         96.8810650000
  1
S 1
```

1	44.0368480000	1.0000000000
S 1 1	20.0167490000	1.0000000000
S 1 1	9.0985220000	1.0000000000
S 1 1	4.1356920000	1.0000000000
5 1 1	1.8798600000	1.0000000000
S 1 1	0.8544820000	1.0000000000
S 1 1	0.3884010000	1.0000000000
S 1 1	0.1765460000	1.0000000000
5 1 1	0.0802480000	1.0000000000
S 1 1	0.0364760000	1.0000000000
S 1 1	0.0165800000	1.0000000000
P 8 1	919065.4160050000	0.0010970615
2	382943.9233360000	0.0011212375
	159559.9680560000	0.0011212373
3		
4	66483.3200240000	0.0102555198
5	27701.3833430000	0.0294418515
6	11542.2430600000	0.0829908583
7	4809.2679420000	0.2513873144
		0.7294086077
8	2003.8616420000	0.7294086077
P 1	834.9423510000	1.0000000000
P 1		
1	347.8926460000	1.0000000000
P 1		
1 P 1	144.9552690000	1.0000000000
1 P 1	60.3980290000	1.0000000000
1 P 1	25.1658450000	1.0000000000
1 P 1	10.4857690000	1.0000000000
1 P 1	4.3690700000	1.0000000000
1 P 1	1.8204460000	1.0000000000
1 P 1	0.7585190000	1.0000000000
1 P 1	0.3160500000	1.0000000000
1 P 1	0.1316870000	1.0000000000
1 D 7	0.0548700000	1.0000000000
1	45453.5554980000	0.0001154384
2	18181.4221990000	0.0003107918
3	7272.5688800000	0.0018578305
4	2909.0275520000	0.0090148321
5	1163.6110210000	0.0507282614
6	465.4444080000	0.2344254017
7	186.1777630000	0.7987645431
D 1		
1 D 1	74.4711050000	1.0000000000
1 D 1	29.7884420000	1.0000000000
1	11.9153770000	1.0000000000
D 1		

```
1
          4.7661510000
                            1.0000000000
D 1
  1
          1.9064600000
                             1.0000000000
D 1
  1
          0.7625840000
                            1.0000000000
D 1
  1
          0.3050340000
                             1.0000000000
D 1
          0.1220130000
                             1.0000000000
  1
D 1
  1
          0.0488050000
                            1.0000000000
F 6
  1
       5137.9626210000
                            0.0000506674
  2
       1976.1394700000
                            0.0004176065
  3
        760.0536420000
                            0.0041066076
  4
        292.3283240000
                            0.0360248602
  5
        112.4339710000
                            0.2310943371
                            0.8309482898
  6
         43.2438350000
F 1
         16.6322440000
                            1.0000000000
  1
F 1
          6.3970170000
  1
                            1.0000000000
F 1
          2.4603910000
                            1.0000000000
  1
F 1
          0.9463040000
                            1.0000000000
  1
F 1
                            1.0000000000
  1
          0.3639630000
F 1
  1
          0.1399860000
                            1.0000000000
 end
# Basis set for element : Bk
NewGTO 97
S 9
                            0.0217560418
 1 65541743.54207900
     29791701.61003600
                            -0.0062142475
  3 13541682.55001600
                            0.0379222736
  4 6155310.250007000
                            0.0182931697
  5 2797868.295458000
                            0.0688079596
                            0.0836914053
    1271758.316117000
  7
     578071.9618710000
                            0.1706219120
  8
     262759.9826690000
                            0.2737295699
  9 119436.3557590000
                            0.5070326595
S 1
  1
      54289.2526180000
                            1.0000000000
S 1
      24676.9330080000
                            1.0000000000
 1
S 1
                             1.0000000000
  1
      11216.7877310000
S 1
       5098.5398780000
                            1.0000000000
  1
S 1
  1
       2317.5181260000
                            1.0000000000
S 1
       1053.4173300000
                            1.0000000000
  1
S 1
        478.8260590000
                            1.0000000000
  1
S 1
        217.6482090000
                            1.0000000000
  1
S 1
         98.9310040000
                            1.0000000000
  1
S 1
                             1.0000000000
  1
         44.9686380000
S 1
  1
         20.4402900000
