| Peak | Assignment | Position (cm$^{-1}$) | Rel. FC factor | Signal |
|---|---|---|---|---|
| 1 | $1_0^0$ | 0.000 | 1 | 1 |
| 2 | $1_0^1 1_1^0$ | 6.900 | 0.550 | 0.264 |
| 3 | $1_0^2 1_2^0$ | 13.800 | 0.302 | 0.070 |
| 4 | $1_0^3 1_3^0$ | 20.700 | 0.166 | 0.018 |
| 5 | $1_0^4 1_4^0$ | 27.600 | 0.091 | 0.005 |
| 6 | $1_0^1 2_1^0$ | 6.900 | 0.450 | 0.216 |
| 7 | $1_0^2 2_2^0$ | 13.800 | 0.202 | 0.047 |
| 8 | $1_0^3 2_3^0$ | 20.700 | 0.091 | 0.010 |
| 9 | $1_0^4 2_4^0$ | 27.600 | 0.041 | 0.002 |
| 10 | $1_0^1 2_0^1 1_2^0$ | 15.200 | 0.495 | 0.114 |
| 11 | $1_0^1 2_0^2 1_3^0$ | 23.500 | 0.334 | 0.037 |
| 12 | $1_0^1 2_0^3 1_4^0$ | 31.800 | 0.200 | 0.011 |
| 13 | $1_0^1 2_0^4 1_5^0$ | 40.100 | 0.112 | 0.003 |
| 14 | $1_0^2 2_0^1 1_3^0$ | 22.100 | 0.408 | 0.045 |
| 15 | $1_0^2 2_0^2 1_4^0$ | 30.400 | 0.367 | 0.019 |
| 16 | $1_0^2 2_0^3 1_5^0$ | 38.700 | 0.275 | 0.007 |
| 17 | $1_0^3 2_0^1 1_4^0$ | 29.000 | 0.299 | 0.016 |
| 18 | $1_0^3 2_0^2 1_5^0$ | 37.300 | 0.336 | 0.009 |
| 19 | $1_0^4 2_0^1 1_5^0$ | 35.900 | 0.205 | 0.005 |
| 20 | $1_1^0 2_1^0 1_0^2$ | 13.800 | 0.495 | 0.114 |
| 21 | $1_1^0 2_2^0 1_0^3$ | 20.700 | 0.334 | 0.037 |
| 22 | $1_1^0 2_3^0 1_0^4$ | 27.600 | 0.200 | 0.011 |
| 23 | $1_2^0 2_1^0 1_0^3$ | 20.700 | 0.408 | 0.045 |
| 24 | $1_2^0 2_2^0 1_0^4$ | 27.600 | 0.367 | 0.020 |
| 25 | $1_2^0 2_3^0 1_0^5$ | 34.500 | 0.275 | 0.007 |
| 26 | $1_3^0 2_1^0 1_0^4$ | 27.600 | 0.299 | 0.016 |
| 27 | $1_3^0 2_2^0 1_0^5$ | 34.500 | 0.336 | 0.009 |
| 28 | $1_3^0 2_3^0 1_0^6$ | 41.400 | 0.302 | 0.004 |
| 29 | $1_0^1 2_0^1 1_1^0 2_1^0$ | 15.200 | 0.010 | 0.002 |
| 30 | $1_0^1 2_0^2 1_1^0 2_2^0$ | 23.500 | 0.067 | 0.007 |

| Peak | Assignment | Position (cm$^{-1}$) | Rel. FC factor | Signal |
|---|---|---|---|---|
| 31 | $1_0^1 2_0^2 1_2^1 2_1^0$ | 23.500 | 0.190 | 0.021 |
| 32 | $1_0^1 2_0^3 1_1^0 2_3^0$ | 31.800 | 0.193 | 0.010 |
| 33 | $1_0^1 2_0^3 1_3^0 2_1^0$ | 31.800 | 0.291 | 0.015 |
| 34 | $1_0^1 2_0^4 1_3^0 2_2^0$ | 40.100 | 0.125 | 0.003 |
| 35 | $1_0^2 2_0^1 1_1^0 2_2^0$ | 22.100 | 0.190 | 0.021 |
| 36 | $1_0^2 2_0^1 1_2^0 2_1^0$ | 22.100 | 0.067 | 0.007 |
| 37 | $1_0^2 2_0^2 1_2^0 2_2^0$ | 30.400 | 0.235 | 0.012 |
| 38 | $1_0^2 2_0^3 1_2^0 2_3^0$ | 38.700 | 0.182 | 0.005 |
| 39 | $1_0^2 2_0^4 1_3^0 2_3^0$ | 47.000 | 0.167 | 0.002 |
| 40 | $1_0^3 2_0^1 1_1^0 2_3^0$ | 29.000 | 0.291 | 0.015 |
| 41 | $1_0^3 2_0^1 1_3^0 2_1^0$ | 29.000 | 0.193 | 0.010 |
