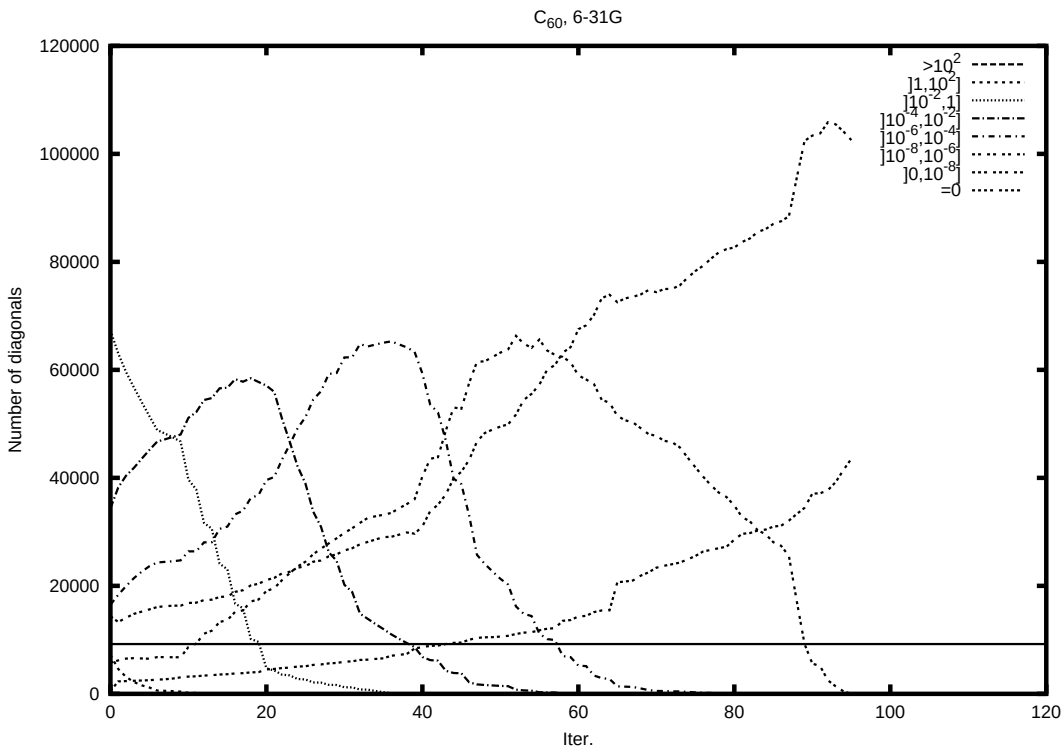
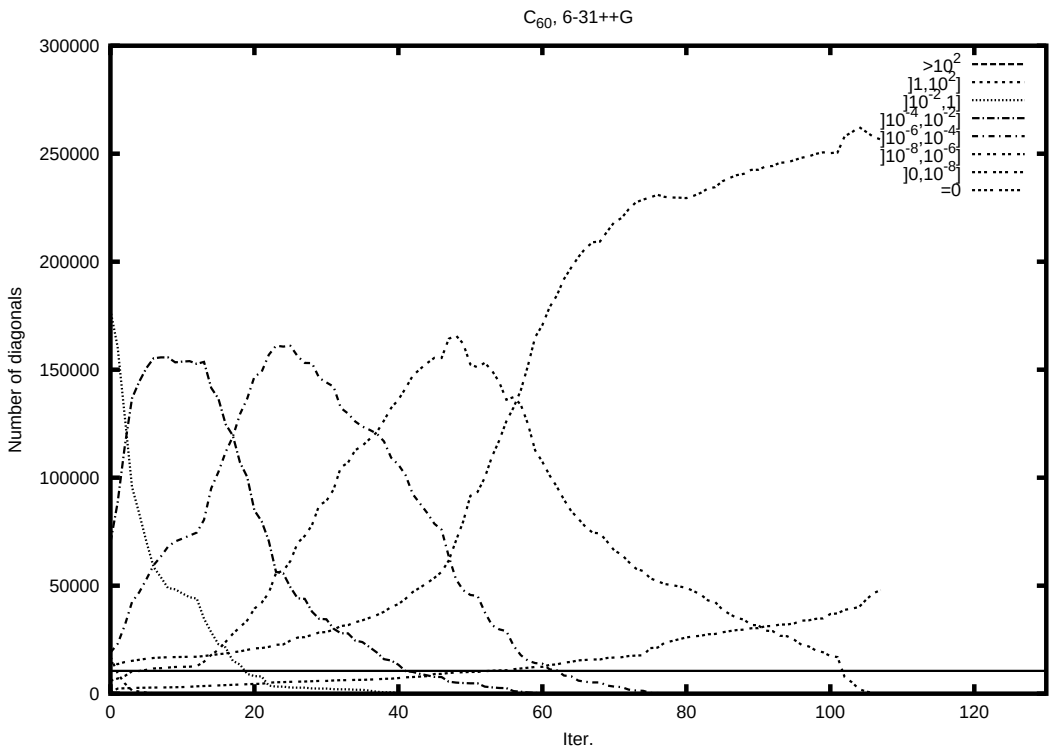
