

```

--- Computing Allowed Magnetic Multipoles (Rank 1..5) for Site 9e / 166.97 ---
Orbit size: 9
Site symmetry operations: 4

===== RANK 1 =====
Allowed Modes: 1

[Mode 1/1]
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -2.047
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -1.772, Y(1,1): 1.023

===== RANK 2 =====
No allowed modes (Forbidden).

===== RANK 3 =====
Allowed Modes: 13

[Mode 1/13]
--- Generator (0.50, 0.00, 0.00) ---
Y(3,-2): 0.116, Y(3,3): 0.173
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(3,-2): -0.058, Y(3,2): 0.101, Y(3,3): 0.173

[Mode 2/13]
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.087, Y(3,-2): 0.108, Y(3,1): -0.093, Y(3,3): -0.155
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.075, Y(1,1): 0.043, Y(3,-2): -0.054, Y(3,-1): -0.080
Y(3,1): 0.046, Y(3,2): 0.094, Y(3,3): -0.155

[Mode 3/13]
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.037, Y(3,-2): 0.148, Y(3,1): -0.039, Y(3,3): 0.025
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.032, Y(1,1): 0.018, Y(3,-2): -0.074, Y(3,-1): -0.034
Y(3,1): 0.020, Y(3,2): 0.128, Y(3,3): 0.025

[Mode 4/13]
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.138, Y(3,-2): 0.204, Y(3,1): -0.148, Y(3,3): -0.110
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.120, Y(1,1): 0.069, Y(3,-2): -0.102, Y(3,-1): -0.128
Y(3,1): 0.074, Y(3,2): 0.176, Y(3,3): -0.110

[Mode 5/13]
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.255, Y(3,-2): -0.338, Y(3,1): -0.272, Y(3,3): 0.047
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.220, Y(1,1): 0.127, Y(3,-2): 0.169, Y(3,-1): -0.236
Y(3,1): 0.136, Y(3,2): -0.293, Y(3,3): 0.047

[Mode 6/13]
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.273, Y(3,-2): 0.162, Y(3,1): -0.292, Y(3,3): 0.067

```

```
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.237, Y(1,1):  0.137, Y(3,-2): -0.081, Y(3,-1): -0.253
Y(3,1):  0.146, Y(3,2):  0.140, Y(3,3):  0.067
```

[Mode 7/13]

```
--- Generator (0.50, 0.00, 0.00) ---
(No projection weights > 1e-4)
--- Atom 0 (0.00, 0.50, 0.00) ---
(No projection weights > 1e-4)
```

[Mode 8/13]

```
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.409, Y(3,1): -0.438
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.354, Y(1,1):  0.205, Y(3,-1): -0.379, Y(3,1):  0.219
```

[Mode 9/13]

```
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.011, Y(3,-2):  0.100, Y(3,1):  0.011, Y(3,3):  0.231
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.009, Y(1,1): -0.005, Y(3,-2): -0.050, Y(3,-1):  0.010
Y(3,1): -0.006, Y(3,2):  0.087, Y(3,3):  0.231
```

[Mode 10/13]

```
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.409, Y(3,1): -0.438
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.354, Y(1,1):  0.205, Y(3,-1): -0.379, Y(3,1):  0.219
```

[Mode 11/13]

```
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -1.228, Y(3,1):  0.328, Y(3,3): -0.424
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -1.063, Y(1,1):  0.614, Y(3,-1):  0.284, Y(3,1): -0.164
Y(3,3): -0.424
```

[Mode 12/13]

```
--- Generator (0.50, 0.00, 0.00) ---
Y(3,-2): -0.346
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(3,-2):  0.173, Y(3,2): -0.300
```

[Mode 13/13]

```
--- Generator (0.50, 0.00, 0.00) ---
Y(3,-2): -0.007, Y(3,3):  0.378
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(3,-2):  0.003, Y(3,2): -0.006, Y(3,3):  0.378
```

===== RANK 4 =====

No allowed modes (Forbidden).

===== RANK 5 =====

Allowed Modes: 121

[Mode 1/121]

```
--- Generator (0.50, 0.00, 0.00) ---
```

```

Y(1,1): -0.034, Y(3,-2): -0.125, Y(3,1): -0.010, Y(3,3): -0.021
Y(5,-4): -0.085, Y(5,-2): 0.038, Y(5,1): 0.010, Y(5,3): -0.005
Y(5,5): -0.011
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.029, Y(1,1): 0.017, Y(3,-2): 0.063, Y(3,-1): -0.009
Y(3,1): 0.005, Y(3,2): -0.109, Y(3,3): -0.021, Y(5,-5): 0.010
Y(5,-4): 0.042, Y(5,-2): -0.019, Y(5,-1): 0.009, Y(5,1): -0.005
Y(5,2): 0.033, Y(5,3): -0.005, Y(5,4): 0.073, Y(5,5): 0.006

```

[Mode 2/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.008, Y(3,-2): 0.002, Y(3,1): -0.034, Y(3,3): 0.054
Y(5,-4): 0.021, Y(5,-2): -0.005, Y(5,1): 0.018, Y(5,3): -0.027
Y(5,5): 0.030
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.007, Y(1,1): 0.004, Y(3,-2): -0.001, Y(3,-1): -0.029
Y(3,1): 0.017, Y(3,2): 0.002, Y(3,3): 0.054, Y(5,-5): -0.026
Y(5,-4): -0.010, Y(5,-2): 0.003, Y(5,-1): 0.016, Y(5,1): -0.009
Y(5,2): -0.004, Y(5,3): -0.027, Y(5,4): -0.018, Y(5,5): -0.015

```

[Mode 3/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): 0.005, Y(3,-2): -0.001, Y(3,1): 0.003, Y(3,3): -0.006
Y(5,-4): -0.030, Y(5,-2): 0.012, Y(5,1): -0.002, Y(5,3): -0.007
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): 0.004, Y(1,1): -0.003, Y(3,-2): 0.001, Y(3,-1): 0.003
Y(3,1): -0.002, Y(3,2): -0.001, Y(3,3): -0.006, Y(5,-4): 0.015
Y(5,-2): -0.006, Y(5,-1): -0.002, Y(5,1): 0.001, Y(5,2): 0.010
Y(5,3): -0.007, Y(5,4): 0.026

```

[Mode 4/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.051, Y(3,-2): -0.010, Y(3,1): -0.033, Y(3,3): -0.078
Y(5,-4): -0.001, Y(5,-2): -0.010, Y(5,1): 0.023, Y(5,3): 0.019
Y(5,5): 0.001
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.044, Y(1,1): 0.025, Y(3,-2): 0.005, Y(3,-1): -0.029
Y(3,1): 0.016, Y(3,2): -0.008, Y(3,3): -0.078, Y(5,-5): -0.001
Y(5,-4): 0.001, Y(5,-2): 0.005, Y(5,-1): 0.020, Y(5,1): -0.012
Y(5,2): -0.008, Y(5,3): 0.019, Y(5,4): 0.001, Y(5,5): -0.001

```

[Mode 5/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.065, Y(3,-2): 0.026, Y(3,1): -0.081, Y(3,3): 0.023
Y(5,-4): -0.004, Y(5,-2): -0.002, Y(5,1): 0.049, Y(5,3): -0.043
Y(5,5): 0.042
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.057, Y(1,1): 0.033, Y(3,-2): -0.013, Y(3,-1): -0.070
Y(3,1): 0.040, Y(3,2): 0.022, Y(3,3): 0.023, Y(5,-5): -0.036
Y(5,-4): 0.002, Y(5,-2): 0.001, Y(5,-1): 0.043, Y(5,1): -0.025
Y(5,2): -0.002, Y(5,3): -0.043, Y(5,4): 0.004, Y(5,5): -0.021

```

[Mode 6/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): 0.027, Y(3,-2): 0.058, Y(3,1): -0.002, Y(3,3): 0.009

```

```

Y(5,-4):  0.000, Y(5,-2): -0.027, Y(5,1): -0.009, Y(5,3): -0.007
Y(5,5):  0.015
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.023, Y(1,1): -0.014, Y(3,-2): -0.029, Y(3,-1): -0.001
Y(3,1):  0.001, Y(3,2):  0.050, Y(3,3):  0.009, Y(5,-5): -0.013
Y(5,-4): -0.000, Y(5,-2):  0.014, Y(5,-1): -0.008, Y(5,1):  0.005
Y(5,2):  -0.023, Y(5,3): -0.007, Y(5,4): -0.000, Y(5,5): -0.008

```

[Mode 7/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.032, Y(3,-2): -0.013, Y(3,1):  0.045, Y(3,3):  0.005
Y(5,-4): -0.022, Y(5,-2):  0.015, Y(5,1): -0.027, Y(5,3):  0.035
Y(5,5): -0.026
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.028, Y(1,1): -0.016, Y(3,-2):  0.006, Y(3,-1):  0.039
Y(3,1): -0.023, Y(3,2): -0.011, Y(3,3):  0.005, Y(5,-5):  0.023
Y(5,-4):  0.011, Y(5,-2): -0.007, Y(5,-1): -0.023, Y(5,1):  0.014
Y(5,2):  0.013, Y(5,3):  0.035, Y(5,4):  0.019, Y(5,5):  0.013

```

[Mode 8/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.063, Y(3,-2):  0.138, Y(3,1):  0.001, Y(3,3): -0.024
Y(5,-4):  0.035, Y(5,-2):  0.011, Y(5,1):  0.014, Y(5,3): -0.001
Y(5,5): -0.038
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.054, Y(1,1):  0.031, Y(3,-2): -0.069, Y(3,-1):  0.001
Y(3,1): -0.001, Y(3,2):  0.119, Y(3,3): -0.024, Y(5,-5):  0.033
Y(5,-4): -0.017, Y(5,-2): -0.006, Y(5,-1):  0.012, Y(5,1): -0.007
Y(5,2):  0.010, Y(5,3): -0.001, Y(5,4): -0.030, Y(5,5):  0.019

```

[Mode 9/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.003, Y(3,-2):  0.013, Y(3,1): -0.041, Y(3,3):  0.061
Y(5,-4): -0.011, Y(5,-2): -0.003, Y(5,1): -0.008, Y(5,3): -0.003
Y(5,5):  0.026
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.003, Y(1,1): -0.002, Y(3,-2): -0.006, Y(3,-1): -0.036
Y(3,1):  0.021, Y(3,2):  0.011, Y(3,3):  0.061, Y(5,-5): -0.022
Y(5,-4):  0.006, Y(5,-2):  0.001, Y(5,-1): -0.007, Y(5,1):  0.004
Y(5,2): -0.002, Y(5,3): -0.003, Y(5,4):  0.010, Y(5,5): -0.013

```

[Mode 10/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.087, Y(3,-2): -0.005, Y(3,1): -0.041, Y(3,3): -0.065
Y(5,-4):  0.024, Y(5,-2): -0.023, Y(5,1):  0.026, Y(5,3): -0.021
Y(5,5): -0.019
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.075, Y(1,1):  0.044, Y(3,-2):  0.003, Y(3,-1): -0.035
Y(3,1):  0.020, Y(3,2): -0.005, Y(3,3): -0.065, Y(5,-5):  0.016
Y(5,-4): -0.012, Y(5,-2):  0.011, Y(5,-1):  0.023, Y(5,1): -0.013
Y(5,2): -0.020, Y(5,3): -0.021, Y(5,4): -0.020, Y(5,5):  0.009

```

[Mode 11/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.057, Y(3,-2): -0.060, Y(3,1):  0.010, Y(3,3): -0.055

