

Terms & Conditions

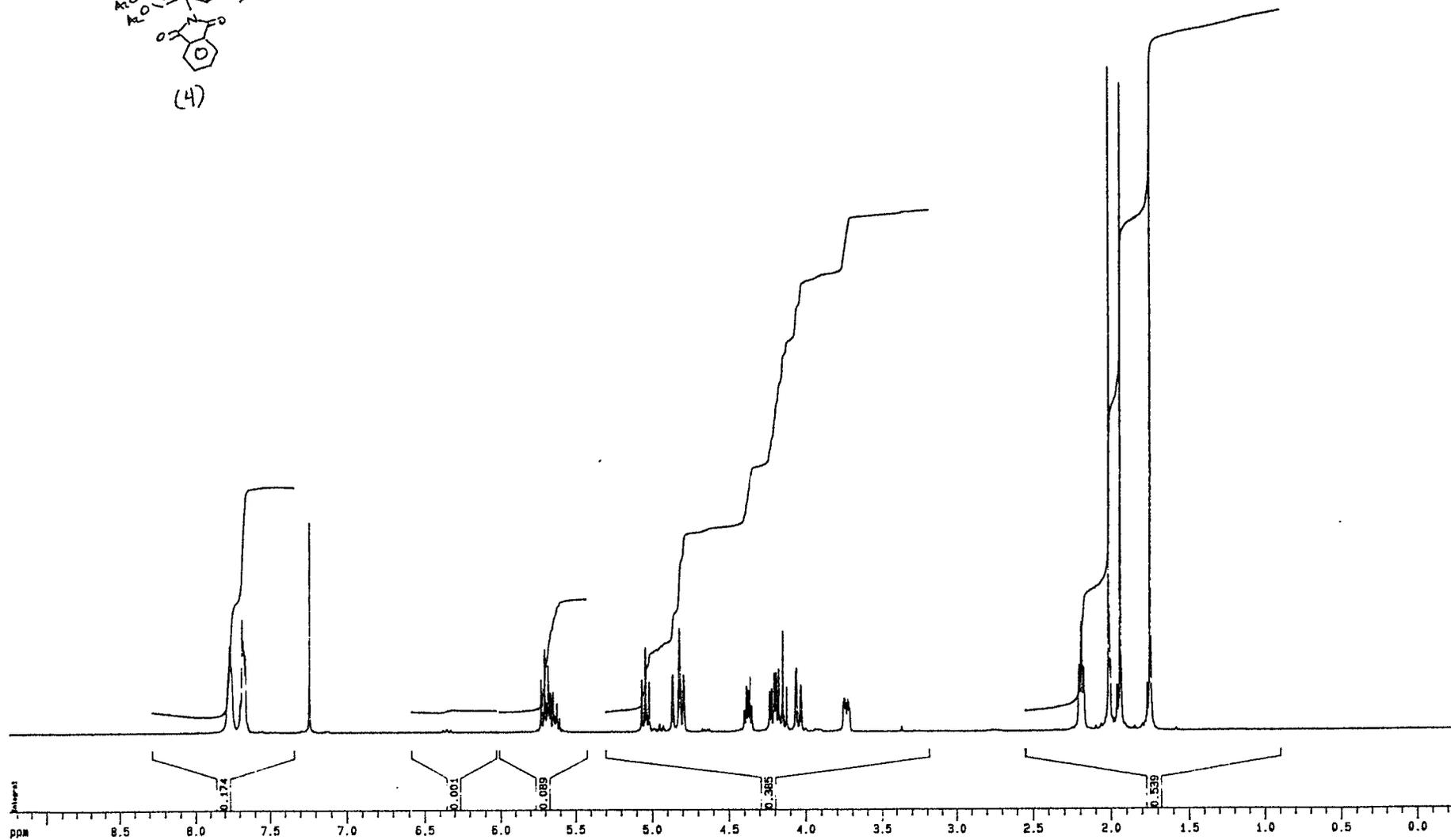
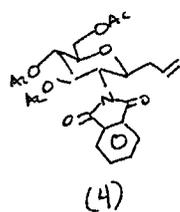
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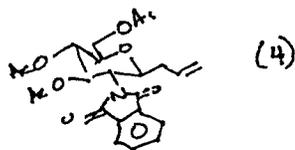


ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

Proton Starting parameters, 11/29/94 RN

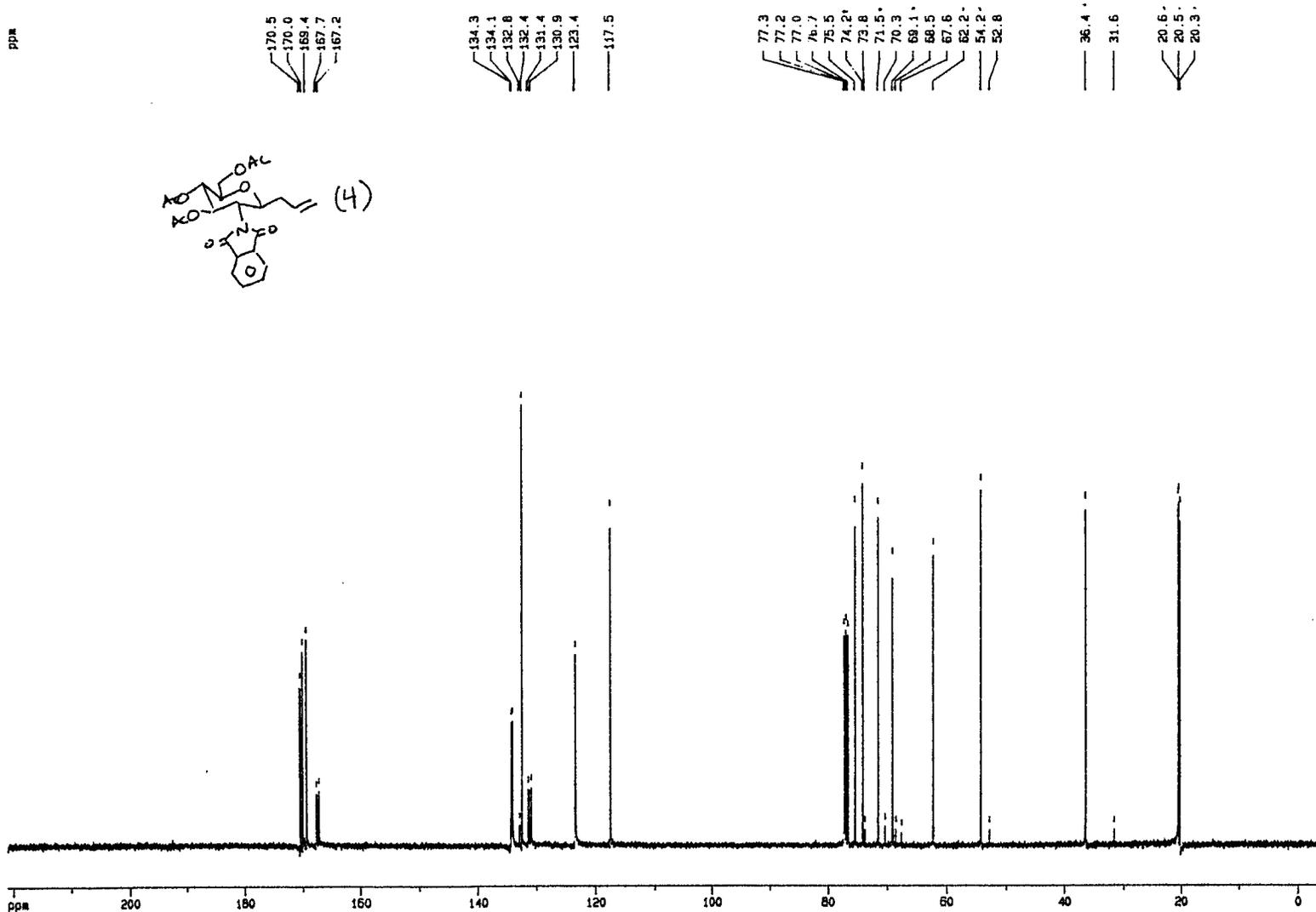




DU=, USER=bert, NAME=barh, EXPNO=1, PROCNO=1
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| # | ADDRESS | FREQUENCY [Hz] | INTENSITY [PPM] |
|----|---------|----------------|-----------------|
| 1 | 8146.3 | 3107.516 | 7.7657 |
| 2 | 8342.1 | 3078.603 | 7.6939 |
| 3 | 8370.6 | 3074.409 | 7.6834 |
| 4 | 8389.8 | 3071.598 | 7.6764 |
| 5 | 8406.9 | 3069.091 | 7.6702 |
| 6 | 8428.2 | 3065.961 | 7.6623 |
| 7 | 8828.0 | 3007.298 | 7.5157 |
| 8 | 9105.6 | 2966.574 | 7.4139 |
| 9 | 9579.8 | 2896.994 | 7.2401 |
| 10 | 9751.1 | 2871.864 | 7.1772 |
| 11 | 10276.9 | 2802.058 | 7.0028 |
| 12 | 10847.9 | 2710.952 | 6.7751 |
| 13 | 11933.6 | 2551.652 | 6.3770 |
| 14 | 11995.3 | 2542.595 | 6.3544 |
| 15 | 12073.4 | 2531.149 | 6.3257 |
| 16 | 12295.3 | 2498.588 | 6.2444 |
| 17 | 13705.4 | 2291.703 | 5.7273 |
| 18 | 13771.1 | 2282.064 | 5.7032 |
| 19 | 13809.7 | 2276.396 | 5.6891 |
| 20 | 13837.5 | 2272.308 | 5.6789 |
| 21 | 13879.1 | 2266.218 | 5.6636 |
| 22 | 13926.3 | 2259.289 | 5.6463 |
| 23 | 13948.7 | 2256.001 | 5.6381 |
| 24 | 13973.8 | 2252.323 | 5.6289 |
| 25 | 13995.8 | 2249.088 | 5.6208 |
| 26 | 14043.2 | 2242.138 | 5.6035 |
| 27 | 15511.2 | 2026.759 | 5.0652 |
| 28 | 15577.1 | 2017.075 | 5.0410 |
| 29 | 15642.3 | 2007.519 | 5.0171 |
| 30 | 15721.9 | 1995.832 | 4.9879 |
| 31 | 15760.1 | 1990.227 | 4.9739 |
| 32 | 15825.9 | 1980.580 | 4.9498 |
| 33 | 15892.2 | 1970.848 | 4.9255 |
| 34 | 16056.9 | 1946.690 | 4.8651 |
| 35 | 16063.9 | 1945.660 | 4.8625 |
| 36 | 16183.7 | 1928.089 | 4.8186 |
| 37 | 16257.3 | 1917.284 | 4.7916 |
| 38 | 16390.1 | 1868.462 | 4.6696 |
