

```

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	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

```

MPI-parallel calculation using      4 processors
Scalapack processors array (row,col):  2  2
Matrix size      313
Optimum Blocksize for setup 158 Excess % 0.128D+01
Optimum Blocksize for diag  16 Excess % 0.386D+01
Base Blocksize   64 Diagonalization 192
    allocate H      0.3 MB      dimensions 185 185
    allocate S      0.3 MB      dimensions 185 185
    allocate spanel  0.1 MB      dimensions 185 64
    allocate hpanel  0.1 MB      dimensions 185 64
    allocate spanelus 0.1 MB      dimensions 185 64
    allocate slen    0.1 MB      dimensions 185 64
    allocate x2      0.1 MB      dimensions 185 64
    allocate legendre 1.2 MB      dimensions 185 13
64
allocate al,bl (row) 0.1 MB      dimensions 185 11
allocate al,bl (col) 0.0 MB      dimensions 64 11
    allocate YL      0.1 MB      dimensions 15 185
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) : 0.01 0.01
Time for us (hamilt, cpu/wall) : 0.01 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) : 0.00 0.00
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

```

```

Time to synchronize (kpt) :          0.0          0.0
Scalapack Workspace size    1.05 Mb
  Seclr4(Transpose of H and S (CPU)) :          0.042
  Seclr4(Transpose of H and S (WALL)) :          0.085
  Seclr4(Cholesky complete (CPU)) :          0.264          38.72
Mflops
  Seclr4(Cholesky complete (WALL)) :          0.267          38.24
Mflops
  Seclr4(Transform to eig.problem (CPU)) :          0.638          48.05
Mflops
  Seclr4(Transform to eig.problem (WALL)) :          0.637          48.12
Mflops
  Seclr4(Compute eigenvalues (CPU)) :          6.135          6.66
Mflops
  Seclr4(Compute eigenvalues (WALL)) :          5.373          7.61
Mflops
  Seclr4(Backtransform (CPU)) :          0.160          8.88
Mflops
  Seclr4(Backtransform (WALL)) :          0.100          14.18
Mflops
  TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          7.4, SYNC =          0.0
  TIME HAMILT (WALL) =          0.1, HNS =          0.0, HORB =          0.0,
DIAG =          6.6, 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
Optimum Blocksize for setup 158 Excess % 0.128D+01
Optimum Blocksize for diag 16 Excess % 0.386D+01
Base Blocksize 64 Diagonalization 192
  allocate H          0.3 MB          dimensions 186 186
  allocate S          0.3 MB          dimensions 186 186
  allocate spanel      0.1 MB          dimensions 186 64

```


allocate hpanel	0.1 MB	dimensions	186	64
allocate spanelus	0.1 MB	dimensions	186	64
allocate slen	0.1 MB	dimensions	186	64
allocate x2	0.1 MB	dimensions	186	64
allocate legendre	1.2 MB	dimensions	186	13
64				
allocate al,bl (row)	0.1 MB	dimensions	186	11
allocate al,bl (col)	0.0 MB	dimensions	64	11
allocate YL	0.1 MB	dimensions	15	186
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) :		0.01	0.01	
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	0.00	
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) :		0.00	0.00	
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		
Time to synchronize (kpt) :	0.1	0.1		
Scalapack Workspace size	1.05 Mb			
Seclr4(Transpose of H and S (CPU)) :		0.000		
Seclr4(Transpose of H and S (WALL)) :		0.000		
Seclr4(Cholesky complete (CPU)) :		0.282		36.59
Mflops				
Seclr4(Cholesky complete (WALL)) :		0.267		38.61
Mflops				
Seclr4(Transform to eig.problem (CPU)) :		0.898		34.47
Mflops				
Seclr4(Transform to eig.problem (WALL)) :		0.854		36.26
Mflops				
Seclr4(Compute eigenvalues (CPU)) :		9.107		4.53
Mflops				
Seclr4(Compute eigenvalues (WALL)) :		11.179		3.69
Mflops				
Seclr4(Backtransform (CPU)) :		0.185		7.74
Mflops				
Seclr4(Backtransform (WALL)) :		0.162		8.83
Mflops				
TIME HAMILT (CPU) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	10.6, SYNC =	0.1		
TIME HAMILT (WALL) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	12.6, SYNC =	0.1		
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
Optimum Blocksize for setup 160 Excess % 0.000D+00
Optimum Blocksize for diag 16 Excess % 0.000D+00
Base Blocksize 64 Diagonalization 192
    allocate H          0.3 MB          dimensions 191 191
    allocate S          0.3 MB          dimensions 191 191
    allocate spanel     0.1 MB          dimensions 191 64
    allocate hpanel     0.1 MB          dimensions 191 64
    allocate spanelus   0.1 MB          dimensions 191 64
    allocate slen       0.1 MB          dimensions 191 64
    allocate x2         0.1 MB          dimensions 191 64
    allocate legendre   1.2 MB          dimensions 191 13
64
    allocate al,bl (row) 0.1 MB          dimensions 191 11
    allocate al,bl (col) 0.0 MB          dimensions 64 11
    allocate YL          0.1 MB          dimensions 15 191
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) : 0.02 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) : 0.00 0.00
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

```

```

Time to synchronize (kpt) :          0.0          0.0
Scalapack Workspace size    1.06 Mb
  Seclr4(Transpose of H and S (CPU)) :          0.000
  Seclr4(Transpose of H and S (WALL)) :          0.000
  Seclr4(Cholesky complete (CPU)) :          0.193          56.02
Mflops
  Seclr4(Cholesky complete (WALL)) :          0.194          55.72
Mflops
  Seclr4(Transform to eig.problem (CPU)) :          0.821          39.53
Mflops
  Seclr4(Transform to eig.problem (WALL)) :          0.820          39.60
Mflops
  Seclr4(Compute eigenvalues (CPU)) :          8.503          5.09
Mflops
  Seclr4(Compute eigenvalues (WALL)) :         12.001          3.61
Mflops
  Seclr4(Backtransform (CPU)) :          0.079          18.61
Mflops
  Seclr4(Backtransform (WALL)) :          0.056          26.49
Mflops
  TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          9.7, SYNC =          0.0
  TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =         13.2, 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
Optimum Blocksize for setup 158 Excess % 0.000D+00
Optimum Blocksize for diag 16 Excess % 0.255D+01
Base Blocksize 64 Diagonalization 192
  allocate H          0.3 MB          dimensions 188 188
  allocate S          0.3 MB          dimensions 188 188
  allocate panel      0.1 MB          dimensions 188 64