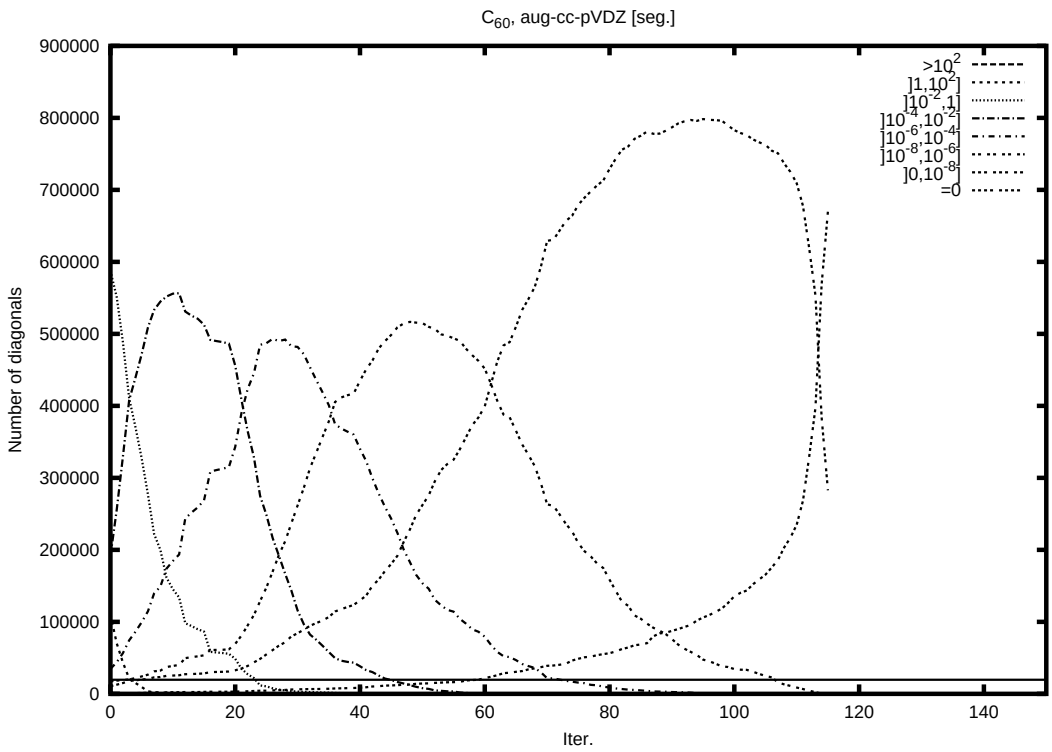
