

# Molecular Insights into Cage Occupancy of Hydrogen Hydrate: A Computational Study

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## Supporting Materials:

1. The atomic coordinates of the hydrates with  $(H_2)_{n=1-6}$  in the small cage and  $(H_2)_{m=1-8}$  in the large cage.

**1. The atomic positions of the hydrates with (H<sub>2</sub>)<sub>n=1~6</sub> in the small cage and (H<sub>2</sub>)<sub>m=1~8</sub> in the large cage.**

**(1) n=1 & m=1**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H23 | 17.2450 | 11.8621 | 4.5118  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H27 | 18.1619 | 9.9696  | 3.6295  |
| 60.0000 | 60.0000 (P1) |         |         |         | H28 | 16.4341 | 11.3722 | 3.2008  |
| O2      | 3.0008       | 1.6787  | 1.2309  |         | H42 | 10.4178 | 6.9441  | 0.0271  |
| O8      | 4.2978       | 5.0498  | 3.6126  |         | H45 | 12.1060 | 7.9550  | 2.8419  |
| O27     | 5.1613       | 2.9200  | 2.1702  |         | H61 | 14.8894 | 9.5149  | 1.8381  |
| H19     | 4.6328       | 4.2702  | 3.0790  |         | H68 | 12.1410 | 7.0353  | 1.5141  |
| H39     | 5.7207       | 3.2233  | 1.3909  |         | O1  | 12.5299 | 7.2111  | 9.7735  |
| H40     | 5.7230       | 2.2964  | 2.7247  |         | O3  | 11.1948 | 6.4779  | 7.5199  |
| H44     | 3.8163       | 2.1457  | 1.5916  |         | O4  | 8.9188  | 5.2451  | 8.2767  |
| H52     | 4.6671       | 5.8691  | 3.1691  |         | O13 | 6.6593  | 6.5030  | 7.4863  |
| H58     | 2.1942       | 2.1767  | 1.5703  |         | O32 | 5.1369  | 4.6353  | 6.1992  |
| O7      | 12.7140      | 2.9772  | 2.0738  |         | H10 | 5.6497  | 3.7738  | 6.1929  |
| O9      | 13.4668      | 5.0486  | 3.6046  |         | H13 | 6.1121  | 5.8443  | 6.9692  |
| O24     | 9.0068       | 0.8182  | 2.3744  |         | H21 | 10.3576 | 5.9974  | 7.7982  |
| H2      | 8.1670       | 0.9925  | 2.8896  |         | H24 | 13.4227 | 6.7560  | 9.7834  |
| H18     | 13.1462      | 5.8932  | 3.1725  |         | H26 | 4.8779  | 4.8193  | 5.2513  |
| H30     | 12.2133      | 2.3266  | 2.6543  |         | H46 | 7.4839  | 6.0117  | 7.7815  |
| H35     | 8.9763       | 1.4104  | 1.5650  |         | H57 | 12.0648 | 6.9227  | 8.9332  |
| H43     | 14.4691      | 5.0753  | 3.5898  |         | H59 | 8.9278  | 5.2095  | 9.2831  |
| H51     | 12.9818      | 3.7534  | 2.6538  |         | H65 | 8.9195  | 4.2910  | 7.9710  |
| O5      | 8.9994       | 9.4606  | 2.1374  |         | H66 | 11.7225 | 5.8200  | 6.9808  |
| O11     | 12.5808      | 11.5381 | 3.6600  |         | O12 | 17.1731 | 7.2652  | 9.7118  |
| O21     | 5.2368       | 7.2750  | 2.3555  |         | O18 | 14.7881 | 4.2572  | 7.6913  |
| O29     | 8.9576       | 7.8546  | -0.0554 |         | O23 | 11.2157 | 2.2054  | 6.0894  |
| O30     | 11.2249      | 9.1756  | 3.6407  |         | O33 | 12.5873 | 4.5670  | 6.1587  |
| H7      | 5.7211       | 6.9827  | 1.5290  |         | O34 | 14.8707 | 5.8368  | 9.8792  |
| H14     | 12.0815      | 10.6694 | 3.6794  |         | H3  | 14.8589 | 5.2471  | 9.0663  |
| H15     | 10.9252      | 8.9357  | 4.5656  |         | H5  | 11.7458 | 1.5609  | 6.6449  |
| H20     | 8.1174       | 7.3098  | -0.0163 |         | H8  | 12.8970 | 4.7938  | 5.2364  |
| H32     | 4.4076       | 7.7443  | 2.0436  |         | H16 | 17.7160 | 6.9506  | 10.4967 |
| H37     | 8.9611       | 10.4099 | 1.8062  |         | H31 | 17.6736 | 6.9738  | 8.8935  |
| H47     | 12.5798      | 11.8993 | 4.5956  |         | H33 | 14.8152 | 3.3044  | 8.0111  |
| H48     | 10.3881      | 9.2918  | 3.0979  |         | H36 | 15.7029 | 6.3918  | 9.8104  |
| H53     | 8.9489       | 8.4388  | 0.7598  |         | H38 | 11.7252 | 3.0686  | 6.1066  |
| H63     | 8.1705       | 9.3228  | 2.6878  |         | H41 | 13.4169 | 4.4389  | 6.7097  |
| O6      | 17.3506      | 11.4831 | 3.5887  |         | H64 | 15.6104 | 4.3911  | 7.1331  |
| O14     | 12.6672      | 7.3047  | 2.3229  |         | O10 | 14.8312 | 12.9463 | 7.4539  |
| O16     | 11.3358      | 6.5451  | 0.0693  |         | O19 | 12.4517 | 12.5757 | 6.1661  |
| O28     | 18.6701      | 9.1059  | 3.6296  |         | O20 | 11.1341 | 10.7609 | 7.6786  |
| O31     | 14.9000      | 8.5675  | 1.5032  |         | O22 | 12.5528 | 9.9375  | 9.8143  |
| H9      | 11.2423      | 5.5463  | 0.0542  |         | O25 | 10.3618 | 8.6696  | 6.1683  |
| H12     | 14.0605      | 8.1195  | 1.8260  |         | O26 | 7.6269  | 8.6739  | 6.1755  |
| H22     | 18.0883      | 8.4261  | 3.1769  |         | H1  | 7.2718  | 8.7635  | 5.2438  |

|     |         |         |        |
|-----|---------|---------|--------|
| H4  | 10.8461 | 9.9761  | 7.1208 |
| H6  | 12.0072 | 10.2125 | 9.0174 |
| H11 | 11.9561 | 11.8984 | 6.7173 |
| H17 | 14.8511 | 12.3431 | 8.2513 |
| H25 | 13.3458 | 12.6857 | 6.6017 |
| H29 | 10.2947 | 11.2081 | 8.0021 |
| H34 | 7.2417  | 7.8411  | 6.5785 |
| H50 | 15.6680 | 12.7615 | 6.9362 |
| H54 | 10.6787 | 7.8335  | 6.6242 |
| H62 | 9.3617  | 8.6361  | 6.1564 |
| H67 | 12.5947 | 8.9378  | 9.7981 |
| O15 | 20.8170 | 12.0143 | 8.5369 |
| O17 | 18.6358 | 10.7904 | 7.5882 |
| H49 | 18.9334 | 9.9841  | 7.0660 |
| H55 | 20.8009 | 11.9999 | 9.5425 |
| H56 | 19.9941 | 11.5356 | 8.2102 |
| H60 | 18.1120 | 10.4595 | 8.3787 |
| end |         |         |        |
| H1  | 8.7999  | 4.8572  | 1.7387 |
| H2  | 8.9374  | 5.5530  | 1.5083 |
| end |         |         |        |
| H1  | 13.3813 | 8.7995  | 7.4352 |
| H2  | 13.3124 | 8.4533  | 6.7780 |
| end |         |         |        |
| H1  | 11.5430 | 0.9831  | 0.2015 |
| H2  | 11.8384 | 0.3309  | 0.4120 |
| end |         |         |        |
| H1  | 3.5715  | 5.7810  | 0.0178 |
| H2  | 3.4835  | 5.4560  | 0.6837 |
| end |         |         |        |
| H1  | 20.3220 | 11.4104 | 5.1909 |
| H2  | 20.5833 | 11.1292 | 4.5510 |
| end |         |         |        |
| H1  | 12.1026 | 10.8038 | 0.7685 |
| H2  | 12.5674 | 10.2201 | 0.7647 |
| end |         |         |        |
| end |         |         |        |

**(2) n=1 & m=2**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H27 | 18.1608 | 9.9900  | 3.6256  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H28 | 16.4302 | 11.3884 | 3.2075  |
| 60.0000 | 60.0000 (P1) |         |         |         | H42 | 10.4159 | 6.9919  | 0.0055  |
| O2      | 2.9875       | 1.7065  | 1.2392  |         | H45 | 12.1034 | 7.9742  | 2.8511  |
| O8      | 4.2748       | 5.0721  | 3.6177  |         | H61 | 14.8853 | 9.5338  | 1.8509  |
| O27     | 5.1542       | 2.9438  | 2.1803  |         | H68 | 12.1353 | 7.0697  | 1.5133  |
| H19     | 4.6230       | 4.2941  | 3.0911  |         | O1  | 12.5350 | 7.2254  | 9.7786  |
| H39     | 5.7130       | 3.2481  | 1.4022  |         | O3  | 11.1796 | 6.5020  | 7.5105  |
| H40     | 5.7159       | 2.3175  | 2.7322  |         | O4  | 8.9099  | 5.2716  | 8.2831  |
| H44     | 3.8016       | 2.1739  | 1.6005  |         | O13 | 6.6523  | 6.5401  | 7.4847  |
| H52     | 4.6484       | 5.8911  | 3.1772  |         | O32 | 5.1343  | 4.6712  | 6.1895  |
| H58     | 2.1795       | 2.2045  | 1.5743  |         | H10 | 5.6459  | 3.8096  | 6.1811  |
| O7      | 12.6947      | 3.0074  | 2.0697  |         | H13 | 6.1096  | 5.8826  | 6.9619  |
| O9      | 13.4498      | 5.0816  | 3.6097  |         | H21 | 10.3471 | 6.0185  | 7.7983  |
| O24     | 8.9996       | 0.8369  | 2.3839  |         | H24 | 13.4215 | 6.7568  | 9.7882  |
| H2      | 8.1574       | 1.0115  | 2.8952  |         | H26 | 4.8689  | 4.8535  | 5.2424  |
| H18     | 13.1323      | 5.9275  | 3.1746  |         | H46 | 7.4765  | 6.0489  | 7.7798  |
| H30     | 12.1958      | 2.3547  | 2.6495  |         | H57 | 12.0651 | 6.9424  | 8.9414  |
| H35     | 8.9715       | 1.4242  | 1.5717  |         | H59 | 8.9169  | 5.2251  | 9.2883  |
| H43     | 14.4526      | 5.1036  | 3.5946  |         | H65 | 8.9068  | 4.3238  | 7.9603  |
| H51     | 12.9618      | 3.7809  | 2.6518  |         | H66 | 11.7099 | 5.8464  | 6.9711  |
| O5      | 8.9919       | 9.4834  | 2.1245  |         | O12 | 17.1520 | 7.3067  | 9.7078  |
| O11     | 12.5715      | 11.5547 | 3.6615  |         | O18 | 14.7835 | 4.2823  | 7.6784  |
| O21     | 5.2246       | 7.2943  | 2.3749  |         | O23 | 11.2067 | 2.2365  | 6.0831  |
| O29     | 8.9464       | 7.9003  | -0.0896 |         | O33 | 12.5772 | 4.6016  | 6.1526  |
| O30     | 11.2121      | 9.1964  | 3.6309  |         | O34 | 14.8681 | 5.8438  | 9.8759  |
| H7      | 5.7098       | 7.0003  | 1.5476  |         | H3  | 14.8569 | 5.2607  | 9.0577  |
| H14     | 12.0705      | 10.6865 | 3.6784  |         | H5  | 11.7351 | 1.5943  | 6.6423  |
| H15     | 10.9128      | 8.9485  | 4.5537  |         | H8  | 12.8805 | 4.8226  | 5.2261  |
| H20     | 8.1144       | 7.3470  | -0.0282 |         | H16 | 17.6954 | 6.9910  | 10.4911 |
| H32     | 4.3986       | 7.7698  | 2.0625  |         | H31 | 17.6528 | 7.0138  | 8.8904  |
| H37     | 8.9502       | 10.4359 | 1.8036  |         | H33 | 14.8142 | 3.3317  | 8.0044  |
| H47     | 12.5692      | 11.9173 | 4.5969  |         | H36 | 15.6947 | 6.4062  | 9.8067  |
| H48     | 10.3762      | 9.3130  | 3.0869  |         | H38 | 11.7133 | 3.1003  | 6.1004  |
| H53     | 8.9473       | 8.4800  | 0.7281  |         | H41 | 13.4099 | 4.4716  | 6.6978  |
| H63     | 8.1657       | 9.3386  | 2.6762  |         | H64 | 15.6071 | 4.4185  | 7.1225  |
| O6      | 17.3479      | 11.5035 | 3.5908  |         | O10 | 14.8173 | 12.9762 | 7.4288  |
| O14     | 12.6614      | 7.3255  | 2.3260  |         | O19 | 12.4423 | 12.6018 | 6.1593  |
| O16     | 11.3333      | 6.5938  | 0.0603  |         | O20 | 11.1301 | 10.7799 | 7.6865  |
| O28     | 18.6663      | 9.1248  | 3.6258  |         | O22 | 12.5396 | 9.9712  | 9.8487  |
| O31     | 14.8976      | 8.5871  | 1.5146  |         | O25 | 10.3507 | 8.6916  | 6.1569  |
| H9      | 11.2379      | 5.5962  | 0.0375  |         | O26 | 7.6175  | 8.7097  | 6.1739  |
| H12     | 14.0594      | 8.1372  | 1.8381  |         | H1  | 7.2675  | 8.7931  | 5.2395  |
| H22     | 18.0801      | 8.4447  | 3.1782  |         | H4  | 10.8351 | 10.0007 | 7.1267  |
| H23     | 17.2423      | 11.8846 | 4.5135  |         | H6  | 12.0027 | 10.2412 | 9.0451  |

|     |         |         |        |     |         |         |        |
|-----|---------|---------|--------|-----|---------|---------|--------|
| H11 | 11.9483 | 11.9291 | 6.7152 | end |         |         |        |
| H17 | 14.8366 | 12.3746 | 8.2284 | H1  | 13.1735 | 7.9864  | 5.4649 |
| H25 | 13.3396 | 12.7140 | 6.5905 | H2  | 13.2158 | 7.2487  | 5.3621 |
| H29 | 10.2933 | 11.2311 | 8.0127 | end |         |         |        |
| H34 | 7.2373  | 7.8742  | 6.5766 | H1  | 11.5644 | 0.9814  | 0.2025 |
| H50 | 15.6555 | 12.7909 | 6.9131 | H2  | 11.8766 | 0.3412  | 0.4252 |
| H54 | 10.6675 | 7.8516  | 6.6044 | end |         |         |        |
| H62 | 9.3505  | 8.6608  | 6.1513 | H1  | 3.5547  | 5.7570  | 0.0261 |
| H67 | 12.5896 | 8.9739  | 9.8275 | H2  | 3.4590  | 5.4245  | 0.6874 |
| O15 | 20.8199 | 12.0454 | 8.5455 | end |         |         |        |
| O17 | 18.6412 | 10.8336 | 7.5846 | H1  | 7.1757  | 5.4608  | 3.0462 |
| H49 | 18.9347 | 10.0261 | 7.0625 | H2  | 7.3336  | 4.7907  | 2.7606 |
| H55 | 20.8009 | 12.0301 | 9.5508 | end |         |         |        |
| H56 | 19.9964 | 11.5695 | 8.2163 | H1  | 20.3323 | 11.4315 | 5.1643 |
| H60 | 18.1088 | 10.5041 | 8.3701 | H2  | 20.5972 | 11.1219 | 4.5392 |
| end |         |         |        | end |         |         |        |
| H1  | 9.5489  | 5.6967  | 5.5738 | H1  | 12.0825 | 10.8465 | 0.7710 |
| H2  | 9.0514  | 5.3994  | 5.1028 | H2  | 12.5252 | 10.2460 | 0.7637 |
| end |         |         |        | end |         |         |        |
| H1  | 15.5039 | 10.0128 | 7.0496 | end |         |         |        |
| H2  | 16.1072 | 9.7227  | 6.7213 |     |         |         |        |

**(3) n=1 & m=3**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H27 | 18.1402 | 9.9541  | 3.6626  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H28 | 16.4126 | 11.3646 | 3.2342  |
| 60.0000 | 60.0000 (P1) |         |         |         | H42 | 10.4237 | 6.9490  | 0.0206  |
| O2      | 2.9709       | 1.6538  | 1.2705  |         | H45 | 12.1042 | 7.9483  | 2.8593  |
| O8      | 4.3000       | 5.0475  | 3.6496  |         | H61 | 14.8905 | 9.5128  | 1.8380  |
| O27     | 5.1276       | 2.9238  | 2.1899  |         | H68 | 12.1410 | 7.0371  | 1.5260  |
| H19     | 4.6264       | 4.2697  | 3.1070  |         | O1  | 12.5168 | 7.2183  | 9.7792  |
| H39     | 5.6882       | 3.2276  | 1.4144  |         | O3  | 11.1665 | 6.4543  | 7.5435  |
| H40     | 5.6904       | 2.2952  | 2.7368  |         | O4  | 8.9223  | 5.2053  | 8.3203  |
| H44     | 3.7866       | 2.1293  | 1.6193  |         | O13 | 6.6816  | 6.4828  | 7.5077  |
| H52     | 4.6710       | 5.8677  | 3.2076  |         | O32 | 5.1575  | 4.6246  | 6.2062  |
| H58     | 2.1658       | 2.1584  | 1.6027  |         | H10 | 5.6651  | 3.7612  | 6.1942  |
| O7      | 12.6886      | 2.9779  | 2.1027  |         | H13 | 6.1374  | 5.8293  | 6.9820  |
| O9      | 13.4614      | 5.0578  | 3.6233  |         | H21 | 10.3388 | 5.9601  | 7.8315  |
| O24     | 8.9879       | 0.8139  | 2.3767  |         | H24 | 13.4105 | 6.7645  | 9.7913  |
| H2      | 8.1467       | 0.9792  | 2.8930  |         | H26 | 4.8847  | 4.8115  | 5.2607  |
| H18     | 13.1473      | 5.9033  | 3.1876  |         | H46 | 7.5032  | 5.9869  | 7.8041  |
| H30     | 12.1873      | 2.3301  | 2.6858  |         | H57 | 12.0433 | 6.9110  | 8.9507  |
| H35     | 8.9635       | 1.4182  | 1.5772  |         | H59 | 8.9179  | 5.1607  | 9.3267  |
| H43     | 14.4631      | 5.0825  | 3.6177  |         | H65 | 8.9224  | 4.2569  | 7.9981  |
| H51     | 12.9626      | 3.7543  | 2.6787  |         | H66 | 11.7056 | 5.8060  | 7.0022  |
| O5      | 8.9773       | 9.4275  | 2.1542  |         | O12 | 17.1771 | 7.2714  | 9.7193  |
| O11     | 12.5511      | 11.5110 | 3.6503  |         | O18 | 14.7998 | 4.2727  | 7.7005  |
| O21     | 5.2294       | 7.2609  | 2.3800  |         | O23 | 11.2292 | 2.2250  | 6.1157  |
| O29     | 8.9581       | 7.8367  | -0.0509 |         | O33 | 12.5901 | 4.5888  | 6.1779  |
| O30     | 11.2020      | 9.1486  | 3.6547  |         | O34 | 14.8642 | 5.8558  | 9.8888  |
| H7      | 5.7173       | 6.9749  | 1.5530  |         | H3  | 14.8601 | 5.2649  | 9.0771  |
| H14     | 12.0512      | 10.6428 | 3.6890  |         | H5  | 11.7578 | 1.5785  | 6.6687  |
| H15     | 10.9103      | 8.9074  | 4.5819  |         | H8  | 12.8923 | 4.8181  | 5.2532  |
| H20     | 8.1181       | 7.2913  | -0.0097 |         | H16 | 17.7105 | 6.9565  | 10.5106 |
| H32     | 4.4030       | 7.7338  | 2.0676  |         | H31 | 17.6807 | 6.9699  | 8.9070  |
| H37     | 8.9399       | 10.3794 | 1.8313  |         | H33 | 14.8232 | 3.3186  | 8.0156  |
| H47     | 12.5772      | 11.8768 | 4.5833  |         | H36 | 15.6972 | 6.4105  | 9.8226  |
| H48     | 10.3606      | 9.2582  | 3.1163  |         | H38 | 11.7363 | 3.0898  | 6.1314  |
| H53     | 8.9467       | 8.4211  | 0.7640  |         | H41 | 13.4235 | 4.4639  | 6.7231  |
| H63     | 8.1487       | 9.2903  | 2.7052  |         | H64 | 15.6242 | 4.4029  | 7.1450  |
| O6      | 17.3288      | 11.4765 | 3.6201  |         | O10 | 14.8476 | 12.9190 | 7.4702  |
| O14     | 12.6714      | 7.3100  | 2.3309  |         | O19 | 12.4687 | 12.5538 | 6.1586  |
| O16     | 11.3420      | 6.5503  | 0.0775  |         | O20 | 11.1395 | 10.7519 | 7.6777  |
| O28     | 18.6497      | 9.0918  | 3.6602  |         | O22 | 12.5455 | 9.9438  | 9.8378  |
| O31     | 14.9046      | 8.5629  | 1.5090  |         | O25 | 10.3519 | 8.6500  | 6.1872  |
| H9      | 11.2482      | 5.5517  | 0.0550  |         | O26 | 7.6220  | 8.6624  | 6.1981  |
| H12     | 14.0577      | 8.1217  | 1.8234  |         | H1  | 7.2636  | 8.7478  | 5.2666  |
| H22     | 18.0655      | 8.4102  | 3.2123  |         | H4  | 10.8465 | 9.9640  | 7.1266  |
| H23     | 17.2288      | 11.8602 | 4.5413  |         | H6  | 12.0085 | 10.2185 | 9.0358  |

|     |         |         |        |     |         |         |         |
|-----|---------|---------|--------|-----|---------|---------|---------|
| H11 | 11.9707 | 11.8811 | 6.7135 | end |         |         |         |
| H17 | 14.8650 | 12.3025 | 8.2587 | H1  | 15.1444 | 8.7279  | 4.7652  |
| H25 | 13.3621 | 12.6639 | 6.5940 | H2  | 14.9681 | 8.5311  | 4.0669  |
| H29 | 10.3026 | 11.2045 | 7.9983 | end |         |         |         |
| H34 | 7.2490  | 7.8237  | 6.6018 | H1  | 15.5397 | 9.7907  | 6.9552  |
| H50 | 15.6867 | 12.7451 | 6.9508 | H2  | 16.2781 | 9.8947  | 6.9690  |
| H54 | 10.6656 | 7.8137  | 6.6441 | end |         |         |         |
| H62 | 9.3512  | 8.6174  | 6.1750 | H1  | 13.1690 | 8.4886  | 7.3949  |
| H67 | 12.5856 | 8.9447  | 9.8168 | H2  | 13.3888 | 8.5506  | 6.6846  |
| O15 | 20.8227 | 12.0201 | 8.5336 | end |         |         |         |
| O17 | 18.6335 | 10.7807 | 7.5983 | H1  | 11.5465 | 0.9918  | 0.1883  |
| H49 | 18.9317 | 9.9692  | 7.0834 | H2  | 11.8131 | 0.3341  | 0.4189  |
| H55 | 20.8093 | 11.9995 | 9.5384 | end |         |         |         |
| H56 | 20.0001 | 11.5406 | 8.2101 | H1  | 3.5717  | 5.7695  | -0.0258 |
| H60 | 18.1129 | 10.4589 | 8.3964 | H2  | 3.4843  | 5.4679  | 0.6511  |
| end |         |         |        | end |         |         |         |
| H1  | 8.7977  | 4.8338  | 1.7267 | H1  | 20.3053 | 11.4106 | 5.1889  |
| H2  | 9.0141  | 5.5057  | 1.4878 | H2  | 20.5528 | 11.1468 | 4.5363  |
| end |         |         |        | end |         |         |         |
| H1  | 9.6516  | 5.6968  | 5.5598 | H1  | 17.5598 | 13.1741 | 9.5937  |
| H2  | 9.1463  | 5.3051  | 5.1744 | H2  | 17.0081 | 13.3187 | 9.1125  |
| end |         |         |        | end |         |         |         |
| H1  | 7.1200  | 4.1107  | 4.0847 | end |         |         |         |
| H2  | 7.7078  | 4.2142  | 3.6388 |     |         |         |         |

**(4) n=1 & m=4**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H27 | 18.0819 | 9.9956  | 3.6271  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H28 | 16.3409 | 11.3730 | 3.2012  |
| 60.0000 | 60.0000 (P1) |         |         |         | H42 | 10.3613 | 6.9889  | -0.0210 |
| O2      | 2.9279       | 1.6997  | 1.2308  |         | H45 | 12.0336 | 7.9337  | 2.8201  |
| O8      | 4.2395       | 5.0880  | 3.6386  |         | H61 | 14.8175 | 9.5035  | 1.8242  |
| O27     | 5.0710       | 2.9661  | 2.1914  |         | H68 | 12.0655 | 7.0387  | 1.4749  |
| H19     | 4.5693       | 4.3062  | 3.1028  |         | O1  | 12.4643 | 7.2375  | 9.7855  |
| H39     | 5.6314       | 3.2602  | 1.4107  |         | O3  | 11.1490 | 6.4912  | 7.5122  |
| H40     | 5.6234       | 2.3193  | 2.7272  |         | O4  | 8.8807  | 5.2535  | 8.2721  |
| H44     | 3.7329       | 2.1802  | 1.5980  |         | O13 | 6.6062  | 6.5076  | 7.4808  |
| H52     | 4.6083       | 5.9046  | 3.1892  |         | O32 | 5.1106  | 4.6242  | 6.1907  |
| H58     | 2.1121       | 2.1868  | 1.5613  |         | H10 | 5.6249  | 3.7646  | 6.1633  |
| O7      | 12.6250      | 2.9935  | 2.0614  |         | H13 | 6.0740  | 5.8441  | 6.9539  |
| O9      | 13.4027      | 5.0688  | 3.5887  |         | H21 | 10.3184 | 6.0018  | 7.7954  |
| O24     | 8.9139       | 0.8167  | 2.3486  |         | H24 | 13.3540 | 6.7769  | 9.7925  |
| H2      | 8.0676       | 0.9807  | 2.8594  |         | H26 | 4.8443  | 4.8305  | 5.2486  |
| H18     | 13.0796      | 5.9082  | 3.1448  |         | H46 | 7.4345  | 6.0246  | 7.7762  |
| H30     | 12.1142      | 2.3509  | 2.6418  |         | H57 | 12.0045 | 6.9526  | 8.9429  |
| H35     | 8.8884       | 1.4099  | 1.5404  |         | H59 | 8.8795  | 5.2117  | 9.2778  |
| H43     | 14.4044      | 5.1057  | 3.5890  |         | H65 | 8.8758  | 4.3035  | 7.9538  |
| H51     | 12.9048      | 3.7644  | 2.6408  |         | H66 | 11.6853 | 5.8376  | 6.9753  |
| O5      | 8.9219       | 9.4722  | 2.1140  |         | O12 | 17.0882 | 7.2896  | 9.7001  |
| O11     | 12.4868      | 11.5072 | 3.6110  |         | O18 | 14.7569 | 4.2554  | 7.6562  |
| O21     | 5.1868       | 7.2874  | 2.3595  |         | O23 | 11.1731 | 2.2401  | 6.0800  |
| O29     | 8.9045       | 7.8913  | -0.0974 |         | O33 | 12.5459 | 4.5974  | 6.1550  |
| O30     | 11.1374      | 9.1567  | 3.6084  |         | O34 | 14.7927 | 5.8278  | 9.8474  |
| H7      | 5.6723       | 6.9929  | 1.5338  |         | H3  | 14.7938 | 5.2468  | 9.0280  |
| H14     | 11.9839      | 10.6395 | 3.6459  |         | H5  | 11.7040 | 1.5923  | 6.6283  |
| H15     | 10.8497      | 8.9178  | 4.5376  |         | H8  | 12.8306 | 4.8167  | 5.2238  |
| H20     | 8.0793       | 7.3302  | -0.0349 |         | H16 | 17.6314 | 6.9744  | 10.4852 |
| H32     | 4.3545       | 7.7499  | 2.0480  |         | H31 | 17.5879 | 6.9929  | 8.8841  |
| H37     | 8.8889       | 10.4252 | 1.7944  |         | H33 | 14.7785 | 3.3052  | 7.9829  |
| H47     | 12.5237      | 11.8679 | 4.5452  |         | H36 | 15.6204 | 6.3881  | 9.7914  |
| H48     | 10.2951      | 9.2819  | 3.0749  |         | H38 | 11.6778 | 3.1054  | 6.1027  |
| H53     | 8.8998       | 8.4720  | 0.7195  |         | H41 | 13.3882 | 4.4612  | 6.6850  |
| H63     | 8.0939       | 9.3333  | 2.6650  |         | H64 | 15.5872 | 4.3858  | 7.1070  |
| O6      | 17.2556      | 11.5064 | 3.5831  |         | O10 | 14.7937 | 12.9623 | 7.4261  |
| O14     | 12.5944      | 7.2954  | 2.2866  |         | O19 | 12.4243 | 12.5561 | 6.1219  |
| O16     | 11.2766      | 6.5798  | 0.0242  |         | O20 | 11.0860 | 10.7669 | 7.6737  |
| O28     | 18.6008      | 9.1391  | 3.6246  |         | O22 | 12.4970 | 9.9552  | 9.8306  |
| O31     | 14.8380      | 8.5533  | 1.4991  |         | O25 | 10.3084 | 8.6699  | 6.1465  |
| H9      | 11.1724      | 5.5837  | 0.0094  |         | O26 | 7.5687  | 8.6674  | 6.1543  |
| H12     | 13.9914      | 8.1073  | 1.8077  |         | H1  | 7.2122  | 8.7610  | 5.2227  |
| H22     | 18.0192      | 8.4490  | 3.1897  |         | H4  | 10.8012 | 9.9832  | 7.1152  |
| H23     | 17.1516      | 11.8900 | 4.5044  |         | H6  | 11.9521 | 10.2334 | 9.0350  |



|     |         |         |        |     |         |         |        |
|-----|---------|---------|--------|-----|---------|---------|--------|
| H11 | 11.9294 | 11.8939 | 6.6891 | H1  | 20.3298 | 11.3647 | 5.1252 |
| H17 | 14.8060 | 12.3523 | 8.2206 | H2  | 20.5872 | 11.1330 | 4.4642 |
| H25 | 13.3200 | 12.6746 | 6.5517 | end |         |         |        |
| H29 | 10.2440 | 11.2148 | 7.9894 | H1  | 17.5306 | 12.9507 | 9.4659 |
| H34 | 7.1804  | 7.8359  | 6.5578 | H2  | 16.9928 | 13.2272 | 9.0292 |
| H50 | 15.6302 | 12.7723 | 6.9081 | end |         |         |        |
| H54 | 10.6337 | 7.8351  | 6.5974 | end |         |         |        |
| H62 | 9.3089  | 8.6293  | 6.1413 |     |         |         |        |
| H67 | 12.5368 | 8.9546  | 9.8062 |     |         |         |        |
| O15 | 20.7647 | 12.0162 | 8.5251 |     |         |         |        |
| O17 | 18.5866 | 10.7921 | 7.5511 |     |         |         |        |
| H49 | 18.8804 | 9.9788  | 7.0365 |     |         |         |        |
| H55 | 20.7428 | 11.9955 | 9.5301 |     |         |         |        |
| H56 | 19.9449 | 11.5411 | 8.1894 |     |         |         |        |
| H60 | 18.0563 | 10.4747 | 8.3440 |     |         |         |        |
| end |         |         |        |     |         |         |        |
| H1  | 9.2080  | 4.9846  | 1.3354 |     |         |         |        |
| H2  | 8.6418  | 5.2938  | 1.7087 |     |         |         |        |
| end |         |         |        |     |         |         |        |
| H1  | 9.8858  | 5.6434  | 5.5309 |     |         |         |        |
| H2  | 9.5977  | 5.1809  | 5.0216 |     |         |         |        |
| end |         |         |        |     |         |         |        |
| H1  | 8.6363  | 3.4238  | 4.3664 |     |         |         |        |
| H2  | 8.8529  | 2.9394  | 3.8433 |     |         |         |        |
| end |         |         |        |     |         |         |        |
| H1  | 15.7530 | 9.1171  | 4.6544 |     |         |         |        |
| H2  | 15.3883 | 8.8167  | 4.0779 |     |         |         |        |
| end |         |         |        |     |         |         |        |
| H1  | 15.5537 | 9.8539  | 6.8969 |     |         |         |        |
| H2  | 16.2809 | 10.0039 | 6.9616 |     |         |         |        |
| end |         |         |        |     |         |         |        |
| H1  | 13.3757 | 9.1259  | 7.6558 |     |         |         |        |
| H2  | 13.4834 | 8.7351  | 7.0305 |     |         |         |        |
| end |         |         |        |     |         |         |        |
| H1  | 13.0289 | 7.8313  | 5.2508 |     |         |         |        |
| H2  | 13.0855 | 7.0980  | 5.1356 |     |         |         |        |
| end |         |         |        |     |         |         |        |
| H1  | 11.3714 | 0.8793  | 0.3427 |     |         |         |        |
| H2  | 11.7095 | 0.3091  | 0.6848 |     |         |         |        |
| end |         |         |        |     |         |         |        |
| H1  | 3.6129  | 5.7633  | 0.0837 |     |         |         |        |
| H2  | 3.4659  | 5.3953  | 0.7159 |     |         |         |        |
| end |         |         |        |     |         |         |        |
| H1  | 6.8913  | 6.1404  | 4.0340 |     |         |         |        |
| H2  | 7.5160  | 6.2115  | 4.4348 |     |         |         |        |
| end |         |         |        |     |         |         |        |

**(5) n=1 & m=5**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H27 | 18.0778 | 10.0222 | 3.6340  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H28 | 16.3354 | 11.4128 | 3.2262  |
| 60.0000 | 60.0000 (P1) |         |         |         | H42 | 10.3491 | 6.9761  | -0.0363 |
| O2      | 2.9334       | 1.7361  | 1.2397  |         | H45 | 12.0233 | 7.9643  | 2.7952  |
| O8      | 4.2189       | 5.0607  | 3.6217  |         | H61 | 14.8296 | 9.5288  | 1.8443  |
| O27     | 5.1130       | 2.9798  | 2.1448  |         | H68 | 12.0588 | 7.0451  | 1.4653  |
| H19     | 4.5542       | 4.2987  | 3.0631  |         | O1  | 12.5430 | 7.2495  | 9.7665  |
| H39     | 5.6878       | 3.2843  | 1.3784  |         | O3  | 11.2027 | 6.5010  | 7.5138  |
| H40     | 5.6649       | 2.3443  | 2.6945  |         | O4  | 8.9034  | 5.2885  | 8.2669  |
| H44     | 3.7542       | 2.2024  | 1.5899  |         | O13 | 6.6535  | 6.5124  | 7.4316  |
| H52     | 4.5909       | 5.8958  | 3.2049  |         | O32 | 5.1473  | 4.5898  | 6.1419  |
| H58     | 2.1301       | 2.2345  | 1.5830  |         | H10 | 5.6764  | 3.7391  | 6.1104  |
| O7      | 12.6341      | 3.0311  | 2.0943  |         | H13 | 6.1218  | 5.8496  | 6.9089  |
| O9      | 13.3888      | 5.1135  | 3.6111  |         | H21 | 10.3701 | 6.0225  | 7.8038  |
| O24     | 8.9457       | 0.8448  | 2.3382  |         | H24 | 13.4310 | 6.7782  | 9.7788  |
| H2      | 8.0942       | 1.0097  | 2.8390  |         | H26 | 4.8403  | 4.7809  | 5.2073  |
| H18     | 13.0724      | 5.9509  | 3.1591  |         | H46 | 7.4822  | 6.0276  | 7.7341  |
| H30     | 12.1166      | 2.3962  | 2.6775  |         | H57 | 12.0754 | 6.9602  | 8.9287  |
| H35     | 8.9303       | 1.4420  | 1.5314  |         | H59 | 8.8843  | 5.2478  | 9.2709  |
| H43     | 14.3911      | 5.1292  | 3.6052  |         | H65 | 8.9073  | 4.3368  | 7.9496  |
| H51     | 12.9020      | 3.8121  | 2.6678  |         | H66 | 11.7291 | 5.8414  | 6.9695  |
| O5      | 8.9200       | 9.4940  | 2.0972  |         | O12 | 17.1533 | 7.3088  | 9.6562  |
| O11     | 12.5116      | 11.5285 | 3.5914  |         | O18 | 14.8144 | 4.2557  | 7.6597  |
| O21     | 5.1665       | 7.3029  | 2.4383  |         | O23 | 11.2178 | 2.2542  | 6.1157  |
| O29     | 8.8933       | 7.8859  | -0.0895 |         | O33 | 12.6035 | 4.6188  | 6.1685  |
| O30     | 11.1476      | 9.1913  | 3.5843  |         | O34 | 14.8582 | 5.8691  | 9.8488  |
| H7      | 5.6643       | 7.0103  | 1.6179  |         | H3  | 14.8504 | 5.2725  | 9.0431  |
| H14     | 11.9974      | 10.6658 | 3.6215  |         | H5  | 11.7535 | 1.6012  | 6.6535  |
| H15     | 10.8847      | 8.9414  | 4.5164  |         | H8  | 12.8812 | 4.8430  | 5.2348  |
| H20     | 8.0599       | 7.3330  | -0.0214 |         | H16 | 17.6839 | 7.0026  | 10.4509 |
| H32     | 4.3446       | 7.7720  | 2.1085  |         | H31 | 17.6501 | 6.9992  | 8.8436  |
| H37     | 8.8821       | 10.4485 | 1.7852  |         | H33 | 14.8346 | 3.3089  | 7.9961  |
| H47     | 12.5530      | 11.8823 | 4.5287  |         | H36 | 15.6816 | 6.4370  | 9.7672  |
| H48     | 10.2940      | 9.3115  | 3.0666  |         | H38 | 11.7311 | 3.1140  | 6.1257  |
| H53     | 8.8856       | 8.4779  | 0.7201  |         | H41 | 13.4485 | 4.4783  | 6.6941  |
| H63     | 8.1012       | 9.3528  | 2.6602  |         | H64 | 15.6379 | 4.3794  | 7.1003  |
| O6      | 17.2503      | 11.5402 | 3.6117  |         | O10 | 14.8092 | 12.9963 | 7.4342  |
| O14     | 12.5840      | 7.3142  | 2.2753  |         | O19 | 12.4789 | 12.5429 | 6.1027  |
| O16     | 11.2668      | 6.5736  | 0.0090  |         | O20 | 11.1482 | 10.7925 | 7.7046  |
| O28     | 18.6065      | 9.1716  | 3.6348  |         | O22 | 12.4930 | 9.9793  | 9.9165  |
| O31     | 14.8437      | 8.5770  | 1.5235  |         | O25 | 10.3758 | 8.7058  | 6.1580  |
| H9      | 11.1768      | 5.5731  | -0.0130 |         | O26 | 7.6357  | 8.6964  | 6.1384  |
| H12     | 13.9894      | 8.1370  | 1.8187  |         | H1  | 7.2549  | 8.8097  | 5.2176  |
| H22     | 18.0223      | 8.4636  | 3.2274  |         | H4  | 10.8566 | 10.0071 | 7.1506  |
| H23     | 17.1533      | 11.9204 | 4.5359  |         | H6  | 11.9764 | 10.2567 | 9.1037  |

|     |         |         |        |     |         |         |        |
|-----|---------|---------|--------|-----|---------|---------|--------|
| H11 | 11.9860 | 11.8986 | 6.6949 | end |         |         |        |
| H17 | 14.8020 | 12.3790 | 8.2215 | H1  | 14.3298 | 8.5295  | 8.3178 |
| H25 | 13.3741 | 12.6808 | 6.5303 | H2  | 14.9346 | 8.8449  | 8.0168 |
| H29 | 10.3089 | 11.2399 | 8.0256 | end |         |         |        |
| H34 | 7.2268  | 7.8744  | 6.5418 | H1  | 13.0649 | 7.9771  | 5.3553 |
| H50 | 15.6559 | 12.8109 | 6.9334 | H2  | 12.9025 | 7.2747  | 5.1707 |
| H54 | 10.6943 | 7.8623  | 6.5964 | end |         |         |        |
| H62 | 9.3779  | 8.6593  | 6.1414 | H1  | 14.5807 | 2.4721  | 4.2909 |
| H67 | 12.5648 | 8.9835  | 9.8714 | H2  | 14.7499 | 2.8104  | 4.9336 |
| O15 | 20.8178 | 12.0341 | 8.5687 | end |         |         |        |
| O17 | 18.6421 | 10.8044 | 7.5870 | H1  | 15.2829 | 5.5161  | 0.7819 |
| H49 | 18.9539 | 10.0043 | 7.0663 | H2  | 15.4107 | 5.9475  | 0.1864 |
| H55 | 20.7853 | 12.0171 | 9.5759 | end |         |         |        |
| H56 | 20.0008 | 11.5562 | 8.2298 | H1  | 6.8789  | 0.2300  | 0.3110 |
| H60 | 18.0885 | 10.4704 | 8.3579 | H2  | 6.4342  | 0.8250  | 0.2411 |
| end |         |         |        | end |         |         |        |
| H1  | 9.1627  | 5.5647  | 1.3505 | H1  | 5.7066  | 9.6163  | 0.0096 |
| H2  | 8.9391  | 4.9705  | 1.7390 | H2  | 6.1344  | 9.4124  | 0.5865 |
| end |         |         |        | end |         |         |        |
| H1  | 9.8162  | 5.2942  | 5.7622 | H1  | 15.0137 | 10.2539 | 5.3630 |
| H2  | 9.6728  | 4.7000  | 5.3372 | H2  | 14.3671 | 10.5485 | 5.1361 |
| end |         |         |        | end |         |         |        |
| H1  | 8.9066  | 2.7935  | 3.8649 | H1  | 8.7523  | 7.3106  | 4.1551 |
| H2  | 8.6352  | 3.3637  | 4.2590 | H2  | 9.0844  | 7.0264  | 3.5528 |
| end |         |         |        | end |         |         |        |
| H1  | 14.9445 | 6.7727  | 5.8985 | H1  | 7.3641  | 5.2727  | 3.1723 |
| H2  | 15.6543 | 6.6210  | 6.0604 | H2  | 6.6943  | 5.0288  | 3.3886 |
| end |         |         |        | end |         |         |        |
| H1  | 16.3802 | 8.7649  | 6.3697 | end |         |         |        |
| H2  | 16.9320 | 9.2508  | 6.4887 | end |         |         |        |

**(6) n=1 & m=6**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H27 | 18.0911 | 10.0159 | 3.6226  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H28 | 16.3659 | 11.4120 | 3.1777  |
| 60.0000 | 60.0000 (P1) |         |         |         | H42 | 10.3959 | 6.9453  | 0.0065  |
| O2      | 3.0752       | 1.6928  | 1.2966  |         | H45 | 12.1065 | 7.9269  | 2.8427  |
| O8      | 4.2983       | 5.1013  | 3.6372  |         | H61 | 14.8320 | 9.5341  | 1.7786  |
| O27     | 5.2228       | 2.9980  | 2.1798  |         | H68 | 12.1218 | 7.0282  | 1.5025  |
| H19     | 4.6465       | 4.3328  | 3.1008  |         | O1  | 12.5850 | 7.2233  | 9.7495  |
| H39     | 5.7814       | 3.2735  | 1.3898  |         | O3  | 11.2072 | 6.4632  | 7.5236  |
| H40     | 5.7513       | 2.3364  | 2.7206  |         | O4  | 8.9556  | 5.2251  | 8.3371  |
| H44     | 3.8841       | 2.1889  | 1.6323  |         | O13 | 6.7163  | 6.4926  | 7.5067  |
| H52     | 4.6625       | 5.9274  | 3.2013  |         | O32 | 5.1629  | 4.6162  | 6.1836  |
| H58     | 2.2595       | 2.1814  | 1.6249  |         | H10 | 5.6657  | 3.7495  | 6.1697  |
| O7      | 12.7537      | 2.9655  | 2.0843  |         | H13 | 6.1679  | 5.8485  | 6.9806  |
| O9      | 13.4821      | 5.0554  | 3.5880  |         | H21 | 10.3886 | 5.9660  | 7.8268  |
| O24     | 8.9589       | 0.8226  | 2.3410  |         | H24 | 13.4775 | 6.7647  | 9.7648  |
| H2      | 8.1284       | 0.9947  | 2.8720  |         | H26 | 4.9003  | 4.8180  | 5.2391  |
| H18     | 13.1451      | 5.8945  | 3.1542  |         | H46 | 7.5321  | 5.9925  | 7.8123  |
| H30     | 12.2122      | 2.3395  | 2.6561  |         | H57 | 12.1139 | 6.9215  | 8.9193  |
| H35     | 8.9305       | 1.4236  | 1.5392  |         | H59 | 8.9752  | 5.1850  | 9.3416  |
| H43     | 14.4834      | 5.1099  | 3.5952  |         | H65 | 8.9299  | 4.2764  | 8.0124  |
| H51     | 13.0171      | 3.7474  | 2.6607  |         | H66 | 11.7294 | 5.8235  | 6.9580  |
| O5      | 8.9783       | 9.4506  | 2.1180  |         | O12 | 17.2097 | 7.2729  | 9.7139  |
| O11     | 12.5378      | 11.4987 | 3.6482  |         | O18 | 14.7955 | 4.2802  | 7.6414  |
| O21     | 5.2037       | 7.3142  | 2.3370  |         | O23 | 11.1585 | 2.2639  | 6.0594  |
| O29     | 8.9498       | 7.8739  | -0.1043 |         | O33 | 12.5860 | 4.5764  | 6.1256  |
| O30     | 11.2006      | 9.1455  | 3.6255  |         | O34 | 14.8979 | 5.8319  | 9.8370  |
| H7      | 5.7052       | 7.0031  | 1.5268  |         | H3  | 14.8850 | 5.2484  | 9.0189  |
| H14     | 12.0360      | 10.6298 | 3.6699  |         | H5  | 11.6753 | 1.5992  | 6.5975  |
| H15     | 10.9155      | 8.8937  | 4.5507  |         | H8  | 12.8827 | 4.7900  | 5.1958  |
| H20     | 8.1137       | 7.3239  | -0.0552 |         | H16 | 17.7603 | 6.9563  | 10.4900 |
| H32     | 4.3811       | 7.7695  | 1.9992  |         | H31 | 17.7023 | 6.9836  | 8.8905  |
| H37     | 8.9882       | 10.4101 | 1.8173  |         | H33 | 14.7992 | 3.3245  | 7.9544  |
| H47     | 12.5523      | 11.8530 | 4.5827  |         | H36 | 15.7357 | 6.3778  | 9.7872  |
| H48     | 10.3561      | 9.2529  | 3.0941  |         | H38 | 11.6881 | 3.1147  | 6.0825  |
| H53     | 8.9352       | 8.4537  | 0.7117  |         | H41 | 13.4234 | 4.4580  | 6.6663  |
| H63     | 8.1492       | 9.3393  | 2.6695  |         | H64 | 15.6263 | 4.4060  | 7.0942  |
| O6      | 17.2789      | 11.5375 | 3.5707  |         | O10 | 14.7837 | 12.9606 | 7.4483  |
| O14     | 12.6623      | 7.2889  | 2.3037  |         | O19 | 12.4381 | 12.5340 | 6.1791  |
| O16     | 11.3187      | 6.5558  | 0.0478  |         | O20 | 11.0768 | 10.7724 | 7.7020  |
| O28     | 18.6150      | 9.1623  | 3.6190  |         | O22 | 12.5395 | 9.9660  | 9.8323  |
| O31     | 14.8480      | 8.5914  | 1.4312  |         | O25 | 10.3495 | 8.6553  | 6.1679  |
| H9      | 11.2411      | 5.5565  | 0.0367  |         | O26 | 7.6146  | 8.6721  | 6.1503  |
| H12     | 14.0223      | 8.1290  | 1.7717  |         | H1  | 7.2386  | 8.7592  | 5.2277  |
| H22     | 18.0414      | 8.4726  | 3.1723  |         | H4  | 10.8116 | 9.9826  | 7.1439  |
| H23     | 17.1628      | 11.9211 | 4.4919  |         | H6  | 11.9866 | 10.2458 | 9.0440  |

|     |         |         |        |     |         |         |         |
|-----|---------|---------|--------|-----|---------|---------|---------|
| H11 | 11.9238 | 11.8761 | 6.7382 | end |         |         |         |
| H17 | 14.8254 | 12.3405 | 8.2355 | H1  | 12.7855 | 7.7318  | 5.3880  |
| H25 | 13.3286 | 12.6548 | 6.6266 | H2  | 12.9404 | 7.0123  | 5.2820  |
| H29 | 10.2266 | 11.2193 | 7.9984 | end |         |         |         |
| H34 | 7.2423  | 7.8392  | 6.5635 | H1  | 15.2337 | 5.5240  | 0.7943  |
| H50 | 15.6097 | 12.7961 | 6.9066 | H2  | 15.3739 | 5.9057  | 0.1689  |
| H54 | 10.6676 | 7.8185  | 6.6183 | end |         |         |         |
| H62 | 9.3505  | 8.6180  | 6.1481 | H1  | 6.0628  | 9.6381  | -0.1515 |
| H67 | 12.6081 | 8.9710  | 9.7923 | H2  | 6.3376  | 9.4131  | 0.5047  |
| O15 | 20.7520 | 12.0422 | 8.4811 | end |         |         |         |
| O17 | 18.5707 | 10.7920 | 7.5450 | H1  | 13.3474 | 10.0965 | 6.2946  |
| H49 | 18.8827 | 9.9860  | 7.0335 | H2  | 13.4596 | 9.4078  | 6.5556  |
| H55 | 20.7332 | 12.0296 | 9.4878 | end |         |         |         |
| H56 | 19.9314 | 11.5628 | 8.1521 | H1  | 9.0723  | 7.1838  | 3.2941  |
| H60 | 18.0623 | 10.4611 | 8.3460 | H2  | 8.9129  | 6.9823  | 3.9925  |
| end |         |         |        | end |         |         |         |
| H1  | 8.6955  | 5.1991  | 1.4546 | H1  | 17.0300 | 7.7093  | 5.2237  |
| H2  | 9.3432  | 5.0804  | 1.1093 | H2  | 16.9335 | 7.0108  | 5.4571  |
| end |         |         |        | end |         |         |         |
| H1  | 9.3180  | 5.0407  | 5.3489 | H1  | 10.8741 | 4.1254  | 3.1488  |
| H2  | 9.6692  | 5.5277  | 5.7888 | H2  | 10.4627 | 4.5530  | 3.5980  |
| end |         |         |        | end |         |         |         |
| H1  | 8.2542  | 3.0765  | 4.5787 | H1  | 3.6464  | 2.5955  | 4.9813  |
| H2  | 8.8924  | 3.1371  | 4.2019 | H2  | 3.5802  | 2.1534  | 4.3841  |
| end |         |         |        | end |         |         |         |
| H1  | 14.7644 | 8.6527  | 4.4998 | H1  | 7.3339  | 5.4697  | 3.0892  |
| H2  | 14.9892 | 8.6866  | 3.7914 | H2  | 6.8539  | 4.9089  | 2.9949  |
| end |         |         |        | end |         |         |         |
| H1  | 16.5586 | 9.9186  | 6.3041 | H1  | 12.7448 | 10.5472 | 0.3702  |
| H2  | 16.0870 | 9.7905  | 5.7427 | H2  | 12.3636 | 11.1780 | 0.2554  |
| end |         |         |        | end |         |         |         |
| H1  | 15.0082 | 7.4041  | 7.7348 | end |         |         |         |
| H2  | 15.3663 | 7.6581  | 7.1320 |     |         |         |         |

(7) n=1 & m=7

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H27 | 18.0950 | 10.0264 | 3.5950  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H28 | 16.3672 | 11.4320 | 3.1468  |
| 60.0000 | 60.0000 (P1) |         |         |         | H42 | 10.3952 | 7.0280  | -0.0286 |
| O2      | 2.9442       | 1.7989  | 1.3028  |         | H45 | 12.0599 | 7.9871  | 2.8229  |
| O8      | 4.2839       | 5.1467  | 3.7181  |         | H61 | 14.8187 | 9.5651  | 1.7529  |
| O27     | 5.1260       | 3.0441  | 2.2091  |         | H68 | 12.0981 | 7.0725  | 1.4943  |
| H19     | 4.6148       | 4.3809  | 3.1653  |         | O1  | 12.4880 | 7.2784  | 9.7690  |
| H39     | 5.6832       | 3.3313  | 1.4246  |         | O3  | 11.1280 | 6.4652  | 7.5724  |
| H40     | 5.6781       | 2.3927  | 2.7375  |         | O4  | 8.8680  | 5.2546  | 8.3490  |
| H44     | 3.7597       | 2.2784  | 1.6473  |         | O13 | 6.6531  | 6.5219  | 7.4691  |
| H52     | 4.6204       | 5.9718  | 3.2626  |         | O32 | 5.1216  | 4.6292  | 6.2576  |
| H58     | 2.1312       | 2.3031  | 1.6183  |         | H10 | 5.6291  | 3.7674  | 6.2235  |
| O7      | 12.6339      | 3.1041  | 2.0685  |         | H13 | 6.0976  | 5.8407  | 6.9890  |
| O9      | 13.4321      | 5.1193  | 3.6546  |         | H21 | 10.2881 | 5.9890  | 7.8570  |
| O24     | 8.9516       | 0.8488  | 2.2614  |         | H24 | 13.3799 | 6.8260  | 9.7621  |
| H2      | 8.1360       | 1.0479  | 2.7982  |         | H26 | 4.8719  | 4.8565  | 5.3148  |
| H18     | 13.1120      | 5.9608  | 3.2182  |         | H46 | 7.4708  | 6.0367  | 7.7936  |
| H30     | 12.1303      | 2.4394  | 2.6305  |         | H57 | 12.0065 | 6.9702  | 8.9449  |
| H35     | 8.9288       | 1.4626  | 1.4703  |         | H59 | 8.8721  | 5.2327  | 9.3551  |
| H43     | 14.4325      | 5.1612  | 3.6675  |         | H65 | 8.8807  | 4.3041  | 8.0305  |
| H51     | 12.9123      | 3.8585  | 2.6708  |         | H66 | 11.6486 | 5.8124  | 7.0253  |
| O5      | 8.9615       | 9.5640  | 2.1424  |         | O12 | 17.1363 | 7.3570  | 9.6513  |
| O11     | 12.5188      | 11.5629 | 3.6242  |         | O18 | 14.7500 | 4.2917  | 7.6650  |
| O21     | 5.1465       | 7.3504  | 2.3449  |         | O23 | 11.2120 | 2.1624  | 6.0786  |
| O29     | 8.9392       | 7.9473  | -0.0367 |         | O33 | 12.5286 | 4.5408  | 6.1791  |
| O30     | 11.1781      | 9.2053  | 3.6313  |         | O34 | 14.8531 | 5.9060  | 9.7912  |
| H7      | 5.6638       | 7.0475  | 1.5448  |         | H3  | 14.8280 | 5.3056  | 8.9829  |
| H14     | 12.0159      | 10.6965 | 3.6527  |         | H5  | 11.7548 | 1.5155  | 6.6174  |
| H15     | 10.9002      | 8.9284  | 4.5503  |         | H8  | 12.8192 | 4.7876  | 5.2568  |
| H20     | 8.1090       | 7.3921  | 0.0102  |         | H16 | 17.6586 | 7.0574  | 10.4548 |
| H32     | 4.3269       | 7.8131  | 2.0023  |         | H31 | 17.6482 | 7.0416  | 8.8489  |
| H37     | 8.9092       | 10.5222 | 1.8410  |         | H33 | 14.7791 | 3.3386  | 7.9872  |
| H47     | 12.5448      | 11.9070 | 4.5639  |         | H36 | 15.6784 | 6.4708  | 9.7156  |
| H48     | 10.3289      | 9.3355  | 3.1094  |         | H38 | 11.7060 | 3.0337  | 6.1004  |
| H53     | 8.9296       | 8.5377  | 0.7742  |         | H41 | 13.3737 | 4.4402  | 6.7148  |
| H63     | 8.1348       | 9.3899  | 2.6828  |         | H64 | 15.5873 | 4.4240  | 7.1237  |
| O6      | 17.2830      | 11.5574 | 3.5266  |         | O10 | 14.8035 | 12.9788 | 7.4674  |
| O14     | 12.6215      | 7.3391  | 2.3025  |         | O19 | 12.4171 | 12.5567 | 6.1633  |
| O16     | 11.3087      | 6.6163  | 0.0004  |         | O20 | 11.0961 | 10.7602 | 7.6546  |
| O28     | 18.5996      | 9.1625  | 3.5995  |         | O22 | 12.5180 | 10.0129 | 9.8283  |
| O31     | 14.8256      | 8.6109  | 1.4332  |         | O25 | 10.3301 | 8.6378  | 6.1734  |
| H9      | 11.2004      | 5.6181  | -0.0223 |         | O26 | 7.6007  | 8.6593  | 6.1035  |
| H12     | 13.9914      | 8.1657  | 1.7738  |         | H1  | 7.2134  | 8.7734  | 5.1859  |
| H22     | 18.0079      | 8.4822  | 3.1580  |         | H4  | 10.8057 | 9.9679  | 7.1101  |
| H23     | 17.1814      | 11.8885 | 4.4677  |         | H6  | 11.9847 | 10.2709 | 9.0189  |

|     |         |         |        |
|-----|---------|---------|--------|
| H11 | 11.9229 | 11.8694 | 6.7066 |
| H17 | 14.8245 | 12.3754 | 8.2673 |
| H25 | 13.3154 | 12.6599 | 6.5883 |
| H29 | 10.2612 | 11.2228 | 7.9722 |
| H34 | 7.2170  | 7.8295  | 6.5150 |
| H50 | 15.6276 | 12.7742 | 6.9435 |
| H54 | 10.6368 | 7.8033  | 6.6386 |
| H62 | 9.3321  | 8.5998  | 6.1361 |
| H67 | 12.5639 | 9.0145  | 9.8170 |
| O15 | 20.7992 | 12.0544 | 8.4849 |
| O17 | 18.6612 | 10.7682 | 7.5447 |
| H49 | 18.9537 | 9.9573  | 7.0282 |
| H55 | 20.7633 | 12.0355 | 9.4910 |
| H56 | 19.9926 | 11.5559 | 8.1482 |
| H60 | 18.1195 | 10.4592 | 8.3333 |
| end |         |         |        |
| H1  | 10.1541 | 5.8491  | 1.9128 |
| H2  | 9.7499  | 5.4732  | 2.4117 |
| end |         |         |        |
| H1  | 8.7889  | 5.6736  | 5.7749 |
| H2  | 9.4002  | 6.0671  | 5.6286 |
| end |         |         |        |
| H1  | 7.3250  | 3.8785  | 4.8798 |
| H2  | 7.6050  | 4.4847  | 4.5561 |
| end |         |         |        |
| H1  | 15.1159 | 8.0974  | 3.9312 |
| H2  | 14.8399 | 7.7687  | 4.5387 |
| end |         |         |        |
| H1  | 16.8802 | 9.4629  | 6.2080 |
| H2  | 16.3106 | 9.3858  | 5.7362 |
| end |         |         |        |
| H1  | 15.3044 | 6.8844  | 7.0136 |
| H2  | 15.9179 | 7.1017  | 6.6548 |
| end |         |         |        |
| H1  | 13.0690 | 6.8571  | 5.7554 |
| H2  | 13.1065 | 7.5978  | 5.8123 |

|     |         |         |        |
|-----|---------|---------|--------|
| end |         |         |        |
| H1  | 6.8292  | 0.2921  | 0.2351 |
| H2  | 6.3777  | 0.8802  | 0.1520 |
| end |         |         |        |
| H1  | 12.9817 | 9.7076  | 5.4152 |
| H2  | 13.1977 | 9.6489  | 6.1224 |
| end |         |         |        |
| H1  | 8.8310  | 7.5594  | 4.0943 |
| H2  | 9.2104  | 7.3534  | 3.4926 |
| end |         |         |        |
| H1  | 15.2342 | 11.4416 | 5.2474 |
| H2  | 14.6078 | 11.1962 | 4.9323 |
| end |         |         |        |
| H1  | 10.2217 | 4.2767  | 4.4627 |
| H2  | 10.4522 | 3.7830  | 3.9569 |
| end |         |         |        |
| H1  | 14.2299 | 9.1545  | 8.2182 |
| H2  | 14.7351 | 8.9194  | 7.7239 |
| end |         |         |        |
| H1  | 8.0573  | 3.6220  | 2.7641 |
| H2  | 8.2708  | 3.4322  | 2.0793 |
| end |         |         |        |
| H1  | 11.1275 | 0.9010  | 0.1901 |
| H2  | 11.6924 | 0.5105  | 0.4776 |
| end |         |         |        |
| H1  | 7.5171  | 6.1996  | 2.8687 |
| H2  | 7.1387  | 5.5712  | 2.7582 |
| end |         |         |        |
| H1  | 20.2618 | 11.5300 | 4.3320 |
| H2  | 19.8912 | 11.8175 | 4.9118 |
| end |         |         |        |
| H1  | 8.5643  | 8.1906  | 9.1394 |
| H2  | 9.0934  | 8.5009  | 8.7140 |
| end |         |         |        |
| end |         |         |        |