```

allocate hpanel	0.1 MB	dimensions	188	64
allocate spanelus	0.1 MB	dimensions	188	64
allocate slen	0.1 MB	dimensions	188	64
allocate x2	0.1 MB	dimensions	188	64
allocate legendre	1.2 MB	dimensions	188	13
64				
allocate al,bl (row)	0.1 MB	dimensions	188	11
allocate al,bl (col)	0.0 MB	dimensions	64	11
allocate YL	0.1 MB	dimensions	15	188
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) :		0.01	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) :		0.00	0.00	
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		
Time to synchronize (kpt) :	0.0	0.0		
Scalapack Workspace size	1.05 Mb			
Seclr4(Transpose of H and S (CPU)) :		0.000		
Seclr4(Transpose of H and S (WALL)) :		0.000		
Seclr4(Cholesky complete (CPU)) :		0.344		30.58
Mflops				
Seclr4(Cholesky complete (WALL)) :		0.351		30.01
Mflops				
Seclr4(Transform to eig.problem (CPU)) :		0.686		46.02
Mflops				
Seclr4(Transform to eig.problem (WALL)) :		0.724		43.60
Mflops				
Seclr4(Compute eigenvalues (CPU)) :		4.559		9.23
Mflops				
Seclr4(Compute eigenvalues (WALL)) :		4.234		9.94
Mflops				
Seclr4(Backtransform (CPU)) :		0.133		11.30
Mflops				
Seclr4(Backtransform (WALL)) :		0.097		15.36
Mflops				
TIME HAMILT (CPU) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	5.9, SYNC =	0.0		
TIME HAMILT (WALL) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	5.6, 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
Optimum Blocksize for setup 156 Excess % 0.000D+00
Optimum Blocksize for diag 26 Excess % 0.000D+00
Base Blocksize 64 Diagonalization 192
    allocate H          0.3 MB          dimensions 184 184
    allocate S          0.3 MB          dimensions 184 184
    allocate spanel      0.1 MB          dimensions 184 64
    allocate hpanel      0.1 MB          dimensions 184 64
    allocate spanelus    0.1 MB          dimensions 184 64
    allocate slen        0.1 MB          dimensions 184 64
    allocate x2          0.1 MB          dimensions 184 64
    allocate legendre    1.2 MB          dimensions 184 13
64
    allocate al,bl (row)  0.1 MB          dimensions 184 11
    allocate al,bl (col)  0.0 MB          dimensions 64 11
    allocate YL          0.1 MB          dimensions 15 184
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) : 0.00 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 0.00
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) : 0.00 0.00
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
Time to synchronize  (kpt) :          0.0          0.0
Scalapack Workspace size      1.05 Mb
  Seclr4(Transpose of H and S (CPU)) :          0.000
  Seclr4(Transpose of H and S (WALL)) :          0.000
  Seclr4(Cholesky complete (CPU)) :          0.286          35.40
Mflops
  Seclr4(Cholesky complete (WALL)) :          0.282          35.90
Mflops
  Seclr4(Transform to eig.problem (CPU)) :          0.719          42.23
Mflops
  Seclr4(Transform to eig.problem (WALL)) :          0.718          42.29
Mflops
  Seclr4(Compute eigenvalues (CPU)) :          5.751          7.04
Mflops
  Seclr4(Compute eigenvalues (WALL)) :          5.284          7.66
Mflops
  Seclr4(Backtransform (CPU)) :          0.098          14.71
Mflops
  Seclr4(Backtransform (WALL)) :          0.072          19.83
Mflops
  TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          7.0, SYNC =          0.0
  TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          6.5, 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
Optimum Blocksize for setup 160 Excess % 0.126D+01
Optimum Blocksize for diag 16 Excess % 0.126D+01
Base Blocksize 64 Diagonalization 192
  allocate H          0.3 MB          dimensions 190 190
  allocate S          0.3 MB          dimensions 190 190

```

allocate spanel	0.1 MB	dimensions	190	64
allocate hpanel	0.1 MB	dimensions	190	64
allocate spanelus	0.1 MB	dimensions	190	64
allocate slen	0.1 MB	dimensions	190	64
allocate x2	0.1 MB	dimensions	190	64
allocate legendre	1.2 MB	dimensions	190	13
64				
allocate al,bl (row)	0.1 MB	dimensions	190	11
allocate al,bl (col)	0.0 MB	dimensions	64	11
allocate YL	0.1 MB	dimensions	15	190
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) :		0.00	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	0.00	
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) :		0.00	0.00	
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		
Time to synchronize (kpt) :	0.0	0.0		
Scalapack Workspace size	1.05 Mb			
Seclr4(Transpose of H and S (CPU)) :		0.000		
Seclr4(Transpose of H and S (WALL)) :		0.000		
Seclr4(Cholesky complete (CPU)) :		0.246	43.66	
Mflops				
Seclr4(Cholesky complete (WALL)) :		0.245	43.84	
Mflops				
Seclr4(Transform to eig.problem (CPU)) :		0.639	50.33	
Mflops				
Seclr4(Transform to eig.problem (WALL)) :		0.636	50.53	
Mflops				
Seclr4(Compute eigenvalues (CPU)) :		4.470	9.59	
Mflops				
Seclr4(Compute eigenvalues (WALL)) :		4.169	10.28	
Mflops				
Seclr4(Backtransform (CPU)) :		0.054	27.35	
Mflops				
Seclr4(Backtransform (WALL)) :		0.054	27.31	
Mflops				
TIME HAMILT (CPU) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	5.5, SYNC =	0.0		
TIME HAMILT (WALL) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	5.2, 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
Optimum Blocksize for setup 160 Excess % 0.126D+01
Optimum Blocksize for diag 16 Excess % 0.126D+01
Base Blocksize 64 Diagonalization 192
allocate H 0.3 MB dimensions 189 189
allocate S 0.3 MB dimensions 189 189
allocate spanel 0.1 MB dimensions 189 64
allocate hpanel 0.1 MB dimensions 189 64
allocate spanelus 0.1 MB dimensions 189 64
allocate slen 0.1 MB dimensions 189 64
allocate x2 0.1 MB dimensions 189 64
allocate legendre 1.2 MB dimensions 189 13
64
allocate al,bl (row) 0.1 MB dimensions 189 11
allocate al,bl (col) 0.0 MB dimensions 64 11
allocate YL 0.1 MB dimensions 15 189
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) : 0.00 0.00
Time for phase (hamilt, cpu/wall) : 0.02 0.00
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) : 0.00 0.00
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
Time to synchronize  (kpt) :          0.0          0.0
Scalapack Workspace size      1.05 Mb
  Seclr4(Transpose of H and S (CPU)) :          0.000
  Seclr4(Transpose of H and S (WALL)) :          0.000
  Seclr4(Cholesky complete (CPU)) :          0.212          49.99
Mflops
  Seclr4(Cholesky complete (WALL)) :          0.212          49.99
Mflops
  Seclr4(Transform to eig.problem (CPU)) :          0.762          41.79
Mflops
  Seclr4(Transform to eig.problem (WALL)) :          0.762          41.79
Mflops
  Seclr4(Compute eigenvalues (CPU)) :          4.212          10.08
Mflops
  Seclr4(Compute eigenvalues (WALL)) :          4.213          10.08
Mflops
  Seclr4(Backtransform (CPU)) :          0.060          24.56
Mflops
  Seclr4(Backtransform (WALL)) :          0.060          24.58
Mflops
  TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          5.4, SYNC =          0.0
  TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          5.4, 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
Optimum Blocksize for setup 160 Excess % 0.126D+01
Optimum Blocksize for diag 16 Excess % 0.126D+01
Base Blocksize 64 Diagonalization 192
  allocate H          0.3 MB          dimensions 190 190
  allocate S          0.3 MB          dimensions 190 190

```

allocate spanel	0.1 MB	dimensions	190	64
allocate hpanel	0.1 MB	dimensions	190	64
allocate spanelus	0.1 MB	dimensions	190	64
allocate slen	0.1 MB	dimensions	190	64
allocate x2	0.1 MB	dimensions	190	64
allocate legendre	1.2 MB	dimensions	190	13
64				
allocate al,bl (row)	0.1 MB	dimensions	190	11
allocate al,bl (col)	0.0 MB	dimensions	64	11
allocate YL	0.1 MB	dimensions	15	190
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) :		0.00	0.00	
Time for phase (hamilt, cpu/wall) :		0.02	0.00	
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) :		0.00	0.00	
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		
Time to synchronize (kpt) :	0.0	0.0		
Scalapack Workspace size	1.05 Mb			
Seclr4(Transpose of H and S (CPU)) :		0.000		
Seclr4(Transpose of H and S (WALL)) :		0.000		
Seclr4(Cholesky complete (CPU)) :		0.221	48.47	
Mflops				
Seclr4(Cholesky complete (WALL)) :		0.221	48.48	
Mflops				
Seclr4(Transform to eig.problem (CPU)) :		0.648	49.62	
Mflops				
Seclr4(Transform to eig.problem (WALL)) :		0.648	49.61	
Mflops				
Seclr4(Compute eigenvalues (CPU)) :		4.061	10.56	
Mflops				
Seclr4(Compute eigenvalues (WALL)) :		4.061	10.56	
Mflops				
Seclr4(Backtransform (CPU)) :		0.090	16.63	
Mflops				
Seclr4(Backtransform (WALL)) :		0.090	16.63	
Mflops				
TIME HAMILT (CPU) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	5.2, SYNC =	0.0		
TIME HAMILT (WALL) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	5.2, 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 -9.000000
*****

```