                             1.0000000000
S 1
  1
          9.2910410000
                            1.0000000000
```

S	1	4.2232000000	1.0000000000
S	1 1	1.9196370000	1.0000000000
S	1	0.8725620000	1.0000000000
S	1		
S	1 1	0.3966190000	1.0000000000
S	1	0.1802810000	1.0000000000
S	1 1	0.0819460000	1.0000000000
S	1	0.0372480000	1.0000000000
	1	0.0169310000	1.0000000000
Р	8		
	1	939440.7605340000	0.0011170680
	2	391433.6502220000	0.0011422566
	3	163097.3542590000	0.0045996610
	4	67957.2309410000	0.0104029576
	5	28315.5128920000	0.0297737266
	6	11798.1303720000	0.0835898642
	7	4915.8876550000	0.2520941835
	8	2048.2865230000	0.7282121380
Р	1	2048.2803230000	0.7282121380
Р	1 1	853.4527180000	1.0000000000
Р	1 1	355.6052990000	1.0000000000
Р	1	148.1688750000	1.0000000000
P	1	61.7370310000	1.0000000000
P	1	25.7237630000	1.0000000000
P	1	10.7182350000	1.0000000000
Р	1 1	4.4659310000	1.0000000000
Р	1 1	1.8608050000	1.0000000000
Р	1 1	0.7753350000	1.0000000000
Р	1 1	0.3230560000	1.0000000000
Р	1 1	0.1346070000	1.0000000000
'		0.050000000	1 000000000
_	1	0.0560860000	1.0000000000
D	7		
	1	46590.6458960000	0.0001173790
	2	18636.2583580000	0.0003153281
	3	7454.5033430000	0.0018765002
	4	2981.8013370000	0.0090653303
	5	1192.7205350000	0.0508438109
	6	477.0882140000	0.2344824183
	7	190.8352860000	0.7986541950
D	1	220.0332000000	31.700511750
υ	1	76.3341140000	1.0000000000
D	1	20 5226460000	1 000000000
D	1 1	30.5336460000	1.0000000000
D	1 1	12.2134580000	1.0000000000
D	1	4.8853830000	1.0000000000
D	1	1.9541530000	1.0000000000
J	1	0.7816610000	1.0000000000

```
D 1
          0.3126650000
                             1.0000000000
  1
D 1
          0.1250660000
                             1.0000000000
  1
D 1
          0.0500260000
                             1.0000000000
  1
F 6
  1
       5327.8457110000
                             0.0000501427
  2
       2049.1714270000
                             0.0004149657
                             0.0040503079
  3
        788.1428570000
  4
        303.1318680000
                             0.0356384948
  5
        116.5891800000
                             0.2296147001
         44.8419920000
  6
                             0.8322276049
F
 1
  1
         17.2469200000
                             1.0000000000
F
  1
          6.6334310000
                             1.0000000000
  1
F 1
                             1.0000000000
          2.5513200000
  1
F 1
          0.9812770000
                             1.0000000000
  1
F 1
                             1.0000000000
  1
          0.3774140000
F 1
  1
          0.1451590000
                             1.0000000000
 end
# Basis set for element : Cf
NewGTO 98
S 9
 1
     66908672.67153500
                            0.0223193024
  2
     30413033.03251600
                            -0.0064087975
  3
    13824105.92387100
                            0.0387696749
  4 6283684.510850000
                            0.0184892425
  5 2856220.232205000
                             0.0698531465
  6 1298281.923729000
                            0.0843416655
  7
     590128.1471500000
                             0.1716349860
     268240.0668860000
  8
                             0.2736468347
    121927.3031300000
                             0.5046617061
S 1
  1
      55421.5014230000
                             1.0000000000
S 1
      25191.5915560000
                             1.0000000000
  1
S 1
     11450.7234340000
  1
                             1.0000000000
S 1
       5204.8742880000
                             1.0000000000
  1
S 1
  1
       2365.8519490000
                             1.0000000000
S 1
  1
       1075.3872500000
                             1.0000000000
S 1
                             1.0000000000
  1
        488.8123860000
S 1
  1
        222.1874480000
                             1.0000000000
S 1
  1
        100.9942950000
                             1.0000000000
S 1
  1
         45.9064980000
                             1.0000000000
S 1
         20.8665900000