| 42 | $1_0^3 2_0^2 1_3^0 2_2^0$ | 37.300 | 0.182 | 0.005 |
| 43 | $1_0^4 2_0^1 1_2^0 2_3^0$ | 35.900 | 0.125 | 0.003 |
| 44 | $1_0^4 2_0^2 1_3^0 2_3^0$ | 44.200 | 0.167 | 0.002 |
| 45 | $1_0^1 2_0^1 2_2^0$ | 15.200 | 0.495 | 0.114 |
| 46 | $1_0^1 2_0^2 2_3^0$ | 23.500 | 0.408 | 0.045 |
| 47 | $1_0^1 2_0^3 2_4^0$ | 31.800 | 0.299 | 0.016 |
| 48 | $1_0^1 2_0^4 2_5^0$ | 40.100 | 0.205 | 0.005 |
| 49 | $1_0^2 2_0^1 2_3^0$ | 22.100 | 0.334 | 0.037 |
| 50 | $1_0^2 2_0^2 2_4^0$ | 30.400 | 0.367 | 0.019 |
| 51 | $1_0^2 2_0^3 2_5^0$ | 38.700 | 0.336 | 0.009 |
| 52 | $1_0^3 2_0^1 2_4^0$ | 29.000 | 0.200 | 0.011 |
| 53 | $1_0^3 2_0^2 2_5^0$ | 37.300 | 0.275 | 0.007 |
| 54 | $1_0^4 2_0^1 2_5^0$ | 35.900 | 0.112 | 0.003 |
| 55 | $1_1^0 2_1^0 2_0^2$ | 16.600 | 0.495 | 0.114 |
| 56 | $1_1^0 2_2^0 2_0^3$ | 24.900 | 0.408 | 0.045 |
| 57 | $1_1^0 2_3^0 2_0^4$ | 33.200 | 0.299 | 0.016 |
| 58 | $1_2^0 2_1^0 2_0^3$ | 24.900 | 0.334 | 0.037 |
| 59 | $1_2^0 2_2^0 2_0^4$ | 33.200 | 0.367 | 0.019 |
| 60 | $1_2^0 2_3^0 2_0^5$ | 41.500 | 0.336 | 0.009 |

| Peak | Assignment | Position (cm$^{-1}$) | Rel. FC factor | Signal |
|------|-----------|---------------------|----------------|--------|
| 61 | $1_3^0 2_1^0 2_0^4$ | 33.200 | 0.200 | 0.011 |
| 62 | $1_3^0 2_2^0 2_0^5$ | 41.500 | 0.275 | 0.007 |
| 63 | $1_3^0 2_3^0 2_0^6$ | 49.800 | 0.302 | 0.004 |
| 64 | $1_0^1 2_0^1 3_0^1 1_2^0$ | 437.000 | 0.289 | 0.067 |
| 65 | $1_0^1 2_0^1 3_0^2 1_2^0$ | 858.800 | 0.085 | 0.020 |
| 66 | $1_0^1 2_0^1 3_0^3 1_2^0$ | 1280.600 | 0.017 | 0.004 |
| 67 | $1_0^1 2_0^2 3_0^1 1_3^0$ | 445.300 | 0.195 | 0.022 |
| 68 | $1_0^1 2_0^2 3_0^2 1_3^0$ | 867.100 | 0.057 | 0.006 |
| 69 | $1_0^1 2_0^3 3_0^1 1_4^0$ | 453.600 | 0.117 | 0.006 |
| 70 | $1_0^1 2_0^3 3_0^2 1_4^0$ | 875.400 | 0.034 | 0.002 |
| 71 | $1_0^2 2_0^1 3_0^1 1_3^0$ | 443.900 | 0.238 | 0.026 |
| 72 | $1_0^2 2_0^1 3_0^2 1_3^0$ | 865.700 | 0.070 | 0.008 |
| 73 | $1_0^2 2_0^2 3_0^1 1_4^0$ | 452.200 | 0.214 | 0.011 |
| 74 | $1_0^2 2_0^2 3_0^2 1_4^0$ | 874.000 | 0.063 | 0.003 |
| 75 | $1_0^2 2_0^3 3_0^1 1_5^0$ | 460.500 | 0.161 | 0.004 |
| 76 | $1_0^3 2_0^1 3_0^1 1_4^0$ | 450.800 | 0.175 | 0.009 |
| 77 | $1_0^3 2_0^1 3_0^2 1_4^0$ | 872.600 | 0.051 | 0.003 |
| 78 | $1_0^3 2_0^2 3_0^1 1_5^0$ | 459.100 | 0.196 | 0.005 |
| 79 | $1_0^1 2_0^2 3_0^1 1_1^0 2_2^0$ | 445.300 | 0.039 | 0.004 |
| 80 | $1_0^1 2_0^2 3_0^1 1_2^0 2_1^0$ | 445.300 | 0.111 | 0.012 |
| 81 | $1_0^1 2_0^2 3_0^2 1_2^0 2_1^0$ | 867.100 | 0.033 | 0.004 |