(8) n=1 & m=8

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H27 | 18.0727 | 10.0602 | 3.5932  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H28 | 16.3395 | 11.4094 | 3.1709  |
| 60.0000 | 60.0000 (P1) |         |         |         | H42 | 10.3199 | 6.9983  | -0.0502 |
| O2      | 2.9990       | 1.8321  | 1.2912  |         | H45 | 12.0092 | 7.9727  | 2.7477  |
| O8      | 4.2503       | 5.1211  | 3.6710  |         | H61 | 14.7617 | 9.4923  | 1.7009  |
| O27     | 5.1817       | 3.0602  | 2.1930  |         | H68 | 12.0210 | 7.0315  | 1.4292  |
| H19     | 4.6102       | 4.3652  | 3.1220  |         | O1  | 12.5616 | 7.2859  | 9.7527  |
| H39     | 5.7455       | 3.3438  | 1.4122  |         | O3  | 11.1641 | 6.5274  | 7.5336  |
| H40     | 5.7099       | 2.3966  | 2.7301  |         | O4  | 8.8914  | 5.3103  | 8.3469  |
| H44     | 3.8153       | 2.3077  | 1.6393  |         | O13 | 6.6556  | 6.5351  | 7.4708  |
| H52     | 4.5794       | 5.9583  | 3.2320  |         | O32 | 5.0679  | 4.6500  | 6.2340  |
| H58     | 2.1774       | 2.3161  | 1.6186  |         | H10 | 5.5673  | 3.7821  | 6.2220  |
| O7      | 12.6598      | 3.0606  | 2.0558  |         | H13 | 6.1117  | 5.8654  | 6.9698  |
| O9      | 13.4368      | 5.1055  | 3.5921  |         | H21 | 10.3376 | 6.0454  | 7.8346  |
| O24     | 8.9378       | 0.7613  | 2.2449  |         | H24 | 13.4365 | 6.8015  | 9.7561  |
| H2      | 8.1322       | 0.9890  | 2.7798  |         | H26 | 4.8355  | 4.8653  | 5.2849  |
| H18     | 13.1184      | 5.9399  | 3.1462  |         | H46 | 7.4706  | 6.0496  | 7.7992  |
| H30     | 12.1331      | 2.4275  | 2.6279  |         | H57 | 12.0736 | 6.9966  | 8.9276  |
| H35     | 8.9392       | 1.3759  | 1.4504  |         | H59 | 8.9088  | 5.2930  | 9.3535  |
| H43     | 14.4406      | 5.1344  | 3.6033  |         | H65 | 8.8769  | 4.3557  | 8.0379  |
| H51     | 12.9231      | 3.8353  | 2.6407  |         | H66 | 11.6764 | 5.8747  | 6.9760  |
| O5      | 8.9397       | 9.5762  | 2.0897  |         | O12 | 17.1108 | 7.3023  | 9.6551  |
| O11     | 12.4802      | 11.5353 | 3.6440  |         | O18 | 14.7129 | 4.2376  | 7.6435  |
| O21     | 5.0853       | 7.3637  | 2.3656  |         | O23 | 11.1385 | 2.2624  | 6.0783  |
| O29     | 8.8823       | 7.9452  | -0.0558 |         | O33 | 12.5169 | 4.6047  | 6.1321  |
| O30     | 11.1583      | 9.1866  | 3.5503  |         | O34 | 14.8644 | 5.8202  | 9.8041  |
| H7      | 5.5999       | 7.0484  | 1.5678  |         | H3  | 14.8220 | 5.2416  | 8.9830  |
| H14     | 11.9755      | 10.6671 | 3.6464  |         | H5  | 11.6734 | 1.6026  | 6.6071  |
| H15     | 10.8862      | 8.9050  | 4.4708  |         | H8  | 12.8125 | 4.8389  | 5.2080  |
| H20     | 8.0449       | 7.4029  | 0.0015  |         | H16 | 17.6535 | 7.0165  | 10.4482 |
| H32     | 4.2559       | 7.8004  | 2.0114  |         | H31 | 17.6235 | 7.0063  | 8.8464  |
| H37     | 8.9256       | 10.5382 | 1.8021  |         | H33 | 14.7419 | 3.2745  | 7.9361  |
| H47     | 12.4659      | 11.8804 | 4.5807  |         | H36 | 15.6914 | 6.3862  | 9.7233  |
| H48     | 10.3064      | 9.3248  | 3.0346  |         | H38 | 11.6534 | 3.1223  | 6.0816  |
| H53     | 8.8900       | 8.5439  | 0.7500  |         | H41 | 13.3537 | 4.4603  | 6.6675  |
| H63     | 8.1090       | 9.4236  | 2.6292  |         | H64 | 15.5436 | 4.3958  | 7.1012  |
| O6      | 17.2458      | 11.5666 | 3.5576  |         | O10 | 14.7543 | 13.0389 | 7.5066  |
| O14     | 12.5575      | 7.3085  | 2.2288  |         | O19 | 12.3319 | 12.5701 | 6.1984  |
| O16     | 11.2256      | 6.5707  | -0.0263 |         | O20 | 11.0471 | 10.7203 | 7.6601  |
| O28     | 18.5859      | 9.2015  | 3.5634  |         | O22 | 12.4449 | 10.0239 | 9.8628  |
| O31     | 14.7694      | 8.5429  | 1.3707  |         | O25 | 10.3210 | 8.6507  | 6.0915  |
| H9      | 11.1126      | 5.5733  | -0.0375 |         | O26 | 7.5718  | 8.6851  | 6.0949  |
| H12     | 13.9317      | 8.0987  | 1.7058  |         | H1  | 7.1823  | 8.7827  | 5.1794  |
| H22     | 17.9809      | 8.5272  | 3.1357  |         | H4  | 10.7741 | 9.9433  | 7.0854  |
| H23     | 17.1237      | 11.9333 | 4.4831  |         | H6  | 11.9234 | 10.2525 | 9.0370  |



|     |         |         |        |     |         |        |         |
|-----|---------|---------|--------|-----|---------|--------|---------|
| H11 | 11.8555 | 11.8663 | 6.7353 | end |         |        |         |
| H17 | 14.7786 | 12.4134 | 8.2895 | H1  | 8.9953  | 7.0957 | 3.3850  |
| H25 | 13.2286 | 12.6875 | 6.6163 | H2  | 8.4323  | 7.4249 | 3.7397  |
| H29 | 10.1974 | 11.1710 | 7.9572 | end |         |        |         |
| H34 | 7.1917  | 7.8549  | 6.5064 | H1  | 17.1811 | 7.3125 | 4.7836  |
| H50 | 15.5741 | 12.8501 | 6.9705 | H2  | 17.0520 | 7.3302 | 5.5137  |
| H54 | 10.6379 | 7.8245  | 6.5646 | end |         |        |         |
| H62 | 9.3235  | 8.6124  | 6.0723 | H1  | 10.4612 | 4.3874 | 3.9594  |
| H67 | 12.5527 | 9.0321  | 9.8529 | H2  | 10.3022 | 3.6781 | 3.8003  |
| O15 | 20.7333 | 11.9965 | 8.4270 | end |         |        |         |
| O17 | 18.5432 | 10.7817 | 7.5084 | H1  | 14.8123 | 9.0741 | 7.9868  |
| H49 | 18.8488 | 9.9763  | 6.9897 | H2  | 14.2874 | 8.8518 | 8.4644  |
| H55 | 20.7011 | 11.9818 | 9.4332 | end |         |        |         |
| H56 | 19.9067 | 11.5275 | 8.0967 | H1  | 8.0096  | 3.5036 | 2.7794  |
| H60 | 18.0165 | 10.4578 | 8.2999 | H2  | 8.2793  | 3.2385 | 2.1425  |
| end |         |         |        | end |         |        |         |
| H1  | 9.0009  | 5.1401  | 1.7085 | H1  | 13.0209 | 9.6935 | 6.2199  |
| H2  | 9.3689  | 5.6961  | 1.3796 | H2  | 13.3275 | 9.9463 | 5.5928  |
| end |         |         |        | end |         |        |         |
| H1  | 9.0054  | 5.8397  | 6.0213 | H1  | 10.7387 | 6.3781 | 4.6451  |
| H2  | 9.0311  | 5.4599  | 5.3844 | H2  | 11.2376 | 6.4025 | 4.0969  |
| end |         |         |        | end |         |        |         |
| H1  | 7.2412  | 3.7396  | 4.7794 | H1  | 3.5744  | 2.5873 | 4.9736  |
| H2  | 7.4053  | 4.4120  | 4.5141 | H2  | 3.4939  | 2.1592 | 4.3680  |
| end |         |         |        | end |         |        |         |
| H1  | 14.9653 | 8.7583  | 3.8560 | H1  | 4.0192  | 5.2862 | 0.2377  |
| H2  | 14.7477 | 8.4745  | 4.5083 | H2  | 3.6242  | 4.7042 | 0.4866  |
| end |         |         |        | end |         |        |         |
| H1  | 16.5457 | 9.7920  | 6.4518 | H1  | 7.2036  | 5.7938 | 2.6165  |
| H2  | 16.0064 | 9.5421  | 6.0033 | H2  | 6.6867  | 5.2849 | 2.7653  |
| end |         |         |        | end |         |        |         |
| H1  | 15.3700 | 7.1843  | 7.3360 | H1  | 11.1374 | 9.7397 | -0.1768 |
| H2  | 15.7882 | 6.6645  | 7.0095 | H2  | 11.6491 | 9.4643 | 0.2910  |
| end |         |         |        | end |         |        |         |
| H1  | 13.1888 | 6.9402  | 5.7215 | H1  | 17.3942 | 4.3314 | 9.2021  |
| H2  | 13.2115 | 7.6831  | 5.7454 | H2  | 18.0804 | 4.0445 | 9.2562  |
| end |         |         |        | end |         |        |         |
| H1  | 15.1308 | 11.7222 | 5.2065 | end |         |        |         |
| H2  | 14.5293 | 11.5500 | 4.8072 |     |         |        |         |

**(9) n=2 & m=1**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H27 | 18.1833 | 9.9474  | 3.6101  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H28 | 16.4890 | 11.4056 | 3.2039  |
| 60.0000 | 60.0000 (P1) |         |         |         | H42 | 10.4182 | 6.9741  | 0.0207  |
| O2      | 2.9904       | 1.6682  | 1.1926  |         | H45 | 12.1199 | 7.9932  | 2.8500  |
| O8      | 4.3212       | 5.0677  | 3.6200  |         | H61 | 14.9293 | 9.5817  | 1.8874  |
| O27     | 5.1312       | 2.9238  | 2.1778  |         | H68 | 12.1723 | 7.0847  | 1.5239  |
| H19     | 4.6302       | 4.2749  | 3.0887  |         | O1  | 12.4933 | 7.1404  | 9.7479  |
| H39     | 5.6902       | 3.1957  | 1.3884  |         | O3  | 11.1480 | 6.4184  | 7.5021  |
| H40     | 5.6893       | 2.3039  | 2.7387  |         | O4  | 8.8702  | 5.1363  | 8.2348  |
| H44     | 3.8052       | 2.1293  | 1.5610  |         | O13 | 6.5997  | 6.4365  | 7.4754  |
| H52     | 4.7024       | 5.8776  | 3.1703  |         | O32 | 5.0974  | 4.6039  | 6.1815  |
| H58     | 2.1951       | 2.1867  | 1.5232  |         | H10 | 5.6124  | 3.7429  | 6.1867  |
| O7      | 12.7389      | 3.0382  | 2.0575  |         | H13 | 6.0373  | 5.7880  | 6.9601  |
| O9      | 13.4939      | 5.0915  | 3.6175  |         | H21 | 10.3160 | 5.9263  | 7.7677  |
| O24     | 9.0205       | 0.9007  | 2.4116  |         | H24 | 13.3972 | 6.7088  | 9.7588  |
| H2      | 8.1773       | 1.0634  | 2.9238  |         | H26 | 4.8635  | 4.8013  | 5.2270  |
| H18     | 13.1789      | 5.9383  | 3.1874  |         | H46 | 7.4130  | 5.9272  | 7.7608  |
| H30     | 12.2519      | 2.3789  | 2.6364  |         | H57 | 12.0259 | 6.8471  | 8.9099  |
| H35     | 8.9864       | 1.4843  | 1.5962  |         | H59 | 8.8999  | 5.1215  | 9.2409  |
| H43     | 14.4962      | 5.1099  | 3.6031  |         | H65 | 8.8797  | 4.1815  | 7.9359  |
| H51     | 13.0176      | 3.8043  | 2.6448  |         | H66 | 11.6879 | 5.7708  | 6.9624  |
| O5      | 8.9816       | 9.4314  | 2.0677  |         | O12 | 17.1846 | 7.3251  | 9.7012  |
| O11     | 12.5628      | 11.5563 | 3.6796  |         | O18 | 14.7777 | 4.2507  | 7.7162  |
| O21     | 5.2761       | 7.2627  | 2.3528  |         | O23 | 11.2475 | 2.1593  | 6.0863  |
| O29     | 8.9003       | 7.8083  | -0.0977 |         | O33 | 12.5859 | 4.5428  | 6.1500  |
| O30     | 11.1882      | 9.1905  | 3.6340  |         | O34 | 14.8821 | 5.8669  | 9.8812  |
| H7      | 5.7381       | 6.9508  | 1.5213  |         | H3  | 14.8779 | 5.2583  | 9.0829  |
| H14     | 12.0621      | 10.6897 | 3.6847  |         | H5  | 11.7866 | 1.5327  | 6.6541  |
| H15     | 10.8710      | 8.9326  | 4.5472  |         | H8  | 12.9061 | 4.7877  | 5.2361  |
| H20     | 8.0798       | 7.2364  | -0.0335 |         | H16 | 17.7323 | 7.0162  | 10.4848 |
| H32     | 4.4597       | 7.7557  | 2.0504  |         | H31 | 17.6697 | 7.0043  | 8.8856  |
| H37     | 8.9430       | 10.3854 | 1.7522  |         | H33 | 14.8109 | 3.2983  | 8.0347  |
| H47     | 12.5371      | 11.9108 | 4.6179  |         | H36 | 15.7034 | 6.4335  | 9.8041  |
| H48     | 10.3652      | 9.2930  | 3.0702  |         | H38 | 11.7378 | 3.0330  | 6.1044  |
| H53     | 8.9005       | 8.4083  | 0.7071  |         | H41 | 13.4069 | 4.4221  | 6.7132  |
| H63     | 8.1683       | 9.2964  | 2.6393  |         | H64 | 15.5898 | 4.3801  | 7.1444  |
| O6      | 17.4145      | 11.4889 | 3.5702  |         | O10 | 14.8221 | 12.8406 | 7.4010  |
| O14     | 12.6969      | 7.3570  | 2.3313  |         | O19 | 12.4029 | 12.5546 | 6.1861  |
| O16     | 11.3401      | 6.5915  | 0.0823  |         | O20 | 11.1187 | 10.6886 | 7.6559  |
| O28     | 18.6866      | 9.0813  | 3.6257  |         | O22 | 12.5353 | 9.8408  | 9.8021  |
| O31     | 14.9478      | 8.6376  | 1.5510  |         | O25 | 10.2953 | 8.6176  | 6.1525  |
| H9      | 11.2564      | 5.5915  | 0.0555  |         | O26 | 7.5696  | 8.6152  | 6.2109  |
| H12     | 14.1057      | 8.1864  | 1.8596  |         | H1  | 7.2268  | 8.7134  | 5.2785  |
| H22     | 18.1153      | 8.4002  | 3.1603  |         | H4  | 10.7995 | 9.9137  | 7.1006  |
| H23     | 17.3239      | 11.8444 | 4.5044  |         | H6  | 11.9896 | 10.1275 | 9.0110  |

|     |         |         |        |     |         |         |        |
|-----|---------|---------|--------|-----|---------|---------|--------|
| H11 | 11.9146 | 11.8569 | 6.7187 | end |         |         |        |
| H17 | 14.8284 | 12.2387 | 8.2015 | H1  | 11.6044 | 1.5159  | 0.1048 |
| H25 | 13.3096 | 12.6371 | 6.5986 | H2  | 11.8711 | 0.8216  | 0.1338 |
| H29 | 10.3030 | 11.1543 | 8.0039 | end |         |         |        |
| H34 | 7.1863  | 7.7771  | 6.6049 | H1  | 3.6682  | 2.3537  | 4.6215 |
| H50 | 15.6696 | 12.6663 | 6.8971 | H2  | 3.8455  | 2.9106  | 5.0818 |
| H54 | 10.6196 | 7.7863  | 6.6085 | end |         |         |        |
| H62 | 9.2948  | 8.5833  | 6.1668 | H1  | 3.5467  | 6.4036  | 0.2223 |
| H67 | 12.5698 | 8.8394  | 9.7771 | H2  | 3.5755  | 5.9484  | 0.8079 |
| O15 | 20.8412 | 12.0078 | 8.5702 | end |         |         |        |
| O17 | 18.6741 | 10.7819 | 7.6154 | H1  | 20.2235 | 11.1819 | 5.1056 |
| H49 | 18.9467 | 9.9615  | 7.1026 | H2  | 20.0438 | 10.6254 | 4.6471 |
| H55 | 20.8206 | 12.0257 | 9.5738 | end |         |         |        |
| H56 | 20.0146 | 11.5305 | 8.2458 | H1  | 12.4109 | 10.9980 | 0.7449 |
| H60 | 18.1340 | 10.4776 | 8.4057 | H2  | 13.0272 | 10.7162 | 1.0513 |
| end |         |         |        | end |         |         |        |
| H1  | 8.7844  | 4.8132  | 1.7465 | H1  | 8.4851  | 7.4148  | 8.8285 |
| H2  | 8.9552  | 5.5030  | 1.5210 | H2  | 8.6118  | 8.0961  | 9.0975 |
| end |         |         |        | end |         |         |        |
| H1  | 13.3440 | 8.7389  | 7.4184 | H1  | 17.2906 | 13.1327 | 9.3134 |
| H2  | 13.3323 | 8.3899  | 6.7590 | H2  | 16.7516 | 13.1855 | 8.8017 |
| end |         |         |        | end |         |         |        |
| H1  | 6.3153  | 8.8431  | 0.0841 | end |         |         |        |
| H2  | 5.6380  | 9.1453  | 0.0470 |     |         |         |        |

**(10) n=2 & m=2**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H27 | 18.1852 | 9.9660  | 3.6073  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H28 | 16.4807 | 11.4238 | 3.2050  |
| 60.0000 | 60.0000 (P1) |         |         |         | H42 | 10.4196 | 7.0225  | 0.0044  |
| O2      | 2.9758       | 1.6944  | 1.2058  |         | H45 | 12.1173 | 8.0122  | 2.8572  |
| O8      | 4.3008       | 5.0975  | 3.6212  |         | H61 | 14.9205 | 9.6083  | 1.8898  |
| O27     | 5.1325       | 2.9528  | 2.1842  |         | H68 | 12.1695 | 7.1194  | 1.5202  |
| H19     | 4.6186       | 4.3038  | 3.0998  |         | O1  | 12.4933 | 7.1572  | 9.7486  |
| H39     | 5.6862       | 3.2174  | 1.3892  |         | O3  | 11.1353 | 6.4277  | 7.4969  |
| H40     | 5.6863       | 2.3253  | 2.7400  |         | O4  | 8.8559  | 5.1612  | 8.2461  |
| H44     | 3.7899       | 2.1581  | 1.5677  |         | O13 | 6.5741  | 6.4683  | 7.4782  |
| H52     | 4.6861       | 5.9053  | 3.1700  |         | O32 | 5.0875  | 4.6310  | 6.1712  |
| H58     | 2.1802       | 2.2125  | 1.5362  |         | H10 | 5.6020  | 3.7706  | 6.1764  |
| O7      | 12.7259      | 3.0731  | 2.0596  |         | H13 | 6.0233  | 5.8156  | 6.9557  |
| O9      | 13.4824      | 5.1339  | 3.6289  |         | H21 | 10.3087 | 5.9326  | 7.7723  |
| O24     | 9.0075       | 0.9240  | 2.4192  |         | H24 | 13.3935 | 6.7175  | 9.7668  |
| H2      | 8.1641       | 1.0868  | 2.9315  |         | H26 | 4.8569  | 4.8342  | 5.2165  |
| H18     | 13.1662      | 5.9781  | 3.1910  |         | H46 | 7.3903  | 5.9692  | 7.7680  |
| H30     | 12.2340      | 2.4124  | 2.6326  |         | H57 | 12.0259 | 6.8616  | 8.9137  |
| H35     | 8.9779       | 1.5093  | 1.6058  |         | H59 | 8.8798  | 5.1366  | 9.2511  |
| H43     | 14.4854      | 5.1499  | 3.6107  |         | H65 | 8.8621  | 4.2113  | 7.9311  |
| H51     | 13.0038      | 3.8341  | 2.6513  |         | H66 | 11.6778 | 5.7830  | 6.9554  |
| O5      | 8.9704       | 9.4513  | 2.0594  |         | O12 | 17.1628 | 7.3645  | 9.6996  |
| O11     | 12.5536      | 11.5715 | 3.6853  |         | O18 | 14.7704 | 4.2739  | 7.7090  |
| O21     | 5.2584       | 7.2897  | 2.3652  |         | O23 | 11.2334 | 2.1848  | 6.0783  |
| O29     | 8.8923       | 7.8474  | -0.1229 |         | O33 | 12.5768 | 4.5690  | 6.1465  |
| O30     | 11.1743      | 9.2070  | 3.6257  |         | O34 | 14.8753 | 5.8847  | 9.8823  |
| H7      | 5.7233       | 6.9659  | 1.5389  |         | H3  | 14.8721 | 5.2803  | 9.0806  |
| H14     | 12.0529      | 10.7053 | 3.6887  |         | H5  | 11.7714 | 1.5604  | 6.6487  |
| H15     | 10.8563      | 8.9337  | 4.5339  |         | H8  | 12.8896 | 4.8185  | 5.2311  |
| H20     | 8.0817       | 7.2665  | -0.0436 |         | H16 | 17.7106 | 7.0585  | 10.4820 |
| H32     | 4.4474       | 7.7874  | 2.0559  |         | H31 | 17.6453 | 7.0368  | 8.8842  |
| H37     | 8.9284       | 10.4086 | 1.7555  |         | H33 | 14.8059 | 3.3224  | 8.0281  |
| H47     | 12.5254      | 11.9287 | 4.6227  |         | H36 | 15.6927 | 6.4556  | 9.8063  |
| H48     | 10.3531      | 9.3096  | 3.0601  |         | H38 | 11.7240 | 3.0571  | 6.0941  |
| H53     | 8.8963       | 8.4413  | 0.6853  |         | H41 | 13.4017 | 4.4502  | 6.7041  |
| H63     | 8.1619       | 9.3079  | 2.6344  |         | H64 | 15.5806 | 4.4041  | 7.1347  |
| O6      | 17.4072      | 11.5137 | 3.5662  |         | O10 | 14.8101 | 12.8750 | 7.3856  |
| O14     | 12.6918      | 7.3787  | 2.3327  |         | O19 | 12.3943 | 12.5775 | 6.1856  |
| O16     | 11.3395      | 6.6377  | 0.0743  |         | O20 | 11.1124 | 10.6989 | 7.6577  |
| O28     | 18.6802      | 9.0965  | 3.6253  |         | O22 | 12.5220 | 9.8681  | 9.8338  |
| O31     | 14.9423      | 8.6648  | 1.5519  |         | O25 | 10.2781 | 8.6194  | 6.1390  |
| H9      | 11.2492      | 5.6395  | 0.0412  |         | O26 | 7.5512  | 8.6400  | 6.2154  |
| H12     | 14.1060      | 8.2084  | 1.8655  |         | H1  | 7.2123  | 8.7341  | 5.2815  |
| H22     | 18.1018      | 8.4193  | 3.1605  |         | H4  | 10.7859 | 9.9284  | 7.1050  |
| H23     | 17.3149      | 11.8671 | 4.5012  |         | H6  | 11.9891 | 10.1522 | 9.0347  |

|     |         |         |         |     |         |         |        |
|-----|---------|---------|---------|-----|---------|---------|--------|
| H11 | 11.9063 | 11.8811 | 6.7175  | end |         |         |        |
| H17 | 14.8133 | 12.2760 | 8.1884  | H1  | 11.6210 | 1.5435  | 0.1174 |
| H25 | 13.3028 | 12.6623 | 6.5955  | H2  | 11.9051 | 0.8626  | 0.2128 |
| H29 | 10.3001 | 11.1661 | 8.0139  | end |         |         |        |
| H34 | 7.1689  | 7.8014  | 6.6096  | H1  | 3.6878  | 2.3492  | 4.6187 |
| H50 | 15.6579 | 12.6947 | 6.8833  | H2  | 3.8794  | 2.9070  | 5.0726 |
| H54 | 10.6031 | 7.7872  | 6.5908  | end |         |         |        |
| H62 | 9.2783  | 8.5907  | 6.1636  | H1  | 3.4631  | 6.4370  | 0.2818 |
| H67 | 12.5622 | 8.8688  | 9.8005  | H2  | 3.4623  | 5.9212  | 0.8158 |
| O15 | 20.8486 | 12.0325 | 8.5787  | end |         |         |        |
| O17 | 18.6790 | 10.8202 | 7.6075  | H1  | 7.4156  | 5.3646  | 3.0821 |
| H49 | 18.9449 | 9.9969  | 7.0962  | H2  | 7.1728  | 4.7321  | 2.7706 |
| H55 | 20.8256 | 12.0576 | 9.5828  | end |         |         |        |
| H56 | 20.0221 | 11.5574 | 8.2544  | H1  | 20.2399 | 11.1953 | 5.0936 |
| H60 | 18.1324 | 10.5197 | 8.3939  | H2  | 20.0612 | 10.6296 | 4.6462 |
| end |         |         |         | end |         |         |        |
| H1  | 9.5202  | 5.7227  | 5.5231  | H1  | 12.4076 | 11.0617 | 0.7032 |
| H2  | 9.0595  | 5.3867  | 5.0409  | H2  | 13.0000 | 10.7703 | 1.0447 |
| end |         |         |         | end |         |         |        |
| H1  | 15.5311 | 9.9653  | 7.0243  | H1  | 8.6305  | 7.3803  | 8.7641 |
| H2  | 16.1756 | 9.6989  | 6.7621  | H2  | 8.5534  | 8.0599  | 9.0562 |
| end |         |         |         | end |         |         |        |
| H1  | 13.1143 | 7.9917  | 5.5184  | H1  | 17.2918 | 13.0955 | 9.2881 |
| H2  | 13.1747 | 7.2693  | 5.3421  | H2  | 16.7549 | 13.2331 | 8.7905 |
| end |         |         |         | end |         |         |        |
| H1  | 6.3254  | 8.8386  | 0.1104  | end |         |         |        |
| H2  | 5.7004  | 9.2130  | -0.0387 |     |         |         |        |

**(11) n=2 & m=3**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H27 | 18.1756 | 9.9359  | 3.6488  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H28 | 16.4934 | 11.3907 | 3.2333  |
| 60.0000 | 60.0000 (P1) |         |         |         | H42 | 10.4333 | 6.9717  | 0.0227  |
| O2      | 2.9795       | 1.6457  | 1.2317  |         | H45 | 12.1319 | 7.9865  | 2.8768  |
| O8      | 4.3390       | 5.0509  | 3.6342  |         | H61 | 14.9344 | 9.5812  | 1.8938  |
| O27     | 5.1334       | 2.9009  | 2.1899  |         | H68 | 12.1825 | 7.0819  | 1.5483  |
| H19     | 4.6443       | 4.2616  | 3.0953  |         | O1  | 12.5061 | 7.1402  | 9.7610  |
| H39     | 5.6959       | 3.1830  | 1.4079  |         | O3  | 11.1412 | 6.3941  | 7.5321  |
| H40     | 5.6955       | 2.2830  | 2.7510  |         | O4  | 8.8793  | 5.1217  | 8.2776  |
| H44     | 3.7984       | 2.1078  | 1.5895  |         | O13 | 6.6183  | 6.4292  | 7.4942  |
| H52     | 4.7185       | 5.8654  | 3.1898  |         | O32 | 5.1242  | 4.5935  | 6.1916  |
| H58     | 2.1871       | 2.1734  | 1.5561  |         | H10 | 5.6335  | 3.7288  | 6.1951  |
| O7      | 12.7341      | 3.0343  | 2.0832  |         | H13 | 6.0649  | 5.7794  | 6.9719  |
| O9      | 13.5043      | 5.0906  | 3.6363  |         | H21 | 10.3136 | 5.8949  | 7.8033  |
| O24     | 9.0274       | 0.8871  | 2.4286  |         | H24 | 13.4078 | 6.7016  | 9.7746  |
| H2      | 8.1824       | 1.0408  | 2.9411  |         | H26 | 4.8806  | 4.7882  | 5.2387  |
| H18     | 13.1946      | 5.9403  | 3.2077  |         | H46 | 7.4321  | 5.9238  | 7.7851  |
| H30     | 12.2502      | 2.3741  | 2.6647  |         | H57 | 12.0295 | 6.8341  | 8.9335  |
| H35     | 8.9925       | 1.4774  | 1.6192  |         | H59 | 8.8978  | 5.0900  | 9.2838  |
| H43     | 14.5061      | 5.1048  | 3.6242  |         | H65 | 8.8885  | 4.1741  | 7.9571  |
| H51     | 13.0149      | 3.8016  | 2.6677  |         | H66 | 11.6899 | 5.7528  | 6.9915  |
| O5      | 8.9769       | 9.4058  | 2.0979  |         | O12 | 17.1945 | 7.3236  | 9.7170  |
| O11     | 12.5616      | 11.5307 | 3.6851  |         | O18 | 14.7995 | 4.2579  | 7.7298  |
| O21     | 5.2781       | 7.2534  | 2.3728  |         | O23 | 11.2561 | 2.1822  | 6.1013  |
| O29     | 8.9216       | 7.8055  | -0.0867 |         | O33 | 12.6027 | 4.5578  | 6.1749  |
| O30     | 11.1863      | 9.1660  | 3.6592  |         | O34 | 14.8901 | 5.8672  | 9.9005  |
| H7      | 5.7473       | 6.9468  | 1.5426  |         | H3  | 14.8924 | 5.2604  | 9.1008  |
| H14     | 12.0607      | 10.6642 | 3.7023  |         | H5  | 11.7840 | 1.5492  | 6.6694  |
| H15     | 10.8733      | 8.9063  | 4.5732  |         | H8  | 12.9174 | 4.8057  | 5.2598  |
| H20     | 8.1051       | 7.2283  | -0.0260 |         | H16 | 17.7395 | 7.0125  | 10.5022 |
| H32     | 4.4635       | 7.7455  | 2.0676  |         | H31 | 17.6782 | 6.9988  | 8.9021  |
| H37     | 8.9378       | 10.3615 | 1.7881  |         | H33 | 14.8285 | 3.3031  | 8.0418  |
| H47     | 12.5470      | 11.8922 | 4.6207  |         | H36 | 15.7095 | 6.4376  | 9.8260  |
| H48     | 10.3604      | 9.2660  | 3.0982  |         | H38 | 11.7519 | 3.0528  | 6.1233  |
| H53     | 8.9125       | 8.3989  | 0.7231  |         | H41 | 13.4269 | 4.4361  | 6.7332  |
| H63     | 8.1618       | 9.2702  | 2.6674  |         | H64 | 15.6127 | 4.3867  | 7.1598  |
| O6      | 17.4180      | 11.4803 | 3.5997  |         | O10 | 14.8272 | 12.8343 | 7.4079  |
| O14     | 12.7121      | 7.3581  | 2.3508  |         | O19 | 12.4145 | 12.5386 | 6.1893  |
| O16     | 11.3548      | 6.5880  | 0.0999  |         | O20 | 11.1316 | 10.6798 | 7.6701  |
| O28     | 18.6792      | 9.0696  | 3.6607  |         | O22 | 12.5466 | 9.8454  | 9.8306  |
| O31     | 14.9478      | 8.6371  | 1.5538  |         | O25 | 10.3002 | 8.6005  | 6.1811  |
| H9      | 11.2703      | 5.5882  | 0.0674  |         | O26 | 7.5766  | 8.6096  | 6.2373  |
| H12     | 14.1013      | 8.1913  | 1.8615  |         | H1  | 7.2318  | 8.7047  | 5.3046  |
| H22     | 18.1047      | 8.3892  | 3.1982  |         | H4  | 10.8112 | 9.9024  | 7.1180  |
| H23     | 17.3257      | 11.8451 | 4.5303  |         | H6  | 12.0057 | 10.1304 | 9.0362  |

|     |         |         |        |     |         |         |        |
|-----|---------|---------|--------|-----|---------|---------|--------|
| H11 | 11.9289 | 11.8433 | 6.7285 | end |         |         |        |
| H17 | 14.8431 | 12.2274 | 8.2043 | H1  | 13.1327 | 8.4720  | 7.3667 |
| H25 | 13.3215 | 12.6284 | 6.6006 | H2  | 13.3268 | 8.5127  | 6.6475 |
| H29 | 10.3155 | 11.1481 | 8.0122 | end |         |         |        |
| H34 | 7.2005  | 7.7663  | 6.6300 | H1  | 6.3483  | 8.8310  | 0.1326 |
| H50 | 15.6731 | 12.6691 | 6.8982 | H2  | 5.6861  | 9.1540  | 0.0400 |
| H54 | 10.6223 | 7.7689  | 6.6370 | end |         |         |        |
| H62 | 9.2991  | 8.5669  | 6.1933 | H1  | 11.5953 | 1.5139  | 0.1138 |
| H67 | 12.5813 | 8.8451  | 9.8035 | H2  | 11.8775 | 0.8265  | 0.1578 |
| O15 | 20.8493 | 12.0078 | 8.5686 | end |         |         |        |
| O17 | 18.6727 | 10.7740 | 7.6295 | H1  | 3.6985  | 2.3327  | 4.6471 |
| H49 | 18.9514 | 9.9516  | 7.1215 | H2  | 3.8697  | 2.8918  | 5.1069 |
| H55 | 20.8267 | 12.0229 | 9.5716 | end |         |         |        |
| H56 | 20.0232 | 11.5299 | 8.2450 | H1  | 3.5496  | 6.3892  | 0.2396 |
| H60 | 18.1412 | 10.4708 | 8.4276 | H2  | 3.5534  | 5.9467  | 0.8355 |
| end |         |         |        | end |         |         |        |
| H1  | 8.7515  | 4.8297  | 1.7290 | H1  | 20.2229 | 11.1792 | 5.1235 |
| H2  | 9.0234  | 5.4756  | 1.4760 | H2  | 20.0389 | 10.6280 | 4.6602 |
| end |         |         |        | end |         |         |        |
| H1  | 9.6268  | 5.7275  | 5.5245 | H1  | 12.4044 | 11.0140 | 0.7871 |
| H2  | 9.1141  | 5.3475  | 5.1373 | H2  | 13.0337 | 10.6966 | 1.0265 |
| end |         |         |        | end |         |         |        |
| H1  | 7.0814  | 4.1467  | 4.0407 | H1  | 8.5936  | 7.3756  | 8.8180 |
| H2  | 7.7283  | 4.2286  | 3.6805 | H2  | 8.5883  | 8.0724  | 9.0777 |
| end |         |         |        | end |         |         |        |
| H1  | 15.1634 | 8.7319  | 4.7997 | H1  | 17.3083 | 13.1751 | 9.3103 |
| H2  | 14.9953 | 8.5196  | 4.1038 | H2  | 16.7721 | 13.1600 | 8.7940 |
| end |         |         |        | end |         |         |        |
| H1  | 15.5572 | 9.8557  | 6.9706 | end |         |         |        |
| H2  | 16.3018 | 9.8510  | 7.0048 |     |         |         |        |

**(12) n=2 & m=4**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.5965 | -4.6838 | 0.0133  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.3446 | 0.2898  | -3.5321 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | -0.0064 | -1.8962 | -2.9745 |
| O1      | 6.5229       | 3.7165  | 0.1018  |         | H12 | -3.8117 | -2.0864 | 1.8394  |
| O2      | 2.9589       | 1.6650  | 1.2356  |         | H13 | 0.0927  | 2.3438  | -2.7541 |
| O3      | 5.1823       | 2.9972  | -2.1700 |         | H14 | 6.0390  | 0.3273  | 3.6941  |
| O4      | 2.9183       | 1.7095  | -1.4307 |         | H15 | 4.8735  | -1.4168 | 4.5500  |
| O5      | 2.9682       | -0.8758 | 2.0859  |         | H16 | -0.1200 | 3.5888  | 0.7626  |
| O6      | -0.4912      | 1.2247  | 3.5768  |         | H17 | 2.8976  | -1.4896 | -1.5053 |
| O7      | 0.8044       | 3.0442  | 2.0524  |         | H18 | 1.2573  | 5.9400  | 3.1545  |
| O8      | 4.2855       | 5.0837  | 3.6323  |         | H19 | 4.6101  | 4.2958  | 3.1019  |
| O9      | 1.5725       | 5.0964  | 3.5944  |         | H20 | 2.1165  | -3.0598 | -0.0203 |
| O10     | 2.8796       | -0.8768 | -2.2982 |         | H21 | 4.3596  | 2.4879  | -1.9032 |
| O11     | 6.5444       | 1.1917  | 3.6870  |         | H22 | 0.1771  | -1.8636 | 3.1743  |
| O12     | -0.6703      | 3.9016  | -0.0194 |         | H23 | -0.5833 | 1.5870  | 4.5084  |
| O13     | 0.6394       | 3.0014  | -2.2328 |         | H24 | 7.4314  | 3.2936  | 0.0969  |
| O14     | -5.1854      | -2.9570 | 2.3004  |         | H25 | 1.3884  | -1.1150 | -3.1051 |
| O15     | -2.9701      | -1.7013 | -1.1556 |         | H26 | -1.0865 | 1.3660  | -4.4823 |
| O16     | -6.5203      | -3.6847 | 0.0357  |         | H27 | 0.2690  | -0.3222 | 3.6271  |
| O17     | -5.1406      | -2.9285 | -2.1242 |         | H28 | -1.4158 | 1.1266  | 3.2136  |
| O18     | -3.0797      | 0.8333  | -2.0236 |         | H29 | -1.6151 | -2.5827 | -1.6906 |
| O19     | 0.4823       | -1.2092 | -3.5200 |         | H30 | 0.3033  | 2.3958  | 2.6321  |
| O20     | -0.8016      | -3.0595 | -2.0266 |         | H31 | -0.1918 | 3.5784  | -0.8388 |
| O21     | -0.7647      | -2.9995 | 2.3518  |         | H32 | -1.5797 | -2.5046 | 2.0468  |
| O22     | 0.5984       | -3.8792 | 0.1501  |         | H33 | -3.0479 | -0.1183 | -1.7020 |
| O23     | -6.6373      | -1.2216 | -3.6247 |         | H34 | -4.7366 | -5.9525 | -3.1091 |
| O24     | -2.9397      | 0.9212  | 2.4094  |         | H35 | -2.9733 | 1.5080  | 1.5974  |
| O25     | -1.6300      | -5.1229 | -3.5430 |         | H36 | -2.1521 | 2.9958  | 0.0771  |
| O26     | -4.3586      | -5.1125 | -3.5053 |         | H37 | 2.9426  | 0.0831  | 1.7836  |
| O27     | 5.0963       | 2.9183  | 2.2257  |         | H38 | -6.1432 | -0.3504 | -3.6063 |
| O28     | 0.7647       | -1.1927 | 3.6317  |         | H39 | 5.6638  | 3.1828  | 1.4402  |
| O29     | 2.9278       | -2.4810 | -0.1011 |         | H40 | 5.6400  | 2.2801  | 2.7816  |
| O30     | 5.1775       | -1.1644 | 3.6310  |         | H41 | -4.4484 | 1.0200  | -3.0181 |
| O31     | -2.9674      | -1.6310 | 1.5384  |         | H42 | -7.4487 | -3.3121 | -0.0160 |
| O32     | -0.8435      | 1.1605  | -3.5319 |         | H43 | 2.5756  | 5.1161  | 3.5904  |
| O33     | -5.2747      | 1.1480  | -3.5724 |         | H44 | 3.7714  | 2.1284  | 1.6085  |
| O34     | -2.9793      | 2.4391  | 0.1546  |         | H45 | -5.7680 | -2.3468 | 2.8437  |
| H1      | -4.7097      | -5.0158 | -4.4346 |         | H46 | 1.4566  | 2.5068  | -1.9360 |
| H2      | -3.7856      | 1.0627  | 2.9241  |         | H47 | 6.5442  | 1.5458  | 4.6247  |
| H3      | -2.9934      | 1.8360  | -0.6470 |         | H48 | 4.3469  | -1.0514 | 3.0797  |
| H4      | -1.1261      | -3.8295 | -2.5854 |         | H49 | -4.8679 | -3.7533 | -2.6301 |
| H5      | -6.0968      | -1.8557 | -3.0699 |         | H50 | 3.7197  | -1.0415 | -2.8155 |
| H6      | 0.0652       | -3.6081 | -0.6546 |         | H51 | 1.0867  | 3.8122  | 2.6356  |
| H7      | -0.2924      | -3.3174 | 1.5278  |         | H52 | 4.6465  | 5.9033  | 3.1843  |
| H8      | -4.9631      | 1.3730  | -4.4939 |         | H53 | 2.9271  | -1.8864 | 0.7067  |



|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.3032 | -5.9491 | -3.0796 | end |         |         |         |
| H55 | -3.0071 | -1.6790 | -0.1531 | H1  | 13.6281 | 8.8609  | 7.8266  |
| H56 | -3.7943 | -2.1742 | -1.4886 | H2  | 13.6921 | 8.5272  | 7.1634  |
| H57 | 6.0607  | 3.4323  | -0.7395 | end |         |         |         |
| H58 | 2.1593  | 2.1867  | 1.5506  | H1  | 12.9435 | 7.8152  | 5.2889  |
| H59 | 2.9363  | 1.6787  | -0.4246 | H2  | 13.0976 | 7.0896  | 5.2229  |
| H60 | -5.6815 | -3.2295 | -1.3302 | end |         |         |         |
| H61 | -2.9838 | -0.6876 | 1.8783  | H1  | 14.2440 | 0.8633  | 5.0718  |
| H62 | -2.6308 | -5.1608 | -3.5341 | H2  | 14.1025 | 0.3007  | 4.6073  |
| H63 | 2.1467  | -1.0102 | 2.6452  | end |         |         |         |
| H64 | -2.2602 | 0.9613  | -2.5849 | H1  | 15.5676 | 2.3459  | 4.6433  |
| H65 | 2.9129  | 0.7610  | -1.7483 | H2  | 15.6950 | 2.8926  | 5.1310  |
| H66 | 5.7225  | 2.3706  | -2.7317 | end |         |         |         |
| H67 | 0.6361  | -4.8808 | 0.1381  | H1  | 8.5859  | -6.3328 | -0.9318 |
| H68 | -5.7129 | -3.2161 | 1.4901  | H2  | 8.5436  | -5.6357 | -0.6758 |
| end |         |         |         | end |         |         |         |
| H1  | -4.7973 | 6.3293  | 3.3497  | H1  | 15.3225 | 6.4020  | 0.2341  |
| H2  | -4.2540 | 5.8295  | 3.4479  | H2  | 15.3881 | 5.9881  | 0.8469  |
| end |         |         |         | end |         |         |         |
| H1  | 9.3529  | 4.8999  | 1.3840  | H1  | 6.3867  | 0.7709  | 0.6997  |
| H2  | 8.8365  | 5.3089  | 1.7319  | H2  | 7.0187  | 0.5244  | 1.0062  |
| end |         |         |         | end |         |         |         |
| H1  | 9.6452  | 5.8687  | 5.5259  | H1  | 5.3953  | -0.6761 | -0.3783 |
| H2  | 9.1774  | 5.4459  | 5.1277  | H2  | 4.8747  | -0.6218 | -0.9078 |
| end |         |         |         | end |         |         |         |
| H1  | 7.8252  | 3.5547  | 4.3795  | H1  | 5.6756  | 11.8107 | 0.1220  |
| H2  | 8.3934  | 3.3996  | 3.9243  | H2  | 5.9387  | 11.1266 | 0.2499  |
| end |         |         |         | end |         |         |         |
| H1  | 15.7248 | 9.0508  | 4.6855  | H1  | 6.2886  | 8.8120  | 0.1289  |
| H2  | 15.3802 | 8.8201  | 4.0659  | H2  | 5.6835  | 9.1885  | -0.0806 |
| end |         |         |         | end |         |         |         |
| H1  | 15.7246 | 9.6350  | 6.8407  | end |         |         |         |
| H2  | 16.4257 | 9.8673  | 6.9412  |     |         |         |         |

**(13) n=2 & m=5**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.6165 | -4.6762 | -0.0476 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.2872 | 0.3050  | -3.5753 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.0453  | -1.8553 | -3.0493 |
| O1      | 6.5822       | 3.7528  | 0.0545  |         | H12 | -3.8417 | -2.1553 | 1.8086  |
| O2      | 2.9111       | 1.7133  | 1.1775  |         | H13 | 0.2031  | 2.4178  | -2.8401 |
| O3      | 5.2314       | 3.0690  | -2.2015 |         | H14 | 6.0384  | 0.3454  | 3.5869  |
| O4      | 2.9550       | 1.7955  | -1.4866 |         | H15 | 4.9271  | -1.3776 | 4.4828  |
| O5      | 2.9668       | -0.8244 | 2.0544  |         | H16 | -0.1182 | 3.6048  | 0.7047  |
| O6      | -0.5601      | 1.2433  | 3.5929  |         | H17 | 2.8601  | -1.4198 | -1.5535 |
| O7      | 0.7506       | 3.0462  | 2.0630  |         | H18 | 1.1838  | 5.9554  | 3.1655  |
| O8      | 4.2159       | 5.0524  | 3.6493  |         | H19 | 4.5318  | 4.2844  | 3.0888  |
| O9      | 1.4833       | 5.1232  | 3.6386  |         | H20 | 2.0756  | -3.0192 | -0.0324 |
| O10     | 2.8766       | -0.8061 | -2.3413 |         | H21 | 4.4006  | 2.5777  | -1.9258 |
| O11     | 6.5497       | 1.2082  | 3.5639  |         | H22 | 0.1711  | -1.8420 | 3.1966  |
| O12     | -0.6263      | 3.9424  | -0.0903 |         | H23 | -0.6565 | 1.6223  | 4.5178  |
| O13     | 0.7462       | 3.0902  | -2.3386 |         | H24 | 7.4922  | 3.3302  | 0.0651  |
| O14     | -5.2357      | -2.9779 | 2.2670  |         | H25 | 1.4359  | -1.0850 | -3.2233 |
| O15     | -2.9560      | -1.6707 | -1.1645 |         | H26 | -1.0945 | 1.3612  | -4.4840 |
| O16     | -6.5485      | -3.6743 | -0.0228 |         | H27 | 0.2487  | -0.2839 | 3.6078  |
| O17     | -5.1268      | -2.9010 | -2.1583 |         | H28 | -1.4788 | 1.1197  | 3.2172  |
| O18     | -3.0083      | 0.8691  | -2.0073 |         | H29 | -1.5913 | -2.5051 | -1.6989 |
| O19     | 0.5295       | -1.1998 | -3.6353 |         | H30 | 0.2334  | 2.4025  | 2.6335  |
| O20     | -0.7595      | -2.9615 | -2.0281 |         | H31 | -0.1361 | 3.6209  | -0.8983 |
| O21     | -0.8011      | -3.0139 | 2.4315  |         | H32 | -1.6243 | -2.5506 | 2.0949  |
| O22     | 0.5646       | -3.8260 | 0.2029  |         | H33 | -2.9917 | -0.0840 | -1.6893 |
| O23     | -6.6292      | -1.1817 | -3.6113 |         | H34 | -4.6417 | -5.8522 | -3.2170 |
| O24     | -2.9261      | 0.8590  | 2.3347  |         | H35 | -2.9278 | 1.4675  | 1.5377  |
| O25     | -1.5291      | -5.0467 | -3.5954 |         | H36 | -2.1029 | 3.0575  | 0.0563  |
| O26     | -4.2546      | -5.0169 | -3.6129 |         | H37 | 2.9297  | 0.1256  | 1.7307  |
| O27     | 5.0719       | 2.9573  | 2.1476  |         | H38 | -6.1301 | -0.3147 | -3.5740 |
| O28     | 0.7642       | -1.1419 | 3.6010  |         | H39 | 5.6494  | 3.2534  | 1.3828  |
| O29     | 2.8987       | -2.4568 | -0.1234 |         | H40 | 5.6229  | 2.3126  | 2.6864  |
| O30     | 5.1940       | -1.1363 | 3.5491  |         | H41 | -4.3927 | 1.0634  | -2.9771 |
| O31     | -2.9889      | -1.7153 | 1.5069  |         | H42 | -7.4753 | -3.2983 | -0.0639 |
| O32     | -0.7860      | 1.1752  | -3.5499 |         | H43 | 2.4840  | 5.1251  | 3.6402  |
| O33     | -5.2407      | 1.1866  | -3.4980 |         | H44 | 3.7281  | 2.1755  | 1.5370  |
| O34     | -2.9181      | 2.4858  | 0.1539  |         | H45 | -5.8085 | -2.3328 | 2.7824  |
| H1      | -4.6366      | -4.9035 | -4.5329 |         | H46 | 1.5726  | 2.6063  | -2.0362 |
| H2      | -3.7887      | 1.0097  | 2.8183  |         | H47 | 6.5637  | 1.5698  | 4.4993  |
| H3      | -2.9300      | 1.8825  | -0.6480 |         | H48 | 4.3441  | -1.0210 | 3.0278  |
| H4      | -1.0584      | -3.7332 | -2.5922 |         | H49 | -4.8231 | -3.7034 | -2.6769 |
| H5      | -6.0851      | -1.8317 | -3.0770 |         | H50 | 3.7371  | -0.9783 | -2.8249 |
| H6      | 0.0594       | -3.5377 | -0.6113 |         | H51 | 1.0113  | 3.8152  | 2.6519  |
| H7      | -0.3090      | -3.3332 | 1.6192  |         | H52 | 4.5883  | 5.8801  | 3.2236  |
| H8      | -4.9703      | 1.4121  | -4.4319 |         | H53 | 2.9026  | -1.8513 | 0.6742  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.2234 | -5.8876 | -3.1429 | end |         |         |         |
| H55 | -2.9855 | -1.6995 | -0.1592 | H1  | 13.0007 | 8.0044  | 5.3818  |
| H56 | -3.7750 | -2.1414 | -1.5063 | H2  | 12.9569 | 7.2896  | 5.1798  |
| H57 | 6.1219  | 3.4742  | -0.7920 | end |         |         |         |
| H58 | 2.1146  | 2.2127  | 1.5317  | H1  | 14.8931 | 0.6940  | 4.9588  |
| H59 | 2.9299  | 1.7657  | -0.4813 | H2  | 14.8749 | 0.2767  | 4.3437  |
| H60 | -5.6781 | -3.2251 | -1.3812 | end |         |         |         |
| H61 | -2.9952 | -0.7652 | 1.8267  | H1  | 14.6026 | 2.7705  | 4.7924  |
| H62 | -2.5284 | -5.0730 | -3.6239 | H2  | 14.9707 | 3.2239  | 5.2524  |
| H63 | 2.1423  | -0.9626 | 2.6067  | end |         |         |         |
| H64 | -2.1895 | 0.9904  | -2.5697 | H1  | 8.7071  | -5.7217 | -0.8581 |
| H65 | 2.9445  | 0.8451  | -1.7973 | H2  | 8.9816  | -5.4835 | -1.5066 |
| H66 | 5.7754  | 2.4065  | -2.7237 | end |         |         |         |
| H67 | 0.6396  | -4.8210 | 0.1507  | H1  | 14.8127 | 5.6069  | 1.4956  |
| H68 | -5.7459 | -3.2311 | 1.4436  | H2  | 14.8403 | 5.7814  | 0.7732  |
| end |         |         |         | end |         |         |         |
| H1  | -4.5131 | 5.2300  | 3.1518  | H1  | 7.0959  | 0.3952  | 0.3154  |
| H2  | -5.1857 | 4.9973  | 3.3716  | H2  | 6.7733  | 1.0646  | 0.3205  |
| end |         |         |         | end |         |         |         |
| H1  | 9.1775  | 5.5555  | 1.3411  | H1  | 5.2737  | -0.5121 | -0.1965 |
| H2  | 8.9842  | 4.9522  | 1.7324  | H2  | 4.6962  | -0.8039 | -0.5639 |
| end |         |         |         | end |         |         |         |
| H1  | 9.9180  | 5.3037  | 5.6261  | H1  | 6.0883  | 11.7044 | -0.7273 |
| H2  | 9.6906  | 4.6845  | 5.2815  | H2  | 5.7554  | 11.2719 | -0.2210 |
| end |         |         |         | end |         |         |         |
| H1  | 8.8721  | 2.7426  | 3.9308  | H1  | 5.9103  | 9.3092  | 0.1340  |
| H2  | 8.5743  | 3.2944  | 4.3317  | H2  | 5.7541  | 8.9724  | 0.7790  |
| end |         |         |         | end |         |         |         |
| H1  | 14.9086 | 6.7970  | 5.9305  | H1  | 15.0235 | 10.3161 | 5.3444  |
| H2  | 15.5939 | 6.5700  | 6.1118  | H2  | 14.3813 | 10.5825 | 5.0747  |
| end |         |         |         | end |         |         |         |
| H1  | 16.3340 | 8.7844  | 6.4213  | H1  | 8.6893  | 7.3048  | 4.1111  |
| H2  | 16.9562 | 9.1869  | 6.4990  | H2  | 9.1088  | 7.0258  | 3.5637  |
| end |         |         |         | end |         |         |         |
| H1  | 14.3332 | 8.5182  | 8.3814  | end |         |         |         |
| H2  | 14.9574 | 8.7657  | 8.0586  | end |         |         |         |

**(14) n=2 & m=6**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H45 | 12.1364 | 7.9705  | 2.7914  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H61 | 14.8770 | 9.6260  | 1.8245  |
| 60.0000 | 60.0000 (P1) |         |         |         | H68 | 12.1765 | 7.0862  | 1.4455  |
| O2      | 2.9895       | 1.6727  | 1.2072  |         | O1  | 12.5429 | 7.1985  | 9.7471  |
| O8      | 4.2659       | 5.0896  | 3.6332  |         | O3  | 11.1616 | 6.4313  | 7.5291  |
| O27     | 5.1100       | 2.9954  | 2.1401  |         | O4  | 8.8954  | 5.1485  | 8.2487  |
| H19     | 4.5985       | 4.3264  | 3.0753  |         | O13 | 6.7179  | 6.5343  | 7.4468  |
| H39     | 5.6865       | 3.2593  | 1.3607  |         | O32 | 5.1911  | 4.6554  | 6.1428  |
| H40     | 5.6446       | 2.3545  | 2.7031  |         | H10 | 5.6901  | 3.7893  | 6.1547  |
| H44     | 3.7976       | 2.1638  | 1.5515  |         | H13 | 6.1556  | 5.9001  | 6.9234  |
| H52     | 4.6288       | 5.9181  | 3.2047  |         | H21 | 10.3373 | 5.9269  | 7.8019  |
| H58     | 2.1828       | 2.1625  | 1.5575  |         | H24 | 13.4475 | 6.7692  | 9.7721  |
| O7      | 12.7201      | 2.9636  | 2.0679  |         | H26 | 4.9097  | 4.8232  | 5.1961  |
| O9      | 13.4369      | 5.0875  | 3.5729  |         | H46 | 7.5226  | 6.0119  | 7.7394  |
| O24     | 8.9322       | 0.9188  | 2.3870  |         | H57 | 12.0804 | 6.8890  | 8.9146  |
| H2      | 8.0758       | 1.0800  | 2.8816  |         | H59 | 8.9081  | 5.1204  | 9.2539  |
| H18     | 13.1389      | 5.9339  | 3.1259  |         | H65 | 8.9021  | 4.2007  | 7.9297  |
| H30     | 12.1897      | 2.3322  | 2.6400  |         | H66 | 11.6961 | 5.8029  | 6.9636  |
| H35     | 8.9334       | 1.5164  | 1.5831  |         | O12 | 17.2414 | 7.3279  | 9.6789  |
| H43     | 14.4384      | 5.1128  | 3.5871  |         | O18 | 14.8343 | 4.3465  | 7.6400  |
| H51     | 12.9717      | 3.7501  | 2.6397  |         | O23 | 11.2484 | 2.2039  | 6.0573  |
| O5      | 9.0036       | 9.4407  | 2.0663  |         | O33 | 12.6005 | 4.5954  | 6.1221  |
| O11     | 12.4725      | 11.5716 | 3.6083  |         | O34 | 14.9280 | 5.9070  | 9.8596  |
| O21     | 5.2043       | 7.2963  | 2.3446  |         | H3  | 14.9114 | 5.3231  | 9.0456  |
| O29     | 8.9548       | 7.8332  | -0.1447 |         | H5  | 11.7904 | 1.5721  | 6.6150  |
| O30     | 11.2049      | 9.1610  | 3.6043  |         | H8  | 12.8812 | 4.8198  | 5.1887  |
| H7      | 5.7003       | 6.9862  | 1.5301  |         | H16 | 17.7639 | 6.9825  | 10.4625 |
| H14     | 12.0045      | 10.6862 | 3.6441  |         | H31 | 17.7251 | 7.0174  | 8.8589  |
| H15     | 10.9194      | 8.9020  | 4.5253  |         | H33 | 14.8594 | 3.3913  | 7.9537  |
| H20     | 8.1237       | 7.2809  | -0.0611 |         | H36 | 15.7562 | 6.4658  | 9.7869  |
| H32     | 4.4130       | 7.8099  | 2.0132  |         | H38 | 11.7400 | 3.0750  | 6.0717  |
| H37     | 8.9680       | 10.3932 | 1.7448  |         | H41 | 13.4436 | 4.4964  | 6.6553  |
| H47     | 12.5122      | 11.9173 | 4.5474  |         | H64 | 15.6553 | 4.4745  | 7.0802  |
| H48     | 10.3640      | 9.2593  | 3.0641  |         | O10 | 14.8356 | 12.8622 | 7.3833  |
| H53     | 8.9628       | 8.4309  | 0.6579  |         | O19 | 12.4533 | 12.5432 | 6.1532  |
| H63     | 8.1756       | 9.3027  | 2.6092  |         | O20 | 11.1396 | 10.7680 | 7.6610  |
| O6      | 17.2951      | 11.4721 | 3.5589  |         | O22 | 12.5334 | 9.9428  | 9.8342  |
| O14     | 12.7070      | 7.3469  | 2.2532  |         | O25 | 10.3460 | 8.6493  | 6.1637  |
| O28     | 18.6555      | 9.0982  | 3.5903  |         | O26 | 7.6264  | 8.6999  | 6.1413  |
| O31     | 14.9214      | 8.6899  | 1.4653  |         | H1  | 7.2656  | 8.7738  | 5.2116  |
| H12     | 14.0940      | 8.2093  | 1.7714  |         | H4  | 10.8317 | 9.9821  | 7.1196  |
| H22     | 18.0598      | 8.4114  | 3.1656  |         | H6  | 12.0066 | 10.2298 | 9.0313  |
| H23     | 17.2303      | 11.8463 | 4.4880  |         | H11 | 11.9411 | 11.8760 | 6.7064  |
| H27     | 18.1404      | 9.9555  | 3.5945  |         | H17 | 14.8550 | 12.2490 | 8.1787  |
| H28     | 16.3638      | 11.3908 | 3.2027  |         | H25 | 13.3581 | 12.6270 | 6.5732  |

|     |         |         |        |     |         |         |        |
|-----|---------|---------|--------|-----|---------|---------|--------|
| H29 | 10.3151 | 11.2436 | 7.9850 | end |         |         |        |
| H34 | 7.2500  | 7.8645  | 6.5543 | H1  | 7.3371  | 0.3178  | 0.4313 |
| H50 | 15.6797 | 12.7031 | 6.8685 | H2  | 6.8099  | 0.7101  | 0.0842 |
| H54 | 10.6523 | 7.8114  | 6.6178 | end |         |         |        |
| H62 | 9.3457  | 8.6203  | 6.1351 | H1  | 6.2167  | 9.5489  | 0.3511 |
| H67 | 12.5845 | 8.9470  | 9.7947 | H2  | 6.4961  | 9.1683  | 0.9259 |
| O15 | 20.8736 | 12.1091 | 8.4974 | end |         |         |        |
| O16 | 17.3167 | 10.0367 | 9.7009 | H1  | 13.8488 | 10.4452 | 5.7236 |
| O17 | 18.7152 | 10.8361 | 7.5641 | H2  | 14.1573 | 9.8465  | 5.4048 |
| H9  | 17.2466 | 9.0367  | 9.6926 | end |         |         |        |
| H42 | 16.3874 | 10.4108 | 9.6542 | H1  | 8.4536  | 7.2981  | 3.6072 |
| H49 | 18.9988 | 10.0244 | 7.0438 | H2  | 8.9219  | 6.7293  | 3.7100 |
| H55 | 20.8486 | 12.1112 | 9.5019 | end |         |         |        |
| H56 | 20.0547 | 11.6210 | 8.1762 | H1  | 16.9362 | 7.6874  | 5.4060 |
| H60 | 18.1703 | 10.5135 | 8.3471 | H2  | 17.1273 | 6.9850  | 5.2642 |
| end |         |         |        | end |         |         |        |
| H1  | 8.7770  | 5.2495  | 1.4445 | H1  | 10.3887 | 3.4448  | 3.3325 |
| H2  | 9.4311  | 5.1195  | 1.1158 | H2  | 10.2134 | 4.1622  | 3.4222 |
| end |         |         |        | end |         |         |        |
| H1  | 9.4894  | 5.0635  | 5.2666 | H1  | 4.0211  | 2.7518  | 5.3234 |
| H2  | 9.8889  | 5.5625  | 5.6482 | H2  | 3.8395  | 2.1238  | 4.9688 |
| end |         |         |        | end |         |         |        |
| H1  | 7.6346  | 3.6091  | 4.7789 | H1  | 7.1416  | 5.5023  | 2.7402 |
| H2  | 8.0329  | 3.8185  | 4.1881 | H2  | 6.7563  | 4.9124  | 2.5085 |
| end |         |         |        | end |         |         |        |
| H1  | 14.6742 | 7.9166  | 4.4117 | H1  | 19.8238 | 11.5224 | 4.8686 |
| H2  | 15.0479 | 8.2197  | 3.8455 | H2  | 19.8077 | 11.1794 | 4.2103 |
| end |         |         |        | end |         |         |        |
| H1  | 16.7805 | 9.6593  | 6.5074 | H1  | 17.0391 | 4.3822  | 8.9048 |
| H2  | 16.0705 | 9.6907  | 6.2858 | H2  | 17.7818 | 4.3627  | 8.9262 |
| end |         |         |        | end |         |         |        |
| H1  | 14.8336 | 7.4761  | 7.8644 | H1  | 8.6356  | 7.8025  | 9.0496 |
| H2  | 15.1887 | 7.8079  | 7.2992 | H2  | 8.8247  | 7.9946  | 8.3579 |
| end |         |         |        | end |         |         |        |
| H1  | 12.8453 | 7.8080  | 5.5330 | H1  | 16.4453 | 13.3411 | 9.1587 |
| H2  | 12.9084 | 7.0676  | 5.5436 | H2  | 16.9533 | 13.3732 | 9.7011 |
| end |         |         |        | end |         |         |        |
| H1  | 15.2884 | 5.9488  | 1.2506 | end |         |         |        |
| H2  | 15.0190 | 5.9737  | 0.5580 | end |         |         |        |