```

```

Y(5,-4): -0.040, Y(5,-2): -0.019, Y(5,1):  0.012, Y(5,3): -0.012
Y(5,5): -0.041
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.049, Y(1,1):  0.028, Y(3,-2):  0.030, Y(3,-1):  0.008
Y(3,1): -0.005, Y(3,2): -0.052, Y(3,3): -0.055, Y(5,-5):  0.036
Y(5,-4):  0.020, Y(5,-2):  0.010, Y(5,-1):  0.010, Y(5,1): -0.006
Y(5,2): -0.017, Y(5,3): -0.012, Y(5,4):  0.034, Y(5,5):  0.021

```

[Mode 12/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.014, Y(3,-2):  0.058, Y(3,1):  0.015, Y(3,3): -0.027
Y(5,-4): -0.003, Y(5,-2):  0.010, Y(5,1):  0.010, Y(5,3): -0.020
Y(5,5):  0.008
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.012, Y(1,1): -0.007, Y(3,-2): -0.029, Y(3,-1):  0.013
Y(3,1): -0.007, Y(3,2):  0.050, Y(3,3): -0.027, Y(5,-5): -0.007
Y(5,-4):  0.001, Y(5,-2): -0.005, Y(5,-1):  0.009, Y(5,1): -0.005
Y(5,2):  0.008, Y(5,3): -0.020, Y(5,4):  0.002, Y(5,5): -0.004

```

[Mode 13/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.036, Y(3,-2): -0.019, Y(3,1): -0.021, Y(3,3):  0.029
Y(5,-4):  0.040, Y(5,-2): -0.037, Y(5,1):  0.009, Y(5,3):  0.007
Y(5,5): -0.006
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.031, Y(1,1):  0.018, Y(3,-2):  0.010, Y(3,-1): -0.018
Y(3,1):  0.010, Y(3,2): -0.016, Y(3,3):  0.029, Y(5,-5):  0.005
Y(5,-4): -0.020, Y(5,-2):  0.018, Y(5,-1):  0.008, Y(5,1): -0.005
Y(5,2): -0.032, Y(5,3):  0.007, Y(5,4): -0.034, Y(5,5):  0.003

```

[Mode 14/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.017, Y(3,-2): -0.007, Y(3,1): -0.060, Y(3,3):  0.036
Y(5,-4): -0.005, Y(5,-2): -0.011, Y(5,1): -0.015, Y(5,3): -0.004
Y(5,5):  0.018
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.015, Y(1,1):  0.009, Y(3,-2):  0.003, Y(3,-1): -0.052
Y(3,1):  0.030, Y(3,2): -0.006, Y(3,3):  0.036, Y(5,-5): -0.016
Y(5,-4):  0.003, Y(5,-2):  0.005, Y(5,-1): -0.013, Y(5,1):  0.008
Y(5,2): -0.009, Y(5,3): -0.004, Y(5,4):  0.005, Y(5,5): -0.009

```

[Mode 15/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.043, Y(3,-2):  0.004, Y(3,1):  0.052, Y(3,3):  0.014
Y(5,-4):  0.023, Y(5,-2):  0.005, Y(5,1):  0.013, Y(5,3):  0.031
Y(5,5):  0.005
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.037, Y(1,1): -0.022, Y(3,-2): -0.002, Y(3,-1):  0.045
Y(3,1): -0.026, Y(3,2):  0.003, Y(3,3):  0.014, Y(5,-5): -0.004
Y(5,-4): -0.012, Y(5,-2): -0.002, Y(5,-1):  0.011, Y(5,1): -0.006
Y(5,2):  0.004, Y(5,3):  0.031, Y(5,4): -0.020, Y(5,5): -0.002

```

[Mode 16/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.079, Y(3,-2):  0.042, Y(3,1):  0.040, Y(3,3): -0.176

```

```

Y(5,-4):  0.028, Y(5,-2): -0.013, Y(5,1): -0.010, Y(5,3):  0.029
Y(5,5): -0.094
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.069, Y(1,1):  0.040, Y(3,-2): -0.021, Y(3,-1):  0.035
Y(3,1): -0.020, Y(3,2):  0.036, Y(3,3): -0.176, Y(5,-5):  0.081
Y(5,-4): -0.014, Y(5,-2):  0.006, Y(5,-1): -0.008, Y(5,1):  0.005
Y(5,2): -0.011, Y(5,3):  0.029, Y(5,4): -0.024, Y(5,5):  0.047

```

[Mode 17/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.091, Y(3,-2):  0.041, Y(3,1):  0.019, Y(3,3):  0.056
Y(5,-4):  0.021, Y(5,-2): -0.020, Y(5,1): -0.021, Y(5,3):  0.005
Y(5,5):  0.040
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.079, Y(1,1): -0.046, Y(3,-2): -0.020, Y(3,-1):  0.016
Y(3,1): -0.009, Y(3,2):  0.035, Y(3,3):  0.056, Y(5,-5): -0.035
Y(5,-4): -0.010, Y(5,-2):  0.010, Y(5,-1): -0.019, Y(5,1):  0.011
Y(5,2): -0.018, Y(5,3):  0.005, Y(5,4): -0.018, Y(5,5): -0.020

```

[Mode 18/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.028, Y(3,-2): -0.035, Y(3,1): -0.004, Y(3,3): -0.024
Y(5,-4): -0.057, Y(5,-2):  0.023, Y(5,1):  0.034, Y(5,3):  0.003
Y(5,5):  0.005
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.025, Y(1,1):  0.014, Y(3,-2):  0.017, Y(3,-1): -0.003
Y(3,1):  0.002, Y(3,2): -0.030, Y(3,3): -0.024, Y(5,-5): -0.004
Y(5,-4):  0.029, Y(5,-2): -0.012, Y(5,-1):  0.029, Y(5,1): -0.017
Y(5,2):  0.020, Y(5,3):  0.003, Y(5,4):  0.049, Y(5,5): -0.002

```

[Mode 19/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.044, Y(3,-2):  0.034, Y(3,1):  0.009, Y(3,3):  0.020
Y(5,-4):  0.031, Y(5,-2): -0.014, Y(5,1):  0.006, Y(5,5):  0.030
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.038, Y(1,1): -0.022, Y(3,-2): -0.017, Y(3,-1):  0.008
Y(3,1): -0.005, Y(3,2):  0.029, Y(3,3):  0.020, Y(5,-5): -0.026
Y(5,-4): -0.015, Y(5,-2):  0.007, Y(5,-1):  0.005, Y(5,1): -0.003
Y(5,2): -0.012, Y(5,4): -0.027, Y(5,5): -0.015

```

[Mode 20/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.103, Y(3,-2):  0.002, Y(3,1): -0.079, Y(3,3): -0.056
Y(5,-4): -0.003, Y(5,-2):  0.011, Y(5,1):  0.064, Y(5,3): -0.059
Y(5,5):  0.022
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.089, Y(1,1):  0.052, Y(3,-2): -0.001, Y(3,-1): -0.068
Y(3,1):  0.039, Y(3,2):  0.002, Y(3,3): -0.056, Y(5,-5): -0.019
Y(5,-4):  0.002, Y(5,-2): -0.005, Y(5,-1):  0.055, Y(5,1): -0.032
Y(5,2):  0.009, Y(5,3): -0.059, Y(5,4):  0.003, Y(5,5): -0.011

```

[Mode 21/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.101, Y(3,-2): -0.011, Y(3,1):  0.045, Y(3,3): -0.018
Y(5,-4): -0.004, Y(5,-2):  0.003, Y(5,1): -0.009, Y(5,3):  0.004

```

```

Y(5,5): -0.113
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.088, Y(1,1):  0.051, Y(3,-2):  0.006, Y(3,-1):  0.039
Y(3,1): -0.023, Y(3,2): -0.010, Y(3,3): -0.018, Y(5,-5):  0.098
Y(5,-4):  0.002, Y(5,-2): -0.002, Y(5,-1): -0.008, Y(5,1):  0.005
Y(5,2):  0.003, Y(5,3):  0.004, Y(5,4):  0.004, Y(5,5):  0.057

```

[Mode 22/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.008, Y(3,-2):  0.014, Y(3,1):  0.003, Y(3,3):  0.034
Y(5,-4):  0.042, Y(5,-2): -0.001, Y(5,1): -0.003, Y(5,3):  0.018
Y(5,5):  0.002
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.007, Y(1,1): -0.004, Y(3,-2): -0.007, Y(3,-1):  0.003
Y(3,1): -0.002, Y(3,2):  0.012, Y(3,3):  0.034, Y(5,-5): -0.002
Y(5,-4): -0.021, Y(5,-2):  0.000, Y(5,-1): -0.002, Y(5,1):  0.001
Y(5,2): -0.001, Y(5,3):  0.018, Y(5,4): -0.037, Y(5,5): -0.001

```

[Mode 23/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.023, Y(3,-2): -0.015, Y(3,1): -0.021, Y(3,3): -0.046
Y(5,-4):  0.031, Y(5,-2): -0.011, Y(5,1): -0.035, Y(5,3):  0.025
Y(5,5):  0.008
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.020, Y(1,1): -0.012, Y(3,-2):  0.008, Y(3,-1): -0.018
Y(3,1):  0.010, Y(3,2): -0.013, Y(3,3): -0.046, Y(5,-5): -0.007
Y(5,-4): -0.016, Y(5,-2):  0.005, Y(5,-1): -0.030, Y(5,1):  0.017
Y(5,2): -0.009, Y(5,3):  0.025, Y(5,4): -0.027, Y(5,5): -0.004

```

[Mode 24/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.126, Y(3,-2):  0.035, Y(3,1): -0.079, Y(3,3): -0.018
Y(5,-4):  0.038, Y(5,-2): -0.032, Y(5,1):  0.023, Y(5,3): -0.046
Y(5,5): -0.023
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.109, Y(1,1):  0.063, Y(3,-2): -0.017, Y(3,-1): -0.068
Y(3,1):  0.039, Y(3,2):  0.030, Y(3,3): -0.018, Y(5,-5):  0.020
Y(5,-4): -0.019, Y(5,-2):  0.016, Y(5,-1):  0.020, Y(5,1): -0.012
Y(5,2): -0.028, Y(5,3): -0.046, Y(5,4): -0.033, Y(5,5):  0.011

```

[Mode 25/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.017, Y(3,-2): -0.016, Y(3,1): -0.011, Y(3,3):  0.083
Y(5,-4): -0.009, Y(5,-2): -0.004, Y(5,1): -0.004, Y(5,3):  0.064
Y(5,5):  0.018
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.015, Y(1,1): -0.008, Y(3,-2):  0.008, Y(3,-1): -0.010
Y(3,1):  0.005, Y(3,2): -0.014, Y(3,3):  0.083, Y(5,-5): -0.015
Y(5,-4):  0.005, Y(5,-2):  0.002, Y(5,-1): -0.003, Y(5,1):  0.002
Y(5,2): -0.004, Y(5,3):  0.064, Y(5,4):  0.008, Y(5,5): -0.009

```

[Mode 26/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.031, Y(3,-2): -0.051, Y(3,1):  0.019, Y(3,3):  0.043
Y(5,-4):  0.026, Y(5,-2): -0.003, Y(5,1): -0.024, Y(5,3):  0.020

```