| 82 | $1_0^1 2_0^3 3_0^1 1_1^0 2_3^0$ | 453.600 | 0.113 | 0.006 |
| 83 | $1_0^1 2_0^3 3_0^1 1_3^0 2_1^0$ | 453.600 | 0.170 | 0.009 |
| 84 | $1_0^1 2_0^3 3_0^2 1_3^0 2_1^0$ | 875.400 | 0.050 | 0.003 |
| 85 | $1_0^2 2_0^1 3_0^1 1_1^0 2_2^0$ | 443.900 | 0.111 | 0.012 |
| 86 | $1_0^2 2_0^1 3_0^1 1_2^0 2_1^0$ | 443.900 | 0.039 | 0.004 |
| 87 | $1_0^2 2_0^1 3_0^2 1_1^0 2_2^0$ | 865.700 | 0.033 | 0.004 |
| 88 | $1_0^2 2_0^2 3_0^1 1_2^0 2_2^0$ | 452.200 | 0.137 | 0.007 |
| 89 | $1_0^2 2_0^2 3_0^2 1_2^0 2_2^0$ | 874.000 | 0.040 | 0.002 |
| 90 | $1_0^2 2_0^3 3_0^1 1_2^0 2_3^0$ | 460.500 | 0.106 | 0.003 |

| Peak | Assignment | Position (cm$^{-1}$) | Rel. FC factor | Signal |
|---|---|---|---|---|
| 91 | $1_0^3 2_0^1 3_0^1 1_1^0 2_3^0$ | 450.800 | 0.170 | 0.009 |
| 92 | $1_0^3 2_0^1 3_0^1 1_3^0 2_1^0$ | 450.800 | 0.113 | 0.006 |
| 93 | $1_0^3 2_0^1 3_0^2 1_1^0 2_3^0$ | 872.600 | 0.050 | 0.003 |
| 94 | $1_0^3 2_0^2 3_0^1 1_3^0 2_2^0$ | 459.100 | 0.106 | 0.003 |
| 95 | $1_2^1 2_1^2 3_1^2$ | 446.300 | 0.111 | 0.004 |
| 96 | $1_2^1 2_1^2 3_1^3$ | 868.100 | 0.063 | 0.002 |
| 97 | $1_1^2 2_2^1 3_1^2$ | 444.900 | 0.111 | 0.004 |
| 98 | $1_1^2 2_2^1 3_1^3$ | 866.700 | 0.063 | 0.002 |
| 99 | $1_2^2 2_2^2 3_1^2$ | 453.200 | 0.137 | 0.002 |
| 100 | $1_0^1 2_0^1 3_0^1 1_2^0 3_1^0$ | 16.200 | 0.085 | 0.006 |
| 101 | $1_0^1 2_0^1 3_0^2 1_2^0 3_1^0$ | 438.000 | 0.289 | 0.020 |
| 102 | $1_0^1 2_0^1 3_0^3 1_2^0 3_1^0$ | 859.800 | 0.165 | 0.011 |
| 103 | $1_0^1 2_0^1 3_0^3 1_2^0 3_2^0$ | 439.000 | 0.193 | 0.004 |
| 104 | $1_0^1 2_0^2 3_0^1 1_3^0 3_1^0$ | 24.500 | 0.057 | 0.002 |
| 105 | $1_0^1 2_0^2 3_0^2 1_3^0 3_1^0$ | 446.300 | 0.195 | 0.006 |
| 106 | $1_0^1 2_0^2 3_0^3 1_3^0 3_1^0$ | 868.100 | 0.111 | 0.004 |
| 107 | $1_0^2 2_0^1 3_0^1 1_3^0 3_1^0$ | 23.100 | 0.070 | 0.002 |
| 108 | $1_0^2 2_0^1 3_0^2 1_3^0 3_1^0$ | 444.900 | 0.238 | 0.008 |
| 109 | $1_0^2 2_0^1 3_0^3 1_3^0 3_1^0$ | 866.700 | 0.136 | 0.004 |
| 110 | $1_1^0 2_1^0 3_1^0 1_0^2 3_0^1$ | 14.800 | 0.085 | 0.006 |
| 111 | $1_1^0 2_1^0 3_1^0 1_0^2 3_0^2$ | 436.600 | 0.289 | 0.020 |
| 112 | $1_1^0 2_1^0 3_1^0 1_0^2 3_0^3$ | 858.400 | 0.165 | 0.011 |
| 113 | $1_1^0 2_1^0 3_1^0 1_0^2 3_0^4$ | 1280.200 | 0.048 | 0.003 |
| 114 | $1_1^0 2_1^0 3_2^0 1_0^2 3_0^3$ | 437.600 | 0.193 | 0.004 |
| 115 | $1_1^0 2_1^0 3_2^0 1_0^2 3_0^4$ | 859.400 | 0.207 | 0.004 |
| 116 | $1_1^0 2_2^0 3_1^0 1_0^1 3_0^1$ | 21.700 | 0.058 | 0.002 |
