

Fobs & Fcalc for C₁₁H₁₇NO₂

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| H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc |
|----|----|----|-----|------|----|-----|----|-----|------|----|-----|----|-----|------|----|----|----|-----|------|
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| -4 | 4 | 10 | -2 | 0 | -4 | 13 | 0 | 2 | 0 | -3 | -11 | 6 | -5 | 0 | -3 | -7 | 8 | 22 | 23 |
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| -4 | 5 | 0 | 47 | 50 | -3 | -16 | 6 | 10 | 6 | -3 | -11 | 8 | -1 | 17 | -3 | -7 | 10 | 169 | 188 |
| -4 | 5 | 1 | 3 | 6 | -3 | -16 | 7 | 0 | 3 | -3 | -11 | 9 | 4 | 2 | -3 | -7 | 11 | 2 | 9 |
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| -4 | 6 | 1 | 123 | 131 | -3 | -15 | 10 | 0 | 1 | -3 | -10 | 4 | 2 | 3 | -3 | -6 | 6 | 127 | 114 |
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| -4 | 6 | 4 | 19 | 13 | -3 | -14 | 1 | 25 | 24 | -3 | -10 | 7 | 24 | 23 | -3 | -6 | 9 | 49 | 50 |
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| -4 | 6 | 7 | 3 | 0 | -3 | -14 | 4 | 1 | 3 | -3 | -10 | 10 | 2 | 1 | -3 | -6 | 12 | 44 | 44 |
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| -4 | 7 | 2 | 135 | 138 | -3 | -14 | 10 | 0 | 0 | -3 | -10 | 16 | 16 | 15 | -3 | -5 | 2 | 359 | 344 |
| -4 | 7 | 3 | 40 | 38 | -3 | -14 | 11 | 1 | 0 | -3 | -9 | 1 | 203 | 202 | -3 | -5 | 3 | -1 | 3 |
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| -4 | 7 | 8 | 2 | 5 | -3 | -13 | 2 | 44 | 41 | -3 | -9 | 6 | 126 | 142 | -3 | -5 | 8 | 422 | 399 |
| -4 | 7 | 9 | 0 | 1 | -3 | -13 | 3 | 15 | 16 | -3 | -9 | 7 | 35 | 42 | -3 | -5 | 9 | 166 | 173 |
| -4 | 8 | 0 | 81 | 83 | -3 | -13 | 4 | -3 | 4 | -3 | -9 | 8 | 34 | 31 | -3 | -5 | 10 | 415 | 420 |
| -4 | 8 | 1 | -2 | 4 | -3 | -13 | 5 | 4 | 8 | -3 | -9 | 9 | -11 | 2 | -3 | -5 | 11 | 7 | 12 |
| -4 | 8 | 2 | 21 | 18 | -3 | -13 | 6 | 11 | 8 | -3 | -9 | 10 | 37 | 33 | -3 | -5 | 12 | 98 | 88 |
| -4 | 8 | 3 | 0 | 1 | -3 | -13 | 7 | 5 | 3 | -3 | -9 | 11 | -2 | 2 | -3 | -5 | 13 | 21 | 22 |
| -4 | 8 | 4 | -2 | 0 | -3 | -13 | 8 | -1 | 1 | -3 | -9 | 12 | -14 | 0 | -3 | -5 | 14 | 8 | 8 |
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| -4 | 8 | 7 | 8 | 6 | -3 | -13 | 11 | 12 | 10 | -3 | -9 | 15 | 6 | 7 | -3 | -4 | 1 | 1 | 1 |
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| -4 | 9 | 0 | -3 | 0 | -3 | -13 | 13 | 0 | 1 | -3 | -8 | 1 | 35 | 27 | -3 | -4 | 3 | 54 | 59 |
| -4 | 9 | 1 | 9 | 8 | -3 | -13 | 14 | 1 | 3 | -3 | -8 | 2 | 8 | 3 | -3 | -4 | 4 | 172 | 158 |
| -4 | 9 | 2 | 29 | 28 | -3 | -13 | 15 | 6 | 2 | -3 | -8 | 3 | 785 | 820 | -3 | -4 | 5 | 23 | 25 |
| -4 | 9 | 3 | 6 | 10 | -3 | -12 | 1 | 30 | 30 | -3 | -8 | 4 | 0 | 2 | -3 | -4 | 6 | -8 | 0 |
| -4 | 9 | 4 | -9 | 0 | -3 | -12 | 2 | 29 | 27 | -3 | -8 | 5 | 324 | 327 | -3 | -4 | 7 | 37 | 42 |
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Reflections flagged with an asterisk were considered unobserved.

F_{obs} & F_{calc} for C₇H₇NO₂

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| H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc |
|----|---|----|-----|------|----|----|----|-----|------|----|-----|----|-----|------|----|-----|----|-----|------|----|----|----|------|------|
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| -3 | 1 | 2 | 93 | 98 | -3 | 5 | 11 | 3 | 4 | -3 | 13 | 2 | 3 | 0 | -2 | -12 | 3 | 16 | 9 | -2 | -8 | 2 | 45 | 50 |
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| -3 | 1 | 6 | -13 | 1 | -3 | 6 | 2 | 154 | 154 | -2 | -17 | 7 | 5 | 2 | -2 | -12 | 7 | 37 | 33 | -2 | -8 | 6 | 28 | 31 |
| -3 | 1 | 7 | -3 | 2 | -3 | 6 | 3 | 201 | 199 | -2 | -17 | 8 | -4 | 0 | -2 | -12 | 8 | 12 | 14 | -2 | -8 | 7 | 164 | 162 |
| -3 | 1 | 8 | 69 | 78 | -3 | 6 | 4 | 0 | 0 | -2 | -17 | 9 | 1 | 0 | -2 | -12 | 9 | 0 | 2 | -2 | -8 | 8 | 41 | 39 |
| -3 | 1 | 9 | 6 | 5 | -3 | 6 | 5 | -9 | 0 | -2 | -17 | 10 | 8 | 5 | -2 | -12 | 10 | 10 | 6 | -2 | -8 | 9 | 25 | 18 |
| -3 | 1 | 10 | 10 | 9 | -3 | 6 | 6 | 10 | 8 | -2 | -16 | 3 | 6 | 5 | -2 | -12 | 11 | 1 | 4 | -2 | -8 | 10 | 0 | 2 |
| -3 | 1 | 11 | 0 | 0 | -3 | 6 | 7 | 4 | 3 | -2 | -16 | 4 | 1 | 1 | -2 | -12 | 12 | 3 | 8 | -2 | -8 | 11 | 23 | 28 |
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| -3 | 4 | 2 | 0 | 13 | -3 | 10 | 0 | 66 | 65 | -2 | -14 | 12 | 0 | 0 | -2 | -10 | 14 | -1 | 2 | -2 | -6 | 12 | 31 | 35 |
| -3 | 4 | 3 | 51 | 61 | -3 | 10 | 1 | 19 | 15 | -2 | -14 | 13 | 10 | 12 | -2 | -10 | 15 | 0 | 0 | -2 | -6 | 13 | 0 | 1 |
| -3 | 4 | 4 | -3 | 3 | -3 | 10 | 2 | 3 | 5 | -2 | -14 | 14 | 3 | 1 | -2 | -10 | 16 | -16 | 2 | -2 | -6 | 14 | -7 | 5 |
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| -3 | 5 | 1 | 39 | 35 | -3 | 11 | 4 | -6 | 1 | -2 | -13 | 9 | 0 | 1 | -2 | -9 | 9 | 111 | 118 | -2 | -5 | 7 | 496 | 510 |
| -3 | 5 | 2 | 79 | 68 | -3 | 11 | 5 | 0 | 0 | -2 | -13 | 10 | 1 | 6 | -2 | -9 | 10 | 6 | 2 | -2 | -5 | 8 | 88 | 84 |
| -3 | 5 | 3 | -13 | 5 | -3 | 11 | 6 | 6 | 7 | -2 | -13 | 11 | 10 | 9 | -2 | -9 | 11 | -5 | 0 | -2 | -5 | 9 | 1 | 6 |
| -3 | 5 | 4 | 6 | 16 | -3 | 12 | 0 | 3 | 1 | -2 | -13 | 12 | 0 | 1 | -2 | -9 | 12 | 10 | 13 | -2 | -5 | 10 | 194 | 192 |
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| -3 | 5 | 7 | -1 | 0 | -3 | 12 | 3 | 3 | 2 | -2 | -13 | 15 | -6 | 0 | -2 | -9 | 15 | 2 | 0 | -2 | -5 | 13 | 2 | 2 |
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Reflections flagged with an asterisk were considered unobserved.