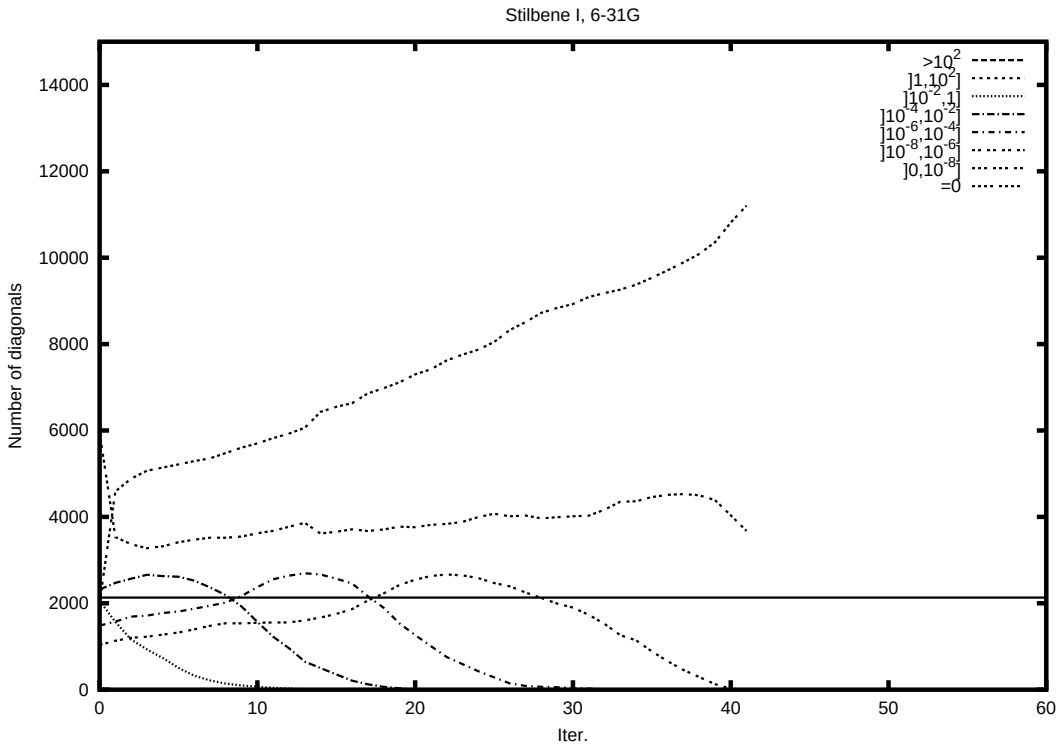
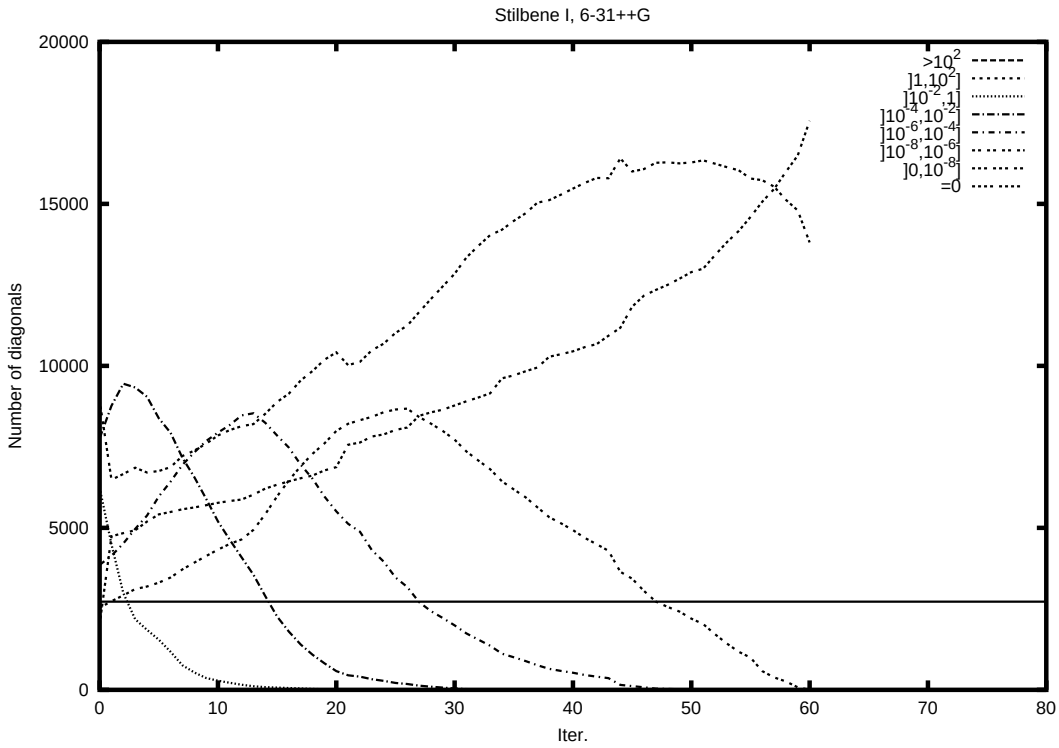
