

```

max number of local orbitals/atom          3
cein3
0      P      TYPE LATTICE ASSUMED
      RELA-CALCULATION

      R-MT TIMES K-MAX IS 7.00
      MAX L IS 10      MAX L IN NONSPHERICAL MATRICELEMENTS:  4
NUMBER OF ATOMS IS      2
  0.11283   0.00000   0.00000
 -0.00000   0.11283   0.00000
 -0.00000  -0.00000   0.11283
  8.86282   0.00000   0.00000
  0.00000   8.86282   0.00000
  0.00000   0.00000   8.86282

      NOT EQUIV ATOM      1      Ce
:E0_0001: E( 0)=      0.3000
      APW+lo
:E0_0001: E( 0)=  -2.0357   E(BOTTOM)=  -2.462   E(TOP)=  -1.609
4  5      162
      LOCAL ORBITAL
:E1_0001: E( 1)=      0.7000
      APW+lo
:E1_0001: E( 1)=  -0.6984   E(BOTTOM)=  -1.392   E(TOP)=  -0.004
3  4      168
      LOCAL ORBITAL
:E3_0001: E( 3)=      0.5828   E(BOTTOM)=      0.416   E(TOP)=      0.750
0  1      131
      APW+lo
:E2_0001: E( 2)=      0.3000   E(BOTTOM)=      0.156   E(TOP)= -200.000
2 -1      93
      APW+lo

      POTENTIAL PARAMETERS
      L      U(R)      U'(R)      DU/DE      DU'/DE
NORM-U'
      0 -0.483019E+00 -0.463201E+00 -0.835366E-01  0.251138E+00
0.961245E-01      5 5 5
      1  0.207355E+00  0.618251E+00  0.266455E+00  0.227643E-01
0.183485E+00      4 4 4
      2  0.438442E+00 -0.503175E-01 -0.144155E+00 -0.348413E+00
0.343374E-01      2 2 2
      3  0.126149E+00 -0.109519E+00 -0.729319E+00 -0.635566E+00
0.122235E+01      0 0 0
      4  0.757913E+00  0.955273E+00 -0.507116E-01 -0.275023E+00
0.335266E-02      0 0 0
      5  0.859617E+00  0.150222E+01 -0.352209E-01 -0.247674E+00
0.129739E-02      0 0 0
      6  0.941607E+00  0.206889E+01 -0.271887E-01 -0.229650E+00
0.663562E-03      0 0 0
      7  0.101354E+01  0.266560E+01 -0.220658E-01 -0.215879E+00
0.386451E-03      0 0 0

```

8	0.107893E+01	0.329450E+01	-0.184734E-01	-0.204679E+00
0.243871E-03	0 0 0			
9	0.113956E+01	0.395564E+01	-0.158065E-01	-0.195239E+00
0.162805E-03	0 0 0			
10	0.119648E+01	0.464839E+01	-0.137481E-01	-0.187095E+00
0.113398E-03	0 0 0			

LOCAL ORBITAL POTENTIAL PARAMETERS

	L	U (R)	U' (R)	NORM U1U2	NORM UE1U2
0 4 0	0	0.160525E+00	-0.221587E+00	0.485359E+00	-0.266139E+00
2 2	2	1.000000	-2.035736	-2.035736	
1	1	-0.206114E+00	0.287863E+00	0.836234E+00	-0.234273E+00
0 3 0	2	2	1.000000	-0.698396	-0.698396
LO COEFFICIENT: 1,A,B,C	0		0.48715	-2.81679	0.00000
LO COEFFICIENT: 1,A,B,C	0		0.27762	0.00000	0.83535
LO COEFFICIENT: 1,A,B,C	1		0.94868	-0.73826	0.00000
LO COEFFICIENT: 1,A,B,C	1		0.52025	0.00000	0.52339
LO COEFFICIENT: 1,A,B,C	2		0.87117	2.64963	0.00000
LO COEFFICIENT: 1,A,B,C	3		0.98220	0.16989	0.00000

131 POSSIBLE NONSPHERICAL CONTRIBUTIONS TO H
NUMBER OF RADIAL INTEGRALS FOR ATOM 1 = 26

NOT EQUIV ATOM 2 In
:E2_0002: E(2)= 0.7000
APW+lo
:E2_0002: E(2)= -0.4293 E(BOTTOM)= -0.609 E(TOP)= -0.249
1 2 154
LOCAL ORBITAL
:E0_0002: E(0)= 0.3000
APW+lo
:E1_0002: E(1)= 0.3000
APW+lo

POTENTIAL PARAMETERS

	L	U (R)	U' (R)	DU/DE	DU'/DE
NORM-U'	0	0.377606E+00	-0.226257E+00	-0.152116E+00	-0.332582E+00
0.365750E-01	4 4 4				
1	1	-0.508655E+00	-0.302565E-01	0.103839E+00	0.320744E+00
0.169877E-01	3 3 3				
2	2	0.448092E+00	0.408820E+00	0.211203E+00	-0.164448E+00
0.341314E+00	2 2 2				
3	3	0.671408E+00	0.613311E+00	-0.753987E-01	-0.307182E+00
0.101470E-01	0 0 0				
4	4	0.795287E+00	0.112607E+01	-0.437561E-01	-0.263137E+00
0.228152E-02	0 0 0				
5	5	0.883008E+00	0.164273E+01	-0.324608E-01	-0.241579E+00
0.104767E-02	0 0 0				
6	6	0.958417E+00	0.219187E+01	-0.257604E-01	-0.225841E+00
0.575608E-03	0 0 0				

7	0.102646E+01	0.277647E+01	-0.212264E-01	-0.213271E+00
0.348762E-03	0 0 0			
8	0.108929E+01	0.339626E+01	-0.179390E-01	-0.202788E+00
0.225601E-03	0 0 0			
9	0.114812E+01	0.405022E+01	-0.154465E-01	-0.193812E+00
0.153139E-03	0 0 0			
10	0.120371E+01	0.473710E+01	-0.134949E-01	-0.185984E+00
0.107932E-03	0 0 0			

LOCAL ORBITAL POTENTIAL PARAMETERS

L	U(R)	U'(R)	NORM U1U2	NORM UE1U2
2	-0.118599E+00	0.124861E+00	0.577781E+00	-0.473732E+00
0 1 0				
2	2	1.000000	-0.429321	-0.429321
LO COEFFICIENT: 1,A,B,C	0	0.90337	2.24248	0.00000
LO COEFFICIENT: 1,A,B,C	1	0.84286	4.12876	0.00000
LO COEFFICIENT: 1,A,B,C	2	0.62791	-1.33218	0.00000
LO COEFFICIENT: 1,A,B,C	2	0.22564	0.00000	0.85252

173 POSSIBLE NONSPHERICAL CONTRIBUTIONS TO H

NUMBER OF RADIAL INTEGRALS FOR ATOM	2	=	36
CPTIME ATPAR	=	0.0	

R-MT= 2.5000000 2.5000000

FRACTIONAL VOLUME WITHIN MT= 0.0940141 0.0940141

ONE/UNIT CELL VOLUME= 0.143642965E-02

LATTICE CONSTANTS ARE: 8.86282 8.86282 8.86282

alloc Warp 0.5 MB

K=	0	0	0	IND= 1				
				1. WAVE=	0	0	0	TAUP= 1.00000
								WARPING= -0.00179
K=	-1	0	0	IND= 6				
				1. WAVE=	1	0	0	TAUP= 1.00000
								WARPING= -0.01983
				2. WAVE=	0	1	0	TAUP= 1.00000
								WARPING= -0.01983
				3. WAVE=	0	0	1	TAUP= 1.00000
								WARPING= -0.01983
				4. WAVE=	0	0	-1	TAUP= 1.00000
								WARPING= -0.01983
				5. WAVE=	0	-1	0	TAUP= 1.00000
								WARPING= -0.01983
				6. WAVE=	-1	0	0	TAUP= 1.00000
								WARPING= -0.01983
K=	-1	-1	0	IND=12				
				1. WAVE=	1	1	0	TAUP= 1.00000
								WARPING= 0.00358
				2. WAVE=	1	0	1	TAUP= 1.00000
								WARPING= 0.00358
				3. WAVE=	1	0	-1	TAUP= 1.00000

					WARPING=	0.00358
				4. WAVE=	1	-1 0
					TAUP=	1.00000
				5. WAVE=	0	1 1
					WARPING=	0.00358
				6. WAVE=	0	1 -1
					TAUP=	1.00000
				7. WAVE=	0	-1 1
					WARPING=	0.00358
				8. WAVE=	0	-1 -1
					TAUP=	1.00000
				9. WAVE=	-1	1 0
					WARPING=	0.00358
				10. WAVE=	-1	0 1
					TAUP=	1.00000
				11. WAVE=	-1	0 -1
					WARPING=	0.00358
				12. WAVE=	-1	-1 0
					TAUP=	1.00000
					WARPING=	0.00358
K=	-1	-1	-1	IND= 8		
				1. WAVE=	1	1 1
					TAUP=	1.00000
				2. WAVE=	1	1 -1
					WARPING=	-0.01366
				3. WAVE=	1	-1 1
					TAUP=	1.00000
				4. WAVE=	1	-1 -1
					WARPING=	-0.01366
				5. WAVE=	-1	1 1
					TAUP=	1.00000
				6. WAVE=	-1	1 -1
					WARPING=	-0.01366
				7. WAVE=	-1	-1 1
					TAUP=	1.00000
				8. WAVE=	-1	-1 -1
					WARPING=	-0.01366
					TAUP=	1.00000
					WARPING=	-0.01366
K=	-2	0	0	IND= 6		
				1. WAVE=	2	0 0
					TAUP=	1.00000
				2. WAVE=	0	2 0
					WARPING=	0.01289
				3. WAVE=	0	0 2
					TAUP=	1.00000
				4. WAVE=	0	0 -2
					WARPING=	0.01289
				5. WAVE=	0	-2 0
					TAUP=	1.00000
				6. WAVE=	-2	0 0
					WARPING=	0.01289
					TAUP=	1.00000
					WARPING=	0.01289
K=	-2	-1	0	IND=24		
				1. WAVE=	2	1 0
					TAUP=	1.00000
					WARPING=	0.00542

2.	WAVE=	2	0	1	TAUP=	1.00000
					WARPING=	0.00542
3.	WAVE=	2	0	-1	TAUP=	1.00000
					WARPING=	0.00542
4.	WAVE=	2	-1	0	TAUP=	1.00000
					WARPING=	0.00542
5.	WAVE=	1	2	0	TAUP=	1.00000
					WARPING=	0.00542
6.	WAVE=	1	0	2	TAUP=	1.00000
					WARPING=	0.00542
7.	WAVE=	1	0	-2	TAUP=	1.00000
					WARPING=	0.00542
8.	WAVE=	1	-2	0	TAUP=	1.00000
					WARPING=	0.00542
9.	WAVE=	0	2	1	TAUP=	1.00000
					WARPING=	0.00542
10.	WAVE=	0	2	-1	TAUP=	1.00000
					WARPING=	0.00542
11.	WAVE=	0	1	2	TAUP=	1.00000
					WARPING=	0.00542
12.	WAVE=	0	1	-2	TAUP=	1.00000
					WARPING=	0.00542
13.	WAVE=	0	-1	2	TAUP=	1.00000
					WARPING=	0.00542
14.	WAVE=	0	-1	-2	TAUP=	1.00000
					WARPING=	0.00542
15.	WAVE=	0	-2	1	TAUP=	1.00000
					WARPING=	0.00542
16.	WAVE=	0	-2	-1	TAUP=	1.00000
					WARPING=	0.00542
17.	WAVE=	-1	2	0	TAUP=	1.00000
					WARPING=	0.00542
18.	WAVE=	-1	0	2	TAUP=	1.00000
					WARPING=	0.00542
19.	WAVE=	-1	0	-2	TAUP=	1.00000
					WARPING=	0.00542
20.	WAVE=	-1	-2	0	TAUP=	1.00000
					WARPING=	0.00542
21.	WAVE=	-2	1	0	TAUP=	1.00000
					WARPING=	0.00542
22.	WAVE=	-2	0	1	TAUP=	1.00000
					WARPING=	0.00542
23.	WAVE=	-2	0	-1	TAUP=	1.00000
					WARPING=	0.00542
24.	WAVE=	-2	-1	0	TAUP=	1.00000
					WARPING=	0.00542
K= -2 -1 -1 IND=24						
1.	WAVE=	2	1	1	TAUP=	1.00000
					WARPING=	0.00490
2.	WAVE=	2	1	-1	TAUP=	1.00000
					WARPING=	0.00490
3.	WAVE=	2	-1	1	TAUP=	1.00000

					WARPING=	0.00490
4.	WAVE=	2	-1	-1	TAUP=	1.00000
					WARPING=	0.00490
5.	WAVE=	1	2	1	TAUP=	1.00000
					WARPING=	0.00490
6.	WAVE=	1	2	-1	TAUP=	1.00000
					WARPING=	0.00490
7.	WAVE=	1	1	2	TAUP=	1.00000
					WARPING=	0.00490
8.	WAVE=	1	1	-2	TAUP=	1.00000
					WARPING=	0.00490
9.	WAVE=	1	-1	2	TAUP=	1.00000
					WARPING=	0.00490
10.	WAVE=	1	-1	-2	TAUP=	1.00000
					WARPING=	0.00490
11.	WAVE=	1	-2	1	TAUP=	1.00000
					WARPING=	0.00490
12.	WAVE=	1	-2	-1	TAUP=	1.00000
					WARPING=	0.00490
13.	WAVE=	-1	2	1	TAUP=	1.00000
					WARPING=	0.00490
14.	WAVE=	-1	2	-1	TAUP=	1.00000
					WARPING=	0.00490
15.	WAVE=	-1	1	2	TAUP=	1.00000
					WARPING=	0.00490
16.	WAVE=	-1	1	-2	TAUP=	1.00000
					WARPING=	0.00490
17.	WAVE=	-1	-1	2	TAUP=	1.00000
					WARPING=	0.00490
18.	WAVE=	-1	-1	-2	TAUP=	1.00000
					WARPING=	0.00490
19.	WAVE=	-1	-2	1	TAUP=	1.00000
					WARPING=	0.00490
20.	WAVE=	-1	-2	-1	TAUP=	1.00000
					WARPING=	0.00490
21.	WAVE=	-2	1	1	TAUP=	1.00000
					WARPING=	0.00490
22.	WAVE=	-2	1	-1	TAUP=	1.00000
					WARPING=	0.00490
23.	WAVE=	-2	-1	1	TAUP=	1.00000
					WARPING=	0.00490
24.	WAVE=	-2	-1	-1	TAUP=	1.00000
					WARPING=	0.00490
K=	-2	-2	0	IND=12		
	1.	WAVE=	2	2	0	TAUP= 1.00000
						WARPING= 0.01257
	2.	WAVE=	2	0	2	TAUP= 1.00000
						WARPING= 0.01257
	3.	WAVE=	2	0	-2	TAUP= 1.00000
						WARPING= 0.01257
	4.	WAVE=	2	-2	0	TAUP= 1.00000
						WARPING= 0.01257

5. WAVE=	0	2	2	TAUP=	1.00000		
				WARPING=	0.01257		
6. WAVE=	0	2	-2	TAUP=	1.00000		
				WARPING=	0.01257		
7. WAVE=	0	-2	2	TAUP=	1.00000		
				WARPING=	0.01257		
8. WAVE=	0	-2	-2	TAUP=	1.00000		
				WARPING=	0.01257		
9. WAVE=	-2	2	0	TAUP=	1.00000		
				WARPING=	0.01257		
10. WAVE=	-2	0	2	TAUP=	1.00000		
				WARPING=	0.01257		
11. WAVE=	-2	0	-2	TAUP=	1.00000		
				WARPING=	0.01257		
12. WAVE=	-2	-2	0	TAUP=	1.00000		
				WARPING=	0.01257		
Matrix size	313						
allocate HS	0.7 MB						
allocate Z	0.7 MB						
allocate spanel	0.3 MB	dimensions	313	128			
allocate hpanel	0.3 MB	dimensions	313	128			
allocate spanelus	0.3 MB	dimensions	313	128			
allocate slen	0.3 MB	dimensions	313	128			
allocate x2	0.3 MB	dimensions	313	128			
allocate legendre	4.0 MB	dimensions	313	13			
128							
allocate al,bl (row)	0.1 MB	dimensions	313	11			
allocate al,bl (col)	0.0 MB	dimensions	128	11			
allocate YL	0.2 MB	dimensions	15	313			
3							
number of local orbitals, nlo (hamilt)	62						
allocate YL	0.2 MB	dimensions	15	313			
3							
allocate phsc	0.0 MB	dimensions	313				
Time for al,bl (hamilt, cpu/wall) :	0.00		0.00				
Time for legendre (hamilt, cpu/wall) :	0.00		0.00				
Time for phase (hamilt, cpu/wall) :	0.00		0.00				
Time for us (hamilt, cpu/wall) :	0.01		0.01				
Time for overlaps (hamilt, cpu/wall) :	0.02		0.02				
Time for distrib (hamilt, cpu/wall) :	0.00		0.00				
Time sum iouter (hamilt, cpu/wall) :	0.02		0.02				
Time for los (hamilt, cpu/wall) :	0.01		0.01				
Time for alm (hns) :	0.0	0.0					
Time for vector (hns) :	0.0	0.0					
Time for vector2 (hns) :	0.0	0.0					
Time for VxV (hns) :	0.0	0.0					
58 Eigenvalues computed							
Seclr4(Cholesky complete (CPU)) :	0.007		1532.91				
Mflops							
Seclr4(Transform to eig.problem (CPU)) :	0.013		2337.75				
Mflops							

```

Seclr4(Compute eigenvalues (CPU)) :          0.044      932.68
Mflops
Seclr4(Backtransform (CPU)) :          0.001      2675.24
Mflops
    TIME HAMILT (CPU) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0
    TIME HAMILT (WALL) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0