```

coors: iplus,nv,n= 0 256 253
Matrix size 315
Optimum Blocksize for setup 158 Excess % 0.000D+00
Optimum Blocksize for diag 16 Excess % 0.255D+01
Base Blocksize 64 Diagonalization 192
allocate H 0.3 MB dimensions 187 187
allocate S 0.3 MB dimensions 187 187
allocate spanel 0.1 MB dimensions 187 64
allocate hpanel 0.1 MB dimensions 187 64
allocate spanelus 0.1 MB dimensions 187 64
allocate slen 0.1 MB dimensions 187 64
allocate x2 0.1 MB dimensions 187 64
allocate legendre 1.2 MB dimensions 187 13
64
allocate al,bl (row) 0.1 MB dimensions 187 11
allocate al,bl (col) 0.0 MB dimensions 64 11
allocate YL 0.1 MB dimensions 15 187
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) : 0.00 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 0.00
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) : 0.00 0.00
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
Time to synchronize  (kpt) :          0.0          0.0
Scalapack Workspace size      1.05 Mb
  Seclr4(Transpose of H and S (CPU)) :          0.000
  Seclr4(Transpose of H and S (WALL)) :          0.000
  Seclr4(Cholesky complete (CPU)) :          0.230          45.29
Mflops
  Seclr4(Cholesky complete (WALL)) :          0.230          45.28
Mflops
  Seclr4(Transform to eig.problem (CPU)) :          0.636          49.14
Mflops
  Seclr4(Transform to eig.problem (WALL)) :          0.636          49.14
Mflops
  Seclr4(Compute eigenvalues (CPU)) :          4.120          10.11
Mflops
  Seclr4(Compute eigenvalues (WALL)) :          4.121          10.11
Mflops
  Seclr4(Backtransform (CPU)) :          0.099          15.05
Mflops
  Seclr4(Backtransform (WALL)) :          0.099          15.03
Mflops
  TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          5.2, SYNC =          0.0
  TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          5.2, 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
Optimum Blocksize for setup 160 Excess % 0.126D+01
Optimum Blocksize for diag 16 Excess % 0.126D+01
Base Blocksize 64 Diagonalization 192
      allocate H          0.3 MB          dimensions 190 190

```

allocate S	0.3 MB	dimensions	190	190
allocate spanel	0.1 MB	dimensions	190	64
allocate hpanel	0.1 MB	dimensions	190	64
allocate spanelus	0.1 MB	dimensions	190	64
allocate slen	0.1 MB	dimensions	190	64
allocate x2	0.1 MB	dimensions	190	64
allocate legendre	1.2 MB	dimensions	190	13
64				
allocate al,bl (row)	0.1 MB	dimensions	190	11
allocate al,bl (col)	0.0 MB	dimensions	64	11
allocate YL	0.1 MB	dimensions	15	190
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) :		0.00	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	0.00	
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) :		0.00	0.00	
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		
Time to synchronize (kpt) :	0.0	0.0		
Scalapack Workspace size	1.05 Mb			
Seclr4(Transpose of H and S (CPU)) :		0.000		
Seclr4(Transpose of H and S (WALL)) :		0.000		
Seclr4(Cholesky complete (CPU)) :		0.122	87.75	
Mflops				
Seclr4(Cholesky complete (WALL)) :		0.122	87.72	
Mflops				
Seclr4(Transform to eig.problem (CPU)) :		0.546	58.93	
Mflops				
Seclr4(Transform to eig.problem (WALL)) :		0.546	58.92	
Mflops				
Seclr4(Compute eigenvalues (CPU)) :		2.173	19.73	
Mflops				
Seclr4(Compute eigenvalues (WALL)) :		2.173	19.73	
Mflops				
Seclr4(Backtransform (CPU)) :		0.202	7.52	
Mflops				
Seclr4(Backtransform (WALL)) :		0.202	7.51	
Mflops				
TIME HAMILT (CPU) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	3.1, SYNC =	0.0		
TIME HAMILT (WALL) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	3.1, 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
Optimum Blocksize for setup 160 Excess % 0.000D+00
Optimum Blocksize for diag 16 Excess % 0.000D+00
Base Blocksize 64 Diagonalization 192
allocate H 0.3 MB dimensions 192 192
allocate S 0.3 MB dimensions 192 192
allocate spanel 0.1 MB dimensions 192 64
allocate hpanel 0.1 MB dimensions 192 64
allocate spanelus 0.1 MB dimensions 192 64
allocate slen 0.1 MB dimensions 192 64
allocate x2 0.1 MB dimensions 192 64
allocate legendre 1.2 MB dimensions 192 13
64
allocate al,bl (row) 0.1 MB dimensions 192 11
allocate al,bl (col) 0.0 MB dimensions 64 11
allocate YL 0.1 MB dimensions 15 192
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) : 0.02 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) : 0.00 0.00
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
Time to synchronize (kpt) :          0.0          0.0
Scalapack Workspace size      1.06 Mb
  Seclr4(Transpose of H and S (CPU)) :          0.000
  Seclr4(Transpose of H and S (WALL)) :          0.000
  Seclr4(Cholesky complete (CPU)) :          0.157          69.73
Mflops
  Seclr4(Cholesky complete (WALL)) :          0.157          69.70
Mflops
  Seclr4(Transform to eig.problem (CPU)) :          0.561          58.44
Mflops
  Seclr4(Transform to eig.problem (WALL)) :          0.561          58.43
Mflops
  Seclr4(Compute eigenvalues (CPU)) :          3.725          11.73
Mflops
  Seclr4(Compute eigenvalues (WALL)) :          3.726          11.73
Mflops
  Seclr4(Backtransform (CPU)) :          0.216          6.99
Mflops
  Seclr4(Backtransform (WALL)) :          0.216          6.99
Mflops
  TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          4.8, SYNC =          0.0
  TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          4.8, 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
Optimum Blocksize for setup 160 Excess % 0.126D+01
Optimum Blocksize for diag 16 Excess % 0.126D+01
Base Blocksize 64 Diagonalization 192

```

allocate H	0.3 MB	dimensions	190	190
allocate S	0.3 MB	dimensions	190	190
allocate spanel	0.1 MB	dimensions	190	64
allocate hpanel	0.1 MB	dimensions	190	64
allocate spanelus	0.1 MB	dimensions	190	64
allocate slen	0.1 MB	dimensions	190	64
allocate x2	0.1 MB	dimensions	190	64
allocate legendre	1.2 MB	dimensions	190	13
64				
allocate al,bl (row)	0.1 MB	dimensions	190	11
allocate al,bl (col)	0.0 MB	dimensions	64	11
allocate YL	0.1 MB	dimensions	15	190
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) :		0.00	0.00	
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) :		0.00	0.00	
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		
Time to synchronize (kpt) :	0.0	0.0		
Scalapack Workspace size	1.05 Mb			
Seclr4(Transpose of H and S (CPU)) :		0.000		
Seclr4(Transpose of H and S (WALL)) :		0.000		
Seclr4(Cholesky complete (CPU)) :		0.287	37.40	
Mflops				
Seclr4(Cholesky complete (WALL)) :		0.287	37.39	
Mflops				
Seclr4(Transform to eig.problem (CPU)) :		0.518	62.10	
Mflops				
Seclr4(Transform to eig.problem (WALL)) :		0.518	62.09	
Mflops				
Seclr4(Compute eigenvalues (CPU)) :		2.388	17.95	
Mflops				
Seclr4(Compute eigenvalues (WALL)) :		2.388	17.95	
Mflops				
Seclr4(Backtransform (CPU)) :		0.237	6.40	
Mflops				
Seclr4(Backtransform (WALL)) :		0.237	6.40	
Mflops				
TIME HAMILT (CPU) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	3.5, SYNC =	0.0		

TIME HAMILT (WALL) = 0.0, HNS = 0.0, HORB = 0.0,
 DIAG = 3.5, 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 -9.000000

coors: iplus,nv,n= 0 256 258
 Matrix size 320
 Optimum Blocksize for setup 160 Excess % 0.000D+00
 Optimum Blocksize for diag 16 Excess % 0.000D+00
 Base Blocksize 64 Diagonalization 192

allocate H	0.3 MB	dimensions	192	192
allocate S	0.3 MB	dimensions	192	192
allocate spanel	0.1 MB	dimensions	192	64
allocate hpanel	0.1 MB	dimensions	192	64
allocate spanelus	0.1 MB	dimensions	192	64
allocate slen	0.1 MB	dimensions	192	64
allocate x2	0.1 MB	dimensions	192	64
allocate legendre	1.2 MB	dimensions	192	13
64				
allocate al,bl (row)	0.1 MB	dimensions	192	11
allocate al,bl (col)	0.0 MB	dimensions	64	11
allocate YL	0.1 MB	dimensions	15	192
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) :			0.00	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) :          0.00          0.00
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
Time to synchronize (kpt) :          0.0          0.0
Scalapack Workspace size      1.06 Mb
  Seclr4(Transpose of H and S (CPU)) :          0.000
  Seclr4(Transpose of H and S (WALL)) :          0.000
  Seclr4(Cholesky complete (CPU)) :          0.213          51.24
Mflops
  Seclr4(Cholesky complete (WALL)) :          0.213          51.23
Mflops
  Seclr4(Transform to eig.problem (CPU)) :          0.618          53.03
Mflops
  Seclr4(Transform to eig.problem (WALL)) :          0.618          53.01
Mflops
  Seclr4(Compute eigenvalues (CPU)) :          5.174          8.44
Mflops
  Seclr4(Compute eigenvalues (WALL)) :          5.174          8.44
Mflops
  Seclr4(Backtransform (CPU)) :          0.281          5.56
Mflops
  Seclr4(Backtransform (WALL)) :          0.281          5.56
Mflops
  TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          6.4, SYNC =          0.0
  TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          6.4, 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

```