                             1.0000000000
  1
S 1
          9.4848140000
                             1.0000000000
  1
S 1
          4.3112790000
                             1.0000000000
  1
S 1
                             1.0000000000
          1.9596720000
  1
S 1
```

1	0.8907600000	1.0000000000
S 1 1	0.4048910000	1.0000000000
S 1		
1 S 1	0.1840410000	1.0000000000
1 S 1	0.0836550000	1.0000000000
1	0.0380250000	1.0000000000
S 1 1	0.0172840000	1.0000000000
P 8 1	060041 2096200000	0.0011374730
	960041.3086390000	
2	400017.2119330000	0.0011635893
3	166673.8383050000	0.0046740948
4	69447.4326270000	0.0105520092
5	28936.4302610000	0.0301085585
6	12056.8459420000	0.0841930164
7	5023.6858090000	0.2528038185
8	2093.2024210000	0.7270071633
	2033.2024210000	0.7270071033
P 1		
1	872.1676750000	1.0000000000
P 1		
	262 4021090000	1 000000000
1	363.4031980000	1.0000000000
P 1		
1	151.4179990000	1.0000000000
	2021.270000	2.000000000
1	63.0908330000	1.0000000000
P 1		
1	26.2878470000	1.0000000000
	20.20/04/0000	1.000000000
P 1		
1	10.9532700000	1.0000000000
	10.3332700000	1.000000000
P 1		
1	4.5638620000	1.0000000000
P 1		
1	1.9016090000	1.0000000000
P 1		
1	0.7923370000	1.0000000000
	0.7525570000	1.000000000
P 1		
1	0.3301410000	1.0000000000
P 1		
1	0.1375590000	1.0000000000
P 1		
1	0.0573160000	1.0000000000
	0.03/3160000	1.000000000
D 7		
1	47740.9667690000	0.0001193500
2	19096.3867080000	0.0003199583
3	7638.5546830000	0.0018955409
4	3055.4218730000	0.0091174251
5	1222.1687490000	0.0509647993
6	488.8675000000	0.2345517512
7	195.5470000000	0.7985305723
D 1		
1	78.2188000000	1.0000000000
D 1		
	24 2075200000	1 000000000
1	31.2875200000	1.0000000000
D 1		
1	12.5150080000	1.0000000000
	12.313000000	1.000000000
D 1		
1	5.0060030000	1.0000000000
D 1		
1	2.0024010000	1.0000000000
D 1		
1	0.8009610000	1.0000000000
	0.0003010000	1.000000000
D 1		
1	0.3203840000	1.0000000000
D 1		
1	0.1281540000	1.0000000000
D 1		
_		

```
1
          0.0512610000
                             1.0000000000
F 6
  1
       5522.2215080000
                             0.0000496296
       2123.9313490000
                             0.0004125745
  2
  3
        816.8966730000
                             0.0039957217
  4
        314.1910280000
                             0.0352630222
  5
        120.8427030000
                             0.2281410123
  6
         46.4779630000
                             0.8334963455
 1
  1
         17.8761400000
                             1.0000000000
F
 1
  1
          6.8754380000
                             1.0000000000
F 1
  1
          2.6443990000
                             1.0000000000
F 1
  1
          1.0170770000
                             1.0000000000
F 1
          0.3911830000
                             1.0000000000
F 1
          0.1504550000
                             1.0000000000
 1
 end
# Basis set for element : Es
NewGTO 99
S 9
    68291966.01786400
                             0.0229010727
                           -0.0066111062
  2 31041802.73539300
     14109910.33426900
                             0.0396423593
  4
    6413595.606486000
                            0.0186852265
  5 2915270.730221000
                            0.0709212952
  6 1325123.059191000
                            0.0849942551
  7
     602328.6632690000
                            0.1726569101
  8
     273785.7560310000
                             0.2735468889
 9
     124448.0709230000
                             0.5022654421
S 1
     56567.3049650000
                             1.00000000000
  1
S 1
                             1.0000000000
      25712.4113480000
  1
S 1
      11687.4597040000
                             1.0000000000
  1
S 1
  1
       5312.4816830000
                             1.0000000000
S 1
  1
       2414.7644020000
                             1.0000000000
S 1
  1
       1097.6201830000
                             1.0000000000
S 1
        498.9182650000
                             1.0000000000
  1
S 1
        226.7810290000
                             1.0000000000