| 117 | $1_1^0 2_2^0 3_1^0 1_0^1 3_0^2$ | 443.500 | 0.195 | 0.006 |
| 118 | $1_1^0 2_2^0 3_1^0 1_0^1 3_0^3$ | 865.300 | 0.111 | 0.004 |
| 119 | $1_2^0 2_1^0 3_1^0 1_0^1 3_0^1$ | 21.700 | 0.070 | 0.002 |
| 120 | $1_2^0 2_1^0 3_1^0 1_0^1 3_0^2$ | 443.500 | 0.238 | 0.008 |

| Peak | Assignment | Position (cm$^{-1}$) | Rel. FC factor | Signal |
|---|---|---|---|---|
| 121 | $1_2^0 2_1^0 3_1^0 1_0^3 3_0^3$ | 865.300 | 0.136 | 0.004 |
| 122 | $1_2^0 2_2^0 3_1^0 1_0^4 3_0^2$ | 450.400 | 0.214 | 0.003 |
| 123 | $1_2^0 2_2^0 3_1^0 1_0^4 3_0^3$ | 872.200 | 0.122 | 0.002 |
| 124 | $1_0^1 2_0^1 3_0^1 2_2^0$ | 437.000 | 0.289 | 0.067 |
| 125 | $1_0^1 2_0^1 3_0^2 2_2^0$ | 858.800 | 0.085 | 0.020 |
| 126 | $1_0^1 2_0^1 3_0^3 2_2^0$ | 1280.600 | 0.017 | 0.004 |
| 127 | $1_0^1 2_0^2 3_0^1 2_3^0$ | 445.300 | 0.238 | 0.026 |
| 128 | $1_0^1 2_0^2 3_0^2 2_3^0$ | 867.100 | 0.070 | 0.008 |
| 129 | $1_0^1 2_0^3 3_0^1 2_4^0$ | 453.600 | 0.175 | 0.009 |
| 130 | $1_0^1 2_0^3 3_0^2 2_4^0$ | 875.400 | 0.051 | 0.003 |
| 131 | $1_0^2 2_0^1 3_0^1 2_3^0$ | 443.900 | 0.195 | 0.022 |
| 132 | $1_0^2 2_0^1 3_0^2 2_3^0$ | 865.700 | 0.057 | 0.006 |
| 133 | $1_0^2 2_0^2 3_0^1 2_4^0$ | 452.200 | 0.214 | 0.011 |
| 134 | $1_0^2 2_0^2 3_0^2 2_4^0$ | 874.000 | 0.063 | 0.003 |
| 135 | $1_0^2 2_0^3 3_0^1 2_5^0$ | 460.500 | 0.196 | 0.005 |
| 136 | $1_0^3 2_0^1 3_0^1 2_4^0$ | 450.800 | 0.117 | 0.006 |
| 137 | $1_0^3 2_0^1 3_0^2 2_4^0$ | 872.600 | 0.034 | 0.002 |
| 138 | $1_0^3 2_0^2 3_0^1 2_5^0$ | 459.100 | 0.161 | 0.004 |
| 139 | $1_0^1 2_0^1 3_0^1 2_2^0 3_1^0$ | 16.200 | 0.085 | 0.006 |
| 140 | $1_0^1 2_0^1 3_0^2 2_2^0 3_1^0$ | 438.000 | 0.289 | 0.020 |
| 141 | $1_0^1 2_0^1 3_0^3 2_2^0 3_1^0$ | 859.800 | 0.165 | 0.011 |
| 142 | $1_0^1 2_0^1 3_0^3 2_2^0 3_2^0$ | 439.000 | 0.192 | 0.004 |
| 143 | $1_0^1 2_0^2 3_0^1 2_3^0 3_1^0$ | 24.500 | 0.070 | 0.002 |
| 144 | $1_0^1 2_0^2 3_0^2 2_3^0 3_1^0$ | 446.300 | 0.238 | 0.008 |
| 145 | $1_0^1 2_0^2 3_0^3 2_3^0 3_1^0$ | 868.100 | 0.136 | 0.004 |
| 146 | $1_0^2 2_0^1 3_0^1 2_3^0 3_1^0$ | 23.100 | 0.057 | 0.002 |
| 147 | $1_0^2 2_0^1 3_0^2 2_3^0 3_1^0$ | 444.900 | 0.195 | 0.006 |
| 148 | $1_0^2 2_0^1 3_0^3 2_3^0 3_1^0$ | 866.700 | 0.111 | 0.004 |
| 149 | $1_1^0 2_1^0 3_1^0 2_0^2 3_0^1$ | 17.600 | 0.085 | 0.006 |
| 150 | $1_1^0 2_1^0 3_1^0 2_0^2 3_0^2$ | 439.400 | 0.289 | 0.020 |

| Peak | Assignment | Position (cm$^{-1}$) | Rel. FC factor | Signal |
|------|-----------|------------------|----------------|--------|