```

K= 0.050000 0.050000 0.050000 1

MATRIX SIZE 313 WEIGHT= 8.00 PGR:

EIGENVALUES ARE:

```

-1.9887407 -0.7316970 -0.7314116 -0.7314116 -0.4183814
-0.4182713 -0.4182713 -0.4118749 -0.4118749 -0.4117753
-0.4011260 -0.4009214 -0.4009214 -0.3835174 -0.3833988
-0.3833988 -0.3742772 -0.3742772 -0.3740127 -0.0424714
 0.3578010  0.3578010  0.4907847  0.5152424  0.5152424
 0.5953098  0.5953098  0.5979380  0.6169011  0.6363571
 0.6410523  0.6410523  0.7051883  0.7051883  0.7254922
 0.8179272  0.8179272  0.8679880  0.9053007  0.9436325

 0.9436325  1.0988937  1.1318279  1.1318279  1.3712929
 1.4010949  1.4010949  1.4651378  1.4651378  1.4741103
 1.5664468  1.6114479  1.6597557  1.6597557  1.9023541
 1.9677049  1.9677049  1.9732887

```

0 EIGENVALUES BELOW THE ENERGY -9.00000

```

coors: iplus,nv,n=          0          251          252
Matrix size          314
    allocate HS          0.8 MB
    allocate Z          0.8 MB
    allocate spanel          0.3 MB          dimensions          314          128
    allocate hpanel          0.3 MB          dimensions          314          128
    allocate spanelus          0.3 MB          dimensions          314          128
    allocate slen          0.3 MB          dimensions          314          128
    allocate x2          0.3 MB          dimensions          314          128
    allocate legendre          4.0 MB          dimensions          314          13
128
    allocate al,bl (row)          0.1 MB          dimensions          314          11
    allocate al,bl (col)          0.0 MB          dimensions          128          11
    allocate YL          0.2 MB          dimensions          15          314
3
    number of local orbitals, nlo (hamilt)          62
    allocate YL          0.2 MB          dimensions          15          314
3
    allocate phsc          0.0 MB          dimensions          314
Time for al,bl (hamilt, cpu/wall) :          0.00          0.00
Time for legendre (hamilt, cpu/wall) :          0.02          0.02
Time for phase (hamilt, cpu/wall) :          0.01          0.00
Time for us (hamilt, cpu/wall) :          0.01          0.00
Time for overlaps (hamilt, cpu/wall) :          0.01          0.02

```


Time for distrib	(hamilt, cpu/wall)	:	0.00	0.00
Time sum iouter	(hamilt, cpu/wall)	:	0.00	0.00
Time for los	(hamilt, cpu/wall)	:	0.01	0.01
Time for alm	(hns)	:	0.0	0.0
Time for vector	(hns)	:	0.0	0.0
Time for vector2	(hns)	:	0.0	0.0
Time for VxV	(hns)	:	0.0	0.0

58 Eigenvalues computed

Seclr4(Cholesky complete (CPU)) :	0.004	2940.09
Mflops		
Seclr4(Transform to eig.problem (CPU)) :	0.007	4231.13
Mflops		
Seclr4(Compute eigenvalues (CPU)) :	0.054	771.52
Mflops		
Seclr4(Backtransform (CPU)) :	0.000	2870.77
Mflops		

TIME HAMILT (CPU) =	0.1,	HNS =	0.0,	HORB =	0.0,
DIAG =	0.1,	SYNC =	0.0		
TIME HAMILT (WALL) =	0.1,	HNS =	0.0,	HORB =	0.0,
DIAG =	0.1,	SYNC =	0.0		

K= 0.050000 0.050000 0.150000 2

MATRIX SIZE 314 WEIGHT=24.00 PGR:

EIGENVALUES ARE:

-1.9886872	-0.7336681	-0.7317722	-0.7316474	-0.4176756
-0.4163637	-0.4162860	-0.4113404	-0.4103471	-0.4100559
-0.4015590	-0.4002015	-0.4000866	-0.3848067	-0.3845244
-0.3833264	-0.3763072	-0.3761357	-0.3740442	-0.0296379
0.3170570	0.3652705	0.4810784	0.5102830	0.5450097
0.5876659	0.5935849	0.5975949	0.6169156	0.6311065
0.6333351	0.6447548	0.6882623	0.7055440	0.7382934
0.7609928	0.8391694	0.9051265	0.9356185	0.9719027

1.0212548	1.0440852	1.1003246	1.1070951	1.3369756
1.4113464	1.4348753	1.4348844	1.4943149	1.5324816
1.5732532	1.6342633	1.6382262	1.6947956	1.8436633
1.9077331	1.9230074	1.9919233		

0 EIGENVALUES BELOW THE ENERGY -9.00000

coors: iplus,nv,n=	0	252	257
Matrix size	319		
allocate HS	0.8 MB		
allocate Z	0.8 MB		
allocate spanel	0.3 MB	dimensions	319 128
allocate hpanel	0.3 MB	dimensions	319 128
allocate spanelus	0.3 MB	dimensions	319 128
allocate slen	0.3 MB	dimensions	319 128
allocate x2	0.3 MB	dimensions	319 128
allocate legendre	4.0 MB	dimensions	319 13
128			
allocate al,bl (row)	0.1 MB	dimensions	319 11

```

allocate al,bl (col)          0.0 MB          dimensions 128   11
      allocate YL              0.2 MB          dimensions 15   319
3
  number of local orbitals, nlo (hamilt)      62
      allocate YL              0.2 MB          dimensions 15   319
3
      allocate phsc            0.0 MB          dimensions 319
Time for al,bl      (hamilt, cpu/wall) :        0.00      0.00
Time for legendre  (hamilt, cpu/wall) :        0.00      0.00
Time for phase     (hamilt, cpu/wall) :        0.01      0.01
Time for us        (hamilt, cpu/wall) :        0.00      0.02
Time for overlaps  (hamilt, cpu/wall) :        0.02      0.02
Time for distrib   (hamilt, cpu/wall) :        0.00      0.00
Time sum iouter    (hamilt, cpu/wall) :        0.00      0.00
Time for los       (hamilt, cpu/wall) :        0.01      0.01
Time for alm       (hns) :          0.0          0.0
Time for vector    (hns) :          0.0          0.0
Time for vector2   (hns) :          0.0          0.0
Time for VxV       (hns) :          0.0          0.0
      58 Eigenvalues computed
      Seclr4(Cholesky complete (CPU)) :          0.004      2465.95
Mflops
      Seclr4(Transform to eig.problem (CPU)) :          0.008      4027.51
Mflops
      Seclr4(Compute eigenvalues (CPU)) :          0.048      910.57
Mflops
      Seclr4(Backtransform (CPU)) :          0.000      3119.52
Mflops
      TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0
      TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0

      K= 0.050000 0.050000 0.250000          3
      MATRIX SIZE 319 WEIGHT=24.00 PGR:
      EIGENVALUES ARE:
      -1.9885968 -0.7369143 -0.7322154 -0.7320259 -0.4169494
      -0.4126783 -0.4126511 -0.4099984 -0.4077660 -0.4070758
      -0.4026002 -0.3990222 -0.3989896 -0.3870602 -0.3869808
      -0.3834202 -0.3805364 -0.3804390 -0.3741468 -0.0047006
      0.2573203 0.3798279 0.4780836 0.4993249 0.5711905
      0.5736846 0.5908137 0.5962086 0.6155604 0.6256325
      0.6264873 0.6495083 0.6818060 0.6910106 0.7335970
      0.7489767 0.8607102 0.9287742 0.9664851 1.0065505

      1.0226115 1.0610432 1.0770887 1.1242944 1.2976716
      1.3522482 1.4671986 1.4866405 1.5507814 1.5615552
      1.5865547 1.6032225 1.6773769 1.6914374 1.7734354
      1.8821450 1.8894418 1.9869524
      0 EIGENVALUES BELOW THE ENERGY -9.00000
      *****

```

```

coors: iplus,nv,n=          0          257          254
Matrix size          316
      allocate HS          0.8 MB
      allocate Z           0.8 MB
      allocate spanel      0.3 MB          dimensions 316 128
      allocate hpanel      0.3 MB          dimensions 316 128
      allocate spanelus    0.3 MB          dimensions 316 128
      allocate slen        0.3 MB          dimensions 316 128
      allocate x2          0.3 MB          dimensions 316 128
      allocate legendre    4.0 MB          dimensions 316 13
128
allocate al,bl (row)      0.1 MB          dimensions 316 11
allocate al,bl (col)     0.0 MB          dimensions 128 11
      allocate YL          0.2 MB          dimensions 15 316
3
  number of local orbitals, nlo (hamilt)      62
      allocate YL          0.2 MB          dimensions 15 316
3
      allocate phsc        0.0 MB          dimensions 316
Time for al,bl (hamilt, cpu/wall) :          0.00          0.00
Time for legendre (hamilt, cpu/wall) :        0.02          0.02
Time for phase (hamilt, cpu/wall) :          0.00          0.00
Time for us (hamilt, cpu/wall) :            0.02          0.02
Time for overlaps (hamilt, cpu/wall) :        0.02          0.02
Time for distrib (hamilt, cpu/wall) :          0.00          0.00
Time sum iouter (hamilt, cpu/wall) :          0.00          0.00
Time for los (hamilt, cpu/wall) :            0.01          0.01
Time for alm (hns) :          0.0          0.0
Time for vector (hns) :          0.0          0.0
Time for vector2 (hns) :          0.0          0.0
Time for VxV (hns) :          0.0          0.0
      60 Eigenvalues computed
Seclr4(Cholesky complete (CPU)) :          0.003          3291.04
Mflops
Seclr4(Transform to eig.problem (CPU)) :        0.007          4455.59
Mflops
Seclr4(Compute eigenvalues (CPU)) :          0.048          868.80
Mflops
Seclr4(Backtransform (CPU)) :          0.000          3032.06
Mflops
      TIME HAMILT (CPU) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0
      TIME HAMILT (WALL) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0

K= 0.050000 0.050000 0.350000          4
MATRIX SIZE 316 WEIGHT=24.00 PGR:
EIGENVALUES ARE:
-1.9884976 -0.7400622 -0.7325763 -0.7323248 -0.4156525
-0.4099339 -0.4078833 -0.4072932 -0.4039858 -0.4036728
-0.4035765 -0.3977329 -0.3975739 -0.3897247 -0.3895725
-0.3858651 -0.3854954 -0.3829871 -0.3740085 0.0309765

```

0.1942693	0.3999989	0.4742733	0.4862633	0.5441789
0.5892993	0.5967451	0.5968215	0.6155866	0.6226947
0.6230004	0.6674734	0.6679748	0.6844413	0.7450150
0.7608045	0.8687776	0.8808361	0.9414139	0.9674767
1.0884243	1.1174848	1.1509231	1.1852057	1.2684802
1.3092703	1.4514435	1.4778670	1.5456171	1.5563538
1.5971631	1.6465088	1.6506902	1.7007298	1.8420169
1.8712248	1.9149934	1.9343204	1.9510479	1.9664726

0 EIGENVALUES BELOW THE ENERGY -9.00000

coors: iplus,nv,n=	0	254	250		
Matrix size	312				
allocate HS	0.7 MB				
allocate Z	0.7 MB				
allocate spanel	0.3 MB	dimensions	312	128	
allocate hpanel	0.3 MB	dimensions	312	128	
allocate spanelus	0.3 MB	dimensions	312	128	
allocate slen	0.3 MB	dimensions	312	128	
allocate x2	0.3 MB	dimensions	312	128	
allocate legendre	4.0 MB	dimensions	312	13	
128					
allocate al,bl (row)	0.1 MB	dimensions	312	11	
allocate al,bl (col)	0.0 MB	dimensions	128	11	
allocate YL	0.2 MB	dimensions	15	312	
3					
number of local orbitals, nlo (hamilt)		62			
allocate YL	0.2 MB	dimensions	15	312	
3					
allocate phsc	0.0 MB	dimensions	312		
Time for al,bl (hamilt, cpu/wall) :		0.00	0.00		
Time for legendre (hamilt, cpu/wall) :		0.02	0.02		
Time for phase (hamilt, cpu/wall) :		0.00	0.00		
Time for us (hamilt, cpu/wall) :		0.02	0.02		
Time for overlaps (hamilt, cpu/wall) :		0.00	0.00		
Time for distrib (hamilt, cpu/wall) :		0.00	0.00		
Time sum iouter (hamilt, cpu/wall) :		0.00	0.00		
Time for los (hamilt, cpu/wall) :		0.01	0.01		
Time for alm (hns) :	0.0	0.0			
Time for vector (hns) :	0.0	0.0			
Time for vector2 (hns) :	0.0	0.0			
Time for VxV (hns) :	0.0	0.0			
59 Eigenvalues computed					
Seclr4(Cholesky complete (CPU)) :		0.003	3309.51		
Mflops					
Seclr4(Transform to eig.problem (CPU)) :		0.007	4474.27		
Mflops					
Seclr4(Compute eigenvalues (CPU)) :		0.047	855.88		
Mflops					

```

Seclr4(Backtransform (CPU)) :          0.000      3190.72
Mflops
    TIME HAMILT (CPU) =      0.1, HNS =      0.0, HORB =      0.0,
DIAG =      0.1, SYNC =      0.0
    TIME HAMILT (WALL) =      0.1, HNS =      0.0, HORB =      0.0,
DIAG =      0.1, SYNC =      0.0

```

```

K=  0.050000  0.050000  0.450000          5
  MATRIX SIZE  312  WEIGHT=24.00  PGR:
EIGENVALUES ARE:
-1.9884479   -0.7419771   -0.7327486   -0.7326889   -0.4146158
-0.4086581   -0.4045779   -0.4036725   -0.4028413   -0.4007033
-0.4005489   -0.3965390   -0.3960539   -0.3926142   -0.3921399
-0.3907342   -0.3900977   -0.3828360   -0.3743996    0.0743758
 0.1363123    0.4195163    0.4708093    0.4767281    0.5181510
 0.5910320    0.5973236    0.6063240    0.6153465    0.6218117
 0.6219258    0.6581221    0.6850375    0.7048537    0.7595769
 0.7715541    0.8149694    0.8922936    0.9112633    0.9196279

 1.1597329    1.1838157    1.2153272    1.2487639    1.2535327
 1.3107742    1.3692677    1.4203073    1.4264847    1.5988679
 1.6364773    1.6787006    1.7263482    1.7450111    1.7896582
 1.8266448    1.8605168    1.9590869    1.9706859

      0 EIGENVALUES BELOW THE ENERGY  -9.00000
*****

```

```

coors:  iplus,nv,n=          0          250          256
Matrix size          318
  allocate HS          0.8 MB
  allocate Z           0.8 MB
  allocate spanel      0.3 MB          dimensions  318   128
  allocate hpanel      0.3 MB          dimensions  318   128
  allocate spanelus    0.3 MB          dimensions  318   128
  allocate slen        0.3 MB          dimensions  318   128
  allocate x2          0.3 MB          dimensions  318   128
  allocate legendre    4.0 MB          dimensions  318   13
128
  allocate al,bl (row)  0.1 MB          dimensions  318   11
  allocate al,bl (col)  0.0 MB          dimensions  128   11
  allocate YL          0.2 MB          dimensions   15   318
3
  number of local orbitals, nlo (hamilt)  62
  allocate YL          0.2 MB          dimensions   15   318
3
  allocate phsc        0.0 MB          dimensions  318
Time for al,bl (hamilt, cpu/wall) :      0.00      0.00
Time for legendre (hamilt, cpu/wall) :      0.02      0.02
Time for phase (hamilt, cpu/wall) :      0.00      0.00
Time for us (hamilt, cpu/wall) :      0.03      0.01
Time for overlaps (hamilt, cpu/wall) :      0.01      0.00
Time for distrib (hamilt, cpu/wall) :      0.00      0.00
Time sum iouter (hamilt, cpu/wall) :      0.00      0.00

