Value of Oscillator strength: 18.426968 for A: 4.000000 Value of V1 = -23.359549Value of V1 = -4.932579Value of V1 = 13.494385Value of V1 = 31.921356Value of V1 = 50.348320Value of V1 = 68.775291Value of V1 = 87.202255! n 1 2j 2tz (2n+1)e hole/p Modelspace 0 0 1 1 0 -23.4 hole outside 0 1 3 1 1 -5.0 particle inside 0 1 1 1 1 -5.0 particle inside 0 2 5 1 2 13.4 particle outside 0 2 3 1 2 13.4 particle outside 1 0 1 1 2 13.4 particle outside 0 3 7 1 3 31.8 particle outside 0 3 5 1 3 31.8 particle outside 1 1 3 1 3 31.8 particle outside 1 1 1 1 3 31.8 particle outside E = (N+1.5)hwValue of Oscillator strength: 13.921007 for A: 16.000000 Value of V1 = -30.118488Value of V1 = -16.197483Value of V1 = -2.276474Value of V1 = 11.644531Value of V1 = 25.565536Value of V1 = 39.486549Value of V1 = 53.407555

```
! n 1 2j 2tz (2n+1)e hole/p Modelspace
0 0 1 1 0 -33.0 hole outside
0 1 3 1 1 -19.0 hole outside
0 1 1 1 1 -19.0 hole outside
0 2 5 1 2 -5.0 particle inside
0 2 3 1 2 -5.0 particle inside
1 0 1 1 2 -5.0 particle inside
0 3 7 1 3 9.0 particle outside
0 3 5 1 3 9.0 particle outside
1 1 3 1 3 9.0 particle outside
1 1 1 1 3 9.0 particle outside
```

Value of Oscillator strength: 11.020609 for A: 40.000000

Value of V1 = -34.469086 Value of V1 = -23.448479 Value of V1 = -12.427868 Value of V1 = -1.407261 Value of V1 = 9.613350 Value of V1 = 20.633957 Value of V1 = 31.654564

! n 1 2j 2tz (2n+l)e hole/p Modelspace 0 0 1 1 0 -43.0 hole outside 0 1 3 1 1 -32.0 hole outside 0 1 1 1 1 -32.0 hole outside 0 2 5 1 2 -21.0 hole outside 0 2 3 1 2 -21.0 hole outside 0 1 1 2 -21.0 hole outside 0 3 7 1 3 -10.0 particle inside 0 3 5 1 3 -10.0 particle inside 1 1 3 1 3 -10.0 particle inside 1 1 1 1 3 -10.0 particle inside 0 4 9 1 4 0.0 particle outside 0 4 7 1 4 0.0 particle outside 1 2 5 1 4 0.0 particle outside 1 2 3 1 4 0.0 particle outside 2 0 1 1 4 0.0 particle outside

# For (N+1.5)hw

Value of Oscillator strength: 10.489394 for A: 48.000000 Value of V1 = -29.765909 Value of V1 = -19.276514 Value of V1 = -8.787121 Value of V1 = 1.702274 Value of V1 = 12.191669 Value of V1 = 22.681061 Value of V1 = 33.170456

#### For (N+0.5)hw

Value of Oscillator strength: 10.489394 for A: 48.000000 Value of V1 = -40.255302 Value of V1 = -29.765909 Value of V1 = -19.276514 Value of V1 = -8.787121 Value of V1 = 1.702274 Value of V1 = 12.191669 Value of V1 = 22.681061

# ! n l 2j 2tz (2n+l)e hole/p Modelspace

```
0 1 -1 0 -41.5 hole
                          outside
  1 3 -1 1 -31.0 hole
                          outside
  1 1 -1 1 -31.0 hole
                          outside
  2 5 -1 2 -20.5 hole
                          outside
  2 3 -1 2 -20.5 hole
                          outside
  0 1 -1 2 -20.5 hole
                          outside
  3 7 -1 3 -10.0 particle inside
  3 5 -1 3 -10.0 particle inside
  1 3 -1 3 -10.0 particle inside
  1 1 -1 3 -10.0 particle inside
  4 9 -1 4 0.5 particle outside
  4 7 -1 4 0.5 particle outside
  2 5 -1 4 0.5 particle outside
  2 3 -1 4 0.5 particle outside
2 0 1 -1 4 0.5 particle outside
0 5 11 -1 5 0.5 particle outside
```

## E = (n+1.5)hw

Value of Oscillator strength: 10.054079 for A: 56.000000 Value of V1 = -35.918880 Value of V1 = -25.864803 Value of V1 = -15.810722 Value of V1 = -5.756645 Value of V1 = 4.297436 Value of V1 = 14.351517

Value of V1 = 24.405594

#### E = (n+0.0)hw

Value of Oscillator strength: 10.054079 for A: 56.000000

Value of V1 = -51.000000 Value of V1 = -40.945923 Value of V1 = -30.891842 Value of V1 = -20.837763 Value of V1 = -10.783684

