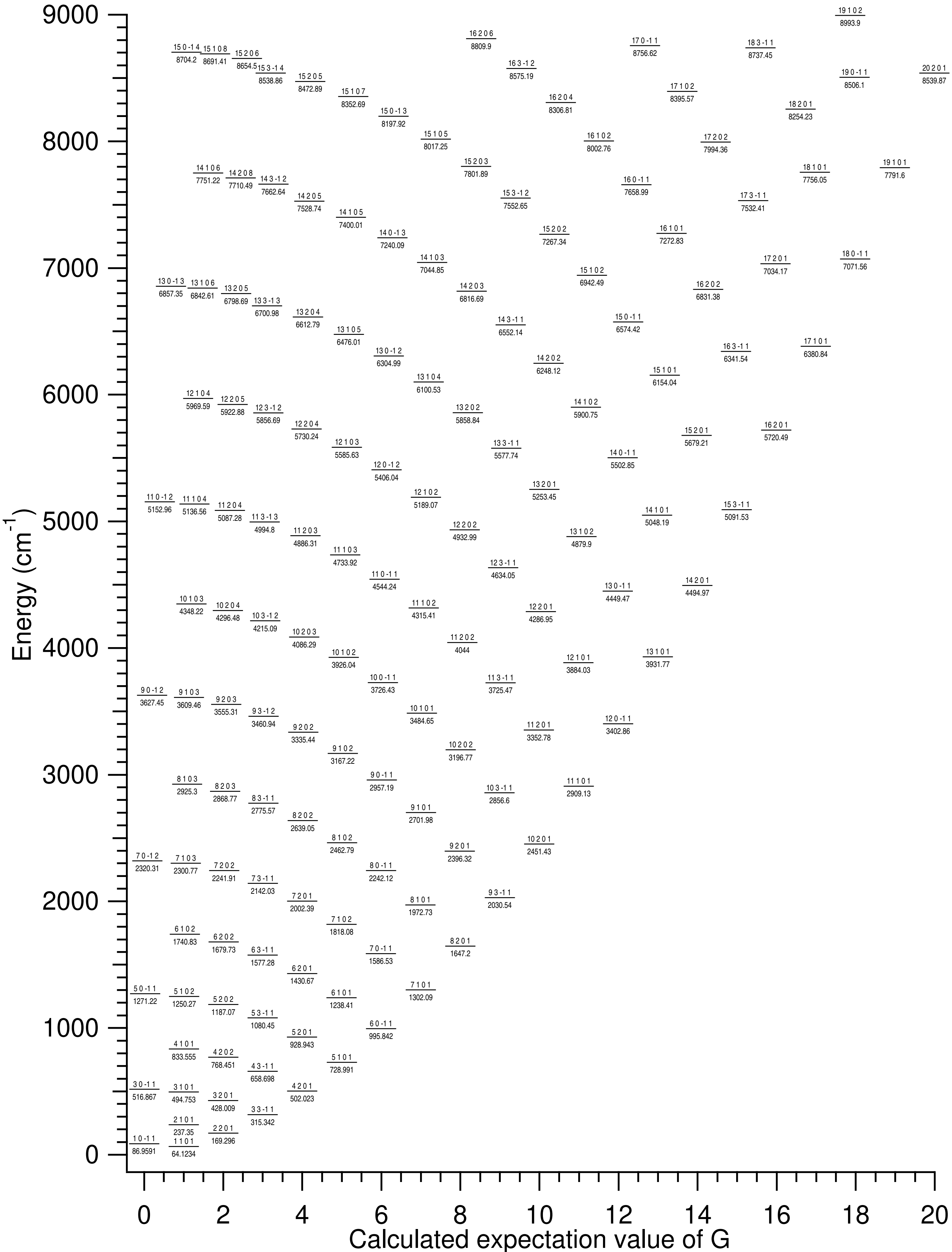
H_3^+ ENERGY LEVEL DIAGRAMS

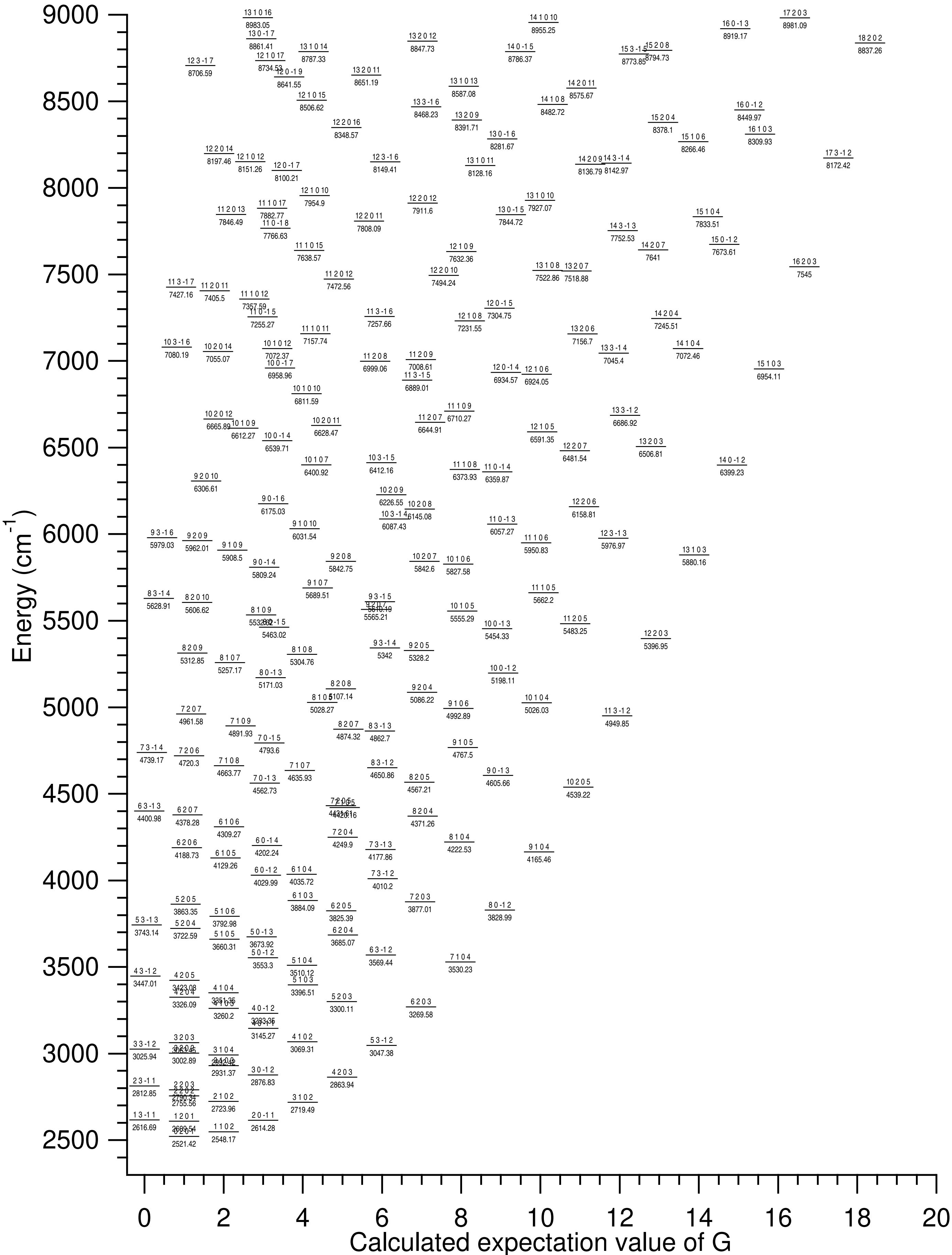
This postscript file contains the energy level diagrams for H_3^+ versus the approximate quantum number G. In the first 12 plots, the energy levels are separated into vibrational bands by rounding the expectation values of v_1, v_2, and ℓ and are plotted versus the expectation value of G. In the second set of plots, the energy levels are separated into the *ideal* bands and plotted versus the *ideal* value of G, each of which was assigned by the authors. See the text for a discussion of these assignments. It is easy to see from these diagrams that G is well behaved at lower energy. At higher energy, however, the states are heavily mixed, and it becomes difficult to identify the G of each level. The vibrational quantum numbers also begin to fail at higher energy as noted by some of the energy levels being assigned to new bands. All of the expectation values and energies used here are from the calculations of Watson. The four numbers above each energy level are the labels used by Watson: J, M, S, n—where J and n are the same as in the text. M and S are related to I and parity as follows:

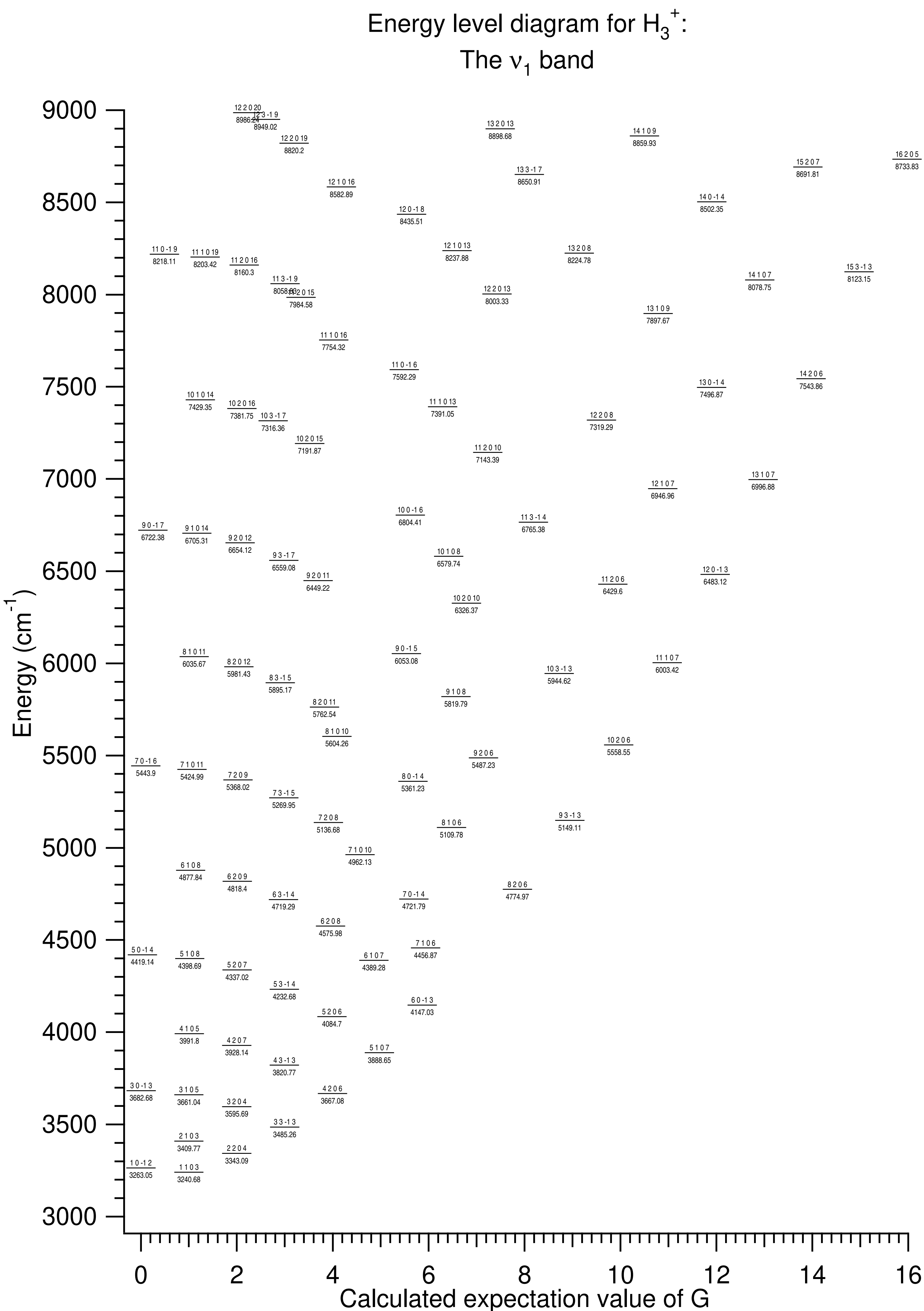
M	S	I	P
0	-1	3/2	$+1$
1	0	1/2	-1
2	0	1/2	$+1$
3	-1	3/2	-1

