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| isomer | neat | inf CDCI3 | lambda | shift at s= | observed | isotope shift | intensity | J | shift at s= | observed | isotope shift | intensity | J | assignment | | | | | | | | | |
|--------|---------|-----------|---------|-------------|--------------------|--------------------|--------------------|-------------|-------------|----------|---------------|-----------|----------|------------|-----------|----------|------|------|------|-----------------|---|---|--|
| C6-A | 135.238 | 135.034 | 0.17 | 135.074427 | 1- ¹³ C | 0.114 | 135.079 | 0.00457332 | 61.4 | 1.46 | | | 135.1309 | 135.1061 | -0.0248 | 13.4 | 71.7 | 43.2 | 1.25 | C ₈ | ¹ J sp ² -sp ² | | |
| | 130.248 | 129.961 | 0.24 | 130.017959 | 2- ¹³ C | 1- ¹³ C | 129.98 | -0.03795896 | 0.68 | 71.65 | 3.32 | | 130.0975 | 130.0893 | -0.0082 | 1073 | 0.4 | | | | C ₉ | | |
| | 43.626 | 43.178 | 0.233 | 43.2526059 | 1- ¹³ C | 1- ¹³ C | 43.258 | 0.00539407 | 47 | 1.52 | 0.48 | | 43.36133 | 43.3456 | -0.01573 | 14.8 | 35 | 35 | 3.5 | | C ₆ | ¹ J sp ² -sp ³ | |
| | 40.928 | 40.41 | 0.245 | 40.493798 | 2- ¹³ C | 2- ¹³ C | 40.479 | -0.01479798 | 0.7 | 43.41 | 34.46 | 1.4 | 40.61685 | 40.6068 | -0.01005 | 1191 | 0.5 | 0.5 | | | C ₇ (CH) | | |
| | 38.144 | 37.733 | 0.213 | 37.8013679 | | | 37.804 | 0.00263215 | 0.69 | s | | | 37.90103 | 37.8875 | -0.01353 | 14 | 35 | 3.4 | | C ₄ | ¹ J sp ³ -sp ³ | | |
| | 36.518 | 36.089 | 0.226 | 36.1607329 | | | 36.165 | 0.0042671 | 0.47 | | 1.77 | | 36.26516 | 36.2563 | -0.00886 | 10 | 35 | 3.3 | | C ₁₅ | | | |
| | 32.607 | 32.258 | 0.202 | 32.3181888 | | | 32.32 | 0.00181119 | 0.91 | s | | | 32.40512 | 32.3872 | -0.01792 | 16 | 43.1 | 4.9 | | C ₁₀ | | | |
| | 32.29 | 31.94 | 0.205 | 32.0006058 | | | 32.006058 | -32.0006058 | | | | | 32.08805 | 32.093 | 0.00495 | 14 | 0.7 | | | C ₁₁ | | | |
| | 30.331 | 30.014 | 0.206 | 30.0709448 | 2- ¹³ C | 2- ¹³ C | 30.05 | -0.02094482 | | | 35 | 35 | 2 | 30.15236 | 30.1429 | -0.00946 | 1179 | 0.72 | | | C ₅ (CH) | | |
| | 29.91 | 29.544 | 0.217 | 29.6076419 | | | 29.614 | 0.00635813 | 0.67 | | 3.04 | 1.73 | 29.69937 | 29.6919 | -0.00747 | 15 | s | | | C ₁₆ | | | |
| | 29.642 | 29.279 | 0.204 | 29.3409868 | | | 29.346 | 0.00501318 | 0.6 | | 2.5 | 2.5 | 29.43074 | 29.421 | -0.00974 | 21 | 0.7 | | | C ₃ | | | |
| | 23.318 | 23.013 | 0.19 | 23.0669608 | | | 23.0669608 | -23.0669608 | | | | | 23.1444 | | -23.1444 | | | | | | C ₁₇ | | |
| | 23.133 | 22.832 | 0.181 | 22.8845957 | | | 22.8845957 | -22.8845957 | | | | | 22.96031 | | -22.96031 | | | | | | C ₂ | | |