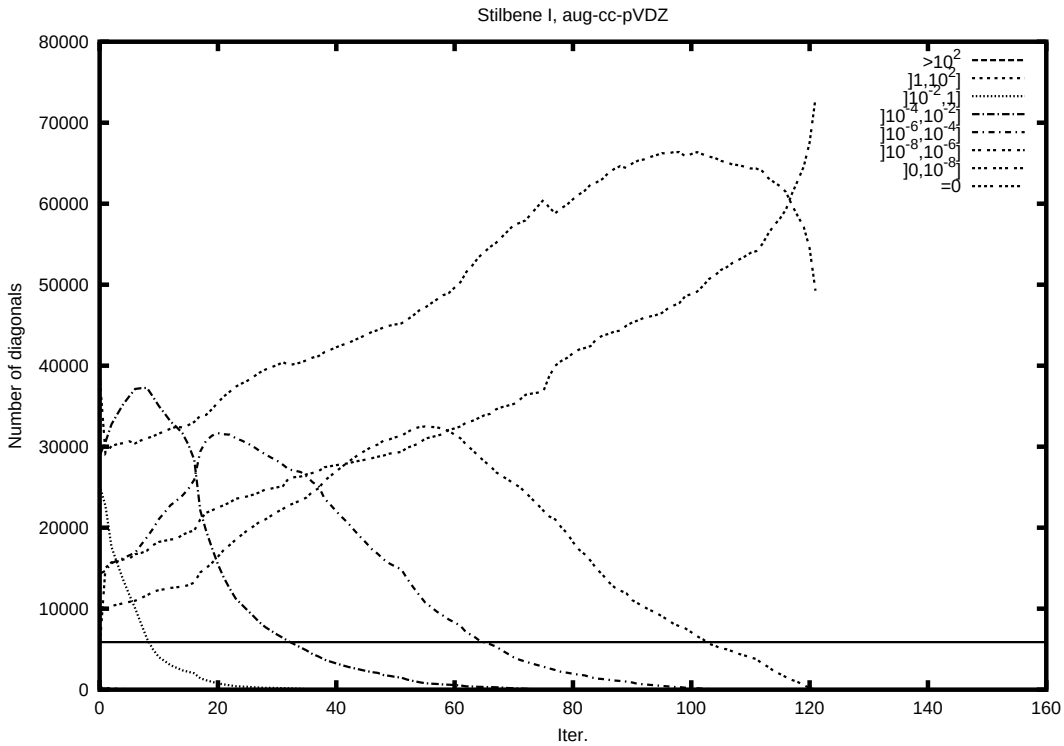