```

Optimum Blocksize for setup 160 Excess % 0.126D+01
Optimum Blocksize for diag 16 Excess % 0.126D+01
Base Blocksize 64 Diagonalization 192
    allocate H          0.3 MB          dimensions 189 189
    allocate S          0.3 MB          dimensions 189 189
    allocate spanel     0.1 MB          dimensions 189 64
    allocate hpanel     0.1 MB          dimensions 189 64
    allocate spanelus   0.1 MB          dimensions 189 64
    allocate slen       0.1 MB          dimensions 189 64
    allocate x2         0.1 MB          dimensions 189 64
    allocate legendre   1.2 MB          dimensions 189 13
64
allocate al,bl (row)    0.1 MB          dimensions 189 11
allocate al,bl (col)    0.0 MB          dimensions 64 11
    allocate YL         0.1 MB          dimensions 15 189
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) : 0.00 0.00
Time for phase (hamilt, cpu/wall) : 0.00 0.01
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) : 0.00 0.00
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
Time to synchronize (kpt) : 0.0 0.0
Scalapack Workspace size 1.05 Mb
    Seclr4(Transpose of H and S (CPU)) : 0.000
    Seclr4(Transpose of H and S (WALL)) : 0.000
    Seclr4(Cholesky complete (CPU)) : 0.230 46.20
Mflops
    Seclr4(Cholesky complete (WALL)) : 0.230 46.21
Mflops
    Seclr4(Transform to eig.problem (CPU)) : 0.561 56.76
Mflops
    Seclr4(Transform to eig.problem (WALL)) : 0.561 56.74
Mflops
    Seclr4(Compute eigenvalues (CPU)) : 5.123 8.29
Mflops
    Seclr4(Compute eigenvalues (WALL)) : 5.124 8.29
Mflops
    Seclr4(Backtransform (CPU)) : 0.289 5.29
Mflops
    Seclr4(Backtransform (WALL)) : 0.289 5.29
Mflops

```

TIME HAMILT (CPU) = 0.0, HNS = 0.0, HORB = 0.0,
 DIAG = 6.3, SYNC = 0.0
 TIME HAMILT (WALL) = 0.0, HNS = 0.0, HORB = 0.0,
 DIAG = 6.3, 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 -9.00000

coors: iplus,nv,n= 0 255 254
 Matrix size 316
 Optimum Blocksize for setup 158 Excess % 0.000D+00
 Optimum Blocksize for diag 16 Excess % 0.255D+01
 Base Blocksize 64 Diagonalization 192

allocate H	0.3 MB	dimensions	188	188
allocate S	0.3 MB	dimensions	188	188
allocate spanel	0.1 MB	dimensions	188	64
allocate hpanel	0.1 MB	dimensions	188	64
allocate spanelus	0.1 MB	dimensions	188	64
allocate slen	0.1 MB	dimensions	188	64
allocate x2	0.1 MB	dimensions	188	64
allocate legendre	1.2 MB	dimensions	188	13

64

allocate al,bl (row)	0.1 MB	dimensions	188	11
allocate al,bl (col)	0.0 MB	dimensions	64	11
allocate YL	0.1 MB	dimensions	15	188

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 0.00
 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) :          0.00          0.00
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
Time to synchronize (kpt) :          0.0          0.0
Scalapack Workspace size      1.05 Mb
  Seclr4(Transpose of H and S (CPU)) :          0.000
  Seclr4(Transpose of H and S (WALL)) :          0.000
  Seclr4(Cholesky complete (CPU)) :          0.203          51.81
Mflops
  Seclr4(Cholesky complete (WALL)) :          0.203          51.81
Mflops
  Seclr4(Transform to eig.problem (CPU)) :          0.624          50.59
Mflops
  Seclr4(Transform to eig.problem (WALL)) :          0.624          50.58
Mflops
  Seclr4(Compute eigenvalues (CPU)) :          5.394          7.80
Mflops
  Seclr4(Compute eigenvalues (WALL)) :          5.395          7.80
Mflops
  Seclr4(Backtransform (CPU)) :          0.128          12.09
Mflops
  Seclr4(Backtransform (WALL)) :          0.128          12.08
Mflops
  TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          6.4, SYNC =          0.0
  TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          6.4, 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
Optimum Blocksize for setup 160 Excess % 0.000D+00
Optimum Blocksize for diag 16 Excess % 0.000D+00
Base Blocksize 64 Diagonalization 192
    allocate H            0.3 MB          dimensions 191 191
    allocate S            0.3 MB          dimensions 191 191
    allocate spanel       0.1 MB          dimensions 191 64
    allocate hpanel       0.1 MB          dimensions 191 64
    allocate spanelus     0.1 MB          dimensions 191 64
    allocate slen         0.1 MB          dimensions 191 64
    allocate x2           0.1 MB          dimensions 191 64
    allocate legendre     1.2 MB          dimensions 191 13
64
allocate al,bl (row)      0.1 MB          dimensions 191 11
allocate al,bl (col)     0.0 MB          dimensions 64 11
    allocate YL           0.1 MB          dimensions 15 191
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) : 0.00 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) : 0.00 0.00
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
Time to synchronize (kpt) : 0.0 0.0
Scalapack Workspace size 1.06 Mb
  Seclr4(Transpose of H and S (CPU)) : 0.000
  Seclr4(Transpose of H and S (WALL)) : 0.000
  Seclr4(Cholesky complete (CPU)) : 0.132 81.67
Mflops
  Seclr4(Cholesky complete (WALL)) : 0.132 81.66
Mflops
  Seclr4(Transform to eig.problem (CPU)) : 0.512 63.46
Mflops
  Seclr4(Transform to eig.problem (WALL)) : 0.512 63.46
Mflops
  Seclr4(Compute eigenvalues (CPU)) : 5.238 8.26
Mflops
  Seclr4(Compute eigenvalues (WALL)) : 5.239 8.26
Mflops
  Seclr4(Backtransform (CPU)) : 0.287 5.06
Mflops

```

```

Seclr4(Backtransform (WALL)) :          0.287          5.06
Mflops
  TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          6.2, SYNC =          0.0
  TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          6.2, 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
Optimum Blocksize for setup 158 Excess % 0.000D+00
Optimum Blocksize for diag 16 Excess % 0.255D+01
Base Blocksize 64 Diagonalization 192
  allocate H          0.3 MB          dimensions 188 188
  allocate S          0.3 MB          dimensions 188 188
  allocate spanel      0.1 MB          dimensions 188 64
  allocate hpanel      0.1 MB          dimensions 188 64
  allocate spanelus    0.1 MB          dimensions 188 64
  allocate slen        0.1 MB          dimensions 188 64
  allocate x2          0.1 MB          dimensions 188 64
  allocate legendre    1.2 MB          dimensions 188 13
64
allocate al,bl (row)    0.1 MB          dimensions 188 11
allocate al,bl (col)    0.0 MB          dimensions 64 11
  allocate YL          0.1 MB          dimensions 15 188
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          0.00

```

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) :	0.00	0.00
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
Time to synchronize (kpt) :	0.0	0.0
Scalapack Workspace size	1.05 Mb	
Seclr4(Transpose of H and S (CPU)) :	0.000	
Seclr4(Transpose of H and S (WALL)) :	0.000	
Seclr4(Cholesky complete (CPU)) :	0.199	52.74
Mflops		
Seclr4(Cholesky complete (WALL)) :	0.199	52.75
Mflops		
Seclr4(Transform to eig.problem (CPU)) :	0.672	46.93
Mflops		
Seclr4(Transform to eig.problem (WALL)) :	0.673	46.91
Mflops		
Seclr4(Compute eigenvalues (CPU)) :	6.020	6.99
Mflops		
Seclr4(Compute eigenvalues (WALL)) :	6.021	6.99
Mflops		
Seclr4(Backtransform (CPU)) :	0.122	12.11
Mflops		
Seclr4(Backtransform (WALL)) :	0.122	12.11
Mflops		
TIME HAMILT (CPU) =	0.0, HNS =	0.0, HORB = 0.0,
DIAG = 7.0, SYNC =	0.0	
TIME HAMILT (WALL) =	0.0, HNS =	0.0, HORB = 0.0,
DIAG = 7.0, 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
Optimum Blocksize for setup 160 Excess % 0.000D+00
Optimum Blocksize for diag 16 Excess % 0.000D+00
Base Blocksize 64 Diagonalization 192
    allocate H            0.3 MB          dimensions 192 192
    allocate S            0.3 MB          dimensions 192 192
    allocate spanel       0.1 MB          dimensions 192 64
    allocate hpanel       0.1 MB          dimensions 192 64
    allocate spanelus     0.1 MB          dimensions 192 64
    allocate slen         0.1 MB          dimensions 192 64
    allocate x2           0.1 MB          dimensions 192 64
    allocate legendre     1.2 MB          dimensions 192 13
64
allocate al,bl (row)      0.1 MB          dimensions 192 11
allocate al,bl (col)     0.0 MB          dimensions 64 11
    allocate YL           0.1 MB          dimensions 15 192
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) : 0.00 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) : 0.00 0.00
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
Time to synchronize (kpt) : 0.0 0.0
Scalapack Workspace size 1.06 Mb
  Seclr4(Transpose of H and S (CPU)) : 0.000
  Seclr4(Transpose of H and S (WALL)) : 0.000
  Seclr4(Cholesky complete (CPU)) : 0.232 47.14
Mflops
  Seclr4(Cholesky complete (WALL)) : 0.232 47.12
Mflops
  Seclr4(Transform to eig.problem (CPU)) : 0.715 45.82
Mflops
  Seclr4(Transform to eig.problem (WALL)) : 0.715 45.82
Mflops
  Seclr4(Compute eigenvalues (CPU)) : 6.136 7.12
Mflops
  Seclr4(Compute eigenvalues (WALL)) : 6.137 7.12
Mflops
  Seclr4(Backtransform (CPU)) : 0.217 6.96
Mflops

```