```

Y(5,5): -0.007
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): 0.027, Y(1,1): -0.016, Y(3,-2): 0.025, Y(3,-1): 0.016
Y(3,1): -0.009, Y(3,2): -0.044, Y(3,3): 0.043, Y(5,-5): 0.006
Y(5,-4): -0.013, Y(5,-2): 0.002, Y(5,-1): -0.021, Y(5,1): 0.012
Y(5,2): -0.003, Y(5,3): 0.020, Y(5,4): -0.023, Y(5,5): 0.003

```

[Mode 27/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): 0.107, Y(3,-2): -0.015, Y(3,1): 0.039, Y(3,3): 0.005
Y(5,-4): 0.018, Y(5,-2): -0.032, Y(5,1): -0.024, Y(5,3): 0.028
Y(5,5): 0.036
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): 0.092, Y(1,1): -0.053, Y(3,-2): 0.008, Y(3,-1): 0.034
Y(3,1): -0.020, Y(3,2): -0.013, Y(3,3): 0.005, Y(5,-5): -0.031
Y(5,-4): -0.009, Y(5,-2): 0.016, Y(5,-1): -0.021, Y(5,1): 0.012
Y(5,2): -0.027, Y(5,3): 0.028, Y(5,4): -0.016, Y(5,5): -0.018

```

[Mode 28/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.015, Y(3,-2): -0.003, Y(3,1): -0.024, Y(3,3): -0.045
Y(5,-4): -0.006, Y(5,-2): 0.017, Y(5,1): -0.039, Y(5,3): 0.032
Y(5,5): -0.021
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.013, Y(1,1): 0.008, Y(3,-2): 0.001, Y(3,-1): -0.021
Y(3,1): 0.012, Y(3,2): -0.002, Y(3,3): -0.045, Y(5,-5): 0.018
Y(5,-4): 0.003, Y(5,-2): -0.008, Y(5,-1): -0.033, Y(5,1): 0.019
Y(5,2): 0.015, Y(5,3): 0.032, Y(5,4): 0.005, Y(5,5): 0.011

```

[Mode 29/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): 0.031, Y(3,-2): -0.033, Y(3,1): -0.006, Y(3,3): 0.037
Y(5,-4): -0.020, Y(5,-2): 0.009, Y(5,1): -0.013, Y(5,3): 0.004
Y(5,5): 0.019
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): 0.027, Y(1,1): -0.016, Y(3,-2): 0.016, Y(3,-1): -0.005
Y(3,1): 0.003, Y(3,2): -0.028, Y(3,3): 0.037, Y(5,-5): -0.016
Y(5,-4): 0.010, Y(5,-2): -0.004, Y(5,-1): -0.011, Y(5,1): 0.006
Y(5,2): 0.008, Y(5,3): 0.004, Y(5,4): 0.017, Y(5,5): -0.009

```

[Mode 30/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): 0.062, Y(3,-2): 0.019, Y(3,1): 0.025, Y(3,3): 0.096
Y(5,-4): -0.007, Y(5,-2): 0.011, Y(5,1): -0.008, Y(5,3): 0.059
Y(5,5): 0.024
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): 0.054, Y(1,1): -0.031, Y(3,-2): -0.010, Y(3,-1): 0.021
Y(3,1): -0.012, Y(3,2): 0.017, Y(3,3): 0.096, Y(5,-5): -0.021
Y(5,-4): 0.003, Y(5,-2): -0.006, Y(5,-1): -0.007, Y(5,1): 0.004
Y(5,2): 0.010, Y(5,3): 0.059, Y(5,4): 0.006, Y(5,5): -0.012

```

[Mode 31/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.107, Y(3,-2): -0.010, Y(3,1): -0.053, Y(3,3): -0.033
Y(5,-4): -0.003, Y(5,-2): -0.032, Y(5,1): 0.024, Y(5,3): -0.002

```

```

Y(5,5): -0.027
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.093, Y(1,1):  0.054, Y(3,-2):  0.005, Y(3,-1): -0.046
Y(3,1):  0.026, Y(3,2): -0.008, Y(3,3): -0.033, Y(5,-5):  0.023
Y(5,-4):  0.002, Y(5,-2):  0.016, Y(5,-1):  0.021, Y(5,1): -0.012
Y(5,2): -0.028, Y(5,3): -0.002, Y(5,4):  0.003, Y(5,5):  0.013

```

[Mode 32/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.080, Y(3,-2): -0.025, Y(3,1):  0.106, Y(3,3): -0.025
Y(5,-4):  0.005, Y(5,-2):  0.003, Y(5,1): -0.004, Y(5,3):  0.004
Y(5,5): -0.017
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.069, Y(1,1): -0.040, Y(3,-2):  0.012, Y(3,-1):  0.092
Y(3,1): -0.053, Y(3,2): -0.021, Y(3,3): -0.025, Y(5,-5):  0.015
Y(5,-4): -0.003, Y(5,-2): -0.002, Y(5,-1): -0.003, Y(5,1):  0.002
Y(5,2):  0.003, Y(5,3):  0.004, Y(5,4): -0.004, Y(5,5):  0.008

```

[Mode 33/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.011, Y(3,-2):  0.024, Y(3,1):  0.043, Y(3,3): -0.019
Y(5,-4): -0.009, Y(5,-2):  0.032, Y(5,1):  0.005, Y(5,3): -0.008
Y(5,5): -0.019
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.009, Y(1,1): -0.005, Y(3,-2): -0.012, Y(3,-1):  0.037
Y(3,1): -0.021, Y(3,2):  0.021, Y(3,3): -0.019, Y(5,-5):  0.016
Y(5,-4):  0.004, Y(5,-2): -0.016, Y(5,-1):  0.004, Y(5,1): -0.002
Y(5,2):  0.028, Y(5,3): -0.008, Y(5,4):  0.008, Y(5,5):  0.009

```

[Mode 34/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.002, Y(3,-2):  0.036, Y(3,1): -0.036, Y(3,3):  0.020
Y(5,-4):  0.011, Y(5,-2): -0.003, Y(5,1): -0.014, Y(5,3): -0.010
Y(5,5):  0.014
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.002, Y(1,1):  0.001, Y(3,-2): -0.018, Y(3,-1): -0.031
Y(3,1):  0.018, Y(3,2):  0.031, Y(3,3):  0.020, Y(5,-5): -0.012
Y(5,-4): -0.006, Y(5,-2):  0.002, Y(5,-1): -0.012, Y(5,1):  0.007
Y(5,2): -0.003, Y(5,3): -0.010, Y(5,4): -0.010, Y(5,5): -0.007

```

[Mode 35/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.056, Y(3,-2): -0.044, Y(3,1): -0.055, Y(3,3): -0.048
Y(5,-4): -0.038, Y(5,-2):  0.014, Y(5,1):  0.030, Y(5,3): -0.040
Y(5,5):  0.017
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.048, Y(1,1):  0.028, Y(3,-2):  0.022, Y(3,-1): -0.048
Y(3,1):  0.028, Y(3,2): -0.038, Y(3,3): -0.048, Y(5,-5): -0.015
Y(5,-4):  0.019, Y(5,-2): -0.007, Y(5,-1):  0.026, Y(5,1): -0.015
Y(5,2):  0.012, Y(5,3): -0.040, Y(5,4):  0.033, Y(5,5): -0.009

```

[Mode 36/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.025, Y(3,-2): -0.046, Y(3,1): -0.009, Y(3,3): -0.033
Y(5,-4):  0.006, Y(5,-2): -0.065, Y(5,1):  0.013, Y(5,3): -0.013

```

```

Y(5,5): -0.004
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.022, Y(1,1):  0.013, Y(3,-2):  0.023, Y(3,-1): -0.008
Y(3,1):  0.004, Y(3,2): -0.039, Y(3,3): -0.033, Y(5,-5):  0.003
Y(5,-4): -0.003, Y(5,-2):  0.032, Y(5,-1):  0.011, Y(5,1): -0.006
Y(5,2): -0.056, Y(5,3): -0.013, Y(5,4): -0.005, Y(5,5):  0.002

```

[Mode 37/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.015, Y(3,-2):  0.071, Y(3,1): -0.038, Y(3,3):  0.031
Y(5,-4): -0.014, Y(5,-2): -0.001, Y(5,1): -0.021, Y(5,3):  0.037
Y(5,5):  0.000
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.013, Y(1,1):  0.008, Y(3,-2): -0.035, Y(3,-1): -0.033
Y(3,1):  0.019, Y(3,2):  0.061, Y(3,3):  0.031, Y(5,-5): -0.000
Y(5,-4):  0.007, Y(5,-2):  0.001, Y(5,-1): -0.018, Y(5,1):  0.011
Y(5,2): -0.001, Y(5,3):  0.037, Y(5,4):  0.012

```

[Mode 38/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.043, Y(3,-2):  0.007, Y(3,1): -0.000, Y(3,3):  0.005
Y(5,-4): -0.002, Y(5,-2): -0.043, Y(5,1):  0.041, Y(5,3): -0.013
Y(5,5): -0.003
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.037, Y(1,1):  0.021, Y(3,-2): -0.004, Y(3,-1): -0.000
Y(3,2):  0.006, Y(3,3):  0.005, Y(5,-5):  0.003, Y(5,-4):  0.001
Y(5,-2):  0.022, Y(5,-1):  0.036, Y(5,1): -0.021, Y(5,2): -0.037
Y(5,3): -0.013, Y(5,4):  0.002, Y(5,5):  0.002

```

[Mode 39/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.077, Y(3,-2): -0.031, Y(3,1):  0.131, Y(3,3): -0.005
Y(5,-4):  0.007, Y(5,-2):  0.004, Y(5,1):  0.055, Y(5,3): -0.008
Y(5,5):  0.004
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.067, Y(1,1): -0.039, Y(3,-2):  0.015, Y(3,-1):  0.114
Y(3,1): -0.066, Y(3,2): -0.026, Y(3,3): -0.005, Y(5,-5): -0.004
Y(5,-4): -0.003, Y(5,-2): -0.002, Y(5,-1):  0.048, Y(5,1): -0.028
Y(5,2):  0.003, Y(5,3): -0.008, Y(5,4): -0.006, Y(5,5): -0.002

```

[Mode 40/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.015, Y(3,-2):  0.012, Y(3,1): -0.008, Y(3,3):  0.016
Y(5,-4):  0.029, Y(5,-2): -0.004, Y(5,1): -0.022, Y(5,3):  0.038
Y(5,5):  0.002
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.013, Y(1,1): -0.008, Y(3,-2): -0.006, Y(3,-1): -0.007
Y(3,1):  0.004, Y(3,2):  0.010, Y(3,3):  0.016, Y(5,-5): -0.002
Y(5,-4): -0.015, Y(5,-2):  0.002, Y(5,-1): -0.019, Y(5,1):  0.011
Y(5,2): -0.003, Y(5,3):  0.038, Y(5,4): -0.025, Y(5,5): -0.001

```

[Mode 41/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.021, Y(3,-2): -0.023, Y(3,1):  0.007, Y(3,3): -0.022
Y(5,-4): -0.036, Y(5,-2): -0.026, Y(5,1):  0.011, Y(5,3):  0.009

```

```

Y(5,5): -0.013
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.018, Y(1,1):  0.010, Y(3,-2):  0.011, Y(3,-1):  0.006
Y(3,1): -0.003, Y(3,2): -0.020, Y(3,3): -0.022, Y(5,-5):  0.011
Y(5,-4):  0.018, Y(5,-2):  0.013, Y(5,-1):  0.010, Y(5,1): -0.006
Y(5,2): -0.023, Y(5,3):  0.009, Y(5,4):  0.031, Y(5,5):  0.006