| | 22.411 | 22.109 | 0.189 | 22.1625178 | | | 22.1625178 | -22.1625178 | | | | | 22.23929 | | -22.23929 | | | | | | C ₁₂ | | |
| | 19.383 | 19.253 | 0.055 | 19.2733752 | 1- ¹³ C | 1- ¹³ C | 19.272 | -0.00137522 | 58.4 | 0.43 | | | 19.30355 | 19.2906 | -0.01295 | 11.4 | 35.3 | 1.4 | | | C ₁₄ | | |
| | 14.283 | 14.172 | 0.049 | 14.1896032 | | | 14.1896032 | -14.1896032 | | | | | 14.21559 | | -14.21559 | | | | | | C ₁ | | |
| | 14.255 | 14.143 | 0.059 | 14.1617272 | | | 14.1617272 | -14.1617272 | | | | | 14.18899 | | -14.18899 | | | | | | C ₁₈ | | |
| | 14.044 | 13.938 | 0.061 | 13.9562452 | | | 13.9562452 | -13.9562452 | | | | | 13.98261 | | -13.98261 | | | | | | C ₁₃ | | |
| | C6-A' | 135.558 | 135.386 | 0.173 | 135.423082 | 1- ¹³ C | 0 | 135.432 | 0.00891831 | 20.9 | 1.43 | | | 135.47393 | 135.451 | -0.02293 | | 71 | 43 | 1.8 | | C ₈ | |
| | | 130.007 | 129.71 | 0.213 | 129.765372 | 2- ¹³ C | 2- ¹³ C | 129.8 | 0.03462815 | 0.27 | 71 | 3.4 | | 129.84383 | 129.8389 | -0.00493 | 373 | 0.4 | | | | C ₉ | |
| 43.965 | | 43.487 | 0.227 | 43.5644199 | 1- ¹³ C | 1- ¹³ C | 43.57 | 0.00558009 | 15.9 | 1.47 | | | 43.67807 | 43.662 | -0.01607 | | 35 | 35 | 3.5 | | C ₆ | | |
| 40.781 | | 40.257 | 0.241 | 40.341078 | 2- ¹³ C | 2- ¹³ C | | -40.341078 | | | | | 40.46481 | 40.4521 | -0.01271 | 422 | 0.5 | 0.5 | | | C ₇ (CH) | | |
| 36.103 | | 35.857 | 0.22 | 35.9072649 | | | 35.906 | -0.00126488 | 0.24 | s | | | 35.977 | | -35.977 | | | | | | C ₄ | | |
| 35.753 | | 35.254 | 0.216 | 35.3327029 | | | 35.337 | 0.00429714 | 0.457 | | 1.66 | | 35.44906 | | -35.44906 | | | | | | C ₁₅ | | |
| 32.65 | | 32.294 | 0.201 | 32.3548858 | | | 32.357 | 0.0021142 | 0.28 | s | | | 32.44301 | 32.427 | -0.01601 | 12 | 43 | 4.5 | | | C ₁₀ | | |
| 32.325 | | 31.94 | 0.2 | 32.0040908 | | | 32.0040908 | -32.0040908 | | | | | 32.0975 | 32.1 | 0.0025 | s | | | | | C ₁₁ | | |
| 30.267 | | 29.927 | 0.201 | 29.9860618 | 2- ¹³ C | 2- ¹³ C | 29.975 | -0.0110618 | 0.2 | | 35 | 35 | 2 | 30.07121 | 30.0606 | -0.01061 | 408 | 0.72 | | | C ₅ (CH) | | |
| 29.823 | | 29.457 | 0.216 | 29.5205409 | | | 29.525 | 0.00445914 | 0.3 | ? | ? | | 29.61216 | 29.6054 | -0.00676 | 6 | s | | | | C ₁₆ | | |
| 29.436 | | 29.056 | 0.202 | 29.1197228 | | | 29.126 | 0.00627719 | 0.25 | | 3.02 | 1.9 | 29.21242 | 29.205 | -0.00742 | 10 | 0.86 | | | | C ₃ | | |
| 23.377 | | 23.039 | 0.177 | 23.0954097 | | | 23.0954097 | -23.0954097 | | | | | 23.17757 | | -23.17757 | | | | | | C ₁₇ | | |
| 23.142 | | 22.85 | 0.178 | 22.9012667 | | | 22.9012667 | -22.9012667 | | | | | 22.97498 | | -22.97498 | | | | | | C ₂ | | |