Fobs & Fcalc for C₁₁H₁₂N₂O₄

| H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc |
|----|----|----|------|------|----|----|----|------|------|----|---|----|------|------|----|----|----|-----|------|
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| -2 | -5 | 16 | -4 | 4 | -2 | -1 | 16 | 1 | 0 | -2 | 4 | 4 | 113 | 107 | -2 | 9 | 7 | 14 | 14 |
| -2 | -5 | 17 | 1 | 3 | -2 | 0 | 1 | -4 | 1 | -2 | 4 | 5 | 479 | 481 | -2 | 9 | 8 | -1 | 4 |
| -2 | -4 | 1 | 191 | 184 | -2 | 0 | 2 | 26 | 32 | -2 | 4 | 6 | 29 | 23 | -2 | 9 | 9 | 2 | 1 |
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| -2 | -4 | 3 | 418 | 383 | -2 | 0 | 4 | 283 | 318 | -2 | 4 | 8 | 47 | 53 | -2 | 10 | 1 | 1 | 2 |
| -2 | -4 | 4 | 1 | 0 | -2 | 0 | 5 | 1 | 1 | -2 | 4 | 9 | -14 | 2 | -2 | 10 | 2 | 74 | 67 |
| -2 | -4 | 5 | 920 | 933 | -2 | 0 | 6 | 55 | 54 | -2 | 4 | 10 | 3 | 4 | -2 | 10 | 3 | 6 | 9 |
| -2 | -4 | 6 | 2971 | 2696 | -2 | 0 | 7 | 114 | 105 | -2 | 4 | 11 | 11 | 15 | -2 | 10 | 4 | 60 | 60 |
| -2 | -4 | 7 | 149 | 164 | -2 | 0 | 8 | 29 | 26 | -2 | 4 | 12 | 20 | 19 | -2 | 10 | 5 | 24 | 26 |
| -2 | -4 | 8 | 1234 | 1212 | -2 | 0 | 9 | 5 | 5 | -2 | 4 | 13 | -1 | 2 | -2 | 10 | 6 | 11 | 13 |
| -2 | -4 | 9 | 40 | 48 | -2 | 0 | 10 | 11 | 11 | -2 | 5 | 0 | 250 | 259 | -2 | 10 | 7 | 8 | 8 |
| -2 | -4 | 10 | -11 | 6 | -2 | 0 | 11 | 8 | 7 | -2 | 5 | 1 | 58 | 60 | -2 | 10 | 8 | 0 | 1 |
| -2 | -4 | 11 | 283 | 279 | -2 | 0 | 12 | 4 | 6 | -2 | 5 | 2 | 178 | 167 | -2 | 11 | 0 | 2 | 6 |
| -2 | -4 | 12 | 3 | 12 | -2 | 0 | 13 | 63 | 61 | -2 | 5 | 3 | -2 | 5 | -2 | 11 | 1 | -7 | 1 |
| -2 | -4 | 13 | 6 | 4 | -2 | 0 | 14 | 38 | 29 | -2 | 5 | 4 | 31 | 20 | -2 | 11 | 2 | 0 | 7 |
| -2 | -4 | 14 | 44 | 39 | -2 | 0 | 15 | -4 | 2 | -2 | 5 | 5 | 34 | 37 | -2 | 11 | 3 | 4 | 11 |
| -2 | -4 | 15 | 0 | 3 | -2 | 1 | 0 | 69 | 72 | -2 | 5 | 6 | 22 | 21 | -2 | 11 | 4 | 3 | 14 |
| -2 | -4 | 16 | 0 | 0 | -2 | 1 | 1 | 387 | 406 | -2 | 5 | 7 | 4 | 4 | -2 | 11 | 5 | 0 | 0 |
| -2 | -4 | 17 | -5 | 3 | -2 | 1 | 2 | 1500 | 1495 | -2 | 5 | 8 | -1 | 0 | -2 | 11 | 6 | 0 | 0 |
| -2 | -3 | 1 | 0 | 0 | -2 | 1 | 3 | 126 | 129 | -2 | 5 | 9 | 2 | 1 | -2 | 11 | 7 | 2 | 4 |
| -2 | -3 | 2 | 483 | 500 | -2 | 1 | 4 | 4 | 7 | -2 | 5 | 10 | 44 | 34 | -2 | 12 | 0 | 9 | 4 |
| -2 | -3 | 3 | 313 | 285 | -2 | 1 | 5 | 85 | 95 | -2 | 5 | 11 | 6 | 5 | -2 | 12 | 1 | -2 | 2 |
| -2 | -3 | 4 | 0 | 5 | -2 | 1 | 6 | 181 | 178 | -2 | 5 | 12 | -2 | 1 | -2 | 12 | 2 | -1 | 4 |
| -2 | -3 | 5 | 897 | 758 | -2 | 1 | 7 | 2 | 6 | -2 | 6 | 0 | 21 | 24 | -2 | 12 | 3 | 2 | 2 |
| -2 | -3 | 6 | 896 | 857 | -2 | 1 | 8 | 1 | 0 | -2 | 6 | 1 | 236 | 236 | -2 | 12 | 4 | 2 | 3 |
| -2 | -3 | 7 | 806 | 783 | -2 | 1 | 9 | 3 | 1 | -2 | 6 | 2 | -6 | 1 | -2 | 12 | 5 | -5 | 0 |
| -2 | -3 | 8 | 583 | 537 | -2 | 1 | 10 | 0 | 2 | -2 | 6 | 3 | 28 | 32 | -2 | 13 | 0 | -2 | 1 |
| -2 | -3 | 9 | 40 | 42 | -2 | 1 | 11 | -1 | 7 | -2 | 6 | 4 | -24* | 2 | -2 | 13 | 1 | 3 | 0 |
| -2 | -3 | 10 | 573 | 570 | -2 | 1 | 12 | 10 | 5 | -2 | 6 | 5 | 15 | 13 | -2 | 13 | 2 | 4 | 3 |
| -2 | -3 | 11 | 1 | 6 | -2 | 1 | 13 | 16 | 8 | -2 | 6 | 6 | -2 | 1 | -2 | 13 | 3 | -7 | 0 |
| -2 | -3 | 12 | -2 | 13 | -2 | 1 | 14 | 4 | 2 | -2 | 6 | 7 | 9 | 11 | -2 | 13 | 4 | 4 | 1 |
| -2 | -3 | 13 | 48 | 35 | -2 | 1 | 15 | 12 | 14 | -2 | 6 | 8 | 10 | 4 | -2 | 14 | 0 | 1 | 5 |
| -2 | -3 | 14 | 1 | 8 | -2 | 2 | 0 | 358 | 430 | -2 | 6 | 9 | 35 | 29 | -2 | 14 | 1 | -4 | 0 |
| -2 | -3 | 15 | 4 | 5 | -2 | 2 | 1 | 86 | 95 | -2 | 6 | 10 | -1 | 2 | -2 | 14 | 2 | 0 | 0 |
| -2 | -3 | 16 | 0 | 3 | -2 | 2 | 2 | 0 | 0 | -2 | 6 | 11 | 3 | 0 | -2 | 15 | 0 | 0 | 1 |
| -2 | -2 | 1 | 1088 | 1082 | -2 | 2 | 3 | 210 | 224 | -2 | 6 | 12 | -3 | 0 | -2 | 15 | 1 | 2 | 2 |
| -2 | -2 | 2 | 368 | 371 | -2 | 2 | 4 | 33 | 34 | -2 | 7 | 0 | 25 | 21 | -1 | 17 | 4 | -1 | 3 |
| -2 | -2 | 3 | 496 | 508 | -2 | 2 | 5 | 918 | 939 | -2 | 7 | 1 | 451 | 477 | -1 | 17 | 5 | 4 | 3 |
| -2 | -2 | 4 | 12 | 13 | -2 | 2 | 6 | 0 | 4 | -2 | 7 | 2 | -1 | 0 | -1 | 17 | 6 | -1 | 2 |
| -2 | -2 | 5 | 935 | 890 | -2 | 2 | 7 | 44 | 37 | -2 | 7 | 3 | 4 | 11 | -1 | 17 | 7 | 4 | 5 |
| -2 | -2 | 6 | 0 | 3 | -2 | 2 | 8 | 7 | 6 | -2 | 7 | 4 | 1 | 3 | -1 | 17 | 8 | -4 | 0 |
| -2 | -2 | 7 | 96 | 88 | -2 | 2 | 9 | 14 | 16 | -2 | 7 | 5 | 44 | 45 | -1 | 17 | 9 | -1 | 0 |
| -2 | -2 | 8 | 50 | 45 | -2 | 2 | 10 | -3 | 0 | -2 | 7 | 6 | 7 | 0 | -1 | 17 | 10 | 1 | 1 |
| -2 | -2 | 9 | 59 | 56 | -2 | 2 | 11 | 12 | 15 | -2 | 7 | 7 | 2 | 0 | -1 | 17 | 11 | 9 | 5 |
| -2 | -2 | 10 | 64 | 78 | -2 | 2 | 12 | 56 | 60 | -2 | 7 | 8 | 2 | 3 | -1 | 17 | 12 | 0 | 1 |
| -2 | -2 | 11 | 6 | 7 | -2 | 2 | 13 | 86 | 88 | -2 | 7 | 9 | 5 | 3 | -1 | 16 | 1 | -4 | 4 |
| -2 | -2 | 12 | 1 | 2 | -2 | 2 | 14 | 15 | 17 | -2 | 7 | 10 | 0 | 1 | -1 | 16 | 2 | 1 | 0 |
| -2 | -2 | 13 | 4 | 0 | -2 | 3 | 0 | -6 | 1 | -2 | 7 | 11 | 3 | 0 | -1 | 16 | 3 | 31 | 30 |
| -2 | -2 | 14 | 13 | 10 | -2 | 3 | 1 | 36 | 36 | -2 | 8 | 0 | 44 | 39 | -1 | 16 | 4 | -5 | 3 |
| -2 | -2 | 15 | -1 | 3 | -2 | 3 | 2 | 388 | 432 | -2 | 8 | 1 | 0 | 1 | -1 | 16 | 5 | 1 | 1 |
| -2 | -2 | 16 | 3 | 0 | -2 | 3 | 3 | 637 | 687 | -2 | 8 | 2 | 135 | 136 | -1 | 16 | 6 | 11 | 9 |
| -2 | -1 | 1 | 21 | 19 | -2 | 3 | 4 | 57 | 52 | -2 | 8 | 3 | 3 | 0 | -1 | 16 | 7 | 6 | 8 |
| -2 | -1 | 2 | 252 | 292 | -2 | 3 | 5 | 175 | 166 | -2 | 8 | 4 | 28 | 31 | -1 | 16 | 8 | -7 | 8 |
| -2 | -1 | 3 | 55 | 50 | -2 | 3 | 6 | -3 | 6 | -2 | 8 | 5 | -6 | 4 | -1 | 16 | 9 | -1 | 2 |
| -2 | -1 | 4 | 284 | 282 | -2 | 3 | 7 | 3 | 20 | -2 | 8 | 6 | 3 | 3 | -1 | 16 | 10 | -2 | 0 |
| -2 | -1 | 5 | 8 | 6 | -2 | 3 | 8 | 1 | 3 | -2 | 8 | 7 | 3 | 1 | -1 | 16 | 11 | 2 | 1 |
| -2 | -1 | 6 | 183 | 168 | -2 | 3 | 9 | -12 | 4 | -2 | 8 | 8 | -5 | 2 | -1 | 16 | 12 | 0 | 4 |
| -2 | -1 | 7 | 79 | 75 | -2 | 3 | 10 | 0 | 0 | -2 | 8 | 9 | 6 | 4 | -1 | 16 | 13 | -2 | 10 |
| -2 | -1 | 8 | 54 | 52 | -2 | 3 | 11 | 0 | 19 | -2 | 8 | 10 | 1 | 0 | -1 | 16 | 14 | 12 | 12 |
| -2 | -1 | 9 | 104 | 106 | -2 | 3 | 12 | -4 | 0 | -2 | 9 | 0 | 39 | 32 | -1 | 15 | 1 | -2 | 1 |
| -2 | -1 | 10 | -4 | 0 | -2 | 3 | 13 | 2 | 1 | -2 | 9 | 1 | 17 | 15 | -1 | 15 | 2 | 2 | 3 |
| -2 | -1 | 11 | 4 | 0 | -2 | 3 | 14 | 13 | 12 | -2 | 9 | 2 | 5 | 16 | -1 | 15 | 3 | -4 | 0 |
| -2 | -1 | 12 | -7 | 1 | -2 | 4 | 0 | 900 | 934 | -2 | 9 | 3 | -2 | 15 | -1 | 15 | 4 | -1 | 0 |
| -2 | -1 | 13 | 0 | 5 | -2 | 4 | 1 | 111 | 116 | -2 | 9 | 4 | 11 | 13 | -1 | 15 | 5 | 12 | 17 |
| -2 | -1 | 14 | 34 | 26 | -2 | 4 | 2 | 1 | 2 | -2 | 9 | 5 | 0 | 0 | -1 | 15 | 6 | 17 | 15 |

Reflections flagged with an asterisk were considered unobserved.