Energy level diagram for H_3^+:
The ground state



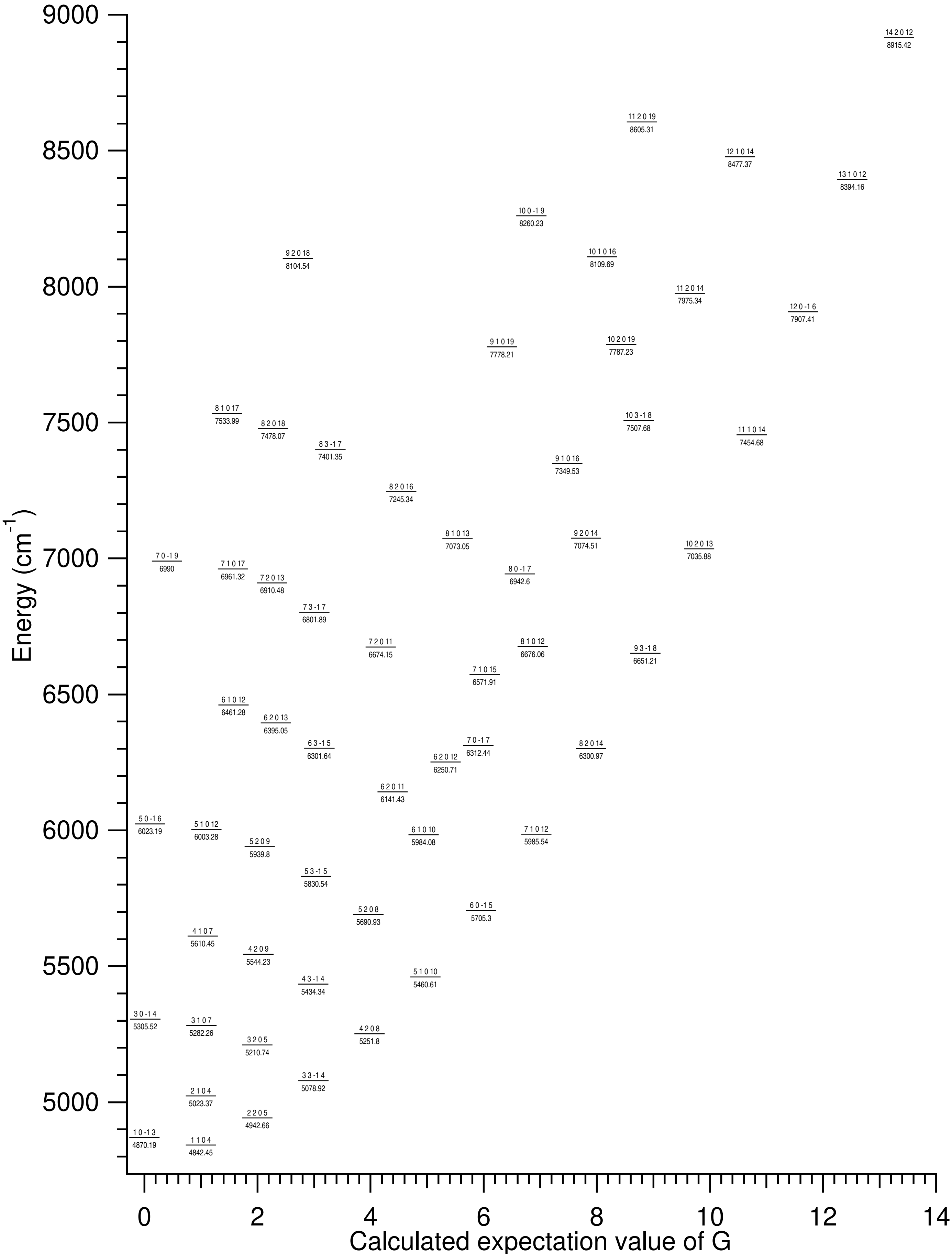
Energy level diagram for H_3^+:
The ν_2 band

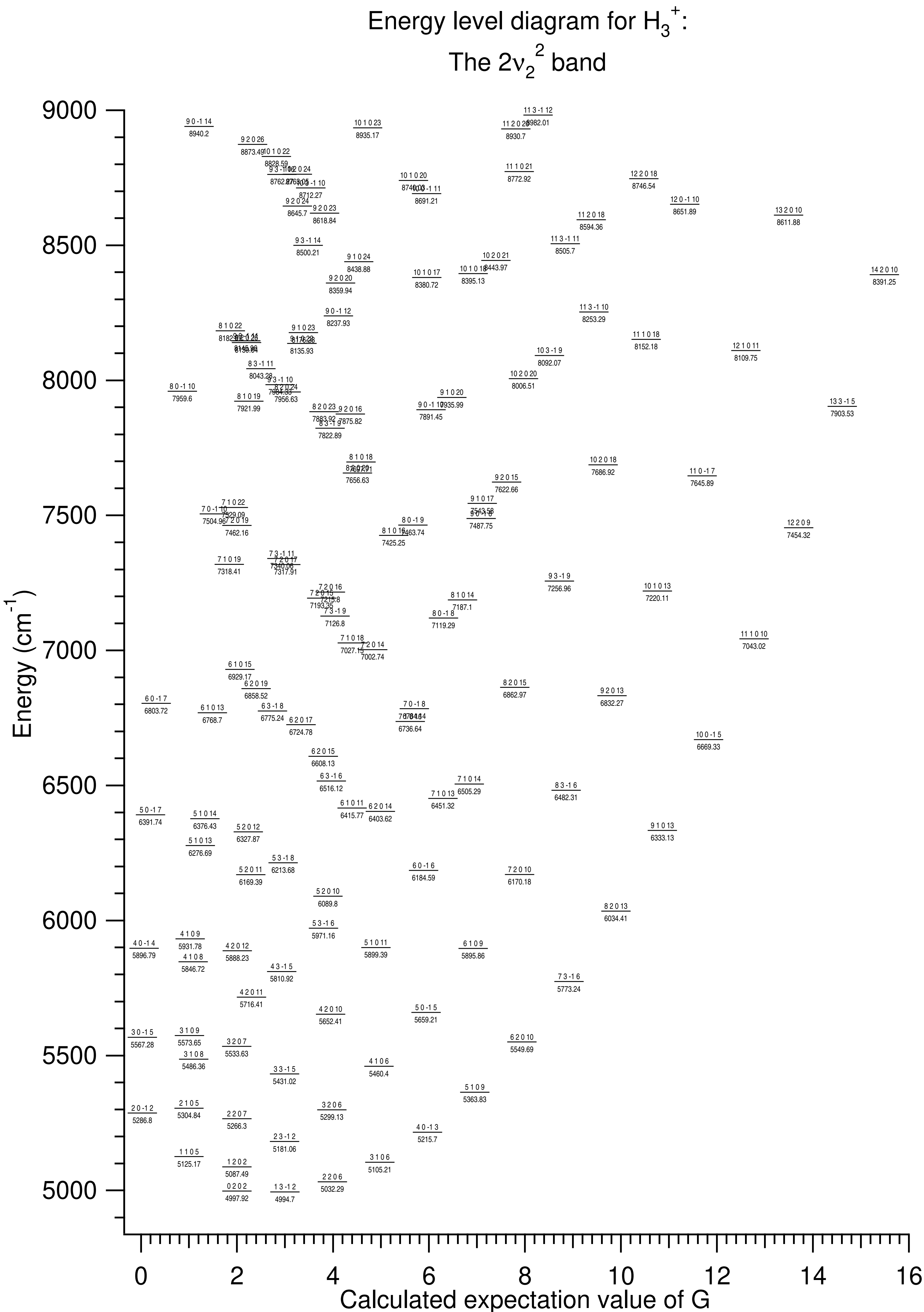


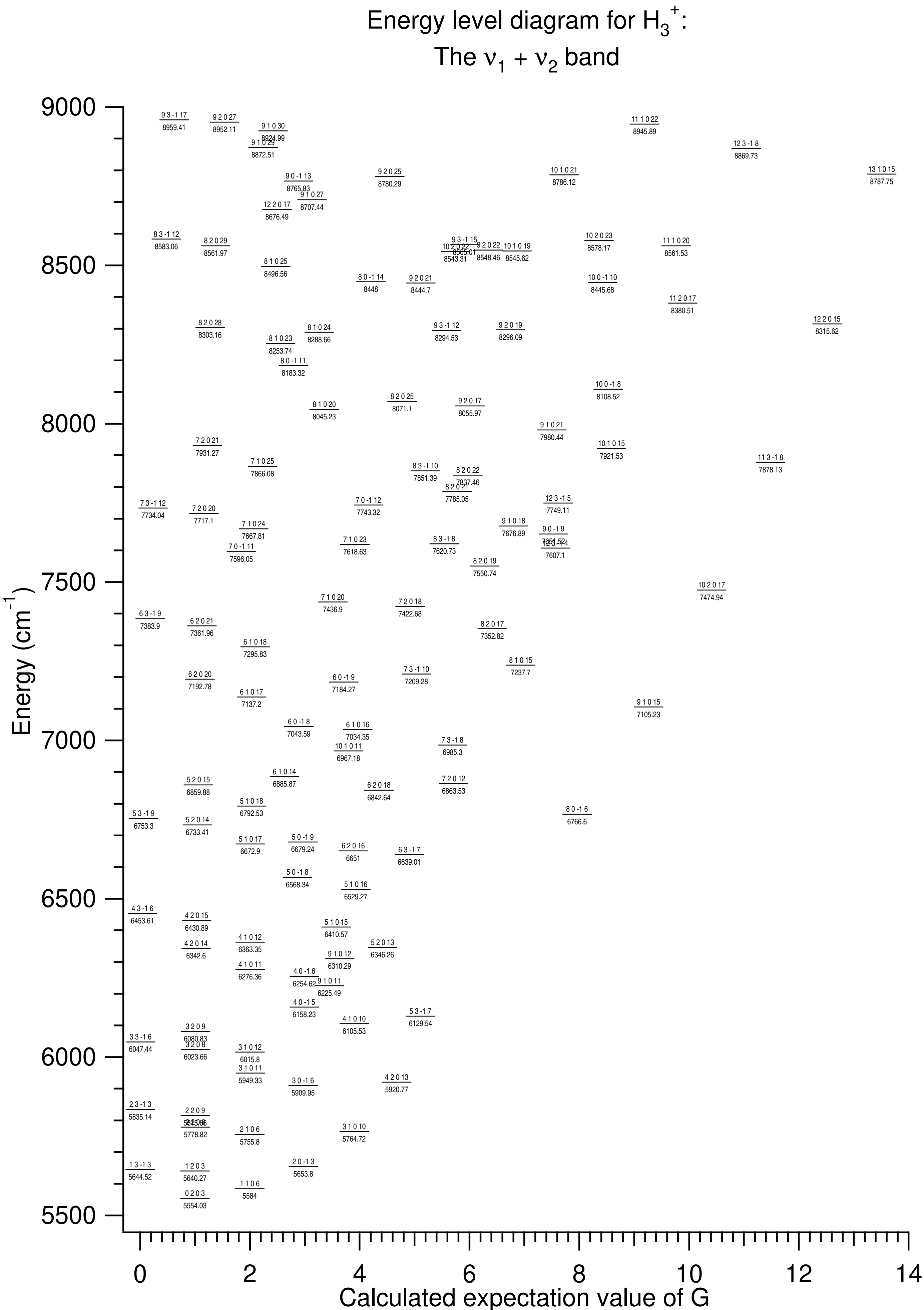


Energy level diagram for H_3^+:
The ν_1 band
Energy (cm^{-1})
Calculated expectation value of G
9000
8500
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
0
2
4
6
8
10
12
14
16
11 0 -1 9
8218.11
9 0 -1 7
6722.38
7 0 -1 6
5443.9
5 0 -1 4
4419.14
3 0 -1 3
3682.68
1 0 -1 2
3263.05
11 1 0 19
8203.42
10 1 0 14
7429.35
9 1 0 14
6705.31
8 1 0 11
6035.67
7 1 0 11
5424.99
6 1 0 8
4877.84
5 1 0 8
4398.69
4 1 0 5
3991.8
3 1 0 5
3661.04
2 1 0 3
3409.77
1 1 0 3
3240.68
12 2 0 20
8986.24
12 3 -1 9
8949.02
11 2 0 16
8160.3
10 2 0 16
7381.75
9 2 0 12
6654.12
8 2 0 12
5981.43
7 2 0 9
5368.02
6 2 0 9
4818.4
5 2 0 7
4337.02
4 2 0 7
3928.14
3 2 0 4
3595.69
2 2 0 4
3343.09
12 2 0 19
8820.2
11 3 -1 9
11 2 0 15
7984.58
10 3 -1 7
7316.36
10 2 0 15
7191.87
9 3 -1 7
6559.08
9 2 0 11
6449.22
8 3 -1 5
5895.17
8 2 0 11
5762.54
7 3 -1 5
5269.95
7 2 0 8
5136.68
6 3 -1 4
4719.29
5 3 -1 4
4232.68
4 3 -1 3
3820.77
3 3 -1 3
3485.26
12 1 0 16
8582.89
11 1 0 16
7754.32
8 1 0 10
5604.26
7 1 0 10
4962.13
6 2 0 8
4575.98
6 1 0 7
4389.28
5 2 0 6
4084.7
5 1 0 7
3888.65
4 2 0 6
3667.08
12 0 -1 8
8435.51
11 0 -1 6
7592.29
10 0 -1 6
6804.41
9 0 -1 5
6053.08
8 0 -1 4
5361.23
7 0 -1 4
4721.79
7 1 0 6
4456.87
6 0 -1 3
4147.03
12 1 0 13
8237.88
11 1 0 13
7391.05
10 1 0 8
6579.74
10 2 0 10
6326.37
9 1 0 8
5819.79
9 2 0 6
5487.23
8 1 0 6
5109.78
13 2 0 13
8898.68
12 2 0 13
8003.33
11 2 0 10
7143.39
13 3 -1 7
8650.91
11 3 -1 4
6765.38
8 2 0 6
4774.97
13 2 0 8
8224.78
12 2 0 8
7319.29
10 3 -1 3
5944.62
9 3 -1 3
5149.11
11 2 0 6
6429.6
10 2 0 6
5558.55
14 1 0 9
8859.93
13 1 0 9
7897.67
12 1 0 7
6946.96
11 1 0 7
6003.42
14 0 -1 4
8502.35
13 0 -1 4
7496.87
12 0 -1 3
6483.12
14 1 0 7
8078.75
13 1 0 7
6996.88
15 2 0 7
8691.81
14 2 0 6
7543.86
15 3 -1 3
8123.15
16 2 0 5
8733.83