| 22.454 | | 22.149 | 0.186 | 22.2025567 | | | 22.2025567 | -22.2025567 | | | | | 22.27956 | | -22.27956 | | | | | | C ₁₂ | | |
| 20.633 | | 20.422 | 0.062 | 20.4523162 | 1- ¹³ C | 1- ¹³ C | 20.453 | 0.00068375 | 18.4 | s | | | 20.49832 | 20.4876 | -0.01072 | 3.8 | 35.2 | 2.9 | | | C ₁₄ | | |
| 14.293 | | 14.18 | 0.055 | 14.1984372 | | | 14.1984372 | -14.1984372 | | | | | 14.22545 | | -14.22545 | | | | | | C ₁ | | |
| 14.254 | | 14.147 | 0.061 | 14.1653592 | | | 14.1653592 | -14.1653592 | | | | | 14.19191 | | -14.19191 | | | | | | C ₁₈ | | |
| 14.064 | | 13.938 | 0.059 | 13.9583232 | | | 13.9583232 | -13.9583232 | | | | | 13.98819 | | -13.98819 | | | | | | C ₁₃ | | |
| C6-B | | 135.484 | 135.503 | 0.178 | 135.518813 | 1- ¹³ C | 0 | 135.5195 | 0.00068729 | 26.5 | 1.28 | | | 135.53468 | 135.5055 | -0.02918 | 10 | 70.1 | 42.9 | 1.8 | | C ₈ | |
| | | 129.319 | 129.097 | 0.2 | 129.142509 | 2- ¹³ C | 2- ¹³ C | 129.107 | -0.0355088 | 0.35 | 70.1 | 3.2 | | 129.2056 | 129.2012 | -0.0044 | 428 | 0.26 | | | | C ₉ | |
| | 44.485 | 43.983 | 0.217 | 44.0621459 | 1- ¹³ C | 1- ¹³ C | 44.068 | 0.00585413 | 20.8 | | 1.3 | | 44.17917 | 44.161 | -0.01817 | | 34.5 | 34.5 | 3 | | C ₆ | | |
| | 36.563 | 36.276 | 0.206 | 36.3295248 | | | 36.3295 | -2.4824E-05 | 0.28 | s | | | 36.40536 | 36.3859 | -0.01946 | 6 | 34.8 | 2.1 | | | C ₄ | | |
| | 36.092 | 35.586 | 0.219 | 35.6658039 | | | 35.67 | 0.00419612 | 0.55 | 1.04? | small | | 35.78379 | ? | #VALUE! | | | | | | C ₁₅ | | |
| | 35.012 | 34.673 | 0.215 | 34.7333619 | 2- ¹³ C | 2- ¹³ C | 34.71 | -0.02336186 | ca 0.6 | | 43 | 34.8 | 3.1 | 34.81985 | 34.8022 | -0.01765 | 490 | 0.6 | | | | C ₇ (CH) | |
| | 32.561 | 32.19 | 0.207 | 32.2532018 | | | 32.28 | 0.02679817 | 0.3 | | 2.16 | | 32.34477 | 32.334 | -0.01077 | 6 | 1.85 | 0.3 | | | C ₁₁ | | |
| | 30.627 | 30.301 | 0.205 | 30.3588698 | 2- ¹³ C | 2- ¹³ C | 30.34 | -0.01886982 | ca 0.6 | | 36 | 35 | 2 | 30.44185 | 30.4316 | -0.01025 | 531 | 0.7 | | | | C ₅ (CH) | |
| | 29.916 | 29.565 | 0.221 | 29.6273359 | | | 29.63 | 0.00266412 | ca 0.6 | | ? | | 29.71671 | 29.7082 | -0.00851 | 6 | s | | | | C ₁₆ | | |
| | 29.668 | 29.27 | 0.169 | 29.3324417 | | | 29.35 | 0.01755832 | ca 0.6 | | ? | | 29.42489 | 29.4006 | -0.02429 | 5 | 0.9 | | | | C ₃ | | |
| | 27.87 | 27.521 | 0.202 | 27.5811888 | | | 27.584 | 0.00281119 | 0.53 | s | | | 27.66812 | 27.667 | -0.00112 | 5 | 42.8 | | | | C ₁₀ | | |
| | 23.468 | 23.148 | 0.19 | 23.2036708 | | | 23.2036708 | -23.2036708 | | | | | 23.2839 | | -23.2839 | | | | | | C ₁₇ | | |

¹J sp²-sp²¹J sp²-sp³¹J sp³-sp³