| 39 | 16628.8 | 1862.779 | 4.6554 |
| 40 | 16667.9 | 1857.038 | 4.6410 |
| 41 | 16707.2 | 1851.281 | 4.6266 |
| 42 | 17322.1 | 1761.052 | 4.4012 |
| 43 | 17360.0 | 1755.491 | 4.3873 |
| 44 | 17394.5 | 1750.437 | 4.3746 |
| 45 | 17429.8 | 1745.255 | 4.3617 |
| 46 | 17467.7 | 1739.692 | 4.3478 |
| 47 | 17773.3 | 1694.854 | 4.2357 |
| 48 | 17806.5 | 1689.990 | 4.2236 |
| 49 | 17856.9 | 1682.598 | 4.2051 |
| 50 | 17889.9 | 1677.754 | 4.1930 |
| 51 | 17936.4 | 1670.934 | 4.1759 |
| 52 | 18006.8 | 1660.392 | 4.1501 |
| 53 | 18077.1 | 1650.290 | 4.1243 |
| 54 | 18239.8 | 1626.407 | 4.0647 |
| 55 | 18253.8 | 1624.366 | 4.0596 |
| 56 | 18323.4 | 1614.142 | 4.0340 |
| 57 | 18337.1 | 1612.137 | 4.0290 |
| 58 | 18425.4 | 1599.177 | 3.9966 |
| 59 | 18594.5 | 1574.379 | 3.9346 |
| 60 | 19069.9 | 1504.627 | 3.7603 |
| 61 | 19084.2 | 1502.519 | 3.7550 |
| 62 | 19102.1 | 1499.892 | 3.7485 |
| 63 | 19116.9 | 1497.720 | 3.7430 |
| 64 | 19138.6 | 1494.541 | 3.7351 |
| 65 | 19153.1 | 1492.409 | 3.7298 |
| 66 | 19171.1 | 1489.780 | 3.7232 |
| 67 | 19185.7 | 1487.629 | 3.7178 |
| 68 | 20143.2 | 1347.146 | 3.3667 |
| 69 | 23304.7 | 883.293 | 2.2075 |
| 70 | 23346.4 | 877.180 | 2.1922 |
| 71 | 23388.8 | 870.957 | 2.1767 |
| 72 | 23602.8 | 839.555 | 2.0982 |
| 73 | 23700.4 | 825.236 | 2.0624 |
| 74 | 23776.5 | 814.071 | 2.0345 |
| 75 | 23840.2 | 804.734 | 2.0112 |
| 76 | 23861.0 | 801.679 | 2.0035 |
| 77 | 23934.0 | 790.971 | 1.9768 |
| 78 | 23979.5 | 784.295 | 1.9601 |
| 79 | 24041.2 | 775.240 | 1.9374 |
| 80 | 24126.3 | 762.755 | 1.9062 |
| 81 | 24287.3 | 739.131 | 1.8472 |
| 82 | 24425.9 | 718.792 | 1.7964 |
| 83 | 24470.5 | 712.248 | 1.7800 |
| 84 | 24512.3 | 706.114 | 1.7647 |
| 85 | 24564.9 | 698.399 | 1.7454 |
| 86 | 25013.0 | 632.660 | 1.5811 |