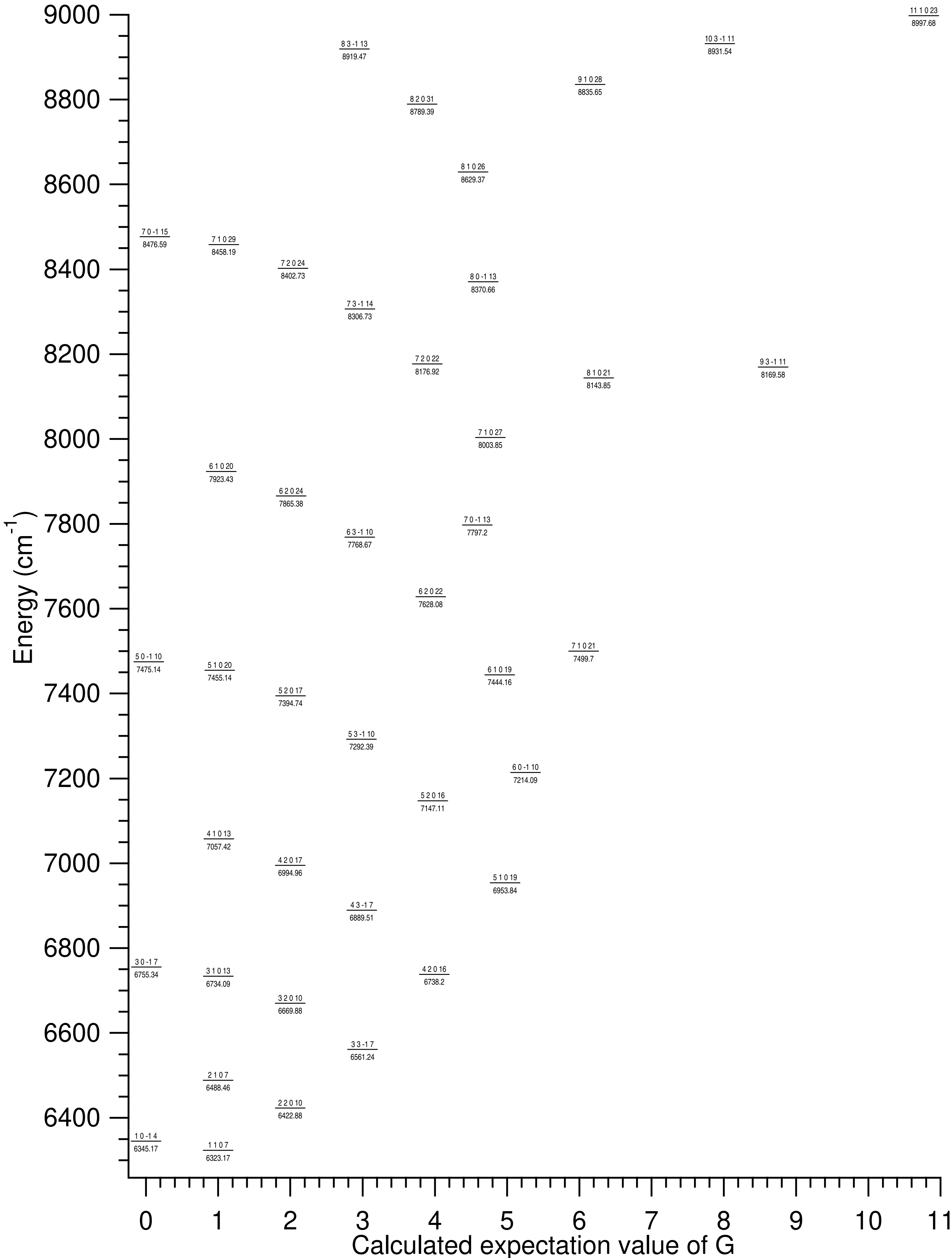
Energy level diagram for H_3^+:
The $2\nu_2^0$ band



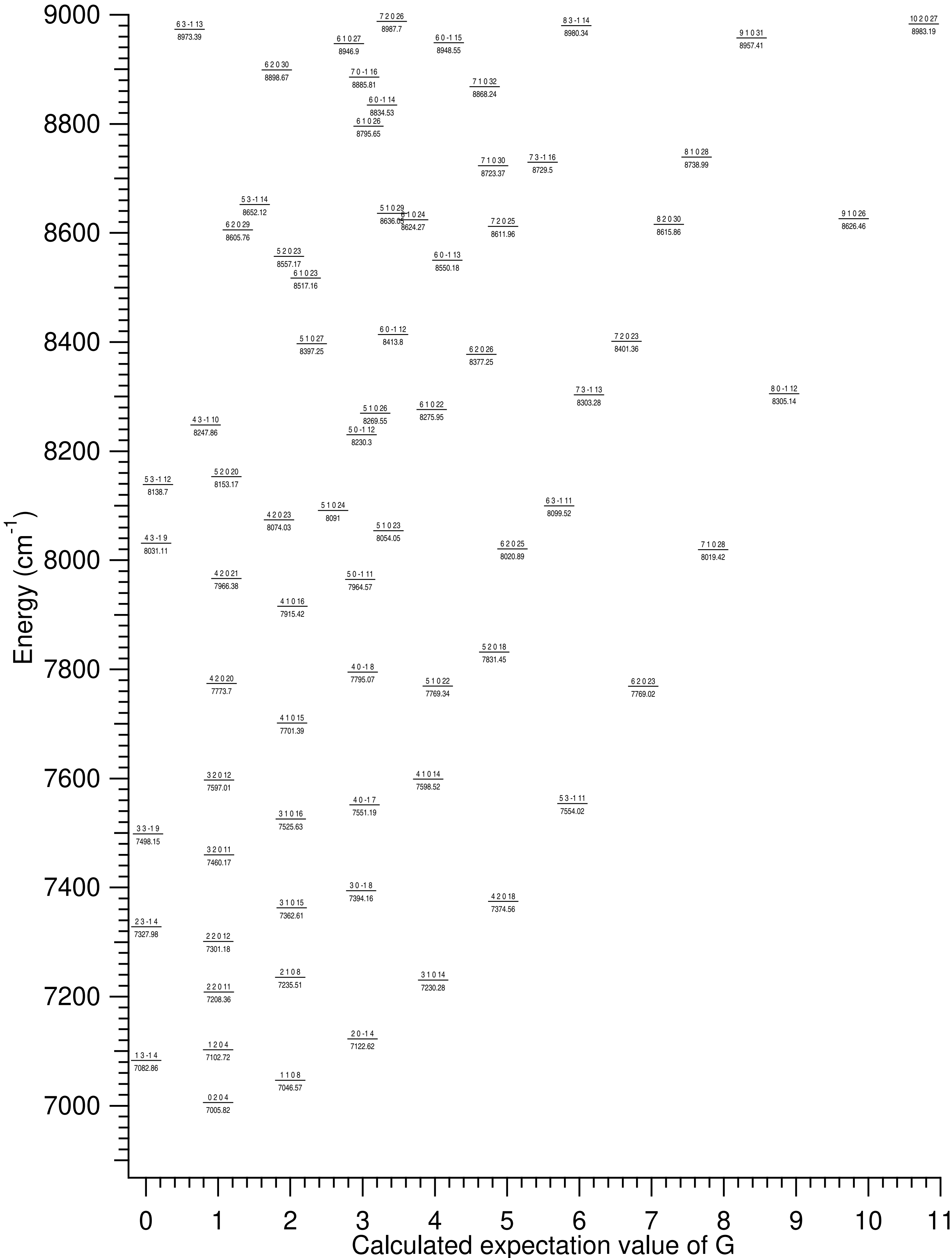

Energy level diagram for H_3^+:
The $2\nu_2^2$ band
Energy (cm^{-1})
Calculated expectation value of G

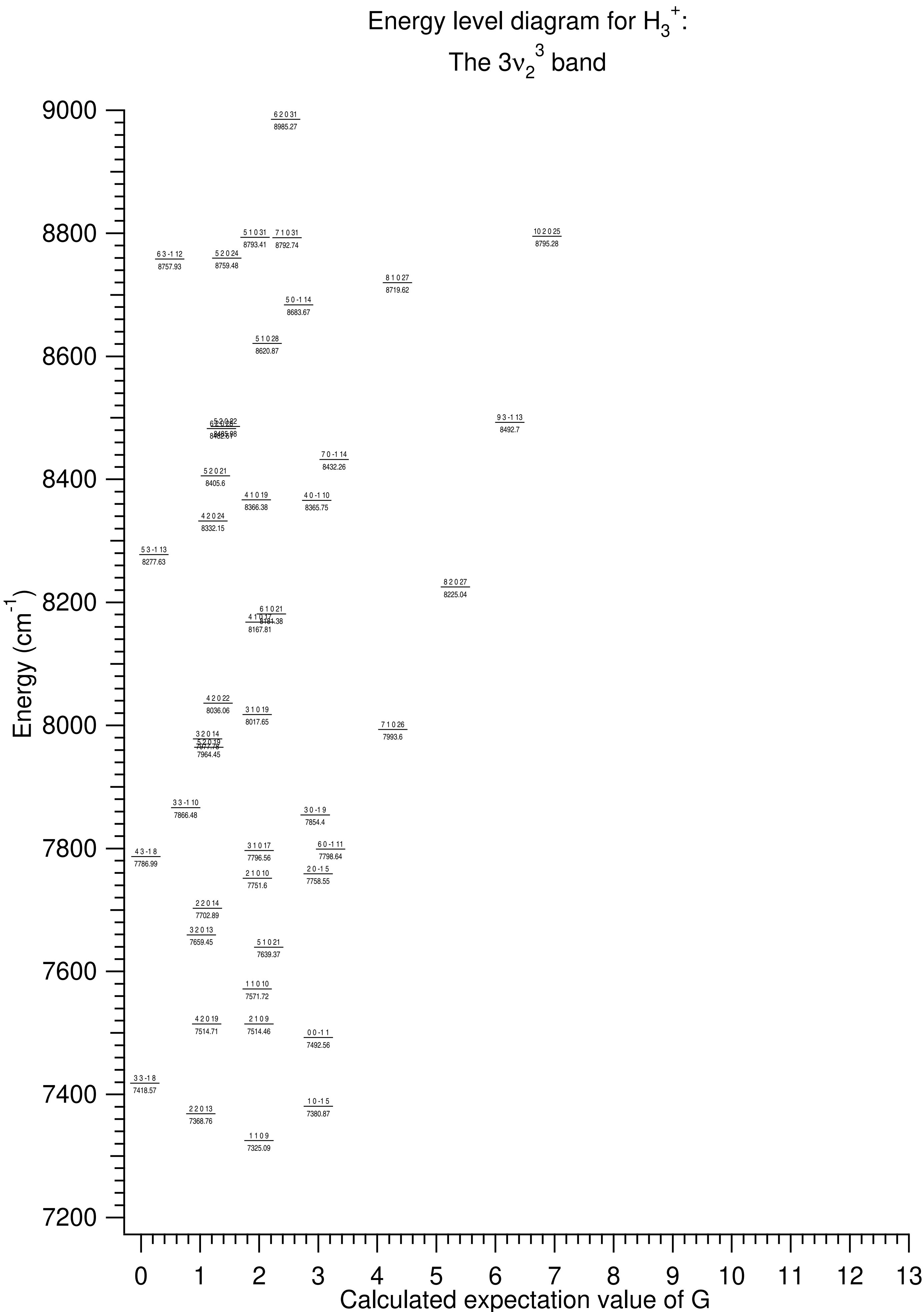

Energy level diagram for H_3^+:
The $\nu_1 + \nu_2$ band
Energy (cm^{-1})
Calculated expectation value of G
9000
8500
8000
7500
7000
6500
6000
5500
0
2
4
6
8
10
12
14