```

[Mode 42/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.072, Y(3,-2): -0.033, Y(3,1):  0.009, Y(3,3):  0.024
Y(5,-4): -0.030, Y(5,-2):  0.001, Y(5,1): -0.042, Y(5,3):  0.016
Y(5,5):  0.019
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.063, Y(1,1): -0.036, Y(3,-2):  0.017, Y(3,-1):  0.008
Y(3,1): -0.005, Y(3,2): -0.029, Y(3,3):  0.024, Y(5,-5): -0.016
Y(5,-4):  0.015, Y(5,-2): -0.001, Y(5,-1): -0.036, Y(5,1):  0.021
Y(5,2):  0.001, Y(5,3):  0.016, Y(5,4):  0.026, Y(5,5): -0.009

```

[Mode 43/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.003, Y(3,-2):  0.019, Y(3,1):  0.020, Y(3,3):  0.040
Y(5,-4):  0.018, Y(5,-2):  0.007, Y(5,1): -0.002, Y(5,3):  0.005
Y(5,5): -0.017
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.002, Y(1,1):  0.001, Y(3,-2): -0.010, Y(3,-1):  0.017
Y(3,1): -0.010, Y(3,2):  0.017, Y(3,3):  0.040, Y(5,-5):  0.015
Y(5,-4): -0.009, Y(5,-2): -0.003, Y(5,-1): -0.002, Y(5,1):  0.001
Y(5,2):  0.006, Y(5,3):  0.005, Y(5,4): -0.016, Y(5,5):  0.009

```

[Mode 44/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.078, Y(3,-2): -0.011, Y(3,1): -0.011, Y(3,3): -0.014
Y(5,-4): -0.022, Y(5,-2): -0.008, Y(5,1):  0.040, Y(5,3): -0.010
Y(5,5): -0.023
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.068, Y(1,1):  0.039, Y(3,-2):  0.005, Y(3,-1): -0.010
Y(3,1):  0.006, Y(3,2): -0.009, Y(3,3): -0.014, Y(5,-5):  0.020
Y(5,-4):  0.011, Y(5,-2):  0.004, Y(5,-1):  0.034, Y(5,1): -0.020
Y(5,2): -0.007, Y(5,3): -0.010, Y(5,4):  0.019, Y(5,5):  0.011

```

[Mode 45/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.877, Y(3,1):  0.365, Y(3,3): -0.471, Y(5,1): -0.066
Y(5,3):  0.071, Y(5,5): -0.095
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.760, Y(1,1):  0.439, Y(3,-1):  0.316, Y(3,1): -0.182
Y(3,3): -0.471, Y(5,-5):  0.082, Y(5,-1): -0.057, Y(5,1):  0.033
Y(5,3):  0.071, Y(5,5):  0.048

```

[Mode 46/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.025, Y(3,-2):  0.025, Y(3,1):  0.050, Y(3,3): -0.003
Y(5,-4): -0.001, Y(5,-2):  0.010, Y(5,1):  0.010, Y(5,3): -0.008
Y(5,5): -0.010
--- Atom 0 (0.00, 0.50, 0.00) ---

```

```

Y(1,-1):  0.021, Y(1,1): -0.012, Y(3,-2): -0.013, Y(3,-1):  0.044
Y(3,1): -0.025, Y(3,2):  0.022, Y(3,3): -0.003, Y(5,-5):  0.008
Y(5,-4):  0.000, Y(5,-2): -0.005, Y(5,-1):  0.009, Y(5,1): -0.005
Y(5,2):  0.008, Y(5,3): -0.008, Y(5,4):  0.001, Y(5,5):  0.005

```

[Mode 47/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.002, Y(3,-2):  0.041, Y(3,1): -0.009, Y(3,3):  0.024
Y(5,-4): -0.003, Y(5,-2): -0.005, Y(5,1):  0.033, Y(5,3): -0.049
Y(5,5):  0.031
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.001, Y(1,1): -0.001, Y(3,-2): -0.021, Y(3,-1): -0.008
Y(3,1):  0.004, Y(3,2):  0.036, Y(3,3):  0.024, Y(5,-5): -0.026
Y(5,-4):  0.001, Y(5,-2):  0.002, Y(5,-1):  0.029, Y(5,1): -0.017
Y(5,2): -0.004, Y(5,3): -0.049, Y(5,4):  0.003, Y(5,5): -0.015

```

[Mode 48/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.100, Y(3,-2): -0.017, Y(3,1):  0.066, Y(3,3):  0.054
Y(5,-4): -0.011, Y(5,-2): -0.007, Y(5,1): -0.036, Y(5,3):  0.020
Y(5,5):  0.003
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.087, Y(1,1): -0.050, Y(3,-2):  0.009, Y(3,-1):  0.057
Y(3,1): -0.033, Y(3,2): -0.015, Y(3,3):  0.054, Y(5,-5): -0.003
Y(5,-4):  0.006, Y(5,-2):  0.004, Y(5,-1): -0.031, Y(5,1):  0.018
Y(5,2): -0.006, Y(5,3):  0.020, Y(5,4):  0.010, Y(5,5): -0.002

```

[Mode 49/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.043, Y(3,-2): -0.011, Y(3,1): -0.048, Y(3,3):  0.018
Y(5,-4):  0.032, Y(5,-2):  0.008, Y(5,1): -0.009, Y(5,3):  0.000
Y(5,5): -0.005
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.038, Y(1,1):  0.022, Y(3,-2):  0.005, Y(3,-1): -0.042
Y(3,1):  0.024, Y(3,2): -0.009, Y(3,3):  0.018, Y(5,-5):  0.004
Y(5,-4): -0.016, Y(5,-2): -0.004, Y(5,-1): -0.008, Y(5,1):  0.004
Y(5,2):  0.007, Y(5,3):  0.000, Y(5,4): -0.028, Y(5,5):  0.002

```

[Mode 50/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.060, Y(3,-2): -0.069, Y(3,1): -0.077, Y(3,3):  0.021
Y(5,-4): -0.033, Y(5,-2):  0.016, Y(5,1):  0.010, Y(5,3):  0.001
Y(5,5):  0.016
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.052, Y(1,1):  0.030, Y(3,-2):  0.034, Y(3,-1): -0.067
Y(3,1):  0.039, Y(3,2): -0.060, Y(3,3):  0.021, Y(5,-5): -0.014
Y(5,-4):  0.017, Y(5,-2): -0.008, Y(5,-1):  0.008, Y(5,1): -0.005
Y(5,2):  0.014, Y(5,3):  0.001, Y(5,4):  0.029, Y(5,5): -0.008

```

[Mode 51/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.027, Y(3,-2):  0.002, Y(3,1): -0.073, Y(3,3):  0.022
Y(5,-4):  0.004, Y(5,-2):  0.008, Y(5,1): -0.010, Y(5,3): -0.048
Y(5,5):  0.024
--- Atom 0 (0.00, 0.50, 0.00) ---

```

```
Y(1,-1): -0.023, Y(1,1):  0.013, Y(3,-2): -0.001, Y(3,-1): -0.063  
Y(3,1):  0.037, Y(3,2):  0.002, Y(3,3):  0.022, Y(5,-5): -0.021  
Y(5,-4): -0.002, Y(5,-2): -0.004, Y(5,-1): -0.009, Y(5,1):  0.005  
Y(5,2):  0.007, Y(5,3): -0.048, Y(5,4): -0.004, Y(5,5): -0.012
```

[Mode 52/121]

```
--- Generator (0.50, 0.00, 0.00) ---  
Y(1,1):  0.016, Y(3,-2):  0.041, Y(3,1):  0.030, Y(3,3):  0.053  
Y(5,-4): -0.009, Y(5,-2): -0.016, Y(5,1):  0.013, Y(5,3):  0.009  
Y(5,5): -0.000  
--- Atom 0 (0.00, 0.50, 0.00) ---  
Y(1,-1):  0.014, Y(1,1): -0.008, Y(3,-2): -0.020, Y(3,-1):  0.026  
Y(3,1): -0.015, Y(3,2):  0.035, Y(3,3):  0.053, Y(5,-5):  0.000  
Y(5,-4):  0.004, Y(5,-2):  0.008, Y(5,-1):  0.011, Y(5,1): -0.006  
Y(5,2): -0.014, Y(5,3):  0.009, Y(5,4):  0.007, Y(5,5):  0.000
```

[Mode 53/121]

```
--- Generator (0.50, 0.00, 0.00) ---  
Y(1,1):  0.072, Y(3,-2): -0.067, Y(3,1):  0.032, Y(3,3):  0.045  
Y(5,-4): -0.017, Y(5,-2): -0.027, Y(5,1): -0.030, Y(5,3):  0.016  
Y(5,5):  0.011  
--- Atom 0 (0.00, 0.50, 0.00) ---  
Y(1,-1):  0.063, Y(1,1): -0.036, Y(3,-2):  0.034, Y(3,-1):  0.028  
Y(3,1): -0.016, Y(3,2): -0.058, Y(3,3):  0.045, Y(5,-5): -0.010  
Y(5,-4):  0.008, Y(5,-2):  0.013, Y(5,-1): -0.026, Y(5,1):  0.015  
Y(5,2): -0.023, Y(5,3):  0.016, Y(5,4):  0.015, Y(5,5): -0.006
```

[Mode 54/121]

```
--- Generator (0.50, 0.00, 0.00) ---  
Y(1,1): -0.058, Y(3,-2): -0.020, Y(3,1): -0.064, Y(3,3): -0.028  
Y(5,-4): -0.012, Y(5,-2):  0.002, Y(5,1):  0.003, Y(5,3): -0.063  
Y(5,5):  0.004  
--- Atom 0 (0.00, 0.50, 0.00) ---  
Y(1,-1): -0.050, Y(1,1):  0.029, Y(3,-2):  0.010, Y(3,-1): -0.056  
Y(3,1):  0.032, Y(3,2): -0.017, Y(3,3): -0.028, Y(5,-5): -0.004  
Y(5,-4):  0.006, Y(5,-2): -0.001, Y(5,-1):  0.003, Y(5,1): -0.002  
Y(5,2):  0.002, Y(5,3): -0.063, Y(5,4):  0.010, Y(5,5): -0.002
```

[Mode 55/121]

```
--- Generator (0.50, 0.00, 0.00) ---  
Y(1,1):  0.022, Y(3,-2):  0.085, Y(3,1): -0.031, Y(3,3):  0.005  
Y(5,-4):  0.010, Y(5,-2):  0.007, Y(5,1): -0.004, Y(5,3): -0.004  
Y(5,5):  0.035  
--- Atom 0 (0.00, 0.50, 0.00) ---  
Y(1,-1):  0.019, Y(1,1): -0.011, Y(3,-2): -0.043, Y(3,-1): -0.027  
Y(3,1):  0.015, Y(3,2):  0.074, Y(3,3):  0.005, Y(5,-5): -0.031  
Y(5,-4): -0.005, Y(5,-2): -0.003, Y(5,-1): -0.004, Y(5,1):  0.002  
Y(5,2):  0.006, Y(5,3): -0.004, Y(5,4): -0.008, Y(5,5): -0.018
```

[Mode 56/121]

```
--- Generator (0.50, 0.00, 0.00) ---  
Y(1,1):  0.042, Y(3,-2): -0.021, Y(3,1):  0.069, Y(3,3):  0.013  
Y(5,-4):  0.004, Y(5,-2): -0.002, Y(5,1):  0.013, Y(5,3):  0.013  
Y(5,5): -0.008  
--- Atom 0 (0.00, 0.50, 0.00) ---
```

```

Y(1,-1):  0.036, Y(1,1): -0.021, Y(3,-2):  0.010, Y(3,-1):  0.060
Y(3,1): -0.035, Y(3,2): -0.018, Y(3,3):  0.013, Y(5,-5):  0.007
Y(5,-4): -0.002, Y(5,-2):  0.001, Y(5,-1):  0.011, Y(5,1): -0.007
Y(5,2): -0.002, Y(5,3):  0.013, Y(5,4): -0.003, Y(5,5):  0.004