Fobs & Fcalc for C₂H₂N₂

| H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc |
|-------|----|---|-----|------|----|----|----|------|------|----|----|----|-------|-------|----|---|----|------|------|
| -1-11 | 8 | | 1 | 5 | -1 | -7 | 4 | 115 | 111 | -1 | -3 | 2 | 1262 | 1291 | -1 | 1 | 2 | 247 | 253 |
| -1-11 | 9 | | 3 | 4 | -1 | -7 | 5 | 1047 | 955 | -1 | -3 | 3 | 1459 | 1378 | -1 | 1 | 3 | 119 | 104 |
| -1-11 | 10 | | 17 | 14 | -1 | -7 | 6 | 126 | 120 | -1 | -3 | 4 | 6484 | 5249 | -1 | 1 | 4 | 297 | 285 |
| -1-11 | 11 | | 30 | 38 | -1 | -7 | 7 | 1 | 3 | -1 | -3 | 5 | 1387 | 1359 | -1 | 1 | 5 | 8 | 12 |
| -1-11 | 12 | | 0 | 0 | -1 | -7 | 8 | 137 | 122 | -1 | -3 | 6 | 237 | 242 | -1 | 1 | 6 | 561 | 516 |
| -1-11 | 13 | | 17 | 17 | -1 | -7 | 9 | 281 | 280 | -1 | -3 | 7 | 68 | 56 | -1 | 1 | 7 | 0 | 6 |
| -1-11 | 14 | | 0 | 1 | -1 | -7 | 10 | -9 | 1 | -1 | -3 | 8 | 79 | 85 | -1 | 1 | 8 | 10 | 13 |
| -1-11 | 15 | | 13 | 14 | -1 | -7 | 11 | 51 | 69 | -1 | -3 | 9 | 32 | 32 | -1 | 1 | 9 | 9 | 7 |
| -1-11 | 16 | | -1 | 1 | -1 | -7 | 12 | 68 | 64 | -1 | -3 | 10 | 35 | 35 | -1 | 1 | 10 | 0 | 0 |
| -1-11 | 17 | | 7 | 5 | -1 | -7 | 13 | 103 | 97 | -1 | -3 | 11 | 12 | 9 | -1 | 1 | 11 | 60 | 72 |
| -1-10 | 1 | | 0 | 0 | -1 | -7 | 14 | 50 | 41 | -1 | -3 | 12 | 101 | 97 | -1 | 1 | 12 | 11 | 13 |
| -1-10 | 2 | | 23 | 26 | -1 | -7 | 15 | -2 | 2 | -1 | -3 | 13 | 0 | 2 | -1 | 1 | 13 | -2 | 1 |
| -1-10 | 3 | | 235 | 230 | -1 | -7 | 16 | 0 | 1 | -1 | -3 | 14 | 45 | 39 | -1 | 1 | 14 | 3 | 2 |
| -1-10 | 4 | | 64 | 55 | -1 | -7 | 17 | -4 | 1 | -1 | -3 | 15 | 4 | 4 | -1 | 1 | 15 | 8 | 10 |
| -1-10 | 5 | | 41 | 48 | -1 | -6 | 1 | 72 | 71 | -1 | -3 | 16 | 3 | 0 | -1 | 2 | 0 | 2331 | 2777 |
| -1-10 | 6 | | 67 | 79 | -1 | -6 | 2 | 86 | 92 | -1 | -3 | 17 | -2 | 0 | -1 | 2 | 1 | 3527 | 3918 |
| -1-10 | 7 | | 15 | 22 | -1 | -6 | 3 | 161 | 142 | -1 | -2 | 1 | 5605 | 5223 | -1 | 2 | 2 | 1699 | 1757 |
| -1-10 | 8 | | 16 | 13 | -1 | -6 | 4 | 171 | 153 | -1 | -2 | 2 | 7683 | 6753 | -1 | 2 | 3 | 372 | 414 |
| -1-10 | 9 | | 43 | 35 | -1 | -6 | 5 | 99 | 87 | -1 | -2 | 3 | 18639 | 14755 | -1 | 2 | 4 | 48 | 45 |
| -1-10 | 10 | | 0 | 1 | -1 | -6 | 6 | 1348 | 1177 | -1 | -2 | 4 | 1939 | 1867 | -1 | 2 | 5 | 1332 | 1299 |
| -1-10 | 11 | | 66 | 65 | -1 | -6 | 7 | 184 | 185 | -1 | -2 | 5 | 234 | 231 | -1 | 2 | 6 | 187 | 207 |
| -1-10 | 12 | | 10 | 14 | -1 | -6 | 8 | 46 | 49 | -1 | -2 | 6 | 222 | 215 | -1 | 2 | 7 | 2 | 7 |
| -1-10 | 13 | | 112 | 115 | -1 | -6 | 9 | 53 | 53 | -1 | -2 | 7 | 979 | 915 | -1 | 2 | 8 | 12 | 10 |
| -1-10 | 14 | | 0 | 1 | -1 | -6 | 10 | 125 | 142 | -1 | -2 | 8 | 102 | 85 | -1 | 2 | 9 | 1 | 0 |
| -1-10 | 15 | | 30 | 26 | -1 | -6 | 11 | 280 | 294 | -1 | -2 | 9 | 18 | 18 | -1 | 2 | 10 | 142 | 155 |
| -1-10 | 16 | | -3 | 3 | -1 | -6 | 12 | 1 | 0 | -1 | -2 | 10 | 37 | 34 | -1 | 2 | 11 | 12 | 16 |
| -1-10 | 17 | | 9 | 9 | -1 | -6 | 13 | 60 | 59 | -1 | -2 | 11 | 0 | 6 | -1 | 2 | 12 | 4 | 2 |
| -1-9 | 1 | | 75 | 73 | -1 | -6 | 14 | 3 | 3 | -1 | -2 | 12 | 150 | 130 | -1 | 2 | 13 | -3 | 0 |
| -1-9 | 2 | | 0 | 2 | -1 | -6 | 15 | 4 | 0 | -1 | -2 | 13 | -1 | 13 | -1 | 2 | 14 | 0 | 1 |
| -1-9 | 3 | | 33 | 31 | -1 | -6 | 16 | 0 | 7 | -1 | -2 | 14 | 4 | 7 | -1 | 2 | 15 | 1 | 0 |
| -1-9 | 4 | | -2 | 2 | -1 | -6 | 17 | -3 | 0 | -1 | -2 | 15 | 2 | 3 | -1 | 3 | 0 | 1440 | 1767 |
| -1-9 | 5 | | 475 | 458 | -1 | -5 | 1 | 214 | 214 | -1 | -2 | 16 | 1 | 2 | -1 | 3 | 1 | 84 | 86 |
| -1-9 | 6 | | 10 | 13 | -1 | -5 | 2 | 10 | 8 | -1 | -1 | 1 | 651 | 642 | -1 | 3 | 2 | 251 | 263 |
| -1-9 | 7 | | 4 | 1 | -1 | -5 | 3 | 291 | 281 | -1 | -1 | 2 | 3108 | 2924 | -1 | 3 | 3 | 170 | 174 |
| -1-9 | 8 | | 4 | 8 | -1 | -5 | 4 | 7 | 9 | -1 | -1 | 3 | 6321 | 5187 | -1 | 3 | 4 | 454 | 466 |
| -1-9 | 9 | | -2 | 0 | -1 | -5 | 5 | 4644 | 4054 | -1 | -1 | 4 | 2816 | 2582 | -1 | 3 | 5 | 204 | 204 |
| -1-9 | 10 | | 43 | 40 | -1 | -5 | 6 | 53 | 53 | -1 | -1 | 5 | 1683 | 1586 | -1 | 3 | 6 | 71 | 70 |
| -1-9 | 11 | | 16 | 18 | -1 | -5 | 7 | 32 | 24 | -1 | -1 | 6 | 325 | 299 | -1 | 3 | 7 | -1 | 2 |
| -1-9 | 12 | | 0 | 1 | -1 | -5 | 8 | 611 | 609 | -1 | -1 | 7 | 79 | 80 | -1 | 3 | 8 | 42 | 39 |
| -1-9 | 13 | | 60 | 68 | -1 | -5 | 9 | 173 | 189 | -1 | -1 | 8 | 154 | 150 | -1 | 3 | 9 | 114 | 115 |
| -1-9 | 14 | | 8 | 3 | -1 | -5 | 10 | 149 | 140 | -1 | -1 | 9 | 77 | 89 | -1 | 3 | 10 | 50 | 51 |
| -1-9 | 15 | | -5 | 0 | -1 | -5 | 11 | 0 | 10 | -1 | -1 | 10 | 1 | 1 | -1 | 3 | 11 | 6 | 3 |
| -1-9 | 16 | | -1 | 4 | -1 | -5 | 12 | 33 | 42 | -1 | -1 | 11 | 3 | 7 | -1 | 3 | 12 | 35 | 31 |
| -1-9 | 17 | | 0 | 1 | -1 | -5 | 13 | 5 | 5 | -1 | -1 | 12 | 120 | 110 | -1 | 3 | 13 | 3 | 4 |
| -1-9 | 18 | | 6 | 3 | -1 | -5 | 14 | 16 | 20 | -1 | -1 | 13 | -5 | 1 | -1 | 3 | 14 | 17 | 11 |
| -1-8 | 1 | | 24 | 19 | -1 | -5 | 15 | -1 | 1 | -1 | -1 | 14 | -6 | 4 | -1 | 4 | 0 | 667 | 759 |
| -1-8 | 2 | | 3 | 5 | -1 | -5 | 16 | 1 | 0 | -1 | -1 | 15 | 0 | 1 | -1 | 4 | 1 | 718 | 788 |
| -1-8 | 3 | | 0 | 2 | -1 | -5 | 17 | 5 | 1 | -1 | -1 | 16 | 0 | 0 | -1 | 4 | 2 | 449 | 437 |
| -1-8 | 4 | | 147 | 152 | -1 | -4 | 1 | 11 | 15 | -1 | 0 | 1 | 16 | 27 | -1 | 4 | 3 | 56 | 72 |
| -1-8 | 5 | | 46 | 46 | -1 | -4 | 2 | 646 | 661 | -1 | 0 | 2 | 2395 | 2240 | -1 | 4 | 4 | 226 | 267 |
| -1-8 | 6 | | 17 | 21 | -1 | -4 | 3 | 598 | 593 | -1 | 0 | 3 | 2225 | 2255 | -1 | 4 | 5 | 8 | 1 |
| -1-8 | 7 | | -3 | 2 | -1 | -4 | 4 | 1572 | 1445 | -1 | 0 | 4 | 715 | 737 | -1 | 4 | 6 | 3 | 4 |
| -1-8 | 8 | | 168 | 187 | -1 | -4 | 5 | 43 | 53 | -1 | 0 | 5 | 95 | 75 | -1 | 4 | 7 | 7 | 5 |
| -1-8 | 9 | | 2 | 1 | -1 | -4 | 6 | 158 | 157 | -1 | 0 | 6 | 170 | 172 | -1 | 4 | 8 | 56 | 62 |
| -1-8 | 10 | | 9 | 8 | -1 | -4 | 7 | 166 | 161 | -1 | 0 | 7 | 24 | 24 | -1 | 4 | 9 | 139 | 136 |
| -1-8 | 11 | | 2 | 3 | -1 | -4 | 8 | 20 | 22 | -1 | 0 | 8 | 47 | 66 | -1 | 4 | 10 | 183 | 187 |
| -1-8 | 12 | | 0 | 10 | -1 | -4 | 9 | 128 | 138 | -1 | 0 | 9 | -2 | 1 | -1 | 4 | 11 | 75 | 79 |
| -1-8 | 13 | | 21 | 21 | -1 | -4 | 10 | 102 | 80 | -1 | 0 | 10 | 0 | 0 | -1 | 4 | 12 | 10 | 11 |
| -1-8 | 14 | | 46 | 43 | -1 | -4 | 11 | 55 | 55 | -1 | 0 | 11 | -1 | 6 | -1 | 4 | 13 | 2 | 3 |
| -1-8 | 15 | | -4 | 2 | -1 | -4 | 12 | 173 | 161 | -1 | 0 | 12 | 15 | 21 | -1 | 5 | 0 | 1327 | 1326 |
| -1-8 | 16 | | 11 | 8 | -1 | -4 | 13 | 2 | 0 | -1 | 0 | 13 | 81 | 74 | -1 | 5 | 1 | 61 | 55 |
| -1-8 | 17 | | -1 | 0 | -1 | -4 | 14 | -5 | 1 | -1 | 0 | 14 | 7 | 8 | -1 | 5 | 2 | 61 | 66 |
| -1-8 | 18 | | 0 | 0 | -1 | -4 | 15 | 1 | 0 | -1 | 0 | 15 | 2 | 0 | -1 | 5 | 3 | 506 | 498 |
| -1-7 | 1 | | 263 | 242 | -1 | -4 | 16 | 5 | 3 | -1 | 0 | 16 | 16 | 15 | -1 | 5 | 4 | 55 | 56 |
| -1-7 | 2 | | 22 | 24 | -1 | -4 | 17 | -8 | 0 | -1 | 1 | 0 | 1125 | 1316 | -1 | 5 | 5 | -5 | 5 |
| -1-7 | 3 | | 31 | 29 | -1 | -3 | 1 | 2337 | 2356 | -1 | 1 | 1 | 9865 | 10526 | -1 | 5 | 6 | 3 | 5 |

Reflections flagged with an asterisk were considered unobserved.