Energy level diagram for H_3^+:
The $2\nu_1$ band



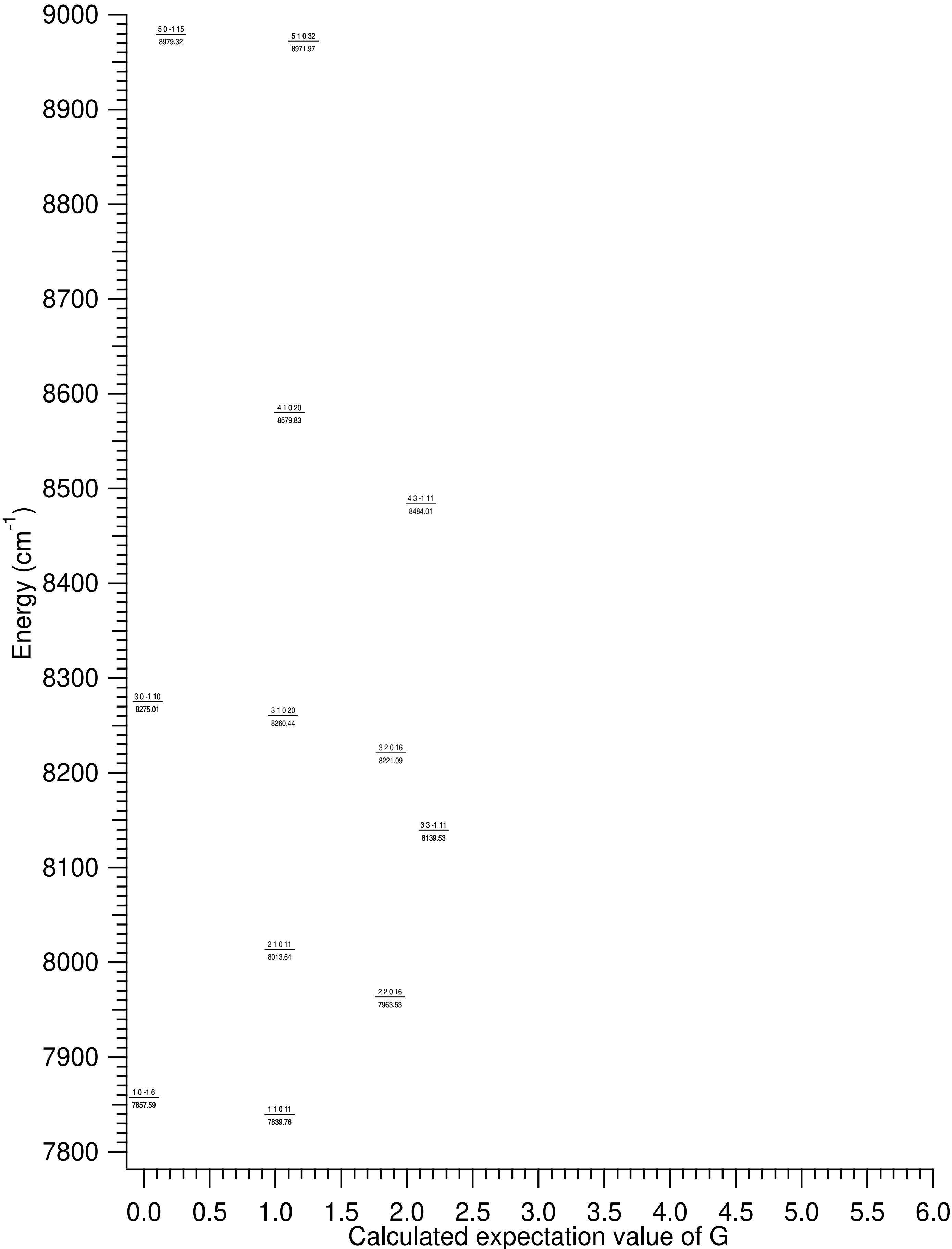
Energy level diagram for H_3^+:
The $3\nu_2^1$ band




Energy level diagram for H_3^+:
The $3\nu_2^3$ band
Energy (cm^{-1})
Calculated expectation value of G
6 2 0 31
8985.27
5 1 0 31
8793.41
7 1 0 31
8792.74
10 2 0 25
8795.28
6 3 -1 12
8757.93
5 2 0 24
8759.48
8 1 0 27
8719.62
5 0 -1 14
8683.67
5 1 0 28
8620.87
9 3 -1 13
8492.7
7 0 -1 14
8432.26
5 2 0 21
8405.6
4 1 0 19
8366.38
4 0 -1 10
8365.75
4 2 0 24
8332.15
5 3 -1 13
8277.63
8 2 0 27
8225.04
6 1 0 21
8167.81
4 2 0 22
8036.06
3 1 0 19
8017.65
7 1 0 26
7993.6
3 2 0 14
7964.45
3 3 -1 10
7866.48
3 0 -1 9
7854.4
4 3 -1 8
7786.99
3 1 0 17
7796.56
6 0 -1 11
7798.64
2 1 0 10
7751.6
2 0 -1 5
7758.55
2 2 0 14
7702.89
3 2 0 13
7659.45
5 1 0 21
7639.37
1 1 0 10
7571.72
4 2 0 19
7514.71
2 1 0 9
7514.46
0 0 -1 1
7492.56
3 3 -1 8
7418.57
2 2 0 13
7368.76
1 0 -1 5
7380.87
1 1 0 9
7325.09

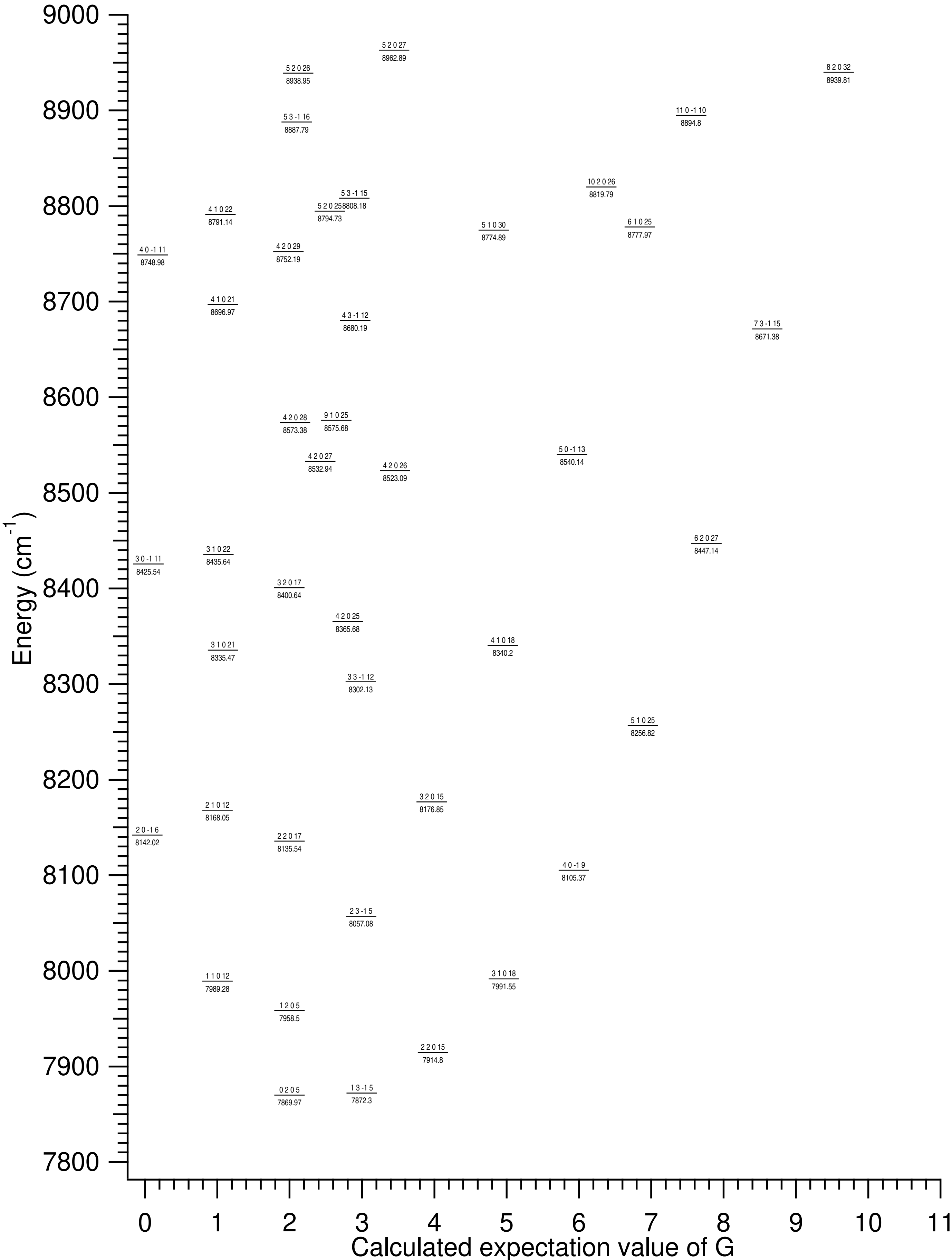
Energy level diagram for H_3^+:

The $\nu_1 + 2\nu_2^0$ band

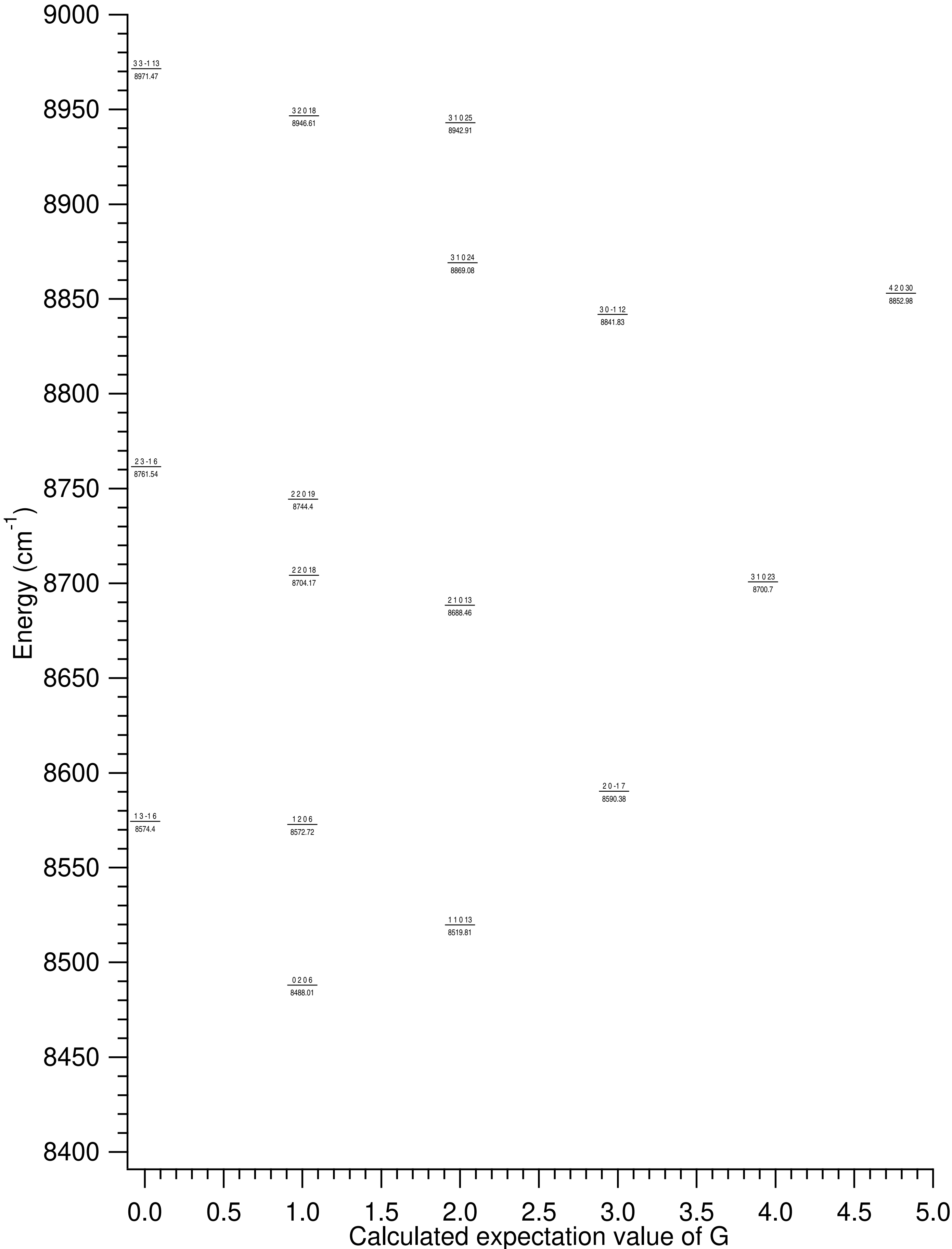


Energy level diagram for H_3^+:

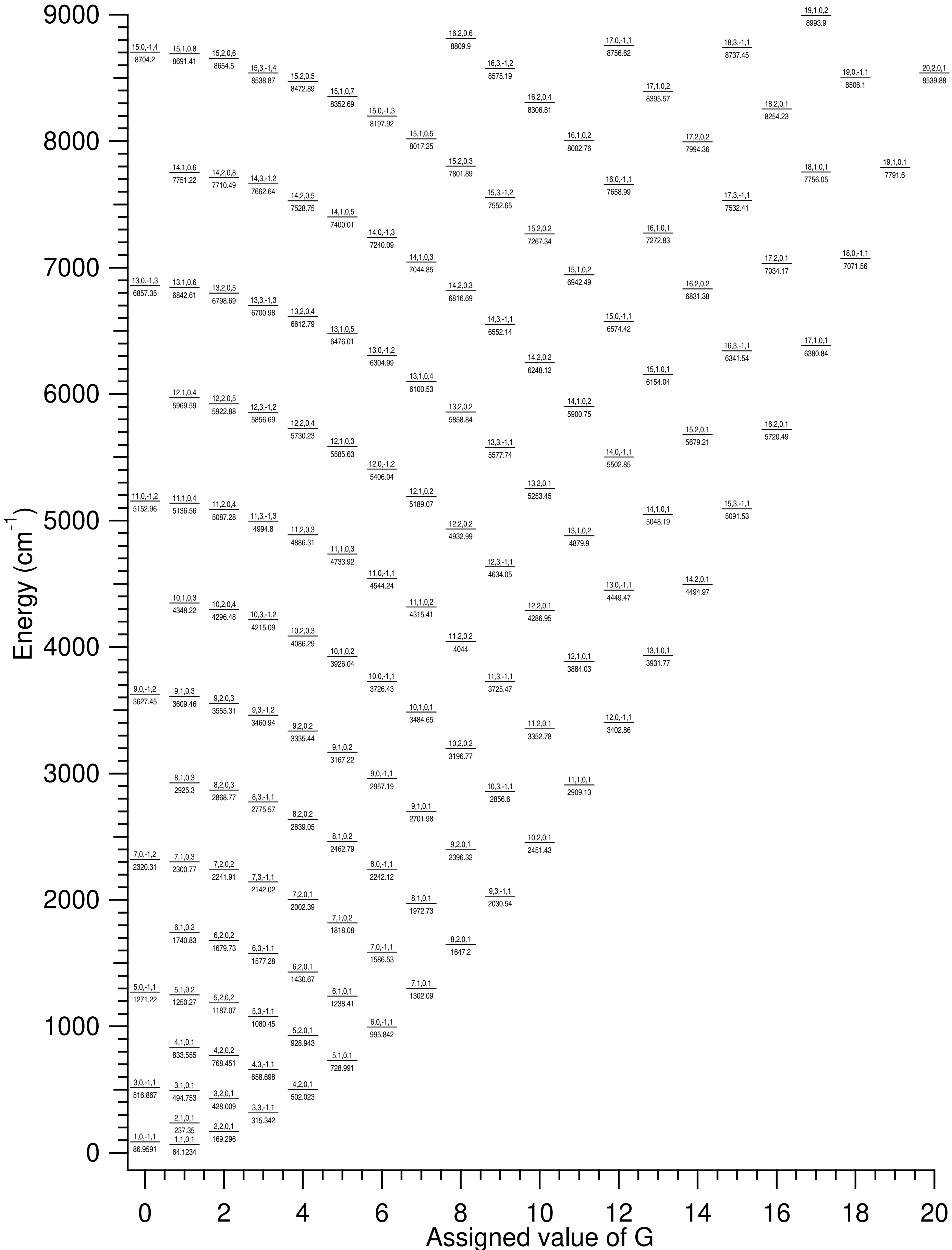
The $\nu_1 + 2\nu_2^2$ band



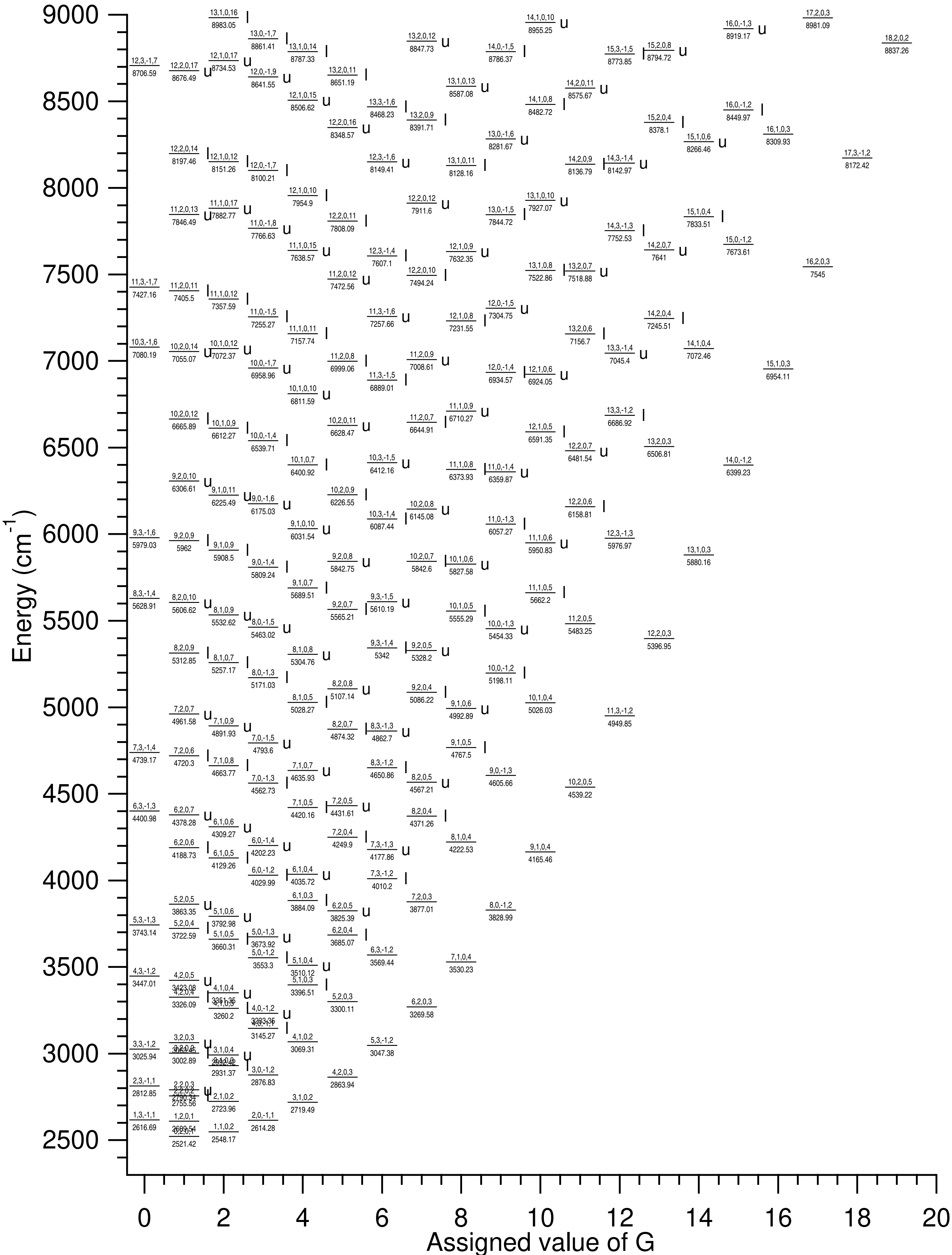
Energy level diagram for H_3^+:
The $2\nu_1 + \nu_2$ band



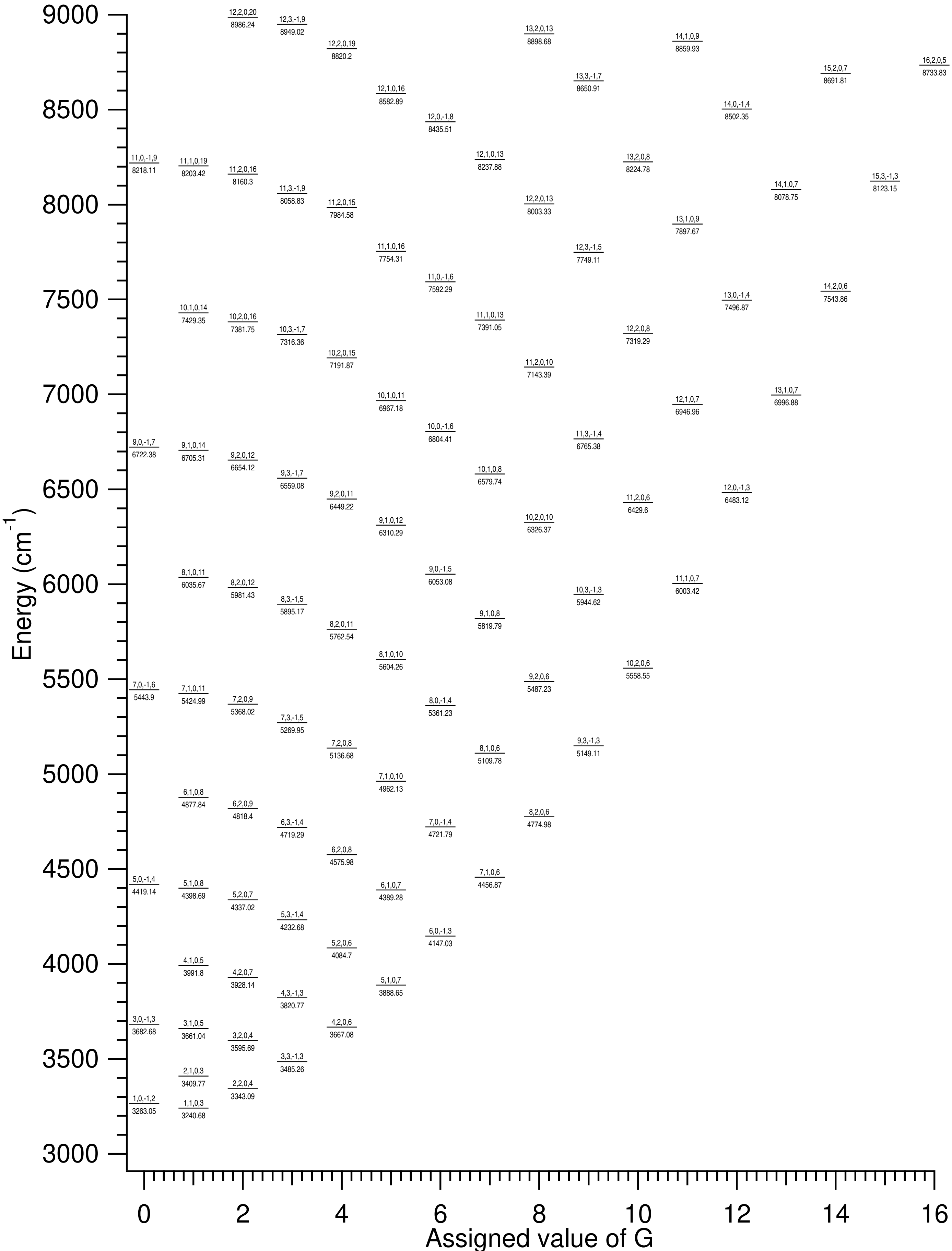
Energy level diagram for H_3^+: The ground state