```

[Mode 57/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.055, Y(3,-2): -0.013, Y(3,1): -0.047, Y(3,3): -0.009
Y(5,-4):  0.018, Y(5,-2):  0.002, Y(5,1):  0.002, Y(5,3):  0.007
Y(5,5): -0.007
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.048, Y(1,1):  0.028, Y(3,-2):  0.006, Y(3,-1): -0.040
Y(3,1):  0.023, Y(3,2): -0.011, Y(3,3): -0.009, Y(5,-5):  0.006
Y(5,-4): -0.009, Y(5,-2): -0.001, Y(5,-1):  0.002, Y(5,1): -0.001
Y(5,2):  0.002, Y(5,3):  0.007, Y(5,4): -0.016, Y(5,5):  0.004

```

[Mode 58/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.026, Y(3,-2): -0.023, Y(3,1):  0.007, Y(3,3): -0.023
Y(5,-4): -0.016, Y(5,-2): -0.017, Y(5,1):  0.029, Y(5,3): -0.023
Y(5,5): -0.005
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.022, Y(1,1):  0.013, Y(3,-2):  0.012, Y(3,-1):  0.006
Y(3,1): -0.004, Y(3,2): -0.020, Y(3,3): -0.023, Y(5,-5):  0.004
Y(5,-4):  0.008, Y(5,-2):  0.009, Y(5,-1):  0.025, Y(5,1): -0.014
Y(5,2): -0.015, Y(5,3): -0.023, Y(5,4):  0.014, Y(5,5):  0.002

```

[Mode 59/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.138, Y(3,-2):  0.063, Y(3,1):  0.093, Y(3,3):  0.062
Y(5,-4): -0.021, Y(5,-2): -0.007, Y(5,1): -0.044, Y(5,3):  0.053
Y(5,5):  0.008
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.120, Y(1,1): -0.069, Y(3,-2): -0.032, Y(3,-1):  0.080
Y(3,1): -0.046, Y(3,2):  0.055, Y(3,3):  0.062, Y(5,-5): -0.007
Y(5,-4):  0.010, Y(5,-2):  0.004, Y(5,-1): -0.038, Y(5,1):  0.022
Y(5,2): -0.006, Y(5,3):  0.053, Y(5,4):  0.018, Y(5,5): -0.004

```

[Mode 60/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.074, Y(3,-2):  0.011, Y(3,1):  0.037, Y(3,3):  0.038
Y(5,-4):  0.005, Y(5,-2): -0.001, Y(5,1):  0.010, Y(5,3): -0.027
Y(5,5):  0.036
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.064, Y(1,1): -0.037, Y(3,-2): -0.006, Y(3,-1):  0.032
Y(3,1): -0.019, Y(3,2):  0.010, Y(3,3):  0.038, Y(5,-5): -0.031
Y(5,-4): -0.002, Y(5,-2):  0.001, Y(5,-1):  0.009, Y(5,1): -0.005
Y(5,2): -0.001, Y(5,3): -0.027, Y(5,4): -0.004, Y(5,5): -0.018

```

[Mode 61/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.049, Y(3,-2):  0.018, Y(3,1): -0.024, Y(3,3):  0.020
Y(5,-4):  0.044, Y(5,-2): -0.000, Y(5,1):  0.029, Y(5,3): -0.006
Y(5,5):  0.000
--- Atom 0 (0.00, 0.50, 0.00) ---

```

```

Y(1,-1): -0.042, Y(1,1):  0.024, Y(3,-2): -0.009, Y(3,-1): -0.021
Y(3,1):  0.012, Y(3,2):  0.016, Y(3,3):  0.020, Y(5,-5): -0.000
Y(5,-4): -0.022, Y(5,-2):  0.000, Y(5,-1):  0.025, Y(5,1): -0.015
Y(5,2): -0.000, Y(5,3): -0.006, Y(5,4): -0.038, Y(5,5): -0.000

```

[Mode 62/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.033, Y(3,-2): -0.025, Y(3,1): -0.066, Y(3,3):  0.087
Y(5,-4): -0.008, Y(5,-2): -0.012, Y(5,1):  0.012, Y(5,3): -0.004
Y(5,5):  0.030
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.028, Y(1,1):  0.016, Y(3,-2):  0.012, Y(3,-1): -0.057
Y(3,1):  0.033, Y(3,2): -0.021, Y(3,3):  0.087, Y(5,-5): -0.026
Y(5,-4):  0.004, Y(5,-2):  0.006, Y(5,-1):  0.010, Y(5,1): -0.006
Y(5,2): -0.010, Y(5,3): -0.004, Y(5,4):  0.007, Y(5,5): -0.015

```

[Mode 63/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.051, Y(3,-2):  0.011, Y(3,1):  0.038, Y(3,3): -0.031
Y(5,-4):  0.042, Y(5,-2): -0.022, Y(5,1): -0.021, Y(5,3):  0.003
Y(5,5): -0.003
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.044, Y(1,1): -0.025, Y(3,-2): -0.005, Y(3,-1):  0.033
Y(3,1): -0.019, Y(3,2):  0.009, Y(3,3): -0.031, Y(5,-5):  0.003
Y(5,-4): -0.021, Y(5,-2):  0.011, Y(5,-1): -0.018, Y(5,1):  0.011
Y(5,2): -0.019, Y(5,3):  0.003, Y(5,4): -0.036, Y(5,5):  0.002

```

[Mode 64/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.024, Y(3,-2):  0.051, Y(3,1): -0.016, Y(3,3): -0.022
Y(5,-4): -0.028, Y(5,-2):  0.004, Y(5,1): -0.059, Y(5,3):  0.023
Y(5,5): -0.047
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.021, Y(1,1):  0.012, Y(3,-2): -0.025, Y(3,-1): -0.014
Y(3,1):  0.008, Y(3,2):  0.044, Y(3,3): -0.022, Y(5,-5):  0.041
Y(5,-4):  0.014, Y(5,-2): -0.002, Y(5,-1): -0.051, Y(5,1):  0.029
Y(5,2):  0.003, Y(5,3):  0.023, Y(5,4):  0.025, Y(5,5):  0.024

```

[Mode 65/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.034, Y(3,-2):  0.039, Y(3,1):  0.022, Y(3,3):  0.046
Y(5,-4):  0.013, Y(5,-2):  0.009, Y(5,1):  0.001, Y(5,3):  0.026
Y(5,5):  0.010
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.029, Y(1,1): -0.017, Y(3,-2): -0.019, Y(3,-1):  0.019
Y(3,1): -0.011, Y(3,2):  0.034, Y(3,3):  0.046, Y(5,-5): -0.009
Y(5,-4): -0.007, Y(5,-2): -0.005, Y(5,-1):  0.001, Y(5,1): -0.000
Y(5,2):  0.008, Y(5,3):  0.026, Y(5,4): -0.011, Y(5,5): -0.005

```

[Mode 66/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.022, Y(3,-2):  0.092, Y(3,1):  0.002, Y(3,3):  0.008
Y(5,-4): -0.001, Y(5,-2):  0.054, Y(5,1): -0.022, Y(5,3):  0.010
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.019, Y(1,1): -0.011, Y(3,-2): -0.046, Y(3,-1):  0.002

```

```
Y(3,1): -0.001, Y(3,2):  0.079, Y(3,3):  0.008, Y(5,-4):  0.001  
Y(5,-2): -0.027, Y(5,-1): -0.019, Y(5,1):  0.011, Y(5,2):  0.047  
Y(5,3):  0.010, Y(5,4):  0.001
```

[Mode 67/121]

```
--- Generator (0.50, 0.00, 0.00) ---  
Y(1,1): -0.009, Y(3,-2): -0.080, Y(3,1):  0.015, Y(3,3): -0.018  
Y(5,-4): -0.006, Y(5,-2): -0.053, Y(5,1):  0.024, Y(5,3): -0.022  
--- Atom 0 (0.00, 0.50, 0.00) ---  
Y(1,-1): -0.007, Y(1,1):  0.004, Y(3,-2):  0.040, Y(3,-1):  0.013  
Y(3,1): -0.008, Y(3,2): -0.070, Y(3,3): -0.018, Y(5,-4):  0.003  
Y(5,-2):  0.027, Y(5,-1):  0.021, Y(5,1): -0.012, Y(5,2): -0.046  
Y(5,3): -0.022, Y(5,4):  0.005
```

[Mode 68/121]

```
--- Generator (0.50, 0.00, 0.00) ---  
Y(1,1): -0.089, Y(3,-2):  0.003, Y(3,1): -0.109, Y(3,3):  0.007  
Y(5,-4): -0.000, Y(5,-2):  0.001, Y(5,1): -0.014, Y(5,3):  0.009  
--- Atom 0 (0.00, 0.50, 0.00) ---  
Y(1,-1): -0.077, Y(1,1):  0.044, Y(3,-2): -0.001, Y(3,-1): -0.094  
Y(3,1):  0.054, Y(3,2):  0.002, Y(3,3):  0.007, Y(5,-4):  0.000  
Y(5,-2): -0.001, Y(5,-1): -0.012, Y(5,1):  0.007, Y(5,2):  0.001  
Y(5,3):  0.009, Y(5,4):  0.000
```

[Mode 69/121]

```
--- Generator (0.50, 0.00, 0.00) ---  
Y(1,1):  0.047, Y(3,-2):  0.004, Y(3,1): -0.025, Y(3,3):  0.034  
Y(5,-4): -0.007, Y(5,-2): -0.004, Y(5,1): -0.076, Y(5,3):  0.041  
--- Atom 0 (0.00, 0.50, 0.00) ---  
Y(1,-1):  0.040, Y(1,1): -0.023, Y(3,-2): -0.002, Y(3,-1): -0.022  
Y(3,1):  0.012, Y(3,2):  0.003, Y(3,3):  0.034, Y(5,-4):  0.003  
Y(5,-2):  0.002, Y(5,-1): -0.065, Y(5,1):  0.038, Y(5,2): -0.003  
Y(5,3):  0.041, Y(5,4):  0.006
```

[Mode 70/121]

```
--- Generator (0.50, 0.00, 0.00) ---  
Y(1,1): -0.079, Y(3,-2):  0.038, Y(3,1): -0.054, Y(3,3):  0.008  
Y(5,-4): -0.001, Y(5,-2):  0.022, Y(5,1):  0.031, Y(5,3):  0.010  
--- Atom 0 (0.00, 0.50, 0.00) ---  
Y(1,-1): -0.069, Y(1,1):  0.040, Y(3,-2): -0.019, Y(3,-1): -0.047  
Y(3,1):  0.027, Y(3,2):  0.033, Y(3,3):  0.008, Y(5,-4):  0.000  
Y(5,-2): -0.011, Y(5,-1):  0.027, Y(5,1): -0.016, Y(5,2):  0.019  
Y(5,3):  0.010, Y(5,4):  0.001
```

[Mode 71/121]

```
--- Generator (0.50, 0.00, 0.00) ---  
Y(1,1):  0.013, Y(3,-2): -0.054, Y(3,1):  0.014, Y(3,3):  0.011  
Y(5,-4): -0.006, Y(5,-2): -0.037, Y(5,3):  0.013  
--- Atom 0 (0.00, 0.50, 0.00) ---  
Y(1,-1):  0.011, Y(1,1): -0.006, Y(3,-2):  0.027, Y(3,-1):  0.012  
Y(3,1): -0.007, Y(3,2): -0.047, Y(3,3):  0.011, Y(5,-4):  0.003  
Y(5,-2):  0.019, Y(5,2): -0.032, Y(5,3):  0.013, Y(5,4):  0.005
```