(15) n=2 & m=7

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H45 | 12.0723 | 8.0119  | 2.8116  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H61 | 14.7914 | 9.6327  | 1.8026  |
| 60.0000 | 60.0000 (P1) |         |         |         | H68 | 12.1206 | 7.0937  | 1.4808  |
| O2      | 2.9733       | 1.8021  | 1.2312  |         | O1  | 12.4816 | 7.3261  | 9.7505  |
| O8      | 4.2734       | 5.1743  | 3.6829  |         | O3  | 11.1423 | 6.4836  | 7.5557  |
| O27     | 5.1136       | 3.0996  | 2.1942  |         | O4  | 8.8843  | 5.1923  | 8.2693  |
| H19     | 4.6090       | 4.4210  | 3.1097  |         | O13 | 6.6672  | 6.5037  | 7.3943  |
| H39     | 5.6830       | 3.3647  | 1.4115  |         | O32 | 5.1094  | 4.6448  | 6.2095  |
| H40     | 5.6544       | 2.4625  | 2.7521  |         | H10 | 5.6416  | 3.7968  | 6.2126  |
| H44     | 3.7734       | 2.2939  | 1.5922  |         | H13 | 6.1008  | 5.8367  | 6.9081  |
| H52     | 4.6169       | 6.0136  | 3.2597  |         | H21 | 10.3138 | 5.9818  | 7.8203  |
| H58     | 2.1538       | 2.2947  | 1.5471  |         | H24 | 13.3771 | 6.8814  | 9.7403  |
| O6      | 11.3350      | 1.2746  | 3.5008  |         | H26 | 4.8719  | 4.8482  | 5.2555  |
| O7      | 12.6515      | 3.0862  | 2.0162  |         | H46 | 7.4719  | 6.0016  | 7.7185  |
| O9      | 13.4303      | 5.1164  | 3.6107  |         | H57 | 12.0008 | 7.0105  | 8.9286  |
| O24     | 8.9063       | 0.9378  | 2.3047  |         | H59 | 8.8911  | 5.2047  | 9.2752  |
| H2      | 8.1045       | 1.1604  | 2.8519  |         | H65 | 8.9145  | 4.2314  | 7.9855  |
| H18     | 13.1140      | 5.9646  | 3.1846  |         | H66 | 11.6708 | 5.8484  | 6.9973  |
| H23     | 11.2582      | 1.5987  | 4.4467  |         | O12 | 17.1755 | 7.3533  | 9.5976  |
| H28     | 10.4105      | 1.1729  | 3.1380  |         | O18 | 14.7308 | 4.3180  | 7.6854  |
| H30     | 12.1412      | 2.4262  | 2.5755  |         | O23 | 11.2453 | 2.1504  | 6.0566  |
| H35     | 8.9004       | 1.5468  | 1.5112  |         | O33 | 12.5253 | 4.5486  | 6.1490  |
| H43     | 14.4303      | 5.1633  | 3.6349  |         | O34 | 14.8510 | 5.9662  | 9.7908  |
| H51     | 12.9187      | 3.8437  | 2.6190  |         | H3  | 14.8247 | 5.3522  | 8.9930  |
| O5      | 8.9990       | 9.5628  | 2.0819  |         | H5  | 11.8057 | 1.5204  | 6.5996  |
| O11     | 12.4868      | 11.6607 | 3.6802  |         | H8  | 12.8189 | 4.7870  | 5.2264  |
| O29     | 8.9694       | 7.8816  | -0.0314 |         | H16 | 17.6993 | 7.0413  | 10.3951 |
| O30     | 11.2010      | 9.2444  | 3.6131  |         | H31 | 17.6783 | 7.0405  | 8.7904  |
| H14     | 12.0184      | 10.7764 | 3.6896  |         | H33 | 14.7656 | 3.3680  | 8.0168  |
| H15     | 10.9101      | 8.9548  | 4.5234  |         | H36 | 15.6906 | 6.5067  | 9.7047  |
| H20     | 8.1281       | 7.3466  | 0.0332  |         | H38 | 11.7130 | 3.0364  | 6.0790  |
| H37     | 8.9488       | 10.5155 | 1.7633  |         | H41 | 13.3653 | 4.4491  | 6.6906  |
| H47     | 12.5093      | 11.9828 | 4.6268  |         | H64 | 15.5561 | 4.4485  | 7.1337  |
| H48     | 10.3592      | 9.3701  | 3.0798  |         | O10 | 14.8713 | 12.8991 | 7.4555  |
| H53     | 8.9759       | 8.4983  | 0.7604  |         | O19 | 12.4395 | 12.5986 | 6.2475  |
| H63     | 8.1654       | 9.3966  | 2.6131  |         | O20 | 11.0879 | 10.7987 | 7.7009  |
| O14     | 12.6342      | 7.3604  | 2.2954  |         | O22 | 12.4975 | 10.0394 | 9.8795  |
| O21     | 17.0369      | 7.4090  | 2.3743  |         | O25 | 10.3385 | 8.6728  | 6.1503  |
| O28     | 18.6318      | 9.1848  | 3.5520  |         | O26 | 7.6090  | 8.6672  | 6.0624  |
| O31     | 14.8310      | 8.6833  | 1.4814  |         | H1  | 7.2240  | 8.7934  | 5.1463  |
| H7      | 17.5330      | 7.0844  | 1.5671  |         | H4  | 10.7991 | 10.0148 | 7.1498  |
| H12     | 14.0041      | 8.2111  | 1.8036  |         | H6  | 11.9785 | 10.3169 | 9.0682  |
| H22     | 18.0234      | 8.5071  | 3.1226  |         | H11 | 11.9380 | 11.9110 | 6.7861  |
| H27     | 18.1275      | 10.0474 | 3.5604  |         | H17 | 14.8784 | 12.2911 | 8.2520  |
| H32     | 16.2188      | 7.8805  | 2.0381  |         | H25 | 13.3494 | 12.6747 | 6.6517  |

|     |         |         |        |     |         |         |        |
|-----|---------|---------|--------|-----|---------|---------|--------|
| H29 | 10.2558 | 11.2678 | 8.0175 | end |         |         |        |
| H34 | 7.2209  | 7.8351  | 6.4652 | H1  | 12.6605 | 9.5879  | 5.8762 |
| H50 | 15.6913 | 12.6964 | 6.9220 | H2  | 13.3431 | 9.8498  | 5.9981 |
| H54 | 10.6365 | 7.8352  | 6.6135 | end |         |         |        |
| H62 | 9.3410  | 8.6336  | 6.1034 | H1  | 8.8419  | 7.5645  | 3.9462 |
| H67 | 12.5247 | 9.0392  | 9.8509 | H2  | 9.1627  | 7.1972  | 3.3874 |
| O15 | 20.8103 | 12.0943 | 8.5354 | end |         |         |        |
| O16 | 17.3004 | 10.0341 | 9.6833 | H1  | 15.2254 | 11.2885 | 5.2500 |
| O17 | 18.7097 | 10.7829 | 7.5320 | H2  | 14.5565 | 11.1119 | 4.9789 |
| H9  | 17.2050 | 9.0337  | 9.6563 | end |         |         |        |
| H42 | 16.3807 | 10.4313 | 9.6600 | H1  | 10.2815 | 4.2508  | 4.3444 |
| H49 | 18.9968 | 9.9740  | 7.0113 | H2  | 10.5117 | 3.6952  | 3.9071 |
| H55 | 20.7614 | 12.0872 | 9.5415 | end |         |         |        |
| H56 | 20.0178 | 11.5869 | 8.1820 | H1  | 14.2444 | 9.0744  | 8.2745 |
| H60 | 18.1553 | 10.4714 | 8.3126 | H2  | 14.8789 | 9.0084  | 7.8912 |
| end |         |         |        | end |         |         |        |
| H1  | 10.0803 | 5.7359  | 1.8131 | H1  | 8.0724  | 3.6152  | 2.7650 |
| H2  | 9.6587  | 5.3096  | 2.2540 | H2  | 8.2341  | 3.4922  | 2.0522 |
| end |         |         |        | end |         |         |        |
| H1  | 8.9918  | 5.6477  | 5.8190 | H1  | 11.3823 | 0.6698  | 0.6717 |
| H2  | 9.3647  | 6.1205  | 5.3861 | H2  | 10.8794 | 1.1967  | 0.5157 |
| end |         |         |        | end |         |         |        |
| H1  | 7.4256  | 3.7874  | 4.9017 | H1  | 3.7507  | 2.0638  | 5.2772 |
| H2  | 7.6577  | 4.4279  | 4.6071 | H2  | 3.9264  | 2.7209  | 5.5794 |
| end |         |         |        | end |         |         |        |
| H1  | 15.2348 | 8.1727  | 4.0229 | H1  | 7.2939  | 6.1470  | 2.9245 |
| H2  | 14.8297 | 7.8503  | 4.5577 | H2  | 7.0861  | 5.4486  | 2.7870 |
| end |         |         |        | end |         |         |        |
| H1  | 16.9224 | 9.5064  | 6.2491 | H1  | 19.9666 | 11.0938 | 4.1334 |
| H2  | 16.3221 | 9.4002  | 5.8209 | H2  | 19.8044 | 11.5931 | 4.6581 |
| end |         |         |        | end |         |         |        |
| H1  | 15.3800 | 7.1150  | 7.1773 | H1  | 12.9348 | 12.6897 | 9.4979 |
| H2  | 15.9183 | 6.8253  | 6.7534 | H2  | 12.4803 | 13.1661 | 9.1539 |
| end |         |         |        | end |         |         |        |
| H1  | 12.9830 | 6.8869  | 5.5888 | H1  | 8.5430  | 8.0953  | 9.0311 |
| H2  | 13.0276 | 7.6183  | 5.7129 | H2  | 8.6564  | 7.6674  | 8.4349 |
| end |         |         |        | end |         |         |        |
| H1  | 15.2946 | 5.8922  | 1.1826 | H1  | 17.5310 | 12.8657 | 9.3112 |
| H2  | 15.3439 | 6.0757  | 0.4641 | H2  | 17.0114 | 12.9300 | 8.7816 |
| end |         |         |        | end |         |         |        |
| H1  | 6.9177  | 0.7866  | 0.9818 | end |         |         |        |
| H2  | 6.3240  | 0.9291  | 0.5572 | end |         |         |        |

**(16) n=2 & m=8**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H45 | 12.0377 | 7.9637  | 2.7720  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H61 | 14.7743 | 9.4767  | 1.6770  |
| 60.0000 | 60.0000 (P1) |         |         |         | H68 | 12.0436 | 7.0450  | 1.4491  |
| O2      | 2.9753       | 1.7943  | 1.2876  |         | O1  | 12.5564 | 7.2273  | 9.7014  |
| O8      | 4.2694       | 5.0773  | 3.6415  |         | O3  | 11.1457 | 6.4922  | 7.5039  |
| O27     | 5.1965       | 2.9904  | 2.1571  |         | O4  | 8.8767  | 5.2882  | 8.3400  |
| H19     | 4.6250       | 4.3181  | 3.0976  |         | O13 | 6.6221  | 6.5104  | 7.4700  |
| H39     | 5.7456       | 3.2685  | 1.3656  |         | O32 | 5.0977  | 4.6072  | 6.2013  |
| H40     | 5.7346       | 2.3383  | 2.6981  |         | H10 | 5.6008  | 3.7395  | 6.1940  |
| H44     | 3.8002       | 2.2606  | 1.6254  |         | H13 | 6.0940  | 5.8326  | 6.9620  |
| H52     | 4.6024       | 5.9061  | 3.1951  |         | H21 | 10.3272 | 6.0050  | 7.8190  |
| H58     | 2.1640       | 2.3025  | 1.6009  |         | H24 | 13.4374 | 6.7522  | 9.6933  |
| O6      | 11.2761      | 1.2658  | 3.4857  |         | H26 | 4.8677  | 4.8214  | 5.2511  |
| O7      | 12.6477      | 3.0852  | 2.0114  |         | H46 | 7.4464  | 6.0401  | 7.7952  |
| O9      | 13.4462      | 5.0828  | 3.5933  |         | H57 | 12.0598 | 6.9353  | 8.8805  |
| O24     | 8.9196       | 0.7560  | 2.2033  |         | H59 | 8.8923  | 5.2694  | 9.3468  |
| H2      | 8.1159       | 0.9721  | 2.7480  |         | H65 | 8.8577  | 4.3335  | 8.0327  |
| H18     | 13.1283      | 5.9229  | 3.1563  |         | H66 | 11.6663 | 5.8372  | 6.9557  |
| H23     | 11.1603      | 1.6176  | 4.4144  |         | O12 | 17.1133 | 7.3579  | 9.6284  |
| H28     | 10.3668      | 1.1076  | 3.1036  |         | O18 | 14.7474 | 4.2186  | 7.6175  |
| H30     | 12.1147      | 2.4413  | 2.5629  |         | O23 | 11.1322 | 2.2336  | 6.0495  |
| H35     | 8.9197       | 1.3815  | 1.4213  |         | O33 | 12.5257 | 4.5776  | 6.1234  |
| H43     | 14.4493      | 5.1040  | 3.5940  |         | O34 | 14.8832 | 5.8432  | 9.7565  |
| H51     | 12.9167      | 3.8406  | 2.6190  |         | H3  | 14.8635 | 5.2558  | 8.9416  |
| O5      | 8.9007       | 9.5366  | 2.1095  |         | H5  | 11.6571 | 1.5801  | 6.5968  |
| O11     | 12.5088      | 11.5039 | 3.6327  |         | H8  | 12.8180 | 4.8109  | 5.1977  |
| O29     | 8.8453       | 7.9240  | -0.0593 |         | H16 | 17.6514 | 7.0587  | 10.4218 |
| O30     | 11.1511      | 9.1734  | 3.5796  |         | H31 | 17.6136 | 7.0325  | 8.8212  |
| H14     | 11.9917      | 10.6432 | 3.6494  |         | H33 | 14.7698 | 3.2576  | 7.9179  |
| H15     | 10.8676      | 8.8915  | 4.4974  |         | H36 | 15.6967 | 6.4262  | 9.6860  |
| H20     | 8.0311       | 7.3456  | -0.0171 |         | H38 | 11.6460 | 3.0931  | 6.0629  |
| H37     | 8.8856       | 10.4959 | 1.8148  |         | H41 | 13.3663 | 4.4352  | 6.6509  |
| H47     | 12.4942      | 11.8662 | 4.5628  |         | H64 | 15.5742 | 4.3668  | 7.0661  |
| H48     | 10.3041      | 9.3000  | 3.0588  |         | O10 | 14.7398 | 13.0153 | 7.4855  |
| H53     | 8.8285       | 8.5100  | 0.7544  |         | O19 | 12.3556 | 12.5378 | 6.1971  |
| H63     | 8.0691       | 9.3925  | 2.6556  |         | O20 | 11.0449 | 10.6776 | 7.6283  |
| O14     | 12.5801      | 7.2951  | 2.2559  |         | O22 | 12.4571 | 9.9381  | 9.8070  |
| O21     | 17.0077      | 7.3328  | 2.3190  |         | O25 | 10.2721 | 8.6210  | 6.0893  |
| O28     | 18.5563      | 9.1986  | 3.5557  |         | H4  | 10.7492 | 9.9047  | 7.0587  |
| O31     | 14.7903      | 8.5217  | 1.3643  |         | H6  | 11.9279 | 10.1924 | 8.9927  |
| H7      | 17.5123      | 7.0092  | 1.5201  |         | H11 | 11.8733 | 11.8317 | 6.7247  |
| H12     | 13.9548      | 8.0803  | 1.7083  |         | H17 | 14.7611 | 12.4002 | 8.2748  |
| H22     | 17.9713      | 8.5204  | 3.1097  |         | H25 | 13.2478 | 12.6575 | 6.6293  |
| H27     | 18.0504      | 10.0622 | 3.5542  |         | H29 | 10.2086 | 11.1385 | 7.9405  |
| H32     | 16.1781      | 7.7746  | 1.9702  |         | H50 | 15.5625 | 12.8259 | 6.9550  |



|     |         |         |        |     |         |         |        |
|-----|---------|---------|--------|-----|---------|---------|--------|
| H54 | 10.5923 | 7.7892  | 6.5495 | end |         |         |        |
| H62 | 9.2738  | 8.5891  | 6.0738 | H1  | 10.4747 | 4.3313  | 3.9733 |
| H67 | 12.5551 | 8.9441  | 9.7797 | H2  | 10.3600 | 3.6115  | 3.8258 |
| O15 | 20.7381 | 11.9816 | 8.4200 | end |         |         |        |
| O16 | 17.1584 | 10.0403 | 9.7032 | H1  | 14.9293 | 9.0137  | 8.0123 |
| O17 | 18.5219 | 10.7947 | 7.5278 | H2  | 14.3471 | 8.8300  | 8.4374 |
| O26 | 19.4186 | 8.6853  | 6.1026 | end |         |         |        |
| H1  | 19.0288 | 8.7942  | 5.1893 | H1  | 8.0837  | 3.4215  | 2.7641 |
| H9  | 17.0589 | 9.0425  | 9.6653 | H2  | 8.2825  | 3.2969  | 2.0614 |
| H34 | 19.0439 | 7.8497  | 6.5042 | end |         |         |        |
| H42 | 16.2462 | 10.4537 | 9.6791 | H1  | 13.0195 | 9.6793  | 6.2267 |
| H49 | 18.8280 | 9.9865  | 7.0166 | H2  | 13.3539 | 9.8893  | 5.5980 |
| H55 | 20.7069 | 11.9604 | 9.4264 | end |         |         |        |
| H56 | 19.9042 | 11.5261 | 8.0891 | H1  | 10.7499 | 6.3069  | 4.6501 |
| H60 | 18.0080 | 10.4775 | 8.3312 | H2  | 11.2207 | 6.3999  | 4.0842 |
| end |         |         |        | end |         |         |        |
| H1  | 9.1154  | 5.2999  | 1.9498 | H1  | 11.2756 | 1.4395  | 0.1039 |
| H2  | 9.6244  | 5.7354  | 1.6267 | H2  | 11.8627 | 0.9838  | 0.1138 |
| end |         |         |        | end |         |         |        |
| H1  | 9.0263  | 5.7798  | 6.0699 | H1  | 4.0116  | 2.5795  | 4.9245 |
| H2  | 8.9254  | 5.5936  | 5.3584 | H2  | 3.8883  | 2.2458  | 4.2721 |
| end |         |         |        | end |         |         |        |
| H1  | 7.3789  | 3.7172  | 4.8265 | H1  | 4.3850  | 5.2267  | 0.5617 |
| H2  | 7.3849  | 4.3410  | 4.4267 | H2  | 3.7613  | 4.8229  | 0.5966 |
| end |         |         |        | end |         |         |        |
| H1  | 14.9642 | 8.7358  | 3.8458 | H1  | 7.0756  | 5.7901  | 2.7235 |
| H2  | 14.7366 | 8.4847  | 4.5081 | H2  | 6.8248  | 5.1120  | 2.5636 |
| end |         |         |        | end |         |         |        |
| H1  | 16.5953 | 9.7637  | 6.4216 | H1  | 19.9731 | 11.3625 | 4.8950 |
| H2  | 16.0784 | 9.4982  | 5.9562 | H2  | 19.2733 | 11.4930 | 5.1077 |
| end |         |         |        | end |         |         |        |
| H1  | 15.3991 | 7.1286  | 7.2944 | H1  | 10.8805 | 9.3226  | 0.8201 |
| H2  | 15.8105 | 6.6213  | 6.9410 | H2  | 11.4960 | 9.4949  | 0.4394 |
| end |         |         |        | end |         |         |        |
| H1  | 13.1983 | 6.9228  | 5.7180 | H1  | 12.8593 | 4.2820  | 8.9346 |
| H2  | 13.2208 | 7.6650  | 5.7609 | H2  | 12.2907 | 4.3690  | 9.4031 |
| end |         |         |        | end |         |         |        |
| H1  | 15.1437 | 11.6862 | 5.1856 | H1  | 12.4349 | 12.3469 | 9.5709 |
| H2  | 14.5510 | 11.4872 | 4.7850 | H2  | 11.8871 | 12.7754 | 9.3098 |
| end |         |         |        | end |         |         |        |
| H1  | 8.7956  | 7.0258  | 3.4019 | H1  | 19.3109 | 8.4964  | 9.2485 |
| H2  | 8.3952  | 7.4132  | 3.8930 | H2  | 19.9642 | 8.8389  | 9.1512 |
| end |         |         |        | end |         |         |        |
| H1  | 17.1928 | 7.2589  | 4.7184 | end |         |         |        |
| H2  | 17.1174 | 7.2750  | 5.4559 | end |         |         |        |

(17) n=3 & m=1

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.5966 | -4.6824 | -0.0015 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.2322 | 0.3773  | -3.5556 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.0788  | -1.7867 | -3.0674 |
| O1      | 6.5584       | 3.7730  | 0.0545  |         | H12 | -3.7520 | -2.2090 | 1.7848  |
| O2      | 2.9255       | 1.5832  | 1.1674  |         | H13 | 0.1900  | 2.4563  | -2.8046 |
| O3      | 5.2733       | 3.0503  | -2.2091 |         | H14 | 6.0807  | 0.2987  | 3.6748  |
| O4      | 2.9934       | 1.8182  | -1.4883 |         | H15 | 4.9681  | -1.4585 | 4.6134  |
| O5      | 3.0042       | -0.9276 | 2.1168  |         | H16 | -0.1316 | 3.5434  | 0.7427  |
| O6      | -0.6099      | 1.1448  | 3.5245  |         | H17 | 2.9368  | -1.3455 | -1.5508 |
| O7      | 0.7539       | 2.9056  | 2.0294  |         | H18 | 1.2294  | 5.7983  | 3.1534  |
| O8      | 4.2745       | 4.9479  | 3.6198  |         | H19 | 4.6043  | 4.1666  | 3.0828  |
| O9      | 1.5281       | 4.9675  | 3.6253  |         | H20 | 2.1984  | -2.9956 | -0.0942 |
| O10     | 2.9286       | -0.7588 | -2.3621 |         | H21 | 4.4389  | 2.5662  | -1.9280 |
| O11     | 6.5759       | 1.1660  | 3.6340  |         | H22 | 0.1864  | -1.9314 | 3.1513  |
| O12     | -0.6532      | 3.9034  | -0.0373 |         | H23 | -0.6678 | 1.5344  | 4.4418  |
| O13     | 0.7248       | 3.1236  | -2.2857 |         | H24 | 7.4631  | 3.3389  | 0.0783  |
| O14     | -5.1484      | -3.0687 | 2.2836  |         | H25 | 1.4778  | -1.0304 | -3.2158 |
| O15     | -2.9367      | -1.6349 | -1.2121 |         | H26 | -1.0437 | 1.3781  | -4.5059 |
| O16     | -6.5064      | -3.6847 | 0.0147  |         | H27 | 0.2357  | -0.3694 | 3.5550  |
| O17     | -5.1440      | -2.8799 | -2.1701 |         | H28 | -1.5395 | 1.0496  | 3.1643  |
| O18     | -2.9648      | 0.9385  | -2.0062 |         | H29 | -1.5410 | -2.4389 | -1.7488 |
| O19     | 0.5811       | -1.1400 | -3.6479 |         | H30 | 0.2138  | 2.2680  | 2.5880  |
| O20     | -0.7134      | -2.9067 | -2.0672 |         | H31 | -0.1823 | 3.5804  | -0.8581 |
| O21     | -0.7492      | -3.1355 | 2.3642  |         | H32 | -1.5530 | -2.6343 | 2.0408  |
| O22     | 0.7053       | -3.8325 | 0.1294  |         | H33 | -2.9539 | -0.0175 | -1.7009 |
| O23     | -6.6227      | -1.2165 | -3.6636 |         | H34 | -4.6420 | -5.8157 | -3.1821 |
| O24     | -3.0057      | 0.8159  | 2.3517  |         | H35 | -2.9940 | 1.4500  | 1.5809  |
| O25     | -1.5408      | -5.0427 | -3.5163 |         | H36 | -2.1371 | 3.0828  | 0.1023  |
| O26     | -4.2636      | -4.9916 | -3.6046 |         | H37 | 2.9736  | 0.0146  | 1.7726  |
| O27     | 5.1064       | 2.8568  | 2.1337  |         | H38 | -6.1012 | -0.3612 | -3.6260 |
| O28     | 0.7568       | -1.2234 | 3.5718  |         | H39 | 5.6755  | 3.1801  | 1.3721  |
| O29     | 2.9950       | -2.3938 | -0.1559 |         | H40 | 5.6540  | 2.2235  | 2.6865  |
| O30     | 5.2704       | -1.2692 | 3.6741  |         | H41 | -4.3783 | 1.0323  | -2.9974 |
| O31     | -2.9155      | -1.7453 | 1.4832  |         | H42 | -7.4221 | -3.2802 | -0.0433 |
| O32     | -0.7461      | 1.2378  | -3.5595 |         | H43 | 2.5270  | 4.9777  | 3.6112  |
| O33     | -5.2215      | 1.1248  | -3.5298 |         | H44 | 3.7318  | 2.0524  | 1.5329  |
| O34     | -2.9620      | 2.5193  | 0.1850  |         | H45 | -5.7108 | -2.4494 | 2.8356  |
| H1      | -4.6328      | -4.9240 | -4.5321 |         | H46 | 1.5463  | 2.6367  | -1.9860 |
| H2      | -3.8553      | 0.9711  | 2.8664  |         | H47 | 6.5951  | 1.5550  | 4.5623  |
| H3      | -2.9604      | 1.9180  | -0.6187 |         | H48 | 4.4370  | -1.1376 | 3.1434  |
| H4      | -1.0267      | -3.6957 | -2.6002 |         | H49 | -4.8347 | -3.6827 | -2.6879 |
| H5      | -6.0997      | -1.8666 | -3.1026 |         | H50 | 3.7773  | -0.9497 | -2.8567 |
| H6      | 0.1602       | -3.5144 | -0.6419 |         | H51 | 1.0413  | 3.6564  | 2.6263  |
| H7      | -0.2387      | -3.3923 | 1.5417  |         | H52 | 4.6293  | 5.7660  | 3.1606  |
| H8      | -4.9384      | 1.3353  | -4.4675 |         | H53 | 2.9762  | -1.8461 | 0.6838  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.2328 | -5.8866 | -3.0695 | end |         |         |         |
| H55 | -2.9670 | -1.6861 | -0.2114 | H1  | 15.6718 | 5.9420  | 0.2664  |
| H56 | -3.7598 | -2.0939 | -1.5556 | H2  | 15.8866 | 6.3772  | -0.2947 |
| H57 | 6.1104  | 3.4802  | -0.7951 | end |         |         |         |
| H58 | 2.1239  | 2.0839  | 1.5097  | H1  | 7.4087  | 0.4775  | 0.3211  |
| H59 | 2.9670  | 1.7427  | -0.4842 | H2  | 7.1158  | 0.4860  | -0.3587 |
| H60 | -5.6533 | -3.2108 | -1.3712 | end |         |         |         |
| H61 | -2.9637 | -0.8004 | 1.8135  | H1  | 5.2382  | -0.8430 | -1.2570 |
| H62 | -2.5418 | -5.0649 | -3.5532 | H2  | 5.4053  | -0.6563 | -0.5580 |
| H63 | 2.1569  | -1.0539 | 2.6402  | end |         |         |         |
| H64 | -2.1506 | 1.0521  | -2.5764 | H1  | 6.2797  | 10.5711 | -1.0400 |
| H65 | 2.9979  | 0.8746  | -1.8250 | H2  | 6.9129  | 10.8673 | -1.2881 |
| H66 | 5.8052  | 2.3896  | -2.7420 | end |         |         |         |
| H67 | 0.7117  | -4.8336 | 0.0732  | H1  | 6.0694  | 8.8957  | 0.1520  |
| H68 | -5.6785 | -3.2877 | 1.4618  | H2  | 5.4001  | 8.9501  | 0.4649  |
| end |         |         |         | end |         |         |         |
| H1  | 10.3698 | 4.7136  | 2.7355  | H1  | -2.8485 | 7.8527  | 11.2582 |
| H2  | 10.5774 | 5.3966  | 2.5202  | H2  | -3.2435 | 7.7764  | 10.6356 |
| end |         |         |         | end |         |         |         |
| H1  | 15.1937 | 9.0460  | 7.7949  | H1  | -8.1734 | 0.8685  | 3.5830  |
| H2  | 14.5460 | 8.7543  | 8.0243  | H2  | -7.9993 | 1.3439  | 4.1240  |
| end |         |         |         | end |         |         |         |
| H1  | 13.8390 | 1.0840  | 4.7373  | H1  | 17.3721 | 14.1993 | 11.0423 |
| H2  | 13.2854 | 1.3088  | 5.1769  | H2  | 17.0999 | 13.5188 | 11.1391 |
| end |         |         |         | end |         |         |         |
| H1  | 15.4347 | 2.1065  | 5.9686  | H1  | 11.2907 | 0.7137  | 0.7839  |
| H2  | 15.7384 | 2.7577  | 5.7911  | H2  | 10.7718 | 1.2166  | 0.6173  |
| end |         |         |         | end |         |         |         |
| H1  | 8.1311  | -5.0050 | -0.8297 | end |         |         |         |
| H2  | 7.5320  | -5.4352 | -0.9144 | end |         |         |         |

**(18) n=3 & m=2**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.5550 | -4.6745 | 0.0015  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.2327 | 0.3778  | -3.5405 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.0716  | -1.7974 | -3.0478 |
| O1      | 6.5289       | 3.7614  | 0.0903  |         | H12 | -3.7490 | -2.1989 | 1.8047  |
| O2      | 2.9208       | 1.5911  | 1.1999  |         | H13 | 0.1957  | 2.4563  | -2.7900 |
| O3      | 5.2425       | 3.0460  | -2.1920 |         | H14 | 6.0761  | 0.2909  | 3.6820  |
| O4      | 2.9844       | 1.8012  | -1.4562 |         | H15 | 4.9720  | -1.4748 | 4.6167  |
| O5      | 3.0030       | -0.9336 | 2.1011  |         | H16 | -0.1196 | 3.5352  | 0.7662  |
| O6      | -0.6085      | 1.1321  | 3.5576  |         | H17 | 2.9291  | -1.3714 | -1.5521 |
| O7      | 0.7499       | 2.9112  | 2.0736  |         | H18 | 1.2269  | 5.8257  | 3.1830  |
| O8      | 4.2444       | 4.9634  | 3.6590  |         | H19 | 4.5761  | 4.1828  | 3.1233  |
| O9      | 1.5133       | 4.9927  | 3.6625  |         | H20 | 2.1759  | -3.0225 | -0.0744 |
| O10     | 2.9268       | -0.7782 | -2.3578 |         | H21 | 4.4134  | 2.5532  | -1.9098 |
| O11     | 6.5641       | 1.1624  | 3.6440  |         | H22 | 0.1898  | -1.9426 | 3.1726  |
| O12     | -0.6341      | 3.9001  | -0.0158 |         | H23 | -0.6726 | 1.5245  | 4.4740  |
| O13     | 0.7329       | 3.1225  | -2.2708 |         | H24 | 7.4428  | 3.3470  | 0.1066  |
| O14     | -5.1220      | -3.0629 | 2.2998  |         | H25 | 1.4688  | -1.0401 | -3.2105 |
| O15     | -2.9238      | -1.6087 | -1.1865 |         | H26 | -1.0437 | 1.3838  | -4.4880 |
| O16     | -6.4716      | -3.6773 | 0.0196  |         | H27 | 0.2443  | -0.3814 | 3.5727  |
| O17     | -5.1106      | -2.8668 | -2.1603 |         | H28 | -1.5351 | 1.0485  | 3.1881  |
| O18     | -2.9643      | 0.9608  | -1.9821 |         | H29 | -1.5446 | -2.4234 | -1.7291 |
| O19     | 0.5693       | -1.1522 | -3.6359 |         | H30 | 0.2156  | 2.2668  | 2.6301  |
| O20     | -0.7190      | -2.9004 | -2.0427 |         | H31 | -0.1597 | 3.5776  | -0.8356 |
| O21     | -0.7641      | -3.1327 | 2.4076  |         | H32 | -1.5578 | -2.6219 | 2.0735  |
| O22     | 0.6862       | -3.8408 | 0.1692  |         | H33 | -2.9563 | 0.0058  | -1.6716 |
| O23     | -6.6147      | -1.2121 | -3.6422 |         | H34 | -4.6295 | -5.8201 | -3.1728 |
| O24     | -3.0087      | 0.8363  | 2.3629  |         | H35 | -2.9965 | 1.4737  | 1.5945  |
| O25     | -1.5403      | -5.0423 | -3.5047 |         | H36 | -2.1340 | 3.0941  | 0.1213  |
| O26     | -4.2604      | -4.9919 | -3.5951 |         | H37 | 2.9644  | 0.0136  | 1.7704  |
| O27     | 5.0956       | 2.8781  | 2.1776  |         | H38 | -6.0951 | -0.3573 | -3.6021 |
| O28     | 0.7687       | -1.2332 | 3.5813  |         | H39 | 5.6573  | 3.1857  | 1.4023  |
| O29     | 2.9799       | -2.4321 | -0.1613 |         | H40 | 5.6398  | 2.2286  | 2.7155  |
| O30     | 5.2716       | -1.2801 | 3.6787  |         | H41 | -4.3758 | 1.0600  | -2.9668 |
| O31     | -2.9138      | -1.7279 | 1.5034  |         | H42 | -7.3911 | -3.2883 | -0.0469 |
| O32     | -0.7405      | 1.2411  | -3.5429 |         | H43 | 2.5139  | 4.9944  | 3.6503  |
| O33     | -5.2212      | 1.1444  | -3.4979 |         | H44 | 3.7282  | 2.0566  | 1.5675  |
| O34     | -2.9656      | 2.5410  | 0.1974  |         | H45 | -5.6862 | -2.4487 | 2.8558  |
| H1      | -4.6255      | -4.9316 | -4.5250 |         | H46 | 1.5525  | 2.6325  | -1.9724 |
| H2      | -3.8582      | 0.9882  | 2.8774  |         | H47 | 6.5818  | 1.5485  | 4.5735  |
| H3      | -2.9602      | 1.9402  | -0.6074 |         | H48 | 4.4397  | -1.1481 | 3.1479  |
| H4      | -1.0347      | -3.6858 | -2.5784 |         | H49 | -4.8119 | -3.6710 | -2.6815 |
| H5      | -6.0914      | -1.8634 | -3.0835 |         | H50 | 3.7799  | -0.9647 | -2.8485 |
| H6      | 0.1444       | -3.5231 | -0.6039 |         | H51 | 1.0331  | 3.6633  | 2.6697  |
| H7      | -0.2498      | -3.4014 | 1.5916  |         | H52 | 4.6061  | 5.7813  | 3.2030  |
| H8      | -4.9420      | 1.3535  | -4.4372 |         | H53 | 2.9775  | -1.8703 | 0.6687  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.2349 | -5.8836 | -3.0514 | end |         |         |         |
| H55 | -2.9551 | -1.6641 | -0.1851 | H1  | 11.2929 | 0.7149  | 0.8095  |
| H56 | -3.7393 | -2.0792 | -1.5340 | H2  | 10.7978 | 1.2423  | 0.6462  |
| H57 | 6.0862  | 3.4734  | -0.7617 | end |         |         |         |
| H58 | 2.1209  | 2.0928  | 1.5451  | H1  | 11.4892 | 10.7454 | 1.3279  |
| H59 | 2.9622  | 1.7248  | -0.4525 | H2  | 11.0711 | 10.1480 | 1.4471  |
| H60 | -5.6273 | -3.1980 | -1.3658 | end |         |         |         |
| H61 | -2.9680 | -0.7833 | 1.8330  | H1  | 14.9545 | 4.4393  | 1.5789  |
| H62 | -2.5415 | -5.0641 | -3.5404 | H2  | 14.5952 | 4.3422  | 0.9377  |
| H63 | 2.1608  | -1.0675 | 2.6306  | end |         |         |         |
| H64 | -2.1525 | 1.0672  | -2.5561 | H1  | 3.3665  | 2.2191  | 5.8075  |
| H65 | 2.9898  | 0.8621  | -1.8022 | H2  | 3.8260  | 2.8022  | 5.8228  |
| H66 | 5.7844  | 2.3925  | -2.7243 | end |         |         |         |
| H67 | 0.6877  | -4.8423 | 0.1191  | H1  | 19.8191 | 11.3554 | 4.7731  |
| H68 | -5.6535 | -3.2785 | 1.4784  | H2  | 19.2436 | 11.5488 | 5.1994  |
| end |         |         |         | end |         |         |         |
| H1  | -4.3354 | 5.0970  | 2.9600  | H1  | 9.6370  | 11.1363 | 3.5976  |
| H2  | -4.9080 | 4.6378  | 2.8253  | H2  | 9.8580  | 11.6250 | 4.1086  |
| end |         |         |         | end |         |         |         |
| H1  | 9.5239  | 5.8585  | 5.4621  | H1  | 6.2583  | 3.6649  | 8.6539  |
| H2  | 9.0077  | 5.4609  | 5.0977  | H2  | 6.8763  | 3.9996  | 8.4162  |
| end |         |         |         | end |         |         |         |
| H1  | 15.4969 | 10.1738 | 7.0162  | H1  | 13.3475 | 3.9354  | 10.0143 |
| H2  | 16.0675 | 9.8111  | 6.7016  | H2  | 13.0265 | 3.9725  | 9.3481  |
| end |         |         |         | end |         |         |         |
| H1  | 13.1903 | 7.8491  | 5.4322  | H1  | 20.0553 | 8.7019  | 8.8741  |
| H2  | 13.2354 | 7.1119  | 5.3273  | H2  | 19.4615 | 8.2692  | 8.7692  |
| end |         |         |         | end |         |         |         |
| H1  | 15.6407 | 5.9788  | 0.3162  | H1  | 17.0988 | 12.8344 | 8.5132  |
| H2  | 15.8547 | 6.4373  | -0.2261 | H2  | 17.3039 | 13.0224 | 9.2016  |
| end |         |         |         | end |         |         |         |
| H1  | 6.0812  | 8.8931  | 0.2198  | end |         |         |         |
| H2  | 5.4036  | 8.9619  | 0.5115  |     |         |         |         |

(19) n=3 & m=3

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.5463 | -4.7162 | 0.0388  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.2221 | 0.3479  | -3.5202 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.0857  | -1.8153 | -3.0453 |
| O1      | 6.5464       | 3.7548  | 0.0894  |         | H12 | -3.7562 | -2.2269 | 1.8274  |
| O2      | 2.9338       | 1.5287  | 1.2157  |         | H13 | 0.2273  | 2.4182  | -2.7720 |
| O3      | 5.2549       | 3.0053  | -2.1672 |         | H14 | 6.0956  | 0.2506  | 3.7161  |
| O4      | 3.0105       | 1.7557  | -1.4307 |         | H15 | 4.9799  | -1.5006 | 4.6658  |
| O5      | 3.0161       | -0.9848 | 2.1564  |         | H16 | -0.0929 | 3.4883  | 0.7759  |
| O6      | -0.6082      | 1.0940  | 3.5693  |         | H17 | 2.9619  | -1.4146 | -1.5240 |
| O7      | 0.7642       | 2.8618  | 2.0858  |         | H18 | 1.2465  | 5.7765  | 3.1974  |
| O8      | 4.2759       | 4.9043  | 3.6709  |         | H19 | 4.6087  | 4.1251  | 3.1313  |
| O9      | 1.5314       | 4.9375  | 3.6652  |         | H20 | 2.1959  | -3.0539 | -0.0618 |
| O10     | 2.9460       | -0.8181 | -2.3261 |         | H21 | 4.4278  | 2.5067  | -1.8840 |
| O11     | 6.5844       | 1.1211  | 3.6623  |         | H22 | 0.1844  | -1.9785 | 3.2038  |
| O12     | -0.6050      | 3.8569  | -0.0072 |         | H23 | -0.6721 | 1.4932  | 4.4823  |
| O13     | 0.7698       | 3.0799  | -2.2534 |         | H24 | 7.4621  | 3.3452  | 0.1019  |
| O14     | -5.1164      | -3.0896 | 2.3354  |         | H25 | 1.4924  | -1.0708 | -3.1815 |
| O15     | -2.9450      | -1.6447 | -1.1680 |         | H26 | -1.0292 | 1.3527  | -4.4673 |
| O16     | -6.4582      | -3.7196 | 0.0585  |         | H27 | 0.2383  | -0.4187 | 3.6073  |
| O17     | -5.1257      | -2.9142 | -2.1408 |         | H28 | -1.5336 | 1.0069  | 3.1989  |
| O18     | -2.9457      | 0.9308  | -1.9756 |         | H29 | -1.5552 | -2.4559 | -1.7194 |
| O19     | 0.5994       | -1.1757 | -3.6230 |         | H30 | 0.2251  | 2.2225  | 2.6437  |
| O20     | -0.7301      | -2.9224 | -2.0438 |         | H31 | -0.1295 | 3.5363  | -0.8268 |
| O21     | -0.7547      | -3.1809 | 2.4063  |         | H32 | -1.5504 | -2.6655 | 2.0876  |
| O22     | 0.6988       | -3.8480 | 0.1388  |         | H33 | -2.9483 | -0.0209 | -1.6601 |
| O23     | -6.6068      | -1.2373 | -3.6317 |         | H34 | -4.6225 | -5.8613 | -3.1493 |
| O24     | -3.0048      | 0.8084  | 2.3622  |         | H35 | -2.9927 | 1.4511  | 1.5999  |
| O25     | -1.5432      | -5.0775 | -3.4654 |         | H36 | -2.1109 | 3.0773  | 0.1162  |
| O26     | -4.2571      | -5.0290 | -3.5697 |         | H37 | 2.9746  | -0.0420 | 1.8127  |
| O27     | 5.0984       | 2.8148  | 2.1803  |         | H38 | -6.0913 | -0.3797 | -3.5982 |
| O28     | 0.7624       | -1.2714 | 3.6131  |         | H39 | 5.6670  | 3.1455  | 1.4234  |
| O29     | 3.0103       | -2.4724 | -0.1134 |         | H40 | 5.6514  | 2.1816  | 2.7280  |
| O30     | 5.2882       | -1.3126 | 3.7286  |         | H41 | -4.3641 | 1.0274  | -2.9589 |
| O31     | -2.9170      | -1.7599 | 1.5275  |         | H42 | -7.3769 | -3.3273 | -0.0131 |
| O32     | -0.7220      | 1.2154  | -3.5226 |         | H43 | 2.5308  | 4.9403  | 3.6602  |
| O33     | -5.2099      | 1.1165  | -3.4876 |         | H44 | 3.7426  | 1.9987  | 1.5782  |
| O34     | -2.9487      | 2.5325  | 0.1976  |         | H45 | -5.6830 | -2.4755 | 2.8906  |
| H1      | -4.6239      | -4.9666 | -4.4990 |         | H46 | 1.5881  | 2.5855  | -1.9554 |
| H2      | -3.8490      | 0.9593  | 2.8873  |         | H47 | 6.6188  | 1.5143  | 4.5876  |
| H3      | -2.9477      | 1.9220  | -0.5992 |         | H48 | 4.4591  | -1.1845 | 3.1915  |
| H4      | -1.0392      | -3.7231 | -2.5639 |         | H49 | -4.8130 | -3.7193 | -2.6552 |
| H5      | -6.0814      | -1.8826 | -3.0694 |         | H50 | 3.7916  | -1.0011 | -2.8308 |
| H6      | 0.1466       | -3.5321 | -0.6289 |         | H51 | 1.0505  | 3.6156  | 2.6797  |
| H7      | -0.2458      | -3.4273 | 1.5817  |         | H52 | 4.6280  | 5.7238  | 3.2114  |
| H8      | -4.9310      | 1.3249  | -4.4270 |         | H53 | 2.9916  | -1.9209 | 0.7232  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.2305 | -5.9184 | -3.0161 | end |         |         |         |
| H55 | -2.9748 | -1.7027 | -0.1675 | H1  | 6.0632  | 8.8757  | 0.2305  |
| H56 | -3.7601 | -2.1152 | -1.5167 | H2  | 5.3833  | 8.9195  | 0.5213  |
| H57 | 6.0981  | 3.4478  | -0.7544 | end |         |         |         |
| H58 | 2.1351  | 2.0336  | 1.5582  | H1  | 11.2681 | 0.6736  | 0.8115  |
| H59 | 2.9838  | 1.6739  | -0.4262 | H2  | 10.7929 | 1.2132  | 0.6300  |
| H60 | -5.6265 | -3.2432 | -1.3351 | end |         |         |         |
| H61 | -2.9738 | -0.8091 | 1.8412  | H1  | 11.5048 | 10.6601 | 1.3939  |
| H62 | -2.5443 | -5.1096 | -3.5118 | H2  | 11.0870 | 10.0515 | 1.4479  |
| H63 | 2.1711  | -1.1154 | 2.6825  | end |         |         |         |
| H64 | -2.1266 | 1.0318  | -2.5423 | H1  | 14.9849 | 4.3770  | 1.5782  |
| H65 | 3.0161  | 0.8174  | -1.7797 | H2  | 14.6160 | 4.2894  | 0.9413  |
| H66 | 5.8006  | 2.3559  | -2.7015 | end |         |         |         |
| H67 | 0.7019  | -4.8494 | 0.0943  | H1  | 3.6539  | 2.0705  | 6.0677  |
| H68 | -5.6529 | -3.3209 | 1.5209  | H2  | 3.7595  | 2.7279  | 5.7434  |
| end |         |         |         | end |         |         |         |
| H1  | 8.9494  | 4.8309  | 1.5628  | H1  | 19.8199 | 11.3349 | 4.7786  |
| H2  | 8.9596  | 5.5711  | 1.4777  | H2  | 19.2120 | 11.4967 | 5.1717  |
| end |         |         |         | end |         |         |         |
| H1  | 9.6384  | 5.7225  | 5.5675  | H1  | 9.6665  | 11.0965 | 3.6345  |
| H2  | 9.1352  | 5.3466  | 5.1642  | H2  | 9.8575  | 11.6068 | 4.1363  |
| end |         |         |         | end |         |         |         |
| H1  | 7.1438  | 4.0195  | 4.0879  | H1  | 6.2616  | 3.6473  | 8.6603  |
| H2  | 7.6018  | 4.2272  | 3.5376  | H2  | 6.8961  | 3.9521  | 8.4257  |
| end |         |         |         | end |         |         |         |
| H1  | 15.2599 | 8.9212  | 4.7903  | H1  | 13.3450 | 3.9312  | 10.0387 |
| H2  | 15.1039 | 8.7172  | 4.0892  | H2  | 13.0438 | 3.9782  | 9.3637  |
| end |         |         |         | end |         |         |         |
| H1  | 15.5280 | 9.9378  | 7.0241  | H1  | 20.0534 | 8.6914  | 8.8986  |
| H2  | 16.2721 | 9.9538  | 6.9855  | H2  | 19.4469 | 8.2749  | 8.8013  |
| end |         |         |         | end |         |         |         |
| H1  | 13.1848 | 8.6003  | 7.3357  | H1  | 17.1238 | 12.8171 | 8.5210  |
| H2  | 13.3163 | 8.7485  | 6.6172  | H2  | 17.3553 | 12.9932 | 9.2040  |
| end |         |         |         | end |         |         |         |
| H1  | 15.6701 | 5.9346  | 0.3217  | end |         |         |         |
| H2  | 15.8673 | 6.4063  | -0.2157 |     |         |         |         |

**(20) n=3 & m=4**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.5805 | -4.7005 | -0.0093 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.2554 | 0.3545  | -3.5297 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.0539  | -1.8279 | -3.0334 |
| O1      | 6.5045       | 3.7445  | 0.1383  |         | H12 | -3.8215 | -2.2024 | 1.8027  |
| O2      | 2.8964       | 1.5360  | 1.2073  |         | H13 | 0.1932  | 2.4366  | -2.7853 |
| O3      | 5.2304       | 3.0365  | -2.1593 |         | H14 | 6.0333  | 0.2316  | 3.6969  |
| O4      | 2.9779       | 1.7845  | -1.4426 |         | H15 | 4.9170  | -1.5344 | 4.6241  |
| O5      | 2.9565       | -0.9895 | 2.1414  |         | H16 | -0.1429 | 3.5178  | 0.7692  |
| O6      | -0.6814      | 1.1587  | 3.5583  |         | H17 | 2.8963  | -1.3846 | -1.5484 |
| O7      | 0.7302       | 2.8893  | 2.0664  |         | H18 | 1.2151  | 5.7874  | 3.1750  |
| O8      | 4.2431       | 4.9454  | 3.6678  |         | H19 | 4.5746  | 4.1600  | 3.1392  |
| O9      | 1.5099       | 4.9613  | 3.6605  |         | H20 | 2.1626  | -3.0521 | -0.0683 |
| O10     | 2.8914       | -0.7888 | -2.3509 |         | H21 | 4.4002  | 2.5386  | -1.8867 |
| O11     | 6.5284       | 1.0962  | 3.6608  |         | H22 | 0.1069  | -1.9242 | 3.1880  |
| O12     | -0.6588      | 3.8796  | -0.0136 |         | H23 | -0.7420 | 1.5409  | 4.4783  |
| O13     | 0.7235       | 3.1080  | -2.2630 |         | H24 | 7.4229  | 3.3415  | 0.1320  |
| O14     | -5.1699      | -3.1045 | 2.3017  |         | H25 | 1.4464  | -1.0671 | -3.2101 |
| O15     | -2.9432      | -1.6091 | -1.1844 |         | H26 | -1.0418 | 1.3781  | -4.4726 |
| O16     | -6.4982      | -3.7029 | 0.0096  |         | H27 | 0.1665  | -0.3645 | 3.5857  |
| O17     | -5.1170      | -2.8882 | -2.1634 |         | H28 | -1.6067 | 1.0596  | 3.1924  |
| O18     | -2.9478      | 0.9488  | -2.0167 |         | H29 | -1.5709 | -2.4472 | -1.7150 |
| O19     | 0.5440       | -1.1865 | -3.6291 |         | H30 | 0.1780  | 2.2621  | 2.6241  |
| O20     | -0.7506      | -2.9291 | -2.0322 |         | H31 | -0.1803 | 3.5609  | -0.8326 |
| O21     | -0.8378      | -3.1311 | 2.3969  |         | H32 | -1.6345 | -2.6214 | 2.0705  |
| O22     | 0.6397       | -3.8608 | 0.1753  |         | H33 | -2.9449 | 0.0007  | -1.6883 |
| O23     | -6.6404      | -1.2135 | -3.6252 |         | H34 | -4.6598 | -5.8429 | -3.1840 |
| O24     | -3.0720      | 0.8351  | 2.3501  |         | H35 | -3.0679 | 1.4660  | 1.5768  |
| O25     | -1.5692      | -5.0690 | -3.4869 |         | H36 | -2.1614 | 3.0648  | 0.1176  |
| O26     | -4.2920      | -5.0145 | -3.6073 |         | H37 | 2.9472  | -0.0421 | 1.8106  |
| O27     | 5.0580       | 2.8197  | 2.2069  |         | H38 | -6.1192 | -0.3595 | -3.5866 |
| O28     | 0.6870       | -1.2179 | 3.5934  |         | H39 | 5.6305  | 3.1403  | 1.4460  |
| O29     | 2.9586       | -2.4551 | -0.1507 |         | H40 | 5.6026  | 2.1738  | 2.7481  |
| O30     | 5.1982       | -1.3454 | 3.6795  |         | H41 | -4.3801 | 1.0543  | -2.9686 |
| O31     | -2.9905      | -1.7248 | 1.5034  |         | H42 | -7.4197 | -3.3153 | -0.0530 |
| O32     | -0.7277      | 1.2373  | -3.5325 |         | H43 | 2.5103  | 4.9678  | 3.6491  |
| O33     | -5.2327      | 1.1284  | -3.4883 |         | H44 | 3.6985  | 2.0014  | 1.5864  |
| O34     | -2.9930      | 2.5112  | 0.1730  |         | H45 | -5.7427 | -2.5058 | 2.8655  |
| H1      | -4.6778      | -4.9410 | -4.5278 |         | H46 | 1.5453  | 2.6242  | -1.9631 |
| H2      | -3.9233      | 0.9665  | 2.8693  |         | H47 | 6.5584  | 1.4862  | 4.5876  |
| H3      | -2.9792      | 1.9258  | -0.6426 |         | H48 | 4.3559  | -1.2360 | 3.1535  |
| H4      | -1.0679      | -3.7170 | -2.5637 |         | H49 | -4.8203 | -3.6935 | -2.6856 |
| H5      | -6.1087      | -1.8684 | -3.0832 |         | H50 | 3.7420  | -0.9758 | -2.8433 |
| H6      | 0.0987       | -3.5485 | -0.6013 |         | H51 | 1.0252  | 3.6365  | 2.6619  |
| H7      | -0.3195      | -3.3897 | 1.5816  |         | H52 | 4.5718  | 5.7670  | 3.1958  |
| H8      | -4.9636      | 1.3351  | -4.4296 |         | H53 | 2.9513  | -1.9101 | 0.6891  |



|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.2606 | -5.9044 | -3.0250 | end |         |         |         |
| H55 | -2.9970 | -1.6578 | -0.1843 | H1  | 15.6106 | 5.9846  | 0.3353  |
| H56 | -3.7523 | -2.0790 | -1.5451 | H2  | 15.7365 | 6.4695  | -0.2116 |
| H57 | 6.0618  | 3.4634  | -0.7151 | end |         |         |         |
| H58 | 2.0954  | 2.0396  | 1.5434  | H1  | 6.0143  | 8.8570  | 0.1965  |
| H59 | 2.9489  | 1.6994  | -0.4393 | H2  | 5.3366  | 8.9374  | 0.4845  |
| H60 | -5.6257 | -3.2175 | -1.3640 | end |         |         |         |
| H61 | -3.0443 | -0.7783 | 1.8305  | H1  | 11.2670 | 0.6988  | 0.8702  |
| H62 | -2.5696 | -5.0935 | -3.5304 | H2  | 10.7567 | 1.2027  | 0.6821  |
| H63 | 2.1039  | -1.0989 | 2.6573  | end |         |         |         |
| H64 | -2.1184 | 1.0557  | -2.5716 | H1  | 11.3550 | 10.7139 | 1.3032  |
| H65 | 2.9743  | 0.8469  | -1.7932 | H2  | 11.1944 | 10.0276 | 1.5272  |
| H66 | 5.7738  | 2.3893  | -2.6948 | end |         |         |         |
| H67 | 0.6447  | -4.8632 | 0.1344  | H1  | 14.9729 | 4.3875  | 1.5594  |
| H68 | -5.6991 | -3.3193 | 1.4784  | H2  | 14.5855 | 4.2990  | 0.9339  |
| end |         |         |         | end |         |         |         |
| H1  | -4.8737 | 6.1291  | 3.5603  | H1  | 3.7130  | 2.1656  | 5.7943  |
| H2  | -4.1319 | 6.1282  | 3.6376  | H2  | 3.3539  | 2.8051  | 5.8994  |
| end |         |         |         | end |         |         |         |
| H1  | 9.3546  | 5.0846  | 1.3518  | H1  | 19.7087 | 11.3440 | 4.6654  |
| H2  | 8.7345  | 5.2826  | 1.7145  | H2  | 19.1626 | 11.5387 | 5.1272  |
| end |         |         |         | end |         |         |         |
| H1  | 9.7060  | 5.8617  | 5.5229  | H1  | 9.7058  | 10.9868 | 3.7279  |
| H2  | 9.2623  | 5.4397  | 5.0967  | H2  | 9.7187  | 11.6751 | 3.9999  |
| end |         |         |         | end |         |         |         |
| H1  | 8.0942  | 3.5755  | 4.1425  | H1  | 6.2476  | 3.6703  | 8.7117  |
| H2  | 8.5532  | 3.1294  | 3.7615  | H2  | 6.8635  | 3.9871  | 8.4456  |
| end |         |         |         | end |         |         |         |
| H1  | 15.7031 | 9.1179  | 4.6177  | H1  | 13.2373 | 4.0826  | 9.9246  |
| H2  | 15.2560 | 8.8426  | 4.0890  | H2  | 12.9308 | 3.9154  | 9.2714  |
| end |         |         |         | end |         |         |         |
| H1  | 15.7685 | 9.7159  | 6.7563  | H1  | 20.0476 | 8.6613  | 8.8658  |
| H2  | 16.4718 | 9.9048  | 6.9133  | H2  | 19.4648 | 8.2354  | 8.6938  |
| end |         |         |         | end |         |         |         |
| H1  | 13.5255 | 8.9952  | 7.7478  | H1  | 17.0637 | 12.8003 | 8.5116  |
| H2  | 13.6682 | 8.5749  | 7.1490  | H2  | 17.2334 | 12.9422 | 9.2202  |
| end |         |         |         | end |         |         |         |
| H1  | 13.0850 | 7.7510  | 5.3639  | end |         |         |         |
| H2  | 13.1601 | 7.0476  | 5.1312  | end |         |         |         |