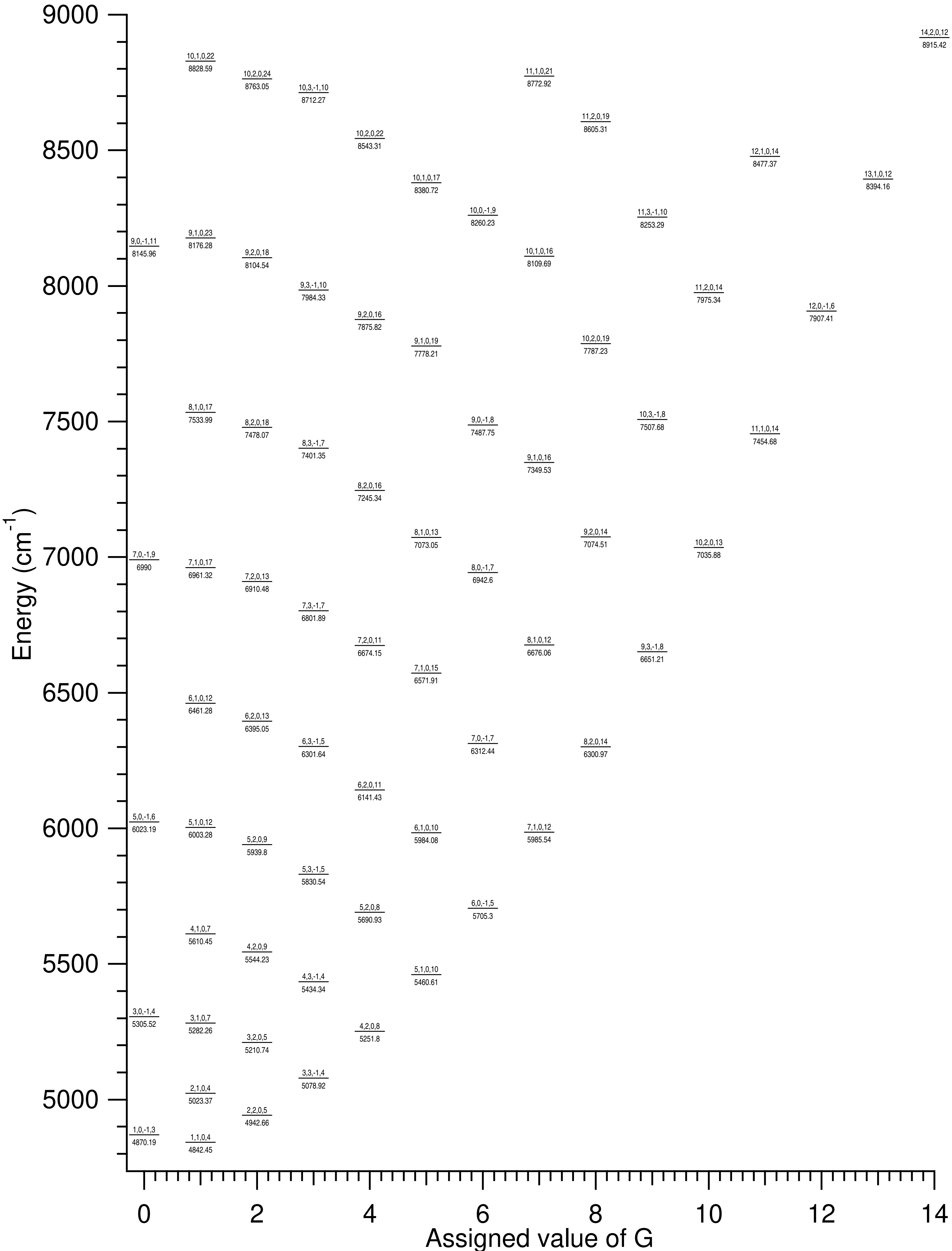
Energy level diagram for H_3^+:
The ν_2 band

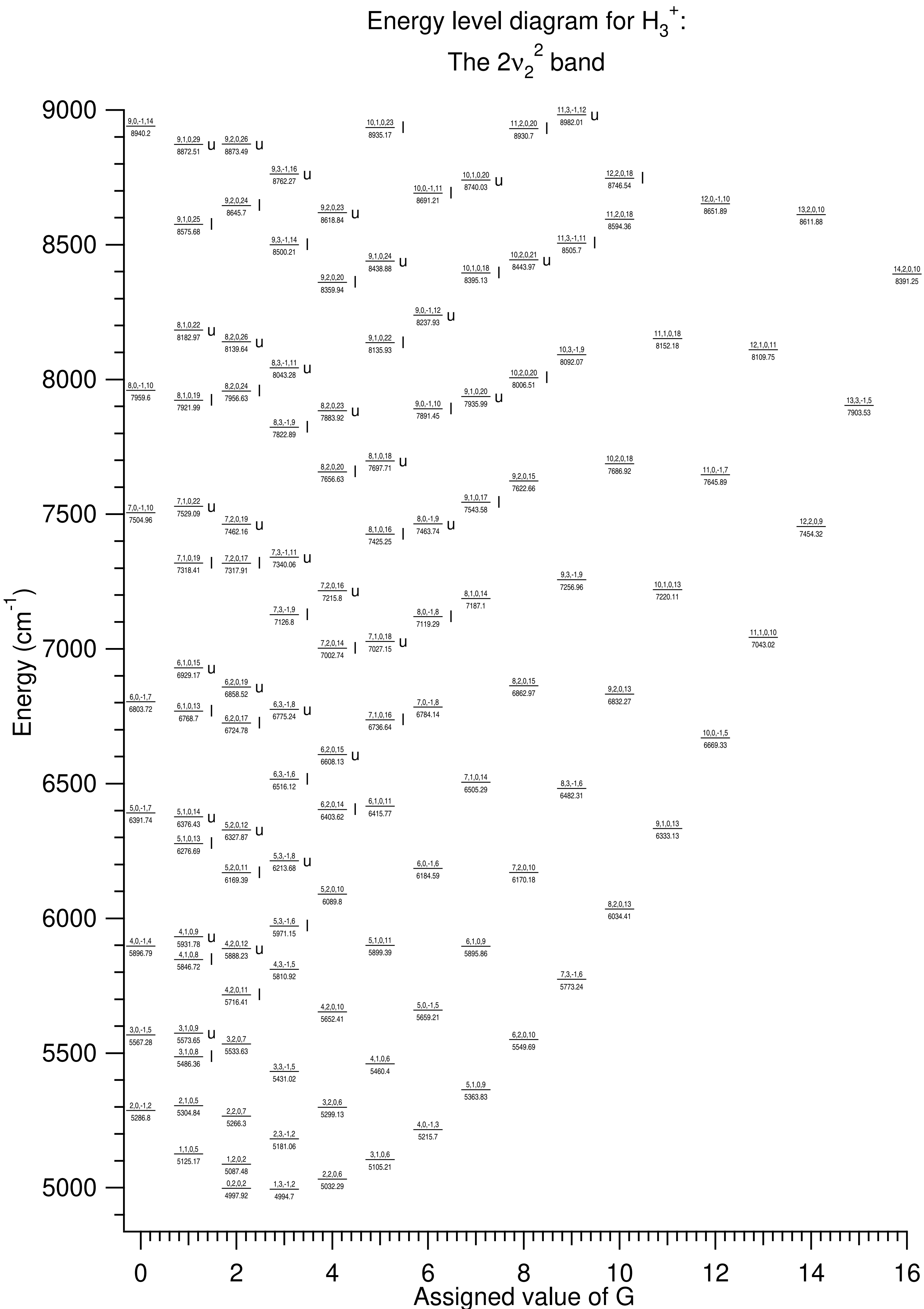


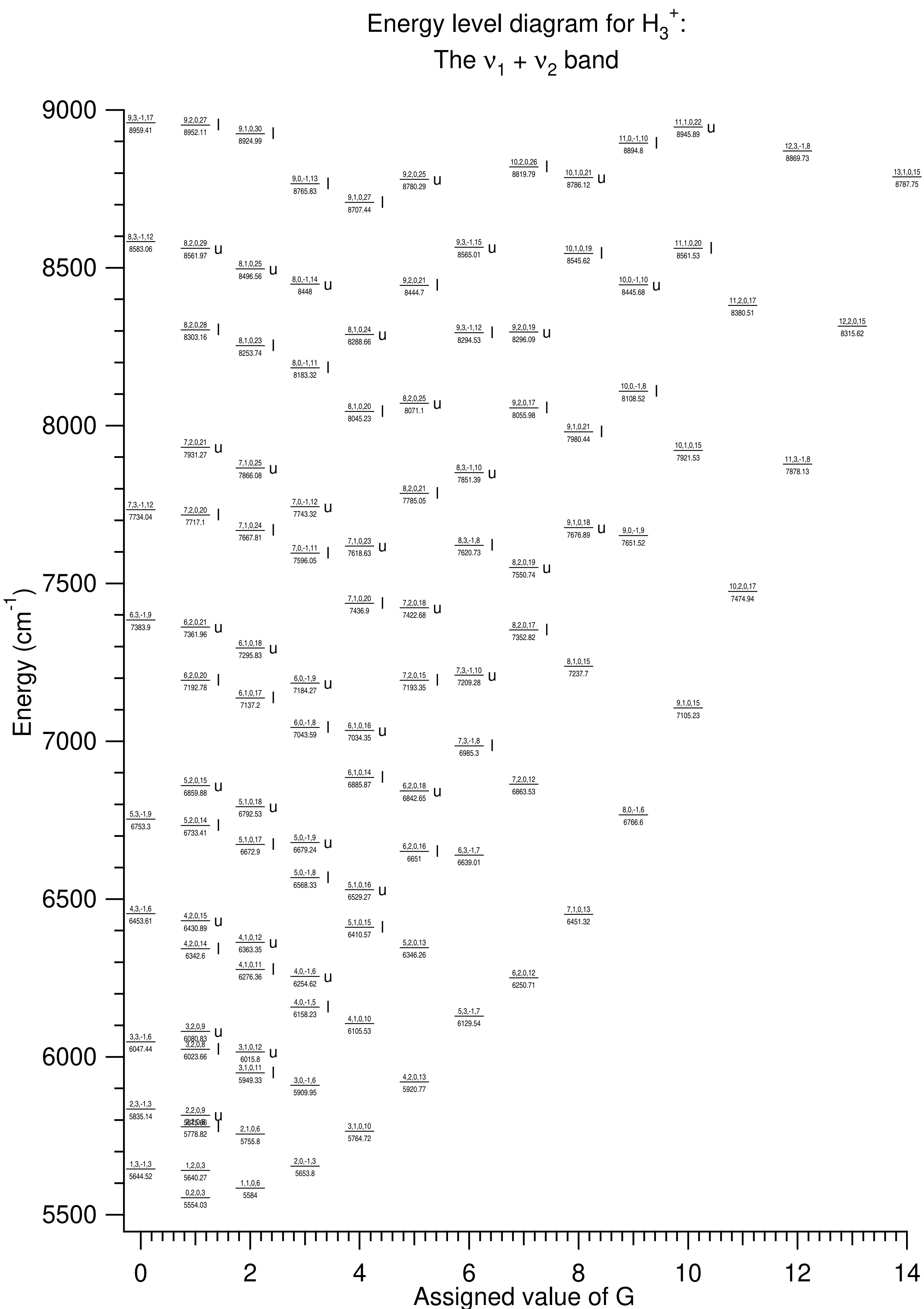
Energy level diagram for H_3^+:
The ν_1 band



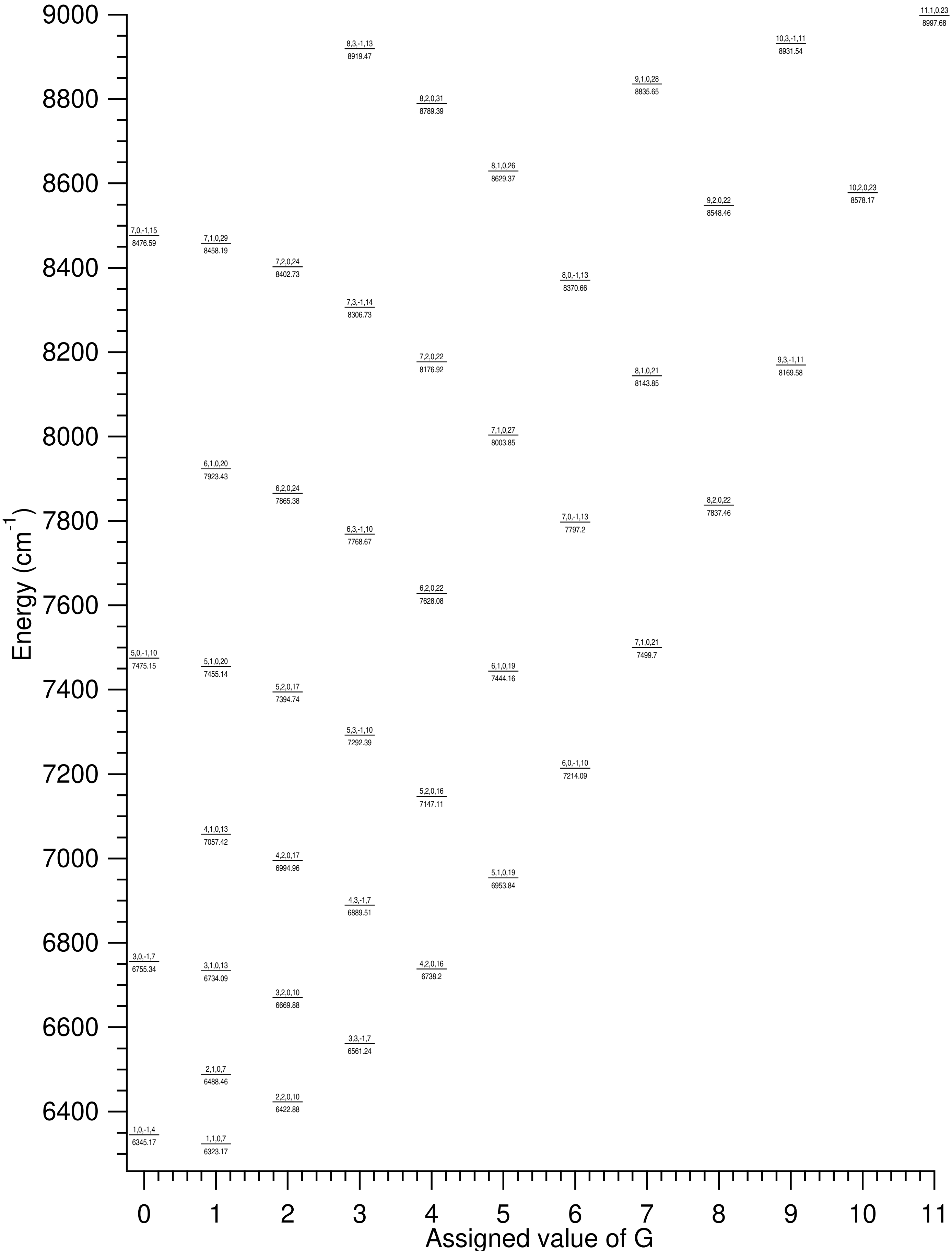
Energy level diagram for H_3^+:
The $2\nu_2^0$ band