[Mode 72/121]

```
--- Generator (0.50, 0.00, 0.00) ---
```

```

Y(1,1):  0.016, Y(3,-2):  0.034, Y(3,1):  0.054, Y(3,3):  0.028
Y(5,-4):  0.000, Y(5,-2):  0.021, Y(5,1):  0.037, Y(5,3):  0.033
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.013, Y(1,1): -0.008, Y(3,-2): -0.017, Y(3,-1):  0.046
Y(3,1): -0.027, Y(3,2):  0.030, Y(3,3):  0.028, Y(5,-2): -0.010
Y(5,-1):  0.032, Y(5,1): -0.019, Y(5,2):  0.018, Y(5,3):  0.033
Y(5,4): -0.000

```

[Mode 73/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.038, Y(3,-2):  0.026, Y(3,1): -0.059, Y(3,3):  0.050
Y(5,-4):  0.007, Y(5,-2):  0.022, Y(5,1): -0.018, Y(5,3):  0.060
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.033, Y(1,1):  0.019, Y(3,-2): -0.013, Y(3,-1): -0.051
Y(3,1):  0.029, Y(3,2):  0.023, Y(3,3):  0.050, Y(5,-4): -0.004
Y(5,-2): -0.011, Y(5,-1): -0.016, Y(5,1):  0.009, Y(5,2):  0.019
Y(5,3):  0.060, Y(5,4): -0.006

```

[Mode 74/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.081, Y(3,-2):  0.031, Y(3,1):  0.052, Y(3,3):  0.036
Y(5,-4):  0.001, Y(5,-2):  0.019, Y(5,1): -0.034, Y(5,3):  0.044
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.070, Y(1,1): -0.040, Y(3,-2): -0.015, Y(3,-1):  0.045
Y(3,1): -0.026, Y(3,2):  0.027, Y(3,3):  0.036, Y(5,-4): -0.001
Y(5,-2): -0.010, Y(5,-1): -0.030, Y(5,1):  0.017, Y(5,2):  0.017
Y(5,3):  0.044, Y(5,4): -0.001

```

[Mode 75/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.026, Y(3,-2): -0.030, Y(3,1): -0.052, Y(3,3):  0.031
Y(5,-4):  0.001, Y(5,-2): -0.017, Y(5,1): -0.025, Y(5,3):  0.038
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.022, Y(1,1):  0.013, Y(3,-2):  0.015, Y(3,-1): -0.045
Y(3,1):  0.026, Y(3,2): -0.026, Y(3,3):  0.031, Y(5,-4): -0.001
Y(5,-2):  0.009, Y(5,-1): -0.021, Y(5,1):  0.012, Y(5,2): -0.015
Y(5,3):  0.038, Y(5,4): -0.001

```

[Mode 76/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.094, Y(3,-2):  0.030, Y(3,1): -0.081, Y(3,3): -0.017
Y(5,-4): -0.008, Y(5,-2):  0.011, Y(5,1):  0.020, Y(5,3): -0.021
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.082, Y(1,1):  0.047, Y(3,-2): -0.015, Y(3,-1): -0.070
Y(3,1):  0.041, Y(3,2):  0.026, Y(3,3): -0.017, Y(5,-4):  0.004
Y(5,-2): -0.006, Y(5,-1):  0.017, Y(5,1): -0.010, Y(5,2):  0.010
Y(5,3): -0.021, Y(5,4):  0.007

```

[Mode 77/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.159, Y(3,-2):  0.052, Y(3,1):  0.159, Y(3,3):  0.014
Y(5,-4):  0.001, Y(5,-2):  0.032, Y(5,1): -0.010, Y(5,3):  0.017
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.137, Y(1,1): -0.079, Y(3,-2): -0.026, Y(3,-1):  0.138
Y(3,1): -0.080, Y(3,2):  0.045, Y(3,3):  0.014, Y(5,-4): -0.000

```

```
Y(5,-2): -0.016, Y(5,-1): -0.009, Y(5,1):  0.005, Y(5,2):  0.027  
Y(5,3):  0.017, Y(5,4): -0.000
```

[Mode 78/121]

```
--- Generator (0.50, 0.00, 0.00) ---  
Y(1,1):  0.014, Y(3,-2):  0.063, Y(3,1): -0.017, Y(3,3): -0.012  
Y(5,-4): -0.009, Y(5,-2):  0.030, Y(5,1): -0.033, Y(5,3): -0.014  
--- Atom 0 (0.00, 0.50, 0.00) ---  
Y(1,-1):  0.013, Y(1,1): -0.007, Y(3,-2): -0.031, Y(3,-1): -0.015  
Y(3,1):  0.009, Y(3,2):  0.054, Y(3,3): -0.012, Y(5,-4):  0.004  
Y(5,-2): -0.015, Y(5,-1): -0.029, Y(5,1):  0.017, Y(5,2):  0.026  
Y(5,3): -0.014, Y(5,4):  0.008
```

[Mode 79/121]

```
--- Generator (0.50, 0.00, 0.00) ---  
Y(1,1): -0.100, Y(3,-2):  0.041, Y(3,1): -0.107, Y(3,3): -0.052  
Y(5,-4):  0.001, Y(5,-2):  0.025, Y(5,1):  0.001, Y(5,3): -0.063  
--- Atom 0 (0.00, 0.50, 0.00) ---  
Y(1,-1): -0.087, Y(1,1):  0.050, Y(3,-2): -0.021, Y(3,-1): -0.092  
Y(3,1):  0.053, Y(3,2):  0.036, Y(3,3): -0.052, Y(5,-4): -0.000  
Y(5,-2): -0.013, Y(5,-1):  0.001, Y(5,1): -0.000, Y(5,2):  0.022  
Y(5,3): -0.063, Y(5,4): -0.001
```

[Mode 80/121]

```
--- Generator (0.50, 0.00, 0.00) ---  
Y(1,1): -0.007, Y(3,-2): -0.003, Y(3,1): -0.023, Y(3,3):  0.003  
Y(5,-4): -0.002, Y(5,-2): -0.003, Y(5,1): -0.016, Y(5,3):  0.004  
--- Atom 0 (0.00, 0.50, 0.00) ---  
Y(1,-1): -0.006, Y(1,1):  0.004, Y(3,-2):  0.001, Y(3,-1): -0.020  
Y(3,1):  0.012, Y(3,2): -0.002, Y(3,3):  0.003, Y(5,-4):  0.001  
Y(5,-2):  0.001, Y(5,-1): -0.014, Y(5,1):  0.008, Y(5,2): -0.003  
Y(5,3):  0.004, Y(5,4):  0.001
```

[Mode 81/121]

```
--- Generator (0.50, 0.00, 0.00) ---  
Y(1,1): -0.041, Y(3,-2): -0.009, Y(3,1): -0.043, Y(3,3):  0.009  
Y(5,-4): -0.010, Y(5,-2): -0.014, Y(5,1):  0.001, Y(5,3):  0.011  
--- Atom 0 (0.00, 0.50, 0.00) ---  
Y(1,-1): -0.035, Y(1,1):  0.020, Y(3,-2):  0.005, Y(3,-1): -0.037  
Y(3,1):  0.021, Y(3,2): -0.008, Y(3,3):  0.009, Y(5,-4):  0.005  
Y(5,-2):  0.007, Y(5,-1):  0.001, Y(5,1): -0.000, Y(5,2): -0.012  
Y(5,3):  0.011, Y(5,4):  0.009
```

[Mode 82/121]

```
--- Generator (0.50, 0.00, 0.00) ---  
Y(1,1): -0.150, Y(3,-2):  0.048, Y(3,1): -0.083, Y(3,3): -0.065  
Y(5,-4): -0.004, Y(5,-2):  0.025, Y(5,1):  0.078, Y(5,3): -0.079  
--- Atom 0 (0.00, 0.50, 0.00) ---  
Y(1,-1): -0.130, Y(1,1):  0.075, Y(3,-2): -0.024, Y(3,-1): -0.072  
Y(3,1):  0.042, Y(3,2):  0.041, Y(3,3): -0.065, Y(5,-4):  0.002  
Y(5,-2): -0.013, Y(5,-1):  0.067, Y(5,1): -0.039, Y(5,2):  0.022  
Y(5,3): -0.079, Y(5,4):  0.004
```

[Mode 83/121]

```
--- Generator (0.50, 0.00, 0.00) ---
```

```

Y(1,1): -0.103, Y(3,-2):  0.001, Y(3,1): -0.141, Y(3,3): -0.005
Y(5,-4): -0.006, Y(5,-2): -0.004, Y(5,1): -0.031, Y(5,3): -0.006
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.089, Y(1,1):  0.051, Y(3,-2): -0.000, Y(3,-1): -0.122
Y(3,1):  0.070, Y(3,2):  0.001, Y(3,3): -0.005, Y(5,-4):  0.003
Y(5,-2):  0.002, Y(5,-1): -0.027, Y(5,1):  0.016, Y(5,2): -0.004
Y(5,3): -0.006, Y(5,4):  0.005

```

[Mode 84/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.013, Y(3,-2):  0.014, Y(3,1): -0.043, Y(3,3):  0.009
Y(5,-4):  0.001, Y(5,-2):  0.010, Y(5,1): -0.029, Y(5,3):  0.011
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.011, Y(1,1):  0.006, Y(3,-2): -0.007, Y(3,-1): -0.037
Y(3,1):  0.021, Y(3,2):  0.012, Y(3,3):  0.009, Y(5,-4): -0.001
Y(5,-2): -0.005, Y(5,-1): -0.025, Y(5,1):  0.015, Y(5,2):  0.008
Y(5,3):  0.011, Y(5,4): -0.001

```

[Mode 85/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.017, Y(3,-2):  0.004, Y(3,1):  0.075, Y(3,3):  0.012
Y(5,-4): -0.005, Y(5,-2): -0.002, Y(5,1):  0.058, Y(5,3):  0.015
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.014, Y(1,1): -0.008, Y(3,-2): -0.002, Y(3,-1):  0.065
Y(3,1): -0.038, Y(3,2):  0.003, Y(3,3):  0.012, Y(5,-4):  0.003
Y(5,-2):  0.001, Y(5,-1):  0.050, Y(5,1): -0.029, Y(5,2): -0.002
Y(5,3):  0.015, Y(5,4):  0.005

```

[Mode 86/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.040, Y(3,-2):  0.042, Y(3,1):  0.085, Y(3,3):  0.008
Y(5,-4): -0.010, Y(5,-2):  0.017, Y(5,1):  0.043, Y(5,3):  0.010
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.035, Y(1,1): -0.020, Y(3,-2): -0.021, Y(3,-1):  0.074
Y(3,1): -0.043, Y(3,2):  0.036, Y(3,3):  0.008, Y(5,-4):  0.005
Y(5,-2): -0.009, Y(5,-1):  0.037, Y(5,1): -0.021, Y(5,2):  0.015
Y(5,3):  0.010, Y(5,4):  0.008

```

[Mode 87/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.175, Y(3,1): -0.109, Y(3,3): -0.047, Y(5,1):  0.079
Y(5,3): -0.057
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.152, Y(1,1):  0.088, Y(3,-1): -0.095, Y(3,1):  0.055
Y(3,3): -0.047, Y(5,-1):  0.068, Y(5,1): -0.039, Y(5,3): -0.057

```

[Mode 88/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.037, Y(3,-2): -0.038, Y(3,1): -0.055, Y(3,3): -0.024
Y(5,-4):  0.028, Y(5,-2): -0.019, Y(5,1): -0.017, Y(5,3): -0.031
Y(5,5): -0.002
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.032, Y(1,1):  0.019, Y(3,-2):  0.019, Y(3,-1): -0.047
Y(3,1):  0.027, Y(3,2): -0.033, Y(3,3): -0.024, Y(5,-5):  0.001
Y(5,-4): -0.014, Y(5,-2):  0.009, Y(5,-1): -0.015, Y(5,1):  0.008