F_{obs} & F_{calc} for C₂₁H₂₇NO₆

| H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc |
|----|-----|----|-----|------|------|----|----|-----|------|----|----|-----|-----|------|----|------|------|------|------|----|-----|-------|-------|------|
| -1 | 11 | 4 | 4 | 1 | 0-14 | 5 | 33 | 26 | 0-10 | 4 | -8 | 5 | 0 | -7 | 17 | -4 | 0 | 0 | -3 | 14 | 3 | 1 | | |
| -1 | 11 | 5 | -7 | 2 | 0-14 | 6 | 58 | 44 | 0-10 | 5 | 25 | 33 | 0 | -7 | 18 | -3 | 2 | 0 | -3 | 15 | -1 | 0 | | |
| -1 | 11 | 6 | 2 | 0 | 0-14 | 7 | 7 | 6 | 0-10 | 6 | 10 | 13 | 0 | -6 | 1 | 77 | 72 | 0 | -3 | 16 | 32 | 37 | | |
| -1 | 11 | 7 | -2 | 3 | 0-14 | 8 | -1 | 0 | 0-10 | 7 | 0 | 5 | 0 | -6 | 2 | 119 | 120 | 0 | -3 | 17 | -4 | 1 | | |
| -1 | 12 | 0 | 42 | 47 | 0-14 | 9 | 66 | 69 | 0-10 | 8 | 53 | 53 | 0 | -6 | 3 | 115 | 125 | 0 | -2 | 1 | 149 | 157 | | |
| -1 | 12 | 1 | 28 | 27 | 0-14 | 10 | 59 | 53 | 0-10 | 9 | 32 | 34 | 0 | -6 | 4 | 1143 | 1098 | 0 | -2 | 2 | 4 | 7 | | |
| -1 | 12 | 2 | 4 | 2 | 0-14 | 11 | -5 | 2 | 0-10 | 10 | 22 | 26 | 0 | -6 | 5 | 349 | 338 | 0 | -2 | 3 | 985 | 1009 | | |
| -1 | 12 | 3 | 12 | 8 | 0-14 | 12 | 16 | 16 | 0-10 | 11 | 6 | 8 | 0 | -6 | 6 | 126 | 129 | 0 | -2 | 4 | 118 | 121 | | |
| -1 | 12 | 4 | -3 | 0 | 0-14 | 13 | 0 | 4 | 0-10 | 12 | 21 | 17 | 0 | -6 | 7 | 39 | 86 | 0 | -2 | 5 | 392 | 397 | | |
| -1 | 12 | 5 | 0 | 2 | 0-14 | 14 | 2 | 2 | 0-10 | 13 | 3 | 24 | 0 | -6 | 8 | 198 | 205 | 0 | -2 | 6 | 53 | 45 | | |
| -1 | 12 | 6 | -1 | 0 | 0-14 | 15 | 0 | 1 | 0-10 | 14 | 95 | 89 | 0 | -6 | 9 | 66 | 72 | 0 | -2 | 7 | 24 | 23 | | |
| -1 | 13 | 0 | 3 | 8 | 0-14 | 16 | 2 | 1 | 0-10 | 15 | 1 | 3 | 0 | -6 | 10 | 54 | 48 | 0 | -2 | 8 | 420 | 443 | | |
| -1 | 13 | 1 | -3 | 1 | 0-13 | 1 | 3 | 0 | 0-10 | 16 | 2 | 1 | 0 | -6 | 11 | -2 | 3 | 0 | -2 | 9 | 764 | 684 | | |
| -1 | 13 | 2 | 11 | 13 | 0-13 | 2 | -8 | 4 | 0-10 | 17 | 22 | 19 | 0 | -6 | 12 | 61 | 65 | 0 | -2 | 10 | 99 | 99 | | |
| -1 | 13 | 3 | 13 | 10 | 0-13 | 3 | 44 | 46 | 0 | -9 | 1 | 18 | 19 | 0 | -6 | 13 | 13 | 21 | 0 | -2 | 11 | 199 | 198 | |
| -1 | 13 | 4 | -2 | 0 | 0-13 | 4 | 54 | 63 | 0 | -9 | 2 | 105 | 112 | 0 | -6 | 14 | -2 | 3 | 0 | -2 | 12 | 203 | 178 | |
| -1 | 14 | 0 | 11 | 9 | 0-13 | 5 | 14 | 3 | 0 | -9 | 3 | 114 | 102 | 0 | -6 | 15 | 0 | 1 | 0 | -2 | 13 | 6 | 12 | |
| -1 | 14 | 1 | 3 | 0 | 0-13 | 6 | 36 | 32 | 0 | -9 | 4 | -1 | 0 | 0 | -6 | 16 | 13 | 14 | 0 | -2 | 14 | 2 | 9 | |
| -1 | 14 | 2 | 0 | 1 | 0-13 | 7 | -1 | 2 | 0 | -9 | 5 | 4 | 0 | 0 | -6 | 17 | 0 | 0 | 0 | -2 | 15 | -1 | 1 | |
| -1 | 14 | 3 | 0 | 0 | 0-13 | 8 | 28 | 23 | 0 | -9 | 6 | 125 | 124 | 0 | -5 | 1 | 14 | 15 | 0 | -2 | 16 | 0 | 2 | |
| -1 | 15 | 0 | -6 | 1 | 0-13 | 9 | 2 | 12 | 0 | -9 | 7 | 121 | 115 | 0 | -5 | 2 | 146 | 160 | 0 | -1 | 1 | 327 | 343 | |
| -1 | 15 | 1 | 2 | 2 | 0-13 | 10 | 22 | 22 | 0 | -9 | 8 | 38 | 36 | 0 | -5 | 3 | 512 | 517 | 0 | -1 | 2 | 752 | 755 | |
| 0 | -17 | 3 | -1 | 0 | 0-13 | 11 | 18 | 29 | 0 | -9 | 9 | 131 | 137 | 0 | -5 | 4 | 137 | 139 | 0 | -1 | 3 | 932 | 984 | |
| 0 | -17 | 4 | 2 | 1 | 0-13 | 12 | 49 | 51 | 0 | -9 | 10 | 0 | 0 | 0 | -5 | 5 | 1096 | 1075 | 0 | -1 | 4 | 32 | 7 | |
| 0 | -17 | 5 | 2 | 3 | 0-13 | 13 | 3 | 2 | 0 | -9 | 11 | 258 | 249 | 0 | -5 | 6 | 1048 | 1038 | 0 | -1 | 5 | 41 | 36 | |
| 0 | -17 | 6 | 0 | 1 | 0-13 | 14 | 4 | 0 | 0 | -9 | 12 | 35 | 38 | 0 | -5 | 7 | 0 | 5 | 0 | -1 | 6 | 315 | 281 | |
| 0 | -17 | 7 | 15 | 11 | 0-13 | 15 | -2 | 0 | 0 | -9 | 13 | 57 | 53 | 0 | -5 | 8 | -1 | 10 | 0 | -1 | 7 | 388 | 368 | |
| 0 | -17 | 8 | 3 | 0 | 0-13 | 16 | 2 | 0 | 0 | -9 | 14 | 21 | 21 | 0 | -5 | 9 | 16 | 18 | 0 | -1 | 8 | 12 | 14 | |
| 0 | -17 | 9 | 8 | 8 | 0-13 | 17 | 10 | 6 | 0 | -9 | 15 | 10 | 9 | 0 | -5 | 10 | -3 | 1 | 0 | -1 | 9 | 69 | 61 | |
| 0 | -17 | 10 | 3 | 0 | 0-12 | 1 | 4 | 4 | 0 | -9 | 16 | 1 | 1 | 0 | -5 | 11 | 67 | 59 | 0 | -1 | 10 | 194 | 193 | |
| 0 | -17 | 11 | 7 | 3 | 0-12 | 2 | 21 | 18 | 0 | -9 | 17 | 22 | 16 | 0 | -5 | 12 | 1 | 3 | 0 | -1 | 11 | 0 | 1 | |
| 0 | -17 | 12 | -1 | 1 | 0-12 | 3 | -3 | 1 | 0 | -9 | 18 | -1 | 1 | 0 | -5 | 13 | 38 | 37 | 0 | -1 | 12 | 83 | 76 | |
| 0 | -17 | 13 | 0 | 1 | 0-12 | 4 | -8 | 0 | 0 | -8 | 1 | 149 | 136 | 0 | -5 | 14 | 7 | 6 | 0 | -1 | 13 | 81 | 81 | |
| 0 | -16 | 1 | 6 | 5 | 0-12 | 5 | 40 | 42 | 0 | -8 | 2 | 123 | 118 | 0 | -5 | 15 | 22 | 19 | 0 | -1 | 14 | 18 | 17 | |
| 0 | -16 | 2 | 2 | 8 | 0-12 | 6 | 0 | 1 | 0 | -8 | 3 | 58 | 55 | 0 | -5 | 16 | 1 | 2 | 0 | -1 | 15 | 6 | 8 | |
| 0 | -16 | 3 | -4 | 0 | 0-12 | 7 | 1 | 0 | 0 | -8 | 4 | 0 | 1 | 0 | -5 | 17 | 5 | 4 | 0 | -1 | 16 | -2 | 1 | |
| 0 | -16 | 4 | 0 | 1 | 0-12 | 8 | 11 | 10 | 0 | -8 | 5 | 8 | 13 | 0 | -4 | 1 | 19 | 15 | 0 | 0 | 1 | 1319 | 1257 | |
| 0 | -16 | 5 | -7 | 0 | 0-12 | 9 | 33 | 29 | 0 | -8 | 6 | 74 | 77 | 0 | -4 | 2 | 1952 | 1936 | 0 | 0 | 2 | 690 | 749 | |
| 0 | -16 | 6 | -2 | 2 | 0-12 | 10 | 82 | 87 | 0 | -8 | 7 | 335 | 338 | 0 | -4 | 3 | 803 | 794 | 0 | 0 | 3 | 24 | 26 | |
| 0 | -16 | 7 | 5 | 3 | 0-12 | 11 | 10 | 14 | 0 | -8 | 8 | 738 | 707 | 0 | -4 | 4 | 74 | 68 | 0 | 0 | 4 | 423 | 447 | |
| 0 | -16 | 8 | 18 | 17 | 0-12 | 12 | 13 | 14 | 0 | -8 | 9 | 62 | 58 | 0 | -4 | 5 | 1231 | 1165 | 0 | 0 | 5 | 426 | 399 | |
| 0 | -16 | 9 | 3 | 1 | 0-12 | 13 | 17 | 14 | 0 | -8 | 10 | 272 | 247 | 0 | -4 | 6 | 18 | 12 | 0 | 0 | 6 | 94 | 101 | |
| 0 | -16 | 10 | 13 | 17 | 0-12 | 14 | 0 | 0 | 0 | -8 | 11 | 217 | 227 | 0 | -4 | 7 | 311 | 283 | 0 | 0 | 7 | 1 | 2 | |
| 0 | -16 | 11 | 32 | 40 | 0-12 | 15 | -6 | 1 | 0 | -8 | 12 | 20 | 28 | 0 | -4 | 8 | 170 | 170 | 0 | 0 | 8 | 0 | 3 | |
| 0 | -16 | 12 | 3 | 4 | 0-12 | 16 | 0 | 1 | 0 | -8 | 13 | 273 | 281 | 0 | -4 | 9 | 40 | 38 | 0 | 0 | 9 | 129 | 141 | |
| 0 | -16 | 13 | 1 | 4 | 0-12 | 17 | 0 | 0 | 0 | -8 | 14 | 8 | 4 | 0 | -4 | 10 | 32 | 34 | 0 | 0 | 10 | 56 | 63 | |
| 0 | -16 | 14 | 3 | 7 | 0-11 | 1 | -3 | 2 | 0 | -8 | 15 | 14 | 8 | 0 | -4 | 11 | -3 | 0 | 0 | 0 | 11 | 15 | 16 | |
| 0 | -15 | 1 | 10 | 7 | 0-11 | 2 | 4 | 3 | 0 | -8 | 16 | 13 | 19 | 0 | -4 | 12 | 1 | 9 | 0 | 0 | 12 | 11 | 12 | |
| 0 | -15 | 2 | -8 | 2 | 0-11 | 3 | 7 | 4 | 0 | -8 | 17 | 16 | 15 | 0 | -4 | 13 | 61 | 60 | 0 | 0 | 13 | 3 | 2 | |
| 0 | -15 | 3 | -1 | 0 | 0-11 | 4 | 26 | 20 | 0 | -8 | 18 | 21 | 26 | 0 | -4 | 14 | 5 | 3 | 0 | 0 | 14 | 17 | 24 | |
| 0 | -15 | 4 | 60 | 54 | 0-11 | 5 | 9 | 7 | 0 | -7 | 1 | 60 | 51 | 0 | -4 | 15 | 14 | 10 | 0 | 0 | 15 | 1 | 1 | |
| 0 | -15 | 5 | 6 | 0 | 0-11 | 6 | 0 | 2 | 0 | -7 | 2 | 916 | 884 | 0 | -4 | 16 | -1 | 2 | 0 | 0 | 16 | -1 | 2 | |
| 0 | -15 | 6 | 25 | 24 | 0-11 | 7 | 42 | 50 | 0 | -7 | 3 | 650 | 626 | 0 | -4 | 17 | 1 | 0 | 0 | 1 | 0 | 183 | 181 | |
| 0 | -15 | 7 | 6 | 4 | 0-11 | 8 | 71 | 68 | 0 | -7 | 4 | 20 | 14 | 0 | -3 | 1 | 0 | 1 | 0 | 1 | 1 | 12 | 8 | |
| 0 | -15 | 8 | 9 | 9 | 0-11 | 9 | 0 | 2 | 0 | -7 | 5 | 497 | 431 | 0 | -3 | 2 | 720 | 696 | 0 | 1 | 2 | 11493 | 11114 | |
| 0 | -15 | 9 | 2 | 2 | 0-11 | 10 | -3 | 1 | 0 | -7 | 6 | 43 | 38 | 0 | -3 | 3 | 515 | 532 | 0 | 1 | 3 | 825 | 805 | |
| 0 | -15 | 10 | -6 | 2 | 0-11 | 11 | 6 | 7 | 0 | -7 | 7 | 133 | 119 | 0 | -3 | 4 | 629 | 603 | 0 | 1 | 4 | 417 | 455 | |
| 0 | -15 | 11 | 11 | 12 | 0-11 | 12 | 31 | 35 | 0 | -7 | 8 | 22 | 24 | 0 | -3 | 5 | 113 | 120 | 0 | 1 | 5 | 1 | 0 | |
| 0 | -15 | 12 | 55 | 46 | 0-11 | 13 | -7 | 1 | 0 | -7 | 9 | 18 | 23 | 0 | -3 | 6 | 203 | 181 | 0 | 1 | 6 | 14 | 12 | |
| 0 | -15 | 13 | 11 | 12 | 0-11 | 14 | 3 | 0 | 0 | -7 | 10 | 214 | 218 | 0 | -3 | 7 | 1 | 1 | 0 | 1 | 7 | 49 | 54 | |
| 0 | -15 | 14 | -4 | 1 | 0-11 | 15 | -7 | 1 | 0 | -7 | 11 | 77 | 70 | 0 | -3 | 8 | 59 | 52 | 0 | 1 | 8 | 5 | 2 | |
| 0 | -15 | 15 | -2 | 2 | 0-11 | 16 | 8 | 8 | 0 | -7 | 12 | -3 | 1 | 0 | -3 | 9 | -9 | 2 | 0 | 1 | 9 | 23 | 18 | |
| 0 | -14 | 1 | 27 | 27 | 0-11 | 17 | 9 | 8 | 0 | -7 | 13 | -3 | 5 | 0 | -3 | 10 | 44 | 35 | 0 | 1 | 10 | 3 | 4 | |
| 0 | -14 | 2 | 51 | 53 | 0-10 | 1 | 4 | 5 | 0 | -7 | 14 | 4 | 0 | 0 | -3 | 11 | 2 | 10 | 0 | 1 | 11 | 0 | 1 | |
| 0 | -14 | 3 | -2 | 1 | 0-10 | 2 | -2 | 3 | 0 | -7 | 15 | 31 | 30 | 0 | -3 | 12 | 3 | 1 | 0 | 1 | 12 | 14 | 11 | |
| 0 | -14 | 4 | 2 | 1 | 0-10 | 3 | -6 | 0 | 0 | -7 | 16 | 9 | 7 | 0 | -3 | 13 | 10 | 10 | 0 | 1 | 13 | 0 | 3 | |

Reflections flagged with an asterisk were considered unobserved.