```

Seclr4(Backtransform (WALL)) :          0.217          6.95
Mflops
  TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          7.4, SYNC =          0.0
  TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          7.4, 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
Optimum Blocksize for setup 160 Excess % 0.000D+00
Optimum Blocksize for diag 16 Excess % 0.000D+00
Base Blocksize 64 Diagonalization 192
  allocate H          0.3 MB          dimensions 191 191
  allocate S          0.3 MB          dimensions 191 191
  allocate spanel      0.1 MB          dimensions 191 64
  allocate hpanel      0.1 MB          dimensions 191 64
  allocate spanelus     0.1 MB          dimensions 191 64
  allocate slen         0.1 MB          dimensions 191 64
  allocate x2           0.1 MB          dimensions 191 64
  allocate legendre     1.2 MB          dimensions 191 13
64
  allocate al,bl (row)  0.1 MB          dimensions 191 11
  allocate al,bl (col)  0.0 MB          dimensions 64 11
  allocate YL           0.1 MB          dimensions 15 191
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) :          0.00          0.00
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) :	0.00	0.00
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
Time to synchronize (kpt) :	0.0	0.0
Scalapack Workspace size	1.06 Mb	
Seclr4(Transpose of H and S (CPU)) :	0.000	
Seclr4(Transpose of H and S (WALL)) :	0.000	
Seclr4(Cholesky complete (CPU)) :	0.235	46.13
Mflops		
Seclr4(Cholesky complete (WALL)) :	0.235	46.12
Mflops		
Seclr4(Transform to eig.problem (CPU)) :	0.543	59.78
Mflops		
Seclr4(Transform to eig.problem (WALL)) :	0.543	59.77
Mflops		
Seclr4(Compute eigenvalues (CPU)) :	6.251	6.92
Mflops		
Seclr4(Compute eigenvalues (WALL)) :	6.252	6.92
Mflops		
Seclr4(Backtransform (CPU)) :	0.215	7.22
Mflops		
Seclr4(Backtransform (WALL)) :	0.215	7.22
Mflops		
TIME HAMILT (CPU) =	0.0, HNS =	0.0, HORB = 0.0,
DIAG =	7.4, SYNC =	0.0
TIME HAMILT (WALL) =	0.0, HNS =	0.0, HORB = 0.0,
DIAG =	7.4, 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
Optimum Blocksize for setup 160 Excess %  0.000D+00
Optimum Blocksize for diag  16 Excess %  0.000D+00
Base Blocksize   64 Diagonalization  192
      allocate H          0.3 MB          dimensions  192   192
      allocate S          0.3 MB          dimensions  192   192
      allocate spanel     0.1 MB          dimensions  192    64
      allocate hpanel     0.1 MB          dimensions  192    64
      allocate spanelus   0.1 MB          dimensions  192    64
      allocate slen       0.1 MB          dimensions  192    64
      allocate x2         0.1 MB          dimensions  192    64
      allocate legendre   1.2 MB          dimensions  192    13
64
allocate al,bl (row)      0.1 MB          dimensions  192    11
allocate al,bl (col)     0.0 MB          dimensions    64    11
      allocate YL         0.1 MB          dimensions    15   192
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) :          0.00          0.00
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
Time to synchronize (kpt) :          0.0          0.0
Scalapack Workspace size  1.06 Mb
  Seclr4(Transpose of H and S (CPU)) :          0.000
  Seclr4(Transpose of H and S (WALL)) :          0.000
  Seclr4(Cholesky complete (CPU)) :          0.227          48.16
Mflops
  Seclr4(Cholesky complete (WALL)) :          0.227          48.14
Mflops
  Seclr4(Transform to eig.problem (CPU)) :          0.735          44.58
Mflops
  Seclr4(Transform to eig.problem (WALL)) :          0.735          44.57
Mflops
  Seclr4(Compute eigenvalues (CPU)) :          6.039          7.24
Mflops
  Seclr4(Compute eigenvalues (WALL)) :          6.039          7.23
Mflops

```

```

Seclr4(Backtransform (CPU)) :          0.281          5.47
Mflops
Seclr4(Backtransform (WALL)) :          0.281          5.46
Mflops
    TIME HAMILT (CPU)  =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          7.4, SYNC =          0.0
    TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          7.4, 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 -9.000000

```

Matrix size          320
Optimum Blocksize for setup 160 Excess % 0.000D+00
Optimum Blocksize for diag 16 Excess % 0.000D+00
Base Blocksize 64 Diagonalization 192
    allocate H          0.3 MB          dimensions 192 192
    allocate S          0.3 MB          dimensions 192 192
    allocate spanel      0.1 MB          dimensions 192 64
    allocate hpanel      0.1 MB          dimensions 192 64
    allocate spanelus    0.1 MB          dimensions 192 64
    allocate slen        0.1 MB          dimensions 192 64
    allocate x2          0.1 MB          dimensions 192 64
    allocate legendre    1.2 MB          dimensions 192 13
64
allocate al,bl (row)    0.1 MB          dimensions 192 11
allocate al,bl (col)    0.0 MB          dimensions 64 11
    allocate YL          0.1 MB          dimensions 15 192
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) :	0.00	0.00
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
Time to synchronize	(kpt) :	0.0	0.0
Scalapack Workspace size	1.06 Mb		
Seclr4(Transpose of H and S (CPU)) :		0.000	
Seclr4(Transpose of H and S (WALL)) :		0.000	
Seclr4(Cholesky complete (CPU)) :		0.183	59.80
Mflops			
Seclr4(Cholesky complete (WALL)) :		0.183	59.78
Mflops			
Seclr4(Transform to eig.problem (CPU)) :		0.589	55.63
Mflops			
Seclr4(Transform to eig.problem (WALL)) :		0.589	55.62
Mflops			
Seclr4(Compute eigenvalues (CPU)) :		6.037	7.24
Mflops			
Seclr4(Compute eigenvalues (WALL)) :		6.038	7.24
Mflops			
Seclr4(Backtransform (CPU)) :		0.293	5.25
Mflops			
Seclr4(Backtransform (WALL)) :		0.292	5.25
Mflops			
TIME HAMILT (CPU) =	0.0, HNS =	0.0, HORB =	0.0,
DIAG =	7.2, SYNC =	0.0	
TIME HAMILT (WALL) =	0.0, HNS =	0.0, HORB =	0.0,
DIAG =	7.2, 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 -9.00000

```

coors: iplus,nv,n=          0          258          260
Matrix size          322
Optimum Blocksize for setup 162 Excess % 0.125D+01
Optimum Blocksize for diag 18 Excess % 0.125D+01
Base Blocksize 64 Diagonalization 192
    allocate H          0.3 MB          dimensions 192 192
    allocate S          0.3 MB          dimensions 192 192
    allocate spanel      0.1 MB          dimensions 192 64
    allocate hpanel      0.1 MB          dimensions 192 64
    allocate spanelus    0.1 MB          dimensions 192 64
    allocate slen        0.1 MB          dimensions 192 64
    allocate x2          0.1 MB          dimensions 192 64
    allocate legendre    1.2 MB          dimensions 192 13
64
allocate al,bl (row)      0.1 MB          dimensions 192 11
allocate al,bl (col)     0.0 MB          dimensions 64 11
    allocate YL          0.1 MB          dimensions 15 192
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 0.00
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) : 0.00 0.00
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
Time to synchronize (kpt) : 0.0 0.0
Scalapack Workspace size 1.06 Mb
    Seclr4(Transpose of H and S (CPU)) : 0.000
    Seclr4(Transpose of H and S (WALL)) : 0.000
    Seclr4(Cholesky complete (CPU)) : 0.304 36.64
Mflops
    Seclr4(Cholesky complete (WALL)) : 0.304 36.63
Mflops
    Seclr4(Transform to eig.problem (CPU)) : 0.725 46.03
Mflops
    Seclr4(Transform to eig.problem (WALL)) : 0.725 46.02
Mflops
    Seclr4(Compute eigenvalues (CPU)) : 5.907 7.54
Mflops

```