Carbon Basic Parameters. Aug 4 92 RN

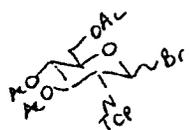


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 EXPNO 2
 PROCNO 1

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 SOLVENT 7.250
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 FIDRES 0.401547 Hz
 DN 19.0 usec
 RG 8192
 NUCLEUS 13C
 HL1 27 dB
 S4 30 dB
 D1 1.5000000 sec
 P31 91.0 usec
 S2 24 dB
 D11 0.0300000 sec
 P0 2.2 usec
 DE 23.8 usec
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 SMH 26315.79 Hz
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 NS 408
 DS 0

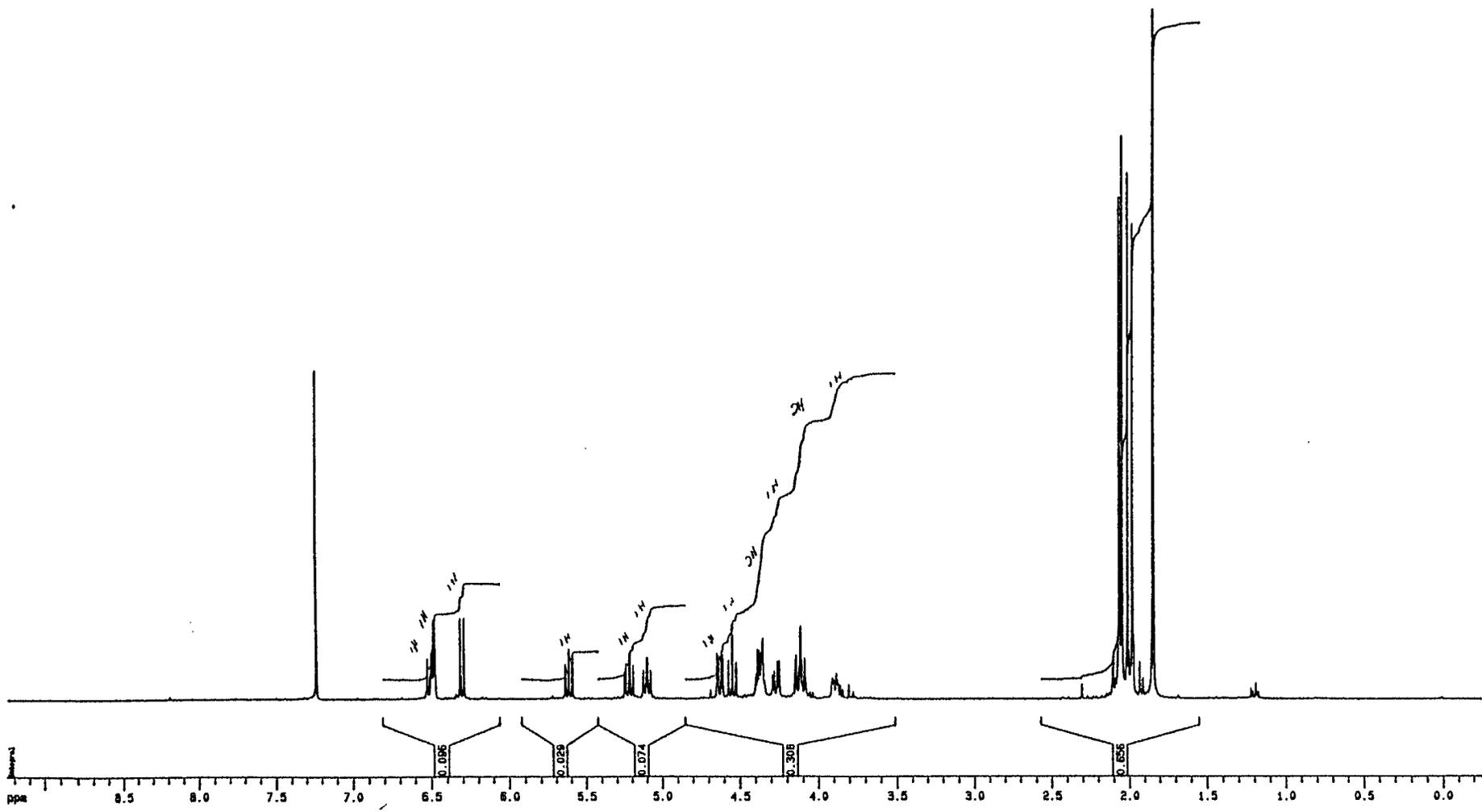
F2 - Processing parameters
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 WDM EM
 SSB 0
 LB 0.75 Hz
 GB 0
 PC 1.50

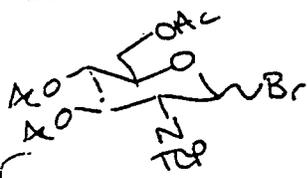
1D NMR plot parameters
 CX 32.14 cm
 F1P 221.000 ppm
 F1 22235.67 Hz
 F2P -4.000 ppm
 F2 -402.46 Hz
 PPMCM 7.00000 ppm/cm
 HZCM 704.29724 Hz/cm