C60, 6-31G
Number of diagonals
Iter.
>10^2
]1,10^2]
]10^-2,1]
]10^-4,10^-2]
]10^-6,10^-4]
]10^-8,10^-6]
]0,10^-8]
=0
0
20000
40000
60000
80000
100000
120000
0
20
40
60
80
100
120

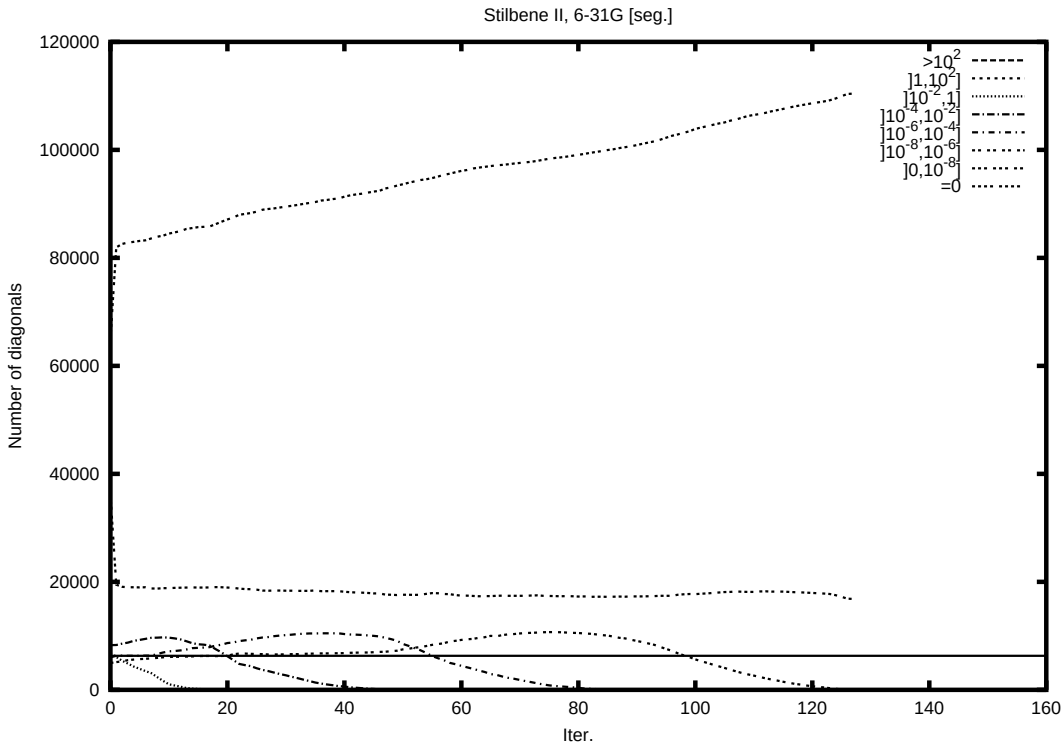

C60, 6-31++G
Number of diagonals
Iter.
>10^2
]1,10^2]
]10^-2,1]
]10^-4,10^-2]
]10^-6,10^-4]
]10^-8,10^-6]
]0,10^-8]
=0
0
50000
100000
150000
200000
250000
300000
0
20
40
60
80
100
120