Fobs & Fcalc for C₁₂H₂₀NO₂

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| H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc | | | |
|---|---|----|------|------|---|----|----|-----|------|------|----|-----|-----|------|------|----|-----|-----|------|----|------|------|
| 0 | 1 | 14 | -2 | 2 | 0 | 6 | 6 | 241 | 245 | 0 | 13 | 2 | -3 | 0 | 1-13 | 2 | 7 | 4 | 1-9 | 1 | 51 | 51 |
| 0 | 1 | 15 | 0 | 0 | 0 | 6 | 7 | 521 | 517 | 0 | 13 | 3 | 4 | 1 | 1-13 | 3 | 8 | 10 | 1-9 | 2 | 158 | 153 |
| 0 | 2 | 0 | 5950 | 5475 | 0 | 6 | 8 | 44 | 57 | 0 | 13 | 4 | 0 | 0 | 1-13 | 4 | 22 | 17 | 1-9 | 3 | 12 | 5 |
| 0 | 2 | 1 | 3309 | 3282 | 0 | 6 | 9 | 42 | 36 | 0 | 13 | 5 | 2 | 5 | 1-13 | 5 | 22 | 20 | 1-9 | 4 | 0 | 0 |
| 0 | 2 | 2 | 4 | 11 | 0 | 6 | 10 | 11 | 11 | 0 | 14 | 0 | 1 | 2 | 1-13 | 6 | 13 | 14 | 1-9 | 5 | 2 | 1 |
| 0 | 2 | 3 | 66 | 61 | 0 | 6 | 11 | 2 | 3 | 0 | 14 | 1 | -2 | 0 | 1-13 | 7 | 29 | 22 | 1-9 | 6 | 166 | 171 |
| 0 | 2 | 4 | 1527 | 1472 | 0 | 6 | 12 | 10 | 8 | 0 | 14 | 2 | 0 | 0 | 1-13 | 8 | -5 | 1 | 1-9 | 7 | 359 | 320 |
| 0 | 2 | 5 | 3 | 1 | 0 | 7 | 0 | 342 | 319 | 0 | 14 | 3 | -3 | 0 | 1-13 | 9 | 15 | 15 | 1-9 | 8 | 4 | 0 |
| 0 | 2 | 6 | 24 | 25 | 0 | 7 | 1 | 5 | 10 | 0 | 15 | 0 | 1 | 2 | 1-13 | 10 | 107 | 112 | 1-9 | 9 | 22 | 22 |
| 0 | 2 | 7 | 2 | 1 | 0 | 7 | 2 | 35 | 39 | 0 | 15 | 1 | 6 | 4 | 1-13 | 11 | -1 | 3 | 1-9 | 10 | 82 | 86 |
| 0 | 2 | 8 | 79 | 91 | 0 | 7 | 3 | -1 | 1 | 1-17 | 3 | 2 | 0 | 0 | 1-13 | 12 | 0 | 1 | 1-9 | 11 | 4 | 2 |
| 0 | 2 | 9 | -6 | 0 | 0 | 7 | 4 | 53 | 58 | 1-17 | 4 | -2 | 1 | 1 | 1-13 | 13 | -2 | 0 | 1-9 | 12 | 47 | 46 |
| 0 | 2 | 10 | 27 | 24 | 0 | 7 | 5 | 31 | 32 | 1-17 | 5 | 1 | 2 | 2 | 1-13 | 14 | 0 | 4 | 1-9 | 13 | -4 | 1 |
| 0 | 2 | 11 | 5 | 3 | 0 | 7 | 6 | 51 | 55 | 1-17 | 6 | 0 | 0 | 0 | 1-13 | 15 | 0 | 5 | 1-9 | 14 | 55 | 64 |
| 0 | 2 | 12 | 1 | 2 | 0 | 7 | 7 | 132 | 121 | 1-17 | 7 | 0 | 0 | 0 | 1-13 | 16 | 4 | 3 | 1-9 | 15 | 16 | 23 |
| 0 | 2 | 13 | -7 | 0 | 0 | 7 | 8 | -3 | 0 | 1-17 | 8 | -4 | 3 | 3 | 1-12 | 1 | -4 | 2 | 1-9 | 16 | -3 | 0 |
| 0 | 2 | 14 | 1 | 2 | 0 | 7 | 9 | 26 | 30 | 1-17 | 9 | 2 | 1 | 1 | 1-12 | 2 | 5 | 4 | 1-9 | 17 | 11 | 13 |
| 0 | 3 | 0 | 1848 | 1852 | 0 | 7 | 10 | 0 | 2 | 1-17 | 10 | 2 | 4 | 4 | 1-12 | 3 | -1 | 0 | 1-8 | 1 | -1 | 2 |
| 0 | 3 | 1 | 309 | 304 | 0 | 7 | 11 | 2 | 3 | 1-17 | 11 | 0 | 0 | 0 | 1-12 | 4 | 27 | 26 | 1-8 | 2 | 266 | 259 |
| 0 | 3 | 2 | 330 | 299 | 0 | 8 | 0 | 501 | 462 | 1-17 | 12 | 3 | 4 | 4 | 1-12 | 5 | -2 | 7 | 1-8 | 3 | 15 | 15 |
| 0 | 3 | 3 | 26 | 24 | 0 | 8 | 1 | 11 | 10 | 1-16 | 1 | 1 | 2 | 2 | 1-12 | 6 | 0 | 0 | 1-8 | 4 | 1 | 11 |
| 0 | 3 | 4 | 1 | 0 | 0 | 8 | 2 | 74 | 70 | 1-16 | 2 | -1 | 3 | 3 | 1-12 | 7 | 140 | 127 | 1-8 | 5 | 83 | 85 |
| 0 | 3 | 5 | 84 | 83 | 0 | 8 | 3 | -4 | 0 | 1-16 | 3 | 0 | 1 | 1 | 1-12 | 8 | 233 | 220 | 1-8 | 6 | 142 | 129 |
| 0 | 3 | 6 | 42 | 38 | 0 | 8 | 4 | 1 | 1 | 1-16 | 4 | 16 | 14 | 3 | 1-12 | 9 | 53 | 52 | 1-8 | 7 | 296 | 290 |
| 0 | 3 | 7 | 421 | 426 | 0 | 8 | 5 | 37 | 28 | 1-16 | 5 | 4 | 3 | 3 | 1-12 | 10 | 6 | 3 | 1-8 | 8 | 34 | 37 |
| 0 | 3 | 8 | -4 | 4 | 0 | 8 | 6 | 42 | 46 | 1-16 | 6 | 0 | 0 | 0 | 1-12 | 11 | 2 | 0 | 1-8 | 9 | 1 | 1 |
| 0 | 3 | 9 | -9 | 5 | 0 | 8 | 7 | 24 | 21 | 1-16 | 7 | -5 | 0 | 0 | 1-12 | 12 | 0 | 4 | 1-8 | 10 | 3 | 2 |
| 0 | 3 | 10 | 2 | 3 | 0 | 8 | 8 | 19 | 21 | 1-16 | 8 | 1 | 0 | 0 | 1-12 | 13 | 0 | 1 | 1-8 | 11 | 139 | 134 |
| 0 | 3 | 11 | -4 | 1 | 0 | 8 | 9 | -1 | 0 | 1-16 | 9 | -2 | 0 | 0 | 1-12 | 14 | 38 | 28 | 1-8 | 12 | 5 | 6 |
| 0 | 3 | 12 | 0 | 0 | 0 | 8 | 10 | 5 | 2 | 1-16 | 10 | 0 | 0 | 0 | 1-12 | 15 | -4 | 1 | 1-8 | 13 | -3 | 5 |
| 0 | 3 | 13 | 1 | 1 | 0 | 9 | 0 | 42 | 28 | 1-16 | 11 | -1 | 1 | 1 | 1-12 | 16 | -6 | 0 | 1-8 | 14 | 35 | 29 |
| 0 | 3 | 14 | 0 | 2 | 0 | 9 | 1 | 12 | 6 | 1-16 | 12 | 0 | 0 | 0 | 1-12 | 17 | 0 | 1 | 1-8 | 15 | 37 | 39 |
| 0 | 4 | 0 | 1117 | 1160 | 0 | 9 | 2 | 2 | 1 | 1-16 | 13 | 1 | 3 | 3 | 1-11 | 1 | 83 | 76 | 1-8 | 16 | 36 | 37 |
| 0 | 4 | 1 | 110 | 121 | 0 | 9 | 3 | 10 | 8 | 1-16 | 14 | -2 | 0 | 0 | 1-11 | 2 | 25 | 25 | 1-8 | 17 | 25 | 21 |
| 0 | 4 | 2 | 9 | 6 | 0 | 9 | 4 | -4 | 12 | 1-15 | 1 | 3 | 11 | 3 | 1-11 | 3 | 1 | 3 | 1-7 | 1 | 17 | 12 |
| 0 | 4 | 3 | 55 | 57 | 0 | 9 | 5 | 22 | 16 | 1-15 | 2 | 0 | 0 | 0 | 1-11 | 4 | 24 | 26 | 1-7 | 2 | 24 | 25 |
| 0 | 4 | 4 | 625 | 662 | 0 | 9 | 6 | -6 | 2 | 1-15 | 3 | 4 | 15 | 3 | 1-11 | 5 | 3 | 1 | 1-7 | 3 | 22 | 28 |
| 0 | 4 | 5 | 76 | 73 | 0 | 9 | 7 | 16 | 10 | 1-15 | 4 | 9 | 10 | 10 | 1-11 | 6 | 0 | 0 | 1-7 | 4 | -1 | 0 |
| 0 | 4 | 6 | 9 | 13 | 0 | 9 | 8 | 4 | 0 | 1-15 | 5 | 16 | 12 | 12 | 1-11 | 7 | 76 | 71 | 1-7 | 5 | 580 | 574 |
| 0 | 4 | 7 | 129 | 143 | 0 | 9 | 9 | 3 | 0 | 1-15 | 6 | -1 | 3 | 3 | 1-11 | 8 | 33 | 33 | 1-7 | 6 | 20 | 21 |
| 0 | 4 | 8 | 0 | 6 | 0 | 10 | 0 | 4 | 3 | 1-15 | 7 | 17 | 14 | 14 | 1-11 | 9 | 6 | 10 | 1-7 | 7 | 5 | 3 |
| 0 | 4 | 9 | 0 | 4 | 0 | 10 | 1 | 17 | 13 | 1-15 | 8 | -1 | 4 | 4 | 1-11 | 10 | -1 | 13 | 1-7 | 8 | 11 | 4 |
| 0 | 4 | 10 | -4 | 0 | 0 | 10 | 2 | 7 | 10 | 1-15 | 9 | -5 | 5 | 5 | 1-11 | 11 | 1 | 0 | 1-7 | 9 | -3 | 2 |
| 0 | 4 | 11 | 3 | 3 | 0 | 10 | 3 | 3 | 5 | 1-15 | 10 | 11 | 19 | 19 | 1-11 | 12 | 21 | 21 | 1-7 | 10 | 1 | 11 |
| 0 | 4 | 12 | -2 | 0 | 0 | 10 | 4 | 3 | 0 | 1-15 | 11 | -1 | 1 | 1 | 1-11 | 13 | 25 | 29 | 1-7 | 11 | 86 | 89 |
| 0 | 4 | 13 | 7 | 5 | 0 | 10 | 5 | 1 | 0 | 1-15 | 12 | 0 | 7 | 7 | 1-11 | 14 | 35 | 34 | 1-7 | 12 | 92 | 104 |
| 0 | 5 | 0 | 37 | 37 | 0 | 10 | 6 | 2 | 0 | 1-15 | 13 | -2 | 4 | 4 | 1-11 | 15 | -7 | 3 | 1-7 | 13 | 3 | 0 |
| 0 | 5 | 1 | 49 | 56 | 0 | 10 | 7 | 13 | 6 | 1-15 | 14 | -3 | 0 | 0 | 1-11 | 16 | 1 | 8 | 1-7 | 14 | 121 | 115 |
| 0 | 5 | 2 | 17 | 23 | 0 | 10 | 8 | -4 | 0 | 1-15 | 15 | 1 | 0 | 0 | 1-11 | 17 | 2 | 2 | 1-7 | 15 | 76 | 79 |
| 0 | 5 | 3 | 306 | 312 | 0 | 11 | 0 | -13 | 3 | 1-14 | 1 | 0 | 1 | 1 | 1-10 | 1 | 10 | 11 | 1-7 | 16 | 3 | 7 |
| 0 | 5 | 4 | 24 | 19 | 0 | 11 | 1 | -6 | 4 | 1-14 | 2 | -6 | 1 | 1 | 1-10 | 2 | 29 | 25 | 1-7 | 17 | 14 | 12 |
| 0 | 5 | 5 | 137 | 130 | 0 | 11 | 2 | 56 | 56 | 1-14 | 3 | 1 | 5 | 5 | 1-10 | 3 | 6 | 7 | 1-6 | 1 | 1 | 3 |
| 0 | 5 | 6 | 77 | 85 | 0 | 11 | 3 | 1 | 9 | 1-14 | 4 | 15 | 16 | 16 | 1-10 | 4 | 3 | 1 | 1-6 | 2 | 23 | 15 |
| 0 | 5 | 7 | 540 | 558 | 0 | 11 | 4 | -4 | 0 | 1-14 | 5 | -1 | 0 | 0 | 1-10 | 5 | 53 | 57 | 1-6 | 3 | 9 | 10 |
| 0 | 5 | 8 | 151 | 162 | 0 | 11 | 5 | 13 | 8 | 1-14 | 6 | -2 | 2 | 2 | 1-10 | 6 | 200 | 195 | 1-6 | 4 | 283 | 286 |
| 0 | 5 | 9 | 34 | 40 | 0 | 11 | 6 | 0 | 0 | 1-14 | 7 | 83 | 76 | 76 | 1-10 | 7 | 12 | 18 | 1-6 | 5 | 0 | 1 |
| 0 | 5 | 10 | 26 | 24 | 0 | 11 | 7 | 1 | 0 | 1-14 | 8 | 106 | 109 | 109 | 1-10 | 8 | 221 | 219 | 1-6 | 6 | 415 | 408 |
| 0 | 5 | 11 | 1 | 1 | 0 | 12 | 0 | 2 | 0 | 1-14 | 9 | 0 | 1 | 1 | 1-10 | 9 | 5 | 5 | 1-6 | 7 | 1627 | 1471 |
| 0 | 5 | 12 | 2 | 4 | 0 | 12 | 1 | 10 | 7 | 1-14 | 10 | 0 | 0 | 0 | 1-10 | 10 | 0 | 0 | 1-6 | 8 | 347 | 338 |
| 0 | 5 | 13 | 12 | 12 | 0 | 12 | 2 | 48 | 44 | 1-14 | 11 | -3 | 0 | 0 | 1-10 | 11 | 233 | 248 | 1-6 | 9 | -1 | 0 |
| 0 | 6 | 0 | -4 | 0 | 0 | 12 | 3 | -1 | 1 | 1-14 | 12 | 14 | 12 | 12 | 1-10 | 12 | -12 | 2 | 1-6 | 10 | 63 | 61 |
| 0 | 6 | 1 | 0 | 5 | 0 | 12 | 4 | -2 | 0 | 1-14 | 13 | -2 | 3 | 3 | 1-10 | 13 | 6 | 4 | 1-6 | 11 | 4 | 4 |
| 0 | 6 | 2 | 382 | 359 | 0 | 12 | 5 | -3 | 0 | 1-14 | 14 | 3 | 0 | 0 | 1-10 | 14 | 12 | 9 | 1-6 | 12 | 137 | 132 |
| 0 | 6 | 3 | 21 | 16 | 0 | 12 | 6 | 0 | 1 | 1-14 | 15 | 0 | 3 | 3 | 1-10 | 15 | 1 | 6 | 1-6 | 13 | 32 | 25 |
| 0 | 6 | 4 | 24 | 24 | 0 | 13 | 0 | -8 | 1 | 1-14 | 16 | 5 | 6 | 6 | 1-10 | 16 | 4 | 1 | 1-6 | 14 | 124 | 124 |
| 0 | 6 | 5 | 73 | 82 | 0 | 13 | 1 | 17 | 23 | 1-13 | 1 | 0 | 4 | 4 | 1-10 | 17 | 0 | 1 | 1-6 | 15 | 106 | 97 |

Reflections flagged with an asterisk were considered unobserved.