(7)

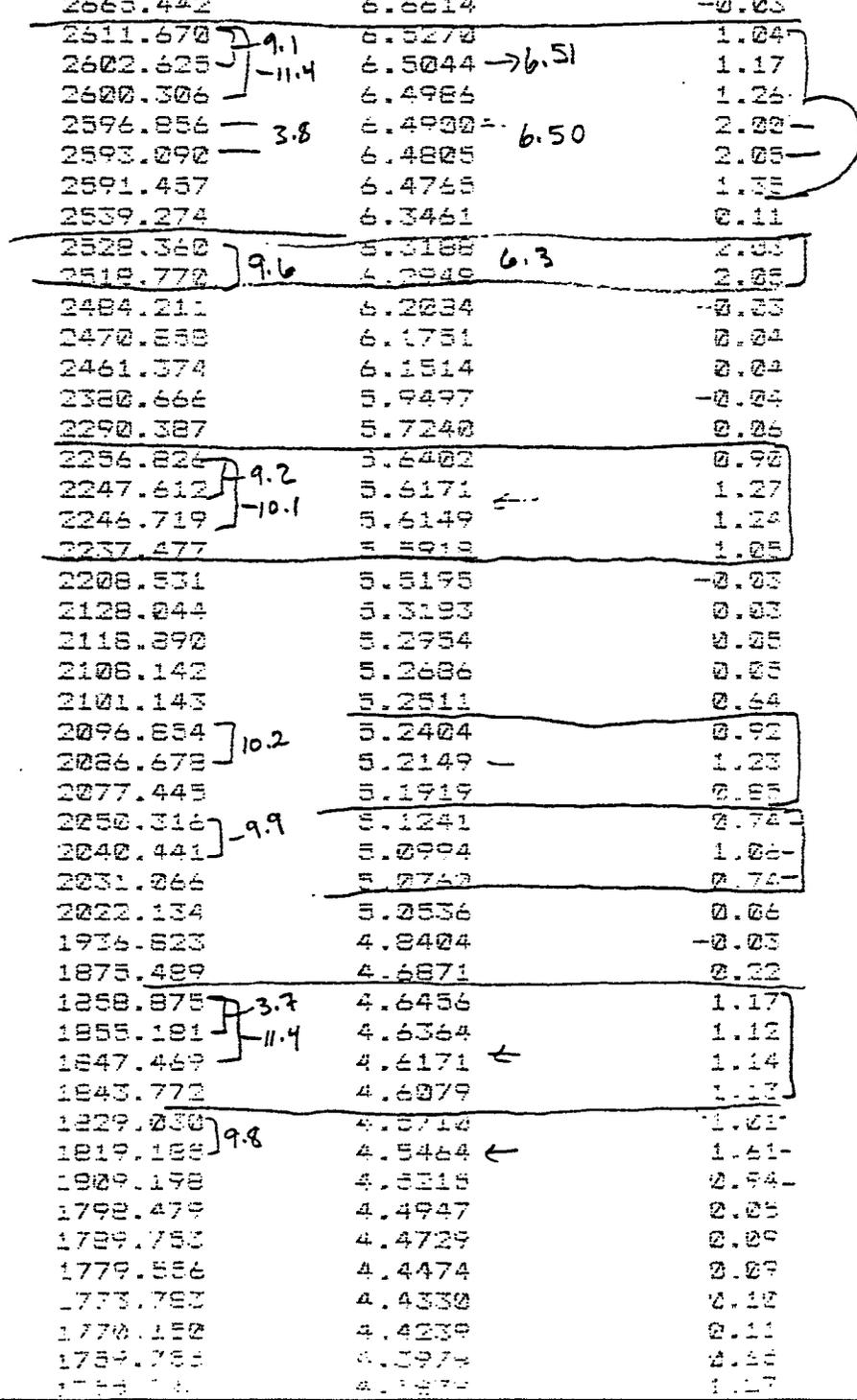
Proton Starting parameters, 11/29/94 RN





ORBITAL NAME=orb, EXPND=1, PRODN=1
 1.25000, FI=-2.25000, MI=0.0000, MAXI=10000.0000, PC=6.200
 ADDRESS ENERGY INTERP.