Value of V1 = -0.729607

Value of V1 = 9.324474

! n 1 2j 2tz (2n+1)e hole/p Modelspace 0 0 1 1 0 -50.0 hole outside 1 3 1 1 -40.0 hole outside 1 1 1 -40.0 hole outside 2 5 1 2 -30.0 hole outside 2 3 1 2 -30.0 hole outside 1 1 2 -30.0 hole outside 3 7 1 3 -20.0 hole outside 3 5 1 4 -10.0 particle inside

```
1 1 3 1 4 -10.0 particle inside

1 1 1 1 4 -10.0 particle inside

0 4 9 1 4 -10.0 particle inside

0 4 7 1 5 0.0 particle outside

1 2 5 1 5 0.0 particle outside

1 2 3 1 5 0.0 particle outside

2 0 1 1 5 0.0 particle outside

0 5 11 1 5 0.0 particle outside

0 5 9 1 6 10.0 particle outside

1 3 7 1 6 10.0 particle outside

1 3 5 1 6 10.0 particle outside

2 1 3 1 6 10.0 particle outside

1 3 7 1 6 10.0 particle outside
```

```
Value of Oscillator strength: 9.162642 for A: 78.000000
Value of V1 = -41.692307
Value of V1 = -32.529663
Value of V1 = -23.367023
Value of V1 = -14.204382
Value of V1 = -5.041740
Value of V1 = 4.120903
Value of V1 = 13.283543
! n 1 2j 2tz (2n+l)e hole/p Modelspace
 0 0 1 -1 0 -46.0 hole
                           outside
   1 3 -1 1 -37.0 hole
                            outside
   1 1 -1 1 -37.0 hole
                            outside
    2 5 -1 2 -28.0 hole
                            outside
    2 3 -1 2 -28.0 hole
                            outside
    0 1 -1 2 -28.0 hole
                            outside
    3 7 -1 3 -19.0 hole
                            outside
      5 -1 4 -10.0 particle inside
       3 -1 4 -10.0 particle inside
      1 -1 4 -10.0 particle inside
       9 -1 4 -10.0 particle inside
    4 7 -1 5 -1.0 particle outside
    2 5 -1 5 -1.0 particle outside
    2 3 -1 5 -1.0 particle outside
    0 1 -1 5 -1.0 particle outside
    5 11 -1 6 8.0 particle outside
       9 -1 6 8.0 particle outside
    3 7 -1 6 8.0 particle outside
    3 5 -1 6 8.0 particle outside
    1 3 -1 6 8.0 particle outside
    1 1 -1 6 8.0 particle outside
    6 13 -1 7 17.0 particle outside
    6 11 -1 7 17.0 particle outside
    4 9 -1 7 17.0 particle outside
    4 7 -1 7 17.0 particle outside
    2 5 -1 7 17.0 particle outside
```

2 3 -1 7 17.0 particle outside

## E = (N+0)hw

```
Value of Oscillator strength: 8.853373 for A: 88.000000 Value of V1 = -46.500000 Value of V1 = -37.646629 Value of V1 = -28.793255 Value of V1 = -19.939882 Value of V1 = -11.086510 Value of V1 = -2.233139 Value of V1 = 6.620235
```

```
! n l 2j 2tz (2n+l)e hole/p Modelspace
 0 0 1 -1 0 -46.0 hole
                           outside
   1 3 -1 1 -37.0 hole
                           outside
      1 -1 1 -37.0 hole
                           outside
    2 5 -1 2 -28.0 hole
                           outside
    2 3 -1 2 -28.0 hole
                           outside
      1 -1 2 -28.0 hole
                           outside
    3 7 -1 3 -19.0 hole
                            outside
    3 5 -1 3 -19.0 hole
                            outside
       3 -1 3 -19.0 hole
                            outside
    1 1 -1 4 -10.0 particle inside
       9 -1 4 -10.0 particle inside
    4 7 -1 5 -1.0 particle outside
    2 5 -1 5 -1.0 particle outside
    2 3 -1 5 -1.0 particle outside
    0 1 -1 5 -1.0 particle outside
   5 11 -1 5 -1.0 particle outside
    5 9 -1 6 8.0 particle outside
    3 7 -1 6 8.0 particle outside
    3 5 -1 6 8.0 particle outside
   1 3 -1 6 8.0 particle outside
   1 1 -1 6 8.0 particle outside
    6 13 -1 6 8.0 particle outside
    6 11 -1 7 17.0 particle outside
    4 9 -1 7 17.0 particle outside
    4 7 -1 7 17.0 particle outside
   2 5 -1 7 17.0 particle outside
   2 3 -1 7 17.0 particle outside
 3 0 1 -1 7 17.0 particle outside
```

```
Value of V1 = -51.000000
Value of V1 = -42.465443
Value of V1 = -33.930885
Value of V1 = -25.396324
Value of V1 = -16.861767
Value of V1 = -8.327209
Value of V1 = 0.207352
! n 1 2j 2tz (2n+1)e hole/p Modelspace
 0 0 1 -1 0 -52.5 hole
                           outside
 0 1 3 -1 1 -44.0 hole
                           outside
   1 1 -1 1 -44.0 hole
                           outside
    2 5 -1 2 -35.5 hole
                            outside
    2 3 -1 2 -35.5 hole
                            outside
    0 1 -1 2 -35.5 hole
                            outside
    3 7 -1 3 -27.0 hole
                            outside
   3 5 -1 4 -18.5 hole
                            outside
    1 3 -1 4 -18.5 hole
                            outside
      1 -1 4 -18.5 hole
                            outside
       9 -1 4 -18.5 hole
                            outside
   4 7 -1 5 -10.0 particle inside
    2 5 -1 5 -10.0 particle inside
    2 3 -1 5 -10.0 particle inside
 2 0 1 -1 5 -10.0 particle inside
   5 11 -1 5 -10.0 particle inside
   5 9 -1 6 -1.5 particle outside
    3 7 -1 6 -1.5 particle outside
   3 5 -1 6 -1.5 particle outside
   1 3 -1 6 -1.5 particle outside
 2 1 1 -1 6 -1.5 particle outside
   6 13 -1 6 -1.5 particle outside
   6 11 -1 7 7.0 particle outside
    4 9 -1 7 7.0 particle outside
   4 7 -1 7 7.0 particle outside
 2
   2 5 -1 7 7.0 particle outside
 2 2 3 -1 7 7.0 particle outside
 3 0 1 -1 7 7.0 particle outside
E = (N-1.0)hw
Value of Oscillator strength: 7.873684 for A: 132.000000
Value of V1 = -50.873684
Value of V1 = -43.000000
Value of V1 = -35.126316
Value of V1 = -27.252632
Value of V1 = -19.378946
```