| 151 | $1_1^0 2_1^0 3_1^0 2_0^2 3_0^3$ | 861.200 | 0.164 | 0.011 |
| 152 | $1_1^0 2_1^0 3_1^0 2_0^2 3_0^4$ | 1283.000 | 0.048 | 0.003 |
| 153 | $1_1^0 2_1^0 3_2^0 2_0^2 3_0^3$ | 440.400 | 0.192 | 0.004 |
| 154 | $1_1^0 2_1^0 3_2^0 2_0^2 3_0^4$ | 862.200 | 0.207 | 0.004 |
| 155 | $1_1^0 2_2^0 3_1^0 2_0^2 3_0^1$ | 25.900 | 0.070 | 0.002 |
| 156 | $1_1^0 2_2^0 3_1^0 2_0^2 3_0^2$ | 447.700 | 0.238 | 0.008 |
| 157 | $1_1^0 2_2^0 3_1^0 2_0^2 3_0^3$ | 869.500 | 0.136 | 0.004 |
| 158 | $1_2^0 2_1^0 3_1^0 2_0^2 3_0^1$ | 25.900 | 0.057 | 0.002 |
| 159 | $1_2^0 2_1^0 3_1^0 2_0^2 3_0^2$ | 447.700 | 0.195 | 0.006 |
| 160 | $1_2^0 2_1^0 3_1^0 2_0^2 3_0^3$ | 869.500 | 0.111 | 0.004 |
| 161 | $1_2^0 2_2^0 3_1^0 2_0^4 3_0^2$ | 456.000 | 0.214 | 0.003 |
| 162 | $1_2^0 2_2^0 3_1^0 2_0^4 3_0^3$ | 877.800 | 0.122 | 0.002 |
| 163 | $1_0^1 3_0^1 1_1^0$ | 428.700 | 0.321 | 0.154 |
| 164 | $1_0^1 3_0^2 1_1^0$ | 850.500 | 0.094 | 0.045 |
| 165 | $1_0^1 3_0^3 1_1^0$ | 1272.300 | 0.019 | 0.009 |
| 166 | $1_0^2 3_0^1 1_2^0$ | 435.600 | 0.177 | 0.041 |
| 167 | $1_0^2 3_0^2 1_2^0$ | 857.400 | 0.052 | 0.012 |
| 168 | $1_0^2 3_0^3 1_2^0$ | 1279.200 | 0.010 | 0.002 |
| 169 | $1_0^3 3_0^1 1_3^0$ | 442.500 | 0.097 | 0.011 |
| 170 | $1_0^3 3_0^2 1_3^0$ | 864.300 | 0.028 | 0.003 |
| 171 | $1_0^4 3_0^1 1_4^0$ | 449.400 | 0.053 | 0.003 |
| 172 | $1_0^2 3_0^1 1_1^0 2_1^0$ | 435.600 | 0.289 | 0.067 |
| 173 | $1_0^2 3_0^2 1_1^0 2_1^0$ | 857.400 | 0.085 | 0.020 |
| 174 | $1_0^2 3_0^3 1_1^0 2_1^0$ | 1279.200 | 0.017 | 0.004 |
| 175 | $1_0^3 3_0^1 1_1^0 2_2^0$ | 442.500 | 0.195 | 0.022 |
| 176 | $1_0^3 3_0^1 1_2^0 2_1^0$ | 442.500 | 0.238 | 0.026 |
| 177 | $1_0^3 3_0^2 1_1^0 2_2^0$ | 864.300 | 0.057 | 0.006 |
| 178 | $1_0^3 3_0^2 1_2^0 2_1^0$ | 864.300 | 0.070 | 0.008 |
| 179 | $1_0^4 3_0^1 1_1^0 2_3^0$ | 449.400 | 0.117 | 0.006 |
| 180 | $1_0^4 3_0^1 1_2^0 2_2^0$ | 449.400 | 0.214 | 0.011 |

| Peak | Assignment | Position (cm$^{-1}$) | Rel. FC factor | Signal |
|------|-----------|---------------------|----------------|--------|
| 181 | $1_0^4 3_0^1 1_3^0 2_1^0$ | 449.400 | 0.175 | 0.009 |
| 182 | $1_0^4 3_0^2 1_1^0 2_3^0$ | 871.200 | 0.034 | 0.002 |
| 183 | $1_0^4 3_0^2 1_2^0 2_2^0$ | 871.200 | 0.063 | 0.003 |
| 184 | $1_0^4 3_0^2 1_3^0 2_1^0$ | 871.200 | 0.051 | 0.003 |
| 185 | $1_0^5 3_0^1 1_2^0 2_3^0$ | 456.300 | 0.161 | 0.004 |
| 186 | $1_0^5 3_0^1 1_3^0 2_2^0$ | 456.300 | 0.196 | 0.005 |