  1
S 1
        103.0822860000
                             1.0000000000
  1
S 1
  1
         46.8555850000
                             1.0000000000
S 1
         21.2979930000
                             1.0000000000
  1
S 1
          9.6809060000
                             1.0000000000
  1
S 1
          4.4004120000
                             1.0000000000
  1
S 1
          2.0001870000
                             1.0000000000
  1
S 1
                             1.0000000000
  1
          0.9091760000
S 1
  1
          0.4132620000
                             1.0000000000
S 1
          0.1878460000
                             1.0000000000
```

S 1 1	0.0853850000	1.0000000000
S 1 1	0.0388110000	1.0000000000
S 1 1	0.0176410000	1.0000000000
P 8	0.0176410000	1.00000000
1	980851.9776920000	0.0011582837
2	408688.3240390000	0.0011852364
3	170286.8016830000	0.0047495845
4	70952.8340340000	0.0107026684
5	29563.6808480000	0.0304463832
6	12318.2003530000	0.0848003791
7	5132.5834810000	0.2535168574
	2138.5764500000	0.7257929891
8	2138.376436666	0.7237323631
P 1	001 0735310000	1 000000000
1	891.0735210000	1.0000000000
P 1		
1	371.2806340000	1.0000000000
P 1		
1	154.7002640000	1.0000000000
P 1		
1	64.4584430000	1.0000000000
P 1		
1	26.8576850000	1.0000000000
P 1		
1	11.1907020000	1.0000000000
P 1		
1	4.6627920000	1.0000000000
P 1		1.000000000
1	1.9428300000	1.0000000000
P 1	1.5420500000	1.000000000
1	0.8095130000	1.0000000000
	0.8093130000	1.0000000000
P 1	0 2272070000	1 000000000
1	0.3372970000	1.0000000000
P 1		
1	0.1405400000	1.0000000000
P 1		
1	0.0585580000	1.0000000000
D 7		
1	48905.6146030000	0.0001213501
2	19562.2458410000	0.0003246886
3	7824.8983360000	0.0019149269
4	3129.9593350000	0.0091711525
5	1251.9837340000	0.0510908974
6	500.7934940000	0.2346346930
7	200.3173970000	0.7983927080
	200.31/39/0000	0.7503527000
D 1	90 126050000	1 000000000
1	80.1269590000	1.0000000000
D 1	22 0507840000	1 000000000
1	32.0507840000	1.0000000000
D 1	12 0202120000	1 000000000
1	12.8203130000	1.0000000000
D 1	F 12012F0000	1 000000000
1	5.1281250000	1.0000000000
D 1	2 0512500000	1 000000000
1	2.0512500000	1.0000000000
D 1	0.030500000	1 000000000
1	0.8205000000	1.0000000000
D 1	a 2202000000	1 000000000
1	0.3282000000	1.0000000000
D 1	Q 1212000000	1 000000000
1	0.1312800000	1.0000000000
D 1	0.050540055	4 00000000
_ 1	0.0525120000	1.0000000000
F 6		
1	5719.1357660000	0.0000491663
2	2199.6676020000	0.0004105704
3	846.0260010000	0.0039450951

```
4
        325.3946160000
                            0.0349132408
  5
        125.1517750000
                            0.2267417726
  6
         48.1352980000
                            0.8346966396
F
 1
                            1.0000000000
  1
         18.5135760000
F 1
  1
          7.1206060000
                            1.0000000000
F 1
          2.7386950000
                            1.0000000000
  1
F 1
  1
          1.0533440000
                             1.0000000000
F 1
  1
          0.4051320000
                            1.0000000000
F 1
          0.1558200000
                            1.0000000000
 1
 end
# Basis set for element : Fm
NewGTO 100
S 9
    69690927.07216800
                            0.0235022496
 1
  2 31677694.12371300
                           -0.0068215675
                            0.0405415180
  3 14398951.87441500
  4
     6544978.124734000
                            0.0188810540
  5 2974990.056697000
                            0.0720134373
  6 1352268.207590000
                            0.0856492145
                            0.1736881277
  7
     614667.3670860000
  8
     279394.2577660000
                            0.2734290222
  9
     126997.3898940000
                            0.4998426122
S 1
  1
      57726.0863150000
                            1.0000000000
S 1
  1
      26239.1301430000
                            1.0000000000
S 1
  1
      11926.8773380000
                            1.0000000000
S 1
  1
       5421.3078810000
                             1.0000000000