```

```

Time for los      (hamilt, cpu/wall) :          0.01          0.01
Time for alm      (hns) :          0.0          0.0
Time for vector   (hns) :          0.0          0.0
Time for vector2  (hns) :          0.0          0.0
Time for VxV      (hns) :          0.0          0.0
      58 Eigenvalues computed
Seclr4(Cholesky complete (CPU)) :          0.004          2887.70
Mflops
Seclr4(Transform to eig.problem (CPU)) :          0.007          4666.58
Mflops
Seclr4(Compute eigenvalues (CPU)) :          0.048          893.39
Mflops
Seclr4(Backtransform (CPU)) :          0.000          3061.16
Mflops
      TIME HAMILT (CPU) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0
      TIME HAMILT (WALL) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0

```

```

K= 0.050000 0.150000 0.150000          6
MATRIX SIZE 318 WEIGHT=24.00 PGR:
EIGENVALUES ARE:
-1.9886350 -0.7343365 -0.7330935 -0.7319402 -0.4161161
-0.4155280 -0.4154024 -0.4103871 -0.4093210 -0.4081281
-0.4014325 -0.4001815 -0.3996798 -0.3859835 -0.3853528
-0.3842236 -0.3777792 -0.3772675 -0.3753611 -0.0171006
0.3146430 0.3370939 0.4646436 0.5169461 0.5674358
0.5778229 0.5907292 0.5989642 0.6157663 0.6271312
0.6313759 0.6466207 0.6743797 0.6842149 0.7657995
0.7879000 0.8086865 0.9365055 0.9539775 0.9760946

1.0142175 1.0453661 1.0988255 1.1164669 1.3602377
1.3890811 1.4004020 1.4562595 1.4875764 1.5310746
1.5858810 1.6338370 1.6854127 1.7567375 1.7931910
1.8671817 1.9109192 1.9572445

0 EIGENVALUES BELOW THE ENERGY -9.000000
*****

```

```

coors: iplus,nv,n=          0          256          255
Matrix size          317
      allocate HS          0.8 MB
      allocate Z          0.8 MB
      allocate spanel          0.3 MB          dimensions          317          128
      allocate hpanel          0.3 MB          dimensions          317          128
      allocate spanelus          0.3 MB          dimensions          317          128
      allocate slen          0.3 MB          dimensions          317          128
      allocate x2          0.3 MB          dimensions          317          128
      allocate legendre          4.0 MB          dimensions          317          13
128
      allocate al,bl (row)          0.1 MB          dimensions          317          11
      allocate al,bl (col)          0.0 MB          dimensions          128          11

```

```

        allocate YL          0.2 MB          dimensions 15 317
3
  number of local orbitals, nlo (hamilt)      62
        allocate YL          0.2 MB          dimensions 15 317
3
        allocate phsc        0.0 MB          dimensions 317
Time for al,bl      (hamilt, cpu/wall) :      0.01      0.01
Time for legendre   (hamilt, cpu/wall) :      0.02      0.02
Time for phase      (hamilt, cpu/wall) :      0.02      0.02
Time for us         (hamilt, cpu/wall) :      0.00      0.00
Time for overlaps   (hamilt, cpu/wall) :      0.00      0.00
Time for distrib    (hamilt, cpu/wall) :      0.00      0.00
Time sum iouter     (hamilt, cpu/wall) :      0.00      0.00
Time for los        (hamilt, cpu/wall) :      0.01      0.01
Time for alm        (hns) :      0.0      0.0
Time for vector     (hns) :      0.0      0.0
Time for vector2    (hns) :      0.0      0.0
Time for VxV        (hns) :      0.0      0.0
        59 Eigenvalues computed
  Seclr4(Cholesky complete (CPU)) :      0.003      3280.30
Mflops
  Seclr4(Transform to eig.problem (CPU)) :      0.007      4544.87
Mflops
  Seclr4(Compute eigenvalues (CPU)) :      0.048      883.85
Mflops
  Seclr4(Backtransform (CPU)) :      0.000      3094.39
Mflops
        TIME HAMILT (CPU) =      0.1, HNS =      0.0, HORB =      0.0,
DIAG =      0.1, SYNC =      0.0
        TIME HAMILT (WALL) =      0.1, HNS =      0.0, HORB =      0.0,
DIAG =      0.1, SYNC =      0.0

K= 0.050000 0.150000 0.250000          7
  MATRIX SIZE 317 WEIGHT=48.00 PGR:
  EIGENVALUES ARE:
-1.9885453 -0.7369076 -0.7336836 -0.7322759 -0.4148885
-0.4132176 -0.4122070 -0.4090138 -0.4067206 -0.4044675
-0.4019192 -0.3992118 -0.3988802 -0.3886334 -0.3871766
-0.3845573 -0.3807662 -0.3801747 -0.3759537 0.0071756
0.2648228 0.3402230 0.4678541 0.5065948 0.5640509
0.5801561 0.5943297 0.5986492 0.6156167 0.6227798
0.6270221 0.6479185 0.6644460 0.6864524 0.7519085
0.7905741 0.8483839 0.9065156 0.9693242 0.9991754

1.0313813 1.0665485 1.0869459 1.1610791 1.3379964
1.3594313 1.4181153 1.4662479 1.5078468 1.5599463
1.5842932 1.6440779 1.6681493 1.7696816 1.8013068
1.8477629 1.8960337 1.9430899 1.9632119
0 EIGENVALUES BELOW THE ENERGY -9.00000
*****
coors: iplus,nv,n=          0          255          256

```

Matrix size	318			
allocate HS	0.8 MB			
allocate Z	0.8 MB			
allocate spanel	0.3 MB	dimensions	318	128
allocate hpanel	0.3 MB	dimensions	318	128
allocate spanelus	0.3 MB	dimensions	318	128
allocate slen	0.3 MB	dimensions	318	128
allocate x2	0.3 MB	dimensions	318	128
allocate legendre	4.0 MB	dimensions	318	13
128				
allocate al,bl (row)	0.1 MB	dimensions	318	11
allocate al,bl (col)	0.0 MB	dimensions	128	11
allocate YL	0.2 MB	dimensions	15	318
3				
number of local orbitals, nlo (hamilt)		62		
allocate YL	0.2 MB	dimensions	15	318
3				
allocate phsc	0.0 MB	dimensions	318	
Time for al,bl (hamilt, cpu/wall) :		0.00	0.00	
Time for legendre (hamilt, cpu/wall) :		0.02	0.02	
Time for phase (hamilt, cpu/wall) :		0.01	0.00	
Time for us (hamilt, cpu/wall) :		0.00	0.00	
Time for overlaps (hamilt, cpu/wall) :		0.01	0.01	
Time for distrib (hamilt, cpu/wall) :		0.01	0.01	
Time sum iouter (hamilt, cpu/wall) :		0.00	0.00	
Time for los (hamilt, cpu/wall) :		0.01	0.01	
Time for alm (hns) :	0.0	0.0		
Time for vector (hns) :	0.0	0.0		
Time for vector2 (hns) :	0.0	0.0		
Time for VxV (hns) :	0.0	0.0		
59 Eigenvalues computed				
Seclr4(Cholesky complete (CPU)) :		0.004	2963.55	
Mflops				
Seclr4(Transform to eig.problem (CPU)) :		0.007	4565.22	
Mflops				
Seclr4(Compute eigenvalues (CPU)) :		0.048	888.32	
Mflops				
Seclr4(Backtransform (CPU)) :		0.000	3180.34	
Mflops				
TIME HAMILT (CPU) =	0.1, HNS =	0.0, HORB =	0.0,	
DIAG =	0.1, SYNC =	0.0		
TIME HAMILT (WALL) =	0.1, HNS =	0.0, HORB =	0.0,	
DIAG =	0.1, SYNC =	0.0		
K=	0.050000 0.150000 0.350000	8		
MATRIX SIZE	318 WEIGHT=48.00 PGR:			
EIGENVALUES ARE:				
-1.9884605	-0.7397754	-0.7339853	-0.7326604	-0.4139909
-0.4103739	-0.4083554	-0.4066016	-0.4034189	-0.4028296
-0.4010999	-0.3980695	-0.3977338	-0.3920323	-0.3896273
-0.3859656	-0.3853644	-0.3834215	-0.3759497	0.0416714
0.2034003	0.3548238	0.4743830	0.4863171	0.5565704

0.5795181	0.5969116	0.6034529	0.6146371	0.6208459
0.6230107	0.6480862	0.6677246	0.6986431	0.7285366
0.8059637	0.8330751	0.9120625	0.9356414	1.0066653

1.0568680	1.0946843	1.1580602	1.2039421	1.3126443
1.3460081	1.4188846	1.4596725	1.5101539	1.5627554
1.5728032	1.6379611	1.7007202	1.7434742	1.8212092
1.8563078	1.8673809	1.9467761	1.9660693	

0 EIGENVALUES BELOW THE ENERGY -9.00000

```

coors: iplus,nv,n=          0          256          253
Matrix size          315
      allocate HS          0.8 MB
      allocate Z           0.8 MB
      allocate spanel      0.3 MB          dimensions 315 128
      allocate hpanel      0.3 MB          dimensions 315 128
      allocate spanelus    0.3 MB          dimensions 315 128
      allocate slen        0.3 MB          dimensions 315 128
      allocate x2          0.3 MB          dimensions 315 128
      allocate legendre    4.0 MB          dimensions 315 13
128
allocate al,bl (row)      0.1 MB          dimensions 315 11
allocate al,bl (col)      0.0 MB          dimensions 128 11
      allocate YL          0.2 MB          dimensions 15 315
3
  number of local orbitals, nlo (hamilt)      62
      allocate YL          0.2 MB          dimensions 15 315
3
      allocate phsc        0.0 MB          dimensions 315
Time for al,bl (hamilt, cpu/wall) :          0.00          0.00
Time for legendre (hamilt, cpu/wall) :          0.02          0.02
Time for phase (hamilt, cpu/wall) :          0.00          0.00
Time for us (hamilt, cpu/wall) :          0.02          0.02
Time for overlaps (hamilt, cpu/wall) :          0.01          0.01
Time for distrib (hamilt, cpu/wall) :          0.00          0.00
Time sum iouter (hamilt, cpu/wall) :          0.00          0.00
Time for los (hamilt, cpu/wall) :          0.01          0.01
Time for alm (hns) :          0.0          0.0
Time for vector (hns) :          0.0          0.0
Time for vector2 (hns) :          0.0          0.0
Time for VxV (hns) :          0.0          0.0
      60 Eigenvalues computed
      Seclr4(Cholesky complete (CPU)) :          0.004          2943.11
Mflops
      Seclr4(Transform to eig.problem (CPU)) :          0.007          4510.23
Mflops
      Seclr4(Compute eigenvalues (CPU)) :          0.048          867.30
Mflops
      Seclr4(Backtransform (CPU)) :          0.000          3107.25
Mflops

```

TIME HAMILT (CPU) = 0.1, HNS = 0.0, HORB = 0.0,
 DIAG = 0.1, SYNC = 0.0
 TIME HAMILT (WALL) = 0.1, HNS = 0.0, HORB = 0.0,
 DIAG = 0.1, SYNC = 0.0

K= 0.050000 0.150000 0.450000 9

MATRIX SIZE 315 WEIGHT=48.00 PGR:

EIGENVALUES ARE:

-1.9884086	-0.7415692	-0.7341532	-0.7328631	-0.4132936
-0.4085915	-0.4056037	-0.4036773	-0.4025090	-0.4004810
-0.3995768	-0.3969712	-0.3959260	-0.3939702	-0.3918247
-0.3906493	-0.3888702	-0.3839566	-0.3758501	0.0825730
0.1479679	0.3673917	0.4690876	0.4764601	0.5590155
0.5752430	0.5969636	0.6083555	0.6143771	0.6197221
0.6218606	0.6491559	0.6717761	0.7085989	0.7336423
0.7805727	0.8344408	0.8908733	0.9429527	0.9698456

1.1045847	1.1521396	1.1839352	1.2665949	1.3070914
1.3432410	1.3793105	1.4258263	1.4524645	1.5335445
1.6405669	1.6701096	1.7275996	1.7701450	1.7917415
1.8343153	1.8488878	1.8976270	1.9644158	1.9988812

0 EIGENVALUES BELOW THE ENERGY -9.00000

coors: iplus,nv,n=	0	253	256
Matrix size	318		
allocate HS	0.8 MB		
allocate Z	0.8 MB		
allocate spanel	0.3 MB	dimensions	318 128
allocate hpanel	0.3 MB	dimensions	318 128
allocate spanelus	0.3 MB	dimensions	318 128
allocate slen	0.3 MB	dimensions	318 128
allocate x2	0.3 MB	dimensions	318 128
allocate legendre	4.0 MB	dimensions	318 13
128			
allocate al,bl (row)	0.1 MB	dimensions	318 11
allocate al,bl (col)	0.0 MB	dimensions	128 11
allocate YL	0.2 MB	dimensions	15 318
3			
number of local orbitals, nlo (hamilt)	62		
allocate YL	0.2 MB	dimensions	15 318
3			
allocate phsc	0.0 MB	dimensions	318
Time for al,bl (hamilt, cpu/wall) :	0.00		0.00
Time for legendre (hamilt, cpu/wall) :	0.02		0.02
Time for phase (hamilt, cpu/wall) :	0.00		0.00
Time for us (hamilt, cpu/wall) :	0.00		0.00
Time for overlaps (hamilt, cpu/wall) :	0.01		0.01
Time for distrib (hamilt, cpu/wall) :	0.00		0.00
Time sum iouter (hamilt, cpu/wall) :	0.00		0.00
Time for los (hamilt, cpu/wall) :	0.01		0.01

Time for alm (hns) : 0.0 0.0
Time for vector (hns) : 0.0 0.0
Time for vector2 (hns) : 0.0 0.0
Time for VxV (hns) : 0.0 0.0

60 Eigenvalues computed
Seclr4(Cholesky complete (CPU)) : 0.004 2985.83
Mflops
Seclr4(Transform to eig.problem (CPU)) : 0.007 4553.59
Mflops
Seclr4(Compute eigenvalues (CPU)) : 0.049 872.66
Mflops
Seclr4(Backtransform (CPU)) : 0.000 3393.42
Mflops
TIME HAMILT (CPU) = 0.1, HNS = 0.0, HORB = 0.0,
DIAG = 0.1, SYNC = 0.0
TIME HAMILT (WALL) = 0.1, HNS = 0.0, HORB = 0.0,
DIAG = 0.1, SYNC = 0.0

K= 0.050000 0.250000 0.250000 10

MATRIX SIZE 318 WEIGHT=24.00 PGR:

EIGENVALUES ARE:

-1.9884680	-0.7374604	-0.7356412	-0.7326585	-0.4130117
-0.4121865	-0.4107914	-0.4074645	-0.4048329	-0.4015948
-0.4011610	-0.3990538	-0.3984324	-0.3916159	-0.3884486
-0.3852714	-0.3822278	-0.3814661	-0.3782866	0.0299646
0.2752364	0.2849415	0.4758874	0.4934338	0.5584571
0.5689416	0.5977491	0.6064281	0.6144786	0.6198513
0.6266034	0.6326341	0.6631193	0.6948641	0.7924228
0.8186886	0.8223027	0.8690295	0.9612392	1.0337463
1.0490053	1.0533931	1.1354313	1.1947762	1.3134988
1.3812448	1.4223228	1.4787452	1.4991156	1.5463846
1.5622697	1.6361179	1.7169387	1.7172340	1.8009029
1.8850898	1.9076473	1.9528175	1.9557580	1.9890130