```

Seclr4(Compute eigenvalues (WALL)) :          5.908          7.54
Mflops
Seclr4(Backtransform (CPU)) :          0.122          13.01
Mflops
Seclr4(Backtransform (WALL)) :          0.122          13.00
Mflops
TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          7.1, SYNC =          0.0
TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          7.1, 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
Optimum Blocksize for setup 162 Excess % 0.000D+00
Optimum Blocksize for diag 18 Excess % 0.000D+00
Base Blocksize 64 Diagonalization 192
allocate H          0.3 MB          dimensions 192 192
allocate S          0.3 MB          dimensions 192 192
allocate spanel      0.1 MB          dimensions 192 64
allocate hpanel      0.1 MB          dimensions 192 64
allocate spanelus    0.1 MB          dimensions 192 64
allocate slen        0.1 MB          dimensions 192 64
allocate x2          0.1 MB          dimensions 192 64
allocate legendre    1.2 MB          dimensions 192 13
64
allocate al,bl (row)  0.1 MB          dimensions 192 11
allocate al,bl (col)  0.0 MB          dimensions 64 11
allocate YL          0.1 MB          dimensions 15 192
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) :	0.00	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	0.00	
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) :	0.00	0.00	
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	
Time to synchronize (kpt) :	0.0	0.0	
Scalapack Workspace size	1.06 Mb		
Seclr4(Transpose of H and S (CPU)) :	0.000		
Seclr4(Transpose of H and S (WALL)) :	0.000		
Seclr4(Cholesky complete (CPU)) :	0.277	40.98	
Mflops			
Seclr4(Cholesky complete (WALL)) :	0.277	40.97	
Mflops			
Seclr4(Transform to eig.problem (CPU)) :	0.767	44.35	
Mflops			
Seclr4(Transform to eig.problem (WALL)) :	0.767	44.34	
Mflops			
Seclr4(Compute eigenvalues (CPU)) :	6.325	7.17	
Mflops			
Seclr4(Compute eigenvalues (WALL)) :	6.326	7.17	
Mflops			
Seclr4(Backtransform (CPU)) :	0.239	6.69	
Mflops			
Seclr4(Backtransform (WALL)) :	0.239	6.69	
Mflops			
TIME HAMILT (CPU) =	0.0, HNS =	0.0, HORB =	0.0,
DIAG =	7.7, SYNC =	0.0	
TIME HAMILT (WALL) =	0.0, HNS =	0.0, HORB =	0.0,
DIAG =	7.7, 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
Optimum Blocksize for setup 162 Excess % 0.125D+01
Optimum Blocksize for diag 18 Excess % 0.125D+01
Base Blocksize 64 Diagonalization 192
      allocate H          0.3 MB          dimensions 192 192
      allocate S          0.3 MB          dimensions 192 192
      allocate spanel     0.1 MB          dimensions 192 64
      allocate hpanel     0.1 MB          dimensions 192 64
      allocate spanelus   0.1 MB          dimensions 192 64
      allocate slen       0.1 MB          dimensions 192 64
      allocate x2         0.1 MB          dimensions 192 64
      allocate legendre   1.2 MB          dimensions 192 13
64
allocate al,bl (row)      0.1 MB          dimensions 192 11
allocate al,bl (col)     0.0 MB          dimensions 64 11
      allocate YL         0.1 MB          dimensions 15 192
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) :      0.02      0.02
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      0.00
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) :      0.00      0.00
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
Time to synchronize (kpt) :      0.0      0.0
Scalapack Workspace size 1.06 Mb
  Seclr4(Transpose of H and S (CPU)) :      0.000
  Seclr4(Transpose of H and S (WALL)) :      0.000
  Seclr4(Cholesky complete (CPU)) :      0.310      35.85
Mflops
  Seclr4(Cholesky complete (WALL)) :      0.310      35.84
Mflops
  Seclr4(Transform to eig.problem (CPU)) :      0.887      37.66
Mflops
  Seclr4(Transform to eig.problem (WALL)) :      0.887      37.66
Mflops

```

```

Seclr4(Compute eigenvalues (CPU)) :          5.790          7.69
Mflops
Seclr4(Compute eigenvalues (WALL)) :          5.791          7.69
Mflops
Seclr4(Backtransform (CPU)) :                0.284          5.58
Mflops
Seclr4(Backtransform (WALL)) :                0.284          5.58
Mflops
TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          7.4, SYNC =          0.0
TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          7.4, 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
Optimum Blocksize for setup 162 Excess % 0.125D+01
Optimum Blocksize for diag 18 Excess % 0.125D+01
Base Blocksize 64 Diagonalization 192
allocate H          0.3 MB          dimensions 192 192
allocate S          0.3 MB          dimensions 192 192
allocate spanel      0.1 MB          dimensions 192 64
allocate hpanel      0.1 MB          dimensions 192 64
allocate spanelus    0.1 MB          dimensions 192 64
allocate slen        0.1 MB          dimensions 192 64
allocate x2          0.1 MB          dimensions 192 64
allocate legendre    1.2 MB          dimensions 192 13
64
allocate al,bl (row) 0.1 MB          dimensions 192 11
allocate al,bl (col) 0.0 MB          dimensions 64 11
allocate YL          0.1 MB          dimensions 15 192
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) :          0.00          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          0.00
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) :          0.00          0.00
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
Time to synchronize (kpt) :          0.0          0.0
Scalapack Workspace size 1.06 Mb
  Seclr4(Transpose of H and S (CPU)) :          0.000
  Seclr4(Transpose of H and S (WALL)) :          0.000
  Seclr4(Cholesky complete (CPU)) :          0.220          50.09
Mflops
  Seclr4(Cholesky complete (WALL)) :          0.220          50.09
Mflops
  Seclr4(Transform to eig.problem (CPU)) :          0.737          44.85
Mflops
  Seclr4(Transform to eig.problem (WALL)) :          0.738          44.84
Mflops
  Seclr4(Compute eigenvalues (CPU)) :          6.445          6.84
Mflops
  Seclr4(Compute eigenvalues (WALL)) :          6.446          6.84
Mflops
  Seclr4(Backtransform (CPU)) :          0.220          7.15
Mflops
  Seclr4(Backtransform (WALL)) :          0.220          7.15
Mflops
  TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          7.7, SYNC =          0.0
  TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          7.7, 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 -9.00000

```

coors: iplus,nv,n=          0          259          251
Matrix size          313
Optimum Blocksize for setup 158 Excess % 0.128D+01
Optimum Blocksize for diag 16 Excess % 0.386D+01
Base Blocksize 64 Diagonalization 192
    allocate H          0.3 MB          dimensions 185 185
    allocate S          0.3 MB          dimensions 185 185
    allocate spanel     0.1 MB          dimensions 185 64
    allocate hpanel     0.1 MB          dimensions 185 64
    allocate spanelus   0.1 MB          dimensions 185 64
    allocate slen       0.1 MB          dimensions 185 64
    allocate x2         0.1 MB          dimensions 185 64
    allocate legendre   1.2 MB          dimensions 185 13
64
allocate al,bl (row)     0.1 MB          dimensions 185 11
allocate al,bl (col)    0.0 MB          dimensions 64 11
    allocate YL          0.1 MB          dimensions 15 185
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) : 0.00 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) : 0.00 0.00
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
Time to synchronize (kpt) : 0.0 0.0
Scalapack Workspace size 1.05 Mb
  Seclr4(Transpose of H and S (CPU)) : 0.000
  Seclr4(Transpose of H and S (WALL)) : 0.000
  Seclr4(Cholesky complete (CPU)) : 0.195 52.30
Mflops
  Seclr4(Cholesky complete (WALL)) : 0.195 52.31
Mflops
  Seclr4(Transform to eig.problem (CPU)) : 0.652 47.06
Mflops

```

```

Seclr4(Transform to eig.problem (WALL)) :      0.652      47.05
Mflops
Seclr4(Compute eigenvalues (CPU)) :           6.301      6.49
Mflops
Seclr4(Compute eigenvalues (WALL)) :           6.302      6.49
Mflops
Seclr4(Backtransform (CPU)) :                 0.282      5.20
Mflops
Seclr4(Backtransform (WALL)) :                 0.283      5.20
Mflops
TIME HAMILT (CPU) =      0.0, HNS =      0.0, HORB =      0.0,
DIAG =      7.6, SYNC =      0.0
TIME HAMILT (WALL) =      0.0, HNS =      0.0, HORB =      0.0,
DIAG =      7.6, 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
Optimum Blocksize for setup 162 Excess % 0.125D+01
Optimum Blocksize for diag 18 Excess % 0.125D+01
Base Blocksize 64 Diagonalization 192
allocate H      0.3 MB      dimensions 192 192
allocate S      0.3 MB      dimensions 192 192
allocate spanel 0.1 MB      dimensions 192 64
allocate hpanel 0.1 MB      dimensions 192 64
allocate spanelus 0.1 MB      dimensions 192 64
allocate slen 0.1 MB      dimensions 192 64
allocate x2 0.1 MB      dimensions 192 64
allocate legendre 1.2 MB      dimensions 192 13
64
allocate al,bl (row) 0.1 MB      dimensions 192 11
allocate al,bl (col) 0.0 MB      dimensions 64 11