| 187 | $1_0^1 3_0^1 1_1^0 3_1^0$ | 7.900 | 0.095 | 0.014 |
| 188 | $1_0^1 3_0^2 1_1^0 3_1^0$ | 429.700 | 0.321 | 0.046 |
| 189 | $1_0^1 3_0^3 1_1^0 3_1^0$ | 851.500 | 0.183 | 0.026 |
| 190 | $1_0^1 3_0^3 1_1^0 3_2^0$ | 430.700 | 0.214 | 0.009 |
| 191 | $1_0^1 3_0^4 1_1^0 3_1^0$ | 1273.300 | 0.054 | 0.008 |
| 192 | $1_0^1 3_0^4 1_1^0 3_2^0$ | 852.500 | 0.230 | 0.010 |
| 193 | $1_0^1 3_0^5 1_1^0 3_2^0$ | 1274.300 | 0.097 | 0.004 |
| 194 | $1_0^1 3_0^5 1_1^0 3_3^0$ | 853.500 | 0.231 | 0.003 |
| 195 | $1_0^2 3_0^1 1_2^0 3_1^0$ | 14.800 | 0.052 | 0.004 |
| 196 | $1_0^2 3_0^2 1_2^0 3_1^0$ | 436.600 | 0.177 | 0.012 |
| 197 | $1_0^2 3_0^3 1_2^0 3_1^0$ | 858.400 | 0.101 | 0.007 |
| 198 | $1_0^2 3_0^3 1_2^0 3_2^0$ | 437.600 | 0.118 | 0.002 |
| 199 | $1_0^2 3_0^4 1_2^0 3_1^0$ | 1280.200 | 0.030 | 0.002 |
| 200 | $1_0^2 3_0^4 1_2^0 3_2^0$ | 859.400 | 0.126 | 0.003 |
| 201 | $1_0^3 3_0^2 1_3^0 3_1^0$ | 443.500 | 0.097 | 0.003 |
| 202 | $1_0^3 3_0^3 1_3^0 3_1^0$ | 865.300 | 0.055 | 0.002 |
| 203 | $1_0^1 3_0^1 2_1^0$ | 428.700 | 0.263 | 0.126 |
| 204 | $1_0^1 3_0^2 2_1^0$ | 850.500 | 0.077 | 0.037 |
| 205 | $1_0^1 3_0^3 2_1^0$ | 1272.300 | 0.015 | 0.007 |
| 206 | $1_0^2 3_0^1 2_2^0$ | 435.600 | 0.118 | 0.027 |
| 207 | $1_0^2 3_0^2 2_2^0$ | 857.400 | 0.035 | 0.008 |
| 208 | $1_0^3 3_0^1 2_3^0$ | 442.500 | 0.053 | 0.006 |
| 209 | $1_0^1 3_0^1 2_1^0 3_1^0$ | 7.900 | 0.078 | 0.011 |
| 210 | $1_0^1 3_0^2 2_1^0 3_1^0$ | 429.700 | 0.263 | 0.038 |

| Peak | Assignment | Position (cm$^{-1}$) | Rel. FC factor | Signal |
|---|---|---|---|---|
| 211 | $1_0^1 3_0^3 2_1^0 3_1^0$ | 851.500 | 0.150 | 0.021 |
| 212 | $1_0^1 3_0^3 2_1^0 3_2^0$ | 430.700 | 0.175 | 0.007 |
| 213 | $1_0^1 3_0^4 2_1^0 3_1^0$ | 1273.300 | 0.044 | 0.006 |
| 214 | $1_0^1 3_0^4 2_1^0 3_2^0$ | 852.500 | 0.188 | 0.008 |
| 215 | $1_0^1 3_0^5 2_1^0 3_2^0$ | 1274.300 | 0.079 | 0.003 |
| 216 | $1_0^1 3_0^5 2_1^0 3_3^0$ | 853.500 | 0.189 | 0.002 |
| 217 | $1_0^2 3_0^1 2_2^0 3_1^0$ | 14.800 | 0.035 | 0.002 |
| 218 | $1_0^2 3_0^2 2_2^0 3_1^0$ | 436.600 | 0.118 | 0.008 |
| 219 | $1_0^2 3_0^3 2_2^0 3_1^0$ | 858.400 | 0.067 | 0.005 |
| 220 | $2_0^1 1_1^0$ | 8.300 | 0.450 | 0.216 |
| 221 | $2_0^2 1_2^0$ | 16.600 | 0.202 | 0.047 |
| 222 | $2_0^3 1_3^0$ | 24.900 | 0.091 | 0.010 |
| 223 | $2_0^4 1_4^0$ | 33.200 | 0.041 | 0.002 |
| 224 | $2_0^1 2_1^0$ | 8.300 | 0.550 | 0.264 |
| 225 | $2_0^2 2_2^0$ | 16.600 | 0.302 | 0.070 |
| 226 | $2_0^3 2_3^0$ | 24.900 | 0.166 | 0.018 |