Fobs & Fcalc for C₁₁H₁₇N₂O₄

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| H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc |
|---|-----|----|------|------|---|-----|----|------|------|---|-----|----|------|------|---|-----|----|-----|------|
| 1 | -6 | 16 | 44 | 39 | 1 | -2 | 15 | 4 | 2 | 1 | 3 | 1 | -1 | 3 | 1 | 8 | 1 | 87 | 79 |
| 1 | -6 | 17 | 2 | 5 | 1 | -2 | 16 | 0 | 1 | 1 | 3 | 2 | 73 | 70 | 1 | 8 | 2 | 13 | 10 |
| 1 | -5 | 1 | 163 | 188 | 1 | -1 | 1 | 78 | 80 | 1 | 3 | 3 | 710 | 696 | 1 | 8 | 3 | 12 | 13 |
| 1 | -5 | 2 | 65 | 69 | 1 | -1 | 2 | 9 | 9 | 1 | 3 | 4 | 171 | 186 | 1 | 8 | 4 | 20 | 22 |
| 1 | -5 | 3 | 37 | 37 | 1 | -1 | 3 | 1896 | 1979 | 1 | 3 | 5 | 4 | 19 | 1 | 8 | 5 | 273 | 277 |
| 1 | -5 | 4 | 290 | 283 | 1 | -1 | 4 | 8 | 9 | 1 | 3 | 6 | 70 | 80 | 1 | 8 | 6 | 143 | 135 |
| 1 | -5 | 5 | 154 | 135 | 1 | -1 | 5 | -2 | 2 | 1 | 3 | 7 | 126 | 149 | 1 | 8 | 7 | -1 | 2 |
| 1 | -5 | 6 | 1215 | 1184 | 1 | -1 | 6 | 472 | 456 | 1 | 3 | 8 | 86 | 86 | 1 | 8 | 8 | 6 | 5 |
| 1 | -5 | 7 | 50 | 48 | 1 | -1 | 7 | 193 | 183 | 1 | 3 | 9 | 14 | 10 | 1 | 8 | 9 | 3 | 0 |
| 1 | -5 | 8 | 194 | 178 | 1 | -1 | 8 | 22 | 27 | 1 | 3 | 10 | -1 | 3 | 1 | 8 | 10 | 4 | 4 |
| 1 | -5 | 9 | 1 | 6 | 1 | -1 | 9 | 0 | 0 | 1 | 3 | 11 | 2 | 0 | 1 | 9 | 0 | 88 | 85 |
| 1 | -5 | 10 | 74 | 82 | 1 | -1 | 10 | 21 | 22 | 1 | 3 | 12 | -3 | 5 | 1 | 9 | 1 | 1 | 6 |
| 1 | -5 | 11 | -3 | 2 | 1 | -1 | 11 | -2 | 3 | 1 | 3 | 13 | -3 | 0 | 1 | 9 | 2 | 31 | 29 |
| 1 | -5 | 12 | -4 | 3 | 1 | -1 | 12 | -2 | 0 | 1 | 3 | 14 | 2 | 1 | 1 | 9 | 3 | 219 | 223 |
| 1 | -5 | 13 | 0 | 5 | 1 | -1 | 13 | 61 | 56 | 1 | 4 | 0 | 383 | 363 | 1 | 9 | 4 | 123 | 113 |
| 1 | -5 | 14 | 71 | 68 | 1 | -1 | 14 | 20 | 15 | 1 | 4 | 1 | 2530 | 2284 | 1 | 9 | 5 | 5 | 0 |
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| 1 | -5 | 16 | 4 | 4 | 1 | -1 | 16 | -2 | 0 | 1 | 4 | 3 | 112 | 97 | 1 | 9 | 7 | 1 | 0 |
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| 1 | -4 | 1 | 1304 | 1392 | 1 | 0 | 1 | 428 | 456 | 1 | 4 | 5 | 234 | 244 | 1 | 9 | 9 | 10 | 8 |
| 1 | -4 | 2 | 60 | 54 | 1 | 0 | 2 | 121 | 130 | 1 | 4 | 6 | 360 | 361 | 1 | 10 | 0 | 3 | 3 |
| 1 | -4 | 3 | 76 | 82 | 1 | 0 | 3 | 53 | 53 | 1 | 4 | 7 | 169 | 171 | 1 | 10 | 1 | 2 | 6 |
| 1 | -4 | 4 | 243 | 237 | 1 | 0 | 4 | 967 | 1016 | 1 | 4 | 8 | 114 | 130 | 1 | 10 | 2 | 35 | 34 |
| 1 | -4 | 5 | 58 | 63 | 1 | 0 | 5 | 1149 | 1230 | 1 | 4 | 9 | 2 | 0 | 1 | 10 | 3 | 9 | 9 |
| 1 | -4 | 6 | 93 | 95 | 1 | 0 | 6 | 728 | 700 | 1 | 4 | 10 | 36 | 33 | 1 | 10 | 4 | 12 | 8 |
| 1 | -4 | 7 | 43 | 40 | 1 | 0 | 7 | 457 | 452 | 1 | 4 | 11 | 0 | 0 | 1 | 10 | 5 | 5 | 6 |
| 1 | -4 | 8 | 95 | 84 | 1 | 0 | 8 | 103 | 98 | 1 | 4 | 12 | 0 | 1 | 1 | 10 | 6 | 0 | 5 |
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| 1 | -4 | 10 | 132 | 134 | 1 | 0 | 10 | 28 | 28 | 1 | 5 | 0 | 8 | 0 | 1 | 10 | 8 | 1 | 0 |
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| 1 | -4 | 14 | 42 | 40 | 1 | 0 | 14 | 20 | 14 | 1 | 5 | 4 | 80 | 74 | 1 | 11 | 3 | 0 | 0 |
| 1 | -4 | 15 | 48 | 53 | 1 | 0 | 15 | 12 | 14 | 1 | 5 | 5 | 278 | 285 | 1 | 11 | 4 | 7 | 3 |
| 1 | -4 | 16 | 0 | 0 | 1 | 1 | 0 | 46 | 38 | 1 | 5 | 6 | 81 | 79 | 1 | 11 | 5 | 0 | 1 |
| 1 | -4 | 17 | 3 | 3 | 1 | 1 | 1 | 12 | 17 | 1 | 5 | 7 | 213 | 195 | 1 | 11 | 6 | 3 | 5 |
| 1 | -3 | 1 | 3809 | 5071 | 1 | 1 | 2 | 126 | 122 | 1 | 5 | 8 | 1 | 8 | 1 | 11 | 7 | 5 | 2 |
| 1 | -3 | 2 | 3131 | 3785 | 1 | 1 | 3 | 281 | 280 | 1 | 5 | 9 | 2 | 10 | 1 | 12 | 0 | 8 | 13 |
| 1 | -3 | 3 | 4007 | 4852 | 1 | 1 | 4 | 1538 | 1529 | 1 | 5 | 10 | 3 | 2 | 1 | 12 | 1 | -2 | 0 |
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| 1 | -3 | 11 | 100 | 119 | 1 | 1 | 12 | 2 | 8 | 1 | 6 | 5 | 64 | 53 | 1 | 13 | 3 | -12 | 3 |
| 1 | -3 | 12 | -6 | 12 | 1 | 1 | 13 | 44 | 48 | 1 | 6 | 6 | 4 | 2 | 1 | 13 | 4 | -4 | 1 |
| 1 | -3 | 13 | 23 | 24 | 1 | 1 | 14 | 2 | 2 | 1 | 6 | 7 | 7 | 5 | 1 | 14 | 0 | -6 | 2 |
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| 1 | -3 | 16 | 1 | 1 | 1 | 2 | 1 | 919 | 939 | 1 | 6 | 10 | 11 | 8 | 1 | 14 | 3 | 0 | 0 |
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| 1 | -2 | 7 | 193 | 170 | 1 | 2 | 8 | 22 | 29 | 1 | 7 | 5 | 52 | 63 | 2 | 17 | 9 | -2 | 0 |
| 1 | -2 | 8 | 14 | 13 | 1 | 2 | 9 | 16 | 16 | 1 | 7 | 6 | 81 | 70 | 2 | 17 | 10 | 0 | 0 |
| 1 | -2 | 9 | -1 | 0 | 1 | 2 | 10 | 23 | 27 | 1 | 7 | 7 | 22 | 12 | 2 | 16 | 2 | -2 | 3 |
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| 1 | -2 | 11 | 2 | 8 | 1 | 2 | 12 | 17 | 14 | 1 | 7 | 9 | 7 | 2 | 2 | 16 | 4 | 2 | 5 |
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| 1 | -2 | 14 | 0 | 2 | 1 | 3 | 0 | 21 | 24 | 1 | 8 | 0 | 35 | 36 | 2 | 16 | 7 | 1 | 2 |
| 2 | -16 | 8 | -2 | 0 | 2 | -16 | 8 | -2 | 0 | 2 | -16 | 9 | 0 | 0 | 2 | -16 | 9 | 0 | 0 |
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| 2 | -16 | 11 | -1 | 1 | 2 | -16 | 12 | -1 | 1 | 2 | -16 | 12 | -1 | 1 | 2 | -16 | 12 | -1 | 1 |
| 2 | -15 | 1 | 0 | 0 | 2 | -15 | 1 | 0 | 0 | 2 | -15 | 2 | 3 | 1 | 2 | -15 | 2 | 3 | 1 |
| 2 | -15 | 2 | 1 | 2 | 2 | -15 | 3 | 1 | 2 | 2 | -15 | 3 | 1 | 2 | 2 | -15 | 3 | 1 | 2 |
| 2 | -15 | 3 | 3 | 0 | 2 | -15 | 4 | 3 | 0 | 2 | -15 | 4 | 3 | 0 | 2 | -15 | 4 | 3 | 0 |
| 2 | -15 | 4 | -1 | 3 | 2 | -15 | 5 | -1 | 3 | 2 | -15 | 5 | -1 | 3 | 2 | -15 | 5 | -1 | 3 |
| 2 | -15 | 5 | 3 | 1 | 2 | -15 | 6 | 3 | 1 | 2 | -15 | 6 | 3 | 1 | 2 | -15 | 6 | 3 | 1 |
| 2 | -15 | 6 | -1 | 1 | 2 | -15 | 7 | -1 | 1 | 2 | -15 | 7 | -1 | 1 | 2 | -15 | 7 | -1 | 1 |
| 2 | -15 | 7 | 13 | 0 | 2 | -15 | 8 | 13 | 0 | 2 | -15 | 8 | 13 | 0 | 2 | -15 | 8 | 13 | 0 |
| 2 | -15 | 8 | -3 | 0 | 2 | -15 | 9 | -3 | 0 | 2 | -15 | 9 | -3 | 0 | 2 | -15 | 9 | -3 | 0 |
| 2 | -15 | 9 | -4 | 0 | 2 | -15 | 10 | -4 | 0 | 2 | -15 | 10 | -4 | 0 | 2 | -15 | 10 | -4 | 0 |
| 2 | -15 | 10 | 5 | 2 | 2 | -15 | 11 | 5 | 2 | 2 | -15 | 11 | 5 | 2 | 2 | -15 | 11 | 5 | 2 |
| 2 | -15 | 11 | 7 | 0 | 2 | -15 | 12 | 7 | 0 | 2 | -15 | 12 | 7 | 0 | 2 | -15 | 12 | 7 | 0 |
| 2 | -15 | 12 | 4 | 0 | 2 | -15 | 13 | 4 | 0 | 2 | -15 | 13 | 4 | 0 | 2 | -15 | 13 | 4 | 0 |
| 2 | -15 | 13 | 4 | 0 | 2 | -15 | 14 | 4 | 0 | 2 | -15 | 14 | 4 | 0 | 2 | -15 | 14 | 4 | 0 |
| 2 | -15 | 14 | 5 | 2 | 2 | -15 | 15 | 5 | 2 | 2 | -15 | 15 | 5 | 2 | 2 | -15 | 15 | 5 | 2 |
| 2 | -15 | 15 | 4 | 0 | 2 | -15 | 16 | 4 | 0 | 2 | -15 | 16 | 4 | 0 | 2 | -15 | 16 | 4 | 0 |
| 2 | -15 | 16 | 3 | 0 | 2 | -15 | 17 | 3 | 0 | 2 | -15 | 17 | 3 | 0 | 2 | -15 | 17 | 3 | 0 |
| 2 | -14 | 1 | 4 | 2 | 2 | -14 | 1 | 4 | 2 | 2 | -14 | 2 | 17 | 19 | 2 | -14 | 1 | 4 | 2 |
| 2 | -14 | 2 | 9 | 13 | 2 | -14 | 2 | 9 | 13 | 2 | -14 | 3 | 9 | 13 | 2 | -14 | 2 | 17 | 19 |
| 2 | -14 | 3 | 12 | 13 | 2 | -14 | 3 | 12 | 13 | 2 | -14 | 4 | 12 | 13 | 2 | -14 | 3 | 9 | 13 |
| 2 | -14 | 4 | -6 | 1 | 2 | -14 | 4 | -6 | 1 | 2 | -14 | 5 | -6 | 1 | 2 | -14 | 4 | 12 | 13 |
| 2 | -14 | 5 | 3 | 0 | 2 | -14 | 5 | 3 | 0 | 2 | -14 | 6 | | | | | | | |