0 EIGENVALUES BELOW THE ENERGY -9.000000

coors: iplus,nv,n=	0	256	258
Matrix size	320		
allocate HS	0.8 MB		
allocate Z	0.8 MB		
allocate spanel	0.3 MB	dimensions	320 128
allocate hpanel	0.3 MB	dimensions	320 128
allocate spanelus	0.3 MB	dimensions	320 128
allocate slen	0.3 MB	dimensions	320 128
allocate x2	0.3 MB	dimensions	320 128
allocate legendre	4.1 MB	dimensions	320 13
128			
allocate al,bl (row)	0.1 MB	dimensions	320 11
allocate al,bl (col)	0.0 MB	dimensions	128 11

```

        allocate YL          0.2 MB          dimensions 15 320
3
  number of local orbitals, nlo (hamilt)      62
        allocate YL          0.2 MB          dimensions 15 320
3
        allocate phsc        0.0 MB          dimensions 320
Time for al,bl      (hamilt, cpu/wall) :      0.00      0.00
Time for legendre  (hamilt, cpu/wall) :      0.02      0.02
Time for phase     (hamilt, cpu/wall) :      0.00      0.00
Time for us        (hamilt, cpu/wall) :      0.02      0.02
Time for overlaps  (hamilt, cpu/wall) :      0.02      0.00
Time for distrib   (hamilt, cpu/wall) :      0.00      0.00
Time sum iouter    (hamilt, cpu/wall) :      0.00      0.00
Time for los       (hamilt, cpu/wall) :      0.01      0.01
Time for alm       (hns) :      0.0      0.0
Time for vector    (hns) :      0.0      0.0
Time for vector2   (hns) :      0.0      0.0
Time for VxV       (hns) :      0.0      0.0
        59 Eigenvalues computed
  Seclr4(Cholesky complete (CPU)) :      0.003      3406.95
Mflops
  Seclr4(Transform to eig.problem (CPU)) :      0.007      4662.49
Mflops
  Seclr4(Compute eigenvalues (CPU)) :      0.049      893.56
Mflops
  Seclr4(Backtransform (CPU)) :      0.000      3283.48
Mflops
        TIME HAMILT (CPU) =      0.1, HNS =      0.0, HORB =      0.0,
DIAG =      0.1, SYNC =      0.0
        TIME HAMILT (WALL) =      0.1, HNS =      0.0, HORB =      0.0,
DIAG =      0.1, SYNC =      0.0

K= 0.050000 0.250000 0.350000      11
  MATRIX SIZE 320 WEIGHT=48.00 PGR:
  EIGENVALUES ARE:
-1.9883936 -0.7394207 -0.7362505 -0.7330056 -0.4112704
-0.4108175 -0.4078285 -0.4056063 -0.4029549 -0.4016169
-0.3998698 -0.3980029 -0.3963653 -0.3948872 -0.3902436
-0.3864730 -0.3860998 -0.3832412 -0.3794195 0.0618122
0.2207459 0.2977248 0.4631233 0.4873297 0.5563846
0.5721245 0.5980111 0.6093579 0.6132096 0.6175382
0.6234437 0.6297824 0.6666927 0.7128820 0.7666705
0.7797554 0.8509060 0.9011886 0.9374456 1.0233328

1.0811308 1.0901288 1.1672363 1.2236841 1.3173678
1.3735426 1.4250511 1.4676003 1.4999656 1.5357179
1.5727485 1.6575106 1.6858282 1.7365845 1.7672856
1.8418914 1.8942779 1.9588513 1.9684555

0 EIGENVALUES BELOW THE ENERGY -9.00000
*****

coors: iplus,nv,n=      0      258      256

```

```

Matrix size      318
    allocate HS      0.8 MB
    allocate Z        0.8 MB
    allocate spanel   0.3 MB      dimensions 318 128
    allocate hpanel   0.3 MB      dimensions 318 128
    allocate spanelus 0.3 MB      dimensions 318 128
    allocate slen      0.3 MB      dimensions 318 128
    allocate x2        0.3 MB      dimensions 318 128
    allocate legendre  4.0 MB      dimensions 318 13
128
allocate al,bl (row)      0.1 MB      dimensions 318 11
allocate al,bl (col)      0.0 MB      dimensions 128 11
    allocate YL          0.2 MB      dimensions 15 318
3
    number of local orbitals, nlo (hamilt)      62
    allocate YL          0.2 MB      dimensions 15 318
3
    allocate phsc        0.0 MB      dimensions 318
Time for al,bl (hamilt, cpu/wall) :      0.00      0.00
Time for legendre (hamilt, cpu/wall) :      0.02      0.02
Time for phase (hamilt, cpu/wall) :      0.00      0.02
Time for us (hamilt, cpu/wall) :      0.01      0.01
Time for overlaps (hamilt, cpu/wall) :      0.00      0.00
Time for distrib (hamilt, cpu/wall) :      0.00      0.00
Time sum iouter (hamilt, cpu/wall) :      0.00      0.00
Time for los (hamilt, cpu/wall) :      0.01      0.01
Time for alm (hns) :      0.0      0.0
Time for vector (hns) :      0.0      0.0
Time for vector2 (hns) :      0.0      0.0
Time for VxV (hns) :      0.0      0.0
    60 Eigenvalues computed
    Seclr4(Cholesky complete (CPU)) :      0.003      3387.85
Mflops
    Seclr4(Transform to eig.problem (CPU)) :      0.007      4480.00
Mflops
    Seclr4(Compute eigenvalues (CPU)) :      0.050      865.09
Mflops
    Seclr4(Backtransform (CPU)) :      0.001      2889.26
Mflops
    TIME HAMILT (CPU) =      0.0, HNS =      0.0, HORB =      0.0,
DIAG =      0.1, SYNC =      0.0
    TIME HAMILT (WALL) =      0.0, HNS =      0.0, HORB =      0.0,
DIAG =      0.1, SYNC =      0.0

K= 0.050000 0.250000 0.450000      12
    MATRIX SIZE 318 WEIGHT=48.00 PGR:
    EIGENVALUES ARE:
-1.9883425 -0.7408237 -0.7363344 -0.7332125 -0.4102862
-0.4090669 -0.4071758 -0.4028753 -0.4016858 -0.4006477
-0.3997288 -0.3974930 -0.3958477 -0.3943276 -0.3912083
-0.3908295 -0.3872904 -0.3844819 -0.3795227 0.0973327
0.1708661 0.3124933 0.4393021 0.4918207 0.5560397

```

0.5845327	0.5954007	0.6109103	0.6123481	0.6172029
0.6219648	0.6300815	0.6862711	0.7181834	0.7378894
0.7507241	0.8503956	0.9145915	0.9745059	0.9954678

1.0739513	1.1442856	1.1698433	1.2843352	1.3132563
1.3843307	1.4042915	1.4212049	1.4843343	1.5142354
1.6270454	1.6582112	1.7172847	1.7356130	1.8001129
1.8121011	1.8427379	1.8982148	1.9328450	1.9774534

0 EIGENVALUES BELOW THE ENERGY -9.00000

```

coors: iplus,nv,n=          0          256          258
Matrix size          320
      allocate HS          0.8 MB
      allocate Z           0.8 MB
      allocate spanel      0.3 MB          dimensions 320 128
      allocate hpanel      0.3 MB          dimensions 320 128
      allocate spanelus    0.3 MB          dimensions 320 128
      allocate slen        0.3 MB          dimensions 320 128
      allocate x2          0.3 MB          dimensions 320 128
      allocate legendre    4.1 MB          dimensions 320 13
128
      allocate al,bl (row)  0.1 MB          dimensions 320 11
      allocate al,bl (col)  0.0 MB          dimensions 128 11
      allocate YL          0.2 MB          dimensions 15 320
3
  number of local orbitals, nlo (hamilt) 62
      allocate YL          0.2 MB          dimensions 15 320
3
      allocate phsc        0.0 MB          dimensions 320
Time for al,bl (hamilt, cpu/wall) :      0.00      0.00
Time for legendre (hamilt, cpu/wall) :      0.02      0.02
Time for phase (hamilt, cpu/wall) :      0.00      0.01
Time for us (hamilt, cpu/wall) :      0.02      0.02
Time for overlaps (hamilt, cpu/wall) :      0.01      0.02
Time for distrib (hamilt, cpu/wall) :      0.00      0.00
Time sum iouter (hamilt, cpu/wall) :      0.00      0.00
Time for los (hamilt, cpu/wall) :      0.01      0.01
Time for alm (hns) :      0.0      0.0
Time for vector (hns) :      0.0      0.0
Time for vector2 (hns) :      0.0      0.0
Time for VxV (hns) :      0.0      0.0
      61 Eigenvalues computed
      Sec1r4(Cholesky complete (CPU)) :      0.003      3409.07
Mflops
      Sec1r4(Transform to eig.problem (CPU)) :      0.007      4527.84
Mflops
      Sec1r4(Compute eigenvalues (CPU)) :      0.050      874.53
Mflops
      Sec1r4(Backtransform (CPU)) :      0.000      3280.67
Mflops

```

TIME HAMILT (CPU) = 0.1, HNS = 0.0, HORB = 0.0,
 DIAG = 0.1, SYNC = 0.0
 TIME HAMILT (WALL) = 0.1, HNS = 0.0, HORB = 0.0,
 DIAG = 0.1, SYNC = 0.0

K= 0.050000 0.350000 0.350000 13

MATRIX SIZE 320 WEIGHT=24.00 PGR:

EIGENVALUES ARE:

-1.9883209	-0.7393632	-0.7381115	-0.7333405	-0.4107552
-0.4076986	-0.4073235	-0.4036951	-0.4031421	-0.4007010
-0.3987460	-0.3981312	-0.3971336	-0.3937652	-0.3911103
-0.3881911	-0.3866448	-0.3842489	-0.3820763	0.0889123
0.2385377	0.2494286	0.4239573	0.5028899	0.5473166
0.5814811	0.5997241	0.6107860	0.6122610	0.6156825
0.6222434	0.6243846	0.6745013	0.7223844	0.7403585
0.8278897	0.8450761	0.8479942	0.9729740	1.0456956

1.0682512	1.1035890	1.2302622	1.2549389	1.2944399
1.3478152	1.4462400	1.4541476	1.5250241	1.5498792
1.5847251	1.6107715	1.7033979	1.7126484	1.7973649
1.8188728	1.8295688	1.9146347	1.9780522	1.9812152
1.9921159				

0 EIGENVALUES BELOW THE ENERGY -9.00000

coors: iplus,nv,n=	0	258	255
Matrix size	317		
allocate HS	0.8 MB		
allocate Z	0.8 MB		
allocate spanel	0.3 MB	dimensions	317 128
allocate hpanel	0.3 MB	dimensions	317 128
allocate spanelus	0.3 MB	dimensions	317 128
allocate slen	0.3 MB	dimensions	317 128
allocate x2	0.3 MB	dimensions	317 128
allocate legendre	4.0 MB	dimensions	317 13
128			
allocate al,bl (row)	0.1 MB	dimensions	317 11
allocate al,bl (col)	0.0 MB	dimensions	128 11
allocate YL	0.2 MB	dimensions	15 317
3			
number of local orbitals, nlo (hamilt)		62	
allocate YL	0.2 MB	dimensions	15 317
3			
allocate phsc	0.0 MB	dimensions	317
Time for al,bl (hamilt, cpu/wall) :	0.00	0.00	
Time for legendre (hamilt, cpu/wall) :	0.02	0.02	
Time for phase (hamilt, cpu/wall) :	0.00	0.00	
Time for us (hamilt, cpu/wall) :	0.02	0.02	
Time for overlaps (hamilt, cpu/wall) :	0.00	0.00	
Time for distrib (hamilt, cpu/wall) :	0.00	0.00	
Time sum iouter (hamilt, cpu/wall) :	0.00	0.00	
Time for los (hamilt, cpu/wall) :	0.01	0.01	

Time for alm	(hns) :	0.0	0.0
Time for vector	(hns) :	0.0	0.0
Time for vector2	(hns) :	0.0	0.0
Time for VxV	(hns) :	0.0	0.0

61 Eigenvalues computed

Seclr4(Cholesky complete (CPU)) :	0.003	3324.46
Mflops		

Seclr4(Transform to eig.problem (CPU)) :	0.007	4564.41
Mflops		

Seclr4(Compute eigenvalues (CPU)) :	0.049	870.05
Mflops		

Seclr4(Backtransform (CPU)) :	0.000	3260.55
Mflops		

TIME HAMILT (CPU) =	0.1,	HNS =	0.0,	HORB =	0.0,
DIAG =	0.1,	SYNC =	0.0		
TIME HAMILT (WALL) =	0.1,	HNS =	0.0,	HORB =	0.0,
DIAG =	0.1,	SYNC =	0.0		

K= 0.050000 0.350000 0.450000 14

MATRIX SIZE 317 WEIGHT=48.00 PGR:

EIGENVALUES ARE:

-1.9882651	-0.7400839	-0.7383144	-0.7335152	-0.4093475
-0.4078007	-0.4061132	-0.4033781	-0.4005685	-0.4004975
-0.3992086	-0.3967727	-0.3958453	-0.3941485	-0.3916777
-0.3908532	-0.3860945	-0.3849609	-0.3832883	0.1159843
0.2024156	0.2657301	0.3923436	0.5113288	0.5422408
0.5938146	0.5992312	0.6088570	0.6133546	0.6154980
0.6212157	0.6246968	0.6910233	0.7192437	0.7389804
0.7894533	0.8199902	0.8972991	0.9782075	1.0212775

1.0964204	1.1399231	1.2476580	1.2578044	1.3097190
1.3641510	1.4097843	1.4295676	1.5143120	1.5536524
1.6165621	1.6551627	1.6740347	1.7115253	1.7888075
1.8263449	1.8397237	1.8771515	1.9214228	1.9508613
1.9617974				

0 EIGENVALUES BELOW THE ENERGY -9.000000

coors: iplus,nv,n=	0	255	254
Matrix size	316		
allocate HS	0.8 MB		
allocate Z	0.8 MB		
allocate spanel	0.3 MB	dimensions	316 128
allocate hpanel	0.3 MB	dimensions	316 128
allocate spanelus	0.3 MB	dimensions	316 128
allocate slen	0.3 MB	dimensions	316 128
allocate x2	0.3 MB	dimensions	316 128
allocate legendre	4.0 MB	dimensions	316 13
128			
allocate al,bl (row)	0.1 MB	dimensions	316 11
allocate al,bl (col)	0.0 MB	dimensions	128 11


```

        allocate YL          0.2 MB          dimensions  15   316
3
  number of local orbitals, nlo (hamilt)      62
        allocate YL          0.2 MB          dimensions  15   316
3
        allocate phsc        0.0 MB          dimensions  316
Time for al,bl      (hamilt, cpu/wall) :      0.00      0.00
Time for legendre  (hamilt, cpu/wall) :      0.00      0.00
Time for phase     (hamilt, cpu/wall) :      0.00      0.00
Time for us        (hamilt, cpu/wall) :      0.00      0.02
Time for overlaps  (hamilt, cpu/wall) :      0.00      0.00
Time for distrib   (hamilt, cpu/wall) :      0.00      0.00
Time sum iouter    (hamilt, cpu/wall) :      0.00      0.00
Time for los       (hamilt, cpu/wall) :      0.01      0.01
Time for alm       (hns) :      0.0      0.0
Time for vector    (hns) :      0.0      0.0
Time for vector2   (hns) :      0.0      0.0
Time for VxV       (hns) :      0.0      0.0
        62 Eigenvalues computed
  Secclr4(Cholesky complete (CPU)) :      0.003      3363.66
Mflops
  Secclr4(Transform to eig.problem (CPU)) :      0.007      4468.84
Mflops
  Secclr4(Compute eigenvalues (CPU)) :      0.050      846.99
Mflops
  Secclr4(Backtransform (CPU)) :      0.000      3307.20
Mflops
        TIME HAMILT (CPU) =      0.0, HNS =      0.0, HORB =      0.0,
DIAG =      0.1, SYNC =      0.0
        TIME HAMILT (WALL) =      0.0, HNS =      0.0, HORB =      0.0,
DIAG =      0.1, SYNC =      0.0

K=  0.050000  0.450000  0.450000          15
MATRIX SIZE  316  WEIGHT=24.00  PGR:
EIGENVALUES ARE:
-1.9882216  -0.7396936  -0.7394932  -0.7337311  -0.4090732
-0.4083102  -0.4046059  -0.4029837  -0.3998484  -0.3998049
-0.3981960  -0.3964180  -0.3956595  -0.3938299  -0.3926065
-0.3916550  -0.3868132  -0.3850855  -0.3844519   0.1323879
 0.2307178   0.2371313   0.3513760   0.5265856   0.5328624
 0.5997438   0.6017696   0.6041312   0.6144737   0.6147995
 0.6203403   0.6244030   0.6822968   0.7428350   0.7478869
 0.8000044   0.8345182   0.8367296   0.9393408   1.0888199

 1.1402508   1.1632019   1.2010860   1.3004415   1.3208117
 1.3447315   1.3524724   1.4680655   1.5470072   1.5521822
 1.6263778   1.6514912   1.6588566   1.7234061   1.7757508
 1.7843219   1.8243623   1.8727794   1.9017749   1.9483192
 1.9600189   1.9851041

      0 EIGENVALUES BELOW THE ENERGY  -9.00000
*****