S 1
       2464.2308550000
                            1.0000000000
  1
S 1
  1
       1120.1049340000
                            1.0000000000
S 1
        509.1386060000
                            1.0000000000
  1
S 1
                            1.0000000000
  1
        231.4266390000
S 1
        105.1939270000
                            1.0000000000
  1
S 1
  1
         47.8154210000
                            1.0000000000
S 1
  1
         21.7342820000
                            1.0000000000
S 1
          9.8792190000
                            1.0000000000
  1
S 1
                            1.0000000000
  1
          4.4905540000
S 1
  1
          2.0411610000
                            1.0000000000
S 1
  1
          0.9278000000
                             1.0000000000
S 1
          0.4217270000
                             1.0000000000
  1
S 1
          0.1916940000
                             1.0000000000
  1
S 1
          0.0871340000
                            1.0000000000
  1
S 1
          0.0396060000
                            1.0000000000
  1
S 1
```

1	0.0180030000	1.0000000000
P 8		
1	1001894.089886000	0.0011795162
2	417455.8707860000	0.0012072133
3	173939.9461610000	0.0012072133
4	72474.9775670000	0.0108549981
5	30197.9073200000	0.0307872246
6	12582.4613830000	0.0854118673
7	5242.6922430000	0.2542324611
8	2184.4551010000	0.7245703942
P 1		
1	910.1896260000	1.0000000000
P 1		
1	379.2456770000	1.0000000000
P 1	373.2430770000	1.000000000
1	159 0100220000	1 000000000
	158.0190320000	1.0000000000
P 1		
1	65.8412630000	1.0000000000
P 1		
1	27.4338600000	1.0000000000
P 1		
1	11.4307750000	1.0000000000
P 1		
1	4.7628230000	1.0000000000
P 1	4.7020250000	1.000000000
	1 094510000	1 000000000
1	1.9845100000	1.0000000000
P 1		
1	0.8268790000	1.0000000000
P 1		
1	0.3445330000	1.0000000000
P 1		
1	0.1435550000	1.0000000000
P 1		
1	0.0598150000	1.0000000000
D 7	0.0338130000	1.000000000
1	F000F 12210F0000	0 0001222707
	50085.1221850000	0.0001233787
2	20034.0488740000	0.0003295164
3	8013.6195500000	0.0019346356
4	3205.4478200000	0.0092263732
5	1282.1791280000	0.0512213626
6	512.8716510000	0.2347290567
7	205.1486600000	0.7982428154
D 1		
1	82.0594640000	1.0000000000
D 1	02.033 .0 .0000	2.000000000
1	32.8237860000	1.0000000000
D 1	32.8237800000	1.000000000
_	12 1205140000	1 000000000
1	13.1295140000	1.0000000000
D 1		
1	5.2518060000	1.0000000000
D 1		
1	2.1007220000	1.0000000000
D 1		
1	0.8402890000	1.0000000000
D 1		
1	0.3361160000	1.0000000000
D 1	0.550220000	2.000000000
1	0.1344460000	1.0000000000
	0.1344400000	1.0000000000
	0.053770000	1 000000000
1	0.0537780000	1.0000000000
F 6		
1	5918.7118140000	0.0000487467
2	2276.4276210000	0.0004089100
3	875.5490850000	0.0038979519
4	336.7496480000	0.0345861496
5	129.5190950000	0.2254078616
6	49.8150370000	0.8358368799
F 1		
1	19.1596290000	1.0000000000
	17.1330230000	1.000000000

```
F 1
          7.3690880000
                            1.0000000000
  1
F 1
  1
          2.8342650000
                            1.0000000000
F 1
          1.0901020000
                            1.0000000000
  1
F 1
  1
          0.4192700000
                            1.0000000000
F 1
  1
          0.1612580000
                            1.0000000000
 end
# Basis set for element : Md
NewGTO 101
S 9
  1 71095290.12593000
                            0.0241234764
  2 32316040.96633200
                           -0.0070405502
  3 14689109.53015100
                            0.0414679822
     6676867.968250000
                            0.0190763794
  5 3034939.985568000
                            0.0731301110
  6 1379518.175258000
                            0.0863059521
  7
     627053.7160270000
                            0.1747286347
  8
     285024.4163760000
                            0.2732923506
  9
     129556.5528980000
                            0.4973935863
S 1
  1
      58889.3422260000
                            1.0000000000
S 1
  1
      26767.8828300000
                            1.0000000000
S 1
     12167.2194680000