```

$\text{Y}(5,2): -0.016, \text{Y}(5,3): -0.031, \text{Y}(5,4): -0.024, \text{Y}(5,5): 0.001$
 [Mode 89/121]
 --- Generator (0.50, 0.00, 0.00) ---
 $\text{Y}(1,1): -0.091, \text{Y}(3,-2): -0.016, \text{Y}(3,1): -0.079, \text{Y}(3,3): 0.002$
 $\text{Y}(5,-4): -0.018, \text{Y}(5,-2): -0.010, \text{Y}(5,1): 0.013, \text{Y}(5,3): 0.003$
 $\text{Y}(5,5): -0.004$
 --- Atom 0 (0.00, 0.50, 0.00) ---
 $\text{Y}(1,-1): -0.079, \text{Y}(1,1): 0.045, \text{Y}(3,-2): 0.008, \text{Y}(3,-1): -0.068$
 $\text{Y}(3,1): 0.039, \text{Y}(3,2): -0.014, \text{Y}(3,3): 0.002, \text{Y}(5,-5): 0.003$
 $\text{Y}(5,-4): 0.009, \text{Y}(5,-2): 0.005, \text{Y}(5,-1): 0.011, \text{Y}(5,1): -0.006$
 $\text{Y}(5,2): -0.008, \text{Y}(5,3): 0.003, \text{Y}(5,4): 0.016, \text{Y}(5,5): 0.002$

 [Mode 90/121]
 --- Generator (0.50, 0.00, 0.00) ---
 $\text{Y}(1,1): 0.021, \text{Y}(3,-2): -0.026, \text{Y}(3,1): 0.049, \text{Y}(5,-4): 0.017$
 $\text{Y}(5,-2): -0.000, \text{Y}(5,1): -0.007, \text{Y}(5,3): -0.008, \text{Y}(5,5): -0.024$
 --- Atom 0 (0.00, 0.50, 0.00) ---
 $\text{Y}(1,-1): 0.018, \text{Y}(1,1): -0.010, \text{Y}(3,-2): 0.013, \text{Y}(3,-1): 0.042$
 $\text{Y}(3,1): -0.024, \text{Y}(3,2): -0.023, \text{Y}(5,-5): 0.021, \text{Y}(5,-4): -0.008$
 $\text{Y}(5,-2): 0.000, \text{Y}(5,-1): -0.006, \text{Y}(5,1): 0.004, \text{Y}(5,2): -0.000$
 $\text{Y}(5,3): -0.008, \text{Y}(5,4): -0.014, \text{Y}(5,5): 0.012$

 [Mode 91/121]
 --- Generator (0.50, 0.00, 0.00) ---
 $\text{Y}(1,1): -0.007, \text{Y}(3,-2): -0.088, \text{Y}(3,1): -0.023, \text{Y}(3,3): -0.002$
 $\text{Y}(5,-4): -0.029, \text{Y}(5,-2): -0.026, \text{Y}(5,1): 0.001, \text{Y}(5,3): -0.012$
 $\text{Y}(5,5): 0.012$
 --- Atom 0 (0.00, 0.50, 0.00) ---
 $\text{Y}(1,-1): -0.006, \text{Y}(1,1): 0.003, \text{Y}(3,-2): 0.044, \text{Y}(3,-1): -0.020$
 $\text{Y}(3,1): 0.011, \text{Y}(3,2): -0.076, \text{Y}(3,3): -0.002, \text{Y}(5,-5): -0.010$
 $\text{Y}(5,-4): 0.015, \text{Y}(5,-2): 0.013, \text{Y}(5,-1): 0.001, \text{Y}(5,1): -0.000$
 $\text{Y}(5,2): -0.023, \text{Y}(5,3): -0.012, \text{Y}(5,4): 0.025, \text{Y}(5,5): -0.006$

 [Mode 92/121]
 --- Generator (0.50, 0.00, 0.00) ---
 $\text{Y}(1,1): 0.029, \text{Y}(3,-2): -0.024, \text{Y}(3,1): 0.049, \text{Y}(3,3): 0.024$
 $\text{Y}(5,-2): -0.015, \text{Y}(5,1): 0.018, \text{Y}(5,3): 0.028$
 --- Atom 0 (0.00, 0.50, 0.00) ---
 $\text{Y}(1,-1): 0.025, \text{Y}(1,1): -0.015, \text{Y}(3,-2): 0.012, \text{Y}(3,-1): 0.042$
 $\text{Y}(3,1): -0.024, \text{Y}(3,2): -0.021, \text{Y}(3,3): 0.024, \text{Y}(5,-2): 0.007$
 $\text{Y}(5,-1): 0.015, \text{Y}(5,1): -0.009, \text{Y}(5,2): -0.013, \text{Y}(5,3): 0.028$

 [Mode 93/121]
 --- Generator (0.50, 0.00, 0.00) ---
 $\text{Y}(1,1): -0.114, \text{Y}(3,-2): -0.046, \text{Y}(3,1): -0.190, \text{Y}(3,3): 0.016$
 $\text{Y}(5,-2): -0.028, \text{Y}(5,1): -0.068, \text{Y}(5,3): 0.020$
 --- Atom 0 (0.00, 0.50, 0.00) ---
 $\text{Y}(1,-1): -0.099, \text{Y}(1,1): 0.057, \text{Y}(3,-2): 0.023, \text{Y}(3,-1): -0.164$
 $\text{Y}(3,1): 0.095, \text{Y}(3,2): -0.040, \text{Y}(3,3): 0.016, \text{Y}(5,-2): 0.014$
 $\text{Y}(5,-1): -0.059, \text{Y}(5,1): 0.034, \text{Y}(5,2): -0.024, \text{Y}(5,3): 0.020$

 [Mode 94/121]
 --- Generator (0.50, 0.00, 0.00) ---
 $\text{Y}(1,1): 0.087, \text{Y}(3,-2): 0.053, \text{Y}(3,1): 0.145, \text{Y}(5,-2): 0.032$

```

Y(5,1):  0.052
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.075, Y(1,1): -0.044, Y(3,-2): -0.026, Y(3,-1):  0.125
Y(3,1): -0.072, Y(3,2):  0.046, Y(5,-2): -0.016, Y(5,-1):  0.045
Y(5,1): -0.026, Y(5,2):  0.028

```

[Mode 95/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.087, Y(3,-2): -0.101, Y(3,1):  0.144, Y(3,3):  0.007
Y(5,-2): -0.061, Y(5,1):  0.052, Y(5,3):  0.009
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.075, Y(1,1): -0.043, Y(3,-2):  0.051, Y(3,-1):  0.125
Y(3,1): -0.072, Y(3,2): -0.088, Y(3,3):  0.007, Y(5,-2):  0.031
Y(5,-1):  0.045, Y(5,1): -0.026, Y(5,2): -0.053, Y(5,3):  0.009

```

[Mode 96/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.038, Y(3,-2): -0.022, Y(3,1): -0.063, Y(3,3): -0.015
Y(5,-2): -0.013, Y(5,1): -0.023, Y(5,3): -0.018
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.033, Y(1,1):  0.019, Y(3,-2):  0.011, Y(3,-1): -0.055
Y(3,1):  0.031, Y(3,2): -0.019, Y(3,3): -0.015, Y(5,-2):  0.007
Y(5,-1): -0.020, Y(5,1):  0.011, Y(5,2): -0.011, Y(5,3): -0.018

```

[Mode 97/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.019, Y(3,-2):  0.059, Y(3,1): -0.032, Y(3,3):  0.002
Y(5,-2):  0.036, Y(5,1): -0.012, Y(5,3):  0.003
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.017, Y(1,1):  0.010, Y(3,-2): -0.030, Y(3,-1): -0.028
Y(3,1):  0.016, Y(3,2):  0.051, Y(3,3):  0.002, Y(5,-2): -0.018
Y(5,-1): -0.010, Y(5,1):  0.006, Y(5,2):  0.031, Y(5,3):  0.003

```

[Mode 98/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.067, Y(3,-2):  0.002, Y(3,1):  0.010, Y(3,3): -0.045
Y(5,-4):  0.007, Y(5,-2):  0.026, Y(5,1):  0.037, Y(5,3): -0.006
Y(5,5): -0.032
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.058, Y(1,1):  0.034, Y(3,-2): -0.001, Y(3,-1):  0.009
Y(3,1): -0.005, Y(3,2):  0.002, Y(3,3): -0.045, Y(5,-5):  0.028
Y(5,-4): -0.003, Y(5,-2): -0.013, Y(5,-1):  0.032, Y(5,1): -0.018
Y(5,2):  0.022, Y(5,3): -0.006, Y(5,4): -0.006, Y(5,5):  0.016

```

[Mode 99/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.042, Y(3,-2):  0.012, Y(3,1): -0.021, Y(3,3):  0.017
Y(5,-4): -0.012, Y(5,-2):  0.021, Y(5,1):  0.029, Y(5,3): -0.007
Y(5,5):  0.003
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.037, Y(1,1):  0.021, Y(3,-2): -0.006, Y(3,-1): -0.018
Y(3,1):  0.011, Y(3,2):  0.010, Y(3,3):  0.017, Y(5,-5): -0.003
Y(5,-4):  0.006, Y(5,-2): -0.010, Y(5,-1):  0.025, Y(5,1): -0.014
Y(5,2):  0.018, Y(5,3): -0.007, Y(5,4):  0.010, Y(5,5): -0.001

```

```

[Mode 100/121]
--- Generator (0.50, 0.00, 0.00) ---
(No projection weights > 1e-4)
--- Atom 0 (0.00, 0.50, 0.00) ---
(No projection weights > 1e-4)

[Mode 101/121]
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.175, Y(3,1): -0.292, Y(5,1): -0.105
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.152, Y(1,1): 0.088, Y(3,-1): -0.253, Y(3,1): 0.146
Y(5,-1): -0.091, Y(5,1): 0.053

[Mode 102/121]
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.088, Y(3,-2): 0.089, Y(3,1): -0.066, Y(3,3): -0.070
Y(5,-4): 0.012, Y(5,-2): 0.035, Y(5,1): 0.034, Y(5,3): -0.058
Y(5,5): 0.004
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.076, Y(1,1): 0.044, Y(3,-2): -0.044, Y(3,-1): -0.057
Y(3,1): 0.033, Y(3,2): 0.077, Y(3,3): -0.070, Y(5,-5): -0.003
Y(5,-4): -0.006, Y(5,-2): -0.018, Y(5,-1): 0.029, Y(5,1): -0.017
Y(5,2): 0.030, Y(5,3): -0.058, Y(5,4): -0.010, Y(5,5): -0.002

[Mode 103/121]
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.175, Y(3,1): -0.292, Y(5,1): -0.105
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.152, Y(1,1): 0.088, Y(3,-1): -0.253, Y(3,1): 0.146
Y(5,-1): -0.091, Y(5,1): 0.053