**(21) n=3 & m=5**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.5805 | -4.7010 | -0.0517 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.2103 | 0.3353  | -3.6028 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.0925  | -1.8131 | -3.0800 |
| O1      | 6.5494       | 3.7999  | 0.0814  |         | H12 | -3.8091 | -2.2084 | 1.8059  |
| O2      | 2.8653       | 1.6084  | 1.1721  |         | H13 | 0.2145  | 2.4415  | -2.8442 |
| O3      | 5.2626       | 3.0568  | -2.1809 |         | H14 | 6.0345  | 0.2929  | 3.6337  |
| O4      | 2.9833       | 1.8182  | -1.4805 |         | H15 | 4.9489  | -1.4577 | 4.5879  |
| O5      | 2.9555       | -0.9078 | 2.1005  |         | H16 | -0.1209 | 3.5436  | 0.7202  |
| O6      | -0.6852      | 1.1558  | 3.5549  |         | H17 | 2.9159  | -1.3782 | -1.5656 |
| O7      | 0.7018       | 2.9324  | 2.0729  |         | H18 | 1.1703  | 5.8344  | 3.1933  |
| O8      | 4.1977       | 4.9185  | 3.6380  |         | H19 | 4.5338  | 4.1580  | 3.0743  |
| O9      | 1.4589       | 5.0075  | 3.6807  |         | H20 | 2.1600  | -3.0256 | -0.0558 |
| O10     | 2.9139       | -0.7766 | -2.3630 |         | H21 | 4.4289  | 2.5682  | -1.9051 |
| O11     | 6.5398       | 1.1545  | 3.5896  |         | H22 | 0.1329  | -1.9220 | 3.2149  |
| O12     | -0.6280      | 3.8964  | -0.0712 |         | H23 | -0.7471 | 1.5464  | 4.4705  |
| O13     | 0.7407       | 3.1142  | -2.3236 |         | H24 | 7.4581  | 3.3726  | 0.0918  |
| O14     | -5.1987      | -3.0651 | 2.2874  |         | H25 | 1.4938  | -1.0731 | -3.2601 |
| O15     | -2.9195      | -1.6111 | -1.1695 |         | H26 | -1.0595 | 1.3423  | -4.5188 |
| O16     | -6.4990      | -3.7020 | -0.0307 |         | H27 | 0.1811  | -0.3540 | 3.5876  |
| O17     | -5.0971      | -2.8782 | -2.1740 |         | H28 | -1.6083 | 1.0540  | 3.1838  |
| O18     | -2.8922      | 0.9507  | -2.0066 |         | H29 | -1.5300 | -2.4165 | -1.7152 |
| O19     | 0.5949       | -1.1899 | -3.6861 |         | H30 | 0.1537  | 2.2942  | 2.6206  |
| O20     | -0.7056      | -2.8865 | -2.0391 |         | H31 | -0.1531 | 3.5697  | -0.8887 |
| O21     | -0.8305      | -3.1297 | 2.4592  |         | H32 | -1.6237 | -2.6219 | 2.1182  |
| O22     | 0.6586       | -3.8085 | 0.2237  |         | H33 | -2.8951 | 0.0024  | -1.6800 |
| O23     | -6.6163      | -1.2041 | -3.6253 |         | H34 | -4.6313 | -5.8171 | -3.2147 |
| O24     | -3.0492      | 0.8339  | 2.3005  |         | H35 | -3.0200 | 1.4777  | 1.5379  |
| O25     | -1.5171      | -5.0202 | -3.5097 |         | H36 | -2.1438 | 3.1225  | 0.0852  |
| O26     | -4.2413      | -4.9957 | -3.6329 |         | H37 | 2.9086  | 0.0356  | 1.7605  |
| O27     | 5.0547       | 2.8742  | 2.1217  |         | H38 | -6.1032 | -0.3472 | -3.5793 |
| O28     | 0.7136       | -1.1999 | 3.5950  |         | H39 | 5.6384  | 3.2052  | 1.3746  |
| O29     | 2.9712       | -2.4450 | -0.1429 |         | H40 | 5.5986  | 2.2329  | 2.6671  |
| O30     | 5.2129       | -1.2573 | 3.6415  |         | H41 | -4.3129 | 1.0603  | -2.9519 |
| O31     | -2.9664      | -1.7466 | 1.5127  |         | H42 | -7.4188 | -3.3094 | -0.0855 |
| O32     | -0.7060      | 1.2056  | -3.5915 |         | H43 | 2.4581  | 4.9994  | 3.6566  |
| O33     | -5.1808      | 1.1462  | -3.4473 |         | H44 | 3.6804  | 2.0719  | 1.5272  |
| O34     | -2.9664      | 2.5557  | 0.1594  |         | H45 | -5.7682 | -2.4378 | 2.8251  |
| H1      | -4.6384      | -4.9025 | -4.5491 |         | H46 | 1.5616  | 2.6291  | -2.0161 |
| H2      | -3.9021      | 0.9879  | 2.8106  |         | H47 | 6.5800  | 1.5394  | 4.5191  |
| H3      | -2.9438      | 1.9568  | -0.6459 |         | H48 | 4.3626  | -1.1359 | 3.1344  |
| H4      | -1.0192      | -3.6792 | -2.5661 |         | H49 | -4.7821 | -3.6762 | -2.6931 |
| H5      | -6.0769      | -1.8568 | -3.0849 |         | H50 | 3.7697  | -0.9550 | -2.8512 |
| H6      | 0.1314       | -3.4956 | -0.5596 |         | H51 | 0.9815  | 3.6812  | 2.6743  |
| H7      | -0.3045      | -3.3871 | 1.6484  |         | H52 | 4.5508  | 5.7564  | 3.2111  |
| H8      | -4.9452      | 1.3619  | -4.3954 |         | H53 | 2.9624  | -1.8736 | 0.6797  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.2058 | -5.8641 | -3.0685 | end |         |         |         |
| H55 | -2.9713 | -1.6779 | -0.1692 | H1  | 8.6874  | 7.2505  | 4.2364  |
| H56 | -3.7301 | -2.0722 | -1.5366 | H2  | 9.0501  | 6.9407  | 3.6649  |
| H57 | 6.0987  | 3.5105  | -0.7669 | end |         |         |         |
| H58 | 2.0717  | 2.1095  | 1.5304  | H1  | 15.6440 | 5.9626  | 0.3199  |
| H59 | 2.9267  | 1.7443  | -0.4776 | H2  | 15.8254 | 6.4212  | -0.2341 |
| H60 | -5.6197 | -3.2164 | -1.3851 | end |         |         |         |
| H61 | -3.0211 | -0.7942 | 1.8192  | H1  | 6.0444  | 8.9471  | 0.2641  |
| H62 | -2.5158 | -5.0569 | -3.5554 | H2  | 5.3879  | 8.9426  | 0.6075  |
| H63 | 2.1168  | -1.0489 | 2.6311  | end |         |         |         |
| H64 | -2.0783 | 1.0488  | -2.5827 | H1  | 11.2932 | 0.7448  | 0.7960  |
| H65 | 2.9879  | 0.8779  | -1.8211 | H2  | 10.8184 | 1.2879  | 0.6236  |
| H66 | 5.8168  | 2.3907  | -2.6854 | end |         |         |         |
| H67 | 0.6846  | -4.8080 | 0.1562  | H1  | 11.4506 | 10.7394 | 1.2393  |
| H68 | -5.7152 | -3.2948 | 1.4612  | H2  | 11.0704 | 10.1440 | 1.4597  |
| end |         |         |         | end |         |         |         |
| H1  | -4.5774 | 5.2032  | 3.0656  | H1  | 14.8848 | 4.4786  | 1.5863  |
| H2  | -5.1915 | 4.9161  | 3.3735  | H2  | 14.5062 | 4.3702  | 0.9581  |
| end |         |         |         | end |         |         |         |
| H1  | 9.2324  | 5.5800  | 1.3988  | H1  | 3.7304  | 2.0117  | 6.0309  |
| H2  | 9.0265  | 4.9896  | 1.8033  | H2  | 3.6295  | 2.7144  | 5.8201  |
| end |         |         |         | end |         |         |         |
| H1  | 10.0045 | 5.2424  | 5.6152  | H1  | 19.7589 | 11.3980 | 4.6907  |
| H2  | 9.7666  | 4.6238  | 5.2767  | H2  | 19.1750 | 11.5762 | 5.1118  |
| end |         |         |         | end |         |         |         |
| H1  | 8.8904  | 2.7600  | 3.8626  | H1  | 9.6523  | 11.1874 | 3.5686  |
| H2  | 8.5873  | 3.3396  | 4.2181  | H2  | 9.7890  | 11.6885 | 4.0964  |
| end |         |         |         | end |         |         |         |
| H1  | 15.0518 | 6.8319  | 5.6733  | H1  | 6.1897  | 3.7207  | 8.6519  |
| H2  | 15.7616 | 6.7149  | 5.8625  | H2  | 6.8477  | 3.8416  | 8.3310  |
| end |         |         |         | end |         |         |         |
| H1  | 16.3868 | 8.8100  | 6.4027  | H1  | 13.2919 | 4.0421  | 9.9109  |
| H2  | 16.9949 | 9.2236  | 6.5205  | H2  | 12.9563 | 4.0104  | 9.2511  |
| end |         |         |         | end |         |         |         |
| H1  | 14.3438 | 8.4789  | 8.3022  | H1  | 20.0734 | 8.6828  | 8.8424  |
| H2  | 14.9536 | 8.7862  | 8.0038  | H2  | 19.4806 | 8.2572  | 8.7067  |
| end |         |         |         | end |         |         |         |
| H1  | 13.1052 | 8.0301  | 5.3831  | H1  | 17.1027 | 12.7913 | 8.5039  |
| H2  | 12.8945 | 7.3243  | 5.2803  | H2  | 17.2934 | 12.9400 | 9.2056  |
| end |         |         |         | end |         |         |         |
| H1  | 15.0062 | 10.2125 | 5.3314  | end |         |         |         |
| H2  | 14.3582 | 10.4952 | 5.0936  | end |         |         |         |

**(22) n=3 & m=6**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.5501 | -4.6583 | -0.0291 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.2481 | 0.3597  | -3.5482 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.0110  | -1.8228 | -3.0513 |
| O1      | 6.5555       | 3.7956  | 0.1118  |         | H12 | -3.7990 | -2.1711 | 1.7322  |
| O2      | 2.9791       | 1.5579  | 1.1911  |         | H13 | 0.2343  | 2.4398  | -2.7628 |
| O3      | 5.2544       | 3.0429  | -2.1407 |         | H14 | 6.0616  | 0.2594  | 3.6840  |
| O4      | 3.0122       | 1.7723  | -1.4500 |         | H15 | 4.9554  | -1.5271 | 4.6029  |
| O5      | 3.0019       | -0.9598 | 2.0879  |         | H16 | -0.0806 | 3.5336  | 0.7802  |
| O6      | -0.6283      | 1.1417  | 3.5285  |         | H17 | 2.9122  | -1.3876 | -1.5947 |
| O7      | 0.8190       | 2.8660  | 2.0528  |         | H18 | 1.2185  | 5.7949  | 3.1633  |
| O8      | 4.2367       | 4.9740  | 3.6571  |         | H19 | 4.5811  | 4.1974  | 3.1283  |
| O9      | 1.5116       | 4.9654  | 3.6409  |         | H20 | 2.1894  | -3.0128 | -0.1330 |
| O10     | 2.8798       | -0.7909 | -2.3996 |         | H21 | 4.4325  | 2.5280  | -1.8733 |
| O11     | 6.5484       | 1.1297  | 3.6477  |         | H22 | 0.1447  | -1.9416 | 3.1244  |
| O12     | -0.6009      | 3.9066  | 0.0068  |         | H23 | -0.6964 | 1.5426  | 4.4418  |
| O13     | 0.7665       | 3.1021  | -2.2364 |         | H24 | 7.4715  | 3.3860  | 0.1248  |
| O14     | -5.1315      | -3.0716 | 2.2661  |         | H25 | 1.4139  | -1.0554 | -3.2068 |
| O15     | -2.9524      | -1.5815 | -1.2665 |         | H26 | -1.0254 | 1.4040  | -4.4874 |
| O16     | -6.4793      | -3.6614 | -0.0317 |         | H27 | 0.2093  | -0.3913 | 3.5528  |
| O17     | -5.1409      | -2.8428 | -2.2166 |         | H28 | -1.5549 | 1.0531  | 3.1607  |
| O18     | -2.9318      | 1.0151  | -1.9785 |         | H29 | -1.6008 | -2.4399 | -1.7789 |
| O19     | 0.5112       | -1.1683 | -3.6293 |         | H30 | 0.2594  | 2.2358  | 2.5976  |
| O20     | -0.7759      | -2.9237 | -2.0873 |         | H31 | -0.1395 | 3.5776  | -0.8172 |
| O21     | -0.8096      | -3.1172 | 2.3381  |         | H32 | -1.5949 | -2.6047 | 1.9982  |
| O22     | 0.6859       | -3.8034 | 0.1032  |         | H33 | -2.9464 | 0.0516  | -1.6979 |
| O23     | -6.6395      | -1.1702 | -3.7006 |         | H34 | -4.6612 | -5.8283 | -3.1721 |
| O24     | -3.0381      | 0.8467  | 2.3493  |         | H35 | -3.0266 | 1.5038  | 1.5985  |
| O25     | -1.5775      | -5.0844 | -3.5164 |         | H36 | -2.1144 | 3.1256  | 0.1523  |
| O26     | -4.3033      | -5.0030 | -3.6084 |         | H37 | 2.9989  | -0.0098 | 1.7595  |
| O27     | 5.1118       | 2.8639  | 2.1781  |         | H38 | -6.1194 | -0.3189 | -3.6391 |
| O28     | 0.7285       | -1.2450 | 3.5463  |         | H39 | 5.6818  | 3.1841  | 1.4153  |
| O29     | 2.9902       | -2.4166 | -0.2112 |         | H40 | 5.6531  | 2.2149  | 2.7200  |
| O30     | 5.2499       | -1.3258 | 3.6659  |         | H41 | -4.3409 | 1.0962  | -2.9778 |
| O31     | -2.9781      | -1.6857 | 1.4133  |         | H42 | -7.4051 | -3.2817 | -0.0906 |
| O32     | -0.7177      | 1.2451  | -3.5474 |         | H43 | 2.5124  | 4.9867  | 3.6406  |
| O33     | -5.1920      | 1.1693  | -3.4998 |         | H44 | 3.7802  | 2.0360  | 1.5609  |
| O34     | -2.9468      | 2.5723  | 0.2069  |         | H45 | -5.7007 | -2.4747 | 2.8366  |
| H1      | -4.6733      | -4.9636 | -4.5349 |         | H46 | 1.5888  | 2.6139  | -1.9410 |
| H2      | -3.8806      | 0.9898  | 2.8791  |         | H47 | 6.5683  | 1.5117  | 4.5757  |
| H3      | -2.9269      | 1.9765  | -0.6019 |         | H48 | 4.4125  | -1.2071 | 3.1384  |
| H4      | -1.0850      | -3.7172 | -2.6169 |         | H49 | -4.8375 | -3.6516 | -2.7273 |
| H5      | -6.1270      | -1.8278 | -3.1421 |         | H50 | 3.7201  | -0.9592 | -2.9138 |
| H6      | 0.1344       | -3.5108 | -0.6727 |         | H51 | 1.0786  | 3.6271  | 2.6502  |
| H7      | -0.2850      | -3.3831 | 1.5298  |         | H52 | 4.5839  | 5.7919  | 3.1965  |
| H8      | -4.9258      | 1.3628  | -4.4460 |         | H53 | 2.9856  | -1.8730 | 0.6297  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.2673 | -5.9103 | -3.0409 | end |         |         |         |
| H55 | -2.9968 | -1.6354 | -0.2652 | H1  | 16.8814 | 7.5782  | 5.0706  |
| H56 | -3.7722 | -2.0420 | -1.6180 | H2  | 16.8934 | 7.0623  | 5.6068  |
| H57 | 6.1069  | 3.4931  | -0.7324 | end |         |         |         |
| H58 | 2.1735  | 2.0560  | 1.5310  | H1  | 10.5595 | 3.5872  | 3.2070  |
| H59 | 3.0004  | 1.6827  | -0.4457 | H2  | 10.1644 | 4.2042  | 3.0804  |
| H60 | -5.6452 | -3.1719 | -1.4131 | end |         |         |         |
| H61 | -3.0310 | -0.7454 | 1.7572  | H1  | 15.6437 | 6.0230  | 0.3164  |
| H62 | -2.5774 | -5.1088 | -3.5601 | H2  | 15.8559 | 6.4408  | -0.2583 |
| H63 | 2.1480  | -1.0731 | 2.5983  | end |         |         |         |
| H64 | -2.1222 | 1.1174  | -2.5567 | H1  | 6.0147  | 8.8582  | 0.1941  |
| H65 | 2.9971  | 0.8407  | -1.8145 | H2  | 5.3153  | 8.9806  | 0.4046  |
| H66 | 5.8041  | 2.4139  | -2.6908 | end |         |         |         |
| H67 | 0.7054  | -4.8048 | 0.0761  | H1  | 11.2648 | 0.7147  | 0.7705  |
| H68 | -5.6691 | -3.2831 | 1.4490  | H2  | 10.7543 | 1.2356  | 0.6362  |
| end |         |         |         | end |         |         |         |
| H1  | -4.7335 | 5.3750  | 2.9365  | H1  | 11.4552 | 10.6936 | 1.2651  |
| H2  | -5.0995 | 4.8432  | 2.5691  | H2  | 11.2985 | 10.0218 | 1.5310  |
| end |         |         |         | end |         |         |         |
| H1  | 8.7825  | 5.3448  | 1.4583  | H1  | 14.9526 | 4.4347  | 1.5565  |
| H2  | 9.4415  | 5.2196  | 1.1385  | H2  | 14.5936 | 4.3645  | 0.9115  |
| end |         |         |         | end |         |         |         |
| H1  | 9.5889  | 4.9358  | 5.3228  | H1  | 3.1317  | 2.4890  | 5.5515  |
| H2  | 9.9904  | 5.4646  | 5.6596  | H2  | 3.6850  | 2.9643  | 5.6919  |
| end |         |         |         | end |         |         |         |
| H1  | 7.8833  | 3.3791  | 4.6147  | H1  | 19.8110 | 11.2981 | 4.7803  |
| H2  | 8.5113  | 3.3887  | 4.2171  | H2  | 19.2092 | 11.5337 | 5.1432  |
| end |         |         |         | end |         |         |         |
| H1  | 14.9635 | 8.3098  | 4.4759  | H1  | 9.6443  | 11.0744 | 3.6451  |
| H2  | 14.9176 | 8.5715  | 3.7809  | H2  | 9.8590  | 11.5774 | 4.1452  |
| end |         |         |         | end |         |         |         |
| H1  | 16.6471 | 9.8403  | 6.2926  | H1  | 6.2832  | 3.6522  | 8.6610  |
| H2  | 15.9651 | 9.8958  | 6.0002  | H2  | 6.8924  | 4.0111  | 8.4365  |
| end |         |         |         | end |         |         |         |
| H1  | 14.9032 | 7.5776  | 7.9206  | H1  | 13.2719 | 4.0010  | 9.9343  |
| H2  | 15.1765 | 7.9644  | 7.3447  | H2  | 13.0314 | 4.1572  | 9.2518  |
| end |         |         |         | end |         |         |         |
| H1  | 12.9659 | 7.7548  | 5.6071  | H1  | 20.0389 | 8.7627  | 8.8659  |
| H2  | 12.9880 | 7.0125  | 5.5682  | H2  | 19.4538 | 8.3203  | 8.7531  |
| end |         |         |         | end |         |         |         |
| H1  | 13.4778 | 10.2076 | 6.2571  | H1  | 17.0305 | 12.9433 | 8.4483  |
| H2  | 13.6923 | 9.6446  | 5.8201  | H2  | 17.3048 | 13.0851 | 9.1239  |
| end |         |         |         | end |         |         |         |
| H1  | 8.5368  | 7.2350  | 3.6162  | end |         |         |         |
| H2  | 8.8617  | 6.6812  | 3.9925  | end |         |         |         |

**(23) n=3 & m=7**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.6272 | -4.6753 | -0.0430 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.2552 | 0.3571  | -3.5187 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.0377  | -1.8183 | -3.0124 |
| O1      | 6.5488       | 3.8289  | 0.0767  |         | H12 | -3.8147 | -2.1909 | 1.7771  |
| O2      | 2.9065       | 1.7140  | 1.2691  |         | H13 | 0.1752  | 2.4207  | -2.7896 |
| O3      | 5.1999       | 3.0634  | -2.1375 |         | H14 | 6.1011  | 0.3763  | 3.6853  |
| O4      | 2.9625       | 1.8446  | -1.3724 |         | H15 | 4.9756  | -1.4461 | 4.5844  |
| O5      | 3.0094       | -0.8222 | 2.1365  |         | H16 | -0.1483 | 3.5951  | 0.7286  |
| O6      | -0.6268      | 1.2187  | 3.5432  |         | H17 | 2.9080  | -1.3272 | -1.4588 |
| O7      | 0.7206       | 3.0318  | 2.0815  |         | H18 | 1.1991  | 5.8780  | 3.2381  |
| O8      | 4.2552       | 5.0415  | 3.6943  |         | H19 | 4.6020  | 4.2763  | 3.1476  |
| O9      | 1.4949       | 5.0492  | 3.7161  |         | H20 | 2.1729  | -2.9498 | -0.0144 |
| O10     | 2.8898       | -0.7341 | -2.2661 |         | H21 | 4.3730  | 2.5788  | -1.8274 |
| O11     | 6.5957       | 1.2419  | 3.6593  |         | H22 | 0.1421  | -1.8500 | 3.1545  |
| O12     | -0.6628      | 3.9096  | -0.0733 |         | H23 | -0.7140 | 1.5566  | 4.4788  |
| O13     | 0.7201       | 3.1066  | -2.3012 |         | H24 | 7.4511  | 3.3948  | 0.0598  |
| O14     | -5.1797      | -3.0436 | 2.3040  |         | H25 | 1.4414  | -1.0518 | -3.1186 |
| O15     | -2.9762      | -1.6105 | -1.2134 |         | H26 | -1.0431 | 1.4018  | -4.4562 |
| O16     | -6.5233      | -3.6797 | -0.0105 |         | H27 | 0.2123  | -0.2974 | 3.5765  |
| O17     | -5.1245      | -2.9144 | -2.1561 |         | H28 | -1.5456 | 1.1003  | 3.1677  |
| O18     | -3.0136      | 0.9417  | -2.0399 |         | H29 | -1.6115 | -2.4287 | -1.7262 |
| O19     | 0.5534       | -1.1595 | -3.5688 |         | H30 | 0.1909  | 2.3805  | 2.6313  |
| O20     | -0.7825      | -2.9038 | -2.0370 |         | H31 | -0.1716 | 3.5796  | -0.8806 |
| O21     | -0.8192      | -3.0476 | 2.3815  |         | H32 | -1.6234 | -2.5679 | 2.0278  |
| O22     | 0.6652       | -3.7641 | 0.1449  |         | H33 | -3.0031 | -0.0095 | -1.7183 |
| O23     | -6.6670      | -1.2692 | -3.6010 |         | H34 | -4.6675 | -5.8563 | -3.2279 |
| O24     | -2.9996      | 0.8214  | 2.2899  |         | H35 | -2.9784 | 1.4528  | 1.5192  |
| O25     | -1.5690      | -5.0465 | -3.5194 |         | H36 | -2.1353 | 3.0814  | 0.0245  |
| O26     | -4.2991      | -5.0202 | -3.6378 |         | H37 | 2.9621  | 0.1254  | 1.8116  |
| O27     | 5.1267       | 2.9669  | 2.1960  |         | H38 | -6.1591 | -0.4059 | -3.5736 |
| O28     | 0.7285       | -1.1540 | 3.5713  |         | H39 | 5.6924  | 3.2745  | 1.4254  |
| O29     | 2.9843       | -2.3683 | -0.0785 |         | H40 | 5.6774  | 2.3323  | 2.7434  |
| O30     | 5.2798       | -1.2039 | 3.6626  |         | H41 | -4.4576 | 1.0259  | -2.9575 |
| O31     | -2.9883      | -1.7211 | 1.4523  |         | H42 | -7.4354 | -3.2654 | -0.0564 |
| O32     | -0.7654      | 1.2190  | -3.5110 |         | H43 | 2.4931  | 5.0648  | 3.7128  |
| O33     | -5.3158      | 1.0927  | -3.4707 |         | H44 | 3.7179  | 2.1823  | 1.6229  |
| O34     | -2.9683      | 2.5292  | 0.1014  |         | H45 | -5.7351 | -2.4053 | 2.8434  |
| H1      | -4.6836      | -4.9200 | -4.5582 |         | H46 | 1.5394  | 2.6328  | -1.9786 |
| H2      | -3.8189      | 1.0276  | 2.8254  |         | H47 | 6.6171  | 1.5965  | 4.5988  |
| H3      | -2.9816      | 1.9231  | -0.7013 |         | H48 | 4.4426  | -1.0578 | 3.1398  |
| H4      | -1.0826      | -3.6929 | -2.5746 |         | H49 | -4.8304 | -3.7157 | -2.6821 |
| H5      | -6.1238      | -1.9188 | -3.0619 |         | H50 | 3.7210  | -0.9445 | -2.7773 |
| H6      | 0.1150       | -3.4688 | -0.6326 |         | H51 | 1.0028  | 3.7766  | 2.6893  |
| H7      | -0.2893      | -3.3278 | 1.5823  |         | H52 | 4.5900  | 5.8702  | 3.2407  |
| H8      | -5.0444      | 1.3218  | -4.4049 |         | H53 | 2.9796  | -1.8009 | 0.7482  |

|     |         |         |         |
|-----|---------|---------|---------|
| H54 | -1.2721 | -5.8823 | -3.0524 |
| H55 | -3.0154 | -1.6576 | -0.2102 |
| H56 | -3.7826 | -2.0993 | -1.5580 |
| H57 | 6.0741  | 3.5345  | -0.7567 |
| H58 | 2.1023  | 2.2209  | 1.5978  |
| H59 | 2.9324  | 1.7913  | -0.3664 |
| H60 | -5.6497 | -3.2397 | -1.3627 |
| H61 | -3.0326 | -0.7725 | 1.7778  |
| H62 | -2.5668 | -5.0747 | -3.5755 |
| H63 | 2.1709  | -0.9753 | 2.6616  |
| H64 | -2.1912 | 1.0503  | -2.6021 |
| H65 | 2.9790  | 0.9023  | -1.7074 |
| H66 | 5.7220  | 2.3990  | -2.6710 |
| H67 | 0.6877  | -4.7643 | 0.1061  |
| H68 | -5.7092 | -3.2819 | 1.4916  |
| end |         |         |         |
| H1  | -4.6157 | 6.0600  | 2.9208  |
| H2  | -4.7120 | 5.3853  | 2.6290  |
| end |         |         |         |
| H1  | 10.0578 | 5.8065  | 1.8426  |
| H2  | 9.6617  | 5.3686  | 2.2956  |
| end |         |         |         |
| H1  | 9.0261  | 5.5241  | 5.5000  |
| H2  | 9.5673  | 5.8600  | 5.8822  |
| end |         |         |         |
| H1  | 7.4967  | 3.8552  | 4.9106  |
| H2  | 7.5706  | 4.4588  | 4.4858  |
| end |         |         |         |
| H1  | 15.2254 | 8.0988  | 4.0248  |
| H2  | 14.7875 | 7.8289  | 4.5628  |
| end |         |         |         |
| H1  | 16.9527 | 9.4064  | 6.1682  |
| H2  | 16.2994 | 9.5123  | 5.8282  |
| end |         |         |         |
| H1  | 15.4451 | 6.8245  | 7.1082  |
| H2  | 15.8514 | 7.1935  | 6.6074  |
| end |         |         |         |
| H1  | 12.9688 | 6.8753  | 5.5009  |
| H2  | 12.9733 | 7.5960  | 5.6817  |
| end |         |         |         |
| H1  | 12.7008 | 9.5948  | 5.7909  |
| H2  | 13.3298 | 9.7675  | 6.1434  |
| end |         |         |         |
| H1  | 8.7794  | 7.4949  | 4.1210  |
| H2  | 9.0328  | 7.2013  | 3.4882  |
| end |         |         |         |

|     |         |         |         |
|-----|---------|---------|---------|
| H1  | 15.1976 | 11.2990 | 5.3152  |
| H2  | 14.5729 | 11.0473 | 5.0013  |
| end |         |         |         |
| H1  | 10.3475 | 4.2727  | 4.3293  |
| H2  | 10.5915 | 3.7329  | 3.8800  |
| end |         |         |         |
| H1  | 14.3006 | 9.1140  | 8.3048  |
| H2  | 14.8623 | 8.8515  | 7.8926  |
| end |         |         |         |
| H1  | 8.1425  | 3.5430  | 2.7828  |
| H2  | 8.3030  | 3.4329  | 2.0671  |
| end |         |         |         |
| H1  | 15.6427 | 5.9670  | 0.2890  |
| H2  | 15.8578 | 6.3894  | -0.2818 |
| end |         |         |         |
| H1  | 5.9709  | 8.9486  | 0.1557  |
| H2  | 5.2940  | 8.9893  | 0.4534  |
| end |         |         |         |
| H1  | 11.3363 | 0.7808  | 0.9315  |
| H2  | 10.9253 | 1.3496  | 0.6937  |
| end |         |         |         |
| H1  | 11.3314 | 10.9227 | 1.3888  |
| H2  | 11.2146 | 10.1948 | 1.4471  |
| end |         |         |         |
| H1  | 14.9270 | 4.5827  | 1.6685  |
| H2  | 14.5557 | 4.4244  | 1.0465  |
| end |         |         |         |
| H1  | 3.4978  | 2.1559  | 5.9980  |
| H2  | 3.8230  | 2.7819  | 5.7735  |
| end |         |         |         |
| H1  | 19.7836 | 11.4164 | 4.7437  |
| H2  | 19.2068 | 11.5448 | 5.1922  |
| end |         |         |         |
| H1  | 9.6744  | 11.2276 | 3.6132  |
| H2  | 9.8624  | 11.6786 | 4.1698  |
| end |         |         |         |
| H1  | 6.2276  | 3.7452  | 8.6830  |
| H2  | 6.8581  | 4.0485  | 8.4374  |
| end |         |         |         |
| H1  | 13.2876 | 4.0759  | 9.9590  |
| H2  | 13.0083 | 3.8733  | 9.3043  |
| end |         |         |         |
| H1  | 20.0754 | 8.6083  | 8.8751  |
| H2  | 19.4620 | 8.2201  | 8.7182  |
| end |         |         |         |
| H1  | 17.1240 | 12.8155 | 8.5157  |

|     |         |         |        |     |
|-----|---------|---------|--------|-----|
| H2  | 17.2417 | 13.0442 | 9.2121 | end |
| end |         |         |        |     |



**(24) n=3 & m=8**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.6446 | -4.7040 | -0.0514 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.3512 | 0.3611  | -3.5485 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | -0.0323 | -1.8780 | -3.0722 |
| O1      | 6.5393       | 3.8168  | 0.0552  |         | H12 | -3.8855 | -2.2661 | 1.6975  |
| O2      | 2.8902       | 1.7224  | 1.2029  |         | H13 | 0.1409  | 2.4182  | -2.7641 |
| O3      | 5.2443       | 3.0671  | -2.2141 |         | H14 | 6.0611  | 0.2850  | 3.6130  |
| O4      | 2.9646       | 1.8374  | -1.4552 |         | H15 | 4.9431  | -1.4639 | 4.4906  |
| O5      | 2.9746       | -0.8062 | 2.0609  |         | H16 | -0.1542 | 3.5982  | 0.7613  |
| O6      | -0.6646      | 1.2028  | 3.5124  |         | H17 | 2.8635  | -1.3642 | -1.5145 |
| O7      | 0.7251       | 3.0117  | 2.0840  |         | H18 | 1.2098  | 5.8275  | 3.2357  |
| O8      | 4.2500       | 5.0422  | 3.6382  |         | H19 | 4.5934  | 4.2680  | 3.1007  |
| O9      | 1.5273       | 5.0129  | 3.7192  |         | H20 | 2.1625  | -2.9723 | -0.0565 |
| O10     | 2.8359       | -0.7562 | -2.3104 |         | H21 | 4.4138  | 2.5839  | -1.9250 |
| O11     | 6.5663       | 1.1499  | 3.5935  |         | H22 | 0.0945  | -1.8395 | 3.0758  |
| O12     | -0.6848      | 3.8990  | -0.0354 |         | H23 | -0.7592 | 1.5564  | 4.4425  |
| O13     | 0.6801       | 3.0847  | -2.2505 |         | H24 | 7.4392  | 3.3749  | 0.0775  |
| O14     | -5.2230      | -3.1105 | 2.2755  |         | H25 | 1.3452  | -1.0801 | -3.2353 |
| O15     | -2.9860      | -1.6765 | -1.3182 |         | H26 | -1.0937 | 1.4325  | -4.4840 |
| O16     | -6.5399      | -3.7069 | -0.0339 |         | H27 | 0.1870  | -0.2965 | 3.5150  |
| O17     | -5.1671      | -2.9432 | -2.2217 |         | H28 | -1.5786 | 1.0644  | 3.1319  |
| O18     | -3.0503      | 0.9064  | -1.9687 |         | H29 | -1.6365 | -2.4901 | -1.8049 |
| O19     | 0.4412       | -1.1911 | -3.6396 |         | H30 | 0.1791  | 2.3611  | 2.6181  |
| O20     | -0.8014      | -2.9681 | -2.1042 |         | H31 | -0.1983 | 3.5714  | -0.8474 |
| O21     | -0.8957      | -3.0318 | 2.3129  |         | H32 | -1.7181 | -2.5835 | 1.9497  |
| O22     | 0.6338       | -3.7753 | 0.1545  |         | H33 | -3.0292 | -0.0632 | -1.7034 |
| O23     | -6.6916      | -1.2496 | -3.6558 |         | H34 | -4.7133 | -5.8756 | -3.2659 |
| O24     | -3.0088      | 0.7364  | 2.2371  |         | H35 | -2.9834 | 1.3974  | 1.4856  |
| O25     | -1.5923      | -5.0654 | -3.6049 |         | H36 | -2.1704 | 3.0650  | 0.0877  |
| O26     | -4.3439      | -5.0482 | -3.6832 |         | H37 | 2.9322  | 0.1469  | 1.7464  |
| O27     | 5.1090       | 2.9533  | 2.1785  |         | H38 | -6.1768 | -0.3911 | -3.6092 |
| O28     | 0.6975       | -1.1562 | 3.4861  |         | H39 | 5.6736  | 3.2595  | 1.4072  |
| O29     | 2.9722       | -2.3919 | -0.1298 |         | H40 | 5.6500  | 2.2943  | 2.7031  |
| O30     | 5.2459       | -1.2310 | 3.5656  |         | H41 | -4.4478 | 0.9895  | -2.9377 |
| O31     | -3.0660      | -1.8055 | 1.3423  |         | H42 | -7.4513 | -3.2912 | -0.0779 |
| O32     | -0.8394      | 1.2323  | -3.5366 |         | H43 | 2.5269  | 5.0328  | 3.6889  |
| O33     | -5.2909      | 1.0755  | -3.4740 |         | H44 | 3.7064  | 2.1699  | 1.5697  |
| O34     | -2.9963      | 2.5053  | 0.1656  |         | H45 | -5.7709 | -2.4433 | 2.7890  |
| H1      | -4.7423      | -4.9552 | -4.5946 |         | H46 | 1.5102  | 2.6043  | -1.9627 |
| H2      | -3.8266      | 0.9406  | 2.7745  |         | H47 | 6.5491  | 1.5188  | 4.5240  |
| H3      | -3.0013      | 1.9022  | -0.6402 |         | H48 | 4.4134  | -1.0789 | 3.0357  |
| H4      | -1.1040      | -3.7512 | -2.6545 |         | H49 | -4.8782 | -3.7521 | -2.7424 |
| H5      | -6.1630      | -1.9032 | -3.1108 |         | H50 | 3.6639  | -0.9501 | -2.8311 |
| H6      | 0.1098       | -3.4836 | -0.6390 |         | H51 | 1.0132  | 3.7438  | 2.7037  |
| H7      | -0.3647      | -3.3448 | 1.5256  |         | H52 | 4.5732  | 5.8706  | 3.1764  |
| H8      | -4.9985      | 1.3096  | -4.4004 |         | H53 | 2.9568  | -1.8027 | 0.6821  |

|     |         |         |         |
|-----|---------|---------|---------|
| H54 | -1.2722 | -5.8992 | -3.1515 |
| H55 | -3.0334 | -1.7441 | -0.3165 |
| H56 | -3.8010 | -2.1468 | -1.6711 |
| H57 | 6.0897  | 3.5206  | -0.7908 |
| H58 | 2.0925  | 2.2226  | 1.5579  |
| H59 | 2.9370  | 1.8050  | -0.4496 |
| H60 | -5.6673 | -3.2588 | -1.4113 |
| H61 | -3.0788 | -0.8630 | 1.6811  |
| H62 | -2.5888 | -5.1116 | -3.6427 |
| H63 | 2.1275  | -0.9691 | 2.5689  |
| H64 | -2.2573 | 1.0461  | -2.5583 |
| H65 | 2.9292  | 0.8859  | -1.7638 |
| H66 | 5.7753  | 2.3926  | -2.7306 |
| H67 | 0.6569  | -4.7757 | 0.1124  |
| H68 | -5.7481 | -3.3474 | 1.4564  |
| end |         |         |         |
| H1  | -4.7440 | 5.8156  | 2.6280  |
| H2  | -5.0877 | 5.2661  | 2.9869  |
| end |         |         |         |
| H1  | 9.0886  | 5.2027  | 1.8818  |
| H2  | 9.5037  | 5.6807  | 1.4906  |
| end |         |         |         |
| H1  | 8.8597  | 5.9747  | 6.0520  |
| H2  | 8.8798  | 6.2208  | 5.3527  |
| end |         |         |         |
| H1  | 7.4386  | 3.8375  | 4.8695  |
| H2  | 7.9641  | 4.3608  | 4.8812  |
| end |         |         |         |
| H1  | 15.0392 | 9.1328  | 4.0188  |
| H2  | 14.7754 | 8.5494  | 4.3975  |
| end |         |         |         |
| H1  | 16.5775 | 9.7429  | 6.6731  |
| H2  | 16.0301 | 9.4853  | 6.2397  |
| end |         |         |         |
| H1  | 15.4463 | 7.1267  | 7.3515  |
| H2  | 15.8545 | 6.6252  | 6.9880  |
| end |         |         |         |
| H1  | 13.3751 | 6.8791  | 5.4268  |
| H2  | 13.3711 | 7.5599  | 5.7274  |
| end |         |         |         |
| H1  | 15.1336 | 11.4944 | 5.2335  |
| H2  | 14.5365 | 11.3009 | 4.8385  |
| end |         |         |         |
| H1  | 8.9146  | 7.0344  | 3.3231  |
| H2  | 8.5951  | 7.5461  | 3.7542  |
| end |         |         |         |

|     |         |         |         |
|-----|---------|---------|---------|
| H1  | 17.1267 | 7.3060  | 4.7191  |
| H2  | 17.0326 | 7.3052  | 5.4550  |
| end |         |         |         |
| H1  | 10.4539 | 4.3330  | 4.0595  |
| H2  | 10.3499 | 3.6274  | 3.8485  |
| end |         |         |         |
| H1  | 14.9440 | 8.9025  | 8.1959  |
| H2  | 14.3917 | 8.6720  | 8.6364  |
| end |         |         |         |
| H1  | 8.0311  | 3.4732  | 2.8925  |
| H2  | 8.2017  | 3.2525  | 2.2057  |
| end |         |         |         |
| H1  | 13.0056 | 9.7353  | 6.4366  |
| H2  | 13.3909 | 9.6758  | 5.8042  |
| end |         |         |         |
| H1  | 10.9012 | 6.2978  | 4.8475  |
| H2  | 11.1856 | 6.3659  | 4.1661  |
| end |         |         |         |
| H1  | 15.6522 | 5.9028  | 0.2176  |
| H2  | 15.9163 | 6.2596  | -0.3769 |
| end |         |         |         |
| H1  | 5.6812  | 9.2352  | -0.0581 |
| H2  | 5.5382  | 8.8303  | 0.5473  |
| end |         |         |         |
| H1  | 11.3842 | 0.7536  | 0.8277  |
| H2  | 11.1557 | 1.4454  | 0.6916  |
| end |         |         |         |
| H1  | 11.3539 | 10.8792 | 1.4013  |
| H2  | 10.9994 | 10.2617 | 1.2024  |
| end |         |         |         |
| H1  | 14.8781 | 4.5929  | 1.6273  |
| H2  | 14.5031 | 4.4216  | 1.0112  |
| end |         |         |         |
| H1  | 2.8489  | 2.7065  | 5.3392  |
| H2  | 3.4367  | 3.1308  | 5.5028  |
| end |         |         |         |
| H1  | 19.7578 | 11.2520 | 4.7192  |
| H2  | 19.1515 | 11.4458 | 5.0994  |
| end |         |         |         |
| H1  | 9.6887  | 11.1318 | 3.7051  |
| H2  | 9.8285  | 11.6689 | 4.1968  |
| end |         |         |         |
| H1  | 6.2739  | 4.0806  | 8.6308  |
| H2  | 6.5478  | 3.6125  | 8.1253  |
| end |         |         |         |
| H1  | 13.3180 | 3.8114  | 10.0402 |

|     |         |        |        |     |         |         |        |
|-----|---------|--------|--------|-----|---------|---------|--------|
| H2  | 13.0280 | 3.9673 | 9.3775 | H1  | 16.9692 | 12.7831 | 8.5845 |
| end |         |        |        | H2  | 17.5035 | 12.8860 | 9.0890 |
| H1  | 19.9985 | 8.6823 | 8.8480 | end |         |         |        |
| H2  | 19.4030 | 8.2577 | 8.7211 | end |         |         |        |
| end |         |        |        |     |         |         |        |

**(25) n=4 & m=1**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.5257 | -4.8067 | 0.0918  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.3755 | 0.3327  | -3.6431 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | -0.0026 | -1.8461 | -3.0878 |
| O1      | 6.7587       | 3.8609  | -0.0872 |         | H12 | -3.7516 | -2.2250 | 1.8689  |
| O2      | 3.0241       | 1.6223  | 1.1025  |         | H13 | 0.0257  | 2.3666  | -2.8555 |
| O3      | 5.1942       | 2.9417  | -2.1468 |         | H14 | 6.0944  | 0.3987  | 3.6494  |
| O4      | 2.8363       | 1.7080  | -1.5766 |         | H15 | 4.9742  | -1.4221 | 4.6807  |
| O5      | 3.1113       | -0.8869 | 2.1805  |         | H16 | -0.0364 | 3.4144  | 0.7951  |
| O6      | -0.6099      | 1.1218  | 3.6582  |         | H17 | 2.8921  | -1.4489 | -1.4887 |
| O7      | 0.8464       | 2.8588  | 2.1524  |         | H18 | 1.2170  | 5.8289  | 3.2525  |
| O8      | 4.2856       | 4.9864  | 3.4980  |         | H19 | 4.6407  | 4.2480  | 2.9226  |
| O9      | 1.5383       | 4.9811  | 3.6801  |         | H20 | 2.2563  | -3.0044 | -0.0242 |
| O10     | 2.8409       | -0.9002 | -2.3224 |         | H21 | 4.3456  | 2.4601  | -1.9212 |
| O11     | 6.5567       | 1.2807  | 3.5965  |         | H22 | 0.2416  | -1.9042 | 3.1399  |
| O12     | -0.5648      | 3.7804  | 0.0264  |         | H23 | -0.6839 | 1.5129  | 4.5758  |
| O13     | 0.5738       | 3.0120  | -2.3215 |         | H24 | 7.6225  | 3.3491  | -0.0604 |
| O14     | -5.1746      | -3.0483 | 2.4321  |         | H25 | 1.3924  | -1.0916 | -3.1790 |
| O15     | -2.9256      | -1.7217 | -1.1536 |         | H26 | -1.1336 | 1.3388  | -4.6483 |
| O16     | -6.4431      | -3.8089 | 0.1171  |         | H27 | 0.2819  | -0.3726 | 3.6175  |
| O17     | -5.1394      | -2.9649 | -2.1409 |         | H28 | -1.5295 | 1.0378  | 3.2751  |
| O18     | -2.9955      | 0.8291  | -2.0550 |         | H29 | -1.5407 | -2.5752 | -1.6614 |
| O19     | 0.5011       | -1.1695 | -3.6267 |         | H30 | 0.3052  | 2.2338  | 2.7151  |
| O20     | -0.7237      | -3.0057 | -2.0476 |         | H31 | -0.1288 | 3.4716  | -0.8221 |
| O21     | -0.7162      | -3.0715 | 2.3218  |         | H32 | -1.5422 | -2.5839 | 2.0157  |
| O22     | 0.7617       | -3.7464 | 0.0867  |         | H33 | -2.9682 | -0.1214 | -1.7407 |
| O23     | -6.6830      | -1.2636 | -3.5385 |         | H34 | -4.7700 | -5.9437 | -3.1644 |
| O24     | -2.9838      | 0.8103  | 2.3680  |         | H35 | -2.9400 | 1.3998  | 1.5623  |
| O25     | -1.5767      | -5.1482 | -3.4416 |         | H36 | -2.0307 | 2.9381  | 0.1063  |
| O26     | -4.3397      | -5.1227 | -3.5474 |         | H37 | 3.0787  | 0.0368  | 1.8013  |
| O27     | 5.2259       | 2.9850  | 1.9302  |         | H38 | -6.1780 | -0.3996 | -3.5166 |
| O28     | 0.8171       | -1.2162 | 3.5837  |         | H39 | 5.8494  | 3.2891  | 1.2040  |
| O29     | 3.1126       | -2.4826 | -0.0798 |         | H40 | 5.7159  | 2.3434  | 2.5211  |
| O30     | 5.2977       | -1.1851 | 3.7643  |         | H41 | -4.4389 | 0.9708  | -2.9485 |
| O31     | -2.9188      | -1.7682 | 1.5581  |         | H42 | -7.3578 | -3.4044 | 0.0417  |
| O32     | -0.8897      | 1.1889  | -3.6853 |         | H43 | 2.5339  | 4.9950  | 3.6046  |
| O33     | -5.2733      | 1.0832  | -3.4937 |         | H44 | 3.8460  | 2.1233  | 1.3743  |
| O34     | -2.8859      | 2.4134  | 0.1301  |         | H45 | -5.7358 | -2.3972 | 2.9518  |
| H1      | -4.6576      | -5.0109 | -4.4869 |         | H46 | 1.4018  | 2.5166  | -2.0547 |
| H2      | -3.8395      | 1.0151  | 2.8500  |         | H47 | 6.5647  | 1.6493  | 4.5314  |
| H3      | -2.8793      | 1.8254  | -0.6817 |         | H48 | 4.4792  | -1.0657 | 3.2022  |
| H4      | -1.0423      | -3.8188 | -2.5418 |         | H49 | -4.8641 | -3.7791 | -2.6616 |
| H5      | -6.1310      | -1.9142 | -3.0066 |         | H50 | 3.7039  | -1.0669 | -2.8060 |
| H6      | 0.2231       | -3.4609 | -0.7105 |         | H51 | 1.0948  | 3.6352  | 2.7357  |
| H7      | -0.2062      | -3.3380 | 1.5053  |         | H52 | 4.6330  | 5.8315  | 3.0862  |
| H8      | -4.9606      | 1.2919  | -4.4219 |         | H53 | 3.1096  | -1.8878 | 0.7215  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.2745 | -5.9946 | -2.9937 | end |         |         |         |
| H55 | -2.9602 | -1.7578 | -0.1534 | H1  | 11.1591 | 10.6031 | 1.6741  |
| H56 | -3.7391 | -2.1981 | -1.4900 | H2  | 11.7900 | 10.3502 | 1.3888  |
| H57 | 6.2119  | 3.5066  | -0.8442 | end |         |         |         |
| H58 | 2.2487  | 2.0986  | 1.5212  | H1  | 14.3975 | 6.2604  | 0.2711  |
| H59 | 2.8830  | 1.6992  | -0.5750 | H2  | 13.6935 | 6.4547  | 0.1563  |
| H60 | -5.6271 | -3.2888 | -1.3307 | end |         |         |         |
| H61 | -2.9633 | -0.8166 | 1.8710  | H1  | 3.1378  | 4.2518  | 1.2883  |
| H62 | -2.5726 | -5.1666 | -3.4921 | H2  | 2.4118  | 4.3807  | 1.2551  |
| H63 | 2.2448  | -1.0097 | 2.6695  | end |         |         |         |
| H64 | -2.2335 | 0.9406  | -2.7005 | H1  | 3.7638  | 1.7686  | 3.8531  |
| H65 | 2.8414  | 0.7450  | -1.8511 | H2  | 3.6409  | 2.4135  | 3.5155  |
| H66 | 5.7320  | 2.3044  | -2.7023 | end |         |         |         |
| H67 | 0.8515  | -4.7398 | 0.0053  | H1  | 7.6721  | 10.3083 | 0.0774  |
| H68 | -5.6906 | -3.3228 | 1.6225  | H2  | 7.1970  | 9.7418  | 0.0921  |
| end |         |         |         | end |         |         |         |
| H1  | 8.7997  | 4.8978  | 1.7103  | H1  | 5.3505  | 3.9698  | 8.2938  |
| H2  | 9.0555  | 5.5648  | 1.4972  | H2  | 6.0587  | 3.8365  | 8.4623  |
| end |         |         |         | end |         |         |         |
| H1  | 13.2534 | 8.3644  | 7.2794  | H1  | 10.1036 | 8.5719  | 9.3971  |
| H2  | 13.1838 | 8.7428  | 6.6401  | H2  | 10.6520 | 8.9133  | 9.7598  |
| end |         |         |         | end |         |         |         |
| H1  | 13.7317 | 2.1398  | 4.5293  | H1  | 13.0381 | 4.4801  | 9.5779  |
| H2  | 13.2755 | 2.3938  | 5.0541  | H2  | 12.4263 | 4.5118  | 9.1623  |
| end |         |         |         | end |         |         |         |
| H1  | 15.4604 | 2.3197  | 5.7843  | H1  | 11.3486 | 12.1285 | 10.1103 |
| H2  | 15.6652 | 1.9319  | 6.3795  | H2  | 11.2191 | 12.5194 | 9.4976  |
| end |         |         |         | end |         |         |         |
| H1  | 11.2971 | 0.8337  | 0.6617  | H1  | 8.3395  | 7.7487  | 8.9048  |
| H2  | 11.3308 | 0.8453  | 1.4007  | H2  | 8.5423  | 7.8272  | 8.1978  |
| end |         |         |         | end |         |         |         |
| H1  | 8.8781  | 10.2438 | 4.5641  | H1  | 16.4545 | 13.5796 | 8.6762  |
| H2  | 8.9253  | 10.6920 | 5.1520  | H2  | 16.7733 | 13.5846 | 9.3441  |
| end |         |         |         | end |         |         |         |
| H1  | 12.4964 | 8.6468  | 0.3381  | end |         |         |         |
| H2  | 12.6700 | 9.2022  | -0.1176 |     |         |         |         |

**(26) n=4 & m=2**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.5208 | -4.7474 | 0.0607  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.3688 | 0.3525  | -3.6584 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.0159  | -1.8245 | -3.0932 |
| O1      | 6.7338       | 3.8498  | -0.0526 |         | H12 | -3.7615 | -2.1902 | 1.8864  |
| O2      | 2.9831       | 1.6404  | 1.1065  |         | H13 | 0.0205  | 2.3862  | -2.8639 |
| O3      | 5.1699       | 2.9861  | -2.1542 |         | H14 | 6.1005  | 0.4325  | 3.6367  |
| O4      | 2.8249       | 1.7443  | -1.5652 |         | H15 | 4.9691  | -1.3862 | 4.6681  |
| O5      | 3.1033       | -0.8741 | 2.1721  |         | H16 | -0.0540 | 3.4613  | 0.7817  |
| O6      | -0.5928      | 1.1435  | 3.6550  |         | H17 | 2.9026  | -1.4204 | -1.5062 |
| O7      | 0.8148       | 2.8939  | 2.1437  |         | H18 | 1.1991  | 5.8738  | 3.2568  |
| O8      | 4.2645       | 4.9899  | 3.4928  |         | H19 | 4.6104  | 4.2475  | 2.9175  |
| O9      | 1.5112       | 5.0232  | 3.6893  |         | H20 | 2.2616  | -2.9834 | -0.0330 |
| O10     | 2.8506       | -0.8764 | -2.3439 |         | H21 | 4.3292  | 2.4991  | -1.9105 |
| O11     | 6.5752       | 1.3090  | 3.5870  |         | H22 | 0.2246  | -1.9062 | 3.1339  |
| O12     | -0.5816      | 3.8293  | 0.0130  |         | H23 | -0.6673 | 1.5368  | 4.5726  |
| O13     | 0.5609       | 3.0326  | -2.3233 |         | H24 | 7.6029  | 3.3452  | -0.0467 |
| O14     | -5.1875      | -3.0173 | 2.4414  |         | H25 | 1.4100  | -1.0672 | -3.1930 |
| O15     | -2.8994      | -1.6784 | -1.1348 |         | H26 | -1.1387 | 1.3511  | -4.6628 |
| O16     | -6.4417      | -3.7499 | 0.0870  |         | H27 | 0.2706  | -0.3697 | 3.6046  |
| O17     | -5.1063      | -2.9303 | -2.1697 |         | H28 | -1.5132 | 1.0600  | 3.2749  |
| O18     | -2.9938      | 0.8538  | -2.0772 |         | H29 | -1.5202 | -2.5432 | -1.6530 |
| O19     | 0.5148       | -1.1476 | -3.6352 |         | H30 | 0.2796  | 2.2593  | 2.7048  |
| O20     | -0.7138      | -2.9854 | -2.0494 |         | H31 | -0.1465 | 3.5136  | -0.8339 |
| O21     | -0.7351      | -3.0786 | 2.3247  |         | H32 | -1.5527 | -2.5771 | 2.0174  |
| O22     | 0.7629       | -3.7608 | 0.0966  |         | H33 | -2.9602 | -0.0904 | -1.7424 |
| O23     | -6.6752      | -1.2339 | -3.5552 |         | H34 | -4.7789 | -5.9334 | -3.1708 |
| O24     | -2.9618      | 0.8395  | 2.3587  |         | H35 | -2.9260 | 1.4185  | 1.5453  |
| O25     | -1.5927      | -5.1139 | -3.4593 |         | H36 | -2.0375 | 2.9642  | 0.0863  |
| O26     | -4.3518      | -5.1135 | -3.5597 |         | H37 | 3.0740  | 0.0531  | 1.8012  |
| O27     | 5.1902       | 2.9667  | 1.9375  |         | H38 | -6.1763 | -0.3683 | -3.5285 |
| O28     | 0.8007       | -1.2166 | 3.5734  |         | H39 | 5.8145  | 3.2862  | 1.2167  |
| O29     | 3.1020       | -2.4409 | -0.0967 |         | H40 | 5.7032  | 2.3612  | 2.5496  |
| O30     | 5.2846       | -1.1372 | 3.7528  |         | H41 | -4.4408 | 1.0157  | -2.9505 |
| O31     | -2.9226      | -1.7444 | 1.5750  |         | H42 | -7.3598 | -3.3514 | 0.0114  |
| O32     | -0.8829      | 1.2085  | -3.7017 |         | H43 | 2.5062  | 5.0210  | 3.6117  |
| O33     | -5.2838      | 1.1308  | -3.4835 |         | H44 | 3.8074  | 2.1328  | 1.3865  |
| O34     | -2.8876      | 2.4308  | 0.1088  |         | H45 | -5.7455 | -2.3667 | 2.9651  |
| H1      | -4.6681      | -5.0089 | -4.5009 |         | H46 | 1.3904  | 2.5417  | -2.0515 |
| H2      | -3.8196      | 1.0425  | 2.8379  |         | H47 | 6.5802  | 1.6754  | 4.5233  |
| H3      | -2.8783      | 1.8495  | -0.7086 |         | H48 | 4.4604  | -1.0184 | 3.1966  |
| H4      | -1.0531      | -3.7870 | -2.5483 |         | H49 | -4.8430 | -3.7508 | -2.6870 |
| H5      | -6.1194      | -1.8852 | -3.0288 |         | H50 | 3.7160  | -1.0398 | -2.8257 |
| H6      | 0.2274       | -3.4705 | -0.6995 |         | H51 | 1.0644  | 3.6631  | 2.7323  |
| H7      | -0.2222      | -3.3506 | 1.5123  |         | H52 | 4.6152  | 5.8324  | 3.0763  |
| H8      | -4.9859      | 1.3398  | -4.4163 |         | H53 | 3.0965  | -1.8541 | 0.7115  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.2877 | -5.9624 | -3.0186 | end |         |         |         |
| H55 | -2.9521 | -1.7202 | -0.1353 | H1  | 12.4145 | 8.5955  | 0.1634  |
| H56 | -3.7056 | -2.1525 | -1.4874 | H2  | 12.7123 | 9.2480  | -0.0160 |
| H57 | 6.1957  | 3.5247  | -0.8281 | end |         |         |         |
| H58 | 2.2074  | 2.1193  | 1.5232  | H1  | 11.3269 | 10.8015 | 1.5314  |
| H59 | 2.8615  | 1.7190  | -0.5625 | H2  | 11.5940 | 10.1132 | 1.5091  |
| H60 | -5.6095 | -3.2468 | -1.3668 | end |         |         |         |
| H61 | -2.9548 | -0.7907 | 1.8833  | H1  | 14.3784 | 6.2960  | 0.2882  |
| H62 | -2.5896 | -5.1414 | -3.5089 | H2  | 13.6864 | 6.5008  | 0.1263  |
| H63 | 2.2345  | -1.0028 | 2.6528  | end |         |         |         |
| H64 | -2.2280 | 0.9596  | -2.7194 | H1  | 3.1151  | 4.2701  | 1.2661  |
| H65 | 2.8357  | 0.7895  | -1.8597 | H2  | 2.3975  | 4.4416  | 1.2648  |
| H66 | 5.7133  | 2.3417  | -2.6958 | end |         |         |         |
| H67 | 0.8341  | -4.7574 | 0.0221  | H1  | 3.7772  | 1.6958  | 3.8872  |
| H68 | -5.6978 | -3.2709 | 1.6232  | H2  | 3.7062  | 2.3308  | 3.5175  |
| end |         |         |         | end |         |         |         |
| H1  | -4.8144 | 5.1350  | 3.2113  | H1  | 7.6634  | 10.3390 | 0.0663  |
| H2  | -4.4208 | 4.9338  | 2.6108  | H2  | 7.2059  | 9.7588  | 0.0433  |
| end |         |         |         | end |         |         |         |
| H1  | 9.5481  | 5.7329  | 5.4996  | H1  | 5.3084  | 3.9973  | 8.3280  |
| H2  | 9.1099  | 5.4399  | 4.9710  | H2  | 6.0203  | 3.8118  | 8.4102  |
| end |         |         |         | end |         |         |         |
| H1  | 15.4351 | 10.1459 | 6.9881  | H1  | 10.0896 | 8.5836  | 9.3804  |
| H2  | 16.0486 | 9.7294  | 6.9076  | H2  | 10.6198 | 8.9275  | 9.7676  |
| end |         |         |         | end |         |         |         |
| H1  | 13.1256 | 7.8390  | 5.6124  | H1  | 13.0336 | 4.6186  | 9.5801  |
| H2  | 13.1732 | 7.1081  | 5.4719  | H2  | 12.4661 | 4.3810  | 9.1684  |
| end |         |         |         | end |         |         |         |
| H1  | 13.7418 | 2.2265  | 4.4993  | H1  | 11.4044 | 12.1361 | 10.1398 |
| H2  | 13.3341 | 2.5373  | 5.0336  | H2  | 11.2129 | 12.5335 | 9.5478  |
| end |         |         |         | end |         |         |         |
| H1  | 15.3898 | 2.2948  | 5.8033  | H1  | 8.3023  | 7.8178  | 8.9085  |
| H2  | 15.7293 | 1.9238  | 6.3449  | H2  | 8.5270  | 7.8081  | 8.2038  |
| end |         |         |         | end |         |         |         |
| H1  | 11.4347 | 0.8531  | 0.6481  | H1  | 16.4459 | 13.6094 | 8.6636  |
| H2  | 11.2562 | 0.9051  | 1.3637  | H2  | 16.7507 | 13.6038 | 9.3387  |
| end |         |         |         | end |         |         |         |
| H1  | 8.7664  | 10.2630 | 4.5834  | end |         |         |         |
| H2  | 8.8037  | 10.7040 | 5.1769  | end |         |         |         |