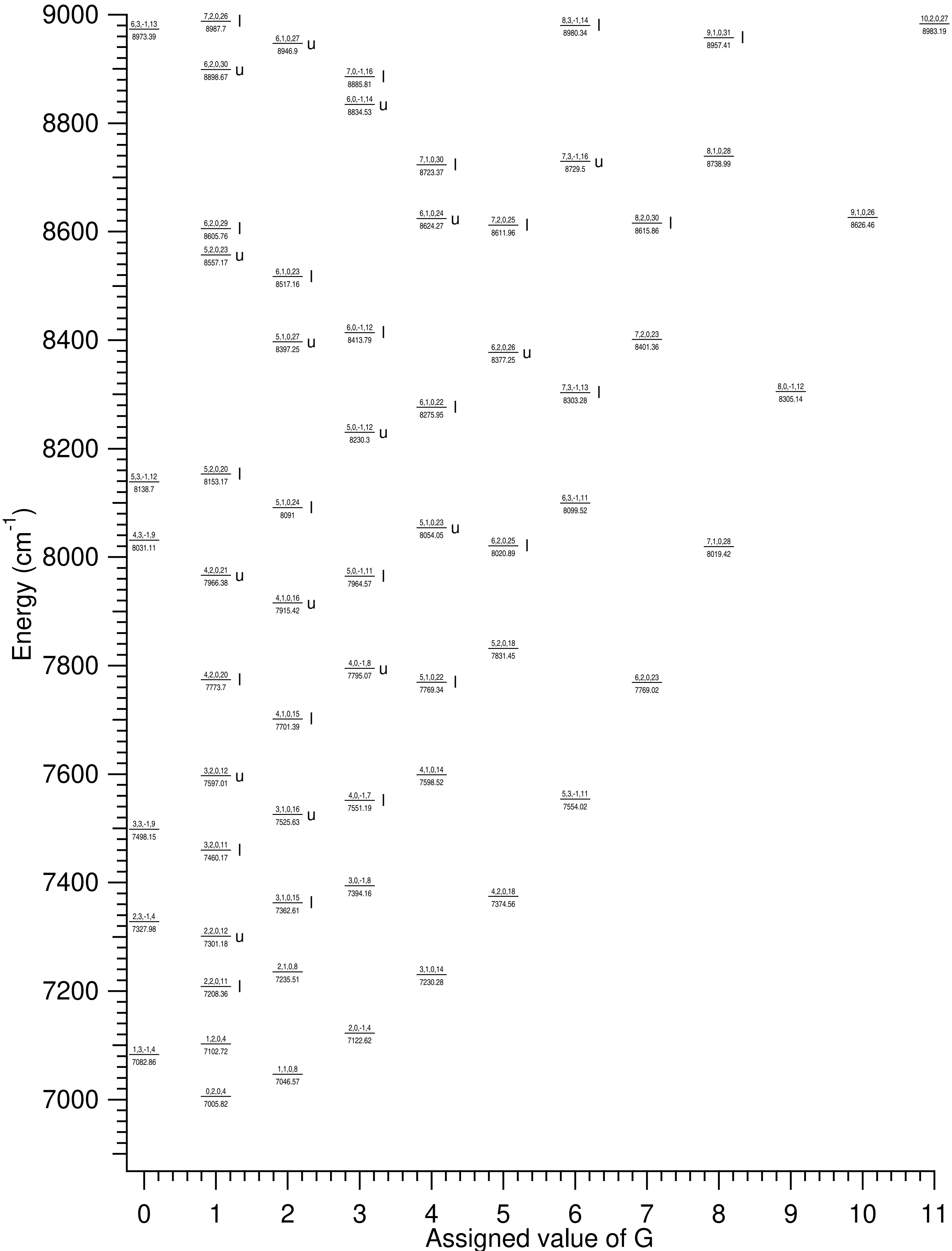

Energy level diagram for H_3^+:
The $2\nu_2^2$ band
Energy (cm^{-1})
Assigned value of G
9000
8500
8000
7500
7000
6500
6000
5500
5000
0
2
4
6
8
10
12
14
16
9,0,-1,14 8940.2
8,0,-1,10 7959.6
7,0,-1,10 7504.96
6,0,-1,7 6803.72
5,0,-1,7 6391.74
4,0,-1,4 5896.79
3,0,-1,5 5567.28
2,0,-1,2 5286.8
9,1,0,29 8872.51 u
9,1,0,25 8575.68 l
8,1,0,22 8182.97 u
8,1,0,19 7921.99 l
7,1,0,22 7529.09 u
7,1,0,19 7318.41 l
6,1,0,15 6929.17 u
6,1,0,13 6768.7 l
5,1,0,14 6376.43 u
5,1,0,13 6276.69 l
4,1,0,9 5931.78 u
4,1,0,8 5846.72 l
3,1,0,9 5573.65 u
3,1,0,8 5486.36 l
2,1,0,5 5304.84
1,1,0,5 5125.17
9,2,0,26 8873.49 u
9,2,0,24 8645.7 l
8,2,0,26 8139.64 u
8,2,0,24 7956.63 l
7,2,0,19 7462.16 u
7,2,0,17 7317.91 l
6,2,0,19 6858.52 u
6,2,0,17 6724.78 l
5,2,0,12 6327.87 u
5,2,0,11 6169.39 l
4,2,0,12 5888.23 u
4,2,0,11 5716.41 l
3,2,0,7 5533.63
2,2,0,7 5266.3
1,2,0,2 5087.48
0,2,0,2 4997.92
9,3,-1,16 8762.27 u
9,3,-1,14 8500.21 l
8,3,-1,11 8043.28 u
8,3,-1,9 7822.89 l
7,3,-1,11 7340.06 u
7,3,-1,9 7126.8 l
6,3,-1,8 6775.24 u
6,3,-1,6 6516.12 l
5,3,-1,8 6213.68 u
5,3,-1,6 5971.15 l
4,3,-1,5 5810.92
3,3,-1,5 5431.02
2,3,-1,2 5181.06
1,3,-1,2 4994.7
9,2,0,23 8618.84 u
9,2,0,20 8359.94 l
8,2,0,23 7883.92 u
8,2,0,20 7656.63 l
7,2,0,16 7215.8 u
7,2,0,14 7002.74 l
6,2,0,15 6608.13 u
6,2,0,14 6403.62 l
5,2,0,10 6089.8
4,2,0,10 5652.41
3,2,0,6 5299.13
2,2,0,6 5032.29
10,1,0,23 8935.17 l
9,1,0,24 8438.88 u
9,1,0,22 8135.93 l
8,1,0,18 7697.71 u
8,1,0,16 7425.25 l
7,1,0,18 7027.15 u
7,1,0,16 6736.64 l
6,1,0,11 6415.77
5,1,0,11 5899.39
4,1,0,6 5460.4
3,1,0,6 5105.21
10,0,-1,11 8691.21 l
9,0,-1,12 8237.93 u
9,0,-1,10 7891.45 l
8,0,-1,9 7463.74 u
8,0,-1,8 7119.29 l
7,0,-1,8 6784.14
6,0,-1,6 6184.59
5,0,-1,5 5659.21
4,0,-1,3 5215.7
10,1,0,20 8740.03 u
10,1,0,18 8395.13 l
9,1,0,20 7935.99 u
9,1,0,17 7543.58 l
8,1,0,14 7187.1
7,1,0,14 6505.29
6,1,0,9 5895.86
5,1,0,9 5363.83
11,2,0,20 8930.7 l
10,2,0,21 8443.97 u
10,2,0,20 8006.51 l
9,2,0,15 7622.66
8,2,0,15 6862.97
7,2,0,10 6170.18
6,2,0,10 5549.69
11,3,-1,12 8982.01 u
11,3,-1,11 8505.7 l
10,3,-1,9 8092.07
9,3,-1,9 7256.96
8,3,-1,6 6482.31
7,3,-1,6 5773.24
12,2,0,18 8746.54 l
11,2,0,18 8594.36
10,2,0,18 7686.92
9,2,0,13 6832.27
8,2,0,13 6034.41
11,1,0,18 8152.18
10,1,0,13 7220.11
9,1,0,13 6333.13
12,0,-1,10 8651.89
11,0,-1,7 7645.89
10,0,-1,5 6669.33
12,1,0,11 8109.75
11,1,0,10 7043.02
13,2,0,10 8611.88
12,2,0,9 7454.32
13,3,-1,5 7903.53
14,2,0,10 8391.25


Energy level diagram for H3+:
The ν1 + ν2 band
Energy (cm-1)
Assigned value of G
9000
8500
8000
7500
7000
6500
6000
5500
0
2
4
6
8
10
12
14
9,3,-1,17 8959.41
8,3,-1,12 8583.06
7,3,-1,12 7734.04
6,3,-1,9 7383.9
5,3,-1,9 6753.3
4,3,-1,6 6453.61
3,3,-1,6 6047.44
2,3,-1,3 5835.14
1,3,-1,3 5644.52
9,2,0,27 8952.11 l
8,2,0,29 8561.97 u
8,2,0,28 8303.16 l
7,2,0,21 7931.27 u
7,2,0,20 7717.1 l
6,2,0,21 7361.96 u
6,2,0,20 7192.78 l
5,2,0,15 6859.88 u
5,2,0,14 6733.41 l
4,2,0,15 6430.89 u
4,2,0,14 6342.6 l
3,2,0,9 6080.83 u
3,2,0,8 6023.66 l
2,2,0,9 u
5778.82 l
1,2,0,3 5640.27
0,2,0,3 5554.03
9,1,0,30 8924.99 l
8,1,0,25 8496.56 u
8,1,0,23 8253.74 l
7,1,0,25 7866.08 u
7,1,0,24 7667.81 l
6,1,0,18 7295.83 u
6,1,0,17 7137.2 l
5,1,0,18 6792.53 u
5,1,0,17 6672.9 l
4,1,0,12 6363.35 u
4,1,0,11 6276.36 l
3,1,0,12 6015.8 u
3,1,0,11 5949.33 l
2,1,0,6 5755.8
1,1,0,6 5584
9,0,-1,13 8765.83 l
8,0,-1,14 8448 u
8,0,-1,11 8183.32 l
7,0,-1,12 7743.32 u
7,0,-1,11 7596.05 l
6,0,-1,9 7184.27 u
6,0,-1,8 7043.59 l
5,0,-1,9 6679.24 u
5,0,-1,8 6568.33 l
4,0,-1,6 6254.62 u
4,0,-1,5 6158.23 l
3,0,-1,6 5909.95
2,0,-1,3 5653.8
9,1,0,27 8707.44 l
8,1,0,24 8288.66 u
8,1,0,20 8045.23 l
7,1,0,23 7618.63 u
7,1,0,20 7436.9 l
6,1,0,16 7034.35 u
6,1,0,14 6885.87 l
5,1,0,16 6529.27 u
5,1,0,15 6410.57 l
4,1,0,10 6105.53
3,1,0,10 5764.72
9,2,0,25 8780.29 u
9,2,0,21 8444.7 l
8,2,0,25 8071.1 u
8,2,0,21 7785.05 l
7,2,0,18 7422.68 u
7,2,0,15 7193.35 l
6,2,0,18 6842.65 u
6,2,0,16 6651 l
5,2,0,13 6346.26
4,2,0,13 5920.77
9,3,-1,15 8565.01 u
9,3,-1,12 8294.53 l
8,3,-1,10 7851.39 u
8,3,-1,8 7620.73 l
7,3,-1,10 7209.28 u
7,3,-1,8 6985.3 l
6,3,-1,7 6639.01
5,3,-1,7 6129.54
10,2,0,26 8819.79 l
9,2,0,19 8296.09 u
9,2,0,17 8055.98 l
8,2,0,19 7550.74 u
8,2,0,17 7352.82 l
7,2,0,12 6863.53
6,2,0,12 6250.71
10,1,0,21 8786.12 u
10,1,0,19 8545.62 l
9,1,0,21 7980.44 l
9,1,0,18 7676.89 u
8,1,0,15 7237.7
7,1,0,13 6451.32
11,0,-1,10 8894.8 l
10,0,-1,10 8445.68 u
10,0,-1,8 8108.52 l
9,0,-1,9 7651.52
8,0,-1,6 6766.6
11,1,0,22 8945.89 u
11,1,0,20 8561.53 l
10,1,0,15 7921.53
9,1,0,15 7105.23
11,2,0,17 8380.51
10,2,0,17 7474.94
12,3,-1,8 8869.73
11,3,-1,8 7878.13
12,2,0,15 8315.62
13,1,0,15 8787.75