```

```

coors: iplus,nv,n=          0          254          257
Matrix size          319
      allocate HS          0.8 MB
      allocate Z           0.8 MB
      allocate spanel      0.3 MB          dimensions 319 128
      allocate hpanel      0.3 MB          dimensions 319 128
      allocate spanelus    0.3 MB          dimensions 319 128
      allocate slen        0.3 MB          dimensions 319 128
      allocate x2          0.3 MB          dimensions 319 128
      allocate legendre    4.0 MB          dimensions 319 13
128
allocate al,bl (row)      0.1 MB          dimensions 319 11
allocate al,bl (col)      0.0 MB          dimensions 128 11
      allocate YL          0.2 MB          dimensions 15 319
3
  number of local orbitals, nlo (hamilt)      62
      allocate YL          0.2 MB          dimensions 15 319
3
      allocate phsc        0.0 MB          dimensions 319
Time for al,bl (hamilt, cpu/wall) :          0.00          0.00
Time for legendre (hamilt, cpu/wall) :          0.02          0.02
Time for phase (hamilt, cpu/wall) :          0.01          0.01
Time for us (hamilt, cpu/wall) :          0.03          0.03
Time for overlaps (hamilt, cpu/wall) :          0.00          0.00
Time for distrib (hamilt, cpu/wall) :          0.00          0.00
Time sum iouter (hamilt, cpu/wall) :          0.00          0.00
Time for los (hamilt, cpu/wall) :          0.01          0.01
Time for alm (hns) :          0.0          0.0
Time for vector (hns) :          0.0          0.0
Time for vector2 (hns) :          0.0          0.0
Time for VxV (hns) :          0.0          0.0
      57 Eigenvalues computed
Seclr4(Cholesky complete (CPU)) :          0.003          3324.30
Mflops
Seclr4(Transform to eig.problem (CPU)) :          0.007          4524.29
Mflops
Seclr4(Compute eigenvalues (CPU)) :          0.039          1122.88
Mflops
Seclr4(Backtransform (CPU)) :          0.001          2526.30
Mflops
      TIME HAMILT (CPU) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.0, SYNC =          0.0
      TIME HAMILT (WALL) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.0, SYNC =          0.0

K= 0.150000 0.150000 0.150000          16
MATRIX SIZE 319 WEIGHT= 8.00 PGR:
EIGENVALUES ARE:
-1.9885851 -0.7349493 -0.7331859 -0.7331859 -0.4153964
-0.4145452 -0.4145452 -0.4083988 -0.4083988 -0.4068034
-0.4017028 -0.3994981 -0.3994981 -0.3875178 -0.3856645
-0.3856645 -0.3787179 -0.3787179 -0.3756935 -0.0048609

```

0.3194375	0.3194375	0.4248020	0.5449822	0.5449822
0.5890467	0.5890467	0.6015703	0.6156737	0.6255990
0.6310510	0.6310510	0.6959182	0.6959182	0.7596065
0.8013572	0.8013572	0.9170192	0.9398796	0.9850882

1.0446632	1.0446632	1.1370972	1.1370972	1.3333478
1.3764149	1.3764149	1.4444736	1.5285889	1.5285889
1.5761803	1.7009317	1.7162493	1.7162493	1.8322969
1.8412459	1.8412459			

0 EIGENVALUES BELOW THE ENERGY -9.00000

```

coors: iplus,nv,n=          0          257          254
Matrix size          316
      allocate HS          0.8 MB
      allocate Z           0.8 MB
      allocate spanel      0.3 MB          dimensions 316 128
      allocate hpanel      0.3 MB          dimensions 316 128
      allocate spanelus    0.3 MB          dimensions 316 128
      allocate slen        0.3 MB          dimensions 316 128
      allocate x2          0.3 MB          dimensions 316 128
      allocate legendre    4.0 MB          dimensions 316 13
128
      allocate al,bl (row)  0.1 MB          dimensions 316 11
      allocate al,bl (col)  0.0 MB          dimensions 128 11
      allocate YL          0.2 MB          dimensions 15 316
3
  number of local orbitals, nlo (hamilt) 62
      allocate YL          0.2 MB          dimensions 15 316
3
      allocate phsc        0.0 MB          dimensions 316
Time for al,bl (hamilt, cpu/wall) :      0.00      0.00
Time for legendre (hamilt, cpu/wall) :      0.02      0.02
Time for phase (hamilt, cpu/wall) :      0.00      0.00
Time for us (hamilt, cpu/wall) :      0.03      0.03
Time for overlaps (hamilt, cpu/wall) :      0.00      0.00
Time for distrib (hamilt, cpu/wall) :      0.00      0.00
Time sum iouter (hamilt, cpu/wall) :      0.00      0.00
Time for los (hamilt, cpu/wall) :      0.01      0.01
Time for alm (hns) :      0.0      0.0
Time for vector (hns) :      0.0      0.0
Time for vector2 (hns) :      0.0      0.0
Time for VxV (hns) :      0.0      0.0
      59 Eigenvalues computed
      Seclr4(Cholesky complete (CPU)) :      0.003      3313.85
Mflops
      Seclr4(Transform to eig.problem (CPU)) :      0.007      4509.72
Mflops
      Seclr4(Compute eigenvalues (CPU)) :      0.048      872.75
Mflops
      Seclr4(Backtransform (CPU)) :      0.000      3081.33
Mflops

```

TIME HAMILT (CPU) = 0.1, HNS = 0.0, HORB = 0.0,
 DIAG = 0.1, SYNC = 0.0
 TIME HAMILT (WALL) = 0.1, HNS = 0.0, HORB = 0.0,
 DIAG = 0.1, SYNC = 0.0

K= 0.150000 0.150000 0.250000 17

MATRIX SIZE 316 WEIGHT=24.00 PGR:

EIGENVALUES ARE:

-1.9884968	-0.7369897	-0.7340975	-0.7332312	-0.4139585
-0.4126805	-0.4125940	-0.4070768	-0.4048753	-0.4038542
-0.4020684	-0.3991608	-0.3984468	-0.3897312	-0.3874920
-0.3857014	-0.3820094	-0.3804596	-0.3762888	0.0187547
0.2712771	0.3280543	0.4224778	0.5132444	0.5529019
0.5900042	0.5990050	0.6027348	0.6150436	0.6226530
0.6254996	0.6325795	0.6929505	0.7091944	0.7666357
0.7780139	0.8289189	0.8821327	0.9732754	1.0055250

1.0281024	1.0779336	1.1466074	1.1938091	1.3182560
1.3345922	1.3871088	1.4454781	1.5153397	1.5971046
1.6065777	1.6560581	1.6586671	1.7645032	1.8112324
1.8441123	1.9076392	1.9249050	1.9364550	

0 EIGENVALUES BELOW THE ENERGY -9.00000

coors: iplus,nv,n=	0	254	258
Matrix size	320		
allocate HS	0.8 MB		
allocate Z	0.8 MB		
allocate spanel	0.3 MB	dimensions	320 128
allocate hpanel	0.3 MB	dimensions	320 128
allocate spanelus	0.3 MB	dimensions	320 128
allocate slen	0.3 MB	dimensions	320 128
allocate x2	0.3 MB	dimensions	320 128
allocate legendre	4.1 MB	dimensions	320 13
128			
allocate al,bl (row)	0.1 MB	dimensions	320 11
allocate al,bl (col)	0.0 MB	dimensions	128 11
allocate YL	0.2 MB	dimensions	15 320
3			
number of local orbitals, nlo (hamilt)	62		
allocate YL	0.2 MB	dimensions	15 320
3			
allocate phsc	0.0 MB	dimensions	320
Time for al,bl (hamilt, cpu/wall) :	0.00	0.00	
Time for legendre (hamilt, cpu/wall) :	0.02	0.02	
Time for phase (hamilt, cpu/wall) :	0.02	0.02	
Time for us (hamilt, cpu/wall) :	0.01	0.01	
Time for overlaps (hamilt, cpu/wall) :	0.01	0.00	
Time for distrib (hamilt, cpu/wall) :	0.00	0.00	
Time sum iouter (hamilt, cpu/wall) :	0.00	0.00	
Time for los (hamilt, cpu/wall) :	0.01	0.01	
Time for alm (hns) :	0.0	0.0	

```

Time for vector      (hns) :          0.0          0.0
Time for vector2     (hns) :          0.0          0.0
Time for VxV         (hns) :          0.0          0.0
      59 Eigenvalues computed
Seclr4(Cholesky complete (CPU)) :          0.003      3507.60
Mflops
Seclr4(Transform to eig.problem (CPU)) :          0.007      4523.47
Mflops
Seclr4(Compute eigenvalues (CPU)) :          0.049      894.33
Mflops
Seclr4(Backtransform (CPU)) :          0.000      3241.20
Mflops
      TIME HAMILT (CPU) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0
      TIME HAMILT (WALL) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0

```

K= 0.150000 0.150000 0.350000 18

MATRIX SIZE 320 WEIGHT=24.00 PGR:

EIGENVALUES ARE:

```

-1.9884246  -0.7395666  -0.7345406  -0.7335252  -0.4130608
-0.4101382  -0.4096245  -0.4058281  -0.4030931  -0.4015597
-0.4002746  -0.3984813  -0.3976777  -0.3928671  -0.3904621
-0.3861891  -0.3856829  -0.3836576  -0.3772518   0.0521023
 0.2122914   0.3379724   0.4412347   0.4856772   0.5458691
 0.5885059   0.6028411   0.6059596   0.6130994   0.6200011
 0.6218728   0.6329439   0.7001652   0.7059641   0.7595734
 0.7724452   0.8046184   0.9446823   0.9614742   0.9753777

```

```

1.0687098  1.0983539  1.2019248  1.2252664  1.2886987
1.2918413  1.4405074  1.4858113  1.5234635  1.5463498
1.5474542  1.6284248  1.7230434  1.7891649  1.8243387
1.8254037  1.8663090  1.8966726  1.9501594

```

0 EIGENVALUES BELOW THE ENERGY -9.00000

```

coors: iplus,nv,n=          0          258          257
Matrix size          319
      allocate HS          0.8 MB
      allocate Z          0.8 MB
      allocate spanel          0.3 MB          dimensions 319 128
      allocate hpanel          0.3 MB          dimensions 319 128
      allocate spanelus          0.3 MB          dimensions 319 128
      allocate slen          0.3 MB          dimensions 319 128
      allocate x2          0.3 MB          dimensions 319 128
      allocate legendre          4.0 MB          dimensions 319 13
128
      allocate al,bl (row)          0.1 MB          dimensions 319 11
      allocate al,bl (col)          0.0 MB          dimensions 128 11
      allocate YL          0.2 MB          dimensions 15 319
3
      number of local orbitals, nlo (hamilt)          62

```

```

        allocate YL          0.2 MB          dimensions 15 319
3
        allocate phsc        0.0 MB          dimensions 319
Time for al,bl (hamilt, cpu/wall) :          0.00          0.00
Time for legendre (hamilt, cpu/wall) :          0.00          0.00
Time for phase (hamilt, cpu/wall) :          0.00          0.00
Time for us (hamilt, cpu/wall) :          0.00          0.00
Time for overlaps (hamilt, cpu/wall) :          0.03          0.03
Time for distrib (hamilt, cpu/wall) :          0.00          0.00
Time sum iouter (hamilt, cpu/wall) :          0.00          0.00
Time for los (hamilt, cpu/wall) :          0.01          0.01
Time for alm (hns) :          0.0          0.0
Time for vector (hns) :          0.0          0.0
Time for vector2 (hns) :          0.0          0.0
Time for VxV (hns) :          0.0          0.0
        61 Eigenvalues computed
        Seclr4(Cholesky complete (CPU)) :          0.003          3214.67
Mflops
        Seclr4(Transform to eig.problem (CPU)) :          0.007          4420.78
Mflops
        Seclr4(Compute eigenvalues (CPU)) :          0.049          881.89
Mflops
        Seclr4(Backtransform (CPU)) :          0.000          3315.93
Mflops
        TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0
        TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0

        K= 0.150000 0.150000 0.450000          19
        MATRIX SIZE 319 WEIGHT=24.00 PGR:
        EIGENVALUES ARE:
        -1.9883724 -0.7411331 -0.7347560 -0.7336019 -0.4123607
        -0.4083428 -0.4060073 -0.4045699 -0.4029746 -0.3996110
        -0.3990124 -0.3985872 -0.3967728 -0.3926759 -0.3923239
        -0.3893069 -0.3886940 -0.3849208 -0.3773088 0.0906726
        0.1594561 0.3453182 0.4607741 0.4698039 0.5337251
        0.5863733 0.6035783 0.6092217 0.6121186 0.6196914
        0.6202776 0.6330843 0.6973085 0.7184152 0.7376759
        0.7820834 0.7974948 0.9353417 0.9373312 1.0160846

        1.0902487 1.1294841 1.2209138 1.2524109 1.2657925
        1.3077662 1.4151423 1.4909539 1.4931094 1.5116347
        1.6187637 1.6226179 1.7323843 1.7460940 1.8170161
        1.8392236 1.8814143 1.9040236 1.9480582 1.9602597
        1.9932226
        0 EIGENVALUES BELOW THE ENERGY -9.00000
        *****

coors: iplus,nv,n=          0          257          258
Matrix size          320
        allocate HS          0.8 MB

```

allocate Z	0.8 MB			
allocate spanel	0.3 MB	dimensions	320	128
allocate hpanel	0.3 MB	dimensions	320	128
allocate spanelus	0.3 MB	dimensions	320	128
allocate slen	0.3 MB	dimensions	320	128
allocate x2	0.3 MB	dimensions	320	128
allocate legendre	4.1 MB	dimensions	320	13
128				
allocate al,bl (row)	0.1 MB	dimensions	320	11
allocate al,bl (col)	0.0 MB	dimensions	128	11
allocate YL	0.2 MB	dimensions	15	320
3				
number of local orbitals, nlo (hamilt)		62		
allocate YL	0.2 MB	dimensions	15	320
3				
allocate phsc	0.0 MB	dimensions	320	
Time for al,bl (hamilt, cpu/wall) :		0.00		0.00
Time for legendre (hamilt, cpu/wall) :		0.02		0.02
Time for phase (hamilt, cpu/wall) :		0.00		0.00
Time for us (hamilt, cpu/wall) :		0.01		0.01
Time for overlaps (hamilt, cpu/wall) :		0.00		0.00
Time for distrib (hamilt, cpu/wall) :		0.00		0.00
Time sum iouter (hamilt, cpu/wall) :		0.00		0.00
Time for los (hamilt, cpu/wall) :		0.01		0.01
Time for alm (hns) :	0.0		0.0	
Time for vector (hns) :	0.0		0.0	
Time for vector2 (hns) :	0.0		0.0	
Time for VxV (hns) :	0.0		0.0	
60 Eigenvalues computed				
Seclr4(Cholesky complete (CPU)) :		0.003		3469.72
Mflops				
Seclr4(Transform to eig.problem (CPU)) :		0.007		4535.36
Mflops				
Seclr4(Compute eigenvalues (CPU)) :		0.049		886.67
Mflops				
Seclr4(Backtransform (CPU)) :		0.000		3467.27
Mflops				
TIME HAMILT (CPU) =	0.1, HNS =	0.0, HORB =		0.0,
DIAG =	0.1, SYNC =	0.0		
TIME HAMILT (WALL) =	0.1, HNS =	0.0, HORB =		0.0,
DIAG =	0.1, SYNC =	0.0		
K=	0.150000 0.250000 0.250000	20		
MATRIX SIZE	320 WEIGHT=24.00	PGR:		
EIGENVALUES ARE:				
-1.9884246	-0.7376030	-0.7354499	-0.7337824	-0.4127147
-0.4120628	-0.4116693	-0.4048295	-0.4040600	-0.4024854
-0.4007337	-0.3987211	-0.3980991	-0.3926923	-0.3886232
-0.3867788	-0.3830091	-0.3828082	-0.3775420	0.0409327
0.2777315	0.2905326	0.4147288	0.4973960	0.5369975
0.5957342	0.6039302	0.6066640	0.6122833	0.6202807
0.6240931	0.6258104	0.7040351	0.7245236	0.7524336

0.8071691	0.8290188	0.8514296	0.9874613	1.0014519
1.0447980	1.1033174	1.2032112	1.2151420	1.2749306
1.3607216	1.3638213	1.4162877	1.5825649	1.5865343
1.5924788	1.6309165	1.7010750	1.7379415	1.7649004
1.8530464	1.9028562	1.9483990	1.9548924	1.9861932