**(27) n=4 & m=3**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.5178 | -4.8012 | 0.0935  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.3550 | 0.3171  | -3.6406 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.0114  | -1.8568 | -3.0901 |
| O1      | 6.7613       | 3.8536  | -0.0685 |         | H12 | -3.7584 | -2.2303 | 1.8840  |
| O2      | 3.0128       | 1.6008  | 1.1411  |         | H13 | 0.0494  | 2.3568  | -2.8456 |
| O3      | 5.1830       | 2.9366  | -2.1239 |         | H14 | 6.0954  | 0.3762  | 3.6555  |
| O4      | 2.8433       | 1.6978  | -1.5330 |         | H15 | 4.9730  | -1.4405 | 4.7055  |
| O5      | 3.0969       | -0.9013 | 2.2139  |         | H16 | -0.0335 | 3.4238  | 0.8054  |
| O6      | -0.6113      | 1.1157  | 3.6716  |         | H17 | 2.9031  | -1.4568 | -1.4810 |
| O7      | 0.8390       | 2.8615  | 2.1683  |         | H18 | 1.2233  | 5.8278  | 3.2725  |
| O8      | 4.2979       | 4.9652  | 3.5081  |         | H19 | 4.6514  | 4.2272  | 2.9304  |
| O9      | 1.5403       | 4.9786  | 3.7012  |         | H20 | 2.2773  | -3.0113 | -0.0102 |
| O10     | 2.8411       | -0.9070 | -2.3129 |         | H21 | 4.3393  | 2.4488  | -1.8886 |
| O11     | 6.5595       | 1.2564  | 3.5928  |         | H22 | 0.2280  | -1.9183 | 3.1753  |
| O12     | -0.5572      | 3.7893  | 0.0333  |         | H23 | -0.6882 | 1.5134  | 4.5859  |
| O13     | 0.5898       | 3.0009  | -2.3034 |         | H24 | 7.6279  | 3.3453  | -0.0475 |
| O14     | -5.1675      | -3.0534 | 2.4556  |         | H25 | 1.4063  | -1.1019 | -3.1797 |
| O15     | -2.9185      | -1.7238 | -1.1439 |         | H26 | -1.1171 | 1.3238  | -4.6445 |
| O16     | -6.4369      | -3.8032 | 0.1299  |         | H27 | 0.2665  | -0.3848 | 3.6480  |
| O17     | -5.1418      | -2.9628 | -2.1392 |         | H28 | -1.5308 | 1.0232  | 3.2913  |
| O18     | -2.9787      | 0.8334  | -2.0473 |         | H29 | -1.5259 | -2.5840 | -1.6559 |
| O19     | 0.5163       | -1.1834 | -3.6313 |         | H30 | 0.2969  | 2.2323  | 2.7259  |
| O20     | -0.7109      | -3.0151 | -2.0429 |         | H31 | -0.1212 | 3.4717  | -0.8122 |
| O21     | -0.7113      | -3.0908 | 2.3383  |         | H32 | -1.5344 | -2.6027 | 2.0305  |
| O22     | 0.7800       | -3.7561 | 0.0953  |         | H33 | -2.9559 | -0.1160 | -1.7315 |
| O23     | -6.6845      | -1.2427 | -3.5356 |         | H34 | -4.7660 | -5.9531 | -3.1417 |
| O24     | -2.9802      | 0.8016  | 2.3705  |         | H35 | -2.9374 | 1.3975  | 1.5701  |
| O25     | -1.5874      | -5.1587 | -3.4224 |         | H36 | -2.0264 | 2.9477  | 0.1191  |
| O26     | -4.3472      | -5.1265 | -3.5264 |         | H37 | 3.0603  | 0.0245  | 1.8390  |
| O27     | 5.2211       | 2.9611  | 1.9431  |         | H38 | -6.1790 | -0.3797 | -3.5085 |
| O28     | 0.8020       | -1.2286 | 3.6169  |         | H39 | 5.8464  | 3.2737  | 1.2235  |
| O29     | 3.1263       | -2.4784 | -0.0600 |         | H40 | 5.7170  | 2.3240  | 2.5347  |
| O30     | 5.2933       | -1.2053 | 3.7876  |         | H41 | -4.4299 | 0.9871  | -2.9328 |
| O31     | -2.9209      | -1.7792 | 1.5751  |         | H42 | -7.3516 | -3.3975 | 0.0465  |
| O32     | -0.8632      | 1.1772  | -3.6832 |         | H43 | 2.5349  | 4.9861  | 3.6245  |
| O33     | -5.2682      | 1.1017  | -3.4703 |         | H44 | 3.8381  | 2.1007  | 1.4050  |
| O34     | -2.8784      | 2.4179  | 0.1391  |         | H45 | -5.7319 | -2.4073 | 2.9791  |
| H1      | -4.6688      | -5.0208 | -4.4662 |         | H46 | 1.4181  | 2.5083  | -2.0321 |
| H2      | -3.8365      | 1.0001  | 2.8555  |         | H47 | 6.5799  | 1.6297  | 4.5252  |
| H3      | -2.8640      | 1.8312  | -0.6731 |         | H48 | 4.4718  | -1.0883 | 3.2301  |
| H4      | -1.0339      | -3.8265 | -2.5368 |         | H49 | -4.8658 | -3.7822 | -2.6533 |
| H5      | -6.1389      | -1.8962 | -3.0043 |         | H50 | 3.7014  | -1.0667 | -2.8032 |
| H6      | 0.2405       | -3.4693 | -0.6999 |         | H51 | 1.0880  | 3.6339  | 2.7563  |
| H7      | -0.1961      | -3.3516 | 1.5245  |         | H52 | 4.6464  | 5.8118  | 3.1001  |
| H8      | -4.9621      | 1.3093  | -4.4012 |         | H53 | 3.1124  | -1.8923 | 0.7473  |



|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.2891 | -6.0037 | -2.9702 | end |         |         |         |
| H55 | -2.9569 | -1.7678 | -0.1450 | H1  | 8.8780  | 10.2434 | 4.5830  |
| H56 | -3.7321 | -2.1946 | -1.4854 | H2  | 8.9189  | 10.6880 | 5.1741  |
| H57 | 6.2120  | 3.4982  | -0.8225 | end |         |         |         |
| H58 | 2.2394  | 2.0879  | 1.5514  | H1  | 12.4726 | 8.6170  | 0.3119  |
| H59 | 2.8814  | 1.6736  | -0.5312 | H2  | 12.7200 | 9.1938  | -0.0780 |
| H60 | -5.6214 | -3.2802 | -1.3222 | end |         |         |         |
| H61 | -2.9637 | -0.8244 | 1.8789  | H1  | 11.1165 | 10.5192 | 1.6727  |
| H62 | -2.5839 | -5.1733 | -3.4749 | H2  | 11.7773 | 10.3436 | 1.3972  |
| H63 | 2.2311  | -1.0284 | 2.7029  | end |         |         |         |
| H64 | -2.2170 | 0.9390  | -2.6929 | H1  | 14.4000 | 6.2598  | 0.2801  |
| H65 | 2.8477  | 0.7410  | -1.8267 | H2  | 13.6957 | 6.4547  | 0.1676  |
| H66 | 5.7263  | 2.3001  | -2.6763 | end |         |         |         |
| H67 | 0.8627  | -4.7506 | 0.0172  | H1  | 3.1435  | 4.2645  | 1.3044  |
| H68 | -5.6839 | -3.3258 | 1.6464  | H2  | 2.4112  | 4.3476  | 1.2616  |
| end |         |         |         | end |         |         |         |
| H1  | 8.7442  | 4.9184  | 1.7220  | H1  | 3.7647  | 1.7634  | 3.8806  |
| H2  | 9.1557  | 5.4829  | 1.4632  | H2  | 3.6711  | 2.4203  | 3.5567  |
| end |         |         |         | end |         |         |         |
| H1  | 9.6749  | 5.6810  | 5.4958  | H1  | 7.6623  | 10.2898 | 0.1050  |
| H2  | 9.1957  | 5.2705  | 5.0970  | H2  | 7.1931  | 9.7184  | 0.1037  |
| end |         |         |         | end |         |         |         |
| H1  | 7.0942  | 4.1709  | 3.9844  | H1  | 5.3580  | 3.9552  | 8.3025  |
| H2  | 7.7178  | 4.1934  | 3.5770  | H2  | 6.0651  | 3.7981  | 8.4548  |
| end |         |         |         | end |         |         |         |
| H1  | 15.2994 | 8.8173  | 4.8136  | H1  | 10.1083 | 8.5816  | 9.4238  |
| H2  | 15.1194 | 8.6532  | 4.1079  | H2  | 10.6618 | 8.9177  | 9.7837  |
| end |         |         |         | end |         |         |         |
| H1  | 15.4826 | 9.8456  | 7.0269  | H1  | 13.0707 | 4.5088  | 9.6339  |
| H2  | 16.2226 | 9.8271  | 7.1117  | H2  | 12.4584 | 4.4503  | 9.2216  |
| end |         |         |         | end |         |         |         |
| H1  | 13.1816 | 8.3994  | 7.2859  | H1  | 11.3677 | 12.1120 | 10.1247 |
| H2  | 13.2630 | 8.6234  | 6.5789  | H2  | 11.1932 | 12.5114 | 9.5290  |
| end |         |         |         | end |         |         |         |
| H1  | 13.7344 | 2.1469  | 4.5432  | H1  | 8.3460  | 7.7597  | 8.9174  |
| H2  | 13.2803 | 2.3806  | 5.0790  | H2  | 8.5600  | 7.8157  | 8.2117  |
| end |         |         |         | end |         |         |         |
| H1  | 15.4697 | 2.3107  | 5.8014  | H1  | 16.4978 | 13.5933 | 8.6502  |
| H2  | 15.6707 | 1.9322  | 6.4035  | H2  | 16.7986 | 13.5555 | 9.3256  |
| end |         |         |         | end |         |         |         |
| H1  | 11.3605 | 0.8417  | 0.6547  | end |         |         |         |
| H2  | 11.2949 | 0.8646  | 1.3913  | end |         |         |         |

**(28) n=4 & m=4**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.5627 | -4.7844 | 0.0455  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.3941 | 0.3352  | -3.6380 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | -0.0135 | -1.8326 | -3.0717 |
| O1      | 6.6992       | 3.8388  | -0.0004 |         | H12 | -3.8354 | -2.1933 | 1.8694  |
| O2      | 2.9503       | 1.6366  | 1.1005  |         | H13 | -0.0286 | 2.3691  | -2.8544 |
| O3      | 5.1705       | 2.9767  | -2.1337 |         | H14 | 6.0439  | 0.3832  | 3.6723  |
| O4      | 2.7956       | 1.7533  | -1.5817 |         | H15 | 4.9032  | -1.4137 | 4.6741  |
| O5      | 3.0496       | -0.8905 | 2.1619  |         | H16 | -0.0950 | 3.4480  | 0.7823  |
| O6      | -0.6403      | 1.1496  | 3.6579  |         | H17 | 2.8629  | -1.4275 | -1.5248 |
| O7      | 0.7689       | 2.8736  | 2.1215  |         | H18 | 1.1658  | 5.8712  | 3.2303  |
| O8      | 4.2308       | 4.9796  | 3.5158  |         | H19 | 4.5634  | 4.2318  | 2.9389  |
| O9      | 1.4821       | 5.0220  | 3.6602  |         | H20 | 2.2367  | -3.0118 | -0.0424 |
| O10     | 2.8225       | -0.8678 | -2.3521 |         | H21 | 4.3256  | 2.4907  | -1.9050 |
| O11     | 6.5276       | 1.2551  | 3.6147  |         | H22 | 0.1657  | -1.9005 | 3.1504  |
| O12     | -0.6357      | 3.8063  | 0.0153  |         | H23 | -0.7224 | 1.5367  | 4.5773  |
| O13     | 0.5100       | 3.0185  | -2.3134 |         | H24 | 7.5723  | 3.3427  | 0.0100  |
| O14     | -5.2524      | -3.0207 | 2.4140  |         | H25 | 1.3812  | -1.0738 | -3.1921 |
| O15     | -2.9450      | -1.6867 | -1.1432 |         | H26 | -1.1591 | 1.3397  | -4.6416 |
| O16     | -6.4759      | -3.7866 | 0.0640  |         | H27 | 0.2030  | -0.3635 | 3.6212  |
| O17     | -5.1131      | -2.9791 | -2.1907 |         | H28 | -1.5569 | 1.0465  | 3.2749  |
| O18     | -3.0388      | 0.8529  | -2.0829 |         | H29 | -1.5564 | -2.5518 | -1.6372 |
| O19     | 0.4800       | -1.1601 | -3.6222 |         | H30 | 0.2244  | 2.2548  | 2.6921  |
| O20     | -0.7483      | -2.9999 | -2.0221 |         | H31 | -0.2027 | 3.4952  | -0.8354 |
| O21     | -0.7832      | -3.0915 | 2.3226  |         | H32 | -1.6006 | -2.5944 | 2.0149  |
| O22     | 0.7218       | -3.7728 | 0.1198  |         | H33 | -3.0112 | -0.0907 | -1.7486 |
| O23     | -6.6979      | -1.2508 | -3.5506 |         | H34 | -4.8261 | -5.9734 | -3.1788 |
| O24     | -3.0220      | 0.8194  | 2.3827  |         | H35 | -2.9865 | 1.4066  | 1.5752  |
| O25     | -1.6270      | -5.1351 | -3.4396 |         | H36 | -2.0788 | 2.9394  | 0.1061  |
| O26     | -4.3841      | -5.1641 | -3.5756 |         | H37 | 3.0259  | 0.0339  | 1.7862  |
| O27     | 5.1611       | 2.9346  | 1.9831  |         | H38 | -6.1991 | -0.3847 | -3.5321 |
| O28     | 0.7428       | -1.2045 | 3.5744  |         | H39 | 5.7831  | 3.2564  | 1.2615  |
| O29     | 3.0711       | -2.4638 | -0.1226 |         | H40 | 5.6719  | 2.3204  | 2.5892  |
| O30     | 5.2156       | -1.1660 | 3.7577  |         | H41 | -4.4625 | 1.0009  | -2.9699 |
| O31     | -2.9889      | -1.7538 | 1.5668  |         | H42 | -7.3917 | -3.3837 | -0.0151 |
| O32     | -0.9131      | 1.1894  | -3.6794 |         | H43 | 2.4795  | 5.0269  | 3.6056  |
| O33     | -5.3138      | 1.1120  | -3.4929 |         | H44 | 3.7752  | 2.1112  | 1.4093  |
| O34     | -2.9236      | 2.3979  | 0.1363  |         | H45 | -5.8137 | -2.3839 | 2.9510  |
| H1      | -4.7125      | -5.0482 | -4.5109 |         | H46 | 1.3409  | 2.5291  | -2.0440 |
| H2      | -3.8841      | 1.0044  | 2.8636  |         | H47 | 6.5425  | 1.6360  | 4.5453  |
| H3      | -2.9312      | 1.8342  | -0.6922 |         | H48 | 4.3932  | -1.0399 | 3.2000  |
| H4      | -1.0847      | -3.7973 | -2.5277 |         | H49 | -4.8501 | -3.8012 | -2.7084 |
| H5      | -6.1347      | -1.9031 | -3.0383 |         | H50 | 3.6833  | -1.0450 | -2.8353 |
| H6      | 0.1760       | -3.4923 | -0.6735 |         | H51 | 1.0298  | 3.6471  | 2.6968  |
| H7      | -0.2644      | -3.3577 | 1.5110  |         | H52 | 4.5764  | 5.8192  | 3.0908  |
| H8      | -5.0305      | 1.3308  | -4.4253 |         | H53 | 3.0680  | -1.8783 | 0.6850  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.3069 | -5.9742 | -2.9914 | end |         |         |         |
| H55 | -3.0084 | -1.7220 | -0.1444 | H1  | 11.1870 | 0.9306  | 0.7633  |
| H56 | -3.7403 | -2.1752 | -1.5019 | H2  | 11.4436 | 0.6857  | 1.4097  |
| H57 | 6.1775  | 3.5154  | -0.7865 | end |         |         |         |
| H58 | 2.1694  | 2.1047  | 1.5214  | H1  | 8.6738  | 10.2350 | 4.6176  |
| H59 | 2.8329  | 1.7249  | -0.5800 | H2  | 8.7835  | 10.6774 | 5.2010  |
| H60 | -5.6149 | -3.2943 | -1.3876 | end |         |         |         |
| H61 | -3.0125 | -0.8027 | 1.8844  | H1  | 12.3475 | 8.5468  | 0.0987  |
| H62 | -2.6230 | -5.1779 | -3.4896 | H2  | 12.6025 | 9.2105  | -0.1059 |
| H63 | 2.1784  | -1.0111 | 2.6397  | end |         |         |         |
| H64 | -2.2651 | 0.9536  | -2.7180 | H1  | 11.3629 | 10.7477 | 1.5664  |
| H65 | 2.8089  | 0.7973  | -1.8747 | H2  | 11.5707 | 10.0435 | 1.4836  |
| H66 | 5.7049  | 2.3391  | -2.6916 | end |         |         |         |
| H67 | 0.7988  | -4.7703 | 0.0559  | H1  | 14.3723 | 6.3224  | 0.2640  |
| H68 | -5.7684 | -3.2824 | 1.6017  | H2  | 13.6472 | 6.4467  | 0.1876  |
| end |         |         |         | end |         |         |         |
| H1  | -4.8850 | 6.0974  | 3.7588  | H1  | 2.9709  | 4.1032  | 1.1338  |
| H2  | -4.2097 | 6.1326  | 4.0745  | H2  | 2.4984  | 4.5796  | 1.4416  |
| end |         |         |         | end |         |         |         |
| H1  | 9.2996  | 5.0416  | 1.3313  | H1  | 3.7051  | 1.6062  | 3.8505  |
| H2  | 8.7229  | 5.2100  | 1.7734  | H2  | 3.6958  | 2.2808  | 3.5518  |
| end |         |         |         | end |         |         |         |
| H1  | 9.8716  | 5.8358  | 5.3411  | H1  | 7.6193  | 10.3325 | 0.0476  |
| H2  | 9.6805  | 5.2921  | 4.8684  | H2  | 7.1861  | 9.7348  | 0.0033  |
| end |         |         |         | end |         |         |         |
| H1  | 8.6439  | 3.5311  | 4.2185  | H1  | 5.2166  | 3.9927  | 8.3418  |
| H2  | 8.8591  | 2.9366  | 3.8219  | H2  | 5.9218  | 3.8735  | 8.5329  |
| end |         |         |         | end |         |         |         |
| H1  | 15.7140 | 8.9890  | 4.6822  | H1  | 10.0487 | 8.5857  | 9.3469  |
| H2  | 15.3421 | 8.7482  | 4.0824  | H2  | 10.5790 | 8.8762  | 9.7751  |
| end |         |         |         | end |         |         |         |
| H1  | 15.7479 | 9.6632  | 6.8416  | H1  | 12.9949 | 4.5224  | 9.6811  |
| H2  | 16.4756 | 9.7933  | 6.9407  | H2  | 12.4917 | 4.4032  | 9.1518  |
| end |         |         |         | end |         |         |         |
| H1  | 13.4208 | 9.3613  | 7.4748  | H1  | 11.3752 | 12.1016 | 10.1281 |
| H2  | 13.6085 | 8.8325  | 6.9854  | H2  | 11.1764 | 12.5317 | 9.5615  |
| end |         |         |         | end |         |         |         |
| H1  | 12.9645 | 7.7179  | 5.4125  | H1  | 8.2031  | 7.9031  | 8.9288  |
| H2  | 13.1313 | 7.0231  | 5.2040  | H2  | 8.4509  | 7.7048  | 8.2603  |
| end |         |         |         | end |         |         |         |
| H1  | 13.7027 | 2.1968  | 4.4868  | H1  | 16.3937 | 13.6221 | 8.6788  |
| H2  | 13.3021 | 2.5458  | 5.0025  | H2  | 16.7102 | 13.7093 | 9.3429  |
| end |         |         |         | end |         |         |         |
| H1  | 15.4183 | 2.2553  | 5.7593  | end |         |         |         |
| H2  | 15.6523 | 1.9478  | 6.3898  | end |         |         |         |

**(29) n=4 & m=5**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.5715 | -4.7830 | 0.0125  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.3601 | 0.3146  | -3.6888 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.0180  | -1.8486 | -3.1175 |
| O1      | 6.7547       | 3.8870  | -0.0272 |         | H12 | -3.7950 | -2.2064 | 1.8798  |
| O2      | 2.9452       | 1.6490  | 1.1126  |         | H13 | 0.0312  | 2.3675  | -2.8984 |
| O3      | 5.2084       | 2.9615  | -2.1065 |         | H14 | 6.0415  | 0.3846  | 3.6122  |
| O4      | 2.8211       | 1.7730  | -1.5619 |         | H15 | 4.9528  | -1.4118 | 4.6602  |
| O5      | 3.0780       | -0.8608 | 2.1613  |         | H16 | -0.0623 | 3.4528  | 0.7434  |
| O6      | -0.6559      | 1.1457  | 3.6387  |         | H17 | 2.8584  | -1.4066 | -1.5546 |
| O7      | 0.7741       | 2.9036  | 2.1363  |         | H18 | 1.1501  | 5.8731  | 3.2478  |
| O8      | 4.2120       | 4.9660  | 3.4945  |         | H19 | 4.5592  | 4.2426  | 2.8971  |
| O9      | 1.4640       | 5.0302  | 3.6904  |         | H20 | 2.2540  | -2.9773 | -0.0443 |
| O10     | 2.8173       | -0.8396 | -2.3767 |         | H21 | 4.3544  | 2.4932  | -1.8726 |
| O11     | 6.5237       | 1.2575  | 3.5468  |         | H22 | 0.2018  | -1.8985 | 3.1813  |
| O12     | -0.5846      | 3.8138  | -0.0310 |         | H23 | -0.7354 | 1.5415  | 4.5541  |
| O13     | 0.5607       | 3.0264  | -2.3628 |         | H24 | 7.6243  | 3.3757  | -0.0111 |
| O14     | -5.2507      | -3.0203 | 2.4035  |         | H25 | 1.4057  | -1.0863 | -3.2490 |
| O15     | -2.8969      | -1.6969 | -1.1321 |         | H26 | -1.1565 | 1.3183  | -4.6694 |
| O16     | -6.4852      | -3.7857 | 0.0540  |         | H27 | 0.2314  | -0.3521 | 3.6106  |
| O17     | -5.1192      | -2.9415 | -2.1660 |         | H28 | -1.5722 | 1.0481  | 3.2569  |
| O18     | -2.9790      | 0.8493  | -2.0670 |         | H29 | -1.4971 | -2.5439 | -1.6383 |
| O19     | 0.5085       | -1.1867 | -3.6849 |         | H30 | 0.2318  | 2.2668  | 2.6855  |
| O20     | -0.6846      | -2.9839 | -2.0225 |         | H31 | -0.1511 | 3.4975  | -0.8786 |
| O21     | -0.7670      | -3.0780 | 2.3893  |         | H32 | -1.5793 | -2.5806 | 2.0670  |
| O22     | 0.7503       | -3.7261 | 0.1674  |         | H33 | -2.9457 | -0.0941 | -1.7346 |
| O23     | -6.6947      | -1.2379 | -3.5669 |         | H34 | -4.7713 | -5.9300 | -3.2023 |
| O24     | -3.0127      | 0.8345  | 2.3008  |         | H35 | -2.9767 | 1.4368  | 1.5013  |
| O25     | -1.5641      | -5.1242 | -3.4323 |         | H36 | -2.0500 | 2.9869  | 0.0731  |
| O26     | -4.3201      | -5.1193 | -3.5828 |         | H37 | 3.0458  | 0.0698  | 1.7979  |
| O27     | 5.1786       | 2.9842  | 1.9240  |         | H38 | -6.2005 | -0.3702 | -3.5240 |
| O28     | 0.7774       | -1.1887 | 3.5883  |         | H39 | 5.8184  | 3.3073  | 1.2187  |
| O29     | 3.0877       | -2.4285 | -0.1393 |         | H40 | 5.6722  | 2.3615  | 2.5323  |
| O30     | 5.2360       | -1.1599 | 3.7359  |         | H41 | -4.4161 | 0.9991  | -2.9404 |
| O31     | -2.9530      | -1.7640 | 1.5758  |         | H42 | -7.3951 | -3.3711 | -0.0289 |
| O32     | -0.8745      | 1.1711  | -3.7172 |         | H43 | 2.4592  | 5.0282  | 3.6150  |
| O33     | -5.2703      | 1.1165  | -3.4556 |         | H44 | 3.7730  | 2.1347  | 1.3869  |
| O34     | -2.9042      | 2.4610  | 0.1119  |         | H45 | -5.8134 | -2.3727 | 2.9276  |
| H1      | -4.6590      | -4.9833 | -4.5139 |         | H46 | 1.3910  | 2.5459  | -2.0735 |
| H2      | -3.8711      | 1.0181  | 2.7854  |         | H47 | 6.5519  | 1.6339  | 4.4789  |
| H3      | -2.9069      | 1.8713  | -0.6974 |         | H48 | 4.3956  | -1.0372 | 3.2037  |
| H4      | -1.0170      | -3.7905 | -2.5156 |         | H49 | -4.8328 | -3.7541 | -2.6792 |
| H5      | -6.1392      | -1.8877 | -3.0432 |         | H50 | 3.6747  | -1.0173 | -2.8649 |
| H6      | 0.2269       | -3.4500 | -0.6412 |         | H51 | 1.0148  | 3.6706  | 2.7313  |
| H7      | -0.2406      | -3.3407 | 1.5827  |         | H52 | 4.5688  | 5.8217  | 3.1113  |
| H8      | -4.9969      | 1.3401  | -4.3910 |         | H53 | 3.0902  | -1.8390 | 0.6642  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.2581 | -5.9700 | -2.9917 | H1  | 13.7187 | 2.1617  | 4.5210  |
| H55 | -2.9569 | -1.7403 | -0.1327 | H2  | 13.2589 | 2.4545  | 5.0224  |
| H56 | -3.7017 | -2.1693 | -1.4871 | end |         |         |         |
| H57 | 6.2225  | 3.5596  | -0.8052 | H1  | 15.4434 | 2.2684  | 5.7707  |
| H58 | 2.1728  | 2.1346  | 1.5281  | H2  | 15.6765 | 1.9342  | 6.3874  |
| H59 | 2.8379  | 1.7368  | -0.5593 | end |         |         |         |
| H60 | -5.6222 | -3.2670 | -1.3643 | H1  | 11.4834 | 0.8559  | 0.6253  |
| H61 | -2.9934 | -0.8043 | 1.8627  | H2  | 11.1669 | 0.9879  | 1.2806  |
| H62 | -2.5596 | -5.1527 | -3.4857 | end |         |         |         |
| H63 | 2.2104  | -0.9989 | 2.6397  | H1  | 8.8072  | 10.2472 | 4.5589  |
| H64 | -2.2174 | 0.9528  | -2.7140 | H2  | 8.9019  | 10.6850 | 5.1483  |
| H65 | 2.8352  | 0.8221  | -1.8682 | end |         |         |         |
| H66 | 5.7393  | 2.3065  | -2.6513 | H1  | 12.5539 | 8.7615  | 0.4003  |
| H67 | 0.8462  | -4.7193 | 0.0914  | H2  | 12.5837 | 9.1258  | -0.2419 |
| H68 | -5.7572 | -3.2884 | 1.5866  | end |         |         |         |
| end |         |         |         | H1  | 11.2742 | 10.1314 | 1.4372  |
| H1  | -4.4747 | 5.2918  | 3.3207  | H2  | 11.4025 | 10.8577 | 1.4705  |
| H2  | -5.1502 | 4.9840  | 3.3847  | end |         |         |         |
| end |         |         |         | H1  | 14.3477 | 6.3089  | 0.3022  |
| H1  | 9.4539  | 5.2921  | 1.4262  | H2  | 13.6468 | 6.4919  | 0.1536  |
| H2  | 8.8248  | 5.0541  | 1.7472  | end |         |         |         |
| end |         |         |         | H1  | 3.0819  | 4.2486  | 1.2317  |
| H1  | 9.8838  | 5.2361  | 5.6815  | H2  | 2.3751  | 4.4535  | 1.2832  |
| H2  | 9.7430  | 4.6398  | 5.2598  | end |         |         |         |
| end |         |         |         | H1  | 3.7629  | 1.7181  | 3.8219  |
| H1  | 8.8791  | 2.7285  | 3.9047  | H2  | 3.6552  | 2.4090  | 3.5854  |
| H2  | 8.6180  | 3.2326  | 4.3856  | end |         |         |         |
| end |         |         |         | H1  | 7.6420  | 10.3376 | 0.0799  |
| H1  | 15.0370 | 6.8827  | 5.5200  | H2  | 7.2002  | 9.7454  | 0.0571  |
| H2  | 15.7520 | 6.7669  | 5.6901  | end |         |         |         |
| end |         |         |         | H1  | 5.3447  | 3.9694  | 8.2934  |
| H1  | 16.3387 | 8.9233  | 6.1444  | H2  | 6.0433  | 3.7369  | 8.3686  |
| H2  | 16.9497 | 9.3250  | 6.2847  | end |         |         |         |
| end |         |         |         | H1  | 10.0683 | 8.6136  | 9.3932  |
| H1  | 14.4708 | 8.5341  | 8.2510  | H2  | 10.6091 | 8.9435  | 9.7788  |
| H2  | 15.0436 | 8.8667  | 7.9087  | end |         |         |         |
| end |         |         |         | H1  | 12.9798 | 4.3133  | 9.5961  |
| H1  | 13.0704 | 8.0089  | 5.5355  | H2  | 12.5226 | 4.7492  | 9.2102  |
| H2  | 12.8317 | 7.3137  | 5.4229  | end |         |         |         |
| end |         |         |         | H1  | 11.3867 | 12.1395 | 10.1805 |
| H1  | 14.8953 | 10.2301 | 5.3118  | H2  | 11.1817 | 12.5634 | 9.6114  |
| H2  | 14.2503 | 10.5077 | 5.0610  | end |         |         |         |
| end |         |         |         | H1  | 8.2616  | 7.8792  | 8.9016  |
| H1  | 8.7464  | 7.2297  | 4.1893  | H2  | 8.5054  | 7.8141  | 8.2063  |
| H2  | 9.1151  | 6.9916  | 3.5883  | end |         |         |         |
| end |         |         |         | H1  | 16.4282 | 13.5382 | 8.6068  |

|     |         |         |        |     |
|-----|---------|---------|--------|-----|
| H2  | 16.8921 | 13.7673 | 9.1367 | end |
| end |         |         |        |     |

**(30) n=4 & m=6**

|         |              |         |          |         |     |         |         |          |
|---------|--------------|---------|----------|---------|-----|---------|---------|----------|
| PBC=ON  |              |         |          |         | H9  | -6.5419 | -4.8076 | 0.03325  |
| PBC     | 11.8900      | 11.8900 | 11.8900  | 60.0000 | H10 | -0.3867 | 0.3659  | -3.65694 |
| 60.0000 | 60.0000 (P1) |         |          |         | H11 | -0.0249 | -1.7981 | -3.04572 |
| O1      | 6.7570       | 3.8803  | -0.03712 |         | H12 | -3.8248 | -2.1950 | 1.83633  |
| O2      | 3.0973       | 1.6301  | 1.14068  |         | H13 | 0.0318  | 2.4035  | -2.86733 |
| O3      | 5.1943       | 2.9777  | -2.11638 |         | H14 | 6.0522  | 0.3718  | 3.70889  |
| O4      | 2.8283       | 1.8002  | -1.51028 |         | H15 | 4.9921  | -1.4520 | 4.66852  |
| O5      | 3.1663       | -0.9008 | 2.13321  |         | H16 | -0.0118 | 3.4051  | 0.76397  |
| O6      | -0.6693      | 1.1898  | 3.62815  |         | H17 | 2.8622  | -1.3828 | -1.50718 |
| O7      | 0.8838       | 2.7940  | 2.10131  |         | H18 | 1.1701  | 5.7772  | 3.24526  |
| O8      | 4.2340       | 5.0359  | 3.49356  |         | H19 | 4.5917  | 4.2877  | 2.93591  |
| O9      | 1.4959       | 4.9317  | 3.67266  |         | H20 | 2.2518  | -2.9654 | -0.09538 |
| O10     | 2.7947       | -0.7984 | -2.31905 |         | H21 | 4.3531  | 2.4934  | -1.86982 |
| O11     | 6.4947       | 1.2666  | 3.65146  |         | H22 | 0.1979  | -1.8395 | 3.05474  |
| O12     | -0.5671      | 3.7723  | 0.01526  |         | H23 | -0.7636 | 1.5690  | 4.54616  |
| O13     | 0.5733       | 3.0628  | -2.34600 |         | H24 | 7.6267  | 3.3799  | -0.02178 |
| O14     | -5.1940      | -3.0820 | 2.41364  |         | H25 | 1.3662  | -1.0164 | -3.14030 |
| O15     | -2.9693      | -1.6819 | -1.18659 |         | H26 | -1.1512 | 1.3875  | -4.65047 |
| O16     | -6.4591      | -3.8105 | 0.03671  |         | H27 | 0.2454  | -0.3144 | 3.54653  |
| O17     | -5.1552      | -2.9612 | -2.22907 |         | H28 | -1.5831 | 1.0803  | 3.23953  |
| O18     | -3.0191      | 0.8550  | -2.08722 |         | H29 | -1.5927 | -2.5288 | -1.69562 |
| O19     | 0.4732       | -1.1186 | -3.58848 |         | H30 | 0.3008  | 2.2005  | 2.66031  |
| O20     | -0.7778      | -2.9683 | -2.08181 |         | H31 | -0.1479 | 3.4856  | -0.85043 |
| O21     | -0.7910      | -3.0231 | 2.27280  |         | H32 | -1.6070 | -2.5280 | 1.96057  |
| O22     | 0.7355       | -3.7183 | 0.04708  |         | H33 | -2.9865 | -0.0960 | -1.76826 |
| O23     | -6.7513      | -1.1846 | -3.55909 |         | H34 | -4.7579 | -5.9029 | -3.26262 |
| O24     | -3.0671      | 0.8344  | 2.38773  |         | H35 | -3.0234 | 1.4358  | 1.59438  |
| O25     | -1.5875      | -5.1360 | -3.47566 |         | H36 | -2.0304 | 2.9410  | 0.09330  |
| O26     | -4.3264      | -5.0946 | -3.66352 |         | H37 | 3.1862  | 0.0334  | 1.77640  |
| O27     | 5.2504       | 3.0019  | 1.98601  |         | H38 | -6.2320 | -0.3294 | -3.51983 |
| O28     | 0.7870       | -1.1494 | 3.47342  |         | H39 | 5.8718  | 3.2980  | 1.25413  |
| O29     | 3.0985       | -2.4331 | -0.16568 |         | H40 | 5.7326  | 2.3717  | 2.59660  |
| O30     | 5.3200       | -1.2091 | 3.75411  |         | H41 | -4.4506 | 1.0036  | -2.96831 |
| O31     | -3.0096      | -1.7121 | 1.51433  |         | H42 | -7.3721 | -3.4052 | -0.03977 |
| O32     | -0.8975      | 1.2255  | -3.69255 |         | H43 | 2.4921  | 4.9843  | 3.63858  |
| O33     | -5.3015      | 1.1205  | -3.48892 |         | H44 | 3.9000  | 2.1602  | 1.42682  |
| O34     | -2.8855      | 2.4163  | 0.12605  |         | H45 | -5.7442 | -2.4357 | 2.95215  |
| H1      | -4.6605      | -4.9912 | -4.59780 |         | H46 | 1.3889  | 2.5710  | -2.04186 |
| H2      | -3.9126      | 1.0369  | 2.89090  |         | H47 | 6.5341  | 1.6378  | 4.58200  |
| H3      | -2.8987      | 1.8364  | -0.69093 |         | H48 | 4.5017  | -1.0885 | 3.19217  |
| H4      | -1.0932      | -3.7808 | -2.57924 |         | H49 | -4.8652 | -3.7591 | -2.76603 |
| H5      | -6.2085      | -1.8571 | -3.05558 |         | H50 | 3.6407  | -0.9658 | -2.83241 |
| H6      | 0.1910       | -3.4567 | -0.75252 |         | H51 | 1.1167  | 3.5830  | 2.67075  |
| H7      | -0.2761      | -3.3011 | 1.46638  |         | H52 | 4.5872  | 5.8770  | 3.08102  |
| H8      | -5.0177      | 1.2938  | -4.43356 |         | H53 | 3.1156  | -1.8609 | 0.65149  |

|     |         |         |          |
|-----|---------|---------|----------|
| H54 | -1.2899 | -5.9697 | -3.00660 |
| H55 | -3.0368 | -1.7125 | -0.18844 |
| H56 | -3.7719 | -2.1548 | -1.54779 |
| H57 | 6.2221  | 3.5389  | -0.80673 |
| H58 | 2.2934  | 2.0695  | 1.55128  |
| H59 | 2.9054  | 1.7438  | -0.51051 |
| H60 | -5.6393 | -3.3071 | -1.42758 |
| H61 | -3.0624 | -0.7666 | 1.84534  |
| H62 | -2.5833 | -5.1617 | -3.55235 |
| H63 | 2.2841  | -0.9901 | 2.59400  |
| H64 | -2.2463 | 0.9795  | -2.71652 |
| H65 | 2.8234  | 0.8516  | -1.82919 |
| H66 | 5.7193  | 2.3437  | -2.68656 |
| H67 | 0.8301  | -4.7143 | 0.00070  |
| H68 | -5.7161 | -3.3315 | 1.60448  |
| end |         |         |          |
| H1  | -4.5817 | 5.4699  | 2.92401  |
| H2  | -5.0779 | 4.9290  | 2.80198  |
| end |         |         |          |
| H1  | 8.6983  | 5.2631  | 1.33209  |
| H2  | 9.3620  | 5.1235  | 1.02955  |
| end |         |         |          |
| H1  | 9.5421  | 4.9553  | 5.20266  |
| H2  | 9.8203  | 5.4578  | 5.67648  |
| end |         |         |          |
| H1  | 8.1351  | 3.1807  | 4.59460  |
| H2  | 8.6992  | 3.1871  | 4.11074  |
| end |         |         |          |
| H1  | 14.9350 | 8.5917  | 4.58759  |
| H2  | 14.8719 | 8.7057  | 3.85534  |
| end |         |         |          |
| H1  | 16.5151 | 9.8774  | 6.42311  |
| H2  | 15.8281 | 9.8748  | 6.13605  |
| end |         |         |          |
| H1  | 15.2067 | 7.3137  | 7.73136  |
| H2  | 15.6204 | 7.6117  | 7.18791  |
| end |         |         |          |
| H1  | 12.9671 | 7.6819  | 5.53893  |
| H2  | 12.9902 | 6.9398  | 5.58596  |
| end |         |         |          |
| H1  | 13.3067 | 10.2062 | 6.28384  |
| H2  | 13.5469 | 9.6121  | 5.90479  |
| end |         |         |          |
| H1  | 8.9674  | 6.8513  | 3.90738  |
| H2  | 9.0704  | 7.1957  | 3.25535  |
| end |         |         |          |

|     |         |         |          |
|-----|---------|---------|----------|
| H1  | 16.8865 | 7.6088  | 4.87704  |
| H2  | 16.9294 | 7.1541  | 5.46209  |
| end |         |         |          |
| H1  | 10.6617 | 3.7452  | 3.05150  |
| H2  | 10.2283 | 4.3347  | 2.91812  |
| end |         |         |          |
| H1  | 13.6770 | 2.0273  | 4.67190  |
| H2  | 13.1211 | 2.1970  | 5.13002  |
| end |         |         |          |
| H1  | 15.2704 | 2.3800  | 5.97110  |
| H2  | 15.7717 | 1.8764  | 6.17378  |
| end |         |         |          |
| H1  | 11.4052 | 0.6016  | 1.22888  |
| H2  | 10.9536 | 1.0762  | 0.88592  |
| end |         |         |          |
| H1  | 9.0556  | 10.3261 | 4.37447  |
| H2  | 8.9547  | 10.6817 | 5.01626  |
| end |         |         |          |
| H1  | 12.3463 | 8.5197  | 0.11176  |
| H2  | 12.5727 | 9.1795  | -0.13278 |
| end |         |         |          |
| H1  | 11.4677 | 10.7631 | 1.58261  |
| H2  | 11.6693 | 10.0602 | 1.47924  |
| end |         |         |          |
| H1  | 14.3961 | 6.3361  | 0.28076  |
| H2  | 13.6832 | 6.4848  | 0.15023  |
| end |         |         |          |
| H1  | 2.7227  | 4.1289  | 0.95464  |
| H2  | 2.8625  | 4.5058  | 1.57457  |
| end |         |         |          |
| H1  | 3.7219  | 2.3231  | 4.01753  |
| H2  | 3.3320  | 2.5603  | 3.43745  |
| end |         |         |          |
| H1  | 7.6342  | 10.3821 | 0.22936  |
| H2  | 7.1141  | 9.8562  | 0.20459  |
| end |         |         |          |
| H1  | 5.3795  | 4.1406  | 8.24678  |
| H2  | 6.0137  | 4.0092  | 8.60408  |
| end |         |         |          |
| H1  | 10.0599 | 8.5849  | 9.31435  |
| H2  | 10.6197 | 8.9090  | 9.67523  |
| end |         |         |          |
| H1  | 12.9723 | 4.4034  | 9.68254  |
| H2  | 12.5459 | 4.5206  | 9.08926  |
| end |         |         |          |
| H1  | 11.3579 | 12.0944 | 9.94947  |



|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H2  | 11.1445 | 12.6770 | 9.54883 | H1  | 16.3935 | 13.6286 | 8.70595 |
| end |         |         |         | H2  | 16.7722 | 13.7497 | 9.33063 |
| H1  | 8.1610  | 8.1771  | 8.72583 | end |         |         |         |
| H2  | 8.4948  | 7.6225  | 8.36665 | end |         |         |         |
| end |         |         |         |     |         |         |         |

**(31) n=4 & m=7**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.5892 | -4.7379 | -0.0078 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.4387 | 0.3413  | -3.6213 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | -0.0488 | -1.8609 | -3.0735 |
| O1      | 6.7404       | 3.9339  | -0.0631 |         | H12 | -3.8055 | -2.2044 | 1.8701  |
| O2      | 2.9810       | 1.7155  | 1.1850  |         | H13 | 0.0355  | 2.3676  | -2.8629 |
| O3      | 5.1547       | 2.9607  | -2.0689 |         | H14 | 6.0866  | 0.4194  | 3.6451  |
| O4      | 2.7974       | 1.7615  | -1.4753 |         | H15 | 4.9657  | -1.4281 | 4.6801  |
| O5      | 3.1062       | -0.7743 | 2.2006  |         | H16 | -0.0855 | 3.5219  | 0.7234  |
| O6      | -0.6271      | 1.2025  | 3.6044  |         | H17 | 2.8495  | -1.3849 | -1.4511 |
| O7      | 0.7815       | 2.9798  | 2.1246  |         | H18 | 1.1840  | 5.8793  | 3.2872  |
| O8      | 4.2863       | 5.0559  | 3.5196  |         | H19 | 4.6534  | 4.3272  | 2.9394  |
| O9      | 1.5097       | 5.0381  | 3.7200  |         | H20 | 2.2490  | -2.9033 | 0.0106  |
| O10     | 2.7849       | -0.8340 | -2.2856 |         | H21 | 4.3004  | 2.4922  | -1.8321 |
| O11     | 6.5513       | 1.2990  | 3.5948  |         | H22 | 0.2127  | -1.8322 | 3.1483  |
| O12     | -0.6065      | 3.8584  | -0.0613 |         | H23 | -0.7297 | 1.5469  | 4.5380  |
| O13     | 0.5926       | 3.0243  | -2.3551 |         | H24 | 7.6067  | 3.4223  | -0.0643 |
| O14     | -5.2281      | -3.0146 | 2.4137  |         | H25 | 1.3401  | -1.0905 | -3.1606 |
| O15     | -2.9460      | -1.7161 | -1.1480 |         | H26 | -1.1536 | 1.3701  | -4.6350 |
| O16     | -6.4843      | -3.7420 | 0.0302  |         | H27 | 0.2512  | -0.2926 | 3.5967  |
| O17     | -5.1217      | -2.9522 | -2.1648 |         | H28 | -1.5379 | 1.0780  | 3.2198  |
| O18     | -3.0731      | 0.8219  | -2.0451 |         | H29 | -1.5845 | -2.5618 | -1.6445 |
| O19     | 0.4508       | -1.1773 | -3.6098 |         | H30 | 0.2486  | 2.3338  | 2.6731  |
| O20     | -0.7586      | -2.9876 | -2.0226 |         | H31 | -0.1545 | 3.5324  | -0.8957 |
| O21     | -0.7442      | -2.9944 | 2.3375  |         | H32 | -1.5744 | -2.5263 | 2.0188  |
| O22     | 0.7505       | -3.6784 | 0.1096  |         | H33 | -3.0193 | -0.1259 | -1.7226 |
| O23     | -6.7431      | -1.2984 | -3.5497 |         | H34 | -4.7693 | -5.9497 | -3.2230 |
| O24     | -2.9996      | 0.8229  | 2.2573  |         | H35 | -2.9638 | 1.4362  | 1.4698  |
| O25     | -1.5855      | -5.1542 | -3.4296 |         | H36 | -2.0491 | 3.0012  | 0.0033  |
| O26     | -4.3436      | -5.1195 | -3.5937 |         | H37 | 3.0589  | 0.1618  | 1.8462  |
| O27     | 5.2256       | 3.0602  | 1.9583  |         | H38 | -6.2544 | -0.4265 | -3.5251 |
| O28     | 0.7893       | -1.1352 | 3.5770  |         | H39 | 5.8484  | 3.3664  | 1.2320  |
| O29     | 3.0898       | -2.3611 | -0.0504 |         | H40 | 5.7181  | 2.4232  | 2.5489  |
| O30     | 5.2690       | -1.1598 | 3.7674  |         | H41 | -4.5181 | 0.9540  | -2.9262 |
| O31     | -2.9715      | -1.7550 | 1.5487  |         | H42 | -7.3898 | -3.3138 | -0.0157 |
| O32     | -0.9440      | 1.2003  | -3.6661 |         | H43 | 2.5030  | 5.0621  | 3.6470  |
| O33     | -5.3615      | 1.0622  | -3.4602 |         | H44 | 3.8066  | 2.2155  | 1.4456  |
| O34     | -2.9089      | 2.4849  | 0.0595  |         | H45 | -5.7887 | -2.3674 | 2.9392  |
| H1      | -4.6815      | -4.9718 | -4.5235 |         | H46 | 1.4077  | 2.5320  | -2.0400 |
| H2      | -3.8200      | 1.0543  | 2.7776  |         | H47 | 6.5544  | 1.6560  | 4.5334  |
| H3      | -2.9398      | 1.8795  | -0.7397 |         | H48 | 4.4343  | -1.0089 | 3.2355  |
| H4      | -1.0614      | -3.8041 | -2.5166 |         | H49 | -4.8506 | -3.7696 | -2.6788 |
| H5      | -6.1723      | -1.9416 | -3.0331 |         | H50 | 3.6243  | -1.0310 | -2.7931 |
| H6      | 0.2009       | -3.4117 | -0.6863 |         | H51 | 1.0362  | 3.7344  | 2.7333  |
| H7      | -0.2229      | -3.2727 | 1.5338  |         | H52 | 4.6298  | 5.9109  | 3.1257  |
| H8      | -5.0586      | 1.2894  | -4.3833 |         | H53 | 3.0908  | -1.7728 | 0.7561  |

|     |         |         |         |
|-----|---------|---------|---------|
| H54 | -1.2942 | -5.9960 | -2.9678 |
| H55 | -2.9996 | -1.7537 | -0.1480 |
| H56 | -3.7542 | -2.1920 | -1.5016 |
| H57 | 6.1877  | 3.5907  | -0.8207 |
| H58 | 2.2003  | 2.2089  | 1.5761  |
| H59 | 2.8415  | 1.7463  | -0.4725 |
| H60 | -5.6331 | -3.2642 | -1.3601 |
| H61 | -3.0163 | -0.7905 | 1.8243  |
| H62 | -2.5799 | -5.1767 | -3.5007 |
| H63 | 2.2437  | -0.9324 | 2.6837  |
| H64 | -2.3146 | 0.9482  | -2.6879 |
| H65 | 2.8113  | 0.8066  | -1.7707 |
| H66 | 5.6666  | 2.3186  | -2.6383 |
| H67 | 0.8320  | -4.6744 | 0.0506  |
| H68 | -5.7348 | -3.2756 | 1.5981  |
| end |         |         |         |
| H1  | -4.4201 | 6.1201  | 2.8907  |
| H2  | -4.7034 | 5.4561  | 2.7195  |
| end |         |         |         |
| H1  | 10.1206 | 5.8142  | 1.8871  |
| H2  | 9.6066  | 5.4697  | 2.3005  |
| end |         |         |         |
| H1  | 8.9314  | 5.5795  | 5.7400  |
| H2  | 9.4747  | 6.0448  | 5.5456  |
| end |         |         |         |
| H1  | 7.3763  | 3.8350  | 4.9076  |
| H2  | 7.7041  | 4.4048  | 4.5629  |
| end |         |         |         |
| H1  | 15.1010 | 7.9613  | 3.9784  |
| H2  | 14.9840 | 7.6735  | 4.6552  |
| end |         |         |         |
| H1  | 16.8990 | 9.4243  | 6.1702  |
| H2  | 16.2762 | 9.5201  | 5.7740  |
| end |         |         |         |
| H1  | 15.3106 | 7.1420  | 7.1036  |
| H2  | 15.8242 | 6.7154  | 6.7755  |
| end |         |         |         |
| H1  | 13.0078 | 6.8304  | 5.7576  |
| H2  | 13.0105 | 7.5691  | 5.8346  |
| end |         |         |         |
| H1  | 12.7430 | 9.5965  | 5.6640  |
| H2  | 13.2924 | 9.7545  | 6.1346  |
| end |         |         |         |
| H1  | 8.7861  | 7.5124  | 4.1088  |
| H2  | 9.1674  | 7.3507  | 3.4944  |
| end |         |         |         |

|     |         |         |         |
|-----|---------|---------|---------|
| H1  | 15.1574 | 11.2799 | 5.2617  |
| H2  | 14.5218 | 11.0732 | 4.9385  |
| end |         |         |         |
| H1  | 10.3364 | 4.2662  | 4.3752  |
| H2  | 10.5850 | 3.7298  | 3.9243  |
| end |         |         |         |
| H1  | 14.3811 | 9.1498  | 8.1798  |
| H2  | 14.9759 | 9.1367  | 7.7327  |
| end |         |         |         |
| H1  | 8.1400  | 3.5674  | 2.7513  |
| H2  | 8.3260  | 3.4261  | 2.0473  |
| end |         |         |         |
| H1  | 13.7253 | 2.1494  | 4.5415  |
| H2  | 13.2242 | 2.4412  | 5.0022  |
| end |         |         |         |
| H1  | 15.4545 | 2.3319  | 5.7985  |
| H2  | 15.6098 | 1.9917  | 6.4348  |
| end |         |         |         |
| H1  | 11.4842 | 0.8175  | 0.6635  |
| H2  | 11.1108 | 1.1673  | 1.1959  |
| end |         |         |         |
| H1  | 8.8718  | 10.3054 | 4.5799  |
| H2  | 8.9618  | 10.7312 | 5.1788  |
| end |         |         |         |
| H1  | 12.5386 | 8.7573  | 0.3582  |
| H2  | 12.5631 | 9.1911  | -0.2388 |
| end |         |         |         |
| H1  | 11.1256 | 10.2504 | 1.5391  |
| H2  | 11.6169 | 10.7937 | 1.4398  |
| end |         |         |         |
| H1  | 14.3169 | 6.2899  | 0.3530  |
| H2  | 13.6357 | 6.4907  | 0.1478  |
| end |         |         |         |
| H1  | 3.1373  | 4.3943  | 1.3412  |
| H2  | 2.4063  | 4.3600  | 1.2500  |
| end |         |         |         |
| H1  | 3.8080  | 1.8337  | 3.8600  |
| H2  | 3.6803  | 2.5372  | 3.6747  |
| end |         |         |         |
| H1  | 7.5948  | 10.3986 | 0.1621  |
| H2  | 7.1559  | 9.8043  | 0.1524  |
| end |         |         |         |
| H1  | 5.3595  | 4.0120  | 8.2949  |
| H2  | 6.0641  | 3.8021  | 8.3742  |
| end |         |         |         |
| H1  | 10.0724 | 8.6728  | 9.4537  |

|     |         |         |         |
|-----|---------|---------|---------|
| H2  | 10.6011 | 9.0111  | 9.8463  |
| end |         |         |         |
| H1  | 12.9893 | 4.3992  | 9.6433  |
| H2  | 12.4684 | 4.7776  | 9.2782  |
| end |         |         |         |
| H1  | 11.3035 | 12.2163 | 10.1520 |
| H2  | 11.1733 | 12.5787 | 9.5249  |
| end |         |         |         |

|     |         |         |        |
|-----|---------|---------|--------|
| H1  | 8.3369  | 7.8319  | 8.9118 |
| H2  | 8.4954  | 7.9247  | 8.1949 |
| end |         |         |        |
| H1  | 16.4586 | 13.6157 | 8.6104 |
| H2  | 16.8432 | 13.7726 | 9.2252 |
| end |         |         |        |
| end |         |         |        |

**(32) n=4 & m=8**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.6212 | -4.7853 | -0.0033 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.4443 | 0.3499  | -3.6110 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | -0.0820 | -1.8449 | -3.0189 |
| O1      | 6.7934       | 3.8990  | -0.0995 |         | H12 | -3.8405 | -2.2386 | 1.8014  |
| O2      | 3.0130       | 1.6851  | 1.1671  |         | H13 | 0.0428  | 2.4108  | -2.8648 |
| O3      | 5.1879       | 2.9813  | -2.1431 |         | H14 | 6.0268  | 0.4274  | 3.6906  |
| O4      | 2.8113       | 1.8033  | -1.4950 |         | H15 | 4.9861  | -1.4194 | 4.6191  |
| O5      | 3.1355       | -0.8332 | 2.1255  |         | H16 | -0.0737 | 3.4681  | 0.7269  |
| O6      | -0.6678      | 1.2124  | 3.6284  |         | H17 | 2.8341  | -1.3580 | -1.4663 |
| O7      | 0.8016       | 2.9190  | 2.1126  |         | H18 | 1.1946  | 5.8458  | 3.2458  |
| O8      | 4.2521       | 5.0533  | 3.4943  |         | H19 | 4.6072  | 4.3177  | 2.9229  |
| O9      | 1.5300       | 5.0099  | 3.6774  |         | H20 | 2.2447  | -2.9208 | -0.0488 |
| O10     | 2.7650       | -0.7861 | -2.2861 |         | H21 | 4.3472  | 2.5112  | -1.8732 |
| O11     | 6.4675       | 1.3243  | 3.6526  |         | H22 | 0.1841  | -1.7764 | 3.0587  |
| O12     | -0.6121      | 3.8019  | -0.0478 |         | H23 | -0.7753 | 1.5586  | 4.5617  |
| O13     | 0.5898       | 3.0725  | -2.3556 |         | H24 | 7.6425  | 3.3643  | -0.0818 |
| O14     | -5.2436      | -3.0392 | 2.3837  |         | H25 | 1.3043  | -1.0522 | -3.1071 |
| O15     | -2.9912      | -1.7493 | -1.2060 |         | H26 | -1.1625 | 1.3847  | -4.6185 |
| O16     | -6.5169      | -3.7895 | 0.0224  |         | H27 | 0.2252  | -0.2505 | 3.5515  |
| O17     | -5.1796      | -2.9871 | -2.2124 |         | H28 | -1.5730 | 1.0729  | 3.2393  |
| O18     | -3.1013      | 0.7935  | -2.0913 |         | H29 | -1.6123 | -2.6025 | -1.6623 |
| O19     | 0.4059       | -1.1432 | -3.5398 |         | H30 | 0.2310  | 2.3058  | 2.6596  |
| O20     | -0.7893      | -3.0388 | -2.0342 |         | H31 | -0.1578 | 3.5080  | -0.8943 |
| O21     | -0.7875      | -2.9746 | 2.2856  |         | H32 | -1.6233 | -2.5183 | 1.9605  |
| O22     | 0.7268       | -3.6765 | 0.0950  |         | H33 | -3.0572 | -0.1567 | -1.7752 |
| O23     | -6.7805      | -1.2551 | -3.5489 |         | H34 | -4.7801 | -5.9170 | -3.2888 |
| O24     | -3.0559      | 0.7612  | 2.2853  |         | H35 | -2.9865 | 1.3680  | 1.4959  |
| O25     | -1.6050      | -5.1382 | -3.5043 |         | H36 | -2.0352 | 2.9167  | 0.0113  |
| O26     | -4.3575      | -5.0964 | -3.6783 |         | H37 | 3.1229  | 0.1075  | 1.7834  |
| O27     | 5.2536       | 3.0386  | 1.9179  |         | H38 | -6.2640 | -0.3992 | -3.5563 |
| O28     | 0.7708       | -1.0860 | 3.4798  |         | H39 | 5.8789  | 3.3321  | 1.1893  |
| O29     | 3.0893       | -2.3874 | -0.1165 |         | H40 | 5.7483  | 2.4315  | 2.5382  |
| O30     | 5.2966       | -1.1510 | 3.7086  |         | H41 | -4.5150 | 0.9499  | -2.9875 |
| O31     | -3.0186      | -1.7715 | 1.4739  |         | H42 | -7.4206 | -3.3567 | -0.0479 |
| O32     | -0.9517      | 1.2106  | -3.6553 |         | H43 | 2.5271  | 5.0399  | 3.6018  |
| O33     | -5.3564      | 1.0746  | -3.5222 |         | H44 | 3.8274  | 2.2010  | 1.4289  |
| O34     | -2.8807      | 2.3775  | 0.0730  |         | H45 | -5.7810 | -2.3669 | 2.9070  |
| H1      | -4.7162      | -4.9606 | -4.5996 |         | H46 | 1.4088  | 2.5846  | -2.0482 |
| H2      | -3.8717      | 1.0230  | 2.7906  |         | H47 | 6.4771  | 1.6760  | 4.5915  |
| H3      | -2.9272      | 1.7991  | -0.7461 |         | H48 | 4.4677  | -1.0202 | 3.1612  |
| H4      | -1.1031      | -3.8323 | -2.5623 |         | H49 | -4.8938 | -3.7882 | -2.7467 |
| H5      | -6.2153      | -1.9107 | -3.0453 |         | H50 | 3.6005  | -0.9787 | -2.8022 |
| H6      | 0.1748       | -3.4444 | -0.7111 |         | H51 | 1.0481  | 3.6876  | 2.7053  |
| H7      | -0.2653      | -3.2649 | 1.4864  |         | H52 | 4.6051  | 5.8982  | 3.0949  |
| H8      | -5.0538      | 1.3152  | -4.4433 |         | H53 | 3.1044  | -1.8044 | 0.6963  |

|     |         |         |         |
|-----|---------|---------|---------|
| H54 | -1.3082 | -5.9835 | -3.0562 |
| H55 | -3.0472 | -1.7700 | -0.2047 |
| H56 | -3.8030 | -2.2214 | -1.5538 |
| H57 | 6.2465  | 3.5663  | -0.8651 |
| H58 | 2.2250  | 2.1557  | 1.5710  |
| H59 | 2.8631  | 1.7797  | -0.4927 |
| H60 | -5.6749 | -3.3192 | -1.4097 |
| H61 | -3.0711 | -0.8179 | 1.7864  |
| H62 | -2.5980 | -5.1685 | -3.5929 |
| H63 | 2.2616  | -0.9539 | 2.5931  |
| H64 | -2.3325 | 0.9231  | -2.7227 |
| H65 | 2.7999  | 0.8458  | -1.7885 |
| H66 | 5.6938  | 2.3317  | -2.7125 |
| H67 | 0.8461  | -4.6649 | 0.0517  |
| H68 | -5.7695 | -3.3048 | 1.5815  |
| end |         |         |         |
| H1  | -4.8520 | 5.7481  | 2.6766  |
| H2  | -5.0617 | 5.0580  | 2.5112  |
| end |         |         |         |
| H1  | 8.9931  | 5.2365  | 1.7620  |
| H2  | 9.5276  | 5.6393  | 1.4373  |
| end |         |         |         |
| H1  | 8.8935  | 5.8644  | 6.0585  |
| H2  | 8.8507  | 5.9464  | 5.3224  |
| end |         |         |         |
| H1  | 7.3913  | 3.7366  | 4.8218  |
| H2  | 7.5012  | 4.3730  | 4.4578  |
| end |         |         |         |
| H1  | 14.8351 | 8.7508  | 3.8983  |
| H2  | 14.6540 | 8.5345  | 4.5865  |
| end |         |         |         |
| H1  | 16.6450 | 9.6823  | 6.3875  |
| H2  | 16.0770 | 9.5933  | 5.9155  |
| end |         |         |         |
| H1  | 15.4065 | 7.1459  | 7.2543  |
| H2  | 15.7690 | 6.5731  | 6.9511  |
| end |         |         |         |
| H1  | 13.2009 | 6.8876  | 5.7050  |
| H2  | 13.1384 | 7.6030  | 5.8965  |
| end |         |         |         |
| H1  | 15.0766 | 11.4775 | 5.2292  |
| H2  | 14.4431 | 11.3420 | 4.8683  |
| end |         |         |         |
| H1  | 8.7073  | 6.9587  | 3.2373  |
| H2  | 8.4273  | 7.3474  | 3.8049  |
| end |         |         |         |

|     |         |         |         |
|-----|---------|---------|---------|
| H1  | 17.1195 | 7.3035  | 4.6459  |
| H2  | 16.9545 | 7.2998  | 5.3693  |
| end |         |         |         |
| H1  | 10.4284 | 4.3179  | 4.0085  |
| H2  | 10.3994 | 3.5982  | 3.8203  |
| end |         |         |         |
| H1  | 14.9812 | 9.0781  | 7.9568  |
| H2  | 14.4524 | 8.7871  | 8.3913  |
| end |         |         |         |
| H1  | 8.0755  | 3.3909  | 2.7655  |
| H2  | 8.2628  | 3.2792  | 2.0580  |
| end |         |         |         |
| H1  | 12.9174 | 9.8706  | 6.3221  |
| H2  | 13.2518 | 9.6519  | 5.6965  |
| end |         |         |         |
| H1  | 10.7694 | 6.2988  | 4.7504  |
| H2  | 11.1691 | 6.3844  | 4.1315  |
| end |         |         |         |
| H1  | 13.5822 | 1.9016  | 4.7715  |
| H2  | 13.2874 | 2.5462  | 4.9867  |
| end |         |         |         |
| H1  | 15.5375 | 2.2748  | 5.7535  |
| H2  | 15.6002 | 1.9489  | 6.4130  |
| end |         |         |         |
| H1  | 11.0646 | 1.0649  | 0.8790  |
| H2  | 11.4986 | 0.6498  | 1.3088  |
| end |         |         |         |
| H1  | 8.8541  | 10.3214 | 4.4406  |
| H2  | 9.0574  | 10.7260 | 5.0271  |
| end |         |         |         |
| H1  | 12.4162 | 8.5796  | 0.1541  |
| H2  | 12.4889 | 9.2293  | -0.1919 |
| end |         |         |         |
| H1  | 11.4530 | 10.8386 | 1.5538  |
| H2  | 11.6240 | 10.1250 | 1.4664  |
| end |         |         |         |
| H1  | 14.3028 | 6.2729  | 0.3121  |
| H2  | 13.6077 | 6.4435  | 0.1275  |
| end |         |         |         |
| H1  | 3.1194  | 4.3401  | 1.2746  |
| H2  | 2.3882  | 4.3091  | 1.1816  |
| end |         |         |         |
| H1  | 3.9990  | 2.2957  | 3.7635  |
| H2  | 3.3052  | 2.5496  | 3.7578  |
| end |         |         |         |
| H1  | 7.5990  | 10.3792 | 0.1472  |

|     |         |        |        |
|-----|---------|--------|--------|
| H2  | 7.1093  | 9.8282 | 0.0846 |
| end |         |        |        |
| H1  | 5.2834  | 4.2297 | 8.2807 |
| H2  | 5.9098  | 4.0766 | 8.6430 |
| end |         |        |        |
| H1  | 10.0972 | 8.6247 | 9.4386 |
| H2  | 10.6219 | 8.9477 | 9.8502 |
| end |         |        |        |
| H1  | 12.8837 | 4.4361 | 9.6681 |
| H2  | 12.5134 | 4.6526 | 9.0655 |
| end |         |        |        |

|     |         |         |        |
|-----|---------|---------|--------|
| H1  | 11.2941 | 12.1651 | 9.9891 |
| H2  | 11.1232 | 12.6396 | 9.4497 |
| end |         |         |        |
| H1  | 8.3077  | 7.9471  | 8.8101 |
| H2  | 8.5791  | 7.9164  | 8.1226 |
| end |         |         |        |
| H1  | 16.3861 | 13.6300 | 8.7011 |
| H2  | 16.7448 | 13.8296 | 9.3169 |
| end |         |         |        |
| end |         |         |        |