| | ADDRESS | ENERGY | ORBITAL | INTERP. |
|----|---------|----------|---------|---------|
| 1 | 6976.1 | 3278.279 | 6.1929 | 0.04 |
| 2 | 7823.3 | 3271.357 | 5.1756 | -0.04 |
| 3 | 8909.1 | 2994.678 | 7.4642 | -0.04 |
| 4 | 9363.0 | 2926.076 | 7.3177 | 0.03 |
| 5 | 9575.5 | 2696.890 | 7.2392 | 0.41 |
| 6 | 9787.0 | 2865.866 | 7.1623 | -0.04 |
| 7 | 10527.7 | 2757.190 | 6.8927 | -0.04 |
| 8 | 10763.8 | 2722.550 | 6.8041 | -0.03 |
| 9 | 11153.1 | 2665.442 | 6.6614 | -0.03 |
| 10 | 11519.6 | 2511.670 | 6.5270 | 1.04 |
| 11 | 11581.2 | 2602.625 | 6.5044 | 1.17 |
| 12 | 11597.0 | 2600.306 | 6.4966 | 1.26 |
| 13 | 11629.5 | 2596.856 | 6.4900 | 2.02 |
| 14 | 11646.2 | 2593.090 | 6.4805 | 2.05 |
| 15 | 11657.3 | 2591.457 | 6.4765 | 1.33 |
| 16 | 12013.0 | 2539.274 | 6.3461 | 0.11 |
| 17 | 12087.4 | 2528.360 | 6.3165 | 2.03 |
| 18 | 12152.7 | 2518.770 | 6.2949 | 2.05 |
| 19 | 12388.3 | 2484.211 | 6.2034 | -0.03 |
| 20 | 12479.7 | 2470.658 | 6.1751 | 0.04 |
| 21 | 12543.9 | 2461.374 | 6.1514 | 0.04 |
| 22 | 13094.0 | 2380.666 | 5.9497 | -0.04 |
| 23 | 13789.3 | 2290.387 | 5.7240 | 0.06 |
| 24 | 13938.1 | 2256.824 | 5.6402 | 0.92 |
| 25 | 14000.9 | 2247.612 | 5.6171 | 1.27 |
| 26 | 14007.0 | 2246.719 | 5.6149 | 1.24 |
| 27 | 14070.0 | 2237.477 | 5.5918 | 1.05 |
| 28 | 14267.2 | 2208.531 | 5.5195 | -0.03 |
| 29 | 14615.8 | 2128.044 | 5.3193 | 0.03 |
| 30 | 14878.2 | 2116.890 | 5.2954 | 0.05 |
| 31 | 14951.5 | 2106.142 | 5.2686 | 0.05 |
| 32 | 14999.2 | 2101.143 | 5.2511 | 0.64 |
| 33 | 15028.4 | 2096.654 | 5.2404 | 0.92 |
| 34 | 15097.8 | 2086.678 | 5.2149 | 1.23 |
| 35 | 15160.7 | 2077.443 | 5.1919 | 0.85 |
| 36 | 15345.6 | 2050.316 | 5.1241 | 0.74 |
| 37 | 15412.9 | 2040.441 | 5.0994 | 1.06 |
| 38 | 15476.3 | 2031.066 | 5.0747 | 0.76 |
| 39 | 15537.7 | 2022.134 | 5.0536 | 0.06 |
| 40 | 16119.1 | 1936.623 | 4.8404 | -0.03 |
| 41 | 16537.2 | 1875.489 | 4.6871 | 0.22 |
| 42 | 16650.4 | 1858.875 | 4.6456 | 1.17 |
| 43 | 16675.6 | 1855.181 | 4.6364 | 1.12 |
| 44 | 16728.2 | 1847.469 | 4.6171 | 1.14 |
| 45 | 16753.3 | 1843.772 | 4.6079 | 1.13 |
| 46 | 16853.2 | 1829.030 | 4.5716 | 1.01 |
| 47 | 16920.9 | 1819.186 | 4.5464 | 1.61 |
| 48 | 16989.0 | 1809.198 | 4.5215 | 0.94 |
| 49 | 17062.1 | 1798.479 | 4.4947 | 0.05 |
| 50 | 17121.5 | 1789.753 | 4.4729 | 0.05 |
| 51 | 17191.0 | 1779.556 | 4.4474 | 0.09 |
| 52 | 17230.4 | 1773.783 | 4.4330 | 0.10 |
| 53 | 17255.1 | 1770.150 | 4.4239 | 0.11 |
| 54 | 17326.0 | 1754.783 | 4.3974 | 0.35 |
| 55 | 17413.0 | 1734.100 | 4.3670 | 1.17 |