| 227 | $2_0^4 2_4^0$ | 33.200 | 0.091 | 0.005 |
| 228 | $2_0^1 3_0^1 1_1^0$ | 430.100 | 0.263 | 0.126 |
| 229 | $2_0^1 3_0^2 1_1^0$ | 851.900 | 0.077 | 0.037 |
| 230 | $2_0^1 3_0^3 1_1^0$ | 1273.700 | 0.015 | 0.007 |
| 231 | $2_0^2 3_0^1 1_2^0$ | 438.400 | 0.118 | 0.027 |
| 232 | $2_0^2 3_0^2 1_2^0$ | 860.200 | 0.035 | 0.008 |
| 233 | $2_0^3 3_0^1 1_3^0$ | 446.700 | 0.053 | 0.006 |
| 234 | $2_0^2 3_0^1 1_1^0 2_1^0$ | 438.400 | 0.289 | 0.067 |
| 235 | $2_0^2 3_0^2 1_1^0 2_1^0$ | 860.200 | 0.085 | 0.020 |
| 236 | $2_0^2 3_0^3 1_1^0 2_1^0$ | 1282.000 | 0.017 | 0.004 |
| 237 | $2_0^3 3_0^1 1_1^0 2_2^0$ | 446.700 | 0.238 | 0.026 |
| 238 | $2_0^3 3_0^1 1_2^0 2_1^0$ | 446.700 | 0.195 | 0.022 |
| 239 | $2_0^3 3_0^2 1_1^0 2_2^0$ | 868.500 | 0.070 | 0.008 |
| 240 | $2_0^3 3_0^2 1_2^0 2_1^0$ | 868.500 | 0.057 | 0.006 |

| Peak | Assignment | Position (cm$^{-1}$) | Rel. FC factor | Signal |
|------|-----------|---------------------|----------------|--------|
| 241 | $2_0^4 3_0^1 1_1^0 2_3^0$ | 455.000 | 0.175 | 0.009 |
| 242 | $2_0^4 3_0^1 1_2^0 2_2^0$ | 455.000 | 0.214 | 0.011 |
| 243 | $2_0^4 3_0^1 1_3^0 2_1^0$ | 455.000 | 0.117 | 0.006 |
| 244 | $2_0^4 3_0^2 1_1^0 2_3^0$ | 876.800 | 0.051 | 0.003 |
| 245 | $2_0^4 3_0^2 1_2^0 2_2^0$ | 876.800 | 0.063 | 0.003 |
| 246 | $2_0^4 3_0^2 1_3^0 2_1^0$ | 876.800 | 0.034 | 0.002 |
| 247 | $2_0^5 3_0^1 1_2^0 2_3^0$ | 463.300 | 0.196 | 0.005 |
| 248 | $2_0^5 3_0^1 1_3^0 2_2^0$ | 463.300 | 0.160 | 0.004 |
| 249 | $2_0^1 3_0^1 1_1^0 3_1^0$ | 9.300 | 0.078 | 0.011 |
| 250 | $2_0^1 3_0^2 1_1^0 3_1^0$ | 431.100 | 0.263 | 0.038 |
| 251 | $2_0^1 3_0^3 1_1^0 3_1^0$ | 852.900 | 0.150 | 0.021 |
| 252 | $2_0^1 3_0^3 1_1^0 3_2^0$ | 432.100 | 0.175 | 0.007 |
| 253 | $2_0^1 3_0^4 1_1^0 3_1^0$ | 1274.700 | 0.044 | 0.006 |
| 254 | $2_0^1 3_0^4 1_1^0 3_2^0$ | 853.900 | 0.188 | 0.008 |
| 255 | $2_0^1 3_0^5 1_1^0 3_2^0$ | 1275.700 | 0.079 | 0.003 |
| 256 | $2_0^1 3_0^5 1_1^0 3_3^0$ | 854.900 | 0.189 | 0.002 |
| 257 | $2_0^2 3_0^1 1_2^0 3_1^0$ | 17.600 | 0.035 | 0.002 |
| 258 | $2_0^2 3_0^2 1_2^0 3_1^0$ | 439.400 | 0.118 | 0.008 |
| 259 | $2_0^2 3_0^3 1_2^0 3_1^0$ | 861.200 | 0.067 | 0.005 |
| 260 | $2_0^1 3_0^1 2_1^0$ | 430.100 | 0.321 | 0.154 |
| 261 | $2_0^1 3_0^2 2_1^0$ | 851.900 | 0.094 | 0.045 |
| 262 | $2_0^1 3_0^3 2_1^0$ | 1273.700 | 0.018 | 0.009 |
| 263 | $2_0^2 3_0^1 2_2^0$ | 438.400 | 0.177 | 0.041 |
| 264 | $2_0^2 3_0^2 2_2^0$ | 860.200 | 0.052 | 0.012 |