0 EIGENVALUES BELOW THE ENERGY -9.00000

```

Matrix size          320
    allocate HS          0.8 MB
    allocate Z           0.8 MB
    allocate spanel      0.3 MB      dimensions 320 128
    allocate hpanel      0.3 MB      dimensions 320 128
    allocate spanelus    0.3 MB      dimensions 320 128
    allocate slen        0.3 MB      dimensions 320 128
    allocate x2          0.3 MB      dimensions 320 128
    allocate legendre    4.1 MB      dimensions 320 13
128
allocate al,bl (row)    0.1 MB      dimensions 320 11
allocate al,bl (col)    0.0 MB      dimensions 128 11
    allocate YL          0.2 MB      dimensions 15 320
3
  number of local orbitals, nlo (hamilt) 62
    allocate YL          0.2 MB      dimensions 15 320
3
    allocate phsc        0.0 MB      dimensions 320
Time for al,bl (hamilt, cpu/wall) :      0.00      0.00
Time for legendre (hamilt, cpu/wall) :      0.00      0.00
Time for phase (hamilt, cpu/wall) :      0.00      0.00
Time for us (hamilt, cpu/wall) :      0.00      0.00
Time for overlaps (hamilt, cpu/wall) :      0.02      0.00
Time for distrib (hamilt, cpu/wall) :      0.00      0.00
Time sum iouter (hamilt, cpu/wall) :      0.00      0.00
Time for los (hamilt, cpu/wall) :      0.01      0.01
Time for alm (hns) :      0.0      0.0
Time for vector (hns) :      0.0      0.0
Time for vector2 (hns) :      0.0      0.0
Time for VxV (hns) :      0.0      0.0
    60 Eigenvalues computed
    Seclr4(Cholesky complete (CPU)) :      0.003      3457.63
Mflops
    Seclr4(Transform to eig.problem (CPU)) :      0.007      4604.19
Mflops
    Seclr4(Compute eigenvalues (CPU)) :      0.049      885.02
Mflops
    Seclr4(Backtransform (CPU)) :      0.000      3459.46
Mflops
    TIME HAMILT (CPU) =      0.0, HNS =      0.0, HORB =      0.0,
DIAG =      0.1, SYNC =      0.0

```


TIME HAMILT (WALL) = 0.0, HNS = 0.0, HORB = 0.0,
 DIAG = 0.1, SYNC = 0.0

K= 0.150000 0.250000 0.350000 21

MATRIX SIZE 320 WEIGHT=48.00 PGR:

EIGENVALUES ARE:

-1.9883508	-0.7391715	-0.7361555	-0.7339442	-0.4112706
-0.4108027	-0.4092717	-0.4047522	-0.4032625	-0.4004631
-0.3986645	-0.3982767	-0.3969766	-0.3949481	-0.3905539
-0.3871573	-0.3859253	-0.3841604	-0.3786884	0.0717960
0.2286693	0.2972186	0.4318363	0.4724849	0.5280251
0.5982969	0.6046202	0.6089242	0.6108084	0.6180948
0.6216063	0.6256408	0.6976908	0.7252843	0.7398039
0.7865827	0.8423391	0.9161553	0.9488236	1.0185622
1.0636064	1.1375593	1.2159647	1.2348792	1.2521170
1.3425589	1.4009937	1.4725305	1.5309019	1.5546181
1.5919780	1.6243854	1.7150784	1.7333632	1.7912375
1.8440027	1.8756831	1.9091471	1.9429332	1.9480584

0 EIGENVALUES BELOW THE ENERGY -9.000000

coors: iplus,nv,n=	0	258	260
Matrix size	322		
allocate HS	0.8 MB		
allocate Z	0.8 MB		
allocate spanel	0.3 MB	dimensions	322 128
allocate hpanel	0.3 MB	dimensions	322 128
allocate spanelus	0.3 MB	dimensions	322 128
allocate slen	0.3 MB	dimensions	322 128
allocate x2	0.3 MB	dimensions	322 128
allocate legendre	4.1 MB	dimensions	322 13
128			
allocate al,bl (row)	0.1 MB	dimensions	322 11
allocate al,bl (col)	0.0 MB	dimensions	128 11
allocate YL	0.2 MB	dimensions	15 322
3			
number of local orbitals, nlo (hamilt)	62		
allocate YL	0.2 MB	dimensions	15 322
3			
allocate phsc	0.0 MB	dimensions	322
Time for al,bl (hamilt, cpu/wall) :	0.00	0.00	
Time for legendre (hamilt, cpu/wall) :	0.00	0.00	
Time for phase (hamilt, cpu/wall) :	0.00	0.00	
Time for us (hamilt, cpu/wall) :	0.00	0.00	
Time for overlaps (hamilt, cpu/wall) :	0.00	0.01	
Time for distrib (hamilt, cpu/wall) :	0.00	0.00	
Time sum iouter (hamilt, cpu/wall) :	0.00	0.00	
Time for los (hamilt, cpu/wall) :	0.01	0.01	
Time for alm (hns) :	0.0	0.0	
Time for vector (hns) :	0.0	0.0	

```

Time for vector2      (hns) :          0.0          0.0
Time for VxV          (hns) :          0.0          0.0
      61 Eigenvalues computed
Seclr4(Cholesky complete (CPU)) :          0.005      2191.56
Mflops
Seclr4(Transform to eig.problem (CPU)) :          0.008      4153.03
Mflops
Seclr4(Compute eigenvalues (CPU)) :          0.050      884.20
Mflops
Seclr4(Backtransform (CPU)) :          0.002      1016.84
Mflops
      TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0
      TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0

```

K= 0.150000 0.250000 0.450000 22

MATRIX SIZE 322 WEIGHT=48.00 PGR:

EIGENVALUES ARE:

```

-1.9883055 -0.7403683 -0.7363571 -0.7340570 -0.4104845
-0.4087561 -0.4071449 -0.4051842 -0.4021858 -0.4007034
-0.3992556 -0.3979131 -0.3968980 -0.3938397 -0.3910635
-0.3891663 -0.3873397 -0.3854545 -0.3795364 0.1056226
0.1812219 0.3061048 0.4450055 0.4663181 0.5126486
0.5996095 0.6044365 0.6064010 0.6116953 0.6174955
0.6199652 0.6254080 0.6841113 0.7305784 0.7487861
0.7598887 0.8563897 0.9135007 0.9781191 1.0200594

1.0882682 1.1401614 1.1979609 1.2284359 1.3048746
1.3379202 1.4145648 1.4614463 1.5126023 1.5443801
1.6113421 1.6493000 1.6755407 1.7320650 1.7978404
1.8439985 1.8605459 1.8921099 1.9252235 1.9553619
1.9896750

```

0 EIGENVALUES BELOW THE ENERGY -9.00000

```

coors: iplus,nv,n=          0          260          262
Matrix size          324
      allocate HS          0.8 MB
      allocate Z          0.8 MB
      allocate spanel          0.3 MB          dimensions 324 128
      allocate hpanel          0.3 MB          dimensions 324 128
      allocate spanelus          0.3 MB          dimensions 324 128
      allocate slen          0.3 MB          dimensions 324 128
      allocate x2          0.3 MB          dimensions 324 128
      allocate legendre          4.1 MB          dimensions 324 13
128
      allocate al,bl (row)          0.1 MB          dimensions 324 11
      allocate al,bl (col)          0.0 MB          dimensions 128 11
      allocate YL          0.2 MB          dimensions 15 324
3
      number of local orbitals, nlo (hamilt)          62

```

```

        allocate YL          0.2 MB          dimensions 15 324
3
        allocate phsc        0.0 MB          dimensions 324
Time for al,bl (hamilt, cpu/wall) :          0.00          0.00
Time for legendre (hamilt, cpu/wall) :          0.02          0.02
Time for phase (hamilt, cpu/wall) :          0.00          0.00
Time for us (hamilt, cpu/wall) :          0.00          0.00
Time for overlaps (hamilt, cpu/wall) :          0.02          0.00
Time for distrib (hamilt, cpu/wall) :          0.00          0.00
Time sum iouter (hamilt, cpu/wall) :          0.00          0.00
Time for los (hamilt, cpu/wall) :          0.01          0.01
Time for alm (hns) :          0.0          0.0
Time for vector (hns) :          0.0          0.0
Time for vector2 (hns) :          0.0          0.0
Time for VxV (hns) :          0.0          0.0
        61 Eigenvalues computed
        Seclr4(Cholesky complete (CPU)) :          0.003          3420.03
Mflops
        Seclr4(Transform to eig.problem (CPU)) :          0.008          4299.36
Mflops
        Seclr4(Compute eigenvalues (CPU)) :          0.051          895.32
Mflops
        Seclr4(Backtransform (CPU)) :          0.002          1025.55
Mflops
        TIME HAMILT (CPU) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0
        TIME HAMILT (WALL) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0

        K= 0.150000 0.350000 0.350000          23
        MATRIX SIZE 324 WEIGHT=24.00 PGR:
        EIGENVALUES ARE:
-1.9882881 -0.7391008 -0.7377484 -0.7342492 -0.4106413
-0.4089377 -0.4084035 -0.4050063 -0.4037491 -0.3996482
-0.3988044 -0.3978891 -0.3968258 -0.3953116 -0.3910498
-0.3872417 -0.3869600 -0.3854712 -0.3804631 0.0983851
0.2475070 0.2500417 0.4206480 0.4669060 0.5236176
0.6005493 0.6019183 0.6050903 0.6128716 0.6161770
0.6203908 0.6221055 0.6697155 0.7241175 0.7432084
0.8323267 0.8571925 0.9170908 0.9204489 1.0655677

1.0906196 1.0921464 1.2263379 1.2641537 1.2761699
1.3628391 1.3985078 1.4606513 1.5064074 1.5637298
1.5869036 1.6596969 1.6880510 1.7033094 1.7991764
1.8361172 1.8696920 1.8890881 1.9116531 1.9348201
1.9622520
        0 EIGENVALUES BELOW THE ENERGY -9.00000
        *****

coors: iplus,nv,n=          0          262          260
Matrix size          322
        allocate HS          0.8 MB

```

allocate Z	0.8 MB			
allocate spanel	0.3 MB	dimensions	322	128
allocate hpanel	0.3 MB	dimensions	322	128
allocate spanelus	0.3 MB	dimensions	322	128
allocate slen	0.3 MB	dimensions	322	128
allocate x2	0.3 MB	dimensions	322	128
allocate legendre	4.1 MB	dimensions	322	13
128				
allocate al,bl (row)	0.1 MB	dimensions	322	11
allocate al,bl (col)	0.0 MB	dimensions	128	11
allocate YL	0.2 MB	dimensions	15	322
3				
number of local orbitals, nlo (hamilt)		62		
allocate YL	0.2 MB	dimensions	15	322
3				
allocate phsc	0.0 MB	dimensions	322	
Time for al,bl (hamilt, cpu/wall) :		0.00		0.00
Time for legendre (hamilt, cpu/wall) :		0.00		0.00
Time for phase (hamilt, cpu/wall) :		0.01		0.01
Time for us (hamilt, cpu/wall) :		0.01		0.01
Time for overlaps (hamilt, cpu/wall) :		0.00		0.00
Time for distrib (hamilt, cpu/wall) :		0.00		0.00
Time sum iouter (hamilt, cpu/wall) :		0.00		0.00
Time for los (hamilt, cpu/wall) :		0.01		0.01
Time for alm (hns) :	0.0		0.0	
Time for vector (hns) :	0.0		0.0	
Time for vector2 (hns) :	0.0		0.0	
Time for VxV (hns) :	0.0		0.0	
61 Eigenvalues computed				
Seclr4(Cholesky complete (CPU)) :		0.003		3417.92
Mflops				
Seclr4(Transform to eig.problem (CPU)) :		0.008		4250.86
Mflops				
Seclr4(Compute eigenvalues (CPU)) :		0.050		885.25
Mflops				
Seclr4(Backtransform (CPU)) :		0.002		1018.15
Mflops				
TIME HAMILT (CPU) =	0.0, HNS =	0.0, HORB =		0.0,
DIAG =	0.1, SYNC =	0.0		
TIME HAMILT (WALL) =	0.0, HNS =	0.0, HORB =		0.0,
DIAG =	0.1, SYNC =	0.0		
K=	0.150000 0.350000 0.450000		24	
MATRIX SIZE	322	WEIGHT=48.00	PGR:	
EIGENVALUES ARE:				
-1.9882389	-0.7396558	-0.7380741	-0.7343130	-0.4094050
-0.4084058	-0.4073054	-0.4060903	-0.4027786	-0.4000921
-0.3997249	-0.3977406	-0.3959282	-0.3952102	-0.3907481
-0.3889291	-0.3862522	-0.3856636	-0.3814643	0.1250612
0.2096291	0.2649823	0.4014119	0.4829383	0.5150392
0.5909954	0.6039225	0.6054502	0.6135496	0.6157161
0.6193619	0.6215766	0.6528940	0.7411756	0.7489763

```

0.8069394    0.8802034    0.8966470    0.9653774    1.0319146

1.1028389    1.1409428    1.1944399    1.2612476    1.3247422
1.3814240    1.3979031    1.4456612    1.4933012    1.5628710
1.5830653    1.6550695    1.6906727    1.7123425    1.8039994
1.8235657    1.8460931    1.8556271    1.8937609    1.9241043
1.9962676

      0 EIGENVALUES BELOW THE ENERGY  -9.00000
*****

coors: iplus,nv,n=          0          260          259
Matrix size          321
      allocate HS          0.8 MB
      allocate Z          0.8 MB
      allocate spanel      0.3 MB          dimensions 321 128
      allocate hpanel      0.3 MB          dimensions 321 128
      allocate spanelus    0.3 MB          dimensions 321 128
      allocate slen        0.3 MB          dimensions 321 128
      allocate x2          0.3 MB          dimensions 321 128
      allocate legendre    4.1 MB          dimensions 321 13
128
allocate al,bl (row)      0.1 MB          dimensions 321 11
allocate al,bl (col)      0.0 MB          dimensions 128 11
      allocate YL          0.2 MB          dimensions 15 321
3
  number of local orbitals, nlo (hamilt) 62
      allocate YL          0.2 MB          dimensions 15 321
3
      allocate phsc        0.0 MB          dimensions 321
Time for al,bl (hamilt, cpu/wall) :      0.00      0.00
Time for legendre (hamilt, cpu/wall) :      0.02      0.02
Time for phase (hamilt, cpu/wall) :      0.02      0.02
Time for us (hamilt, cpu/wall) :      0.03      0.02
Time for overlaps (hamilt, cpu/wall) :      0.00      0.00
Time for distrib (hamilt, cpu/wall) :      0.00      0.00
Time sum iouter (hamilt, cpu/wall) :      0.00      0.00
Time for los (hamilt, cpu/wall) :      0.01      0.01
Time for alm (hns) :      0.0      0.0
Time for vector (hns) :      0.0      0.0
Time for vector2 (hns) :      0.0      0.0
Time for VxV (hns) :      0.0      0.0
      61 Eigenvalues computed
Seclr4(Cholesky complete (CPU)) :      0.003      3482.43
Mflops
Seclr4(Transform to eig.problem (CPU)) :      0.008      4207.63
Mflops
Seclr4(Compute eigenvalues (CPU)) :      0.049      891.99
Mflops
Seclr4(Backtransform (CPU)) :      0.002      1013.14
Mflops
      TIME HAMILT (CPU) =      0.1, HNS =      0.0, HORB =      0.0,
DIAG =      0.1, SYNC =      0.0

```

TIME HAMILT (WALL) = 0.1, HNS = 0.0, HORB = 0.0,
 DIAG = 0.1, SYNC = 0.0

K= 0.150000 0.450000 0.450000 25

MATRIX SIZE 321 WEIGHT=24.00 PGR:

EIGENVALUES ARE:

-1.9881959	-0.7392916	-0.7390171	-0.7344497	-0.4091349
-0.4085727	-0.4071549	-0.4046415	-0.4028669	-0.3994632
-0.3992180	-0.3990201	-0.3975775	-0.3935883	-0.3903821
-0.3893863	-0.3857645	-0.3848503	-0.3831170	0.1428367
0.2332603	0.2366412	0.3667793	0.5042714	0.5163816
0.5683970	0.6055291	0.6060748	0.6145810	0.6151999
0.6186537	0.6211137	0.6412166	0.7519844	0.7605785
0.8483867	0.8522471	0.8766646	0.9579599	1.0443435

1.1372261	1.1659175	1.1735000	1.3046767	1.3066328
1.3435024	1.4273923	1.4619012	1.5031248	1.5592612
1.6065352	1.6073054	1.6558853	1.7113919	1.7865194
1.8197917	1.8492676	1.8620691	1.8743534	1.9543427
1.9789477				