| | | | | |
|-----|---------|----------|--------|-------|
| 57 | 17419.1 | 1745.271 | 4.3333 | 1.17 |
| 58 | 17414.2 | 1742.411 | 4.3345 | 1.33 |
| 59 | 17476.5 | 1737.378 | 4.3333 | 0.48 |
| 60 | 17537.8 | 1728.879 | 4.3333 | 0.18 |
| 61 | 17637.6 | 1724.326 | 4.3393 | 0.18 |
| 62 | 17615.7 | 1717.327 | 4.3413 | 0.37 |
| 63 | 17647.0 | 1712.617 | 4.3521 | 0.71 |
| 64 | 17721.3 | 1704.385 | 4.3633 | 0.77 |
| 65 | 17733.2 | 1702.459 | 4.3637 | 0.58 |
| 66 | 17813.7 | 1688.231 | 4.3791 | 0.26 |
| 67 | 18237.7 | 1659.734 | 4.4479 | 0.48 |
| 68 | 18021.5 | 1637.714 | 4.4409 | 1.12 |
| 69 | 18093.4 | 1647.156 | 4.4163 | 1.83 |
| 70 | 18167.2 | 1636.339 | 4.3893 | 1.64 |
| 71 | 18187.4 | 1633.363 | 4.3823 | 0.44 |
| 72 | 18264.5 | 1622.363 | 4.3838 | 0.17 |
| 73 | 18313.2 | 1614.917 | 4.3859 | 0.16 |
| 74 | 18361.2 | 1607.776 | 4.3811 | 0.24 |
| 75 | 18543.2 | 1581.166 | 3.9516 | 0.24 |
| 76 | 18646.0 | 1566.086 | 3.9139 | 0.45 |
| 77 | 18660.2 | 1564.000 | 3.9087 | 0.54 |
| 78 | 18677.2 | 1561.581 | 3.9024 | 0.53 |
| 79 | 18691.5 | 1559.408 | 3.8972 | 0.44 |
| 80 | 18729.2 | 1553.873 | 3.8834 | 0.65 |
| 81 | 18747.3 | 1551.226 | 3.8768 | 0.49 |
| 82 | 18761.8 | 1549.094 | 3.8714 | 0.42 |
| 83 | 18799.9 | 1543.589 | 3.8573 | 0.36 |
| 84 | 18838.2 | 1537.881 | 3.8434 | 0.28 |
| 85 | 18946.1 | 1522.852 | 3.8259 | 0.37 |
| 86 | 19020.1 | 1511.194 | 3.7767 | 0.18 |
| 87 | 22017.0 | 1071.492 | 2.6773 | -0.03 |
| 88 | 22797.2 | 957.023 | 2.3918 | 0.63 |
| 89 | 23028.7 | 923.263 | 2.3869 | 0.37 |
| 90 | 23129.1 | 908.327 | 2.2781 | 0.67 |
| 91 | 23235.0 | 892.788 | 2.2312 | 0.88 |
| 92 | 23288.8 | 885.336 | 2.2126 | 0.06 |
| 93 | 23384.4 | 878.868 | 2.1764 | 0.87 |
| 94 | 23464.1 | 859.173 | 2.1472 | 0.13 |
| 95 | 23512.2 | 852.128 | 2.1296 | 0.15 |
| 96 | 23566.8 | 844.109 | 2.1096 | 0.78 |
| 97 | 23681.3 | 841.976 | 2.1042 | 1.87 |
| 98 | 23618.7 | 836.500 | 2.0925 | 0.52 |
| 99 | 23673.8 | 828.538 | 2.0786 | 12.41 |
| 100 | 23723.8 | 821.078 | 2.0528 | 14.08 |
| 101 | 23769.1 | 814.429 | 2.0354 | 0.56 |
| 102 | 23779.2 | 812.261 | 2.0313 | 0.54 |
| 103 | 23824.3 | 806.332 | 2.0152 | 13.86 |
| 104 | 23869.3 | 799.733 | 1.9987 | 0.79 |
| 105 | 23906.6 | 794.247 | 1.9858 | 11.64 |
| 106 | 23932.3 | 790.479 | 1.9755 | 1.63 |
| 107 | 24043.0 | 774.235 | 1.9349 | 0.94 |
| 108 | 24065.1 | 772.845 | 1.9265 | 0.22 |
| 109 | 24106.6 | 764.983 | 1.9116 | 0.54 |
| 110 | 24171.7 | 755.357 | 1.8873 | 0.17 |
| 111 | 24278.7 | 739.653 | 1.8463 | 17.11 |
| 112 | 24282.7 | 739.271 | 1.8471 | 16.48 |
| 113 | 24738.6 | 571.969 | 1.6543 | 0.08 |
| 114 | 25986.3 | 469.119 | 1.2224 | 0.23 |
| 115 | 25925.3 | 463.437 | 1.2352 | 0.19 |
| 116 | 26073.8 | 476.252 | 1.1983 | 0.41 |
| 117 | 26122.5 | 469.137 | 1.1724 | 0.19 |
| 118 | 26668.9 | 92.925 | 0.2424 | -0.03 |
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4.3
11.6