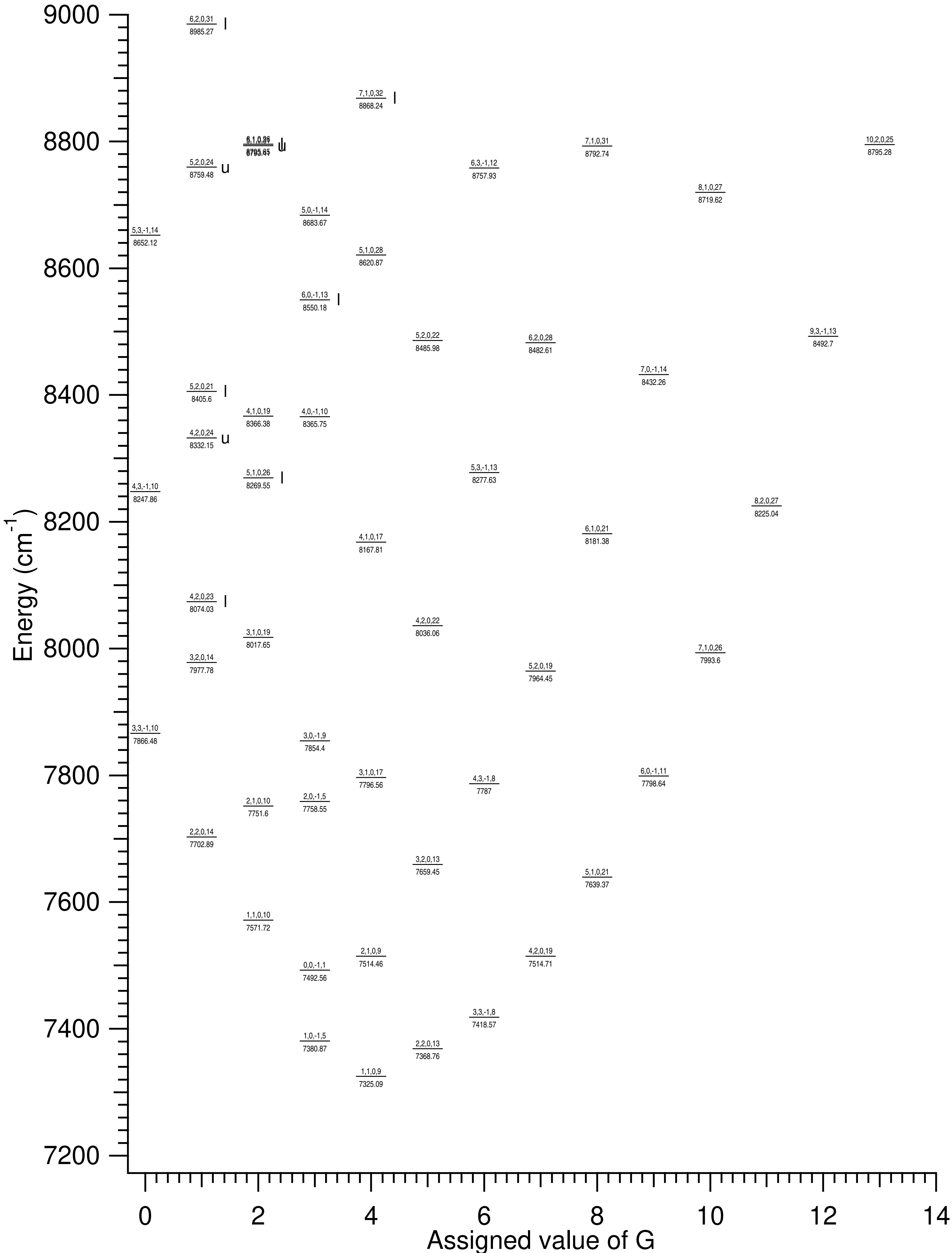
Energy level diagram for H_3^+:
The $2\nu_1$ band

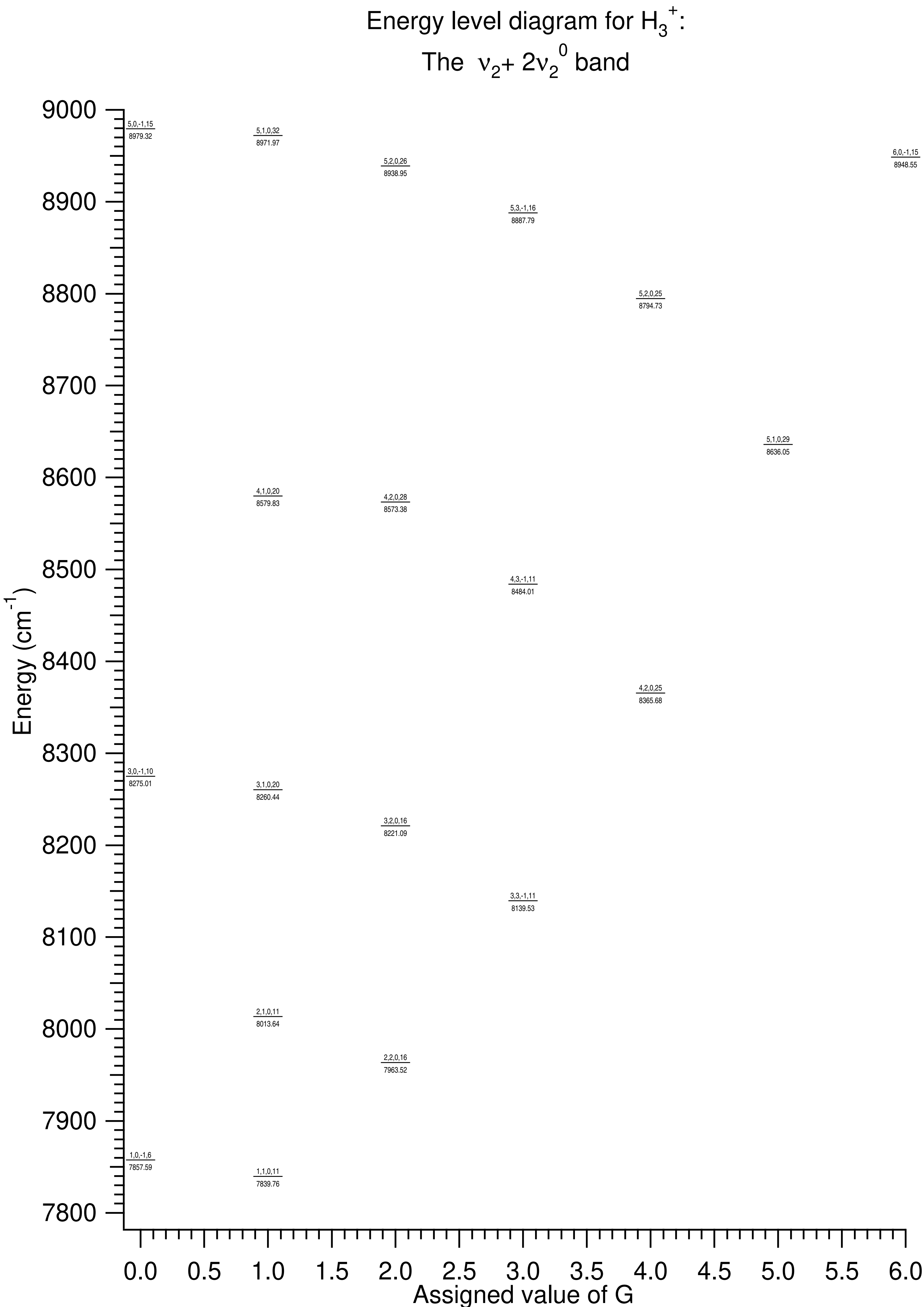


Energy level diagram for H_3^+:
The $3\nu_2^1$ band



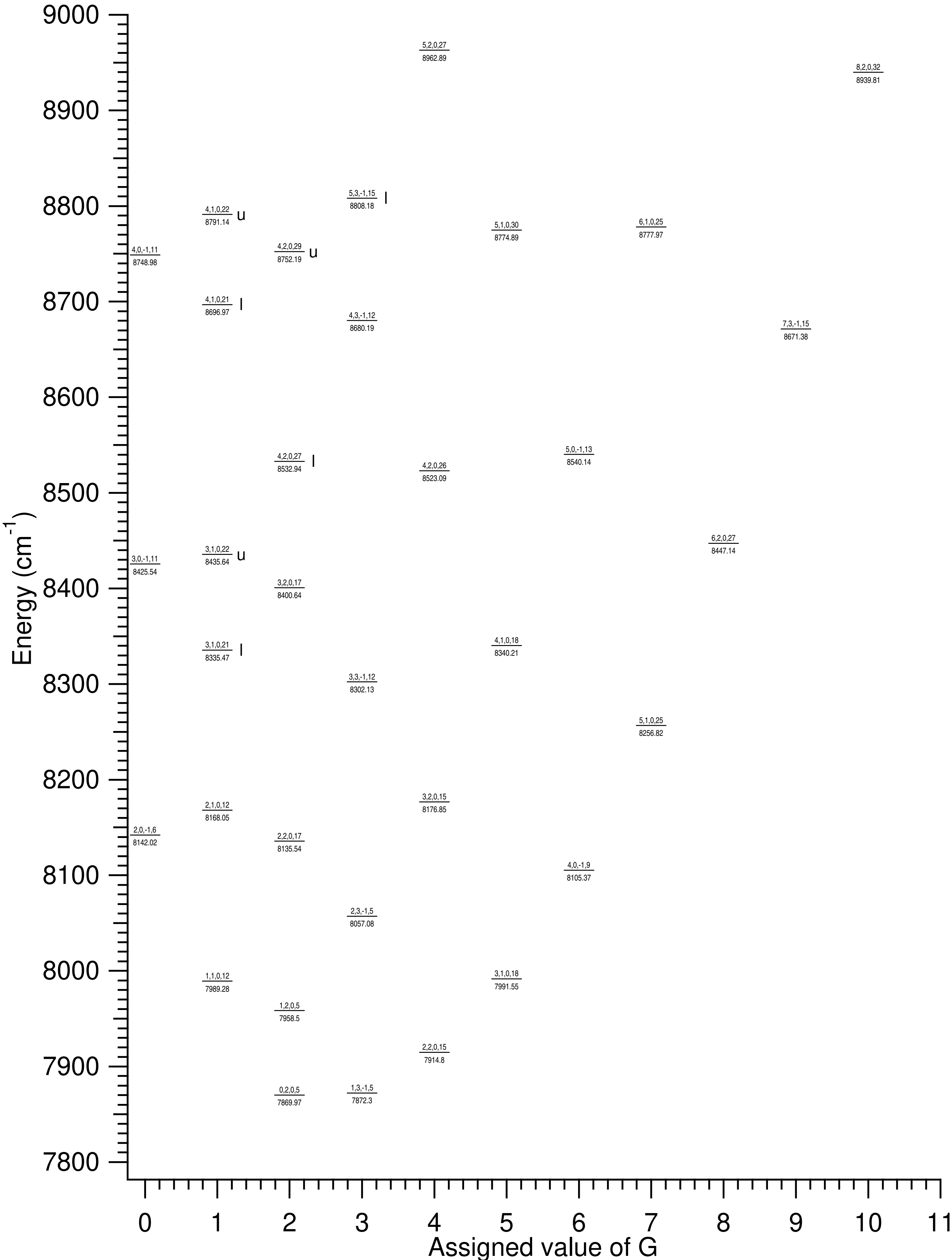
Energy level diagram for H_3^+:
The $3\nu_2^3$ band





Energy level diagram for H_3^+:
The $\nu_2 + 2\nu_2^0$ band
Energy (cm^{-1})
Assigned value of G
9000
8900
8800
8700
8600
8500
8400
8300
8200
8100
8000
7900
7800
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
5,0,-1,15
8979.32
5,1,0,32
8971.97
5,2,0,26
8938.95
6,0,-1,15
8948.55
5,3,-1,16
8887.79
5,2,0,25
8794.73
5,1,0,29
8636.05
4,1,0,20
8579.83
4,2,0,28
8573.38
4,3,-1,11
8484.01
4,2,0,25
8365.68
3,0,-1,10
8275.01
3,1,0,20
8260.44
3,2,0,16
8221.09
3,3,-1,11
8139.53
2,1,0,11
8013.64
2,2,0,16
7963.52
1,0,-1,6
7857.59
1,1,0,11
7839.76

Energy level diagram for H_3^+:
The $\nu_1+2\nu_2^2$ band



Energy level diagram for H_3^+:
The $2\nu_1 + \nu_2$ band