**(33) n=5 & m=1**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.5720 | -4.8021 | -0.0101 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.2840 | 0.3856  | -3.5740 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.0371  | -1.8789 | -3.0573 |
| O1      | 6.7240       | 3.7963  | 0.1338  |         | H12 | -3.6752 | -2.2371 | 1.8917  |
| O2      | 2.9352       | 1.7234  | 1.2096  |         | H13 | 0.2158  | 2.4668  | -2.8907 |
| O3      | 5.2898       | 3.0390  | -2.2466 |         | H14 | 6.1542  | 0.3682  | 3.6972  |
| O4      | 2.9839       | 1.7828  | -1.5275 |         | H15 | 5.0316  | -1.4130 | 4.6403  |
| O5      | 3.0038       | -0.8745 | 2.1085  |         | H16 | -0.1193 | 3.5336  | 0.6977  |
| O6      | -0.7223      | 1.2246  | 3.5613  |         | H17 | 2.8696  | -1.4092 | -1.5208 |
| O7      | 0.6843       | 2.9797  | 2.0921  |         | H18 | 1.2177  | 5.8708  | 3.2501  |
| O8      | 4.2592       | 5.1462  | 3.6907  |         | H19 | 4.5846  | 4.3585  | 3.1617  |
| O9      | 1.5366       | 5.0118  | 3.6688  |         | H20 | 2.2678  | -3.0857 | -0.0782 |
| O10     | 2.8144       | -0.8156 | -2.3237 |         | H21 | 4.4646  | 2.5595  | -1.9480 |
| O11     | 6.6003       | 1.2624  | 3.6699  |         | H22 | 0.2105  | -1.8097 | 3.1468  |
| O12     | -0.6366      | 3.8517  | -0.0996 |         | H23 | -0.7865 | 1.5867  | 4.4926  |
| O13     | 0.7557       | 3.1591  | -2.4045 |         | H24 | 7.5960  | 3.2952  | 0.1071  |
| O14     | -5.1477      | -3.0563 | 2.4462  |         | H25 | 1.3971  | -1.0573 | -3.1488 |
| O15     | -2.8417      | -1.7570 | -1.2180 |         | H26 | -1.0338 | 1.4681  | -4.5178 |
| O16     | -6.4767      | -3.8062 | 0.0702  |         | H27 | 0.1999  | -0.2434 | 3.5599  |
| O17     | -5.2545      | -2.9400 | -2.1671 |         | H28 | -1.6481 | 1.1003  | 3.1915  |
| O18     | -2.9886      | 0.8964  | -2.1116 |         | H29 | -1.4706 | -2.6261 | -1.7563 |
| O19     | 0.5049       | -1.1735 | -3.5974 |         | H30 | 0.1216  | 2.3655  | 2.6518  |
| O20     | -0.6447      | -3.0876 | -2.0758 |         | H31 | -0.1249 | 3.5632  | -0.9059 |
| O21     | -0.6393      | -3.0497 | 2.4150  |         | H32 | -1.4532 | -2.5633 | 2.0808  |
| O22     | 0.8660       | -3.8568 | 0.1523  |         | H33 | -2.9526 | -0.0490 | -1.8079 |
| O23     | -6.7527      | -1.2285 | -3.6358 |         | H34 | -4.6586 | -5.8000 | -3.2851 |
| O24     | -3.0396      | 0.8015  | 2.3431  |         | H35 | -2.9937 | 1.3841  | 1.5303  |
| O25     | -1.4977      | -5.1571 | -3.5568 |         | H36 | -2.0714 | 2.9391  | 0.0591  |
| O26     | -4.2610      | -4.9691 | -3.6804 |         | H37 | 3.0082  | 0.0614  | 1.7673  |
| O27     | 5.1647       | 3.0814  | 2.2419  |         | H38 | -6.2104 | -0.3895 | -3.6200 |
| O28     | 0.7543       | -1.0757 | 3.5614  |         | H39 | 5.7510  | 3.3546  | 1.4783  |
| O29     | 3.0943       | -2.5144 | -0.1718 |         | H40 | 5.6857  | 2.4187  | 2.7791  |
| O30     | 5.3308       | -1.1676 | 3.7111  |         | H41 | -4.5056 | 1.0334  | -3.0406 |
| O31     | -2.8430      | -1.7695 | 1.6027  |         | H42 | -7.3844 | -3.3842 | -0.0025 |
| O32     | -0.7396      | 1.2759  | -3.5736 |         | H43 | 2.5372  | 5.0593  | 3.6745  |
| O33     | -5.3264      | 1.1603  | -3.5899 |         | H44 | 3.7026  | 2.1879  | 1.6340  |
| O34     | -2.9011      | 2.3836  | 0.1354  |         | H45 | -5.7099 | -2.3830 | 2.9357  |
| H1      | -4.6348      | -4.8499 | -4.6041 |         | H46 | 1.5876  | 2.6937  | -2.1119 |
| H2      | -3.8806      | 1.0195  | 2.8484  |         | H47 | 6.6111  | 1.6150  | 4.6162  |
| H3      | -2.9353      | 1.8225  | -0.6964 |         | H48 | 4.4950  | -1.0000 | 3.2012  |
| H4      | -0.9653      | -3.8568 | -2.6354 |         | H49 | -4.9224 | -3.7169 | -2.7052 |
| H5      | -6.2310      | -1.8940 | -3.0953 |         | H50 | 3.6560  | -0.9808 | -2.8400 |
| H6      | 0.2963       | -3.5878 | -0.6163 |         | H51 | 0.9997  | 3.7239  | 2.6826  |
| H7      | -0.1321      | -3.3318 | 1.6063  |         | H52 | 4.6522  | 5.9460  | 3.2303  |
| H8      | -4.9919      | 1.3539  | -4.5192 |         | H53 | 3.0861  | -1.9340 | 0.6340  |



|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.1973 | -6.0051 | -3.0910 | end |         |         |         |
| H55 | -2.8936 | -1.7636 | -0.2271 | H1  | 14.2043 | 6.6209  | 0.2767  |
| H56 | -3.6709 | -2.2094 | -1.5231 | H2  | 13.4961 | 6.7292  | 0.1162  |
| H57 | 6.2219  | 3.5247  | -0.6763 | end |         |         |         |
| H58 | 2.1048  | 2.1831  | 1.5277  | H1  | 14.6733 | 4.4317  | 1.0745  |
| H59 | 2.9691  | 1.7810  | -0.5295 | H2  | 14.2616 | 4.8572  | 1.5174  |
| H60 | -5.7275 | -3.3047 | -1.3598 | end |         |         |         |
| H61 | -2.9164 | -0.8164 | 1.9088  | H1  | 11.0945 | 3.3430  | 8.9441  |
| H62 | -2.4921 | -5.1536 | -3.6160 | H2  | 11.0220 | 2.8950  | 8.3596  |
| H63 | 2.1573  | -0.9483 | 2.6408  | end |         |         |         |
| H64 | -2.1546 | 1.0364  | -2.6477 | H1  | 3.5236  | 2.6790  | 4.7069  |
| H65 | 2.9348  | 0.8211  | -1.8016 | H2  | 3.7562  | 3.1893  | 5.1900  |
| H66 | 5.7813  | 2.3827  | -2.8285 | end |         |         |         |
| H67 | 0.9054  | -4.8606 | 0.1282  | H1  | 4.1563  | 5.9105  | 0.5057  |
| H68 | -5.6560 | -3.3047 | 1.6289  | H2  | 4.2646  | 6.2398  | -0.1468 |
| end |         |         |         | end |         |         |         |
| H1  | 8.8683  | 4.8419  | 1.8391  | H1  | 13.8950 | 2.6050  | 6.0848  |
| H2  | 9.2990  | 5.3639  | 1.5257  | H2  | 13.5619 | 2.0626  | 6.4487  |
| end |         |         |         | end |         |         |         |
| H1  | 13.4669 | 8.8973  | 7.3453  | H1  | 18.2812 | 5.0240  | 9.8068  |
| H2  | 13.3814 | 8.2990  | 6.9082  | H2  | 18.7110 | 5.1748  | 9.2293  |
| end |         |         |         | end |         |         |         |
| H1  | 13.5384 | 1.4804  | 3.7794  | H1  | 10.8678 | 8.7847  | 1.2972  |
| H2  | 13.7672 | 1.3451  | 4.4693  | H2  | 11.3898 | 8.7212  | 0.7855  |
| end |         |         |         | end |         |         |         |
| H1  | 5.7311  | 8.6413  | 0.1855  | H1  | 9.5750  | 11.2980 | 3.5255  |
| H2  | 5.0529  | 8.3629  | 0.1508  | H2  | 10.2798 | 11.4626 | 3.6542  |
| end |         |         |         | end |         |         |         |
| H1  | 11.0558 | 0.2034  | 0.8182  | H1  | 5.2722  | 3.0921  | 8.4082  |
| H2  | 11.2772 | 0.4431  | 1.4819  | H2  | 5.4265  | 3.8140  | 8.4248  |
| end |         |         |         | end |         |         |         |
| H1  | 9.4321  | 11.1554 | 5.7337  | H1  | 12.8062 | 4.6603  | 9.2040  |
| H2  | 8.9780  | 10.6016 | 5.9139  | H2  | 12.4908 | 4.9669  | 8.6144  |
| end |         |         |         | end |         |         |         |
| H1  | 13.2744 | 9.5306  | 0.4803  | H1  | 13.4754 | 13.0936 | 9.9407  |
| H2  | 12.9263 | 9.5918  | -0.1679 | H2  | 13.0844 | 13.4226 | 9.4067  |
| end |         |         |         | end |         |         |         |
| H1  | 10.0989 | 7.4711  | 9.3605  | H1  | 20.1603 | 8.3244  | 8.8150  |
| H2  | 10.1370 | 6.8543  | 9.7584  | H2  | 20.3686 | 8.3541  | 8.1060  |
| end |         |         |         | end |         |         |         |
| H1  | 5.5646  | 0.3888  | 1.1599  | end |         |         |         |
| H2  | 5.4803  | 1.1232  | 1.1846  | end |         |         |         |

**(34) n=5 & m=2**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.6027 | -4.7773 | -0.0248 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.3090 | 0.4208  | -3.5820 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.0302  | -1.8547 | -3.0482 |
| O1      | 6.7326       | 3.8006  | 0.1459  |         | H12 | -3.6720 | -2.2489 | 1.8714  |
| O2      | 2.9222       | 1.7469  | 1.2405  |         | H13 | 0.2107  | 2.5083  | -2.8821 |
| O3      | 5.2607       | 3.0761  | -2.2462 |         | H14 | 6.1724  | 0.3836  | 3.6946  |
| O4      | 2.9788       | 1.8099  | -1.4947 |         | H15 | 5.0506  | -1.4133 | 4.6045  |
| O5      | 3.0042       | -0.8551 | 2.0983  |         | H16 | -0.1524 | 3.5516  | 0.7313  |
| O6      | -0.7201      | 1.2274  | 3.5881  |         | H17 | 2.8613  | -1.3692 | -1.5333 |
| O7      | 0.6624       | 3.0014  | 2.1239  |         | H18 | 1.2282  | 5.8893  | 3.2393  |
| O8      | 4.2677       | 5.1717  | 3.6639  |         | H19 | 4.5949  | 4.3761  | 3.1492  |
| O9      | 1.5501       | 5.0427  | 3.6808  |         | H20 | 2.2695  | -3.0514 | -0.0973 |
| O10     | 2.8007       | -0.7705 | -2.3323 |         | H21 | 4.4428  | 2.5913  | -1.9350 |
| O11     | 6.6196       | 1.2773  | 3.6787  |         | H22 | 0.2172  | -1.8010 | 3.1471  |
| O12     | -0.6762      | 3.8621  | -0.0651 |         | H23 | -0.7986 | 1.6024  | 4.5142  |
| O13     | 0.7488       | 3.1907  | -2.3838 |         | H24 | 7.5932  | 3.2798  | 0.1109  |
| O14     | -5.1429      | -3.0627 | 2.4111  |         | H25 | 1.3822  | -1.0206 | -3.1495 |
| O15     | -2.8564      | -1.7299 | -1.2325 |         | H26 | -1.0453 | 1.5005  | -4.5345 |
| O16     | -6.4880      | -3.7831 | 0.0272  |         | H27 | 0.2075  | -0.2385 | 3.5776  |
| O17     | -5.2709      | -2.9154 | -2.1868 |         | H28 | -1.6392 | 1.0945  | 3.2069  |
| O18     | -3.0158      | 0.9068  | -2.1302 |         | H29 | -1.4756 | -2.6210 | -1.7560 |
| O19     | 0.4885       | -1.1488 | -3.5931 |         | H30 | 0.1106  | 2.3808  | 2.6876  |
| O20     | -0.6513      | -3.0865 | -2.0716 |         | H31 | -0.1599 | 3.5796  | -0.8693 |
| O21     | -0.6210      | -3.0283 | 2.4097  |         | H32 | -1.4409 | -2.5531 | 2.0744  |
| O22     | 0.8579       | -3.8380 | 0.1633  |         | H33 | -2.9726 | -0.0407 | -1.8308 |
| O23     | -6.7717      | -1.1839 | -3.6391 |         | H34 | -4.6402 | -5.7691 | -3.2744 |
| O24     | -3.0275      | 0.7864  | 2.3459  |         | H35 | -2.9858 | 1.3605  | 1.5270  |
| O25     | -1.4955      | -5.1321 | -3.5952 |         | H36 | -2.0849 | 2.9169  | 0.0602  |
| O26     | -4.2506      | -4.9418 | -3.6826 |         | H37 | 2.9969  | 0.0831  | 1.7627  |
| O27     | 5.1601       | 3.0733  | 2.2536  |         | H38 | -6.2278 | -0.3465 | -3.6217 |
| O28     | 0.7627       | -1.0701 | 3.5664  |         | H39 | 5.7460  | 3.3488  | 1.4922  |
| O29     | 3.0866       | -2.4703 | -0.1871 |         | H40 | 5.6872  | 2.4181  | 2.7952  |
| O30     | 5.3558       | -1.1616 | 3.6791  |         | H41 | -4.5235 | 1.0716  | -3.0356 |
| O31     | -2.8388      | -1.7793 | 1.5864  |         | H42 | -7.3909 | -3.3480 | -0.0330 |
| O32     | -0.7632      | 1.3106  | -3.5861 |         | H43 | 2.5511  | 5.0892  | 3.6749  |
| O33     | -5.3441      | 1.2017  | -3.5866 |         | H44 | 3.6924  | 2.2084  | 1.6651  |
| O34     | -2.9125      | 2.3565  | 0.1301  |         | H45 | -5.6937 | -2.3846 | 2.9070  |
| H1      | -4.6293      | -4.8385 | -4.6068 |         | H46 | 1.5766  | 2.7180  | -2.0920 |
| H2      | -3.8631      | 1.0167  | 2.8534  |         | H47 | 6.6163  | 1.6301  | 4.6248  |
| H3      | -2.9474      | 1.8069  | -0.7103 |         | H48 | 4.5217  | -0.9848 | 3.1710  |
| H4      | -0.9751      | -3.8426 | -2.6467 |         | H49 | -4.9264 | -3.6883 | -2.7235 |
| H5      | -6.2544      | -1.8530 | -3.1014 |         | H50 | 3.6370  | -0.9397 | -2.8563 |
| H6      | 0.2935       | -3.5750 | -0.6116 |         | H51 | 0.9884  | 3.7417  | 2.7123  |
| H7      | -0.1132      | -3.3163 | 1.6011  |         | H52 | 4.6762  | 5.9667  | 3.2073  |
| H8      | -5.0045      | 1.3920  | -4.5136 |         | H53 | 3.0741  | -1.8989 | 0.6253  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.2066 | -5.9767 | -3.1182 | end |         |         |         |
| H55 | -2.9075 | -1.7395 | -0.2410 | H1  | 5.5583  | 0.3855  | 1.1659  |
| H56 | -3.6860 | -2.1801 | -1.5397 | H2  | 5.4614  | 1.1170  | 1.2149  |
| H57 | 6.2142  | 3.5342  | -0.6543 | end |         |         |         |
| H58 | 2.0913  | 2.2048  | 1.5586  | H1  | 14.2012 | 6.6287  | 0.2243  |
| H59 | 2.9646  | 1.7992  | -0.4974 | H2  | 13.4883 | 6.7241  | 0.0751  |
| H60 | -5.7417 | -3.2864 | -1.3785 | end |         |         |         |
| H61 | -2.9109 | -0.8307 | 1.9054  | H1  | 14.5991 | 4.4095  | 1.0306  |
| H62 | -2.4912 | -5.1193 | -3.6487 | H2  | 14.2103 | 4.8512  | 1.4788  |
| H63 | 2.1631  | -0.9385 | 2.6373  | end |         |         |         |
| H64 | -2.1838 | 1.0576  | -2.6669 | H1  | 11.0943 | 3.3340  | 8.9466  |
| H65 | 2.9300  | 0.8522  | -1.7846 | H2  | 11.0031 | 2.8741  | 8.3744  |
| H66 | 5.7555  | 2.4231  | -2.8287 | end |         |         |         |
| H67 | 0.8976  | -4.8401 | 0.1460  | H1  | 3.4676  | 2.7258  | 4.6561  |
| H68 | -5.6570 | -3.3018 | 1.5955  | H2  | 3.7011  | 3.2483  | 5.1257  |
| end |         |         |         | end |         |         |         |
| H1  | -4.5851 | 5.3953  | 3.2828  | H1  | 4.1316  | 5.9172  | 0.5786  |
| H2  | -4.4879 | 4.8136  | 2.8269  | H2  | 4.2804  | 6.2330  | -0.0728 |
| end |         |         |         | end |         |         |         |
| H1  | 9.6023  | 5.7202  | 5.5129  | H1  | 13.8566 | 2.6369  | 6.0518  |
| H2  | 9.1024  | 5.4573  | 5.0250  | H2  | 13.5429 | 2.0806  | 6.4122  |
| end |         |         |         | end |         |         |         |
| H1  | 15.3360 | 9.9851  | 6.8309  | H1  | 18.2781 | 5.0604  | 9.8379  |
| H2  | 16.0667 | 9.9485  | 6.9776  | H2  | 18.7211 | 5.2242  | 9.2748  |
| end |         |         |         | end |         |         |         |
| H1  | 13.2822 | 7.8941  | 5.5096  | H1  | 10.8697 | 8.7785  | 1.2789  |
| H2  | 13.3135 | 7.1649  | 5.3561  | H2  | 11.4067 | 8.7306  | 0.7817  |
| end |         |         |         | end |         |         |         |
| H1  | 13.5421 | 1.4318  | 3.7669  | H1  | 9.6162  | 11.2940 | 3.5022  |
| H2  | 13.8075 | 1.3237  | 4.4486  | H2  | 10.2941 | 11.4700 | 3.7254  |
| end |         |         |         | end |         |         |         |
| H1  | 5.7172  | 8.6804  | 0.1410  | H1  | 5.2091  | 3.1833  | 8.4398  |
| H2  | 5.0472  | 8.3803  | 0.1465  | H2  | 5.4269  | 3.8890  | 8.4287  |
| end |         |         |         | end |         |         |         |
| H1  | 11.0858 | 0.2213  | 0.8544  | H1  | 12.7958 | 4.6881  | 9.1701  |
| H2  | 11.3265 | 0.4411  | 1.5183  | H2  | 12.3974 | 4.9686  | 8.6187  |
| end |         |         |         | end |         |         |         |
| H1  | 9.4432  | 11.2073 | 5.7603  | H1  | 13.4602 | 13.1143 | 9.8950  |
| H2  | 8.9940  | 10.6464 | 5.9298  | H2  | 13.0702 | 13.4690 | 9.3772  |
| end |         |         |         | end |         |         |         |
| H1  | 13.2774 | 9.5870  | 0.4973  | H1  | 20.2302 | 8.3960  | 8.7490  |
| H2  | 12.9419 | 9.6274  | -0.1590 | H2  | 20.5288 | 8.3012  | 8.0792  |
| end |         |         |         | end |         |         |         |
| H1  | 10.1201 | 7.4872  | 9.4105  | end |         |         |         |
| H2  | 10.1438 | 6.8572  | 9.7877  | end |         |         |         |

**(35) n=5 & m=3**

|         |              |         |         |         |     |         |        |         |
|---------|--------------|---------|---------|---------|-----|---------|--------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.5533 | -4.778 | -0.0101 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.2463 | 0.365  | -3.5771 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.0622  | -1.893 | -3.0528 |
| O1      | 6.7027       | 3.773   | 0.1621  |         | H12 | -3.6898 | -2.220 | 1.8907  |
| O2      | 2.9352       | 1.690   | 1.2425  |         | H13 | 0.2563  | 2.456  | -2.8811 |
| O3      | 5.2701       | 3.018   | -2.2112 |         | H14 | 6.1479  | 0.342  | 3.7184  |
| O4      | 2.9869       | 1.762   | -1.4811 |         | H15 | 5.0194  | -1.444 | 4.6638  |
| O5      | 2.9940       | -0.902  | 2.1391  |         | H16 | -0.1092 | 3.552  | 0.7020  |
| O6      | -0.7361      | 1.226   | 3.5681  |         | H17 | 2.8866  | -1.422 | -1.5136 |
| O7      | 0.6828       | 2.989   | 2.1038  |         | H18 | 1.2271  | 5.893  | 3.2548  |
| O8      | 4.2682       | 5.130   | 3.7100  |         | H19 | 4.5753  | 4.339  | 3.1762  |
| O9      | 1.5375       | 5.034   | 3.6809  |         | H20 | 2.2815  | -3.098 | -0.0720 |
| O10     | 2.8266       | -0.824  | -2.3124 |         | H21 | 4.4521  | 2.524  | -1.9124 |
| O11     | 6.5868       | 1.239   | 3.6776  |         | H22 | 0.1891  | -1.819 | 3.1758  |
| O12     | -0.6215      | 3.875   | -0.0960 |         | H23 | -0.7965 | 1.591  | 4.4981  |
| O13     | 0.7877       | 3.146   | -2.3847 |         | H24 | 7.5821  | 3.286  | 0.1257  |
| O14     | -5.1396      | -3.038  | 2.4459  |         | H25 | 1.4236  | -1.072 | -3.1464 |
| O15     | -2.8124      | -1.747  | -1.2121 |         | H26 | -1.0001 | 1.452  | -4.5179 |
| O16     | -6.4597      | -3.782  | 0.0726  |         | H27 | 0.1755  | -0.252 | 3.5820  |
| O17     | -5.2407      | -2.936  | -2.1647 |         | H28 | -1.6631 | 1.102  | 3.2026  |
| O18     | -2.9475      | 0.913   | -2.1135 |         | H29 | -1.4515 | -2.629 | -1.7531 |
| O19     | 0.5304       | -1.191  | -3.5945 |         | H30 | 0.1124  | 2.377  | 2.6569  |
| O20     | -0.6300      | -3.098  | -2.0731 |         | H31 | -0.1105 | 3.579  | -0.8996 |
| O21     | -0.6487      | -3.064  | 2.4187  |         | H32 | -1.4566 | -2.570 | 2.0870  |
| O22     | 0.8706       | -3.873  | 0.1544  |         | H33 | -2.9165 | -0.029 | -1.8045 |
| O23     | -6.7419      | -1.211  | -3.6311 |         | H34 | -4.6504 | -5.815 | -3.2586 |
| O24     | -3.0531      | 0.810   | 2.3417  |         | H35 | -3.0033 | 1.399  | 1.5344  |
| O25     | -1.5073      | -5.177  | -3.5283 |         | H36 | -2.0646 | 2.964  | 0.0626  |
| O26     | -4.2663      | -4.977  | -3.6562 |         | H37 | 2.9977  | 0.033  | 1.7973  |
| O27     | 5.1294       | 3.046   | 2.2668  |         | H38 | -6.2003 | -0.373 | -3.6116 |
| O28     | 0.7312       | -1.084  | 3.5874  |         | H39 | 5.7220  | 3.328  | 1.5128  |
| O29     | 3.1007       | -2.516  | -0.1519 |         | H40 | 5.6539  | 2.385  | 2.8046  |
| O30     | 5.3169       | -1.193  | 3.7357  |         | H41 | -4.4782 | 1.061  | -3.0361 |
| O31     | -2.8519      | -1.758  | 1.6076  |         | H42 | -7.3700 | -3.364 | -0.0055 |
| O32     | -0.6894      | 1.261   | -3.5783 |         | H43 | 2.5376  | 5.073  | 3.6924  |
| O33     | -5.3077      | 1.187   | -3.5713 |         | H44 | 3.7072  | 2.156  | 1.6613  |
| O34     | -2.8906      | 2.403   | 0.1351  |         | H45 | -5.7086 | -2.378 | 2.9461  |
| H1      | -4.6479      | -4.861  | -4.5764 |         | H46 | 1.6180  | 2.680  | -2.0865 |
| H2      | -3.8962      | 1.019   | 2.8477  |         | H47 | 6.6186  | 1.596  | 4.6215  |
| H3      | -2.9140      | 1.842   | -0.6964 |         | H48 | 4.4798  | -1.032 | 3.2252  |
| H4      | -0.9576      | -3.867  | -2.6274 |         | H49 | -4.9109 | -3.721 | -2.6948 |
| H5      | -6.2223      | -1.880  | -3.0960 |         | H50 | 3.6657  | -0.981 | -2.8346 |
| H6      | 0.3044       | -3.599  | -0.6155 |         | H51 | 0.9944  | 3.732  | 2.6969  |
| H7      | -0.1359      | -3.336  | 1.6105  |         | H52 | 4.6590  | 5.928  | 3.2451  |
| H8      | -4.9892      | 1.389   | -4.5040 |         | H53 | 3.0821  | -1.949 | 0.6629  |

|     |         |        |         |     |         |        |         |
|-----|---------|--------|---------|-----|---------|--------|---------|
| H54 | -1.2138 | -6.022 | -3.0541 | H1  | 13.2642 | 9.492  | 0.4462  |
| H55 | -2.8740 | -1.757 | -0.2217 | H2  | 12.9185 | 9.558  | -0.2028 |
| H56 | -3.6412 | -2.192 | -1.5255 | end |         |        |         |
| H57 | 6.1968  | 3.493  | -0.6429 | H1  | 10.0807 | 7.450  | 9.3845  |
| H58 | 2.1094  | 2.161  | 1.5519  | H2  | 10.1169 | 6.835  | 9.7861  |
| H59 | 2.9672  | 1.745  | -0.4827 | end |         |        |         |
| H60 | -5.7068 | -3.291 | -1.3485 | H1  | 5.5952  | 0.400  | 1.1534  |
| H61 | -2.9230 | -0.803 | 1.9098  | H2  | 5.5262  | 1.136  | 1.1555  |
| H62 | -2.5018 | -5.167 | -3.5899 | end |         |        |         |
| H63 | 2.1471  | -0.975 | 2.6693  | H1  | 14.2254 | 6.625  | 0.2905  |
| H64 | -2.1105 | 1.046  | -2.6457 | H2  | 13.5180 | 6.746  | 0.1354  |
| H65 | 2.9403  | 0.807  | -1.7757 | end |         |        |         |
| H66 | 5.7773  | 2.376  | -2.7962 | H1  | 14.6860 | 4.456  | 1.0956  |
| H67 | 0.8892  | -4.876 | 0.1434  | H2  | 14.2673 | 4.865  | 1.5484  |
| H68 | -5.6499 | -3.290 | 1.6308  | end |         |        |         |
| end |         |        |         | H1  | 11.1109 | 3.379  | 8.9366  |
| H1  | 8.8465  | 4.864  | 1.8423  | H2  | 11.0235 | 2.920  | 8.3630  |
| H2  | 9.3093  | 5.341  | 1.5056  | end |         |        |         |
| end |         |        |         | H1  | 3.5697  | 2.663  | 4.7513  |
| H1  | 9.7383  | 5.632  | 5.5209  | H2  | 3.7940  | 3.172  | 5.2394  |
| H2  | 9.1954  | 5.300  | 5.1313  | end |         |        |         |
| end |         |        |         | H1  | 4.1862  | 5.915  | 0.4903  |
| H1  | 7.1359  | 4.164  | 4.0396  | H2  | 4.2659  | 6.201  | -0.1866 |
| H2  | 7.7907  | 4.203  | 3.6862  | end |         |        |         |
| end |         |        |         | H1  | 13.9162 | 2.628  | 6.1158  |
| H1  | 15.1920 | 8.711  | 4.8363  | H2  | 13.5612 | 2.092  | 6.4685  |
| H2  | 15.0180 | 8.526  | 4.1338  | end |         |        |         |
| end |         |        |         | H1  | 18.2708 | 5.025  | 9.8308  |
| H1  | 15.5573 | 9.621  | 6.8777  | H2  | 18.6994 | 5.186  | 9.2553  |
| H2  | 16.2567 | 9.842  | 7.0150  | end |         |        |         |
| end |         |        |         | H1  | 10.8670 | 8.811  | 1.3098  |
| H1  | 13.3823 | 8.662  | 7.4542  | H2  | 11.3801 | 8.743  | 0.7896  |
| H2  | 13.3940 | 8.357  | 6.7742  | end |         |        |         |
| end |         |        |         | H1  | 9.5586  | 11.306 | 3.5401  |
| H1  | 13.5034 | 1.477  | 3.8153  | H2  | 10.2640 | 11.417 | 3.7140  |
| H2  | 13.7649 | 1.368  | 4.4985  | end |         |        |         |
| end |         |        |         | H1  | 5.2866  | 3.082  | 8.4179  |
| H1  | 5.7278  | 8.647  | 0.2135  | H2  | 5.4625  | 3.799  | 8.4272  |
| H2  | 5.0670  | 8.335  | 0.1447  | end |         |        |         |
| end |         |        |         | H1  | 12.8511 | 4.657  | 9.2134  |
| H1  | 11.0419 | 0.211  | 0.8246  | H2  | 12.5437 | 4.948  | 8.6121  |
| H2  | 11.2569 | 0.430  | 1.4975  | end |         |        |         |
| end |         |        |         | H1  | 13.4713 | 13.083 | 9.9603  |
| H1  | 9.4105  | 11.166 | 5.7980  | H2  | 13.0885 | 13.429 | 9.4311  |
| H2  | 8.9722  | 10.586 | 5.9262  | end |         |        |         |
| end |         |        |         | H1  | 20.1459 | 8.342  | 8.8576  |

|     |         |       |        |     |
|-----|---------|-------|--------|-----|
| H2  | 20.3721 | 8.312 | 8.1543 | end |
| end |         |       |        |     |

**(36) n=5 & m=4**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.5837 | -4.7713 | -0.0400 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.2990 | 0.3987  | -3.5885 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.0203  | -1.8785 | -3.0503 |
| O1      | 6.6964       | 3.7991  | 0.1985  |         | H12 | -3.7506 | -2.2312 | 1.8533  |
| O2      | 2.9103       | 1.7053  | 1.2564  |         | H13 | 0.2232  | 2.4877  | -2.8890 |
| O3      | 5.2675       | 3.0762  | -2.2017 |         | H14 | 6.1133  | 0.3049  | 3.6969  |
| O4      | 2.9736       | 1.7983  | -1.4838 |         | H15 | 4.9924  | -1.4649 | 4.6223  |
| O5      | 2.9335       | -0.8940 | 2.1291  |         | H16 | -0.1210 | 3.5394  | 0.7039  |
| O6      | -0.7898      | 1.2530  | 3.5788  |         | H17 | 2.8248  | -1.3930 | -1.5339 |
| O7      | 0.6508       | 2.9710  | 2.0992  |         | H18 | 1.1685  | 5.8577  | 3.2075  |
| O8      | 4.2062       | 5.1470  | 3.6997  |         | H19 | 4.5451  | 4.3561  | 3.1833  |
| O9      | 1.4859       | 5.0161  | 3.6606  |         | H20 | 2.2319  | -3.0847 | -0.0718 |
| O10     | 2.7727       | -0.7884 | -2.3270 |         | H21 | 4.4506  | 2.5849  | -1.9001 |
| O11     | 6.5646       | 1.1959  | 3.6741  |         | H22 | 0.1099  | -1.7967 | 3.1663  |
| O12     | -0.6425      | 3.8678  | -0.0877 |         | H23 | -0.8574 | 1.6274  | 4.5053  |
| O13     | 0.7595       | 3.1800  | -2.4025 |         | H24 | 7.5778  | 3.3177  | 0.1463  |
| O14     | -5.1870      | -3.0795 | 2.3780  |         | H25 | 1.3738  | -1.0549 | -3.1671 |
| O15     | -2.8620      | -1.7175 | -1.2461 |         | H26 | -1.0509 | 1.4844  | -4.5249 |
| O16     | -6.4947      | -3.7743 | 0.0090  |         | H27 | 0.1209  | -0.2369 | 3.5939  |
| O17     | -5.2679      | -2.9012 | -2.2034 |         | H28 | -1.7113 | 1.1097  | 3.2073  |
| O18     | -3.0078      | 0.9384  | -2.1466 |         | H29 | -1.4870 | -2.6093 | -1.7513 |
| O19     | 0.4801       | -1.1856 | -3.6097 |         | H30 | 0.0758  | 2.3699  | 2.6607  |
| O20     | -0.6615      | -3.0865 | -2.0463 |         | H31 | -0.1396 | 3.5813  | -0.8993 |
| O21     | -0.7352      | -3.0354 | 2.4278  |         | H32 | -1.5425 | -2.5494 | 2.0781  |
| O22     | 0.8177       | -3.8529 | 0.2191  |         | H33 | -2.9786 | -0.0064 | -1.8414 |
| O23     | -6.8020      | -1.1827 | -3.6415 |         | H34 | -4.6691 | -5.7625 | -3.2850 |
| O24     | -3.0860      | 0.8080  | 2.3207  |         | H35 | -3.0367 | 1.3946  | 1.5122  |
| O25     | -1.5158      | -5.1450 | -3.5568 |         | H36 | -2.0781 | 2.9406  | 0.0424  |
| O26     | -4.2805      | -4.9370 | -3.6974 |         | H37 | 2.9489  | 0.0461  | 1.7985  |
| O27     | 5.1377       | 3.0544  | 2.3035  |         | H38 | -6.2684 | -0.3404 | -3.6219 |
| O28     | 0.6690       | -1.0713 | 3.5730  |         | H39 | 5.7328  | 3.3321  | 1.5494  |
| O29     | 3.0506       | -2.5094 | -0.1720 |         | H40 | 5.6487  | 2.3786  | 2.8349  |
| O30     | 5.2704       | -1.2264 | 3.6852  |         | H41 | -4.5313 | 1.0887  | -3.0554 |
| O31     | -2.9163      | -1.7581 | 1.5734  |         | H42 | -7.4126 | -3.3708 | -0.0314 |
| O32     | -0.7433      | 1.2932  | -3.5844 |         | H43 | 2.4866  | 5.0704  | 3.6819  |
| O33     | -5.3659      | 1.2167  | -3.5837 |         | H44 | 3.6761  | 2.1673  | 1.6873  |
| O34     | -2.9188      | 2.4024  | 0.1125  |         | H45 | -5.7533 | -2.4262 | 2.8880  |
| H1      | -4.6725      | -4.8365 | -4.6158 |         | H46 | 1.5920  | 2.7170  | -2.1083 |
| H2      | -3.9317      | 1.0097  | 2.8257  |         | H47 | 6.5858  | 1.5569  | 4.6160  |
| H3      | -2.9684      | 1.8565  | -0.7286 |         | H48 | 4.4238  | -1.0475 | 3.1965  |
| H4      | -0.9832      | -3.8466 | -2.6152 |         | H49 | -4.9261 | -3.6794 | -2.7364 |
| H5      | -6.2701      | -1.8473 | -3.1134 |         | H50 | 3.6105  | -0.9496 | -2.8506 |
| H6      | 0.2580       | -3.5851 | -0.5560 |         | H51 | 0.9683  | 3.7186  | 2.6837  |
| H7      | -0.2083      | -3.3222 | 1.6332  |         | H52 | 4.5853  | 5.9517  | 3.2370  |
| H8      | -5.0539      | 1.3938  | -4.5225 |         | H53 | 3.0411  | -1.9401 | 0.6408  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.2194 | -5.9824 | -3.0729 | H1  | 11.0300 | 0.2453  | 0.8349  |
| H55 | -2.9271 | -1.7289 | -0.2565 | H2  | 11.2665 | 0.4468  | 1.5062  |
| H56 | -3.6855 | -2.1720 | -1.5618 | end |         |         |         |
| H57 | 6.1933  | 3.5416  | -0.6143 | H1  | 9.3679  | 11.2225 | 5.8422  |
| H58 | 2.0777  | 2.1671  | 1.5644  | H2  | 8.9614  | 10.6185 | 5.9660  |
| H59 | 2.9527  | 1.7758  | -0.4867 | end |         |         |         |
| H60 | -5.7508 | -3.2660 | -1.4008 | H1  | 13.1799 | 9.4954  | 0.4224  |
| H61 | -2.9838 | -0.8069 | 1.8880  | H2  | 12.8607 | 9.5406  | -0.2416 |
| H62 | -2.5095 | -5.1426 | -3.6251 | end |         |         |         |
| H63 | 2.0840  | -0.9657 | 2.6547  | H1  | 10.0928 | 7.4517  | 9.4361  |
| H64 | -2.1642 | 1.0737  | -2.6703 | H2  | 10.1189 | 6.8355  | 9.8354  |
| H65 | 2.9186  | 0.8444  | -1.7801 | end |         |         |         |
| H66 | 5.7565  | 2.4328  | -2.7996 | H1  | 5.5501  | 0.3951  | 1.1416  |
| H67 | 0.8561  | -4.8576 | 0.1972  | H2  | 5.4965  | 1.1288  | 1.2181  |
| H68 | -5.6939 | -3.3083 | 1.5522  | end |         |         |         |
| end |         |         |         | H1  | 14.1848 | 6.6176  | 0.2022  |
| H1  | -4.8073 | 6.1744  | 3.6280  | H2  | 13.4773 | 6.7364  | 0.0440  |
| H2  | -4.2097 | 5.7641  | 3.4556  | end |         |         |         |
| end |         |         |         | H1  | 14.5931 | 4.4487  | 1.0277  |
| H1  | 9.3745  | 4.8395  | 1.4707  | H2  | 14.1782 | 4.8560  | 1.4850  |
| H2  | 8.9015  | 5.3562  | 1.7223  | end |         |         |         |
| end |         |         |         | H1  | 11.0810 | 3.4565  | 8.9167  |
| H1  | 9.7959  | 5.8089  | 5.5336  | H2  | 10.8660 | 2.9357  | 8.4377  |
| H2  | 9.3286  | 5.4546  | 5.0733  | end |         |         |         |
| end |         |         |         | H1  | 3.5090  | 2.6761  | 4.6985  |
| H1  | 8.1581  | 3.5513  | 4.2646  | H2  | 3.7335  | 3.1998  | 5.1711  |
| H2  | 8.6972  | 3.1353  | 3.9613  | end |         |         |         |
| end |         |         |         | H1  | 4.1137  | 5.9162  | 0.5163  |
| H1  | 15.6547 | 9.1051  | 4.6773  | H2  | 4.2537  | 6.2078  | -0.1478 |
| H2  | 15.3360 | 8.8380  | 4.0587  | end |         |         |         |
| end |         |         |         | H1  | 13.8457 | 2.6674  | 6.0437  |
| H1  | 15.6660 | 9.6063  | 6.8204  | H2  | 13.5327 | 2.1162  | 6.4121  |
| H2  | 16.3573 | 9.8645  | 6.9321  | end |         |         |         |
| end |         |         |         | H1  | 18.2607 | 5.0230  | 9.7997  |
| H1  | 13.5934 | 8.9109  | 7.7769  | H2  | 18.6857 | 5.1931  | 9.2255  |
| H2  | 13.6019 | 8.4214  | 7.2156  | end |         |         |         |
| end |         |         |         | H1  | 10.8141 | 8.7888  | 1.2952  |
| H1  | 13.2114 | 7.8004  | 5.2988  | H2  | 11.3173 | 8.7365  | 0.7640  |
| H2  | 13.1627 | 7.0635  | 5.2065  | end |         |         |         |
| end |         |         |         | H1  | 9.5381  | 11.2612 | 3.5528  |
| H1  | 13.4746 | 1.4053  | 3.8038  | H2  | 10.2407 | 11.3879 | 3.7288  |
| H2  | 13.7208 | 1.3118  | 4.4940  | end |         |         |         |
| end |         |         |         | H1  | 5.2107  | 3.1092  | 8.4166  |
| H1  | 5.6827  | 8.6657  | 0.2040  | H2  | 5.4099  | 3.8202  | 8.4196  |
| H2  | 5.0191  | 8.3556  | 0.1548  | end |         |         |         |
| end |         |         |         | H1  | 12.8044 | 4.6193  | 9.1790  |



|     |         |         |        |     |         |        |        |
|-----|---------|---------|--------|-----|---------|--------|--------|
| H2  | 12.4952 | 5.0002  | 8.6309 | H1  | 20.1616 | 8.3872 | 8.7331 |
| end |         |         |        | H2  | 20.5186 | 8.2401 | 8.1025 |
| H1  | 13.4316 | 13.1073 | 9.9550 | end |         |        |        |
| H2  | 13.0617 | 13.4083 | 9.3880 | end |         |        |        |
| end |         |         |        |     |         |        |        |

**(37) n=5 & m=5**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.6108 | -4.7773 | -0.0884 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.2683 | 0.3611  | -3.6259 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.0581  | -1.8939 | -3.0659 |
| O1      | 6.7387       | 3.8109  | 0.1351  |         | H12 | -3.7195 | -2.2169 | 1.8814  |
| O2      | 2.8974       | 1.7520  | 1.1918  |         | H13 | 0.2489  | 2.4820  | -2.9406 |
| O3      | 5.3064       | 3.0815  | -2.2209 |         | H14 | 6.0880  | 0.3362  | 3.6512  |
| O4      | 2.9789       | 1.8393  | -1.5316 |         | H15 | 4.9930  | -1.4178 | 4.6029  |
| O5      | 2.9471       | -0.8467 | 2.0832  |         | H16 | -0.1281 | 3.5594  | 0.6555  |
| O6      | -0.7667      | 1.2422  | 3.5677  |         | H17 | 2.8283  | -1.3620 | -1.5924 |
| O7      | 0.6435       | 2.9935  | 2.0808  |         | H18 | 1.1813  | 5.8888  | 3.2259  |
| O8      | 4.2073       | 5.1412  | 3.6842  |         | H19 | 4.5405  | 4.3669  | 3.1448  |
| O9      | 1.5052       | 5.0411  | 3.6602  |         | H20 | 2.2406  | -3.0759 | -0.0869 |
| O10     | 2.7937       | -0.7599 | -2.3878 |         | H21 | 4.4757  | 2.6044  | -1.9369 |
| O11     | 6.5492       | 1.2237  | 3.6284  |         | H22 | 0.1638  | -1.7961 | 3.1903  |
| O12     | -0.6376      | 3.8799  | -0.1437 |         | H23 | -0.8301 | 1.6219  | 4.4921  |
| O13     | 0.7707       | 3.1831  | -2.4512 |         | H24 | 7.6089  | 3.3041  | 0.0997  |
| O14     | -5.2051      | -3.0486 | 2.4072  |         | H25 | 1.4002  | -1.0573 | -3.2332 |
| O15     | -2.8216      | -1.7399 | -1.2076 |         | H26 | -1.0371 | 1.4590  | -4.5371 |
| O16     | -6.5242      | -3.7800 | -0.0220 |         | H27 | 0.1486  | -0.2243 | 3.5820  |
| O17     | -5.2391      | -2.9166 | -2.1994 |         | H28 | -1.6902 | 1.1184  | 3.1998  |
| O18     | -2.9557      | 0.9152  | -2.1263 |         | H29 | -1.4331 | -2.6122 | -1.7253 |
| O19     | 0.4970       | -1.2061 | -3.6491 |         | H30 | 0.0756  | 2.3824  | 2.6372  |
| O20     | -0.6070      | -3.0814 | -2.0314 |         | H31 | -0.1308 | 3.5841  | -0.9492 |
| O21     | -0.6942      | -3.0310 | 2.4805  |         | H32 | -1.4979 | -2.5486 | 2.1235  |
| O22     | 0.8289       | -3.8378 | 0.2764  |         | H33 | -2.9187 | -0.0278 | -1.8181 |
| O23     | -6.7337      | -1.1834 | -3.6454 |         | H34 | -4.6430 | -5.7652 | -3.3140 |
| O24     | -3.0764      | 0.8209  | 2.3098  |         | H35 | -3.0230 | 1.4089  | 1.5024  |
| O25     | -1.4783      | -5.1260 | -3.5633 |         | H36 | -2.0786 | 2.9810  | 0.0300  |
| O26     | -4.2362      | -4.9419 | -3.7152 |         | H37 | 2.9494  | 0.0921  | 1.7516  |
| O27     | 5.1569       | 3.0906  | 2.2287  |         | H38 | -6.1853 | -0.3502 | -3.6262 |
| O28     | 0.7124       | -1.0497 | 3.5761  |         | H39 | 5.7549  | 3.3641  | 1.4748  |
| O29     | 3.0494       | -2.4934 | -0.2233 |         | H40 | 5.6602  | 2.4087  | 2.7579  |
| O30     | 5.2547       | -1.1751 | 3.6619  |         | H41 | -4.4732 | 1.0915  | -3.0364 |
| O31     | -2.8833      | -1.7556 | 1.5964  |         | H42 | -7.4365 | -3.3649 | -0.0926 |
| O32     | -0.7071      | 1.2588  | -3.6080 |         | H43 | 2.5076  | 5.0888  | 3.6657  |
| O33     | -5.3012      | 1.2141  | -3.5765 |         | H44 | 3.6677  | 2.2080  | 1.6180  |
| O34     | -2.8973      | 2.4107  | 0.1070  |         | H45 | -5.7745 | -2.3768 | 2.8917  |
| H1      | -4.6399      | -4.8105 | -4.6268 |         | H46 | 1.6015  | 2.7255  | -2.1393 |
| H2      | -3.9287      | 1.0179  | 2.8038  |         | H47 | 6.5682  | 1.5806  | 4.5735  |
| H3      | -2.9196      | 1.8527  | -0.7275 |         | H48 | 4.4035  | -1.0154 | 3.1735  |
| H4      | -0.9305      | -3.8388 | -2.6017 |         | H49 | -4.8874 | -3.6875 | -2.7317 |
| H5      | -6.2110      | -1.8567 | -3.1181 |         | H50 | 3.6353  | -0.9390 | -2.8956 |
| H6      | 0.2789       | -3.5775 | -0.5080 |         | H51 | 0.9566  | 3.7347  | 2.6740  |
| H7      | -0.1660      | -3.3251 | 1.6869  |         | H52 | 4.6091  | 5.9547  | 3.2539  |
| H8      | -4.9853      | 1.4048  | -4.5121 |         | H53 | 3.0586  | -1.9143 | 0.5808  |

|     |         |         |         |
|-----|---------|---------|---------|
| H54 | -1.1775 | -5.9720 | -3.0977 |
| H55 | -2.8889 | -1.7459 | -0.2167 |
| H56 | -3.6476 | -2.1873 | -1.5232 |
| H57 | 6.2284  | 3.5529  | -0.6753 |
| H58 | 2.0684  | 2.2107  | 1.5150  |
| H59 | 2.9437  | 1.8154  | -0.5337 |
| H60 | -5.7443 | -3.2866 | -1.4116 |
| H61 | -2.9521 | -0.8005 | 1.8960  |
| H62 | -2.4719 | -5.1202 | -3.6169 |
| H63 | 2.1073  | -0.9314 | 2.6213  |
| H64 | -2.1251 | 1.0544  | -2.6671 |
| H65 | 2.9338  | 0.8876  | -1.8331 |
| H66 | 5.7961  | 2.4321  | -2.8111 |
| H67 | 0.8919  | -4.8377 | 0.2343  |
| H68 | -5.6975 | -3.2916 | 1.5817  |
| end |         |         |         |
| H1  | -4.5525 | 5.3901  | 3.2224  |
| H2  | -5.0729 | 4.8575  | 3.2103  |
| end |         |         |         |
| H1  | 9.5540  | 5.3312  | 1.4952  |
| H2  | 8.9903  | 4.9942  | 1.8475  |
| end |         |         |         |
| H1  | 9.5008  | 5.4172  | 5.3213  |
| H2  | 9.9033  | 4.8190  | 5.5027  |
| end |         |         |         |
| H1  | 8.7791  | 2.7378  | 3.9327  |
| H2  | 8.7491  | 3.3349  | 4.3759  |
| end |         |         |         |
| H1  | 15.0381 | 6.7472  | 5.9033  |
| H2  | 15.7084 | 6.7318  | 6.2233  |
| end |         |         |         |
| H1  | 16.3719 | 8.7984  | 6.2410  |
| H2  | 16.9283 | 9.2686  | 6.3965  |
| end |         |         |         |
| H1  | 14.3848 | 8.4761  | 8.3004  |
| H2  | 14.9925 | 8.7394  | 7.9593  |
| end |         |         |         |
| H1  | 13.2269 | 7.9788  | 5.4881  |
| H2  | 12.8985 | 7.3719  | 5.2119  |
| end |         |         |         |
| H1  | 14.9922 | 10.3108 | 5.3847  |
| H2  | 14.3534 | 10.5830 | 5.1134  |
| end |         |         |         |
| H1  | 8.6705  | 7.3423  | 4.1412  |
| H2  | 9.0150  | 7.0101  | 3.5710  |
| end |         |         |         |

|     |         |         |         |
|-----|---------|---------|---------|
| H1  | 13.4720 | 1.4460  | 3.8241  |
| H2  | 13.7241 | 1.3451  | 4.5116  |
| end |         |         |         |
| H1  | 5.7302  | 8.6829  | 0.2214  |
| H2  | 5.0618  | 8.3791  | 0.2125  |
| end |         |         |         |
| H1  | 11.0565 | 0.2422  | 0.8189  |
| H2  | 11.2825 | 0.4857  | 1.4800  |
| end |         |         |         |
| H1  | 9.4531  | 11.2209 | 5.7724  |
| H2  | 9.0345  | 10.6324 | 5.9272  |
| end |         |         |         |
| H1  | 13.2079 | 9.4759  | 0.4418  |
| H2  | 12.8719 | 9.5535  | -0.2112 |
| end |         |         |         |
| H1  | 10.1081 | 7.5284  | 9.3906  |
| H2  | 10.1362 | 6.8981  | 9.7675  |
| end |         |         |         |
| H1  | 5.5242  | 0.3925  | 1.1483  |
| H2  | 5.4577  | 1.1287  | 1.1476  |
| end |         |         |         |
| H1  | 14.1551 | 6.6315  | 0.2607  |
| H2  | 13.4557 | 6.7493  | 0.0691  |
| end |         |         |         |
| H1  | 14.5942 | 4.4637  | 1.0200  |
| H2  | 14.2247 | 4.8611  | 1.5230  |
| end |         |         |         |
| H1  | 11.0363 | 3.3611  | 8.9505  |
| H2  | 10.9565 | 2.9658  | 8.3298  |
| end |         |         |         |
| H1  | 3.4978  | 2.6930  | 4.6794  |
| H2  | 3.7319  | 3.2073  | 5.1568  |
| end |         |         |         |
| H1  | 4.1084  | 5.9592  | 0.5560  |
| H2  | 4.2321  | 6.2844  | -0.0959 |
| end |         |         |         |
| H1  | 13.8883 | 2.6538  | 6.0842  |
| H2  | 13.5862 | 2.1034  | 6.4624  |
| end |         |         |         |
| H1  | 18.2402 | 5.0414  | 9.7435  |
| H2  | 18.6850 | 5.2004  | 9.1802  |
| end |         |         |         |
| H1  | 10.8170 | 8.7980  | 1.2802  |
| H2  | 11.3170 | 8.7256  | 0.7483  |
| end |         |         |         |
| H1  | 9.5112  | 11.3267 | 3.5039  |

|     |         |         |        |
|-----|---------|---------|--------|
| H2  | 10.2235 | 11.4580 | 3.6287 |
| end |         |         |        |
| H1  | 5.2440  | 3.0650  | 8.4013 |
| H2  | 5.4307  | 3.7788  | 8.3784 |
| end |         |         |        |
| H1  | 12.8652 | 4.6111  | 9.1385 |
| H2  | 12.4723 | 4.9832  | 8.6398 |
| end |         |         |        |

|     |         |         |        |
|-----|---------|---------|--------|
| H1  | 13.4727 | 13.1408 | 9.8976 |
| H2  | 13.0805 | 13.4473 | 9.3514 |
| end |         |         |        |
| H1  | 20.1202 | 8.4476  | 8.7373 |
| H2  | 20.4703 | 8.2467  | 8.1178 |
| end |         |         |        |
| end |         |         |        |

(38) n=5 & m=6

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.5945 | -4.8337 | -0.0941 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.3141 | 0.3947  | -3.5980 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | -0.0044 | -1.8698 | -3.0971 |
| O1      | 6.7543       | 3.7957  | 0.1321  |         | H12 | -3.6924 | -2.2596 | 1.7746  |
| O2      | 2.9601       | 1.7302  | 1.2517  |         | H13 | 0.2314  | 2.4870  | -2.8856 |
| O3      | 5.2608       | 3.0920  | -2.2469 |         | H14 | 6.1681  | 0.3011  | 3.6732  |
| O4      | 2.9985       | 1.8016  | -1.4685 |         | H15 | 5.0446  | -1.4665 | 4.5583  |
| O5      | 3.0079       | -0.8732 | 2.0696  |         | H16 | -0.1069 | 3.5131  | 0.7021  |
| O6      | -0.7716      | 1.2343  | 3.5745  |         | H17 | 2.8227  | -1.3952 | -1.5757 |
| O7      | 0.6838       | 2.9652  | 2.1301  |         | H18 | 1.2417  | 5.8456  | 3.2010  |
| O8      | 4.2778       | 5.1695  | 3.6375  |         | H19 | 4.6154  | 4.3732  | 3.1339  |
| O9      | 1.5777       | 5.0156  | 3.6590  |         | H20 | 2.2531  | -3.0906 | -0.1549 |
| O10     | 2.7489       | -0.7700 | -2.3535 |         | H21 | 4.4586  | 2.5928  | -1.9218 |
| O11     | 6.6171       | 1.1957  | 3.6597  |         | H22 | 0.1802  | -1.8077 | 3.1175  |
| O12     | -0.6301      | 3.8130  | -0.0953 |         | H23 | -0.8593 | 1.6236  | 4.4930  |
| O13     | 0.7708       | 3.1600  | -2.3767 |         | H24 | 7.6220  | 3.2863  | 0.0980  |
| O14     | -5.1307      | -3.1011 | 2.3517  |         | H25 | 1.3442  | -1.0316 | -3.1811 |
| O15     | -2.8565      | -1.7310 | -1.3111 |         | H26 | -1.0233 | 1.4970  | -4.5408 |
| O16     | -6.5013      | -3.8364 | -0.0489 |         | H27 | 0.1791  | -0.2538 | 3.5571  |
| O17     | -5.2696      | -2.9227 | -2.2507 |         | H28 | -1.6849 | 1.1062  | 3.1787  |
| O18     | -3.0186      | 0.9110  | -2.1691 |         | H29 | -1.5071 | -2.6344 | -1.8079 |
| O19     | 0.4531       | -1.1570 | -3.6325 |         | H30 | 0.1139  | 2.3543  | 2.6863  |
| O20     | -0.6838      | -3.1087 | -2.1190 |         | H31 | -0.1180 | 3.5273  | -0.9042 |
| O21     | -0.6747      | -3.0252 | 2.3549  |         | H32 | -1.4828 | -2.5482 | 1.9991  |
| O22     | 0.8427       | -3.8454 | 0.1325  |         | H33 | -2.9790 | -0.0404 | -1.8803 |
| O23     | -6.8041      | -1.1475 | -3.6612 |         | H34 | -4.6591 | -5.7942 | -3.3020 |
| O24     | -3.0457      | 0.7667  | 2.2834  |         | H35 | -2.9988 | 1.3644  | 1.4817  |
| O25     | -1.5246      | -5.1556 | -3.6488 |         | H36 | -2.0613 | 2.9117  | 0.0316  |
| O26     | -4.2802      | -4.9732 | -3.7299 |         | H37 | 3.0163  | 0.0712  | 1.7513  |
| O27     | 5.2160       | 3.0548  | 2.2625  |         | H38 | -6.2559 | -0.3123 | -3.6491 |
| O28     | 0.7359       | -1.0798 | 3.5254  |         | H39 | 5.7937  | 3.3261  | 1.4926  |
| O29     | 3.0780       | -2.5215 | -0.2676 |         | H40 | 5.7311  | 2.3784  | 2.7895  |
| O30     | 5.3555       | -1.2165 | 3.6339  |         | H41 | -4.5327 | 1.0842  | -3.0567 |
| O31     | -2.8790      | -1.7769 | 1.4553  |         | H42 | -7.4113 | -3.4191 | -0.1133 |
| O32     | -0.7498      | 1.2953  | -3.5966 |         | H43 | 2.5783  | 5.0788  | 3.6567  |
| O33     | -5.3562      | 1.2111  | -3.6046 |         | H44 | 3.7283  | 2.1902  | 1.6793  |
| O34     | -2.8955      | 2.3592  | 0.0907  |         | H45 | -5.6865 | -2.4312 | 2.8535  |
| H1      | -4.6712      | -4.8827 | -4.6502 |         | H46 | 1.5931  | 2.6845  | -2.0770 |
| H2      | -3.8757      | 0.9839  | 2.8050  |         | H47 | 6.6110  | 1.5535  | 4.6008  |
| H3      | -2.9309      | 1.8129  | -0.7522 |         | H48 | 4.5211  | -1.0389 | 3.1266  |
| H4      | -1.0080      | -3.8589 | -2.7006 |         | H49 | -4.9313 | -3.6959 | -2.7920 |
| H5      | -6.2793      | -1.8232 | -3.1453 |         | H50 | 3.5773  | -0.9206 | -2.8927 |
| H6      | 0.2736       | -3.5992 | -0.6426 |         | H51 | 1.0090  | 3.7043  | 2.7206  |
| H7      | -0.1505      | -3.3178 | 1.5600  |         | H52 | 4.6628  | 5.9706  | 3.1684  |
| H8      | -5.0178      | 1.3876  | -4.5329 |         | H53 | 3.0881  | -1.9463 | 0.5380  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.2322 | -5.9835 | -3.1480 | H1  | 16.7311 | 7.7982  | 5.4853  |
| H55 | -2.9128 | -1.7393 | -0.3177 | H2  | 16.7723 | 7.1410  | 5.1407  |
| H56 | -3.6863 | -2.1792 | -1.6198 | end |         |         |         |
| H57 | 6.2418  | 3.5262  | -0.6708 | H1  | 10.8780 | 4.3332  | 3.4103  |
| H58 | 2.1271  | 2.1847  | 1.5674  | H2  | 10.5652 | 4.6810  | 3.9886  |
| H59 | 2.9946  | 1.7819  | -0.4704 | end |         |         |         |
| H60 | -5.7484 | -3.3022 | -1.4532 | H1  | 13.5438 | 1.3828  | 3.7278  |
| H61 | -2.9483 | -0.8358 | 1.7961  | H2  | 13.7703 | 1.2834  | 4.4242  |
| H62 | -2.5201 | -5.1448 | -3.7007 | end |         |         |         |
| H63 | 2.1677  | -0.9552 | 2.6069  | H1  | 5.7062  | 8.6620  | 0.1030  |
| H64 | -2.1849 | 1.0628  | -2.7039 | H2  | 5.0313  | 8.3745  | 0.0807  |
| H65 | 2.9330  | 0.8501  | -1.7706 | end |         |         |         |
| H66 | 5.7536  | 2.4486  | -2.8399 | H1  | 11.0871 | 0.2025  | 0.8285  |
| H67 | 0.9071  | -4.8467 | 0.1225  | H2  | 11.2905 | 0.4194  | 1.5057  |
| H68 | -5.6488 | -3.3442 | 1.5414  | end |         |         |         |
| end |         |         |         | H1  | 9.3593  | 11.2083 | 5.7911  |
| H1  | -4.4872 | 5.4050  | 3.0507  | H2  | 8.9454  | 10.6103 | 5.9174  |
| H2  | -5.0109 | 4.8762  | 3.0720  | end |         |         |         |
| end |         |         |         | H1  | 13.2322 | 9.5000  | 0.3521  |
| H1  | 8.8662  | 5.0533  | 1.6120  | H2  | 12.8682 | 9.6139  | -0.2801 |
| H2  | 9.4803  | 5.1760  | 1.2107  | end |         |         |         |
| end |         |         |         | H1  | 10.1712 | 7.4834  | 9.4488  |
| H1  | 9.0008  | 5.2434  | 5.2718  | H2  | 10.1448 | 6.8500  | 9.8196  |
| H2  | 9.2919  | 5.6422  | 5.8279  | end |         |         |         |
| end |         |         |         | H1  | 5.5905  | 0.3407  | 1.1540  |
| H1  | 8.2957  | 2.9624  | 4.4386  | H2  | 5.4848  | 1.0698  | 1.2216  |
| H2  | 9.0009  | 3.1053  | 4.2530  | end |         |         |         |
| end |         |         |         | H1  | 14.1823 | 6.6348  | 0.1475  |
| H1  | 14.6043 | 8.6963  | 4.3633  | H2  | 13.4692 | 6.6775  | -0.0241 |
| H2  | 14.9572 | 9.2453  | 4.0084  | end |         |         |         |
| end |         |         |         | H1  | 14.5156 | 4.4676  | 0.9055  |
| H1  | 16.4983 | 9.9545  | 6.4511  | H2  | 14.2168 | 4.7887  | 1.5016  |
| H2  | 15.9294 | 9.7659  | 6.0090  | end |         |         |         |
| end |         |         |         | H1  | 11.0100 | 3.3572  | 8.9493  |
| H1  | 14.6802 | 8.0471  | 8.2370  | H2  | 10.9157 | 2.9565  | 8.3344  |
| H2  | 15.0029 | 8.5002  | 7.7411  | end |         |         |         |
| end |         |         |         | H1  | 3.4655  | 2.7131  | 4.6325  |
| H1  | 13.1024 | 7.7497  | 5.5650  | H2  | 3.6766  | 3.2547  | 5.0912  |
| H2  | 13.1598 | 7.0516  | 5.3129  | end |         |         |         |
| end |         |         |         | H1  | 4.1102  | 5.9307  | 0.5337  |
| H1  | 13.2215 | 9.9579  | 6.4375  | H2  | 4.2561  | 6.2158  | -0.1322 |
| H2  | 13.5802 | 9.8548  | 5.7943  | end |         |         |         |
| end |         |         |         | H1  | 13.7933 | 2.6576  | 5.9726  |
| H1  | 8.8488  | 6.9854  | 3.8914  | H2  | 13.5181 | 2.0914  | 6.3486  |
| H2  | 9.0008  | 7.2812  | 3.2260  | end |         |         |         |
| end |         |         |         | H1  | 18.3309 | 5.0169  | 9.8623  |

|     |         |         |        |
|-----|---------|---------|--------|
| H2  | 18.7684 | 5.1770  | 9.2943 |
| end |         |         |        |
| H1  | 10.8602 | 8.7387  | 1.2275 |
| H2  | 11.3789 | 8.6792  | 0.7119 |
| end |         |         |        |
| H1  | 9.6180  | 11.2457 | 3.5586 |
| H2  | 10.3066 | 11.4487 | 3.7193 |
| end |         |         |        |
| H1  | 5.2461  | 3.1847  | 8.3978 |
| H2  | 5.4566  | 3.8922  | 8.4282 |
| end |         |         |        |

|     |         |         |        |
|-----|---------|---------|--------|
| H1  | 12.8027 | 4.6988  | 9.1430 |
| H2  | 12.3796 | 4.9620  | 8.6015 |
| end |         |         |        |
| H1  | 13.4497 | 13.0969 | 9.9726 |
| H2  | 13.1001 | 13.4031 | 9.3976 |
| end |         |         |        |
| H1  | 20.2550 | 8.5001  | 8.6150 |
| H2  | 20.6043 | 8.1163  | 8.0884 |
| end |         |         |        |
| end |         |         |        |