F_{obs} & F_{calc} for C₇H₇NO₂

| H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc |
|------|----|---|-----|------|-----|----|---|------|------|-----|----|---|------|------|-----|----|---|------|------|
| 2-11 | 2 | | -6 | 0 | 2-7 | 3 | | 24 | 20 | 2-3 | 5 | | 1 | 0 | 2-1 | 8 | | 154 | 157 |
| 2-11 | 3 | | 97 | 91 | 2-7 | 4 | | -1 | 2 | 2-3 | 6 | | 29 | 17 | 2-1 | 9 | | 98 | 106 |
| 2-11 | 4 | | 171 | 170 | 2-7 | 5 | | -3 | 0 | 2-3 | 7 | | 174 | 177 | 2-1 | 10 | | 179 | 184 |
| 2-11 | 5 | | 1 | 6 | 2-7 | 6 | | 22 | 20 | 2-3 | 8 | | -1 | 0 | 2-1 | 11 | | 10 | 27 |
| 2-11 | 6 | | 22 | 19 | 2-7 | 7 | | 0 | 0 | 2-3 | 9 | | 3 | 5 | 2-1 | 12 | | 0 | 0 |
| 2-11 | 7 | | 3 | 2 | 2-7 | 8 | | 4 | 1 | 2-3 | 10 | | 0 | 5 | 2-1 | 13 | | 1 | 2 |
| 2-11 | 8 | | -1 | 1 | 2-7 | 9 | | 2 | 0 | 2-3 | 11 | | 2 | 3 | 2-1 | 14 | | -3 | 1 |
| 2-11 | 9 | | 3 | 1 | 2-7 | 10 | | 36 | 44 | 2-3 | 12 | | -4 | 1 | 2-2 | 0 | | 320 | 344 |
| 2-11 | 10 | | 22 | 18 | 2-7 | 11 | | 91 | 97 | 2-3 | 13 | | 3 | 0 | 2-2 | 1 | | 65 | 64 |
| 2-11 | 11 | | 23 | 24 | 2-7 | 12 | | 14 | 15 | 2-3 | 14 | | 4 | 4 | 2-2 | 2 | | 563 | 543 |
| 2-11 | 12 | | 3 | 3 | 2-7 | 13 | | 103 | 104 | 2-3 | 15 | | 0 | 3 | 2-2 | 3 | | 124 | 119 |
| 2-11 | 13 | | 4 | 6 | 2-7 | 14 | | 1 | 4 | 2-3 | 16 | | 8 | 4 | 2-2 | 4 | | 764 | 755 |
| 2-11 | 14 | | 2 | 3 | 2-7 | 15 | | 23 | 20 | 2-2 | 1 | | 240 | 252 | 2-2 | 5 | | 323 | 290 |
| 2-11 | 15 | | 0 | 0 | 2-7 | 16 | | 12 | 9 | 2-2 | 2 | | 1 | 5 | 2-2 | 6 | | 65 | 60 |
| 2-11 | 16 | | -6 | 1 | 2-6 | 1 | | 14 | 18 | 2-2 | 3 | | 952 | 934 | 2-2 | 7 | | 58 | 68 |
| 2-10 | 1 | | -7 | 1 | 2-6 | 2 | | 34 | 32 | 2-2 | 4 | | 216 | 214 | 2-2 | 8 | | 219 | 214 |
| 2-10 | 2 | | 0 | 0 | 2-6 | 3 | | 211 | 215 | 2-2 | 5 | | 62 | 61 | 2-2 | 9 | | 2 | 2 |
| 2-10 | 3 | | 14 | 12 | 2-6 | 4 | | 7 | 8 | 2-2 | 6 | | -3 | 0 | 2-2 | 10 | | 66 | 74 |
| 2-10 | 4 | | 20 | 23 | 2-6 | 5 | | 92 | 96 | 2-2 | 7 | | 57 | 50 | 2-2 | 11 | | 13 | 15 |
| 2-10 | 5 | | 122 | 115 | 2-6 | 6 | | 4 | 4 | 2-2 | 8 | | 12 | 13 | 2-2 | 12 | | 0 | 3 |
| 2-10 | 6 | | 364 | 357 | 2-6 | 7 | | -2 | 1 | 2-2 | 9 | | 58 | 64 | 2-2 | 13 | | 2 | 4 |
| 2-10 | 7 | | 20 | 15 | 2-6 | 8 | | 179 | 177 | 2-2 | 10 | | 37 | 29 | 2-3 | 0 | | 1034 | 1042 |
| 2-10 | 8 | | 3 | 3 | 2-6 | 9 | | 105 | 96 | 2-2 | 11 | | 6 | 13 | 2-3 | 1 | | 699 | 681 |
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| 2-10 | 10 | | 30 | 27 | 2-6 | 11 | | 34 | 38 | 2-2 | 13 | | 34 | 32 | 2-3 | 3 | | 285 | 275 |
| 2-10 | 11 | | 10 | 13 | 2-6 | 12 | | 116 | 120 | 2-2 | 14 | | 0 | 0 | 2-3 | 4 | | 123 | 117 |
| 2-10 | 12 | | -2 | 1 | 2-6 | 13 | | 340 | 318 | 2-2 | 15 | | 3 | 1 | 2-3 | 5 | | 97 | 104 |
| 2-10 | 13 | | 16 | 14 | 2-6 | 14 | | 1 | 2 | 2-1 | 1 | | 892 | 930 | 2-3 | 6 | | 64 | 64 |
| 2-10 | 14 | | 2 | 3 | 2-6 | 15 | | 15 | 12 | 2-1 | 2 | | 43 | 49 | 2-3 | 7 | | 47 | 59 |
| 2-10 | 15 | | 5 | 3 | 2-6 | 16 | | 15 | 8 | 2-1 | 3 | | 725 | 788 | 2-3 | 8 | | 4 | 12 |
| 2-10 | 16 | | 2 | 2 | 2-5 | 1 | | 621 | 886 | 2-1 | 4 | | 38 | 39 | 2-3 | 9 | | 84 | 81 |
| 2-9 | 1 | | 3 | 1 | 2-5 | 2 | | 95 | 100 | 2-1 | 5 | | 20 | 17 | 2-3 | 10 | | 18 | 21 |
| 2-9 | 2 | | -3 | 1 | 2-5 | 3 | | 3450 | 3583 | 2-1 | 6 | | 185 | 180 | 2-3 | 11 | | 52 | 50 |
| 2-9 | 3 | | -1 | 7 | 2-5 | 4 | | 33 | 26 | 2-1 | 7 | | 93 | 108 | 2-3 | 12 | | 12 | 12 |
| 2-9 | 4 | | 43 | 35 | 2-5 | 5 | | 39 | 40 | 2-1 | 8 | | 8 | 2 | 2-3 | 13 | | -1 | 3 |
| 2-9 | 5 | | 10 | 10 | 2-5 | 6 | | 101 | 94 | 2-1 | 9 | | 50 | 57 | 2-4 | 0 | | 162 | 178 |
| 2-9 | 6 | | 125 | 116 | 2-5 | 7 | | 7 | 8 | 2-1 | 10 | | 26 | 27 | 2-4 | 1 | | 1104 | 1091 |
| 2-9 | 7 | | 48 | 41 | 2-5 | 8 | | 0 | 1 | 2-1 | 11 | | 19 | 20 | 2-4 | 2 | | 10 | 10 |
| 2-9 | 8 | | 59 | 56 | 2-5 | 9 | | 64 | 65 | 2-1 | 12 | | -1 | 2 | 2-4 | 3 | | 290 | 288 |
| 2-9 | 9 | | 0 | 6 | 2-5 | 10 | | 1 | 5 | 2-1 | 13 | | 1 | 0 | 2-4 | 4 | | 241 | 220 |
| 2-9 | 10 | | 109 | 106 | 2-5 | 11 | | 458 | 435 | 2-1 | 14 | | 6 | 6 | 2-4 | 5 | | 3 | 14 |
| 2-9 | 11 | | 89 | 93 | 2-5 | 12 | | 50 | 43 | 2-1 | 15 | | 0 | 2 | 2-4 | 6 | | 51 | 56 |
| 2-9 | 12 | | 13 | 5 | 2-5 | 13 | | 96 | 105 | 2-0 | 0 | | 1380 | 1487 | 2-4 | 7 | | -4 | 4 |
| 2-9 | 13 | | 1 | 0 | 2-5 | 14 | | 1 | 1 | 2-0 | 1 | | 52 | 49 | 2-4 | 8 | | 4 | 7 |
| 2-9 | 14 | | 3 | 3 | 2-5 | 15 | | 25 | 32 | 2-0 | 2 | | 25 | 27 | 2-4 | 9 | | 5 | 11 |
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| 2-9 | 16 | | -1 | 0 | 2-4 | 1 | | 503 | 559 | 2-0 | 4 | | 429 | 416 | 2-4 | 11 | | 18 | 15 |
| 2-8 | 1 | | 0 | 3 | 2-4 | 2 | | 803 | 858 | 2-0 | 5 | | 720 | 751 | 2-4 | 12 | | -1 | 2 |
| 2-8 | 2 | | 15 | 17 | 2-4 | 3 | | 195 | 215 | 2-0 | 6 | | 33 | 34 | 2-5 | 0 | | 202 | 202 |
| 2-8 | 3 | | -7 | 2 | 2-4 | 4 | | 557 | 558 | 2-0 | 7 | | 45 | 58 | 2-5 | 1 | | 228 | 243 |
| 2-8 | 4 | | 55 | 52 | 2-4 | 5 | | 1814 | 1734 | 2-0 | 8 | | 31 | 27 | 2-5 | 2 | | 6 | 5 |
| 2-8 | 5 | | 25 | 22 | 2-4 | 6 | | 143 | 158 | 2-0 | 9 | | 34 | 33 | 2-5 | 3 | | 0 | 5 |
| 2-8 | 6 | | 117 | 95 | 2-4 | 7 | | 14 | 11 | 2-0 | 10 | | 25 | 26 | 2-5 | 4 | | -9 | 4 |
| 2-8 | 7 | | 60 | 52 | 2-4 | 8 | | -8 | 2 | 2-0 | 11 | | 34 | 30 | 2-5 | 5 | | 26 | 25 |
| 2-8 | 8 | | -2 | 5 | 2-4 | 9 | | 51 | 43 | 2-0 | 12 | | 0 | 1 | 2-5 | 6 | | 36 | 39 |
| 2-8 | 9 | | 119 | 120 | 2-4 | 10 | | 38 | 31 | 2-0 | 13 | | 1 | 3 | 2-5 | 7 | | 10 | 11 |
| 2-8 | 10 | | 39 | 40 | 2-4 | 11 | | 52 | 51 | 2-0 | 14 | | 4 | 4 | 2-5 | 8 | | 0 | 1 |
| 2-8 | 11 | | 119 | 121 | 2-4 | 12 | | 59 | 60 | 2-0 | 15 | | 2 | 0 | 2-5 | 9 | | -1 | 1 |
| 2-8 | 12 | | 53 | 59 | 2-4 | 13 | | 289 | 279 | 2-1 | 0 | | 1 | 1 | 2-5 | 10 | | 0 | 1 |
| 2-8 | 13 | | 9 | 8 | 2-4 | 14 | | -4 | 5 | 2-1 | 1 | | -5 | 3 | 2-5 | 11 | | 2 | 0 |
| 2-8 | 14 | | 3 | 0 | 2-4 | 15 | | 2 | 1 | 2-1 | 2 | | 622 | 605 | 2-5 | 12 | | -3 | 0 |
| 2-8 | 15 | | 3 | 4 | 2-4 | 16 | | 1 | 0 | 2-1 | 3 | | 715 | 685 | 2-6 | 0 | | 45 | 38 |
| 2-8 | 16 | | 3 | 2 | 2-3 | 1 | | 338 | 358 | 2-1 | 4 | | 43 | 40 | 2-6 | 1 | | 108 | 102 |
| 2-8 | 17 | | 0 | 0 | 2-3 | 2 | | 266 | 271 | 2-1 | 5 | | 0 | 16 | 2-6 | 2 | | 18 | 17 |
| 2-7 | 1 | | 13 | 8 | 2-3 | 3 | | 2226 | 2173 | 2-1 | 6 | | 7 | 12 | 2-6 | 3 | | -2 | 3 |
| 2-7 | 2 | | 38 | 39 | 2-3 | 4 | | 234 | 235 | 2-1 | 7 | | 23 | 26 | 2-6 | 4 | | 3 | 6 |

Reflections flagged with an asterisk were considered unobserved.