                            1.0000000000
  1
S 1
  1
      5530.5543040000
                            1.0000000000
S 1
       2513.8883200000
                            1.0000000000
  1
S 1
                            1.0000000000
      1142.6765090000
  1
S 1
        519.3984130000
                            1.0000000000
  1
S 1
        236.0901880000
                            1.0000000000
  1
S 1
  1
        107.3137220000
                            1.0000000000
S 1
  1
         48.7789640000
                            1.0000000000
S 1
         22.1722570000
                             1.0000000000
S 1
         10.0782980000
                            1.0000000000
  1
S 1
          4.5810450000
                             1.0000000000
  1
S 1
          2.0822930000
                            1.0000000000
  1
S 1
          0.9464970000
  1
                            1.0000000000
S 1
          0.4302260000
                            1.0000000000
  1
S 1
          0.1955570000
                            1.0000000000
  1
S 1
          0.0888900000
                            1.0000000000
  1
S 1
          0.0404040000
                            1.0000000000
  1
S 1
                             1.0000000000
  1
          0.0183660000
P 8
  1 1023192.458988000
                            0.0012011861
  2 426330.1912450000
                            0.0012295340
  3 177637.5796850000
                            0.0049038851
```

4	74015.6582020000	0.0110090538
5	30839.8575840000	0.0311311096
6	12849.9406600000	0.0860274159
7	5354.1419420000	0.2549499790
8	2230.8924760000	0.7233399697
P 1		
1	020 520522000	1 000000000
	929.5385320000	1.0000000000
P 1		
1	387.3077210000	1.0000000000
P 1		
1	161.3782170000	1.0000000000
P 1		
	67 2400240000	1 000000000
1	67.2409240000	1.0000000000
P 1		
1	28.0170520000	1.0000000000
P 1		
1	11.6737720000	1.0000000000
P 1		
1	4.8640710000	1.0000000000
	4.8640/10000	1.000000000
P 1		
1	2.0266960000	1.0000000000
P 1		
1	0.8444570000	1.0000000000
P 1		
1	0 3519570000	1.0000000000
	0.3518570000	1.000000000
P 1		
1	0.1466070000	1.0000000000
P 1		
1	0.0610860000	1.0000000000
D 7		
1	F1279 F20F940000	0 0001254275
	51278.5205840000	0.0001254375
2	20511.4082340000	0.0003344454
3	8204.5632930000	0.0019546919
4	3281.8253170000	0.0092832009
5	1312.7301270000	0.0513567754
6	525.0920510000	0.2348365466
	210.0368200000	0.7980791512
7	210.0368200000	0.7980791312
D 1		
1	84.0147280000	1.0000000000
D 1		
1	33.6058910000	1.0000000000
D 1		
1	13.4423570000	1.0000000000
D 1	13:4423370000	1.000000000
	F 3760430000	1 000000000
1	5.3769430000	1.0000000000
D 1		
1	2.1507770000	1.0000000000
D 1		
1	0.8603110000	1.0000000000
D 1		
1	0.3441240000	1.0000000000
	0.3441240000	1.000000000
D 1		
1	0.1376500000	1.0000000000
D 1		
1	0.0550600000	1.0000000000
F 6		
1	6120.8574960000	0.0000483690
2	2354.1759600000	0.0004075722
3	905.4522920000	0.0038541090
4	348.2508820000	0.0342806437
5	133.9426470000	0.2241375640
6	51.5164030000	0.8369190545
F 1		
1	19.8140010000	1.0000000000
	19.0140010000	1.00000000000
F 1		
1	7.6207700000	1.0000000000
F 1		
1	2.9310650000	1.0000000000
F 1		

```
1
          1.1273330000
                            1.0000000000
F 1
          0.4335900000
                             1.0000000000
F 1
  1
          0.1667650000
                            1.0000000000
 end
# Basis set for element : No
NewGTO 102
S 9
  1
     72522948.25117100
                            0.0247663050
  2 32964976.47780500
                            -0.0072685813
  3 14984080.21718400
                            0.0424238448
  4
     6810945.553265000
                            0.0192716088
  5
     3095884.342393000
                            0.0742734509
    1407220.155633000
                            0.0869656042
  6
     639645.5252880000
  7
                            0.1757797970
    290747.9660400000
  8
                            0.2731361884
  9
     132158.1663820000
                            0.4949140363
S 1
      60071.8938100000
  1