**(39) n=5 & m=7**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.6621 | -4.7433 | -0.0800 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.3619 | 0.3798  | -3.5589 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | -0.0268 | -1.9285 | -2.9844 |
| O1      | 6.7771       | 3.8654  | 0.1071  |         | H12 | -3.7254 | -2.2429 | 1.8641  |
| O2      | 2.9111       | 1.8702  | 1.2540  |         | H13 | 0.1840  | 2.4711  | -2.8875 |
| O3      | 5.2741       | 3.0962  | -2.2032 |         | H14 | 6.1587  | 0.4052  | 3.7004  |
| O4      | 2.9581       | 1.8445  | -1.4684 |         | H15 | 5.0085  | -1.4019 | 4.5905  |
| O5      | 2.9769       | -0.7373 | 2.0748  |         | H16 | -0.1796 | 3.6205  | 0.6991  |
| O6      | -0.7503      | 1.3106  | 3.5865  |         | H17 | 2.8125  | -1.3372 | -1.4828 |
| O7      | 0.6263       | 3.0860  | 2.1230  |         | H18 | 1.2106  | 5.9019  | 3.3028  |
| O8      | 4.2661       | 5.2349  | 3.6920  |         | H19 | 4.6166  | 4.4663  | 3.1549  |
| O9      | 1.5459       | 5.0591  | 3.7344  |         | H20 | 2.2413  | -2.9865 | -0.0597 |
| O10     | 2.7406       | -0.7378 | -2.2831 |         | H21 | 4.4558  | 2.6183  | -1.8921 |
| O11     | 6.6149       | 1.2930  | 3.7106  |         | H22 | 0.1808  | -1.7092 | 3.1633  |
| O12     | -0.6994      | 3.9051  | -0.1074 |         | H23 | -0.8370 | 1.6533  | 4.5237  |
| O13     | 0.7184       | 3.1670  | -2.4051 |         | H24 | 7.6265  | 3.3296  | 0.0724  |
| O14     | -5.1817      | -3.0549 | 2.4264  |         | H25 | 1.3087  | -1.0573 | -3.0854 |
| O15     | -2.9040      | -1.7458 | -1.2466 |         | H26 | -1.0605 | 1.4888  | -4.5188 |
| O16     | -6.5354      | -3.7495 | -0.0261 |         | H27 | 0.1848  | -0.1519 | 3.5966  |
| O17     | -5.2368      | -2.9336 | -2.1877 |         | H28 | -1.6661 | 1.1426  | 3.2181  |
| O18     | -3.0674      | 0.8635  | -2.1218 |         | H29 | -1.5562 | -2.6405 | -1.7238 |
| O19     | 0.4166       | -1.2051 | -3.5227 |         | H30 | 0.0787  | 2.4546  | 2.6783  |
| O20     | -0.7206      | -3.1118 | -2.0066 |         | H31 | -0.1827 | 3.6053  | -0.9048 |
| O21     | -0.6672      | -2.9380 | 2.4342  |         | H32 | -1.4891 | -2.4908 | 2.0711  |
| O22     | 0.8390       | -3.7760 | 0.1975  |         | H33 | -3.0114 | -0.0852 | -1.8223 |
| O23     | -6.7950      | -1.2019 | -3.5912 |         | H34 | -4.6606 | -5.7868 | -3.3019 |
| O24     | -3.0443      | 0.7696  | 2.3161  |         | H35 | -2.9874 | 1.3611  | 1.5132  |
| O25     | -1.5080      | -5.1358 | -3.5833 |         | H36 | -2.0753 | 2.9318  | 0.0040  |
| O26     | -4.2573      | -4.9604 | -3.6971 |         | H37 | 2.9658  | 0.2073  | 1.7593  |
| O27     | 5.2378       | 3.1746  | 2.2578  |         | H38 | -6.2641 | -0.3550 | -3.5826 |
| O28     | 0.7381       | -0.9836 | 3.5755  |         | H39 | 5.8118  | 3.4337  | 1.4818  |
| O29     | 3.0584       | -2.4060 | -0.1587 |         | H40 | 5.7614  | 2.5194  | 2.7964  |
| O30     | 5.3081       | -1.1390 | 3.6688  |         | H41 | -4.5555 | 1.0361  | -2.9871 |
| O31     | -2.9035      | -1.7683 | 1.5543  |         | H42 | -7.4340 | -3.3017 | -0.0658 |
| O32     | -0.8085      | 1.2722  | -3.5677 |         | H43 | 2.5448  | 5.1270  | 3.7356  |
| O33     | -5.3826      | 1.1614  | -3.5339 |         | H44 | 3.6861  | 2.3173  | 1.6788  |
| O34     | -2.8940      | 2.3597  | 0.0918  |         | H45 | -5.7397 | -2.3694 | 2.9042  |
| H1      | -4.6619      | -4.8130 | -4.6044 |         | H46 | 1.5461  | 2.7061  | -2.0976 |
| H2      | -3.8565      | 1.0299  | 2.8392  |         | H47 | 6.5868  | 1.6129  | 4.6655  |
| H3      | -2.9480      | 1.8026  | -0.7432 |         | H48 | 4.4754  | -0.9467 | 3.1652  |
| H4      | -1.0160      | -3.8700 | -2.5929 |         | H49 | -4.9056 | -3.7128 | -2.7247 |
| H5      | -6.2509      | -1.8651 | -3.0772 |         | H50 | 3.5595  | -0.9244 | -2.8214 |
| H6      | 0.2619       | -3.5336 | -0.5756 |         | H51 | 0.9540  | 3.8093  | 2.7315  |
| H7      | -0.1445      | -3.2485 | 1.6465  |         | H52 | 4.6556  | 6.0534  | 3.2625  |
| H8      | -5.0486      | 1.3559  | -4.4593 |         | H53 | 3.0500  | -1.8180 | 0.6417  |



|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.2107 | -5.9788 | -3.1111 | H1  | 15.1568 | 11.1656 | 5.3642  |
| H55 | -2.9578 | -1.7536 | -0.2549 | H2  | 14.5228 | 11.1200 | 4.9816  |
| H56 | -3.7351 | -2.1978 | -1.5587 | end |         |         |         |
| H57 | 6.2479  | 3.5939  | -0.6856 | H1  | 10.4341 | 4.4337  | 4.3307  |
| H58 | 2.0823  | 2.3341  | 1.5704  | H2  | 10.6726 | 3.9560  | 3.8139  |
| H59 | 2.9397  | 1.8617  | -0.4707 | end |         |         |         |
| H60 | -5.7492 | -3.2900 | -1.3955 | H1  | 14.3416 | 9.0541  | 8.1939  |
| H61 | -2.9744 | -0.8159 | 1.8693  | H2  | 14.9671 | 9.0265  | 7.7923  |
| H62 | -2.5033 | -5.1360 | -3.6335 | end |         |         |         |
| H63 | 2.1453  | -0.8427 | 2.6209  | H1  | 8.3363  | 3.5063  | 2.8506  |
| H64 | -2.2450 | 1.0257  | -2.6684 | H2  | 8.4569  | 3.3775  | 2.1304  |
| H65 | 2.8998  | 0.8799  | -1.7366 | end |         |         |         |
| H66 | 5.7561  | 2.4377  | -2.7875 | H1  | 13.5773 | 1.5037  | 3.6558  |
| H67 | 0.9117  | -4.7757 | 0.1761  | H2  | 13.7550 | 1.3940  | 4.3647  |
| H68 | -5.6808 | -3.2985 | 1.6066  | end |         |         |         |
| end |         |         |         | H1  | 5.6754  | 8.7217  | 0.1541  |
| H1  | -4.6425 | 5.9124  | 3.0088  | H2  | 5.0079  | 8.4172  | 0.1324  |
| H2  | -4.7958 | 5.2018  | 2.8614  | end |         |         |         |
| end |         |         |         | H1  | 11.0794 | 0.2508  | 0.8752  |
| H1  | 9.9331  | 5.8552  | 1.7490  | H2  | 11.3133 | 0.4583  | 1.5452  |
| H2  | 9.4249  | 5.4707  | 2.1340  | end |         |         |         |
| end |         |         |         | H1  | 9.4252  | 11.2265 | 5.6438  |
| H1  | 9.2459  | 5.7807  | 5.9072  | H2  | 9.0461  | 10.6406 | 5.8858  |
| H2  | 9.1649  | 6.0882  | 5.2361  | end |         |         |         |
| end |         |         |         | H1  | 13.2378 | 9.5796  | 0.4516  |
| H1  | 7.6217  | 3.6115  | 4.9184  | H2  | 12.8820 | 9.6605  | -0.1902 |
| H2  | 7.9485  | 4.2631  | 4.7814  | end |         |         |         |
| end |         |         |         | H1  | 10.2062 | 7.5951  | 9.4827  |
| H1  | 15.1930 | 8.2197  | 3.9868  | H2  | 10.1417 | 6.9277  | 9.7825  |
| H2  | 15.0655 | 7.9395  | 4.6644  | end |         |         |         |
| end |         |         |         | H1  | 5.5089  | 0.4238  | 1.2175  |
| H1  | 16.8337 | 9.5797  | 6.2869  | H2  | 5.4539  | 1.1591  | 1.2814  |
| H2  | 16.3857 | 9.2743  | 5.7770  | end |         |         |         |
| end |         |         |         | H1  | 14.1479 | 6.5892  | 0.2669  |
| H1  | 15.4027 | 7.1589  | 7.0720  | H2  | 13.4531 | 6.7106  | 0.0606  |
| H2  | 15.9182 | 6.6984  | 6.7980  | end |         |         |         |
| end |         |         |         | H1  | 14.5830 | 4.5286  | 1.0173  |
| H1  | 13.2022 | 6.8483  | 5.6856  | H2  | 14.3054 | 4.8330  | 1.6318  |
| H2  | 13.1966 | 7.5834  | 5.7913  | end |         |         |         |
| end |         |         |         | H1  | 11.0315 | 3.4078  | 8.9898  |
| H1  | 12.6504 | 9.5459  | 5.8832  | H2  | 10.9073 | 2.9840  | 8.3957  |
| H2  | 13.3548 | 9.7676  | 5.9373  | end |         |         |         |
| end |         |         |         | H1  | 3.4006  | 2.7896  | 4.5779  |
| H1  | 8.6867  | 7.6213  | 3.9323  | H2  | 3.6151  | 3.2965  | 5.0721  |
| H2  | 8.9662  | 7.2275  | 3.3689  | end |         |         |         |
| end |         |         |         | H1  | 4.1147  | 6.0078  | 0.6264  |

|     |         |         |         |
|-----|---------|---------|---------|
| H2  | 4.2571  | 6.2877  | -0.0427 |
| end |         |         |         |
| H1  | 13.7973 | 2.6283  | 5.9945  |
| H2  | 13.5481 | 2.0340  | 6.3446  |
| end |         |         |         |
| H1  | 18.2695 | 5.1079  | 9.8850  |
| H2  | 18.6863 | 5.2701  | 9.3021  |
| end |         |         |         |
| H1  | 10.8434 | 8.8084  | 1.2866  |
| H2  | 11.3890 | 8.7522  | 0.8000  |
| end |         |         |         |
| H1  | 9.6321  | 11.3450 | 3.5168  |
| H2  | 10.3166 | 11.5860 | 3.6339  |
| end |         |         |         |

|     |         |         |        |
|-----|---------|---------|--------|
| H1  | 5.2248  | 3.2361  | 8.4371 |
| H2  | 5.3493  | 3.9616  | 8.4971 |
| end |         |         |        |
| H1  | 12.8032 | 4.7375  | 9.2102 |
| H2  | 12.3615 | 5.0070  | 8.6873 |
| end |         |         |        |
| H1  | 13.4206 | 13.1910 | 9.9256 |
| H2  | 13.0374 | 13.4905 | 9.3688 |
| end |         |         |        |
| H1  | 20.1034 | 8.5040  | 8.6619 |
| H2  | 20.4729 | 8.0117  | 8.2520 |
| end |         |         |        |
| end |         |         |        |

**(40) n=5 & m=8**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.7044 | -4.7964 | -0.0583 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.4229 | 0.3650  | -3.5693 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | -0.1133 | -1.9551 | -2.9873 |
| O1      | 6.7858       | 3.8907  | 0.0561  |         | H12 | -3.7844 | -2.2753 | 1.7851  |
| O2      | 2.9298       | 1.8286  | 1.2117  |         | H13 | 0.1799  | 2.4758  | -2.8756 |
| O3      | 5.2706       | 3.1464  | -2.3273 |         | H14 | 6.1257  | 0.3884  | 3.6716  |
| O4      | 2.9694       | 1.8624  | -1.5135 |         | H15 | 5.0034  | -1.3707 | 4.5212  |
| O5      | 3.0247       | -0.7502 | 2.0374  |         | H16 | -0.1905 | 3.5536  | 0.7240  |
| O6      | -0.7808      | 1.2752  | 3.5805  |         | H17 | 2.7550  | -1.3184 | -1.5042 |
| O7      | 0.6478       | 3.0104  | 2.1182  |         | H18 | 1.2373  | 5.8709  | 3.2360  |
| O8      | 4.2765       | 5.1880  | 3.6252  |         | H19 | 4.6305  | 4.4180  | 3.0907  |
| O9      | 1.5679       | 5.0327  | 3.6725  |         | H20 | 2.2065  | -2.9735 | -0.0588 |
| O10     | 2.6629       | -0.7245 | -2.3032 |         | H21 | 4.4645  | 2.6618  | -1.9987 |
| O11     | 6.5811       | 1.2802  | 3.7013  |         | H22 | 0.1691  | -1.7319 | 3.0856  |
| O12     | -0.7273      | 3.8406  | -0.0710 |         | H23 | -0.8680 | 1.6393  | 4.5090  |
| O13     | 0.7122       | 3.1648  | -2.3854 |         | H24 | 7.6232  | 3.3362  | 0.0407  |
| O14     | -5.2057      | -3.0788 | 2.3644  |         | H25 | 1.2077  | -1.0662 | -3.1149 |
| O15     | -2.9639      | -1.7854 | -1.2899 |         | H26 | -1.0811 | 1.4882  | -4.5272 |
| O16     | -6.5676      | -3.8034 | -0.0282 |         | H27 | 0.1976  | -0.1886 | 3.5318  |
| O17     | -5.2943      | -2.9431 | -2.2146 |         | H28 | -1.6955 | 1.1054  | 3.2127  |
| O18     | -3.1163      | 0.8209  | -2.1258 |         | H29 | -1.6125 | -2.6768 | -1.7278 |
| O19     | 0.3119       | -1.2282 | -3.5337 |         | H30 | 0.0764  | 2.4053  | 2.6781  |
| O20     | -0.7814      | -3.1612 | -2.0079 |         | H31 | -0.2133 | 3.5655  | -0.8777 |
| O21     | -0.7422      | -2.9482 | 2.3853  |         | H32 | -1.5692 | -2.5087 | 2.0224  |
| O22     | 0.7801       | -3.7444 | 0.2180  |         | H33 | -3.0619 | -0.1355 | -1.8451 |
| O23     | -6.8498      | -1.1774 | -3.6190 |         | H34 | -4.7117 | -5.7806 | -3.3420 |
| O24     | -3.0758      | 0.7339  | 2.3054  |         | H35 | -3.0202 | 1.3144  | 1.4926  |
| O25     | -1.5811      | -5.0970 | -3.6763 |         | H36 | -2.1069 | 2.8711  | 0.0139  |
| O26     | -4.3196      | -4.9534 | -3.7401 |         | H37 | 3.0013  | 0.1938  | 1.7136  |
| O27     | 5.2349       | 3.1304  | 2.2045  |         | H38 | -6.3126 | -0.3360 | -3.6245 |
| O28     | 0.7495       | -1.0166 | 3.4805  |         | H39 | 5.8209  | 3.4136  | 1.4497  |
| O29     | 3.0384       | -2.4191 | -0.1702 |         | H40 | 5.7579  | 2.4805  | 2.7551  |
| O30     | 5.3242       | -1.1208 | 3.6013  |         | H41 | -4.5711 | 1.0259  | -3.0282 |
| O31     | -2.9698      | -1.7942 | 1.4645  |         | H42 | -7.4604 | -3.3485 | -0.0725 |
| O32     | -0.8409      | 1.2715  | -3.5777 |         | H43 | 2.5693  | 5.0797  | 3.6601  |
| O33     | -5.3873      | 1.1654  | -3.5880 |         | H44 | 3.6983  | 2.2934  | 1.6304  |
| O34     | -2.9379      | 2.3148  | 0.0953  |         | H45 | -5.7411 | -2.3760 | 2.8415  |
| H1      | -4.6945      | -4.8403 | -4.6631 |         | H46 | 1.5462  | 2.7088  | -2.0848 |
| H2      | -3.8824      | 1.0062  | 2.8291  |         | H47 | 6.5128  | 1.5983  | 4.6544  |
| H3      | -2.9985      | 1.7561  | -0.7382 |         | H48 | 4.4997  | -0.9167 | 3.0847  |
| H4      | -1.0904      | -3.8899 | -2.6254 |         | H49 | -4.9659 | -3.7131 | -2.7687 |
| H5      | -6.3077      | -1.8376 | -3.1014 |         | H50 | 3.4744  | -0.9064 | -2.8502 |
| H6      | 0.2071       | -3.5282 | -0.5655 |         | H51 | 0.9646  | 3.7523  | 2.7080  |
| H7      | -0.2087      | -3.2492 | 1.5970  |         | H52 | 4.6333  | 6.0156  | 3.1828  |
| H8      | -5.0418      | 1.3591  | -4.5074 |         | H53 | 3.0566  | -1.8224 | 0.6258  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.2545 | -5.9354 | -3.2169 | H1  | 17.1343 | 7.3956  | 4.7388  |
| H55 | -3.0250 | -1.7745 | -0.2964 | H2  | 16.9640 | 7.4754  | 5.4564  |
| H56 | -3.7973 | -2.2365 | -1.6017 | end |         |         |         |
| H57 | 6.2644  | 3.6255  | -0.7416 | H1  | 10.4727 | 4.4673  | 3.9884  |
| H58 | 2.0934  | 2.2692  | 1.5414  | H2  | 10.2595 | 3.7829  | 3.7893  |
| H59 | 2.9663  | 1.8727  | -0.5157 | end |         |         |         |
| H60 | -5.7863 | -3.3166 | -1.4216 | H1  | 14.9302 | 8.9659  | 8.0329  |
| H61 | -3.0270 | -0.8582 | 1.8234  | H2  | 14.4060 | 8.6765  | 8.4732  |
| H62 | -2.5775 | -5.1313 | -3.7295 | end |         |         |         |
| H63 | 2.1855  | -0.8688 | 2.5694  | H1  | 8.0593  | 3.5793  | 2.7488  |
| H64 | -2.2951 | 0.9969  | -2.6665 | H2  | 8.2965  | 3.2404  | 2.1342  |
| H65 | 2.8819  | 0.9015  | -1.7824 | end |         |         |         |
| H66 | 5.7608  | 2.4756  | -2.8901 | H1  | 12.8832 | 9.7558  | 6.3483  |
| H67 | 0.8904  | -4.7383 | 0.1891  | H2  | 13.3246 | 9.6099  | 5.7694  |
| H68 | -5.7222 | -3.3264 | 1.5531  | end |         |         |         |
| end |         |         |         | H1  | 10.9659 | 6.4334  | 4.7974  |
| H1  | -4.4711 | 5.7180  | 2.9722  | H2  | 11.2590 | 6.4091  | 4.1177  |
| H2  | -5.0849 | 5.5266  | 3.3437  | end |         |         |         |
| end |         |         |         | H1  | 13.5529 | 1.4271  | 3.6498  |
| H1  | 8.9977  | 5.1539  | 1.6618  | H2  | 13.7466 | 1.2862  | 4.3483  |
| H2  | 9.2558  | 5.7877  | 1.3717  | end |         |         |         |
| end |         |         |         | H1  | 5.5939  | 8.7166  | 0.0900  |
| H1  | 8.7494  | 5.9002  | 5.8705  | H2  | 4.9115  | 8.4477  | 0.1133  |
| H2  | 9.0128  | 5.8940  | 5.1768  | end |         |         |         |
| end |         |         |         | H1  | 11.0616 | 0.2642  | 0.8474  |
| H1  | 7.6507  | 3.4338  | 4.7609  | H2  | 11.2875 | 0.4721  | 1.5199  |
| H2  | 7.8966  | 4.1184  | 4.9003  | end |         |         |         |
| end |         |         |         | H1  | 9.3480  | 11.3679 | 5.6996  |
| H1  | 14.9077 | 9.2244  | 4.1709  | H2  | 9.1766  | 10.6724 | 5.8767  |
| H2  | 14.7489 | 8.5253  | 4.3665  | end |         |         |         |
| end |         |         |         | H1  | 13.2393 | 9.6504  | 0.3826  |
| H1  | 16.5763 | 9.7542  | 6.5445  | H2  | 12.8907 | 9.7910  | -0.2525 |
| H2  | 16.0352 | 9.4689  | 6.1210  | end |         |         |         |
| end |         |         |         | H1  | 10.1750 | 7.5354  | 9.3944  |
| H1  | 15.4680 | 7.1102  | 7.3306  | H2  | 10.2245 | 6.8835  | 9.7283  |
| H2  | 15.8823 | 6.5846  | 7.0103  | end |         |         |         |
| end |         |         |         | H1  | 5.5704  | 0.4021  | 1.1441  |
| H1  | 13.4315 | 6.8515  | 5.5382  | H2  | 5.4205  | 1.1160  | 1.2662  |
| H2  | 13.4179 | 7.5560  | 5.7747  | end |         |         |         |
| end |         |         |         | H1  | 14.1257 | 6.5510  | 0.1995  |
| H1  | 15.0904 | 11.3455 | 5.2991  | H2  | 13.4108 | 6.5729  | 0.0288  |
| H2  | 14.4559 | 11.2636 | 4.9252  | end |         |         |         |
| end |         |         |         | H1  | 14.6061 | 4.3825  | 0.9788  |
| H1  | 9.2365  | 7.5364  | 3.3795  | H2  | 14.2652 | 4.7621  | 1.5143  |
| H2  | 8.6255  | 7.2242  | 3.6596  | end |         |         |         |
| end |         |         |         | H1  | 10.9923 | 3.3876  | 8.9314  |

|     |         |        |         |
|-----|---------|--------|---------|
| H2  | 10.9133 | 2.9885 | 8.3126  |
| end |         |        |         |
| H1  | 3.3203  | 2.8104 | 4.5534  |
| H2  | 3.5011  | 3.3332 | 5.0446  |
| end |         |        |         |
| H1  | 4.0764  | 5.9394 | 0.5943  |
| H2  | 4.2209  | 6.2070 | -0.0793 |
| end |         |        |         |
| H1  | 13.6487 | 2.6120 | 5.9136  |
| H2  | 13.5127 | 2.0119 | 6.3122  |
| end |         |        |         |
| H1  | 18.3123 | 5.0831 | 9.8806  |
| H2  | 18.7230 | 5.2359 | 9.2909  |
| end |         |        |         |
| H1  | 10.8945 | 8.7965 | 1.1995  |
| H2  | 11.4204 | 8.7362 | 0.6918  |
| end |         |        |         |

|     |         |         |        |
|-----|---------|---------|--------|
| H1  | 9.6215  | 11.3650 | 3.4866 |
| H2  | 10.2950 | 11.6011 | 3.6627 |
| end |         |         |        |
| H1  | 5.1974  | 3.2681  | 8.4143 |
| H2  | 5.3391  | 3.9881  | 8.4972 |
| end |         |         |        |
| H1  | 12.6549 | 4.8577  | 9.2301 |
| H2  | 12.3231 | 5.0299  | 8.5969 |
| end |         |         |        |
| H1  | 13.3665 | 13.0928 | 9.9173 |
| H2  | 12.9910 | 13.4757 | 9.4094 |
| end |         |         |        |
| H1  | 20.2227 | 8.4561  | 8.6255 |
| H2  | 20.5302 | 8.0664  | 8.0775 |
| end |         |         |        |
| end |         |         |        |

**(41) n=6 & m=1**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.6723 | -4.8672 | -0.0059 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.4242 | 0.4058  | -3.4771 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.2539  | -1.8721 | -3.0227 |
| O1      | 6.7826       | 3.8586  | 0.1262  |         | H12 | -3.7270 | -2.3710 | 1.9239  |
| O2      | 3.0239       | 1.9164  | 1.2371  |         | H13 | 0.0065  | 2.3941  | -2.7714 |
| O3      | 5.3787       | 3.1756  | -2.3196 |         | H14 | 6.2391  | 0.5350  | 3.7036  |
| O4      | 3.0387       | 2.0259  | -1.5661 |         | H15 | 5.1538  | -1.3601 | 4.4328  |
| O5      | 3.1413       | -0.7355 | 2.1303  |         | H16 | -0.2433 | 3.5599  | 0.7532  |
| O6      | -0.5606      | 1.2718  | 3.4466  |         | H17 | 3.0908  | -1.2647 | -1.5373 |
| O7      | 0.7383       | 3.1958  | 2.1073  |         | H18 | 1.1712  | 5.9767  | 3.3532  |
| O8      | 4.3888       | 5.2435  | 3.7532  |         | H19 | 4.7283  | 4.4664  | 3.2179  |
| O9      | 1.4746       | 5.1466  | 3.8450  |         | H20 | 2.3868  | -2.9595 | -0.0673 |
| O10     | 3.0553       | -0.7184 | -2.3674 |         | H21 | 4.5190  | 2.7913  | -1.9838 |
| O11     | 6.7395       | 1.3972  | 3.7149  |         | H22 | 0.2943  | -1.7778 | 3.0530  |
| O12     | -0.8100      | 3.7820  | -0.0431 |         | H23 | -0.6401 | 1.5741  | 4.3999  |
| O13     | 0.5281       | 3.1242  | -2.3161 |         | H24 | 7.6052  | 3.2754  | 0.1224  |
| O14     | -5.1787      | -3.1006 | 2.4317  |         | H25 | 1.6430  | -1.0547 | -3.1230 |
| O15     | -3.0484      | -1.8785 | -1.2441 |         | H26 | -1.1447 | 1.4839  | -4.4246 |
| O16     | -6.4849      | -3.8836 | 0.0324  |         | H27 | 0.3322  | -0.2105 | 3.4605  |
| O17     | -5.2191      | -3.1868 | -2.2568 |         | H28 | -1.4901 | 1.1001  | 3.1131  |
| O18     | -3.2660      | 0.7442  | -2.0529 |         | H29 | -1.4622 | -2.7398 | -1.8023 |
| O19     | 0.7245       | -1.1548 | -3.5296 |         | H30 | 0.2165  | 2.5038  | 2.6176  |
| O20     | -0.6343      | -3.1352 | -2.1730 |         | H31 | -0.2940 | 3.5075  | -0.8581 |
| O21     | -0.5527      | -2.9989 | 2.3821  |         | H32 | -1.4245 | -2.6005 | 2.0756  |
| O22     | 0.9737       | -3.7939 | 0.0908  |         | H33 | -3.2047 | -0.1968 | -1.7259 |
| O23     | -6.6707      | -1.3820 | -3.7471 |         | H34 | -4.7614 | -5.9874 | -3.3685 |
| O24     | -2.9573      | 0.7621  | 2.4162  |         | H35 | -2.9603 | 1.3465  | 1.6039  |
| O25     | -1.4134      | -5.1753 | -3.8138 |         | H36 | -2.1555 | 2.8244  | 0.0695  |
| O26     | -4.2789      | -5.2132 | -3.7723 |         | H37 | 3.0836  | 0.1972  | 1.7949  |
| O27     | 5.2438       | 3.1736  | 2.2730  |         | H38 | -6.1720 | -0.5175 | -3.6637 |
| O28     | 0.8523       | -1.0665 | 3.4899  |         | H39 | 5.8069  | 3.4356  | 1.4892  |
| O29     | 3.2260       | -2.4098 | -0.1390 |         | H40 | 5.7704  | 2.4996  | 2.7907  |
| O30     | 5.4797       | -1.0633 | 3.5293  |         | H41 | -4.6715 | 0.9128  | -2.9518 |
| O31     | -2.8816      | -1.9259 | 1.6234  |         | H42 | -7.3586 | -3.3855 | -0.0244 |
| O32     | -0.9491      | 1.2440  | -3.4624 |         | H43 | 2.4624  | 5.1566  | 3.8473  |
| O33     | -5.4845      | 1.0608  | -3.5192 |         | H44 | 3.8112  | 2.3797  | 1.6380  |
| O34     | -2.9868      | 2.2713  | 0.1825  |         | H45 | -5.7001 | -2.3370 | 2.8413  |
| H1      | -4.6590      | -5.0108 | -4.6769 |         | H46 | 1.3885  | 2.7178  | -2.0386 |
| H2      | -3.7570      | 1.0286  | 2.9680  |         | H47 | 6.7592  | 1.7228  | 4.6725  |
| H3      | -3.0725      | 1.6808  | -0.6212 |         | H48 | 4.6467  | -0.8963 | 3.0054  |
| H4      | -0.9376      | -3.8691 | -2.7806 |         | H49 | -4.8808 | -3.9739 | -2.7825 |
| H5      | -6.1544      | -2.0467 | -3.2107 |         | H50 | 3.8602  | -0.9959 | -2.8992 |
| H6      | 0.4124       | -3.6012 | -0.7019 |         | H51 | 1.0088  | 3.9138  | 2.7489  |
| H7      | -0.0799      | -3.2924 | 1.5591  |         | H52 | 4.8035  | 6.0404  | 3.3113  |
| H8      | -5.1216      | 1.3356  | -4.4152 |         | H53 | 3.2255  | -1.8090 | 0.6519  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.0739 | -5.9809 | -3.3024 | H1  | 15.0017 | 4.7887  | 1.9689  |
| H55 | -3.1148 | -1.9273 | -0.2579 | H2  | 14.6959 | 4.5375  | 1.3469  |
| H56 | -3.8216 | -2.3953 | -1.6126 | end |         |         |         |
| H57 | 6.2672  | 3.6137  | -0.6816 | H1  | 12.5517 | 1.7729  | 0.3157  |
| H58 | 2.2156  | 2.3878  | 1.5861  | H2  | 12.1024 | 1.1981  | 0.4103  |
| H59 | 3.0275  | 2.0235  | -0.5724 | end |         |         |         |
| H60 | -5.7109 | -3.5246 | -1.4518 | H1  | 12.3583 | 2.3743  | 8.1843  |
| H61 | -2.9300 | -0.9808 | 1.9235  | H2  | 12.0067 | 3.0194  | 8.2543  |
| H62 | -2.4007 | -5.2428 | -3.8633 | end |         |         |         |
| H63 | 2.3018  | -0.8662 | 2.6668  | H1  | 7.7591  | 0.0652  | 0.6172  |
| H64 | -2.4341 | 0.8910  | -2.5843 | H2  | 7.4152  | -0.2480 | 0.0468  |
| H65 | 3.0684  | 1.0706  | -1.8389 | end |         |         |         |
| H66 | 5.7960  | 2.4135  | -2.8304 | H1  | 7.3176  | 9.4321  | 0.5837  |
| H67 | 1.0379  | -4.7949 | 0.1163  | H2  | 6.9949  | 9.6959  | -0.0269 |
| H68 | -5.6529 | -3.3836 | 1.6072  | end |         |         |         |
| end |         |         |         | H1  | 13.6268 | 1.9179  | 5.7658  |
| H1  | 8.8181  | 4.9338  | 1.9183  | H2  | 13.8340 | 2.4880  | 6.1813  |
| H2  | 9.3470  | 5.3626  | 1.6135  | end |         |         |         |
| end |         |         |         | H1  | 9.9370  | 12.7666 | 5.7817  |
| H1  | 13.6456 | 8.8938  | 6.7728  | H2  | 10.1883 | 12.3199 | 6.3094  |
| H2  | 13.2268 | 8.3952  | 7.1375  | end |         |         |         |
| end |         |         |         | H1  | 19.8990 | 11.2459 | 3.9865  |
| H1  | 15.1489 | 3.2281  | 3.9142  | H2  | 19.5549 | 11.7050 | 3.5277  |
| H2  | 14.5674 | 3.0779  | 4.3388  | end |         |         |         |
| end |         |         |         | H1  | 9.8981  | 10.5870 | -0.0784 |
| H1  | 16.1262 | 5.9295  | 0.6771  | H2  | 10.3835 | 10.0582 | -0.2333 |
| H2  | 16.2695 | 6.3067  | 0.0616  | end |         |         |         |
| end |         |         |         | H1  | 16.6923 | 10.3151 | 1.4143  |
| H1  | 20.1338 | 9.8031  | 10.1528 | H2  | 17.2814 | 9.8778  | 1.3667  |
| H2  | 19.4757 | 9.8677  | 9.8286  | end |         |         |         |
| end |         |         |         | H1  | 10.3234 | 11.7366 | 4.0402  |
| H1  | 8.7066  | 10.3610 | 5.7868  | H2  | 9.9543  | 11.3406 | 3.5424  |
| H2  | 9.2549  | 10.7378 | 5.4720  | end |         |         |         |
| end |         |         |         | H1  | 6.8388  | 3.7591  | 7.7817  |
| H1  | 11.7055 | 9.0682  | 0.9628  | H2  | 6.9891  | 4.2694  | 8.2865  |
| H2  | 11.6598 | 8.5456  | 0.4476  | end |         |         |         |
| end |         |         |         | H1  | 4.7109  | 3.1145  | 8.7241  |
| H1  | 8.8895  | 9.1812  | 8.3617  | H2  | 4.9925  | 3.7911  | 8.6531  |
| H2  | 9.2689  | 8.8936  | 7.7987  | end |         |         |         |
| end |         |         |         | H1  | 11.8942 | 5.0318  | 8.7939  |
| H1  | 5.9645  | 0.6349  | 1.6629  | H2  | 12.1169 | 4.7136  | 9.4204  |
| H2  | 5.2644  | 0.7163  | 1.4538  | end |         |         |         |
| end |         |         |         | H1  | 10.7566 | 11.7104 | 9.8380  |
| H1  | 4.1911  | 4.2242  | -0.4229 | H2  | 11.4573 | 11.8166 | 9.6579  |
| H2  | 4.2134  | 3.6309  | 0.0094  | end |         |         |         |
| end |         |         |         | H1  | 19.3469 | 7.6313  | 9.5764  |

|     |         |        |        |     |
|-----|---------|--------|--------|-----|
| H2  | 19.9429 | 7.4865 | 9.1695 | end |
| end |         |        |        |     |



**(42) n=6 & m=2**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.6886 | -4.9211 | 0.0104  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.4210 | 0.4962  | -3.4981 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.1205  | -1.8408 | -3.2006 |
| O1      | 6.6904       | 3.9624  | 0.1384  |         | H12 | -3.6793 | -2.3529 | 1.7314  |
| O2      | 3.1098       | 1.9052  | 1.3532  |         | H13 | 0.0482  | 2.4298  | -2.6899 |
| O3      | 5.2472       | 3.2097  | -2.2756 |         | H14 | 6.4238  | 0.4049  | 3.6562  |
| O4      | 2.9551       | 1.9662  | -1.4370 |         | H15 | 5.1644  | -1.4432 | 4.3722  |
| O5      | 3.1913       | -0.7701 | 2.1608  |         | H16 | -0.2304 | 3.4902  | 0.8314  |
| O6      | -0.4511      | 1.2469  | 3.5248  |         | H17 | 2.9422  | -1.2894 | -1.5178 |
| O7      | 0.8257       | 3.2027  | 2.2121  |         | H18 | 1.2460  | 6.0339  | 3.2832  |
| O8      | 4.4542       | 5.3093  | 3.7592  |         | H19 | 4.8274  | 4.5127  | 3.2837  |
| O9      | 1.5327       | 5.2511  | 3.8581  |         | H20 | 2.3491  | -2.9401 | -0.0742 |
| O10     | 2.8645       | -0.7141 | -2.3267 |         | H21 | 4.4058  | 2.7938  | -1.9367 |
| O11     | 6.9391       | 1.2557  | 3.6544  |         | H22 | 0.3128  | -1.8911 | 3.0172  |
| O12     | -0.8004      | 3.7129  | 0.0416  |         | H23 | -0.6427 | 1.5842  | 4.4490  |
| O13     | 0.5798       | 3.1188  | -2.1855 |         | H24 | 7.5216  | 3.3888  | 0.1141  |
| O14     | -5.1043      | -3.0951 | 2.2999  |         | H25 | 1.4930  | -1.0196 | -3.1931 |
| O15     | -3.0557      | -1.8257 | -1.3873 |         | H26 | -1.0912 | 1.6207  | -4.4123 |
| O16     | -6.5204      | -3.9335 | 0.0006  |         | H27 | 0.4093  | -0.3662 | 3.5094  |
| O17     | -5.3627      | -3.1381 | -2.3207 |         | H28 | -1.3397 | 1.1050  | 3.0860  |
| O18     | -3.2765      | 0.8369  | -2.1169 |         | H29 | -1.5132 | -2.7056 | -1.9843 |
| O19     | 0.6171       | -1.1188 | -3.6775 |         | H30 | 0.3370  | 2.5041  | 2.7420  |
| O20     | -0.6839      | -3.1318 | -2.3197 |         | H31 | -0.2724 | 3.4541  | -0.7760 |
| O21     | -0.5670      | -3.0257 | 2.2407  |         | H32 | -1.4177 | -2.5986 | 1.9119  |
| O22     | 0.9105       | -3.7181 | 0.0460  |         | H33 | -3.2174 | -0.1223 | -1.8483 |
| O23     | -6.8459      | -1.2905 | -3.7248 |         | H34 | -4.7141 | -5.9891 | -3.2581 |
| O24     | -2.7677      | 0.7346  | 2.2930  |         | H35 | -2.8604 | 1.3447  | 1.5066  |
| O25     | -1.4885      | -5.2027 | -3.8970 |         | H36 | -2.2270 | 2.8741  | 0.0767  |
| O26     | -4.3029      | -5.2094 | -3.7263 |         | H37 | 3.1375  | 0.1928  | 1.9187  |
| O27     | 5.3755       | 3.1821  | 2.3846  |         | H38 | -6.3259 | -0.4441 | -3.6496 |
| O28     | 0.8916       | -1.2349 | 3.5119  |         | H39 | 5.8652  | 3.4616  | 1.5569  |
| O29     | 3.2118       | -2.4317 | -0.1545 |         | H40 | 5.9279  | 2.4831  | 2.8300  |
| O30     | 5.5092       | -1.1238 | 3.4840  |         | H41 | -4.7012 | 1.0145  | -2.9725 |
| O31     | -2.8344      | -1.9127 | 1.4202  |         | H42 | -7.4016 | -3.4495 | -0.0424 |
| O32     | -0.9181      | 1.3510  | -3.4555 |         | H43 | 2.5199  | 5.2396  | 3.8533  |
| O33     | -5.5232      | 1.1596  | -3.5291 |         | H44 | 3.9081  | 2.3413  | 1.7538  |
| O34     | -3.1042      | 2.3900  | 0.1611  |         | H45 | -5.6332 | -2.3570 | 2.7414  |
| H1      | -4.6833      | -5.1199 | -4.6491 |         | H46 | 1.4195  | 2.6680  | -1.8912 |
| H2      | -3.5510      | 0.9447  | 2.8901  |         | H47 | 6.8557  | 1.6471  | 4.5830  |
| H3      | -3.1837      | 1.7934  | -0.6337 |         | H48 | 4.6766  | -0.9539 | 2.9534  |
| H4      | -0.9917      | -3.8668 | -2.9237 |         | H49 | -5.0032 | -3.9182 | -2.8387 |
| H5      | -6.3322      | -1.9673 | -3.1997 |         | H50 | 3.6707  | -0.9459 | -2.8797 |
| H6      | 0.3469       | -3.4855 | -0.7319 |         | H51 | 1.0769  | 3.9433  | 2.8318  |
| H7      | -0.0470      | -3.3024 | 1.4316  |         | H52 | 4.8272  | 6.0863  | 3.2442  |
| H8      | -5.1608      | 1.4452  | -4.4180 |         | H53 | 3.2506  | -1.8299 | 0.6309  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.1754 | -5.9771 | -3.3290 | H1  | 5.7931  | 0.7126  | 1.7798  |
| H55 | -3.0382 | -1.8892 | -0.3974 | H2  | 5.2273  | 0.6437  | 1.3159  |
| H56 | -3.8482 | -2.3397 | -1.6967 | end |         |         |         |
| H57 | 6.1519  | 3.7045  | -0.6499 | H1  | 4.1762  | 4.2079  | -0.3145 |
| H58 | 2.3138  | 2.3974  | 1.7036  | H2  | 4.1624  | 3.6315  | 0.1409  |
| H59 | 3.0238  | 1.9517  | -0.4456 | end |         |         |         |
| H60 | -5.8131 | -3.4977 | -1.5020 | H1  | 15.1391 | 5.0282  | 1.9682  |
| H61 | -2.8633 | -0.9687 | 1.7286  | H2  | 14.7662 | 4.8562  | 1.3541  |
| H62 | -2.4823 | -5.2319 | -3.9010 | end |         |         |         |
| H63 | 2.3658  | -0.9516 | 2.6981  | H1  | 12.6814 | 1.6968  | 0.4347  |
| H64 | -2.4565 | 1.0060  | -2.6599 | H2  | 12.1699 | 1.2020  | 0.6200  |
| H65 | 2.9540  | 1.0157  | -1.7302 | end |         |         |         |
| H66 | 5.7014  | 2.4720  | -2.7876 | H1  | 12.3434 | 2.4348  | 8.1446  |
| H67 | 0.9330  | -4.7260 | 0.0665  | H2  | 12.0644 | 3.1167  | 8.1767  |
| H68 | -5.6192 | -3.4014 | 1.5071  | end |         |         |         |
| end |         |         |         | H1  | 7.6770  | 0.1321  | 0.6178  |
| H1  | -4.0354 | 5.2317  | 3.2231  | H2  | 7.4754  | -0.2350 | 0.0117  |
| H2  | -4.6242 | 4.7867  | 3.1089  | end |         |         |         |
| end |         |         |         | H1  | 7.5179  | 9.5685  | 0.6427  |
| H1  | 9.6725  | 5.7413  | 5.4466  | H2  | 7.1756  | 9.7519  | 0.0154  |
| H2  | 9.1251  | 5.4438  | 5.0359  | end |         |         |         |
| end |         |         |         | H1  | 13.5824 | 1.9379  | 5.5832  |
| H1  | 15.1436 | 10.0506 | 6.9611  | H2  | 13.5371 | 2.6387  | 5.8067  |
| H2  | 15.8506 | 9.8171  | 7.0054  | end |         |         |         |
| end |         |         |         | H1  | 9.7912  | 12.9530 | 5.8021  |
| H1  | 13.2627 | 8.0015  | 5.5584  | H2  | 10.0037 | 12.5983 | 6.4090  |
| H2  | 13.3122 | 7.3302  | 5.2353  | end |         |         |         |
| end |         |         |         | H1  | 20.2096 | 11.1743 | 3.8770  |
| H1  | 15.2102 | 3.3386  | 3.8956  | H2  | 19.5844 | 11.4653 | 3.6180  |
| H2  | 14.6272 | 2.9242  | 4.0716  | end |         |         |         |
| end |         |         |         | H1  | 9.8094  | 10.4399 | -0.0363 |
| H1  | 16.1469 | 6.1434  | 0.4366  | H2  | 10.3686 | 10.1128 | -0.3818 |
| H2  | 16.1808 | 6.3593  | -0.2667 | end |         |         |         |
| end |         |         |         | H1  | 16.9574 | 10.0023 | 1.7497  |
| H1  | 20.1281 | 9.8730  | 9.8666  | H2  | 17.5183 | 9.6828  | 1.3990  |
| H2  | 19.4245 | 9.8829  | 9.6507  | end |         |         |         |
| end |         |         |         | H1  | 10.2218 | 11.8275 | 4.1577  |
| H1  | 8.6718  | 10.4057 | 5.9487  | H2  | 10.4147 | 11.1197 | 4.0764  |
| H2  | 9.1872  | 10.8964 | 5.7593  | end |         |         |         |
| end |         |         |         | H1  | 6.6996  | 3.6809  | 7.8812  |
| H1  | 11.7440 | 9.0953  | 0.8336  | H2  | 6.4203  | 4.1771  | 8.3484  |
| H2  | 11.5773 | 8.5300  | 0.3937  | end |         |         |         |
| end |         |         |         | H1  | 4.5744  | 3.6533  | 9.5777  |
| H1  | 8.7800  | 8.8135  | 8.2392  | H2  | 4.4676  | 4.0997  | 9.0028  |
| H2  | 9.3734  | 8.7591  | 7.8058  | end |         |         |         |
| end |         |         |         | H1  | 11.8430 | 5.1083  | 8.8432  |

|     |         |         |        |
|-----|---------|---------|--------|
| H2  | 12.1490 | 4.7208  | 9.3918 |
| end |         |         |        |
| H1  | 11.0011 | 11.8192 | 9.6025 |
| H2  | 11.4369 | 12.2048 | 9.1541 |
| end |         |         |        |

|     |         |        |        |
|-----|---------|--------|--------|
| H1  | 19.3586 | 7.6161 | 9.7177 |
| H2  | 19.9729 | 7.3441 | 9.4183 |
| end |         |        |        |
| end |         |        |        |

**(43) n=6 & m=3**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.6611 | -4.9594 | 0.0228  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.4070 | 0.4281  | -3.5481 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.1498  | -1.9193 | -3.1585 |
| O1      | 6.6968       | 3.9118  | 0.1440  |         | H12 | -3.6451 | -2.3409 | 1.7993  |
| O2      | 3.0982       | 1.8688  | 1.3473  |         | H13 | 0.0403  | 2.3544  | -2.7345 |
| O3      | 5.2364       | 3.1420  | -2.2664 |         | H14 | 6.3759  | 0.4130  | 3.6611  |
| O4      | 2.9384       | 1.8933  | -1.4500 |         | H15 | 5.1392  | -1.4475 | 4.4118  |
| O5      | 3.1882       | -0.7772 | 2.1824  |         | H16 | -0.1920 | 3.4656  | 0.8036  |
| O6      | -0.4952      | 1.2768  | 3.5368  |         | H17 | 2.9797  | -1.3440 | -1.4897 |
| O7      | 0.8197       | 3.1793  | 2.1815  |         | H18 | 1.2185  | 6.0190  | 3.3284  |
| O8      | 4.4309       | 5.2963  | 3.7226  |         | H19 | 4.7888  | 4.4995  | 3.2374  |
| O9      | 1.4953       | 5.2069  | 3.8650  |         | H20 | 2.3717  | -2.9915 | -0.0531 |
| O10     | 2.8993       | -0.7675 | -2.2977 |         | H21 | 4.3937  | 2.7279  | -1.9278 |
| O11     | 6.8860       | 1.2676  | 3.6523  |         | H22 | 0.3444  | -1.8528 | 3.0642  |
| O12     | -0.7694      | 3.6826  | 0.0150  |         | H23 | -0.6609 | 1.6107  | 4.4673  |
| O13     | 0.5703       | 3.0417  | -2.2264 |         | H24 | 7.5385  | 3.3555  | 0.1118  |
| O14     | -5.0820      | -3.0792 | 2.3573  |         | H25 | 1.5224  | -1.0925 | -3.1684 |
| O15     | -3.0371      | -1.8636 | -1.3432 |         | H26 | -1.0951 | 1.5532  | -4.4588 |
| O16     | -6.4969      | -3.9709 | 0.0480  |         | H27 | 0.3980  | -0.3278 | 3.5596  |
| O17     | -5.3072      | -3.1812 | -2.2558 |         | H28 | -1.3930 | 1.1257  | 3.1187  |
| O18     | -3.2452      | 0.7832  | -2.1213 |         | H29 | -1.5026 | -2.7580 | -1.9273 |
| O19     | 0.6407       | -1.1948 | -3.6395 |         | H30 | 0.3062  | 2.4990  | 2.7126  |
| O20     | -0.6718      | -3.1781 | -2.2658 |         | H31 | -0.2610 | 3.3986  | -0.8056 |
| O21     | -0.4966      | -3.0153 | 2.2763  |         | H32 | -1.3487 | -2.5848 | 1.9652  |
| O22     | 0.9234       | -3.7491 | 0.0543  |         | H33 | -3.1848 | -0.1724 | -1.8397 |
| O23     | -6.7989      | -1.2899 | -3.6959 |         | H34 | -4.7461 | -6.0339 | -3.2440 |
| O24     | -2.8030      | 0.7530  | 2.3069  |         | H35 | -2.8777 | 1.3637  | 1.5163  |
| O25     | -1.4862      | -5.2401 | -3.8505 |         | H36 | -2.1884 | 2.8629  | 0.0831  |
| O26     | -4.3160      | -5.2456 | -3.6826 |         | H37 | 3.1438  | 0.1807  | 1.9143  |
| O27     | 5.3264       | 3.1388  | 2.3636  |         | H38 | -6.2816 | -0.4371 | -3.6293 |
| O28     | 0.8991       | -1.1855 | 3.5707  |         | H39 | 5.8398  | 3.4127  | 1.5490  |
| O29     | 3.2350       | -2.4802 | -0.1243 |         | H40 | 5.8696  | 2.4426  | 2.8301  |
| O30     | 5.4859       | -1.1308 | 3.5228  |         | H41 | -4.6788 | 0.9765  | -2.9662 |
| O31     | -2.8014      | -1.8977 | 1.4921  |         | H42 | -7.3778 | -3.4872 | -0.0096 |
| O32     | -0.9166      | 1.2749  | -3.5055 |         | H43 | 2.4815  | 5.2003  | 3.8665  |
| O33     | -5.5039      | 1.1264  | -3.5165 |         | H44 | 3.8980  | 2.3161  | 1.7388  |
| O34     | -3.0644      | 2.3713  | 0.1578  |         | H45 | -5.6291 | -2.3454 | 2.7853  |
| H1      | -4.6947      | -5.1107 | -4.6012 |         | H46 | 1.4142  | 2.5964  | -1.9366 |
| H2      | -3.5961      | 0.9594  | 2.8916  |         | H47 | 6.8347  | 1.6384  | 4.5919  |
| H3      | -3.1195      | 1.7611  | -0.6269 |         | H48 | 4.6565  | -0.9773 | 2.9804  |
| H4      | -0.9750      | -3.9231 | -2.8605 |         | H49 | -4.9538 | -3.9677 | -2.7734 |
| H5      | -6.2765      | -1.9620 | -3.1807 |         | H50 | 3.7166  | -0.9779 | -2.8424 |
| H6      | 0.3591       | -3.5253 | -0.7280 |         | H51 | 1.0642  | 3.9250  | 2.7991  |
| H7      | -0.0023      | -3.2987 | 1.4536  |         | H52 | 4.8435  | 6.0756  | 3.2440  |
| H8      | -5.1514      | 1.4159  | -4.4128 |         | H53 | 3.2592  | -1.8729 | 0.6569  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.1808 | -6.0324 | -3.3039 | H1  | 11.8609 | 9.0505  | 0.8202  |
| H55 | -3.0229 | -1.9048 | -0.3538 | H2  | 11.6304 | 8.4912  | 0.4017  |
| H56 | -3.8342 | -2.3792 | -1.6461 | end |         |         |         |
| H57 | 6.1583  | 3.6417  | -0.6394 | H1  | 8.8363  | 8.9326  | 8.3275  |
| H58 | 2.3015  | 2.3539  | 1.7076  | H2  | 9.3554  | 8.7874  | 7.8257  |
| H59 | 2.9909  | 1.8912  | -0.4577 | end |         |         |         |
| H60 | -5.7655 | -3.5368 | -1.4396 | H1  | 5.9137  | 0.6740  | 1.7176  |
| H61 | -2.8476 | -0.9462 | 1.7786  | H2  | 5.2782  | 0.5777  | 1.3608  |
| H62 | -2.4786 | -5.2719 | -3.8664 | end |         |         |         |
| H63 | 2.3694  | -0.9274 | 2.7404  | H1  | 4.1572  | 4.2038  | -0.3049 |
| H64 | -2.4338 | 0.9437  | -2.6790 | H2  | 4.1446  | 3.5794  | 0.0842  |
| H65 | 2.9433  | 0.9371  | -1.7346 | end |         |         |         |
| H66 | 5.6966  | 2.4040  | -2.7765 | H1  | 15.0652 | 4.9359  | 1.9596  |
| H67 | 0.9501  | -4.7537 | 0.0768  | H2  | 14.6620 | 4.7053  | 1.3855  |
| H68 | -5.5816 | -3.4005 | 1.5628  | end |         |         |         |
| end |         |         |         | H1  | 12.7626 | 1.6709  | 0.3862  |
| H1  | 8.7389  | 4.9841  | 1.8996  | H2  | 12.2073 | 1.2215  | 0.5598  |
| H2  | 9.2891  | 5.3381  | 1.5420  | end |         |         |         |
| end |         |         |         | H1  | 12.3762 | 2.4115  | 8.1512  |
| H1  | 9.7245  | 5.5785  | 5.5396  | H2  | 12.0882 | 3.0881  | 8.2011  |
| H2  | 9.2302  | 5.4616  | 4.9938  | end |         |         |         |
| end |         |         |         | H1  | 7.7193  | 0.1221  | 0.5880  |
| H1  | 7.5453  | 4.5101  | 4.3635  | H2  | 7.5213  | -0.2469 | -0.0174 |
| H2  | 7.0515  | 4.2792  | 3.8550  | end |         |         |         |
| end |         |         |         | H1  | 7.5241  | 9.5186  | 0.6468  |
| H1  | 15.7324 | 8.7313  | 4.6618  | H2  | 7.1810  | 9.6982  | 0.0183  |
| H2  | 15.4922 | 8.5705  | 3.9738  | end |         |         |         |
| end |         |         |         | H1  | 13.5805 | 1.8968  | 5.6556  |
| H1  | 15.2878 | 10.0025 | 6.8887  | H2  | 13.5974 | 2.5663  | 5.9616  |
| H2  | 16.0190 | 9.9317  | 7.0159  | end |         |         |         |
| end |         |         |         | H1  | 9.8321  | 12.8683 | 5.8592  |
| H1  | 13.6567 | 8.6274  | 6.9170  | H2  | 10.0497 | 12.4873 | 6.4473  |
| H2  | 13.0497 | 8.2642  | 7.1538  | end |         |         |         |
| end |         |         |         | H1  | 20.1682 | 11.2440 | 3.8876  |
| H1  | 15.2059 | 3.3358  | 3.9320  | H2  | 19.5477 | 11.5412 | 3.6258  |
| H2  | 14.6306 | 2.9767  | 4.2193  | end |         |         |         |
| end |         |         |         | H1  | 9.8621  | 10.4280 | -0.0369 |
| H1  | 16.1639 | 6.0585  | 0.5607  | H2  | 10.4144 | 10.0320 | -0.3154 |
| H2  | 16.1954 | 6.3504  | -0.1147 | end |         |         |         |
| end |         |         |         | H1  | 16.9970 | 10.0330 | 1.8053  |
| H1  | 20.1321 | 9.8372  | 10.0198 | H2  | 17.5339 | 9.7114  | 1.4202  |
| H2  | 19.4606 | 9.8739  | 9.7209  | end |         |         |         |
| end |         |         |         | H1  | 10.1746 | 11.8318 | 4.1414  |
| H1  | 8.6834  | 10.3461 | 5.9288  | H2  | 10.3655 | 11.1368 | 3.9857  |
| H2  | 9.1900  | 10.8428 | 5.7308  | end |         |         |         |
| end |         |         |         | H1  | 6.6159  | 3.5709  | 7.8588  |

|     |         |        |        |
|-----|---------|--------|--------|
| H2  | 6.4910  | 4.1195 | 8.3343 |
| end |         |        |        |
| H1  | 4.5718  | 3.7253 | 9.6460 |
| H2  | 4.4951  | 4.0060 | 8.9701 |
| end |         |        |        |
| H1  | 11.8520 | 5.0578 | 8.8361 |
| H2  | 12.1651 | 4.7023 | 9.4019 |
| end |         |        |        |

|     |         |         |        |
|-----|---------|---------|--------|
| H1  | 10.9770 | 11.7962 | 9.6659 |
| H2  | 11.4275 | 12.1780 | 9.2294 |
| end |         |         |        |
| H1  | 19.3437 | 7.6475  | 9.5825 |
| H2  | 19.9678 | 7.3392  | 9.3444 |
| end |         |         |        |
| end |         |         |        |