0 EIGENVALUES BELOW THE ENERGY -9.000000

coors: iplus,nv,n=	0	259	251
Matrix size	313		
allocate HS	0.7 MB		
allocate Z	0.7 MB		
allocate spanel	0.3 MB	dimensions	313 128
allocate hpanel	0.3 MB	dimensions	313 128
allocate spanelus	0.3 MB	dimensions	313 128
allocate slen	0.3 MB	dimensions	313 128
allocate x2	0.3 MB	dimensions	313 128
allocate legendre	4.0 MB	dimensions	313 13
128			
allocate al,bl (row)	0.1 MB	dimensions	313 11
allocate al,bl (col)	0.0 MB	dimensions	128 11
allocate YL	0.2 MB	dimensions	15 313
3			
number of local orbitals, nlo (hamilt)	62		
allocate YL	0.2 MB	dimensions	15 313
3			
allocate phsc	0.0 MB	dimensions	313
Time for al,bl (hamilt, cpu/wall) :	0.00	0.00	
Time for legendre (hamilt, cpu/wall) :	0.02	0.02	
Time for phase (hamilt, cpu/wall) :	0.02	0.02	
Time for us (hamilt, cpu/wall) :	0.00	0.00	
Time for overlaps (hamilt, cpu/wall) :	0.01	0.00	
Time for distrib (hamilt, cpu/wall) :	0.00	0.00	
Time sum iouter (hamilt, cpu/wall) :	0.00	0.00	
Time for los (hamilt, cpu/wall) :	0.01	0.01	
Time for alm (hns) :	0.0	0.0	
Time for vector (hns) :	0.0	0.0	

```

Time for vector2      (hns) :          0.0          0.0
Time for VxV          (hns) :          0.0          0.0
      60 Eigenvalues computed
Seclr4(Cholesky complete (CPU)) :          0.003      3291.93
Mflops
Seclr4(Transform to eig.problem (CPU)) :          0.007      4466.11
Mflops
Seclr4(Compute eigenvalues (CPU)) :          0.039      1052.72
Mflops
Seclr4(Backtransform (CPU)) :          0.000      3126.67
Mflops
      TIME HAMILT (CPU) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.0, SYNC =          0.0
      TIME HAMILT (WALL) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.0, SYNC =          0.0

```

```

K= 0.250000 0.250000 0.250000          26
MATRIX SIZE 313 WEIGHT= 8.00 PGR:
EIGENVALUES ARE:
-1.9883409 -0.7379322 -0.7351410 -0.7351410 -0.4120775
-0.4111602 -0.4111602 -0.4048659 -0.4019204 -0.4019204
-0.3987546 -0.3978896 -0.3978896 -0.3944311 -0.3882164
-0.3882164 -0.3838170 -0.3838170 -0.3766154 0.0618519
0.2819554 0.2819554 0.3808486 0.5035038 0.5035038
0.6072120 0.6073004 0.6079558 0.6079558 0.6220259
0.6226966 0.6226966 0.6981123 0.7550627 0.7550627
0.8267044 0.8267044 0.8270938 1.0076621 1.0283625

1.0283625 1.1265665 1.2423969 1.2585081 1.2585081
1.3437921 1.3437921 1.3793949 1.5495106 1.6216381
1.6216381 1.7126583 1.7126583 1.7147910 1.7551723
1.7551723 1.8295036 1.9641586 1.9684679 1.9684679

```

```

      0 EIGENVALUES BELOW THE ENERGY -9.00000
*****

```

```

coors: iplus,nv,n=          0          251          259
Matrix size          321
      allocate HS          0.8 MB
      allocate Z          0.8 MB
      allocate spanel          0.3 MB          dimensions 321 128
      allocate hpanel          0.3 MB          dimensions 321 128
      allocate spanelus          0.3 MB          dimensions 321 128
      allocate slen          0.3 MB          dimensions 321 128
      allocate x2          0.3 MB          dimensions 321 128
      allocate legendre          4.1 MB          dimensions 321 13
128
      allocate al,bl (row)          0.1 MB          dimensions 321 11
      allocate al,bl (col)          0.0 MB          dimensions 128 11
      allocate YL          0.2 MB          dimensions 15 321
3
number of local orbitals, nlo (hamilt)          62

```

```

        allocate YL          0.2 MB          dimensions 15 321
3
        allocate phsc        0.0 MB          dimensions 321
Time for al,bl (hamilt, cpu/wall) :          0.00          0.00
Time for legendre (hamilt, cpu/wall) :          0.02          0.02
Time for phase (hamilt, cpu/wall) :          0.02          0.02
Time for us (hamilt, cpu/wall) :          0.02          0.02
Time for overlaps (hamilt, cpu/wall) :          0.00          0.00
Time for distrib (hamilt, cpu/wall) :          0.00          0.00
Time sum iouter (hamilt, cpu/wall) :          0.00          0.00
Time for los (hamilt, cpu/wall) :          0.01          0.01
Time for alm (hns) :          0.0          0.0
Time for vector (hns) :          0.0          0.0
Time for vector2 (hns) :          0.0          0.0
Time for VxV (hns) :          0.0          0.0
        61 Eigenvalues computed
        Seclr4(Cholesky complete (CPU)) :          0.003          3419.79
Mflops
        Seclr4(Transform to eig.problem (CPU)) :          0.008          4236.73
Mflops
        Seclr4(Compute eigenvalues (CPU)) :          0.050          887.61
Mflops
        Seclr4(Backtransform (CPU)) :          0.002          1013.79
Mflops
        TIME HAMILT (CPU) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0
        TIME HAMILT (WALL) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0

        K= 0.250000 0.250000 0.350000          27
        MATRIX SIZE 321 WEIGHT=24.00 PGR:
        EIGENVALUES ARE:
        -1.9882843 -0.7388523 -0.7363150 -0.7350678 -0.4110412
        -0.4102405 -0.4098756 -0.4058347 -0.4023058 -0.4003676
        -0.3985607 -0.3984036 -0.3965909 -0.3962846 -0.3898448
        -0.3878234 -0.3858292 -0.3848800 -0.3784675 0.0907094
        0.2413598 0.2862157 0.3970671 0.4780942 0.5002572
        0.5955997 0.6072037 0.6080380 0.6114769 0.6181075
        0.6200999 0.6223892 0.6625205 0.7526886 0.7779316
        0.8124189 0.8229561 0.8956819 1.0048227 1.0231663

        1.0559579 1.1318800 1.2494685 1.2566140 1.2632341
        1.3188732 1.3861148 1.4259920 1.5297868 1.5886924
        1.5946099 1.6830556 1.7157607 1.7159129 1.7807533
        1.8017995 1.8098500 1.9067971 1.9319735 1.9349320
        1.9831134
        0 EIGENVALUES BELOW THE ENERGY -9.00000
        *****

coors: iplus,nv,n=          0          259          257
Matrix size          319
        allocate HS          0.8 MB

```


allocate Z	0.8 MB			
allocate spanel	0.3 MB	dimensions	319	128
allocate hpanel	0.3 MB	dimensions	319	128
allocate spanelus	0.3 MB	dimensions	319	128
allocate slen	0.3 MB	dimensions	319	128
allocate x2	0.3 MB	dimensions	319	128
allocate legendre	4.0 MB	dimensions	319	13
128				
allocate al,bl (row)	0.1 MB	dimensions	319	11
allocate al,bl (col)	0.0 MB	dimensions	128	11
allocate YL	0.2 MB	dimensions	15	319
3				
number of local orbitals, nlo (hamilt)		62		
allocate YL	0.2 MB	dimensions	15	319
3				
allocate phsc	0.0 MB	dimensions	319	
Time for al,bl (hamilt, cpu/wall) :		0.00		0.00
Time for legendre (hamilt, cpu/wall) :		0.00		0.00
Time for phase (hamilt, cpu/wall) :		0.02		0.02
Time for us (hamilt, cpu/wall) :		0.02		0.02
Time for overlaps (hamilt, cpu/wall) :		0.00		0.00
Time for distrib (hamilt, cpu/wall) :		0.00		0.00
Time sum iouter (hamilt, cpu/wall) :		0.00		0.00
Time for los (hamilt, cpu/wall) :		0.01		0.01
Time for alm (hns) :	0.0		0.0	
Time for vector (hns) :	0.0		0.0	
Time for vector2 (hns) :	0.0		0.0	
Time for VxV (hns) :	0.0		0.0	
62 Eigenvalues computed				
Seclr4(Cholesky complete (CPU)) :		0.003		3373.00
Mflops				
Seclr4(Transform to eig.problem (CPU)) :		0.007		4519.25
Mflops				
Seclr4(Compute eigenvalues (CPU)) :		0.050		872.56
Mflops				
Seclr4(Backtransform (CPU)) :		0.000		3199.38
Mflops				
TIME HAMILT (CPU) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	0.1, SYNC =	0.0		
TIME HAMILT (WALL) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	0.1, SYNC =	0.0		
K=	0.250000 0.250000 0.450000	28		
MATRIX SIZE	319	WEIGHT=24.00	PGR:	
EIGENVALUES ARE:				
-1.9882384	-0.7396498	-0.7366840	-0.7348887	-0.4101378
-0.4086037	-0.4075614	-0.4070006	-0.4025826	-0.4024389
-0.3986652	-0.3985624	-0.3954991	-0.3954435	-0.3894719
-0.3877709	-0.3867877	-0.3854020	-0.3790987	0.1212808
0.1995023	0.2890682	0.4351256	0.4647108	0.4754847
0.5859646	0.6072969	0.6088994	0.6133156	0.6169797
0.6188188	0.6231049	0.6478358	0.7496332	0.7884081

```

0.8053852    0.8237447    0.9389033    0.9894763    1.0347096

1.1021177    1.1065240    1.2235797    1.2407067    1.2886324
1.3426027    1.4119427    1.4286001    1.5463219    1.5630989
1.6025693    1.6627163    1.6741001    1.7207944    1.7407642
1.8259679    1.8662383    1.8772844    1.9030558    1.9236042
1.9820964    1.9963516

      0 EIGENVALUES BELOW THE ENERGY  -9.00000
*****

coors: iplus,nv,n=          0          257          259
Matrix size          321
      allocate HS          0.8 MB
      allocate Z          0.8 MB
      allocate spanel      0.3 MB          dimensions 321 128
      allocate hpanel      0.3 MB          dimensions 321 128
      allocate spanelus    0.3 MB          dimensions 321 128
      allocate slen        0.3 MB          dimensions 321 128
      allocate x2          0.3 MB          dimensions 321 128
      allocate legendre    4.1 MB          dimensions 321 13
128
allocate al,bl (row)      0.1 MB          dimensions 321 11
allocate al,bl (col)      0.0 MB          dimensions 128 11
      allocate YL          0.2 MB          dimensions 15 321
3
  number of local orbitals, nlo (hamilt)      62
      allocate YL          0.2 MB          dimensions 15 321
3
      allocate phsc          0.0 MB          dimensions 321
Time for al,bl (hamilt, cpu/wall) :          0.00          0.00
Time for legendre (hamilt, cpu/wall) :          0.02          0.02
Time for phase (hamilt, cpu/wall) :          0.00          0.00
Time for us (hamilt, cpu/wall) :          0.02          0.02
Time for overlaps (hamilt, cpu/wall) :          0.00          0.00
Time for distrib (hamilt, cpu/wall) :          0.00          0.00
Time sum iouter (hamilt, cpu/wall) :          0.00          0.00
Time for los (hamilt, cpu/wall) :          0.01          0.01
Time for alm (hns) :          0.0          0.0
Time for vector (hns) :          0.0          0.0
Time for vector2 (hns) :          0.0          0.0
Time for VxV (hns) :          0.0          0.0
      62 Eigenvalues computed
      Seclr4(Cholesky complete (CPU)) :          0.003          3421.91
Mflops
      Seclr4(Transform to eig.problem (CPU)) :          0.008          4143.32
Mflops
      Seclr4(Compute eigenvalues (CPU)) :          0.050          881.22
Mflops
      Seclr4(Backtransform (CPU)) :          0.002          1025.78
Mflops
      TIME HAMILT (CPU) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0

```

TIME HAMILT (WALL) = 0.1, HNS = 0.0, HORB = 0.0,
 DIAG = 0.1, SYNC = 0.0

K= 0.250000 0.350000 0.350000 29

MATRIX SIZE 321 WEIGHT=24.00 PGR:

EIGENVALUES ARE:

-1.9882215	-0.7387215	-0.7371535	-0.7353881	-0.4104511
-0.4096347	-0.4092246	-0.4072013	-0.4032780	-0.3996869
-0.3995564	-0.3985657	-0.3982493	-0.3947419	-0.3893512
-0.3877759	-0.3855893	-0.3851870	-0.3790165	0.1163725
0.2510264	0.2576690	0.3974188	0.4645272	0.4971187
0.5666434	0.6087300	0.6099160	0.6133605	0.6167703
0.6185557	0.6204502	0.6405783	0.7687327	0.7730993
0.8376999	0.8688183	0.8752244	0.9980097	1.0687725

1.0777592	1.0882189	1.2277147	1.2934277	1.3057232
1.3473869	1.3608323	1.4154932	1.5187089	1.5897370
1.6039204	1.6430301	1.6913358	1.7439122	1.7553322
1.7769307	1.8223655	1.8764348	1.9056612	1.9426873
1.9692180	1.9733813			

0 EIGENVALUES BELOW THE ENERGY -9.000000

coors: iplus,nv,n=	0	259	263
Matrix size	325		
allocate HS	0.8 MB		
allocate Z	0.8 MB		
allocate spanel	0.3 MB	dimensions	325 128
allocate hpanel	0.3 MB	dimensions	325 128
allocate spanelus	0.3 MB	dimensions	325 128
allocate slen	0.3 MB	dimensions	325 128
allocate x2	0.3 MB	dimensions	325 128
allocate legendre	4.1 MB	dimensions	325 13
128			
allocate al,bl (row)	0.1 MB	dimensions	325 11
allocate al,bl (col)	0.0 MB	dimensions	128 11
allocate YL	0.2 MB	dimensions	15 325
3			
number of local orbitals, nlo (hamilt)	62		
allocate YL	0.2 MB	dimensions	15 325
3			
allocate phsc	0.0 MB	dimensions	325
Time for al,bl (hamilt, cpu/wall) :	0.00	0.00	
Time for legendre (hamilt, cpu/wall) :	0.02	0.02	
Time for phase (hamilt, cpu/wall) :	0.00	0.00	
Time for us (hamilt, cpu/wall) :	0.02	0.02	
Time for overlaps (hamilt, cpu/wall) :	0.01	0.01	
Time for distrib (hamilt, cpu/wall) :	0.00	0.00	
Time sum iouter (hamilt, cpu/wall) :	0.00	0.00	
Time for los (hamilt, cpu/wall) :	0.01	0.01	
Time for alm (hns) :	0.0	0.0	
Time for vector (hns) :	0.0	0.0	

```

Time for vector2      (hns) :          0.0          0.0
Time for VxV          (hns) :          0.0          0.0
      61 Eigenvalues computed
Seclr4(Cholesky complete (CPU)) :          0.003      3540.44
Mflops
Seclr4(Transform to eig.problem (CPU)) :          0.008      4310.95
Mflops
Seclr4(Compute eigenvalues (CPU)) :          0.050          909.11
Mflops
Seclr4(Backtransform (CPU)) :          0.002      1029.25
Mflops
      TIME HAMILT (CPU) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0
      TIME HAMILT (WALL) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0

```

K= 0.250000 0.350000 0.450000 30

MATRIX SIZE 325 WEIGHT=48.00 PGR:

EIGENVALUES ARE:

```

-1.9881874   -0.7389815   -0.7376475   -0.7353962   -0.4099378
-0.4091886   -0.4081878   -0.4075958   -0.4047204   -0.4027530
-0.3990786   -0.3989214   -0.3983016   -0.3937028   -0.3892473
-0.3881112   -0.3859097   -0.3839676   -0.3803749    0.1423350
 0.2205855    0.2617485    0.4148716    0.4558438    0.4858247
 0.5472592    0.6090008    0.6100642    0.6140665    0.6155519
 0.6172373    0.6198692    0.6339828    0.7616605    0.7828674
 0.8372986    0.8635864    0.9194043    0.9893671    1.0325732

 1.1158382    1.1297048    1.2006757    1.2665635    1.3376082
 1.3485143    1.3889180    1.4278211    1.5166561    1.5769053
 1.5840650    1.6449617    1.6812849    1.7052052    1.7401924
 1.7586142    1.8448636    1.8724388    1.8943696    1.9274803
 1.9475462