| 265 | $2_0^2 3_0^3 2_2^0$ | 1282.000 | 0.010 | 0.002 |
| 266 | $2_0^3 3_0^1 2_3^0$ | 446.700 | 0.097 | 0.011 |
| 267 | $2_0^3 3_0^2 2_3^0$ | 868.500 | 0.028 | 0.003 |
| 268 | $2_0^4 3_0^1 2_4^0$ | 455.000 | 0.053 | 0.003 |
| 269 | $2_0^1 3_0^1 2_1^0 3_1^0$ | 9.300 | 0.095 | 0.014 |
| 270 | $2_0^1 3_0^2 2_1^0 3_1^0$ | 431.100 | 0.321 | 0.046 |

| Peak | Assignment | Position (cm$^{-1}$) | Rel. FC factor | Signal |
| --- | --- | --- | --- | --- |
| 271 | $2_0^1 3_0^3 2_1^0 3_1^0$ | 852.900 | 0.183 | 0.026 |
| 272 | $2_0^1 3_0^3 2_1^0 3_2^0$ | 432.100 | 0.214 | 0.009 |
| 273 | $2_0^1 3_0^4 2_1^0 3_1^0$ | 1274.700 | 0.054 | 0.008 |
| 274 | $2_0^1 3_0^4 2_1^0 3_2^0$ | 853.900 | 0.230 | 0.010 |
| 275 | $2_0^1 3_0^5 2_1^0 3_2^0$ | 1275.700 | 0.097 | 0.004 |
| 276 | $2_0^1 3_0^5 2_1^0 3_3^0$ | 854.900 | 0.231 | 0.003 |
| 277 | $2_0^2 3_0^1 2_2^0 3_1^0$ | 17.600 | 0.052 | 0.004 |
| 278 | $2_0^2 3_0^2 2_2^0 3_1^0$ | 439.400 | 0.177 | 0.012 |
| 279 | $2_0^2 3_0^3 2_2^0 3_1^0$ | 861.200 | 0.101 | 0.007 |
| 280 | $2_0^2 3_0^3 2_2^0 3_2^0$ | 440.400 | 0.118 | 0.002 |
| 281 | $2_0^2 3_0^4 2_2^0 3_1^0$ | 1283.000 | 0.030 | 0.002 |
| 282 | $2_0^2 3_0^4 2_2^0 3_2^0$ | 862.200 | 0.126 | 0.003 |
| 283 | $2_0^3 3_0^2 2_3^0 3_1^0$ | 447.700 | 0.097 | 0.003 |
| 284 | $2_0^3 3_0^3 2_3^0 3_1^0$ | 869.500 | 0.055 | 0.002 |
| 285 | $3_0^1$ | 421.800 | 0.584 | 0.584 |
| 286 | $3_0^2$ | 843.600 | 0.171 | 0.171 |
| 287 | $3_0^3$ | 1265.400 | 0.034 | 0.034 |
| 288 | $3_0^4$ | 1687.200 | 0.005 | 0.005 |
| 289 | $3_0^1 3_1^0$ | 1.000 | 0.172 | 0.051 |
| 290 | $3_0^2 3_1^0$ | 422.800 | 0.584 | 0.174 |
| 291 | $3_0^3 3_1^0$ | 844.600 | 0.332 | 0.099 |
| 292 | $3_0^3 3_2^0$ | 423.800 | 0.389 | 0.035 |
| 293 | $3_0^3 3_3^0$ | 3.000 | 0.076 | 0.002 |
| 294 | $3_0^4 3_1^0$ | 1266.400 | 0.098 | 0.029 |
| 295 | $3_0^4 3_2^0$ | 845.600 | 0.417 | 0.037 |
| 296 | $3_0^4 3_3^0$ | 424.800 | 0.189 | 0.005 |
| 297 | $3_0^5 3_1^0$ | 1688.200 | 0.019 | 0.006 |
| 298 | $3_0^5 3_2^0$ | 1267.400 | 0.176 | 0.016 |
| 299 | $3_0^5 3_3^0$ | 846.600 | 0.421 | 0.011 |
| 300 | $3_0^6 3_2^0$ | 1689.200 | 0.045 | 0.004 |

| Peak | Assignment | Position ($\mathrm{cm}^{-1}$) | Rel. FC factor | Signal |
|---|---|---|---|---|
| 301 | $3_0^6 3_3^0$ | 1268.400 | 0.249 | 0.007 |
| 302 | $3_0^6 3_4^0$ | 847.600 | 0.364 | 0.003 |
| 303 | $3_0^7 3_3^0$ | 1690.200 | 0.080 | 0.002 |
| 304 | $3_0^7 3_4^0$ | 1269.400 | 0.305 | 0.002 |