[Mode 104/121]
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): 0.077, Y(3,-2): -0.017, Y(3,1): 0.061, Y(3,3): 0.038
Y(5,-4): -0.001, Y(5,-2): -0.008, Y(5,1): -0.018, Y(5,3): 0.016
Y(5,5): 0.002
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): 0.066, Y(1,1): -0.038, Y(3,-2): 0.008, Y(3,-1): 0.053
Y(3,1): -0.031, Y(3,2): -0.015, Y(3,3): 0.038, Y(5,-5): -0.002
Y(5,-4): 0.000, Y(5,-2): 0.004, Y(5,-1): -0.016, Y(5,1): 0.009
Y(5,2): -0.007, Y(5,3): 0.016, Y(5,4): 0.000, Y(5,5): -0.001

[Mode 105/121]
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.078, Y(3,-2): -0.003, Y(3,1): -0.014, Y(3,3): -0.070
Y(5,-4): 0.041, Y(5,-2): -0.026, Y(5,1): 0.046, Y(5,3): 0.004
Y(5,5): -0.016
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.067, Y(1,1): 0.039, Y(3,-2): 0.002, Y(3,-1): -0.012
Y(3,1): 0.007, Y(3,2): -0.003, Y(3,3): -0.070, Y(5,-5): 0.014
Y(5,-4): -0.020, Y(5,-2): 0.013, Y(5,-1): 0.040, Y(5,1): -0.023
Y(5,2): -0.022, Y(5,3): 0.004, Y(5,4): -0.035, Y(5,5): 0.008

[Mode 106/121]
--- Generator (0.50, 0.00, 0.00) ---
```

```

Y(1,1): -0.013, Y(3,-2):  0.107, Y(3,1): -0.008, Y(3,3):  0.003
Y(5,-4): -0.012, Y(5,-2): -0.025, Y(5,1):  0.006, Y(5,3):  0.004
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.011, Y(1,1):  0.007, Y(3,-2): -0.054, Y(3,-1): -0.007
Y(3,1):  0.004, Y(3,2):  0.093, Y(3,3):  0.003, Y(5,-4):  0.006
Y(5,-2):  0.013, Y(5,-1):  0.005, Y(5,1): -0.003, Y(5,2): -0.022
Y(5,3):  0.004, Y(5,4):  0.011

```

[Mode 107/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.001, Y(3,-2): -0.016, Y(3,1):  0.015, Y(3,3): -0.027
Y(5,-4): -0.003, Y(5,-2): -0.019, Y(5,1): -0.008, Y(5,3):  0.009
Y(5,5): -0.017
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.001, Y(1,1):  0.001, Y(3,-2):  0.008, Y(3,-1):  0.013
Y(3,1): -0.008, Y(3,2): -0.014, Y(3,3): -0.027, Y(5,-5):  0.015
Y(5,-4):  0.001, Y(5,-2):  0.009, Y(5,-1): -0.007, Y(5,1):  0.004
Y(5,2): -0.016, Y(5,3):  0.009, Y(5,4):  0.002, Y(5,5):  0.009

```

[Mode 108/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.053, Y(3,-2): -0.009, Y(3,1):  0.045, Y(3,3): -0.034
Y(5,-4): -0.026, Y(5,-2): -0.012, Y(5,1): -0.013, Y(5,3): -0.030
Y(5,5): -0.001
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.046, Y(1,1): -0.026, Y(3,-2):  0.004, Y(3,-1):  0.039
Y(3,1): -0.023, Y(3,2): -0.008, Y(3,3): -0.034, Y(5,-5):  0.001
Y(5,-4):  0.013, Y(5,-2):  0.006, Y(5,-1): -0.011, Y(5,1):  0.006
Y(5,2): -0.010, Y(5,3): -0.030, Y(5,4):  0.022, Y(5,5):  0.001

```

[Mode 109/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.108, Y(3,-2):  0.021, Y(3,1): -0.037, Y(3,3): -0.063
Y(5,-4): -0.024, Y(5,-2):  0.002, Y(5,1):  0.021, Y(5,3): -0.003
Y(5,5): -0.040
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.093, Y(1,1):  0.054, Y(3,-2): -0.010, Y(3,-1): -0.032
Y(3,1):  0.018, Y(3,2):  0.018, Y(3,3): -0.063, Y(5,-5):  0.035
Y(5,-4):  0.012, Y(5,-2): -0.001, Y(5,-1):  0.018, Y(5,1): -0.011
Y(5,2):  0.002, Y(5,3): -0.003, Y(5,4):  0.021, Y(5,5):  0.020

```

[Mode 110/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.043, Y(3,-2): -0.051, Y(3,1):  0.028, Y(3,3):  0.008
Y(5,-4): -0.015, Y(5,-2): -0.031, Y(5,1): -0.018, Y(5,3):  0.010
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.038, Y(1,1): -0.022, Y(3,-2):  0.026, Y(3,-1):  0.024
Y(3,1): -0.014, Y(3,2): -0.044, Y(3,3):  0.008, Y(5,-4):  0.008
Y(5,-2):  0.015, Y(5,-1): -0.016, Y(5,1):  0.009, Y(5,2): -0.027
Y(5,3):  0.010, Y(5,4):  0.013

```

[Mode 111/121]

```

--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.003, Y(3,-2): -0.084, Y(3,1): -0.002, Y(3,3):  0.007
Y(5,-4): -0.086, Y(5,-2):  0.037, Y(5,1):  0.001, Y(5,3):  0.009

```

--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.003, Y(1,1): 0.002, Y(3,-2): 0.042, Y(3,-1): -0.002
Y(3,1): 0.001, Y(3,2): -0.073, Y(3,3): 0.007, Y(5,-4): 0.043
Y(5,-2): -0.018, Y(5,-1): 0.001, Y(5,1): -0.001, Y(5,2): 0.032
Y(5,3): 0.009, Y(5,4): 0.074

[Mode 112/121]
--- Generator (0.50, 0.00, 0.00) ---
Y(3,-2): -0.115, Y(5,-2): -0.070
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(3,-2): 0.058, Y(3,2): -0.100, Y(5,-2): 0.035, Y(5,2): -0.060

[Mode 113/121]
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.030, Y(3,-2): -0.094, Y(3,1): -0.051, Y(3,3): 0.035
Y(5,-4): -0.013, Y(5,-2): 0.010, Y(5,1): 0.007, Y(5,3): -0.003
Y(5,5): 0.018
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.026, Y(1,1): 0.015, Y(3,-2): 0.047, Y(3,-1): -0.044
Y(3,1): 0.025, Y(3,2): -0.081, Y(3,3): 0.035, Y(5,-5): -0.015
Y(5,-4): 0.006, Y(5,-2): -0.005, Y(5,-1): 0.006, Y(5,1): -0.004
Y(5,2): 0.009, Y(5,3): -0.003, Y(5,4): 0.011, Y(5,5): -0.009

[Mode 114/121]
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): 0.049, Y(3,-2): -0.028, Y(3,1): 0.050, Y(3,3): -0.052
Y(5,-4): -0.021, Y(5,-2): 0.013, Y(5,1): -0.032, Y(5,3): 0.032
Y(5,5): -0.020
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): 0.042, Y(1,1): -0.024, Y(3,-2): 0.014, Y(3,-1): 0.043
Y(3,1): -0.025, Y(3,2): -0.024, Y(3,3): -0.052, Y(5,-5): 0.018
Y(5,-4): 0.011, Y(5,-2): -0.007, Y(5,-1): -0.027, Y(5,1): 0.016
Y(5,2): 0.011, Y(5,3): 0.032, Y(5,4): 0.018, Y(5,5): 0.010

[Mode 115/121]
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.017, Y(3,-2): 0.013, Y(3,1): 0.011, Y(3,3): -0.036
Y(5,-4): -0.040, Y(5,-2): 0.002, Y(5,1): -0.003, Y(5,3): 0.007
Y(5,5): -0.022
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.014, Y(1,1): 0.008, Y(3,-2): -0.007, Y(3,-1): 0.009
Y(3,1): -0.005, Y(3,2): 0.011, Y(3,3): -0.036, Y(5,-5): 0.019
Y(5,-4): 0.020, Y(5,-2): -0.001, Y(5,-1): -0.003, Y(5,1): 0.002
Y(5,2): 0.002, Y(5,3): 0.007, Y(5,4): 0.034, Y(5,5): 0.011

[Mode 116/121]
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): 0.019, Y(3,-2): -0.048, Y(3,1): 0.047, Y(3,3): 0.004
Y(5,-4): -0.009, Y(5,-2): -0.030, Y(5,1): 0.012, Y(5,3): -0.010
Y(5,5): -0.011
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): 0.016, Y(1,1): -0.009, Y(3,-2): 0.024, Y(3,-1): 0.041
Y(3,1): -0.024, Y(3,2): -0.041, Y(3,3): 0.004, Y(5,-5): 0.009
Y(5,-4): 0.005, Y(5,-2): 0.015, Y(5,-1): 0.010, Y(5,1): -0.006
Y(5,2): -0.026, Y(5,3): -0.010, Y(5,4): 0.008, Y(5,5): 0.005

```

[Mode 117/121]
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.020, Y(3,-2):  0.045, Y(3,1):  0.013, Y(3,3):  0.012
Y(5,-4):  0.049, Y(5,-2):  0.004, Y(5,1): -0.009, Y(5,3):  0.014
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.017, Y(1,1): -0.010, Y(3,-2): -0.022, Y(3,-1):  0.011
Y(3,1): -0.006, Y(3,2):  0.039, Y(3,3):  0.012, Y(5,-4): -0.025
Y(5,-2): -0.002, Y(5,-1): -0.008, Y(5,1):  0.005, Y(5,2):  0.004
Y(5,3):  0.014, Y(5,4): -0.042

[Mode 118/121]
--- Generator (0.50, 0.00, 0.00) ---
Y(3,-2):  0.083, Y(3,3):  0.019, Y(5,-2):  0.050, Y(5,3):  0.023
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(3,-2): -0.042, Y(3,2):  0.072, Y(3,3):  0.019, Y(5,-2): -0.025
Y(5,2):  0.043, Y(5,3):  0.023

[Mode 119/121]
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1):  0.031, Y(3,-2):  0.022, Y(3,1):  0.013, Y(3,3):  0.040
Y(5,-4): -0.023, Y(5,-2):  0.007, Y(5,1):  0.035, Y(5,3):  0.003
Y(5,5):  0.038
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1):  0.027, Y(1,1): -0.015, Y(3,-2): -0.011, Y(3,-1):  0.011
Y(3,1): -0.007, Y(3,2):  0.019, Y(3,3):  0.040, Y(5,-5): -0.033
Y(5,-4):  0.012, Y(5,-2): -0.004, Y(5,-1):  0.030, Y(5,1): -0.017
Y(5,2):  0.006, Y(5,3):  0.003, Y(5,4):  0.020, Y(5,5): -0.019

[Mode 120/121]
--- Generator (0.50, 0.00, 0.00) ---
Y(1,1): -0.117, Y(3,-2): -0.033, Y(3,1): -0.071, Y(3,3): -0.031
Y(5,-4):  0.016, Y(5,-2): -0.006, Y(5,1):  0.054, Y(5,3): -0.038
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(1,-1): -0.101, Y(1,1):  0.058, Y(3,-2):  0.016, Y(3,-1): -0.062
Y(3,1):  0.036, Y(3,2): -0.028, Y(3,3): -0.031, Y(5,-4): -0.008
Y(5,-2):  0.003, Y(5,-1):  0.046, Y(5,1): -0.027, Y(5,2): -0.005
Y(5,3): -0.038, Y(5,4): -0.014

[Mode 121/121]
--- Generator (0.50, 0.00, 0.00) ---
Y(3,3):  0.043, Y(5,3):  0.052
--- Atom 0 (0.00, 0.50, 0.00) ---
Y(3,3):  0.043, Y(5,3):  0.052

```