```

0 EIGENVALUES BELOW THE ENERGY -9.00000

```

coors: iplus,nv,n=          0          263          265
Matrix size          327
      allocate HS          0.8 MB
      allocate Z          0.8 MB
      allocate spanel          0.3 MB          dimensions 327 128
      allocate hpanel          0.3 MB          dimensions 327 128
      allocate spanelus          0.3 MB          dimensions 327 128
      allocate slen          0.3 MB          dimensions 327 128
      allocate x2          0.3 MB          dimensions 327 128
      allocate legendre          4.2 MB          dimensions 327 13
128
      allocate al,bl (row)          0.1 MB          dimensions 327 11
      allocate al,bl (col)          0.0 MB          dimensions 128 11
      allocate YL          0.2 MB          dimensions 15 327
3
      number of local orbitals, nlo (hamilt)          62

```

```

        allocate YL              0.2 MB          dimensions 15 327
3
        allocate phsc            0.0 MB          dimensions 327
Time for al,bl (hamilt, cpu/wall) :          0.00          0.00
Time for legendre (hamilt, cpu/wall) :          0.00          0.00
Time for phase (hamilt, cpu/wall) :          0.01          0.01
Time for us (hamilt, cpu/wall) :          0.02          0.02
Time for overlaps (hamilt, cpu/wall) :          0.00          0.00
Time for distrib (hamilt, cpu/wall) :          0.01          0.01
Time sum iouter (hamilt, cpu/wall) :          0.00          0.00
Time for los (hamilt, cpu/wall) :          0.01          0.01
Time for alm (hns) :          0.0          0.0
Time for vector (hns) :          0.0          0.0
Time for vector2 (hns) :          0.0          0.0
Time for VxV (hns) :          0.0          0.0
        61 Eigenvalues computed
        Seclr4(Cholesky complete (CPU)) :          0.003          3499.03
Mflops
        Seclr4(Transform to eig.problem (CPU)) :          0.008          4290.28
Mflops
        Seclr4(Compute eigenvalues (CPU)) :          0.050          923.81
Mflops
        Seclr4(Backtransform (CPU)) :          0.002          1043.96
Mflops
        TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0
        TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0

        K= 0.250000 0.450000 0.450000          31
        MATRIX SIZE 327 WEIGHT=24.00 PGR:
        EIGENVALUES ARE:
-1.9881478 -0.7385831 -0.7383544 -0.7354507 -0.4108096
-0.4087967 -0.4085179 -0.4064824 -0.4055291 -0.4027856
-0.4025131 -0.3994025 -0.3976774 -0.3924060 -0.3895737
-0.3889406 -0.3841652 -0.3831262 -0.3812924 0.1627097
0.2358050 0.2362622 0.3960645 0.4684150 0.4957015
0.5123417 0.6097276 0.6097792 0.6142806 0.6153247
0.6161468 0.6189852 0.6305497 0.7651858 0.7776198
0.8675355 0.8781772 0.9071190 0.9645276 1.0366423

1.1435334 1.1707197 1.1887681 1.2768323 1.3172096
1.3405731 1.4140127 1.4416207 1.5349986 1.5424887
1.6095735 1.6206154 1.6446381 1.6667865 1.7179982
1.7351403 1.8375279 1.8689088 1.8924802 1.9705717
1.9805657
        0 EIGENVALUES BELOW THE ENERGY -9.00000
        *****

Matrix size          327
        allocate HS          0.8 MB
        allocate Z          0.8 MB

```

allocate spanel	0.3 MB	dimensions	327	128
allocate hpanel	0.3 MB	dimensions	327	128
allocate spanelus	0.3 MB	dimensions	327	128
allocate slen	0.3 MB	dimensions	327	128
allocate x2	0.3 MB	dimensions	327	128
allocate legendre	4.2 MB	dimensions	327	13
128				
allocate al,bl (row)	0.1 MB	dimensions	327	11
allocate al,bl (col)	0.0 MB	dimensions	128	11
allocate YL	0.2 MB	dimensions	15	327
3				
number of local orbitals, nlo (hamilt)		62		
allocate YL	0.2 MB	dimensions	15	327
3				
allocate phsc	0.0 MB	dimensions	327	
Time for al,bl (hamilt, cpu/wall) :		0.00	0.00	
Time for legendre (hamilt, cpu/wall) :		0.00	0.00	
Time for phase (hamilt, cpu/wall) :		0.02	0.00	
Time for us (hamilt, cpu/wall) :		0.01	0.01	
Time for overlaps (hamilt, cpu/wall) :		0.02	0.02	
Time for distrib (hamilt, cpu/wall) :		0.00	0.00	
Time sum iouter (hamilt, cpu/wall) :		0.00	0.00	
Time for los (hamilt, cpu/wall) :		0.01	0.01	
Time for alm (hns) :	0.0	0.0		
Time for vector (hns) :	0.0	0.0		
Time for vector2 (hns) :	0.0	0.0		
Time for VxV (hns) :	0.0	0.0		
62 Eigenvalues computed				
Seclr4(Cholesky complete (CPU)) :		0.003	3502.18	
Mflops				
Seclr4(Transform to eig.problem (CPU)) :		0.008	4345.73	
Mflops				
Seclr4(Compute eigenvalues (CPU)) :		0.042	1113.23	
Mflops				
Seclr4(Backtransform (CPU)) :		0.002	1049.65	
Mflops				
TIME HAMILT (CPU) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	0.1, SYNC =	0.0		
TIME HAMILT (WALL) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	0.1, SYNC =	0.0		
K=	0.350000 0.350000 0.350000	32		
MATRIX SIZE	327	WEIGHT= 8.00	PGR:	
EIGENVALUES ARE:				
-1.9881691	-0.7383934	-0.7366988	-0.7366988	-0.4113680
-0.4094952	-0.4094952	-0.4084092	-0.4029549	-0.4026683
-0.4026683	-0.3987720	-0.3987720	-0.3934465	-0.3884758
-0.3884758	-0.3843677	-0.3843677	-0.3795779	0.1408526
0.2518290	0.2518290	0.3902252	0.4767823	0.4767823
0.5179504	0.6103799	0.6125628	0.6125628	0.6165484
0.6175581	0.6175581	0.6309204	0.7886504	0.7886504
0.8485786	0.8720377	0.8720377	1.0094196	1.0848190

1.0848190	1.1016210	1.2719033	1.2719033	1.3283336
1.3414862	1.3414862	1.3958501	1.5296259	1.6231396
1.6231396	1.6471777	1.6471777	1.6496513	1.6846577
1.7897851	1.7897851	1.9088944	1.9088944	1.9292948
1.9706973	1.9706973			

0 EIGENVALUES BELOW THE ENERGY -9.00000

coors: iplus,nv,n=	0	265	267		
Matrix size	329				
allocate HS	0.8 MB				
allocate Z	0.8 MB				
allocate spanel	0.3 MB	dimensions	329	128	
allocate hpanel	0.3 MB	dimensions	329	128	
allocate spanelus	0.3 MB	dimensions	329	128	
allocate slen	0.3 MB	dimensions	329	128	
allocate x2	0.3 MB	dimensions	329	128	
allocate legendre	4.2 MB	dimensions	329	13	
128					
allocate al,bl (row)	0.1 MB	dimensions	329	11	
allocate al,bl (col)	0.0 MB	dimensions	128	11	
allocate YL	0.2 MB	dimensions	15	329	
3					
number of local orbitals, nlo (hamilt)		62			
allocate YL	0.2 MB	dimensions	15	329	
3					
allocate phsc	0.0 MB	dimensions	329		
Time for al,bl (hamilt, cpu/wall) :		0.00	0.00		
Time for legendre (hamilt, cpu/wall) :		0.02	0.02		
Time for phase (hamilt, cpu/wall) :		0.01	0.01		
Time for us (hamilt, cpu/wall) :		0.01	0.00		
Time for overlaps (hamilt, cpu/wall) :		0.00	0.00		
Time for distrib (hamilt, cpu/wall) :		0.00	0.00		
Time sum iouter (hamilt, cpu/wall) :		0.00	0.00		
Time for los (hamilt, cpu/wall) :		0.01	0.01		
Time for alm (hns) :	0.0	0.0			
Time for vector (hns) :	0.0	0.0			
Time for vector2 (hns) :	0.0	0.0			
Time for VxV (hns) :	0.0	0.0			
61 Eigenvalues computed					
Seclr4(Cholesky complete (CPU)) :		0.004	2647.29		
Mflops					
Seclr4(Transform to eig.problem (CPU)) :		0.008	4275.58		
Mflops					
Seclr4(Compute eigenvalues (CPU)) :		0.051	931.34		
Mflops					
Seclr4(Backtransform (CPU)) :		0.002	1050.72		
Mflops					
TIME HAMILT (CPU) =	0.1, HNS =	0.0, HORB =	0.0,		
DIAG =	0.1, SYNC =	0.0			

TIME HAMILT (WALL) = 0.1, HNS = 0.0, HORB = 0.0,
 DIAG = 0.1, SYNC = 0.0

K= 0.350000 0.350000 0.450000 33

MATRIX SIZE 329 WEIGHT=24.00 PGR:

EIGENVALUES ARE:

-1.9881341	-0.7382905	-0.7373135	-0.7363960	-0.4122449
-0.4092747	-0.4085036	-0.4080447	-0.4056466	-0.4051729
-0.4022358	-0.3986899	-0.3986234	-0.3921645	-0.3895085
-0.3887907	-0.3835970	-0.3822483	-0.3800879	0.1657039
0.2304445	0.2522945	0.4144906	0.4548208	0.4660325
0.5038961	0.6107672	0.6117537	0.6140012	0.6150721
0.6166307	0.6176609	0.6289811	0.7741186	0.8000518
0.8512887	0.8699084	0.9120872	0.9611323	1.0873800

1.1414006	1.1479967	1.2303073	1.2575937	1.3225921
1.3547263	1.3724195	1.3974838	1.5595111	1.5704320
1.5875491	1.6218306	1.6448609	1.6733188	1.6984574
1.7054513	1.7515798	1.9235844	1.9308302	1.9679371
1.9876062				

0 EIGENVALUES BELOW THE ENERGY -9.00000

coors: iplus,nv,n=	0	267	266		
Matrix size	328				
allocate HS	0.8 MB				
allocate Z	0.8 MB				
allocate spanel	0.3 MB	dimensions	328	128	
allocate hpanel	0.3 MB	dimensions	328	128	
allocate spanelus	0.3 MB	dimensions	328	128	
allocate slen	0.3 MB	dimensions	328	128	
allocate x2	0.3 MB	dimensions	328	128	
allocate legendre	4.2 MB	dimensions	328	13	
128					
allocate al,bl (row)	0.1 MB	dimensions	328	11	
allocate al,bl (col)	0.0 MB	dimensions	128	11	
allocate YL	0.2 MB	dimensions	15	328	
3					
number of local orbitals, nlo (hamilt)		62			
allocate YL	0.2 MB	dimensions	15	328	
3					
allocate phsc	0.0 MB	dimensions	328		
Time for al,bl (hamilt, cpu/wall) :		0.00	0.00		
Time for legendre (hamilt, cpu/wall) :		0.02	0.02		
Time for phase (hamilt, cpu/wall) :		0.00	0.00		
Time for us (hamilt, cpu/wall) :		0.03	0.03		
Time for overlaps (hamilt, cpu/wall) :		0.00	0.00		
Time for distrib (hamilt, cpu/wall) :		0.00	0.00		
Time sum iouter (hamilt, cpu/wall) :		0.00	0.00		
Time for los (hamilt, cpu/wall) :		0.01	0.01		
Time for alm (hns) :	0.0	0.0			
Time for vector (hns) :	0.0	0.0			


```

Time for vector2      (hns) :          0.0          0.0
Time for VxV         (hns) :          0.0          0.0
      60 Eigenvalues computed
Seclr4(Cholesky complete (CPU)) :          0.003      3682.69
Mflops
Seclr4(Transform to eig.problem (CPU)) :          0.009      4139.79
Mflops
Seclr4(Compute eigenvalues (CPU)) :          0.050          940.16
Mflops
Seclr4(Backtransform (CPU)) :          0.002      1031.82
Mflops
      TIME HAMILT (CPU) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0
      TIME HAMILT (WALL) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0

```

```

K=  0.350000  0.450000  0.450000          34
MATRIX SIZE  328  WEIGHT=24.00  PGR:
EIGENVALUES ARE:
-1.9880889   -0.7377920   -0.7376148   -0.7363412   -0.4135910
-0.4087353   -0.4085194   -0.4075041   -0.4070631   -0.4055510
-0.4051246   -0.3989494   -0.3979990   -0.3909387   -0.3895661
-0.3892048   -0.3815145   -0.3810001   -0.3799463    0.1892568
 0.2349777    0.2374536    0.4147293    0.4375588    0.4789780
 0.4802514    0.6122670    0.6122841    0.6143127    0.6156166
 0.6160237    0.6177776    0.6271474    0.7780688    0.7890060
 0.8661415    0.8976841    0.8992335    0.9266334    1.1310639

 1.1664233    1.2023797    1.2050575    1.2519300    1.3315296
 1.3377441    1.3854324    1.3921712    1.5207118    1.5794241
 1.5949544    1.5965427    1.6079615    1.6384265    1.6977913
 1.6988506    1.7080639    1.9191810    1.9814736    1.9821331

```

```

      0 EIGENVALUES BELOW THE ENERGY  -9.000000
*****

```

```

coors: iplus,nv,n=          0          266          280
Matrix size          342
      allocate HS          0.9 MB
      allocate Z          0.9 MB
      allocate spanel          0.3 MB          dimensions  342  128
      allocate hpanel          0.3 MB          dimensions  342  128
      allocate spanelus          0.3 MB          dimensions  342  128
      allocate slen          0.3 MB          dimensions  342  128
      allocate x2          0.3 MB          dimensions  342  128
      allocate legendre          4.3 MB          dimensions  342  13
128
      allocate al,bl (row)          0.1 MB          dimensions  342  11
      allocate al,bl (col)          0.0 MB          dimensions  128  11
      allocate YL          0.3 MB          dimensions   15  342
3
      number of local orbitals, nlo (hamilt)          62

```

```

3      allocate YL          0.3 MB          dimensions 15 342
      allocate phsc         0.0 MB          dimensions 342
Time for al,bl (hamilt, cpu/wall) :          0.00          0.00
Time for legendre (hamilt, cpu/wall) :          0.02          0.02
Time for phase (hamilt, cpu/wall) :          0.01          0.01
Time for us (hamilt, cpu/wall) :          0.02          0.01
Time for overlaps (hamilt, cpu/wall) :          0.00          0.00
Time for distrib (hamilt, cpu/wall) :          0.00          0.00
Time sum iouter (hamilt, cpu/wall) :          0.00          0.00
Time for los (hamilt, cpu/wall) :          0.01          0.01
Time for alm (hns) :          0.0          0.0
Time for vector (hns) :          0.0          0.0
Time for vector2 (hns) :          0.0          0.0
Time for VxV (hns) :          0.0          0.0
      60 Eigenvalues computed
      Seclr4(Cholesky complete (CPU)) :          0.004          3515.40
Mflops
      Seclr4(Transform to eig.problem (CPU)) :          0.009          4362.23
Mflops
      Seclr4(Compute eigenvalues (CPU)) :          0.044          1220.72
Mflops
      Seclr4(Backtransform (CPU)) :          0.002          1085.68
Mflops
      TIME HAMILT (CPU) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0
      TIME HAMILT (WALL) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          0.1, SYNC =          0.0

      K= 0.450000 0.450000 0.450000          35
      MATRIX SIZE 342 WEIGHT= 8.00 PGR:
      EIGENVALUES ARE:
      -1.9880917 -0.7375413 -0.7372773 -0.7372773 -0.4154496
      -0.4090005 -0.4090005 -0.4083151 -0.4079178 -0.4071901
      -0.4071901 -0.3992369 -0.3992369 -0.3908334 -0.3902748
      -0.3902748 -0.3810003 -0.3810003 -0.3802687 0.2148056
      0.2343481 0.2343481 0.3791938 0.4616821 0.4698281
      0.4698281 0.6116865 0.6120601 0.6120601 0.6152047
      0.6152047 0.6152073 0.6241481 0.7857919 0.7857919
      0.8328706 0.9082818 0.9082818 0.9183162 1.1961501

      1.2048813 1.2048813 1.2360206 1.2360206 1.3460411
      1.3460411 1.3627738 1.3880888 1.5125317 1.5175312
      1.5175312 1.5728367 1.5827428 1.5827428 1.7020484
      1.7403347 1.7403347 1.9533146 1.9533146 1.9664893

      0 EIGENVALUES BELOW THE ENERGY -9.00000
      *****

      NUMBER OF K-POINTS:          35
      ==> TOTAL CPU          TIME:          0.2 (INIT =          0.0 + K-POINTS =
0.1)

```

```
> SUM OF WALL CLOCK TIMES:      0.2 (INIT =      0.0 + K-POINTS =
0.1)
    Maximum WALL clock time:    6.926699999999998
    Maximum CPU time:           6.912309000000000
```