                            1.0000000000
S 1
  1
      27305.4062770000
                            1.0000000000
S 1
      12411.5483080000
 1
                            1.0000000000
S 1
       5641.6128670000
                            1.0000000000
  1
S 1
  1
       2564.3694850000
                            1.0000000000
S 1
  1
       1165.6224930000
                            1.0000000000
S 1
  1
        529.8284060000
                            1.0000000000
S 1
        240.8310940000
                            1.0000000000
S 1
        109.4686790000
                             1.0000000000
  1
S 1
         49.7584900000
                            1.0000000000
  1
S 1
  1
         22.6174960000
                            1.0000000000
S 1
         10.2806800000
                            1.0000000000
  1
S 1
          4.6730360000
  1
                            1.0000000000
S 1
                            1.0000000000
  1
          2.1241070000
S 1
  1
          0.9655030000
                            1.0000000000
S 1
  1
          0.4388650000
                            1.0000000000
S 1
          0.1994840000
                            1.0000000000
  1
S 1
                            1.0000000000
  1
          0.0906750000
S 1
  1
          0.0412160000
                            1.0000000000
S 1
  1
          0.0187340000
                            1.0000000000
P 8
  1 1044695.317505000
                            0.0012233006
  2 435289.7156270000
                            0.0012521977
     181370.7148450000
                            0.0049827454
  3
  4
      75571.1311850000
                            0.0111648253
      31487.9713270000
                            0.0314781128
  5
      13119.9880530000
                            0.0866472012
       5466.6616890000
                            0.2556705674
  7
  8
       2277.7757040000
                            0.7221004452
```

_			
Р	1 1	949.0732100000	1.0000000000
P	1 1	395.4471710000	1.0000000000
Р	1		
Р	1 1	164.7696540000	1.0000000000
ь	1 1	68.6540230000	1.0000000000
Р	1	28.6058430000	1.0000000000
P	1	11.9191010000	1.0000000000
P _	1	4.9662920000	1.0000000000
Р	1 1	2.0692880000	1.0000000000
Р	1 1	0.8622030000	1.0000000000
Р	1 1	0.3592510000	1.0000000000
Р	1 1	0.1496880000	1.0000000000
Р	1 1	0.0623700000	1.0000000000
D	7		
	1	52485.5878850000	0.0001275273
	2	20994.2351540000	0.0003394764
	3	8397.6940620000	0.0019751020
	4	3359.0776250000	0.0093416460
	5	1343.6310500000	0.0514971814
	6	537.4524200000	0.2349572730
	7	214.9809680000	0.7979015879
D	1		
_		05 0022070000	1 000000000
	1	85.9923870000	1.0000000000
D	1		
	1	34.3969550000	1.0000000000
D	1		
D	1 1	13.7587820000	1.0000000000
D	1	5.5035130000	1.0000000000
D	1 1	2.2014050000	1.0000000000
D	1 1	0.8805620000	1.0000000000
D	1	0.3522250000	1.0000000000
D	1	0.1408900000	1.000000000
D	1		
F	1 6	0.0563560000	1.0000000000
	1	6334.4566490000	0.0000479235
	2	2436.3294800000	0.0004059586
	3	937.0498000000	0.0038062252
	4	360.4037690000	0.0339464480
	5	138.6168340000	0.2227302689
	6	53.3141670000	0.8381146240
F	1		
	1	20.5054490000	1.0000000000
F	1		
F	1 1	7.8867110000	1.0000000000
	1	3.0333500000	1.0000000000
F	1	1.1666730000	1.0000000000
F	1	0.4487200000	1.0000000000
F	1 1	0.1725850000	1.0000000000

```
# Basis set for element : Lr
NewGTO 103
S 9
  1
     73963782.78320600
                             0.0254314704
  2
     33619901.26509300
                            -0.0075060780
  3 15281773.30231500
                            0.0434100498
  4 6946260.591961000
                            0.0194663593
     3157391.178164000
                            0.0754440633
  6
     1435177.808256000
                            0.0876275137
  7
     652353.5492070000
                            0.1768416025
  8
     296524.3405490000
                             0.2729595270
  9
    134783.7911590000
                             0.4924043577
S 1
      61265.3596180000
                             1.0000000000
  1
S 1
                             1.0000000000