```

```

        allocate YL          0.1 MB          dimensions    15    192
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) :      0.00      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      0.02
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) :      0.00      0.00
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
Time to synchronize (kpt) :      0.0      0.0
Scalapack Workspace size      1.06 Mb
  Seclr4(Transpose of H and S (CPU)) :      0.000
  Seclr4(Transpose of H and S (WALL)) :      0.000
  Seclr4(Cholesky complete (CPU)) :      0.259      42.63
Mflops
  Seclr4(Cholesky complete (WALL)) :      0.259      42.62
Mflops
  Seclr4(Transform to eig.problem (CPU)) :      0.821      40.27
Mflops
  Seclr4(Transform to eig.problem (WALL)) :      0.821      40.27
Mflops
  Seclr4(Compute eigenvalues (CPU)) :      6.182      7.13
Mflops
  Seclr4(Compute eigenvalues (WALL)) :      6.183      7.13
Mflops
  Seclr4(Backtransform (CPU)) :      0.201      7.81
Mflops
  Seclr4(Backtransform (WALL)) :      0.201      7.81
Mflops
  TIME HAMILT (CPU) =      0.0, HNS =      0.0, HORB =      0.0,
DIAG =      7.6, SYNC =      0.0
  TIME HAMILT (WALL) =      0.0, HNS =      0.0, HORB =      0.0,
DIAG =      7.6, 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
Optimum Blocksize for setup 160 Excess %  0.000D+00
Optimum Blocksize for diag  16 Excess %  0.000D+00
Base Blocksize   64 Diagonalization  192
      allocate H          0.3 MB          dimensions  191  191
      allocate S          0.3 MB          dimensions  191  191
      allocate spanel      0.1 MB          dimensions  191   64
      allocate hpanel      0.1 MB          dimensions  191   64
      allocate spanelus    0.1 MB          dimensions  191   64
      allocate slen        0.1 MB          dimensions  191   64
      allocate x2          0.1 MB          dimensions  191   64
      allocate legendre    1.2 MB          dimensions  191   13
64
allocate al,bl (row)      0.1 MB          dimensions  191   11
allocate al,bl (col)      0.0 MB          dimensions   64   11
      allocate YL          0.1 MB          dimensions   15  191
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) :          0.00           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) :               0.00           0.00
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
Time to synchronize (kpt) :         0.0           0.0
Scalapack Workspace size      1.06 Mb
  Seclr4(Transpose of H and S (CPU)) :           0.000
  Seclr4(Transpose of H and S (WALL)) :           0.000
  Seclr4(Cholesky complete (CPU)) :           0.192           56.34
Mflops

```



```

Seclr4(Cholesky complete (WALL)) :          0.192          56.33
Mflops
Seclr4(Transform to eig.problem (CPU)) :      0.508          63.94
Mflops
Seclr4(Transform to eig.problem (WALL)) :      0.508          63.94
Mflops
Seclr4(Compute eigenvalues (CPU)) :           5.196           8.33
Mflops
Seclr4(Compute eigenvalues (WALL)) :           5.197           8.33
Mflops
Seclr4(Backtransform (CPU)) :                 0.232           6.81
Mflops
Seclr4(Backtransform (WALL)) :                 0.232           6.81
Mflops
TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          6.2, SYNC =          0.0
TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          6.2, 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  -9.000000
*****

```

```

coors: iplus,nv,n=          0          257          259
Matrix size          321
Optimum Blocksize for setup 162 Excess %  0.125D+01
Optimum Blocksize for diag  18 Excess %  0.125D+01
Base Blocksize   64 Diagonalization  192
      allocate H          0.3 MB          dimensions  192  192
      allocate S          0.3 MB          dimensions  192  192
      allocate spanel      0.1 MB          dimensions  192   64
      allocate hpanel      0.1 MB          dimensions  192   64
      allocate spanelus    0.1 MB          dimensions  192   64
      allocate slen        0.1 MB          dimensions  192   64
      allocate x2          0.1 MB          dimensions  192   64

```

allocate legendre	1.2 MB	dimensions	192	13
64				
allocate al,bl (row)	0.1 MB	dimensions	192	11
allocate al,bl (col)	0.0 MB	dimensions	64	11
allocate YL	0.1 MB	dimensions	15	192
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) :		0.00	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) :		0.00	0.00	
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		
Time to synchronize (kpt) :	0.0	0.0		
Scalapack Workspace size	1.06 Mb			
Seclr4(Transpose of H and S (CPU)) :		0.000		
Seclr4(Transpose of H and S (WALL)) :		0.000		
Seclr4(Cholesky complete (CPU)) :		0.170	64.92	
Mflops				
Seclr4(Cholesky complete (WALL)) :		0.170	64.93	
Mflops				
Seclr4(Transform to eig.problem (CPU)) :		0.808	40.92	
Mflops				
Seclr4(Transform to eig.problem (WALL)) :		0.808	40.92	
Mflops				
Seclr4(Compute eigenvalues (CPU)) :		6.157	7.16	
Mflops				
Seclr4(Compute eigenvalues (WALL)) :		6.158	7.16	
Mflops				
Seclr4(Backtransform (CPU)) :		0.247	6.46	
Mflops				
Seclr4(Backtransform (WALL)) :		0.247	6.46	
Mflops				
TIME HAMILT (CPU) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	7.4, SYNC =	0.0		
TIME HAMILT (WALL) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	7.4, 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 -9.00000

```

coors: iplus,nv,n=          0          259          263
Matrix size          325
Optimum Blocksize for setup 164 Excess % 0.123D+01
Optimum Blocksize for diag 24 Excess % 0.623D+01
Base Blocksize 64 Diagonalization 192
    allocate H          0.3 MB          dimensions 192 192
    allocate S          0.3 MB          dimensions 192 192
    allocate spanel     0.1 MB          dimensions 192 64
    allocate hpanel     0.1 MB          dimensions 192 64
    allocate spanelus   0.1 MB          dimensions 192 64
    allocate slen       0.1 MB          dimensions 192 64
    allocate x2         0.1 MB          dimensions 192 64
    allocate legendre   1.2 MB          dimensions 192 13
64
allocate al,bl (row)    0.1 MB          dimensions 192 11
allocate al,bl (col)    0.0 MB          dimensions 64 11
    allocate YL         0.1 MB          dimensions 15 192
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) : 0.00 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 0.00
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) : 0.00 0.00
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
Time to synchronize (kpt) : 0.0 0.0
Scalapack Workspace size 1.06 Mb
Sec1r4(Transpose of H and S (CPU)) : 0.000

```

```

Seclr4(Transpose of H and S (WALL)) :          0.000
Seclr4(Cholesky complete (CPU)) :             0.266          42.99
Mflops
Seclr4(Cholesky complete (WALL)) :             0.266          42.99
Mflops
Seclr4(Transform to eig.problem (CPU)) :         0.828          41.44
Mflops
Seclr4(Transform to eig.problem (WALL)) :         0.828          41.43
Mflops
Seclr4(Compute eigenvalues (CPU)) :             6.211           7.37
Mflops
Seclr4(Compute eigenvalues (WALL)) :             6.212           7.37
Mflops
Seclr4(Backtransform (CPU)) :                   0.255           6.32
Mflops
Seclr4(Backtransform (WALL)) :                   0.255           6.32
Mflops
TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          7.7, SYNC =          0.0
TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          7.7, 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
Optimum Blocksize for setup 164 Excess % 0.000D+00
Optimum Blocksize for diag 24 Excess % 0.494D+01
Base Blocksize 64 Diagonalization 192
allocate H          0.3 MB          dimensions 192 192
allocate S          0.3 MB          dimensions 192 192
allocate spanel     0.1 MB          dimensions 192 64
allocate hpanel     0.1 MB          dimensions 192 64
allocate spanelus   0.1 MB          dimensions 192 64

```

allocate slen	0.1 MB	dimensions	192	64
allocate x2	0.1 MB	dimensions	192	64
allocate legendre	1.2 MB	dimensions	192	13
64				
allocate al,bl (row)	0.1 MB	dimensions	192	11
allocate al,bl (col)	0.0 MB	dimensions	64	11
allocate YL	0.1 MB	dimensions	15	192
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) :		0.00	0.00	
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) :		0.00	0.00	
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		
Time to synchronize (kpt) :	0.0	0.0		
Scalapack Workspace size	1.07 Mb			
Seclr4(Transpose of H and S (CPU)) :		0.000		
Seclr4(Transpose of H and S (WALL)) :		0.000		
Seclr4(Cholesky complete (CPU)) :		0.297	39.30	
Mflops				
Seclr4(Cholesky complete (WALL)) :		0.297	39.28	
Mflops				
Seclr4(Transform to eig.problem (CPU)) :		0.784	44.61	
Mflops				
Seclr4(Transform to eig.problem (WALL)) :		0.784	44.60	
Mflops				
Seclr4(Compute eigenvalues (CPU)) :		6.144	7.59	
Mflops				
Seclr4(Compute eigenvalues (WALL)) :		6.145	7.59	
Mflops				
Seclr4(Backtransform (CPU)) :		0.274	5.95	
Mflops				
Seclr4(Backtransform (WALL)) :		0.274	5.95	
Mflops				
TIME HAMILT (CPU) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	7.5, SYNC =	0.0		
TIME HAMILT (WALL) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	7.5, 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
Optimum Blocksize for setup 164 Excess % 0.000D+00
Optimum Blocksize for diag 24 Excess % 0.494D+01
Base Blocksize 64 Diagonalization 192
    allocate H          0.3 MB          dimensions 192 192
    allocate S          0.3 MB          dimensions 192 192
    allocate spanel     0.1 MB          dimensions 192 64
    allocate hpanel     0.1 MB          dimensions 192 64
    allocate spanelus   0.1 MB          dimensions 192 64
    allocate slen       0.1 MB          dimensions 192 64
    allocate x2         0.1 MB          dimensions 192 64
    allocate legendre   1.2 MB          dimensions 192 13
64
allocate al,bl (row)    0.1 MB          dimensions 192 11
allocate al,bl (col)    0.0 MB          dimensions 64 11
    allocate YL         0.1 MB          dimensions 15 192
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) :      0.00      0.00
Time for us (hamilt, cpu/wall) :      0.00      0.00
Time for overlaps (hamilt, cpu/wall) :      0.00      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) :      0.00      0.00
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
Time to synchronize (kpt) :      0.0      0.0
Scalapack Workspace size 1.07 Mb

```