**(44) n=6 & m=4**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.6698 | -4.8477 | -0.0267 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.3960 | 0.4313  | -3.5403 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.2460  | -1.8659 | -3.0279 |
| O1      | 6.6793       | 3.8849  | 0.1813  |         | H12 | -3.8112 | -2.3411 | 1.9127  |
| O2      | 2.9429       | 1.8599  | 1.2591  |         | H13 | 0.0272  | 2.3999  | -2.8058 |
| O3      | 5.2956       | 3.2199  | -2.3072 |         | H14 | 6.1461  | 0.4614  | 3.6941  |
| O4      | 3.0050       | 1.9688  | -1.5590 |         | H15 | 5.0396  | -1.3994 | 4.4074  |
| O5      | 3.0400       | -0.7361 | 2.1169  |         | H16 | -0.2523 | 3.5546  | 0.7252  |
| O6      | -0.6700      | 1.2487  | 3.4561  |         | H17 | 3.0966  | -1.3252 | -1.5374 |
| O7      | 0.6504       | 3.1398  | 2.0888  |         | H18 | 1.0797  | 5.9597  | 3.2811  |
| O8      | 4.2835       | 5.2362  | 3.7546  |         | H19 | 4.6654  | 4.4692  | 3.2307  |
| O9      | 1.3746       | 5.1345  | 3.7943  |         | H20 | 2.3679  | -2.9614 | -0.0296 |
| O10     | 3.0443       | -0.7627 | -2.3574 |         | H21 | 4.4513  | 2.7970  | -1.9812 |
| O11     | 6.6606       | 1.3121  | 3.7029  |         | H22 | 0.1998  | -1.7887 | 3.1274  |
| O12     | -0.8130      | 3.7952  | -0.0724 |         | H23 | -0.7325 | 1.5854  | 4.3996  |
| O13     | 0.5456       | 3.1159  | -2.3228 |         | H24 | 7.5184  | 3.3327  | 0.1502  |
| O14     | -5.2356      | -3.1180 | 2.3831  |         | H25 | 1.6471  | -1.0880 | -3.1593 |
| O15     | -3.0432      | -1.8514 | -1.2745 |         | H26 | -1.1546 | 1.5125  | -4.4630 |
| O16     | -6.4845      | -3.8633 | 0.0011  |         | H27 | 0.2810  | -0.2443 | 3.5571  |
| O17     | -5.2223      | -3.1546 | -2.2707 |         | H28 | -1.6010 | 1.0680  | 3.1200  |
| O18     | -3.2189      | 0.8154  | -2.1048 |         | H29 | -1.4650 | -2.6879 | -1.8088 |
| O19     | 0.7298       | -1.1788 | -3.5676 |         | H30 | 0.1182  | 2.4556  | 2.5963  |
| O20     | -0.6197      | -3.0813 | -2.1447 |         | H31 | -0.3077 | 3.5055  | -0.8893 |
| O21     | -0.6889      | -2.9625 | 2.4715  |         | H32 | -1.5425 | -2.5426 | 2.1372  |
| O22     | 0.9332       | -3.7762 | 0.1835  |         | H33 | -3.1748 | -0.1247 | -1.7833 |
| O23     | -6.6700      | -1.3226 | -3.7712 |         | H34 | -4.7353 | -5.9709 | -3.3319 |
| O24     | -3.0318      | 0.7740  | 2.3776  |         | H35 | -3.0122 | 1.3713  | 1.5769  |
| O25     | -1.4378      | -5.0958 | -3.7849 |         | H36 | -2.1888 | 2.8808  | 0.0431  |
| O26     | -4.2842      | -5.1793 | -3.7385 |         | H37 | 2.9950  | 0.2129  | 1.8133  |
| O27     | 5.1716       | 3.1469  | 2.3285  |         | H38 | -6.1765 | -0.4573 | -3.6774 |
| O28     | 0.7966       | -1.0962 | 3.5462  |         | H39 | 5.7287  | 3.4089  | 1.5399  |
| O29     | 3.2046       | -2.4139 | -0.1220 |         | H40 | 5.6935  | 2.4586  | 2.8312  |
| O30     | 5.3477       | -1.1426 | 3.4845  |         | H41 | -4.6508 | 1.0174  | -2.9817 |
| O31     | -2.9657      | -1.8845 | 1.6231  |         | H42 | -7.3657 | -3.3777 | -0.0305 |
| O32     | -0.9082      | 1.2761  | -3.5102 |         | H43 | 2.3624  | 5.1481  | 3.8096  |
| O33     | -5.4873      | 1.1394  | -3.5169 |         | H44 | 3.7170  | 2.3189  | 1.6836  |
| O34     | -3.0311      | 2.3443  | 0.1528  |         | H45 | -5.7799 | -2.3825 | 2.8175  |
| H1      | -4.6718      | -5.0076 | -4.6488 |         | H46 | 1.4022  | 2.6975  | -2.0492 |
| H2      | -3.8439      | 1.0187  | 2.9217  |         | H47 | 6.7159  | 1.6431  | 4.6569  |
| H3      | -3.1023      | 1.7541  | -0.6510 |         | H48 | 4.5105  | -0.9959 | 2.9575  |
| H4      | -0.9023      | -3.8087 | -2.7705 |         | H49 | -4.8918 | -3.9526 | -2.7908 |
| H5      | -6.1543      | -1.9872 | -3.2376 |         | H50 | 3.8479  | -1.0050 | -2.9057 |
| H6      | 0.3824       | -3.5551 | -0.6075 |         | H51 | 0.9146  | 3.8605  | 2.7275  |
| H7      | -0.1958      | -3.2670 | 1.6685  |         | H52 | 4.6704  | 6.0549  | 3.3255  |
| H8      | -5.1708      | 1.3848  | -4.4396 |         | H53 | 3.1818  | -1.7777 | 0.6408  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.1186 | -5.9115 | -3.2793 | H1  | 20.1678 | 9.7970  | 10.0760 |
| H55 | -3.1329 | -1.8977 | -0.2914 | H2  | 19.4813 | 9.8854  | 9.8195  |
| H56 | -3.8136 | -2.3644 | -1.6531 | end |         |         |         |
| H57 | 6.1832  | 3.6657  | -0.6459 | H1  | 8.7547  | 10.4289 | 6.0111  |
| H58 | 2.1231  | 2.3296  | 1.5869  | H2  | 9.1713  | 10.8482 | 5.5751  |
| H59 | 2.9934  | 1.9441  | -0.5681 | end |         |         |         |
| H60 | -5.7160 | -3.4831 | -1.4623 | H1  | 11.8136 | 9.0920  | 0.9359  |
| H61 | -3.0266 | -0.9301 | 1.9027  | H2  | 11.6489 | 8.5853  | 0.4293  |
| H62 | -2.4284 | -5.1350 | -3.7978 | end |         |         |         |
| H63 | 2.2066  | -0.8776 | 2.6589  | H1  | 8.9113  | 8.9978  | 8.3895  |
| H64 | -2.3793 | 0.9528  | -2.6284 | H2  | 9.4673  | 8.8940  | 7.9161  |
| H65 | 3.0216  | 1.0180  | -1.8505 | end |         |         |         |
| H66 | 5.7464  | 2.4805  | -2.8189 | H1  | 6.0586  | 0.7355  | 1.6596  |
| H67 | 0.9548  | -4.7816 | 0.2004  | H2  | 5.4091  | 0.7140  | 1.3159  |
| H68 | -5.7013 | -3.3848 | 1.5455  | end |         |         |         |
| end |         |         |         | H1  | 4.1075  | 4.1121  | -0.3354 |
| H1  | -4.7542 | 6.2520  | 3.6920  | H2  | 4.1503  | 3.4990  | 0.0604  |
| H2  | -4.2320 | 5.7766  | 3.4553  | end |         |         |         |
| end |         |         |         | H1  | 14.9116 | 4.6637  | 1.9809  |
| H1  | 9.2047  | 4.7667  | 1.5813  | H2  | 14.5784 | 4.4648  | 1.3541  |
| H2  | 9.0726  | 5.4667  | 1.7971  | end |         |         |         |
| end |         |         |         | H1  | 12.4405 | 1.7918  | 0.1812  |
| H1  | 9.7913  | 5.8837  | 5.4828  | H2  | 12.2220 | 1.1214  | 0.3920  |
| H2  | 9.3584  | 5.4519  | 5.0568  | end |         |         |         |
| end |         |         |         | H1  | 12.3074 | 2.3723  | 8.2203  |
| H1  | 8.2444  | 3.4940  | 4.2533  | H2  | 12.0254 | 3.0471  | 8.1331  |
| H2  | 8.8773  | 3.2618  | 3.9379  | end |         |         |         |
| end |         |         |         | H1  | 7.7349  | 0.1313  | 0.5201  |
| H1  | 15.7471 | 9.1182  | 4.7128  | H2  | 7.4754  | -0.2454 | -0.0557 |
| H2  | 15.4013 | 8.8404  | 4.1137  | end |         |         |         |
| end |         |         |         | H1  | 7.2225  | 9.3820  | 0.4801  |
| H1  | 15.5636 | 9.7891  | 6.8894  | H2  | 7.0204  | 9.6129  | -0.1927 |
| H2  | 16.2833 | 9.9596  | 6.9993  | end |         |         |         |
| end |         |         |         | H1  | 13.6502 | 1.9928  | 5.8319  |
| H1  | 13.5862 | 8.9831  | 7.7268  | H2  | 13.8155 | 2.6305  | 6.1565  |
| H2  | 13.5833 | 8.4633  | 7.1938  | end |         |         |         |
| end |         |         |         | H1  | 9.9377  | 12.8853 | 5.7567  |
| H1  | 13.1798 | 7.8799  | 5.3106  | H2  | 10.2133 | 12.4104 | 6.2456  |
| H2  | 13.1624 | 7.1727  | 5.0785  | end |         |         |         |
| end |         |         |         | H1  | 19.8891 | 11.3138 | 4.0669  |
| H1  | 15.0347 | 3.2627  | 3.7866  | H2  | 19.3469 | 11.6521 | 3.7056  |
| H2  | 14.5353 | 3.0290  | 4.2734  | end |         |         |         |
| end |         |         |         | H1  | 9.9197  | 10.5576 | -0.0147 |
| H1  | 16.0918 | 5.8529  | 0.8265  | H2  | 10.4314 | 10.0918 | -0.2626 |
| H2  | 16.3360 | 6.1333  | 0.1904  | end |         |         |         |
| end |         |         |         | H1  | 16.8032 | 10.0229 | 1.1256  |



|     |         |         |        |
|-----|---------|---------|--------|
| H2  | 17.1516 | 10.2433 | 1.7343 |
| end |         |         |        |
| H1  | 10.0956 | 11.7732 | 4.0066 |
| H2  | 9.9761  | 11.1481 | 3.6368 |
| end |         |         |        |
| H1  | 6.8225  | 3.7258  | 7.7150 |
| H2  | 6.9016  | 4.2599  | 8.2095 |
| end |         |         |        |
| H1  | 4.6806  | 3.0606  | 8.7653 |
| H2  | 4.9976  | 3.7252  | 8.7307 |
| end |         |         |        |

|     |         |         |        |
|-----|---------|---------|--------|
| H1  | 11.9363 | 5.0897  | 8.7222 |
| H2  | 12.1687 | 4.7296  | 9.3252 |
| end |         |         |        |
| H1  | 10.6984 | 11.5920 | 9.8516 |
| H2  | 11.3834 | 11.8328 | 9.8134 |
| end |         |         |        |
| H1  | 19.3202 | 7.7504  | 9.4128 |
| H2  | 19.9164 | 7.3605  | 9.2282 |
| end |         |         |        |
| end |         |         |        |

**(45) n=6 & m=5**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.7047 | -4.9239 | -0.0196 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.4128 | 0.3780  | -3.5879 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.2019  | -1.9009 | -3.1663 |
| O1      | 6.7249       | 3.9373  | 0.0670  |         | H12 | -3.6582 | -2.2796 | 1.8279  |
| O2      | 3.0677       | 1.9494  | 1.2895  |         | H13 | 0.0141  | 2.3188  | -2.7595 |
| O3      | 5.2822       | 3.1472  | -2.3203 |         | H14 | 6.2529  | 0.4873  | 3.6217  |
| O4      | 2.9448       | 1.9579  | -1.4922 |         | H15 | 5.1029  | -1.3728 | 4.4017  |
| O5      | 3.1559       | -0.6741 | 2.1371  |         | H16 | -0.2423 | 3.5101  | 0.7670  |
| O6      | -0.5684      | 1.2653  | 3.5034  |         | H17 | 2.9755  | -1.3149 | -1.5674 |
| O7      | 0.7149       | 3.2396  | 2.1519  |         | H18 | 1.1416  | 6.1115  | 3.2856  |
| O8      | 4.3701       | 5.3034  | 3.6912  |         | H19 | 4.6971  | 4.5154  | 3.1684  |
| O9      | 1.4389       | 5.2929  | 3.8048  |         | H20 | 2.3404  | -2.9471 | -0.0818 |
| O10     | 2.9122       | -0.7266 | -2.3684 |         | H21 | 4.4345  | 2.7475  | -1.9791 |
| O11     | 6.7916       | 1.3271  | 3.6028  |         | H22 | 0.3385  | -1.8045 | 3.1054  |
| O12     | -0.8108      | 3.6992  | -0.0367 |         | H23 | -0.7172 | 1.5917  | 4.4388  |
| O13     | 0.5356       | 3.0142  | -2.2568 |         | H24 | 7.5546  | 3.3598  | 0.0536  |
| O14     | -5.1481      | -2.9736 | 2.3557  |         | H25 | 1.5711  | -1.0646 | -3.2185 |
| O15     | -3.0624      | -1.8711 | -1.3099 |         | H26 | -1.1191 | 1.5021  | -4.4968 |
| O16     | -6.5334      | -3.9387 | 0.0111  |         | H27 | 0.4068  | -0.2859 | 3.6259  |
| O17     | -5.2969      | -3.1933 | -2.2771 |         | H28 | -1.4718 | 1.0855  | 3.1002  |
| O18     | -3.2836      | 0.7282  | -2.1250 |         | H29 | -1.4969 | -2.7461 | -1.8997 |
| O19     | 0.6745       | -1.1825 | -3.6683 |         | H30 | 0.2078  | 2.5604  | 2.6844  |
| O20     | -0.6660      | -3.1506 | -2.2551 |         | H31 | -0.2913 | 3.4193  | -0.8516 |
| O21     | -0.5262      | -2.9562 | 2.3367  |         | H32 | -1.3790 | -2.5334 | 2.0076  |
| O22     | 0.9089       | -3.7319 | 0.0899  |         | H33 | -3.2356 | -0.2299 | -1.8426 |
| O23     | -6.7859      | -1.2885 | -3.7306 |         | H34 | -4.7374 | -6.0669 | -3.2735 |
| O24     | -2.8745      | 0.7584  | 2.3126  |         | H35 | -2.9183 | 1.3530  | 1.5102  |
| O25     | -1.4788      | -5.2156 | -3.8411 |         | H36 | -2.2251 | 2.8442  | 0.0181  |
| O26     | -4.2791      | -5.2857 | -3.6935 |         | H37 | 3.0844  | 0.2813  | 1.8671  |
| O27     | 5.2859       | 3.2019  | 2.2654  |         | H38 | -6.2653 | -0.4360 | -3.6692 |
| O28     | 0.9129       | -1.1392 | 3.5952  |         | H39 | 5.8219  | 3.4653  | 1.4628  |
| O29     | 3.1944       | -2.4257 | -0.1815 |         | H40 | 5.8162  | 2.5126  | 2.7567  |
| O30     | 5.4189       | -1.0403 | 3.5101  |         | H41 | -4.6535 | 0.9667  | -3.0111 |
| O31     | -2.8079      | -1.8583 | 1.5138  |         | H42 | -7.4110 | -3.4546 | -0.0501 |
| O32     | -0.9342      | 1.2180  | -3.5479 |         | H43 | 2.4255  | 5.3058  | 3.7967  |
| O33     | -5.4803      | 1.1161  | -3.5629 |         | H44 | 3.8641  | 2.4107  | 1.6803  |
| O34     | -3.0877      | 2.3384  | 0.1083  |         | H45 | -5.6943 | -2.2395 | 2.7912  |
| H1      | -4.6534      | -5.1222 | -4.6100 |         | H46 | 1.3829  | 2.5791  | -1.9602 |
| H2      | -3.6816      | 0.9832  | 2.8693  |         | H47 | 6.7874  | 1.6875  | 4.5462  |
| H3      | -3.1500      | 1.7227  | -0.6747 |         | H48 | 4.5797  | -0.8898 | 2.9794  |
| H4      | -0.9684      | -3.8994 | -2.8460 |         | H49 | -4.9274 | -3.9832 | -2.7699 |
| H5      | -6.2676      | -1.9594 | -3.2132 |         | H50 | 3.7262  | -0.9489 | -2.9141 |
| H6      | 0.3352       | -3.4943 | -0.6799 |         | H51 | 0.9592  | 3.9955  | 2.7568  |
| H7      | -0.0275      | -3.2557 | 1.5262  |         | H52 | 4.8047  | 6.0928  | 3.2505  |
| H8      | -5.1447      | 1.4264  | -4.4567 |         | H53 | 3.2096  | -1.7912 | 0.5767  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.1377 | -6.0105 | -3.3163 | H1  | 15.1081 | 3.5462  | 4.3062  |
| H55 | -3.0727 | -1.8958 | -0.3189 | H2  | 14.6515 | 2.9897  | 4.1470  |
| H56 | -3.8531 | -2.3889 | -1.6253 | end |         |         |         |
| H57 | 6.1947  | 3.6734  | -0.7248 | H1  | 16.1310 | 6.0732  | 0.6230  |
| H58 | 2.2628  | 2.4211  | 1.6319  | H2  | 16.1917 | 6.3576  | -0.0534 |
| H59 | 2.9900  | 1.9532  | -0.4986 | end |         |         |         |
| H60 | -5.7825 | -3.5372 | -1.4707 | H1  | 20.0980 | 9.8479  | 10.0626 |
| H61 | -2.8357 | -0.9052 | 1.8079  | H2  | 19.4293 | 9.9013  | 9.7587  |
| H62 | -2.4704 | -5.2712 | -3.8352 | end |         |         |         |
| H63 | 2.3500  | -0.8536 | 2.7007  | H1  | 8.6401  | 10.3158 | 5.7228  |
| H64 | -2.4601 | 0.8935  | -2.6572 | H2  | 9.1928  | 10.7597 | 5.5218  |
| H65 | 2.9666  | 1.0057  | -1.7785 | end |         |         |         |
| H66 | 5.7250  | 2.4016  | -2.8351 | H1  | 11.7454 | 9.0635  | 0.8146  |
| H67 | 0.9456  | -4.7384 | 0.0831  | H2  | 11.5441 | 8.5473  | 0.3315  |
| H68 | -5.6429 | -3.2860 | 1.5577  | end |         |         |         |
| end |         |         |         | H1  | 8.8276  | 9.0532  | 8.3440  |
| H1  | -4.3345 | 5.4240  | 3.9654  | H2  | 9.3323  | 8.8966  | 7.8310  |
| H2  | -4.9552 | 5.0612  | 3.7681  | end |         |         |         |
| end |         |         |         | H1  | 5.8445  | 0.7210  | 1.6581  |
| H1  | 9.3007  | 5.1357  | 1.3273  | H2  | 5.1748  | 0.5737  | 1.3946  |
| H2  | 8.7759  | 5.0627  | 1.8505  | end |         |         |         |
| end |         |         |         | H1  | 4.1752  | 4.2409  | -0.3841 |
| H1  | 9.5970  | 5.5544  | 5.6940  | H2  | 4.1599  | 3.6271  | 0.0200  |
| H2  | 9.4150  | 4.9872  | 5.2482  | end |         |         |         |
| end |         |         |         | H1  | 14.9858 | 4.9067  | 1.9255  |
| H1  | 9.2615  | 2.9047  | 3.9816  | H2  | 14.6639 | 4.6299  | 1.3222  |
| H2  | 8.7240  | 3.4070  | 4.0921  | end |         |         |         |
| end |         |         |         | H1  | 12.6183 | 1.7506  | 0.3526  |
| H1  | 14.7163 | 6.7552  | 6.3411  | H2  | 12.4775 | 1.0696  | 0.5949  |
| H2  | 15.3599 | 6.3902  | 6.4104  | end |         |         |         |
| end |         |         |         | H1  | 12.3525 | 2.4152  | 8.1484  |
| H1  | 16.3182 | 8.4527  | 5.8596  | H2  | 12.0722 | 3.0967  | 8.1640  |
| H2  | 16.9460 | 8.8435  | 5.9480  | end |         |         |         |
| end |         |         |         | H1  | 7.6777  | 0.1004  | 0.6257  |
| H1  | 14.5260 | 8.7913  | 8.2413  | H2  | 7.4231  | -0.2074 | 0.0074  |
| H2  | 15.1737 | 8.7109  | 7.8828  | end |         |         |         |
| end |         |         |         | H1  | 7.2482  | 9.4256  | 0.6344  |
| H1  | 13.2564 | 8.3129  | 5.3637  | H2  | 7.2729  | 9.5502  | -0.0912 |
| H2  | 13.1256 | 7.6079  | 5.1651  | end |         |         |         |
| end |         |         |         | H1  | 13.6097 | 1.8106  | 5.8415  |
| H1  | 15.0900 | 10.3559 | 5.4386  | H2  | 13.6086 | 2.5405  | 5.9300  |
| H2  | 14.4733 | 10.6760 | 5.1690  | end |         |         |         |
| end |         |         |         | H1  | 9.7431  | 12.8066 | 5.9305  |
| H1  | 9.2829  | 7.3296  | 3.7612  | H2  | 10.1501 | 12.3596 | 6.3472  |
| H2  | 9.1779  | 6.9638  | 3.1216  | end |         |         |         |
| end |         |         |         | H1  | 20.0517 | 11.3464 | 3.8608  |

|     |         |         |         |
|-----|---------|---------|---------|
| H2  | 19.4810 | 11.6526 | 3.5108  |
| end |         |         |         |
| H1  | 9.7958  | 10.4608 | -0.0601 |
| H2  | 10.3673 | 10.1247 | -0.3746 |
| end |         |         |         |
| H1  | 17.1261 | 9.8095  | 1.2558  |
| H2  | 17.3646 | 10.1807 | 1.8414  |
| end |         |         |         |
| H1  | 10.2139 | 11.9194 | 4.1574  |
| H2  | 10.1681 | 11.3504 | 3.6927  |
| end |         |         |         |
| H1  | 6.6719  | 3.5860  | 7.8147  |
| H2  | 6.4987  | 4.0733  | 8.3388  |
| end |         |         |         |

|     |         |         |        |
|-----|---------|---------|--------|
| H1  | 4.4583  | 3.6319  | 9.0622 |
| H2  | 4.6964  | 4.2163  | 9.4402 |
| end |         |         |        |
| H1  | 11.8626 | 5.0790  | 8.8110 |
| H2  | 12.0559 | 4.7026  | 9.4151 |
| end |         |         |        |
| H1  | 10.8662 | 11.7793 | 9.6640 |
| H2  | 11.4029 | 12.1479 | 9.3231 |
| end |         |         |        |
| H1  | 19.3261 | 7.7080  | 9.5143 |
| H2  | 19.9307 | 7.3845  | 9.2456 |
| end |         |         |        |
| end |         |         |        |

**(46) n=6 & m=6**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.6550 | -4.9929 | 0.0784  |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.4210 | 0.4955  | -3.5500 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | -0.0588 | -1.8185 | -3.3483 |
| O1      | 6.6197       | 4.0523  | 0.0569  |         | H12 | -3.6507 | -2.3330 | 1.6883  |
| O2      | 3.1370       | 1.7463  | 1.3046  |         | H13 | 0.0357  | 2.4263  | -2.6691 |
| O3      | 5.1585       | 3.2036  | -2.3121 |         | H14 | 6.4137  | 0.3004  | 3.5829  |
| O4      | 2.9028       | 1.8309  | -1.4429 |         | H15 | 5.1493  | -1.4958 | 4.3909  |
| O5      | 3.2610       | -0.8749 | 2.0865  |         | H16 | -0.2088 | 3.4281  | 0.9080  |
| O6      | -0.4682      | 1.1648  | 3.6743  |         | H17 | 2.8292  | -1.3553 | -1.5318 |
| O7      | 0.8129       | 3.0297  | 2.2677  |         | H18 | 1.3519  | 5.8938  | 3.2641  |
| O8      | 4.5374       | 5.2551  | 3.6733  |         | H19 | 4.8854  | 4.4533  | 3.1907  |
| O9      | 1.6302       | 5.0986  | 3.8241  |         | H20 | 2.3880  | -2.9813 | -0.1538 |
| O10     | 2.7038       | -0.7886 | -2.3376 |         | H21 | 4.3382  | 2.7566  | -1.9714 |
| O11     | 6.9074       | 1.1653  | 3.5599  |         | H22 | 0.3386  | -1.9550 | 2.9586  |
| O12     | -0.7909      | 3.6547  | 0.1281  |         | H23 | -0.6883 | 1.5608  | 4.5660  |
| O13     | 0.5594       | 3.0988  | -2.1370 |         | H24 | 7.4686  | 3.5067  | 0.0665  |
| O14     | -4.9998      | -3.1717 | 2.3316  |         | H25 | 1.3385  | -1.0748 | -3.2819 |
| O15     | -3.0923      | -1.7638 | -1.4139 |         | H26 | -1.0577 | 1.6282  | -4.4647 |
| O16     | -6.4849      | -4.0061 | 0.0759  |         | H27 | 0.4670  | -0.4726 | 3.5325  |
| O17     | -5.3998      | -3.1036 | -2.2767 |         | H28 | -1.3332 | 1.0518  | 3.1851  |
| O18     | -3.2466      | 0.9233  | -2.1054 |         | H29 | -1.6670 | -2.6486 | -2.0178 |
| O19     | 0.4969       | -1.1397 | -3.8205 |         | H30 | 0.3344  | 2.3650  | 2.8513  |
| O20     | -0.8387      | -3.0754 | -2.3658 |         | H31 | -0.2841 | 3.3869  | -0.6981 |
| O21     | -0.5980      | -3.0202 | 2.1275  |         | H32 | -1.4444 | -2.5798 | 1.8088  |
| O22     | 0.8902       | -3.6364 | -0.1084 |         | H33 | -3.2257 | -0.0434 | -1.8705 |
| O23     | -6.9221      | -1.2024 | -3.6341 |         | H34 | -4.7565 | -5.9947 | -3.2265 |
| O24     | -2.7354      | 0.7634  | 2.2984  |         | H35 | -2.8306 | 1.3909  | 1.5297  |
| O25     | -1.5918      | -5.1843 | -3.9051 |         | H36 | -2.2683 | 2.9412  | 0.1476  |
| O26     | -4.3695      | -5.2133 | -3.7098 |         | H37 | 3.2052  | 0.0883  | 1.8323  |
| O27     | 5.3741       | 3.0924  | 2.2720  |         | H38 | -6.4038 | -0.3536 | -3.5846 |
| O28     | 0.9427       | -1.3381 | 3.4715  |         | H39 | 5.8413  | 3.4302  | 1.4525  |
| O29     | 3.2706       | -2.5000 | -0.1628 |         | H40 | 5.9698  | 2.4290  | 2.7156  |
| O30     | 5.5461       | -1.2314 | 3.5069  |         | H41 | -4.7111 | 1.0707  | -2.9755 |
| O31     | -2.8491      | -1.8556 | 1.3219  |         | H42 | -7.3658 | -3.5219 | 0.0112  |
| O32     | -0.9016      | 1.3608  | -3.5063 |         | H43 | 2.6178  | 5.0929  | 3.8214  |
| O33     | -5.5176      | 1.2026  | -3.5515 |         | H44 | 3.9399  | 2.1941  | 1.6829  |
| O34     | -3.1668      | 2.4926  | 0.2030  |         | H45 | -5.5430 | -2.4679 | 2.8086  |
| H1      | -4.7218      | -5.1859 | -4.6462 |         | H46 | 1.3943  | 2.6341  | -1.8535 |
| H2      | -3.5501      | 0.9315  | 2.8698  |         | H47 | 6.8076  | 1.5746  | 4.4769  |
| H3      | -3.2209      | 1.8935  | -0.5872 |         | H48 | 4.7446  | -1.0745 | 2.9301  |
| H4      | -1.1420      | -3.8292 | -2.9496 |         | H49 | -5.0800 | -3.8819 | -2.8169 |
| H5      | -6.4128      | -1.8645 | -3.0920 |         | H50 | 3.5386  | -0.9462 | -2.8764 |
| H6      | 0.3072       | -3.3850 | -0.8657 |         | H51 | 1.1235  | 3.7809  | 2.8484  |
| H7      | -0.0751      | -3.2656 | 1.3125  |         | H52 | 4.8627  | 6.0394  | 3.1424  |
| H8      | -5.1332      | 1.4338  | -4.4456 |         | H53 | 3.2685  | -1.9310 | 0.6529  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.2785 | -5.9591 | -3.3387 | H1  | 16.5436 | 7.7928  | 5.1230  |
| H55 | -3.0431 | -1.8135 | -0.4189 | H2  | 16.8818 | 7.4287  | 5.6761  |
| H56 | -3.8895 | -2.2903 | -1.6912 | end |         |         |         |
| H57 | 6.0945  | 3.7519  | -0.7250 | H1  | 10.9648 | 4.1578  | 3.5536  |
| H58 | 2.3456  | 2.2030  | 1.6959  | H2  | 10.4970 | 4.5163  | 4.0075  |
| H59 | 2.9737  | 1.7959  | -0.4510 | end |         |         |         |
| H60 | -5.8112 | -3.4803 | -1.4486 | H1  | 15.3569 | 3.0895  | 3.5642  |
| H61 | -2.8699 | -0.9237 | 1.6670  | H2  | 14.7635 | 2.8924  | 3.9539  |
| H62 | -2.5881 | -5.2160 | -3.9020 | end |         |         |         |
| H63 | 2.4362  | -1.0602 | 2.6199  | H1  | 16.1592 | 6.0825  | 0.3256  |
| H64 | -2.4326 | 1.0792  | -2.6611 | H2  | 16.2367 | 6.2979  | -0.3752 |
| H65 | 2.8551  | 0.8858  | -1.7571 | end |         |         |         |
| H66 | 5.6392  | 2.4925  | -2.8369 | H1  | 20.1758 | 9.8902  | 9.6877  |
| H67 | 0.8759  | -4.6441 | -0.0792 | H2  | 19.4408 | 9.8869  | 9.6504  |
| H68 | -5.5464 | -3.4753 | 1.5593  | end |         |         |         |
| end |         |         |         | H1  | 8.5332  | 10.4297 | 6.0136  |
| H1  | -4.1722 | 5.8918  | 3.3139  | H2  | 9.0328  | 10.9224 | 5.7922  |
| H2  | -4.8844 | 5.6768  | 3.3383  | end |         |         |         |
| end |         |         |         | H1  | 12.1363 | 8.9664  | 0.5692  |
| H1  | 8.6449  | 5.1332  | 1.5866  | H2  | 11.7941 | 8.3847  | 0.2750  |
| H2  | 9.2044  | 4.9964  | 1.1175  | end |         |         |         |
| end |         |         |         | H1  | 8.6905  | 8.5182  | 8.2221  |
| H1  | 8.6896  | 5.4954  | 5.2204  | H2  | 9.3083  | 8.6405  | 7.8407  |
| H2  | 8.9975  | 5.8726  | 5.7827  | end |         |         |         |
| end |         |         |         | H1  | 5.6816  | 0.6745  | 1.7371  |
| H1  | 8.1391  | 3.3035  | 4.4190  | H2  | 5.2692  | 0.2671  | 1.2852  |
| H2  | 8.8386  | 3.2747  | 4.1696  | end |         |         |         |
| end |         |         |         | H1  | 4.0530  | 4.1167  | -0.2433 |
| H1  | 14.6059 | 8.7283  | 4.3103  | H2  | 4.1297  | 3.4749  | 0.1056  |
| H2  | 14.9975 | 9.2889  | 4.0180  | end |         |         |         |
| end |         |         |         | H1  | 15.1724 | 5.1209  | 1.9049  |
| H1  | 16.0982 | 10.0667 | 6.8811  | H2  | 14.7007 | 5.0352  | 1.3434  |
| H2  | 15.3629 | 10.0726 | 6.7653  | end |         |         |         |
| end |         |         |         | H1  | 12.7826 | 1.3089  | 0.0131  |
| H1  | 14.8169 | 7.4623  | 7.9621  | H2  | 12.5512 | 1.6110  | 0.6419  |
| H2  | 15.0605 | 7.9796  | 7.4843  | end |         |         |         |
| end |         |         |         | H1  | 12.5927 | 2.6950  | 7.9750  |
| H1  | 13.1135 | 7.7016  | 5.5808  | H2  | 12.1091 | 3.2030  | 8.1963  |
| H2  | 13.1998 | 7.0415  | 5.2473  | end |         |         |         |
| end |         |         |         | H1  | 7.6358  | 0.2647  | 0.6374  |
| H1  | 13.0324 | 9.8704  | 6.4622  | H2  | 7.5560  | -0.0137 | -0.0389 |
| H2  | 13.4767 | 9.7375  | 5.8814  | end |         |         |         |
| end |         |         |         | H1  | 7.6540  | 9.6308  | 0.4947  |
| H1  | 9.8770  | 7.0273  | 3.2792  | H2  | 7.1314  | 9.5126  | -0.0117 |
| H2  | 9.7383  | 6.5930  | 2.6918  | end |         |         |         |
| end |         |         |         | H1  | 13.5893 | 2.0596  | 5.4103  |

|     |         |         |         |
|-----|---------|---------|---------|
| H2  | 13.3388 | 2.7516  | 5.4788  |
| end |         |         |         |
| H1  | 9.8283  | 12.9881 | 5.7270  |
| H2  | 9.7577  | 12.6514 | 6.3767  |
| end |         |         |         |
| H1  | 20.2709 | 11.0708 | 3.7676  |
| H2  | 19.6175 | 11.3656 | 3.6024  |
| end |         |         |         |
| H1  | 10.3065 | 10.5174 | -0.4794 |
| H2  | 10.3340 | 9.7855  | -0.4046 |
| end |         |         |         |
| H1  | 17.0237 | 10.0383 | 1.7002  |
| H2  | 17.7110 | 9.9657  | 1.4463  |
| end |         |         |         |
| H1  | 10.2539 | 11.6490 | 4.2625  |
| H2  | 10.4363 | 10.9356 | 4.2100  |
| end |         |         |         |

|     |         |         |        |
|-----|---------|---------|--------|
| H1  | 6.7413  | 3.6401  | 7.9304 |
| H2  | 6.0651  | 3.8106  | 8.1671 |
| end |         |         |        |
| H1  | 4.7915  | 4.1405  | 9.6662 |
| H2  | 4.2952  | 4.1048  | 9.1213 |
| end |         |         |        |
| H1  | 11.7706 | 5.1888  | 8.8952 |
| H2  | 12.0262 | 4.8305  | 9.4882 |
| end |         |         |        |
| H1  | 11.1290 | 12.0978 | 9.6372 |
| H2  | 11.2963 | 12.3266 | 8.9590 |
| end |         |         |        |
| H1  | 19.3590 | 7.7097  | 9.6032 |
| H2  | 19.8385 | 7.1697  | 9.7450 |
| end |         |         |        |
| end |         |         |        |

(47) n=6 & m=7

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.7015 | -4.8426 | -0.0779 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.4557 | 0.4172  | -3.4807 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.2081  | -1.9358 | -3.0087 |
| O1      | 6.7281       | 3.9598  | 0.0783  |         | H12 | -3.7251 | -2.2720 | 1.8494  |
| O2      | 3.0464       | 1.9964  | 1.3377  |         | H13 | 0.0331  | 2.3877  | -2.7351 |
| O3      | 5.2464       | 3.2153  | -2.2687 |         | H14 | 6.2425  | 0.5513  | 3.6726  |
| O4      | 2.9460       | 2.0109  | -1.4188 |         | H15 | 5.0885  | -1.4002 | 4.4084  |
| O5      | 3.1038       | -0.6374 | 2.1855  |         | H16 | -0.2881 | 3.5934  | 0.7490  |
| O6      | -0.6077      | 1.3461  | 3.4950  |         | H17 | 3.0459  | -1.2758 | -1.4463 |
| O7      | 0.7065       | 3.2761  | 2.1427  |         | H18 | 1.1583  | 6.0428  | 3.3356  |
| O8      | 4.4124       | 5.3188  | 3.7437  |         | H19 | 4.7782  | 4.5547  | 3.2096  |
| O9      | 1.4544       | 5.2285  | 3.8607  |         | H20 | 2.3760  | -2.8780 | -0.0118 |
| O10     | 2.9779       | -0.7117 | -2.2656 |         | H21 | 4.4196  | 2.8015  | -1.8925 |
| O11     | 6.7687       | 1.3897  | 3.7146  |         | H22 | 0.2514  | -1.7195 | 3.1038  |
| O12     | -0.8408      | 3.7802  | -0.0625 |         | H23 | -0.7320 | 1.6503  | 4.4444  |
| O13     | 0.5698       | 3.0890  | -2.2612 |         | H24 | 7.5458  | 3.3708  | 0.0577  |
| O14     | -5.1665      | -3.0596 | 2.3893  |         | H25 | 1.5862  | -1.1017 | -3.0765 |
| O15     | -3.0475      | -1.8290 | -1.3372 |         | H26 | -1.1274 | 1.5244  | -4.4297 |
| O16     | -6.4992      | -3.8622 | -0.0577 |         | H27 | 0.3192  | -0.1980 | 3.6210  |
| O17     | -5.2083      | -3.1572 | -2.3004 |         | H28 | -1.5178 | 1.1531  | 3.1198  |
| O18     | -3.3368      | 0.7555  | -2.1308 |         | H29 | -1.5493 | -2.6750 | -1.8596 |
| O19     | 0.6805       | -1.2061 | -3.5032 |         | H30 | 0.1844  | 2.5921  | 2.6556  |
| O20     | -0.7109      | -3.1056 | -2.1745 |         | H31 | -0.3017 | 3.4974  | -0.8624 |
| O21     | -0.6074      | -2.8858 | 2.3487  |         | H32 | -1.4620 | -2.4774 | 2.0098  |
| O22     | 0.9275       | -3.6760 | 0.0937  |         | H33 | -3.2655 | -0.1996 | -1.8388 |
| O23     | -6.7523      | -1.3150 | -3.7083 |         | H34 | -4.7313 | -6.0209 | -3.2970 |
| O24     | -2.9435      | 0.7507  | 2.3526  |         | H35 | -2.9804 | 1.3180  | 1.5336  |
| O25     | -1.4644      | -5.1520 | -3.8012 |         | H36 | -2.2303 | 2.8663  | 0.0031  |
| O26     | -4.2796      | -5.2425 | -3.7324 |         | H37 | 3.0508  | 0.3156  | 1.9053  |
| O27     | 5.3087       | 3.2333  | 2.2974  |         | H38 | -6.2774 | -0.4333 | -3.6568 |
| O28     | 0.8265       | -1.0526 | 3.5890  |         | H39 | 5.8353  | 3.4904  | 1.4876  |
| O29     | 3.2284       | -2.3497 | -0.0582 |         | H40 | 5.8520  | 2.5634  | 2.8028  |
| O30     | 5.3989       | -1.0994 | 3.5029  |         | H41 | -4.7391 | 0.9726  | -2.9716 |
| O31     | -2.8982      | -1.8074 | 1.5330  |         | H42 | -7.3697 | -3.3583 | -0.0570 |
| O32     | -0.9716      | 1.2590  | -3.4692 |         | H43 | 2.4405  | 5.2382  | 3.8516  |
| O33     | -5.5723      | 1.1087  | -3.5163 |         | H44 | 3.8347  | 2.4601  | 1.7357  |
| O34     | -3.0770      | 2.3393  | 0.1162  |         | H45 | -5.7221 | -2.3247 | 2.8113  |
| H1      | -4.6987      | -5.0546 | -4.6232 |         | H46 | 1.4132  | 2.6504  | -1.9571 |
| H2      | -3.7286      | 1.0211  | 2.9182  |         | H47 | 6.7702  | 1.6842  | 4.6799  |
| H3      | -3.1525      | 1.7314  | -0.6704 |         | H48 | 4.5534  | -0.9421 | 2.9895  |
| H4      | -0.9912      | -3.8490 | -2.7804 |         | H49 | -4.8631 | -3.9581 | -2.7987 |
| H5      | -6.1896      | -1.9603 | -3.2027 |         | H50 | 3.7735  | -0.9604 | -2.8220 |
| H6      | 0.3466       | -3.4561 | -0.6770 |         | H51 | 0.9584  | 4.0028  | 2.7809  |
| H7      | -0.0922      | -3.1826 | 1.5526  |         | H52 | 4.7913  | 6.1341  | 3.3050  |
| H8      | -5.2286      | 1.3886  | -4.4137 |         | H53 | 3.2081  | -1.7317 | 0.7177  |



|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.1510 | -5.9539 | -3.2667 | H1  | 15.2786 | 11.0647 | 5.3225  |
| H55 | -3.0977 | -1.8523 | -0.3503 | H2  | 14.6281 | 10.9531 | 4.9835  |
| H56 | -3.8297 | -2.3522 | -1.6791 | end |         |         |         |
| H57 | 6.1885  | 3.7121  | -0.7140 | H1  | 10.3736 | 4.3229  | 4.3514  |
| H58 | 2.2314  | 2.4636  | 1.6712  | H2  | 10.5297 | 3.8085  | 3.8385  |
| H59 | 2.9499  | 2.0145  | -0.4234 | end |         |         |         |
| H60 | -5.7162 | -3.4840 | -1.4988 | H1  | 14.5021 | 9.2214  | 8.1123  |
| H61 | -2.9270 | -0.8712 | 1.8897  | H2  | 15.1098 | 9.1860  | 7.6835  |
| H62 | -2.4532 | -5.2132 | -3.8464 | end |         |         |         |
| H63 | 2.2864  | -0.8042 | 2.7377  | H1  | 8.3984  | 3.5473  | 2.8997  |
| H64 | -2.5075 | 0.9354  | -2.6526 | H2  | 8.4355  | 3.3140  | 2.1973  |
| H65 | 2.9830  | 1.0587  | -1.6990 | end |         |         |         |
| H66 | 5.6798  | 2.4748  | -2.7873 | H1  | 15.2132 | 3.4776  | 4.1833  |
| H67 | 0.9652  | -4.6778 | 0.1086  | H2  | 14.6305 | 3.0299  | 4.1376  |
| H68 | -5.6337 | -3.3525 | 1.5686  | end |         |         |         |
| end |         |         |         | H1  | 16.1393 | 6.1561  | 0.6222  |
| H1  | -4.5269 | 5.9349  | 2.7719  | H2  | 16.1942 | 6.3794  | -0.0776 |
| H2  | -4.7572 | 5.2518  | 2.5994  | end |         |         |         |
| end |         |         |         | H1  | 20.1147 | 9.9049  | 10.0746 |
| H1  | 10.0309 | 5.7884  | 1.7676  | H2  | 19.4509 | 9.9691  | 9.7630  |
| H2  | 9.5112  | 5.4113  | 2.1431  | end |         |         |         |
| end |         |         |         | H1  | 8.6236  | 10.3623 | 5.6681  |
| H1  | 9.0247  | 5.5566  | 5.4430  | H2  | 9.2051  | 10.7912 | 5.5269  |
| H2  | 9.5416  | 5.9478  | 5.8043  | end |         |         |         |
| end |         |         |         | H1  | 11.7478 | 9.1202  | 0.9725  |
| H1  | 7.3704  | 3.9857  | 5.0301  | H2  | 11.5831 | 8.5899  | 0.4911  |
| H2  | 7.4376  | 4.5224  | 4.5211  | end |         |         |         |
| end |         |         |         | H1  | 8.7968  | 9.1044  | 8.3356  |
| H1  | 15.1310 | 8.0666  | 3.9016  | H2  | 9.2928  | 8.8920  | 7.8340  |
| H2  | 14.9818 | 7.8253  | 4.5893  | end |         |         |         |
| end |         |         |         | H1  | 6.1637  | 0.7141  | 1.5005  |
| H1  | 16.9244 | 9.3252  | 6.1194  | H2  | 5.4363  | 0.8081  | 1.5590  |
| H2  | 16.3949 | 9.0620  | 5.6675  | end |         |         |         |
| end |         |         |         | H1  | 4.1565  | 4.3075  | -0.3288 |
| H1  | 15.3082 | 7.1219  | 7.2408  | H2  | 4.1399  | 3.6973  | 0.0807  |
| H2  | 15.7023 | 6.5337  | 7.0147  | end |         |         |         |
| end |         |         |         | H1  | 15.0330 | 4.9834  | 1.9766  |
| H1  | 13.2022 | 6.8823  | 5.5394  | H2  | 14.6484 | 4.7471  | 1.3923  |
| H2  | 13.1105 | 7.5008  | 5.9403  | end |         |         |         |
| end |         |         |         | H1  | 12.5977 | 1.8479  | 0.3396  |
| H1  | 12.6905 | 9.4948  | 5.7408  | H2  | 12.4449 | 1.1644  | 0.5667  |
| H2  | 13.3288 | 9.7753  | 5.9903  | end |         |         |         |
| end |         |         |         | H1  | 12.2752 | 2.3678  | 8.2822  |
| H1  | 8.7302  | 7.5107  | 3.9013  | H2  | 11.8692 | 2.9772  | 8.2047  |
| H2  | 9.0406  | 7.2040  | 3.3003  | end |         |         |         |
| end |         |         |         | H1  | 7.8087  | -0.1250 | 0.4597  |

|     |         |         |         |
|-----|---------|---------|---------|
| H2  | 7.3641  | 0.0947  | -0.0822 |
| end |         |         |         |
| H1  | 7.3174  | 9.5656  | 0.6440  |
| H2  | 7.2460  | 9.6688  | -0.0828 |
| end |         |         |         |
| H1  | 13.6686 | 1.9005  | 5.7973  |
| H2  | 13.6256 | 2.6169  | 5.9569  |
| end |         |         |         |
| H1  | 9.7263  | 12.7846 | 5.9110  |
| H2  | 10.2496 | 12.3731 | 6.2221  |
| end |         |         |         |
| H1  | 20.0365 | 11.4013 | 3.8536  |
| H2  | 19.4333 | 11.7092 | 3.5665  |
| end |         |         |         |
| H1  | 9.9493  | 10.6704 | 0.0647  |
| H2  | 10.3562 | 10.1116 | -0.1827 |
| end |         |         |         |
| H1  | 17.3281 | 10.2593 | 1.8113  |
| H2  | 16.9919 | 9.9620  | 1.2305  |
| end |         |         |         |

|     |         |         |        |
|-----|---------|---------|--------|
| H1  | 10.1568 | 11.9129 | 4.0275 |
| H2  | 10.1691 | 11.2517 | 3.7044 |
| end |         |         |        |
| H1  | 6.7430  | 3.6910  | 7.8237 |
| H2  | 6.6391  | 4.2202  | 8.3228 |
| end |         |         |        |
| H1  | 4.4882  | 3.6394  | 8.9707 |
| H2  | 4.7360  | 4.2575  | 9.2841 |
| end |         |         |        |
| H1  | 12.1609 | 5.0451  | 8.7516 |
| H2  | 11.7796 | 4.7423  | 9.3035 |
| end |         |         |        |
| H1  | 10.8563 | 11.8118 | 9.7043 |
| H2  | 11.4346 | 12.1622 | 9.4182 |
| end |         |         |        |
| H1  | 19.3091 | 7.6929  | 9.6317 |
| H2  | 19.9265 | 7.4743  | 9.2954 |
| end |         |         |        |
| end |         |         |        |

**(48) n=6 & m=8**

|         |              |         |         |         |     |         |         |         |
|---------|--------------|---------|---------|---------|-----|---------|---------|---------|
| PBC=ON  |              |         |         |         | H9  | -6.7137 | -4.8699 | -0.0431 |
| PBC     | 11.8900      | 11.8900 | 11.8900 | 60.0000 | H10 | -0.4504 | 0.4008  | -3.5045 |
| 60.0000 | 60.0000 (P1) |         |         |         | H11 | 0.1034  | -1.9694 | -3.0690 |
| O1      | 6.6796       | 3.9743  | 0.0516  |         | H12 | -3.7089 | -2.2619 | 1.7656  |
| O2      | 3.0492       | 1.9423  | 1.2975  |         | H13 | 0.0390  | 2.3671  | -2.7303 |
| O3      | 5.2232       | 3.2231  | -2.3387 |         | H14 | 6.2250  | 0.4612  | 3.6288  |
| O4      | 2.9418       | 1.9593  | -1.4483 |         | H15 | 5.1094  | -1.4285 | 4.3757  |
| O5      | 3.1230       | -0.6704 | 2.1489  |         | H16 | -0.2672 | 3.5667  | 0.7854  |
| O6      | -0.6457      | 1.3276  | 3.4984  |         | H17 | 2.9909  | -1.3128 | -1.4493 |
| O7      | 0.7131       | 3.2249  | 2.1514  |         | H18 | 1.2630  | 6.0065  | 3.3072  |
| O8      | 4.4162       | 5.2623  | 3.7089  |         | H19 | 4.7864  | 4.5034  | 3.1729  |
| O9      | 1.5185       | 5.1935  | 3.8479  |         | H20 | 2.3419  | -2.9098 | -0.0092 |
| O10     | 2.8985       | -0.7523 | -2.2691 |         | H21 | 4.3976  | 2.8018  | -1.9711 |
| O11     | 6.7314       | 1.3173  | 3.6501  |         | H22 | 0.2228  | -1.7472 | 3.0767  |
| O12     | -0.8272      | 3.7604  | -0.0222 |         | H23 | -0.7660 | 1.6380  | 4.4441  |
| O13     | 0.5631       | 3.0576  | -2.2261 |         | H24 | 7.5107  | 3.4037  | 0.0262  |
| O14     | -5.0868      | -3.0831 | 2.3526  |         | H25 | 1.5034  | -1.1719 | -3.1255 |
| O15     | -3.0749      | -1.8216 | -1.4041 |         | H26 | -1.1010 | 1.5163  | -4.4559 |
| O16     | -6.5238      | -3.8863 | -0.0234 |         | H27 | 0.3193  | -0.2365 | 3.5973  |
| O17     | -5.2788      | -3.1397 | -2.2857 |         | H28 | -1.5570 | 1.1466  | 3.1203  |
| O18     | -3.3218      | 0.7815  | -2.1626 |         | H29 | -1.5908 | -2.7015 | -1.9087 |
| O19     | 0.6111       | -1.2661 | -3.5722 |         | H30 | 0.1690  | 2.5613  | 2.6691  |
| O20     | -0.7508      | -3.1336 | -2.2172 |         | H31 | -0.3031 | 3.4637  | -0.8263 |
| O21     | -0.6580      | -2.9045 | 2.3124  |         | H32 | -1.4988 | -2.4823 | 1.9564  |
| O22     | 0.8603       | -3.6709 | 0.1228  |         | H33 | -3.2682 | -0.1774 | -1.8821 |
| O23     | -6.7935      | -1.2779 | -3.7071 |         | H34 | -4.7859 | -6.0223 | -3.2623 |
| O24     | -2.9480      | 0.7547  | 2.2919  |         | H35 | -2.9924 | 1.3404  | 1.4859  |
| O25     | -1.5094      | -5.1418 | -3.8591 |         | H36 | -2.2406 | 2.9056  | 0.0136  |
| O26     | -4.3449      | -5.2440 | -3.7092 |         | H37 | 3.0541  | 0.2787  | 1.8546  |
| O27     | 5.2883       | 3.1730  | 2.2617  |         | H38 | -6.3009 | -0.4059 | -3.6632 |
| O28     | 0.8124       | -1.0967 | 3.5654  |         | H39 | 5.8117  | 3.4462  | 1.4550  |
| O29     | 3.1960       | -2.3880 | -0.0632 |         | H40 | 5.8291  | 2.4911  | 2.7565  |
| O30     | 5.4529       | -1.1524 | 3.4727  |         | H41 | -4.7489 | 0.9983  | -2.9972 |
| O31     | -2.8952      | -1.7874 | 1.4277  |         | H42 | -7.3988 | -3.3895 | -0.0275 |
| O32     | -0.9485      | 1.2534  | -3.4952 |         | H43 | 2.5056  | 5.1538  | 3.8500  |
| O33     | -5.5795      | 1.1320  | -3.5440 |         | H44 | 3.8429  | 2.4028  | 1.6921  |
| O34     | -3.1014      | 2.3922  | 0.0918  |         | H45 | -5.6475 | -2.3603 | 2.7916  |
| H1      | -4.7652      | -5.0884 | -4.6029 |         | H46 | 1.4099  | 2.6162  | -1.9354 |
| H2      | -3.7438      | 0.9943  | 2.8554  |         | H47 | 6.7314  | 1.6254  | 4.6101  |
| H3      | -3.1502      | 1.7843  | -0.6949 |         | H48 | 4.6248  | -0.9816 | 2.9430  |
| H4      | -1.0284      | -3.8664 | -2.8403 |         | H49 | -4.9419 | -3.9417 | -2.7860 |
| H5      | -6.2483      | -1.9322 | -3.1952 |         | H50 | 3.7080  | -0.9612 | -2.8203 |
| H6      | 0.2991       | -3.4447 | -0.6588 |         | H51 | 0.9815  | 3.9500  | 2.7822  |
| H7      | -0.1255      | -3.2041 | 1.5243  |         | H52 | 4.7654  | 6.0853  | 3.2629  |
| H8      | -5.2277      | 1.4076  | -4.4382 |         | H53 | 3.1791  | -1.7608 | 0.7074  |

|     |         |         |         |     |         |         |         |
|-----|---------|---------|---------|-----|---------|---------|---------|
| H54 | -1.1935 | -5.9478 | -3.3310 | H1  | 17.2256 | 7.3564  | 4.8312  |
| H55 | -3.0933 | -1.8348 | -0.4141 | H2  | 16.9508 | 7.4052  | 5.5163  |
| H56 | -3.8734 | -2.3382 | -1.7157 | end |         |         |         |
| H57 | 6.1479  | 3.7319  | -0.7471 | H1  | 10.2770 | 4.3501  | 4.1197  |
| H58 | 2.2382  | 2.4101  | 1.6386  | H2  | 10.1839 | 3.6292  | 3.9638  |
| H59 | 2.9654  | 1.9558  | -0.4529 | end |         |         |         |
| H60 | -5.7713 | -3.4703 | -1.4763 | H1  | 15.0243 | 9.0613  | 7.9787  |
| H61 | -2.9196 | -0.8533 | 1.7912  | H2  | 14.4284 | 8.9854  | 8.4164  |
| H62 | -2.4976 | -5.1967 | -3.8891 | end |         |         |         |
| H63 | 2.3067  | -0.8448 | 2.6953  | H1  | 8.1833  | 3.4941  | 2.8292  |
| H64 | -2.4975 | 0.9499  | -2.6973 | H2  | 8.3335  | 3.2752  | 2.1384  |
| H65 | 2.9436  | 1.0067  | -1.7317 | end |         |         |         |
| H66 | 5.6610  | 2.4820  | -2.8586 | H1  | 13.2019 | 9.9910  | 6.0621  |
| H67 | 0.8935  | -4.6744 | 0.1254  | H2  | 13.1494 | 9.3197  | 5.7502  |
| H68 | -5.5811 | -3.3852 | 1.5501  | end |         |         |         |
| end |         |         |         | H1  | 10.6637 | 6.4148  | 4.4812  |
| H1  | -4.6031 | 5.8611  | 2.7375  | H2  | 11.1648 | 6.3043  | 3.9467  |
| H2  | -4.9655 | 5.2173  | 2.6865  | end |         |         |         |
| end |         |         |         | H1  | 15.2107 | 3.2534  | 3.7874  |
| H1  | 9.1900  | 5.2591  | 1.9346  | H2  | 14.5878 | 3.0287  | 4.1076  |
| H2  | 9.6825  | 5.7038  | 1.5990  | end |         |         |         |
| end |         |         |         | H1  | 16.1187 | 6.1571  | 0.5302  |
| H1  | 8.7653  | 6.2624  | 5.6622  | H2  | 16.1527 | 6.3811  | -0.1707 |
| H2  | 8.9654  | 5.5730  | 5.4754  | end |         |         |         |
| end |         |         |         | H1  | 20.1022 | 9.8917  | 9.9981  |
| H1  | 7.2805  | 3.8056  | 4.8936  | H2  | 19.4362 | 9.9525  | 9.6919  |
| H2  | 7.4680  | 4.4151  | 4.5147  | end |         |         |         |
| end |         |         |         | H1  | 8.5555  | 10.3751 | 5.7486  |
| H1  | 14.9813 | 8.5910  | 3.7913  | H2  | 9.0966  | 10.8412 | 5.5688  |
| H2  | 14.8294 | 8.5477  | 4.5177  | end |         |         |         |
| end |         |         |         | H1  | 11.8847 | 9.0967  | 0.8432  |
| H1  | 16.6133 | 9.6359  | 6.4274  | H2  | 11.6921 | 8.5314  | 0.4135  |
| H2  | 16.0035 | 9.5198  | 6.0180  | end |         |         |         |
| end |         |         |         | H1  | 8.7463  | 8.9446  | 8.3046  |
| H1  | 15.3624 | 7.1470  | 7.3500  | H2  | 9.2844  | 8.8641  | 7.8081  |
| H2  | 15.7431 | 6.5893  | 7.0418  | end |         |         |         |
| end |         |         |         | H1  | 6.0377  | 0.7059  | 1.5391  |
| H1  | 13.3270 | 6.9170  | 5.4329  | H2  | 5.3074  | 0.6351  | 1.4937  |
| H2  | 13.2368 | 7.3652  | 6.0187  | end |         |         |         |
| end |         |         |         | H1  | 4.1247  | 4.2697  | -0.3522 |
| H1  | 15.1908 | 11.3965 | 5.2425  | H2  | 4.1415  | 3.6371  | 0.0217  |
| H2  | 14.5900 | 11.1328 | 4.8995  | end |         |         |         |
| end |         |         |         | H1  | 15.0419 | 4.9959  | 1.9437  |
| H1  | 8.9390  | 7.1386  | 3.2422  | H2  | 14.6987 | 4.7555  | 1.3358  |
| H2  | 8.4929  | 7.5458  | 3.6719  | end |         |         |         |
| end |         |         |         | H1  | 12.6209 | 1.8310  | 0.2612  |

|     |         |         |         |
|-----|---------|---------|---------|
| H2  | 12.5136 | 1.1519  | 0.5236  |
| end |         |         |         |
| H1  | 12.3299 | 2.4735  | 8.2072  |
| H2  | 11.9134 | 3.0785  | 8.1605  |
| end |         |         |         |
| H1  | 7.7821  | -0.0690 | 0.4192  |
| H2  | 7.3467  | 0.2093  | -0.1026 |
| end |         |         |         |
| H1  | 7.2247  | 9.4973  | 0.5929  |
| H2  | 7.2597  | 9.6588  | -0.1251 |
| end |         |         |         |
| H1  | 13.5529 | 1.9870  | 5.5980  |
| H2  | 13.6353 | 2.6401  | 5.9266  |
| end |         |         |         |
| H1  | 9.7949  | 12.8507 | 5.7198  |
| H2  | 10.0571 | 12.4451 | 6.2740  |
| end |         |         |         |
| H1  | 19.9548 | 11.2979 | 3.8629  |
| H2  | 19.4439 | 11.6686 | 3.4868  |
| end |         |         |         |
| H1  | 9.9173  | 10.5471 | -0.0283 |
| H2  | 10.3857 | 10.0084 | -0.1981 |
| end |         |         |         |
| H1  | 17.1200 | 9.8311  | 1.2681  |
| H2  | 17.3062 | 10.3125 | 1.7905  |
| end |         |         |         |
| H1  | 10.2658 | 11.7313 | 4.1002  |
| H2  | 10.0341 | 11.1748 | 3.6778  |
| end |         |         |         |
| H1  | 6.7769  | 3.6819  | 7.8010  |
| H2  | 6.4332  | 4.1287  | 8.2731  |
| end |         |         |         |
| H1  | 4.4275  | 3.7852  | 8.9256  |
| H2  | 4.7294  | 4.2064  | 9.4483  |
| end |         |         |         |
| H1  | 11.9525 | 5.1235  | 8.7515  |
| H2  | 11.7045 | 4.7762  | 9.3517  |
| end |         |         |         |
| H1  | 10.8648 | 11.8278 | 9.6244  |
| H2  | 11.3752 | 12.2411 | 9.2948  |
| end |         |         |         |
| H1  | 19.3132 | 7.7105  | 9.5972  |
| H2  | 19.9144 | 7.3645  | 9.3512  |
| end |         |         |         |
| end |         |         |         |