10.5

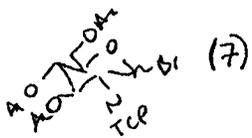
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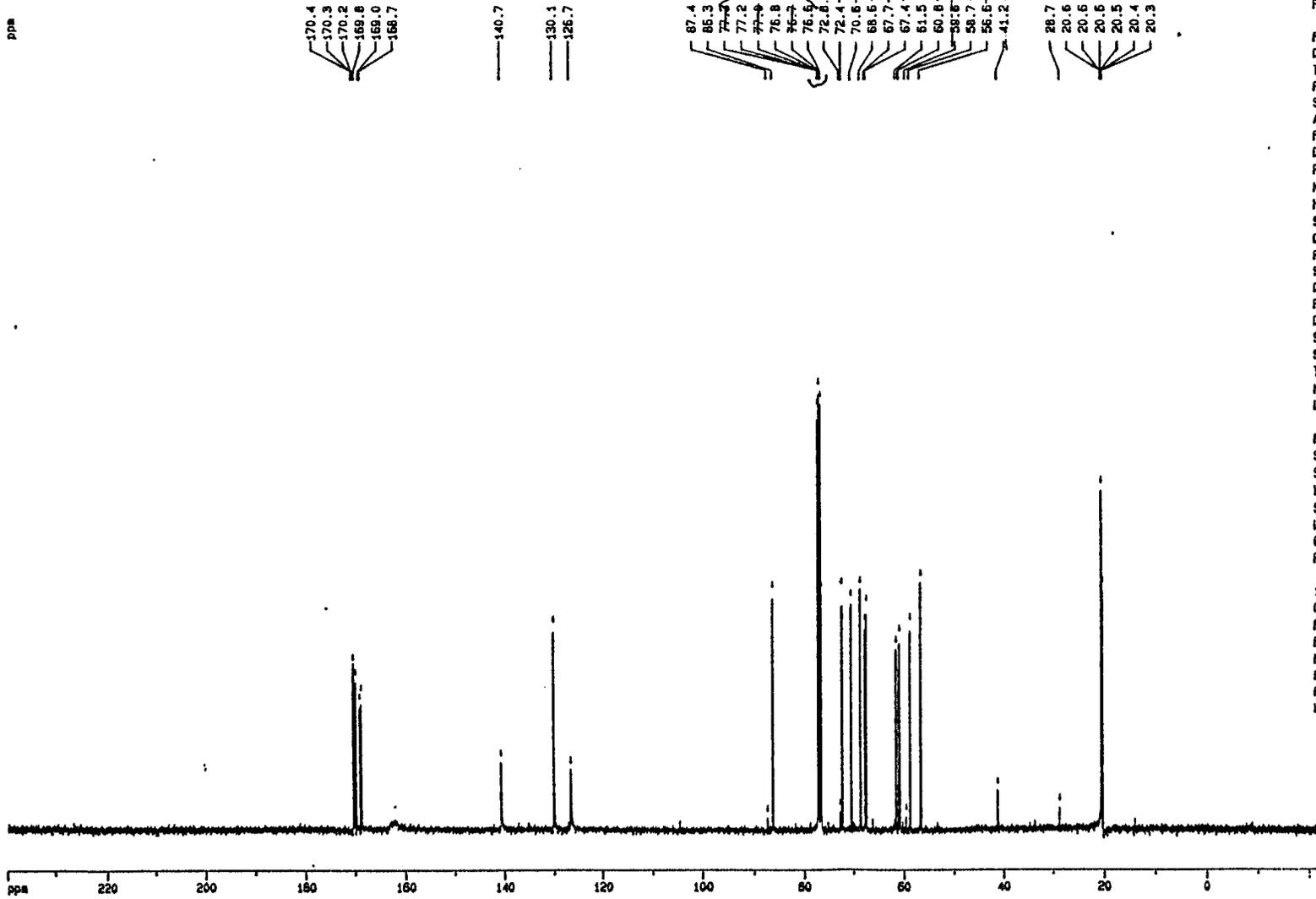
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Carbon Basic Parameters, Aug 4 92 PM



Current Data Parameters
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 PROCNO 1

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 FIDRES 0.401547 Hz
 DN 19.0 usec
 RG 8192
 NUCLEUS 13C
 HL1 27 dB
 S4 30 dB
 O1 1.5000000 sec
 P31 91.0 usec
 S2 24 dB
 D11 0.0300000 sec
 P0 2.2 usec
 DE 23.8 usec
 SF01 100.6248799 MHz
 SMH 26315.79 Hz
 TD 65536
 NS 1587
 DS 0

F2 - Processing parameters
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 SF 100.6138833 MHz
 MDW EM
 SSB 0
 LB 0.75 Hz
 GB 0
 PC 1.50

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 F1 24154.49 Hz
 F2P -21.481 ppm
 F2 -2161.30 Hz
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 HZCM 818.71350 Hz/cm