```

Seclr4(Transpose of H and S (CPU)) :          0.000
Seclr4(Transpose of H and S (WALL)) :          0.000
Seclr4(Cholesky complete (CPU)) :             0.308          37.81
Mflops
Seclr4(Cholesky complete (WALL)) :             0.308          37.80
Mflops
Seclr4(Transform to eig.problem (CPU)) :         0.642          54.45
Mflops
Seclr4(Transform to eig.problem (WALL)) :         0.642          54.45
Mflops
Seclr4(Compute eigenvalues (CPU)) :             5.831           7.99
Mflops
Seclr4(Compute eigenvalues (WALL)) :             5.832           7.99
Mflops
Seclr4(Backtransform (CPU)) :                   0.143          11.57
Mflops
Seclr4(Backtransform (WALL)) :                   0.143          11.57
Mflops
TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          7.1, SYNC =          0.0
TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          7.1, 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
Optimum Blocksize for setup 166 Excess % 0.122D+01
Optimum Blocksize for diag 24 Excess % 0.367D+01
Base Blocksize 64 Diagonalization 192
allocate H          0.3 MB          dimensions 192 192
allocate S          0.3 MB          dimensions 192 192
allocate spanel     0.1 MB          dimensions 192 64
allocate hpanel     0.1 MB          dimensions 192 64

```

allocate spanelus	0.1 MB	dimensions	192	64
allocate slen	0.1 MB	dimensions	192	64
allocate x2	0.1 MB	dimensions	192	64
allocate legendre	1.2 MB	dimensions	192	13
64				
allocate al,bl (row)	0.1 MB	dimensions	192	11
allocate al,bl (col)	0.0 MB	dimensions	64	11
allocate YL	0.1 MB	dimensions	15	192
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) :		0.00	0.00	
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) :		0.00	0.00	
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		
Time to synchronize (kpt) :	0.0	0.0		
Scalapack Workspace size	1.07 Mb			
Seclr4(Transpose of H and S (CPU)) :		0.000		
Seclr4(Transpose of H and S (WALL)) :		0.000		
Seclr4(Cholesky complete (CPU)) :		0.301	39.41	
Mflops				
Seclr4(Cholesky complete (WALL)) :		0.301	39.40	
Mflops				
Seclr4(Transform to eig.problem (CPU)) :		1.012	35.19	
Mflops				
Seclr4(Transform to eig.problem (WALL)) :		1.012	35.19	
Mflops				
Seclr4(Compute eigenvalues (CPU)) :		6.424	7.39	
Mflops				
Seclr4(Compute eigenvalues (WALL)) :		6.425	7.39	
Mflops				
Seclr4(Backtransform (CPU)) :		0.248	6.66	
Mflops				
Seclr4(Backtransform (WALL)) :		0.248	6.66	
Mflops				
TIME HAMILT (CPU) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	8.2, SYNC =	0.0		
TIME HAMILT (WALL) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	8.2, 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
Optimum Blocksize for setup 164 Excess % 0.000D+00
Optimum Blocksize for diag 24 Excess % 0.494D+01
Base Blocksize 64 Diagonalization 192
    allocate H          0.3 MB          dimensions 192 192
    allocate S          0.3 MB          dimensions 192 192
    allocate spanel      0.1 MB          dimensions 192 64
    allocate hpanel      0.1 MB          dimensions 192 64
    allocate spanelus    0.1 MB          dimensions 192 64
    allocate slen        0.1 MB          dimensions 192 64
    allocate x2          0.1 MB          dimensions 192 64
    allocate legendre    1.2 MB          dimensions 192 13
64
    allocate al,bl (row)  0.1 MB          dimensions 192 11
    allocate al,bl (col)  0.0 MB          dimensions 64 11
    allocate YL          0.1 MB          dimensions 15 192
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) : 0.00 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 0.00
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) : 0.00 0.00
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

```

```

Time to synchronize (kpt) :          0.0          0.0
Scalapack Workspace size    1.07 Mb
  Seclr4(Transpose of H and S (CPU)) :          0.000
  Seclr4(Transpose of H and S (WALL)) :          0.000
  Seclr4(Cholesky complete (CPU)) :          0.303          38.79
Mflops
  Seclr4(Cholesky complete (WALL)) :          0.303          38.78
Mflops
  Seclr4(Transform to eig.problem (CPU)) :          0.829          42.56
Mflops
  Seclr4(Transform to eig.problem (WALL)) :          0.829          42.55
Mflops
  Seclr4(Compute eigenvalues (CPU)) :          8.010          5.87
Mflops
  Seclr4(Compute eigenvalues (WALL)) :         10.447          4.50
Mflops
  Seclr4(Backtransform (CPU)) :          0.038          42.80
Mflops
  Seclr4(Backtransform (WALL)) :          0.047          34.56
Mflops
  TIME HAMILT (CPU) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =          9.3, SYNC =          0.0
  TIME HAMILT (WALL) =          0.0, HNS =          0.0, HORB =          0.0,
DIAG =         11.8, 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 -9.00000
*****

```

```

coors: iplus,nv,n=          0          266          280
Matrix size          342
Optimum Blocksize for setup 172 Excess % 0.117D+01
Optimum Blocksize for diag 16 Excess % 0.593D+01
Base Blocksize 64 Diagonalization 192
  allocate H          0.3 MB          dimensions 192 192
  allocate S          0.3 MB          dimensions 192 192

```

allocate spanel	0.1 MB	dimensions	192	64
allocate hpanel	0.1 MB	dimensions	192	64
allocate spanelus	0.1 MB	dimensions	192	64
allocate slen	0.1 MB	dimensions	192	64
allocate x2	0.1 MB	dimensions	192	64
allocate legendre	1.2 MB	dimensions	192	13
64				
allocate al,bl (row)	0.1 MB	dimensions	192	11
allocate al,bl (col)	0.0 MB	dimensions	64	11
allocate YL	0.1 MB	dimensions	15	192
3				
number of local orbitals, nlo (hamilt)		62		
allocate YL	0.3 MB	dimensions	15	342
3				
allocate phsc	0.0 MB	dimensions	342	
Time for al,bl (hamilt, cpu/wall) :		0.00	0.00	
Time for legendre (hamilt, cpu/wall) :		0.00	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	0.00	
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) :		0.00	0.00	
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		
Time to synchronize (kpt) :	0.0	0.0		
Scalapack Workspace size	1.09 Mb			
Seclr4(Transpose of H and S (CPU)) :		0.000		
Seclr4(Transpose of H and S (WALL)) :		0.000		
Seclr4(Cholesky complete (CPU)) :		0.245		54.37
Mflops				
Seclr4(Cholesky complete (WALL)) :		0.245		54.36
Mflops				
Seclr4(Transform to eig.problem (CPU)) :		0.970		41.25
Mflops				
Seclr4(Transform to eig.problem (WALL)) :		0.970		41.24
Mflops				
Seclr4(Compute eigenvalues (CPU)) :		8.011		6.66
Mflops				
Seclr4(Compute eigenvalues (WALL)) :		8.012		6.66
Mflops				
Seclr4(Backtransform (CPU)) :		0.114		15.41
Mflops				
Seclr4(Backtransform (WALL)) :		0.114		15.40
Mflops				
TIME HAMILT (CPU) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	9.4, SYNC =	0.0		
TIME HAMILT (WALL) =	0.0, HNS =	0.0, HORB =	0.0,	
DIAG =	9.4, 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: 9.5 (INIT = 0.0 + K-POINTS =
 9.5)
 > SUM OF WALL CLOCK TIMES: 9.5 (INIT = 0.1 + K-POINTS =
 9.5)
 Maximum WALL clock time: 255.822799999998
 Maximum CPU time: 249.875403000000