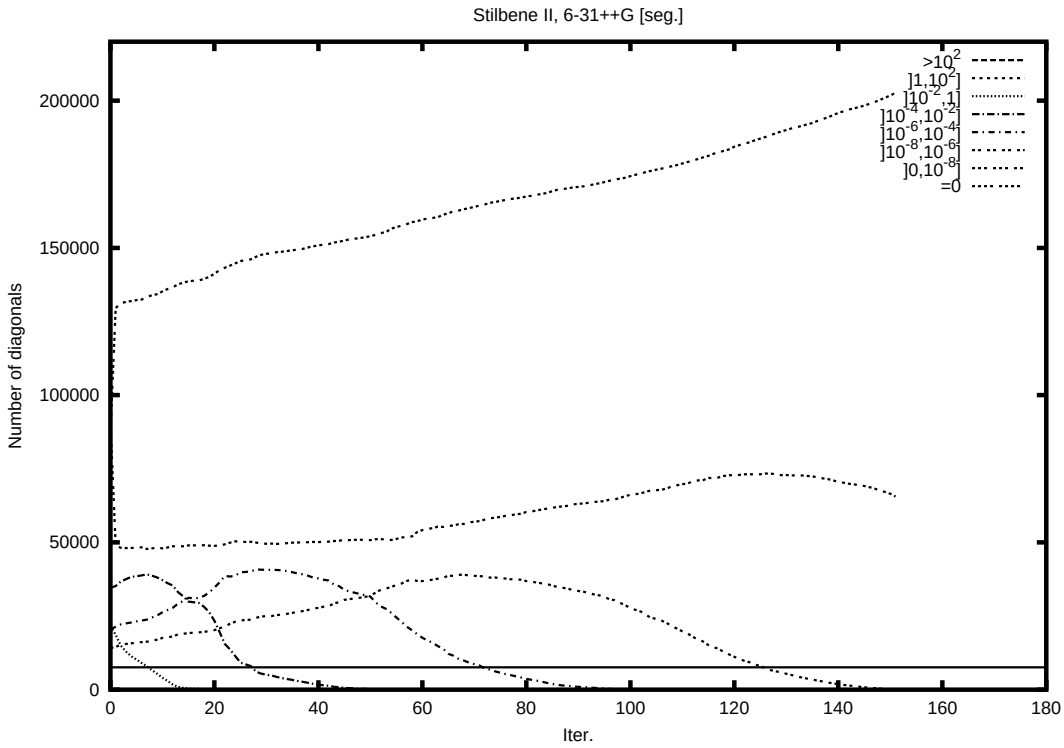

C60, aug-cc-pVDZ [seg.]
Number of diagonals
Iter.
>10^2
]1,10^2]
]10^-2,1]
]10^-4,10^-2]
]10^-6,10^-4]
]10^-8,10^-6]
]0,10^-8]
=0

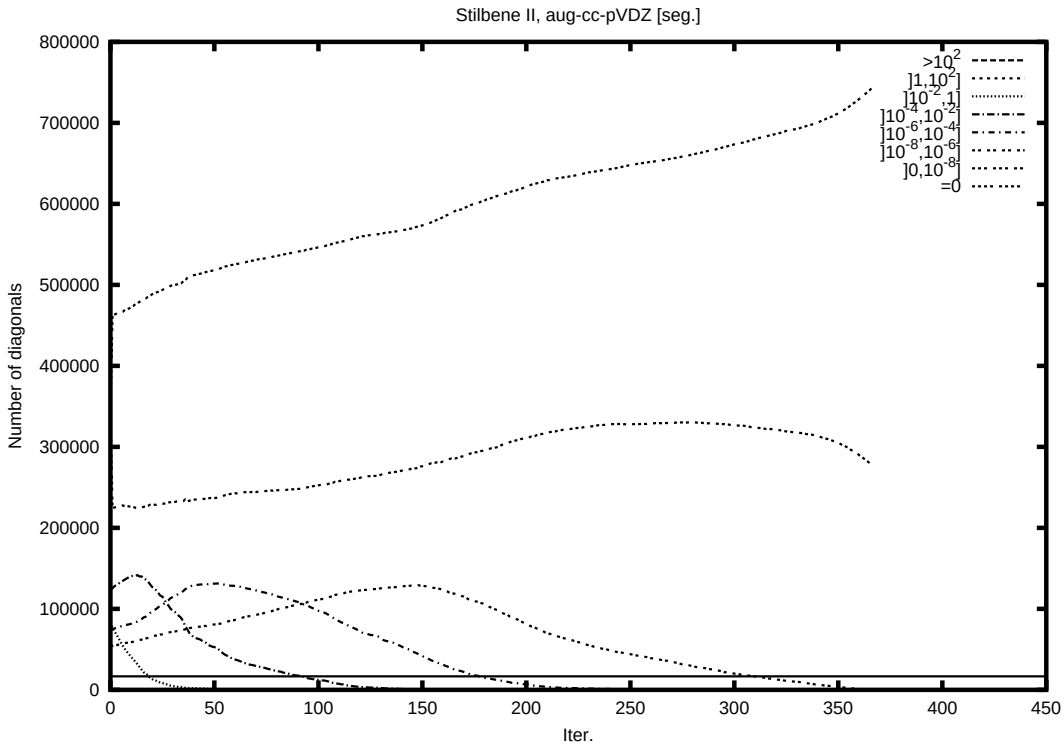

Stilbene I, 6-31G
Number of diagonals
Iter.
>10^2
]1,10^2]
]10^-2,1]
]10^-4,10^-2]
]10^-6,10^-4]
]10^-8,10^-6]
]0,10^-8]
=0