     27847.8907350000
  1
S 1
      12658.1321520000
                             1.0000000000
  1
S 1
  1
       5753.6964330000
                             1.0000000000
S 1
  1
       2615.3165600000
                             1.0000000000
S 1
       1188.7802550000
                             1.0000000000
S 1
        540.3546610000
                             1.0000000000
  1
S 1
        245.6157550000
                             1.0000000000
  1
S 1
  1
        111.6435250000
                             1.0000000000
S 1
         50.7470570000
                             1.0000000000
  1
S 1
         23.0668440000
                             1.0000000000
  1
S 1
         10.4849290000
                             1.0000000000
  1
S 1
          4.7658770000
                             1.0000000000
  1
S 1
  1
          2.1663080000
                             1.0000000000
S 1
  1
          0.9846850000
                             1.0000000000
S 1
          0.4475840000
                             1.0000000000
S 1
          0.2034470000
                             1.0000000000
  1
S 1
                             1.0000000000
  1
          0.0924760000
S 1
          0.0420350000
                             1.0000000000
  1
S 1
                             1.0000000000
  1
          0.0191070000
P 8
     1066386.172543000
                             0.0012458711
  1
  2
     444327.5718930000
                             0.0012752099
     185136.4882890000
                             0.0050627758
  3
  4
      77140.2034540000
                             0.0113223370
      32141.7514390000
                             0.0318283161
  6
      13392.3964330000
                             0.0872713846
  7
       5580.1651800000
                             0.2563948402
  8
       2325.0688250000
                             0.7208510570
P 1
        968.7786770000
                             1.0000000000
  1
P 1
        403.6577820000
                             1.00000000000
  1
P 1
```

1	168.1907430000	1.0000000000
P 1 1	70.0794760000	1.0000000000
P 1	70.0754700000	1.000000000
1 P 1	29.1997820000	1.0000000000
1	12.1665760000	1.0000000000
P 1	F 0604070000	1 000000000
1 P 1	5.0694070000	1.0000000000
1 P 1	2.1122530000	1.0000000000
1	0.8801050000	1.0000000000
P 1 1	0.3667110000	1.0000000000
P 1 1	0.1527960000	1.0000000000
P 1	0.1327300000	1.000000000
1 D 7	0.0636650000	1.0000000000
	F2706 0042F60000	0.0001206502
1	53706.9942560000	0.0001296503
2	21482.7977020000	0.0003446003
3	8593.1190810000	0.0019958902
4	3437.2476320000	0.0094015674
5	1374.8990530000	0.0516425050
6	549.9596210000	0.2350882183
7	219.9838480000	0.7977127450
	219.9636460000	0.7377127430
D 1 1	87.9935390000	1.0000000000
D 1		
1 D 1	35.1974160000	1.0000000000
1 D 1	14.0789660000	1.0000000000
1 D 1	5.6315870000	1.0000000000
1 D 1	2.2526350000	1.0000000000
1 D 1	0.9010540000	1.0000000000
1	0.3604220000	1.0000000000
D 1 1	0.1441690000	1.0000000000
D 1	0.0576670000	1 000000000
1 F 6	0.0576670000	1.0000000000
1	6543.7113860000	0.0000475960
2	2516.8120720000	0.0004051086
3	968.0046430000	0.0037668407
4	372.3094780000	0.0336701482
5	143.1959530000	0.2215290610
6 F 1	55.0753670000	0.8391305662
1	21.1828330000	1.0000000000
F 1	8.1472440000	1.0000000000
F 1 1	3.1335550000	1.0000000000
F 1	1 2052140000	1 000000000
1 F 1	1.2052140000	1.0000000000
1 F 1	0.4635440000	1.0000000000
1 end	0.1782860000	1.0000000000

Polarization functions

# SARC g polarization function for actinides		
Ac: G 1 1	0.7100250000	1.0000000000
Th: G 1 1	0.7422170000	1.0000000000
Pa: G 1 1	0.7746840000	1.0000000000
U : G 1 1	0.8077110000	1.0000000000
Np: G 1 1	0.8412210000	1.0000000000
Pu: G 1 1	0.8751860000	1.0000000000
Am: G 1 1	0.9097580000	1.0000000000
Cm: G 1 1	0.9449040000	1.0000000000
Bk: G 1 1	0.9798240000	1.0000000000
Cf: G 1 1	1.0155710000	1.0000000000
Es: G 1 1	1.0517850000	1.0000000000
Fm: G 1 1	1.0884900000	1.0000000000
Md: G 1 1	1.1256660000	1.0000000000
No: G 1 1	1.1649470000	1.0000000000
Lr: G 1 1	1.2034310000	1.0000000000