Value of V1 = -11.505262Value of V1 = -3.631577

Value of Oscillator strength: 8.534558 for A: 100.000000

! n 1 2j 2tz (2n+l)e hole/p Modelspace 0 0 1 -1 0 -50.0 hole outside outside 3 -1 1 -42.0 hole 1 -42 0 hole outside 2 5 -1 2 -34.0 hole outside 2 3 -1 2 -34.0 hole outside 1 -1 2 -34.0 hole outside 7 -1 3 -26.0 hole outside 5 -1 4 -18.0 hole outside 3 -1 4 -18.0 hole outside 1 -1 4 -18.0 hole outside 9 -1 4 -18.0 hole outside 7 -1 5 -10.0 particle inside 2 5 -1 5 -10.0 particle inside 2 3 -1 5 -10.0 particle inside 0 1 -1 5 -10.0 particle inside 5 11 -1 5 -10.0 particle inside 9 -1 6 -2.0 particle outside 7 -1 6 -2.0 particle outside 3 5 -1 6 -2.0 particle outside 1 3 -1 6 -2.0 particle outside 1 1 -1 6 -2.0 particle outside 6 13 -1 6 -2.0 particle outside 6 11 -1 7 6.0 particle outside 4 9 -1 7 6.0 particle outside 4 7 -1 7 6.0 particle outside 2 5 -1 7 6.0 particle outside 2 3 -1 7 6.0 particle outside 0 1 -1 7 6.0 particle outside 0 7 15 -1 8 14.0 particle outside

### E = (N-1.0)hw

```
Value of Oscillator strength: 6.882808 for A: 208.000000

Value of V1 = -50.902039

Value of V1 = -44.019230

Value of V1 = -37.136421

Value of V1 = -30.253613

Value of V1 = -23.370806

Value of V1 = -16.487997

Value of V1 = -9.605190
```

```
! n 1 2j 2tz (2n+1)e hole/p Modelspace
0 0 1 -1 0 -52.0 hole outside
0 1 3 -1 1 -45.0 hole outside
0 1 1 -1 1 -45.0 hole outside
0 2 5 -1 2 -38.0 hole outside
```

0	2	3 -1	2 -38.0	hole	outside
1	0	1 -1	2 -38.0	hole	outside
0	3	7 -1	3 -31.0	hole	outside
0	3	5 -1	4 -24.0	hole	outside
1	1	3 -1	4 -24.0	hole	outside
1	1	1 -1	4 -24.0	hole	outside
0	4	9 -1	4 -24.0	hole	outside
0	4	7 -1	5 -17.0	hole	outside
1	2	5 -1	5 -17.0	hole	outside
1	2	3 -1	5 -17.0	hole	outside
2	0	1 -1	5 -17.0	hole	outside
0	5	11 -1	5 -17.0	hole	outside
0	5	9 -1	6 -10.0	particle	inside
1	3	7 -1	6 -10.0	particle	inside
1	3	5 -1	6 -10.0	particle	inside
2	1	3 -1	6 -10.0	particle	inside
2	1	1 -1	6 -10.0	particle	inside
0	6	13 -1	6 -10.0	particle	e inside
0	6	11 -1	7 -3.0	particle	outside
1	4	9 -1	7 -3.0 p	particle	outside
1	4	7 -1	7 -3.0 p	particle	outside
2	2	5 -1	7 -3.0 p	particle	outside
2	2	3 -1	7 -3.0 p	particle	outside
3	0	1 -1	7 -3.0 p	particle	outside
0	7	15 -1		article	