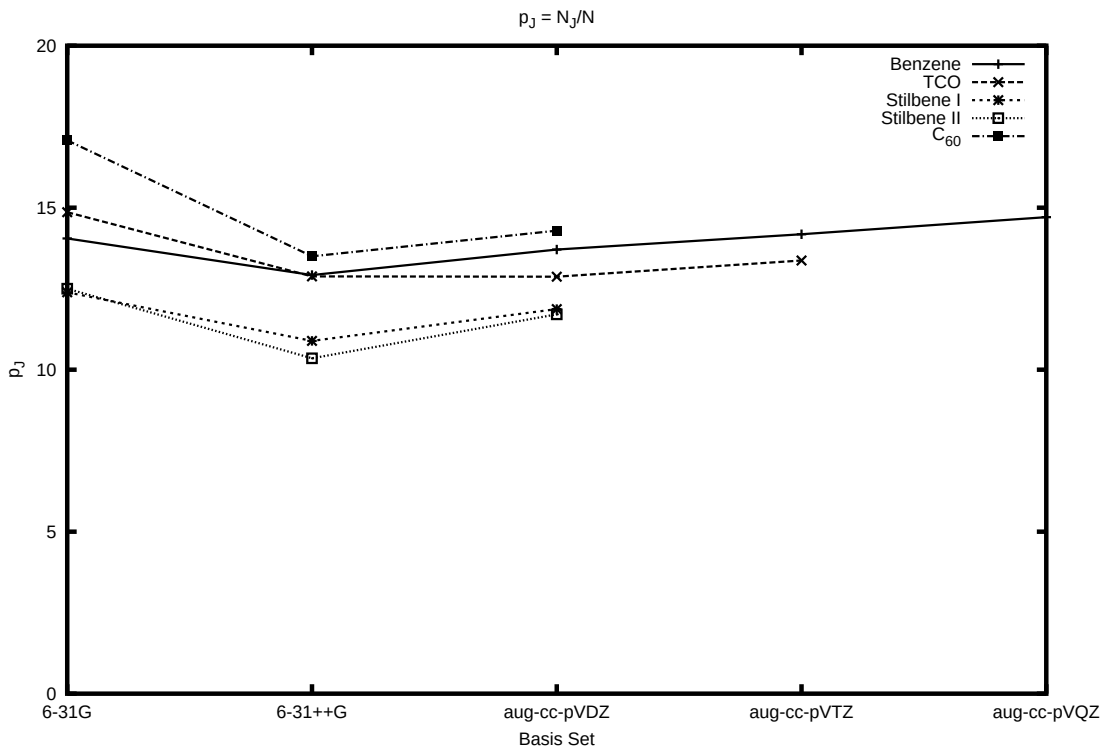

Stilbene I, 6-31++G
Number of diagonals
Iter.
0
5000
10000
15000
20000
0
10
20
30
40
50
60
70
80
>10^2
]1,10^2]
]10^-2,1]
]10^-4,10^-2]
]10^-6,10^-4]
]10^-8,10^-6]
]0,10^-8]
=0


Stilbene I, aug-cc-pVDZ
Number of diagonals
Iter.
0
10000
20000
30000
40000
50000
60000
70000
80000
0
20
40
60
80
100
120
140
160
>10^2
]1,10^2]
]10^-2,1]
]10^-4,10^-2]
]10^-6,10^-4]
]10^-8,10^-6]
]0,10^-8]
=0


Stilbene II, 6-31G [seg.]
Number of diagonals
Iter.
>10^2
]1,10^2]
]10^-2,1]
]10^-4,10^-2]
]10^-6,10^-4]
]10^-8,10^-6]
]0,10^-8]
=0


Stilbene II, 6-31++G [seg.]
Number of diagonals
Iter.
>10^2
]1,10^2]
]10^-2,1]
]10^-4,10^-2]
]10^-6,10^-4]
]10^-8,10^-6]
]0,10^-8]
=0


Stilbene II, aug-cc-pVDZ [seg.]
Number of diagonals
Iter.
>10^2
]1,10^2]
]10^-2,1]
]10^-4,10^-2]
]10^-6,10^-4]
]10^-8,10^-6]
]0,10^-8]
=0
0
100000
200000
300000
400000
500000
600000
700000
800000
0
50
100
150
200
250
300
350
400
450


p_J = N_J/N
p_J
Basis Set
Benzene
TCO
Stilbene I
Stilbene II
C60
0
5
10
15
20
6-31G
6-31++G
aug-cc-pVDZ
aug-cc-pVTZ
aug-cc-pVQZ