Obs & Calc for C₂₀H₁₂NO₂

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| H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc | | | | | |
|------|----|---|-----|------|------|----|---|-----|------|-----|----|---|-----|------|-----|----|---|-----|------|-----|----|--|-----|-----|
| 3-16 | 4 | | 0 | 0 | 3-11 | 7 | | 3 | 2 | 3-7 | 13 | | 8 | 9 | 3-2 | 4 | | 48 | 56 | 3-3 | 0 | | 462 | 467 |
| 3-16 | 5 | | -3 | 2 | 3-11 | 8 | | -1 | 1 | 3-7 | 14 | | 16 | 11 | 3-2 | 5 | | 107 | 93 | 3-3 | 1 | | 50 | 52 |
| 3-16 | 6 | | -5 | 1 | 3-11 | 9 | | 45 | 43 | 3-7 | 15 | | -5 | 4 | 3-2 | 6 | | -3 | 1 | 3-3 | 2 | | 36 | 29 |
| 3-16 | 7 | | 1 | 0 | 3-11 | 10 | | 0 | 6 | 3-6 | 1 | | 58 | 63 | 3-2 | 7 | | 3 | 2 | 3-3 | 3 | | 14 | 28 |
| 3-16 | 8 | | 0 | 1 | 3-11 | 11 | | 6 | 2 | 3-6 | 2 | | 279 | 249 | 3-2 | 8 | | 2 | 10 | 3-3 | 4 | | 1 | 2 |
| 3-16 | 9 | | 0 | 0 | 3-11 | 12 | | -1 | 5 | 3-6 | 3 | | -3 | 0 | 3-2 | 9 | | 144 | 138 | 3-3 | 5 | | 10 | 11 |
| 3-16 | 10 | | 2 | 2 | 3-11 | 13 | | 4 | 2 | 3-6 | 4 | | 0 | 0 | 3-2 | 10 | | 106 | 89 | 3-3 | 6 | | 3 | 1 |
| 3-15 | 1 | | 1 | 3 | 3-11 | 14 | | 2 | 0 | 3-6 | 5 | | 13 | 16 | 3-2 | 11 | | 0 | 0 | 3-3 | 7 | | 4 | 18 |
| 3-15 | 2 | | 0 | 0 | 3-11 | 15 | | 0 | 1 | 3-6 | 6 | | 0 | 3 | 3-2 | 12 | | 5 | 5 | 3-3 | 8 | | 132 | 149 |
| 3-15 | 3 | | 0 | 3 | 3-10 | 1 | | 3 | 9 | 3-6 | 7 | | 0 | 9 | 3-2 | 13 | | 0 | 2 | 3-3 | 9 | | 4 | 4 |
| 3-15 | 4 | | 2 | 0 | 3-10 | 2 | | 114 | 116 | 3-6 | 8 | | 1 | 3 | 3-2 | 14 | | 2 | 1 | 3-3 | 10 | | 3 | 7 |
| 3-15 | 5 | | -5 | 1 | 3-10 | 3 | | 69 | 70 | 3-6 | 9 | | -1 | 0 | 3-1 | 1 | | 558 | 532 | 3-3 | 11 | | -1 | 0 |
| 3-15 | 6 | | 1 | 0 | 3-10 | 4 | | 52 | 56 | 3-6 | 10 | | 7 | 5 | 3-1 | 2 | | 0 | 2 | 3-3 | 12 | | -2 | 0 |
| 3-15 | 7 | | -1 | 3 | 3-10 | 5 | | 2 | 2 | 3-6 | 11 | | 15 | 17 | 3-1 | 3 | | 26 | 24 | 3-4 | 0 | | 151 | 149 |
| 3-15 | 8 | | 0 | 1 | 3-10 | 6 | | 12 | 12 | 3-6 | 12 | | 68 | 57 | 3-1 | 4 | | 25 | 32 | 3-4 | 1 | | 31 | 34 |
| 3-15 | 9 | | 7 | 7 | 3-10 | 7 | | 2 | 2 | 3-6 | 13 | | 4 | 9 | 3-1 | 5 | | 40 | 40 | 3-4 | 2 | | 27 | 28 |
| 3-15 | 10 | | 2 | 0 | 3-10 | 8 | | 0 | 0 | 3-6 | 14 | | -2 | 0 | 3-1 | 6 | | 140 | 132 | 3-4 | 3 | | 34 | 40 |
| 3-15 | 11 | | 3 | 6 | 3-10 | 9 | | 31 | 31 | 3-6 | 15 | | 0 | 2 | 3-1 | 7 | | 6 | 2 | 3-4 | 4 | | 36 | 34 |
| 3-15 | 12 | | -1 | 1 | 3-10 | 10 | | 21 | 17 | 3-5 | 1 | | 272 | 264 | 3-1 | 8 | | 48 | 42 | 3-4 | 5 | | 116 | 116 |
| 3-14 | 1 | | 0 | 0 | 3-10 | 11 | | 7 | 11 | 3-5 | 2 | | 3 | 1 | 3-1 | 9 | | 100 | 102 | 3-4 | 6 | | 78 | 86 |
| 3-14 | 2 | | -1 | 5 | 3-10 | 12 | | 0 | 5 | 3-5 | 3 | | 26 | 29 | 3-1 | 10 | | 188 | 186 | 3-4 | 7 | | 19 | 12 |
| 3-14 | 3 | | -7 | 2 | 3-10 | 13 | | 2 | 1 | 3-5 | 4 | | 21 | 19 | 3-1 | 11 | | 51 | 59 | 3-4 | 8 | | -8 | 1 |
| 3-14 | 4 | | -1 | 0 | 3-10 | 14 | | -4 | 0 | 3-5 | 5 | | 237 | 235 | 3-1 | 12 | | 2 | 1 | 3-4 | 9 | | 3 | 5 |
| 3-14 | 5 | | 0 | 1 | 3-10 | 15 | | 1 | 0 | 3-5 | 6 | | -2 | 0 | 3-1 | 13 | | 20 | 17 | 3-4 | 10 | | -6 | 5 |
| 3-14 | 6 | | 3 | 0 | 3-9 | 1 | | 184 | 175 | 3-5 | 7 | | 18 | 16 | 3-1 | 14 | | -2 | 0 | 3-4 | 11 | | 0 | 1 |
| 3-14 | 7 | | 5 | 5 | 3-9 | 2 | | 103 | 110 | 3-5 | 8 | | 76 | 74 | 3-0 | 0 | | 16 | 12 | 3-5 | 0 | | 383 | 343 |
| 3-14 | 8 | | -1 | 0 | 3-9 | 3 | | -6 | 4 | 3-5 | 9 | | 195 | 195 | 3-0 | 1 | | 1 | 5 | 3-5 | 1 | | 82 | 83 |
| 3-14 | 9 | | -3 | 1 | 3-9 | 4 | | -10 | 4 | 3-5 | 10 | | 91 | 71 | 3-0 | 2 | | 6 | 4 | 3-5 | 2 | | 60 | 62 |
| 3-14 | 10 | | 8 | 8 | 3-9 | 5 | | 3 | 0 | 3-5 | 11 | | -1 | 1 | 3-0 | 3 | | 251 | 237 | 3-5 | 3 | | 0 | 0 |
| 3-14 | 11 | | 5 | 2 | 3-9 | 6 | | -7 | 1 | 3-5 | 12 | | -2 | 1 | 3-0 | 4 | | 61 | 56 | 3-5 | 4 | | 2 | 2 |
| 3-14 | 12 | | -3 | 0 | 3-9 | 7 | | 0 | 2 | 3-5 | 13 | | 1 | 0 | 3-0 | 5 | | 197 | 211 | 3-5 | 5 | | 5 | 11 |
| 3-14 | 13 | | 2 | 4 | 3-9 | 8 | | 39 | 31 | 3-5 | 14 | | 0 | 3 | 3-0 | 6 | | -5 | 1 | 3-5 | 6 | | 59 | 60 |
| 3-13 | 1 | | 2 | 2 | 3-9 | 9 | | 0 | 10 | 3-5 | 15 | | 0 | 0 | 3-0 | 7 | | 22 | 19 | 3-5 | 7 | | -9 | 0 |
| 3-13 | 2 | | 0 | 0 | 3-9 | 10 | | 60 | 66 | 3-4 | 1 | | 83 | 70 | 3-0 | 8 | | 212 | 223 | 3-5 | 8 | | 42 | 41 |
| 3-13 | 3 | | 0 | 0 | 3-9 | 11 | | 38 | 31 | 3-4 | 2 | | 279 | 248 | 3-0 | 9 | | 54 | 55 | 3-5 | 9 | | -3 | 6 |
| 3-13 | 4 | | 1 | 1 | 3-9 | 12 | | 0 | 2 | 3-4 | 3 | | 57 | 63 | 3-0 | 10 | | 22 | 19 | 3-5 | 10 | | -5 | 0 |
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| 3-13 | 6 | | -3 | 0 | 3-9 | 14 | | 5 | 8 | 3-4 | 5 | | 174 | 172 | 3-0 | 12 | | -3 | 3 | 3-6 | 1 | | 59 | 50 |
| 3-13 | 7 | | -2 | 1 | 3-9 | 15 | | 0 | 1 | 3-4 | 6 | | 255 | 262 | 3-0 | 13 | | 10 | 8 | 3-6 | 2 | | 0 | 0 |
| 3-13 | 8 | | -7 | 4 | 3-8 | 1 | | 4 | 15 | 3-4 | 7 | | 93 | 93 | 3-1 | 0 | | 15 | 20 | 3-6 | 3 | | 2 | 3 |
| 3-13 | 9 | | 1 | 1 | 3-8 | 2 | | 118 | 135 | 3-4 | 8 | | 58 | 58 | 3-1 | 1 | | 30 | 30 | 3-6 | 4 | | 0 | 1 |
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| 3-13 | 11 | | 3 | 2 | 3-8 | 4 | | 4 | 2 | 3-4 | 10 | | 63 | 54 | 3-1 | 3 | | 73 | 74 | 3-6 | 6 | | -4 | 2 |
| 3-13 | 12 | | 12 | 13 | 3-8 | 5 | | 26 | 21 | 3-4 | 11 | | 141 | 133 | 3-1 | 4 | | 133 | 144 | 3-6 | 7 | | 15 | 17 |
| 3-13 | 13 | | 0 | 2 | 3-8 | 6 | | 83 | 73 | 3-4 | 12 | | 0 | 0 | 3-1 | 5 | | 3 | 4 | 3-6 | 8 | | -2 | 0 |
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| 3-12 | 5 | | 14 | 16 | 3-8 | 12 | | 45 | 37 | 3-3 | 3 | | 27 | 19 | 3-1 | 11 | | 11 | 11 | 3-7 | 3 | | 23 | 29 |
| 3-12 | 6 | | -3 | 3 | 3-8 | 13 | | -6 | 0 | 3-3 | 4 | | 379 | 352 | 3-1 | 12 | | 4 | 6 | 3-7 | 4 | | 48 | 44 |
| 3-12 | 7 | | 1 | 0 | 3-8 | 14 | | 0 | 4 | 3-3 | 5 | | 12 | 8 | 3-1 | 13 | | -4 | 1 | 3-7 | 5 | | 0 | 2 |
| 3-12 | 8 | | 5 | 2 | 3-8 | 15 | | 0 | 0 | 3-3 | 6 | | 9 | 4 | 3-2 | 0 | | 36 | 34 | 3-7 | 6 | | 2 | 6 |
| 3-12 | 9 | | 7 | 12 | 3-7 | 1 | | 26 | 18 | 3-3 | 7 | | 15 | 19 | 3-2 | 1 | | 42 | 43 | 3-7 | 7 | | 20 | 23 |
| 3-12 | 10 | | 0 | 1 | 3-7 | 2 | | 3 | 0 | 3-3 | 8 | | 473 | 474 | 3-2 | 2 | | 178 | 188 | 3-7 | 8 | | 17 | 19 |
| 3-12 | 11 | | -4 | 1 | 3-7 | 3 | | 71 | 68 | 3-3 | 9 | | 465 | 462 | 3-2 | 3 | | -4 | 0 | 3-7 | 9 | | 5 | 4 |
| 3-12 | 12 | | 5 | 7 | 3-7 | 4 | | 44 | 39 | 3-3 | 10 | | 171 | 166 | 3-2 | 4 | | 0 | 0 | 3-8 | 0 | | 1 | 8 |
| 3-12 | 13 | | 14 | 14 | 3-7 | 5 | | 1 | 6 | 3-3 | 11 | | 6 | 3 | 3-2 | 5 | | 181 | 180 | 3-8 | 1 | | 2 | 1 |
| 3-12 | 14 | | 2 | 1 | 3-7 | 6 | | 127 | 117 | 3-3 | 12 | | 0 | 0 | 3-2 | 6 | | 4 | 8 | 3-8 | 2 | | 17 | 18 |
| 3-11 | 1 | | -3 | 2 | 3-7 | 7 | | 4 | 8 | 3-3 | 13 | | 0 | 8 | 3-2 | 7 | | -1 | 1 | 3-8 | 3 | | 0 | 7 |
| 3-11 | 2 | | 46 | 39 | 3-7 | 8 | | 42 | 38 | 3-3 | 14 | | 4 | 3 | 3-2 | 8 | | 28 | 35 | 3-8 | 4 | | 57 | 63 |
| 3-11 | 3 | | -10 | 0 | 3-7 | 9 | | 51 | 43 | 3-3 | 15 | | 1 | 0 | 3-2 | 9 | | -6 | 1 | 3-8 | 5 | | 1 | 0 |
| 3-11 | 4 | | 2 | 0 | 3-7 | 10 | | 41 | 32 | 3-2 | 1 | | 374 | 384 | 3-2 | 10 | | -1 | 1 | 3-8 | 6 | | 5 | 11 |
| 3-11 | 5 | | 9 | 10 | 3-7 | 11 | | 12 | 12 | 3-2 | 2 | | 324 | 304 | 3-2 | 11 | | 0 | 4 | 3-8 | 7 | | 16 | 12 |
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Reflections flagged with an asterisk were considered unobserved.

Fobs & Fcalc for C₁₂H₇N₃O

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| H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc | | | |
|------|----|----|-----|------|------|----|----|-----|------|----|-----|-----|-----|------|-----|-----|-----|------|------|-----|-----|----|
| 3 | 9 | 0 | 13 | 20 | 4-11 | 5 | 1 | 4 | 4-6 | 3 | -11 | 0 | 4-1 | 2 | 171 | 160 | 4 | 4 | 6 | 20 | 25 | |
| 3 | 9 | 1 | 0 | 0 | 4-11 | 6 | 5 | 13 | 4-6 | 4 | -3 | 9 | 4-1 | 3 | 234 | 236 | 4 | 4 | 7 | 1 | 1 | |
| 3 | 9 | 2 | -7 | 0 | 4-11 | 7 | 0 | 5 | 4-6 | 5 | -4 | 0 | 4-1 | 4 | 149 | 142 | 4 | 4 | 8 | 0 | 0 | |
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| 3 | 9 | 4 | 9 | 9 | 4-11 | 9 | 7 | 7 | 4-6 | 7 | 7 | 6 | 4-1 | 6 | 462 | 462 | 4 | 4 | 10 | 30 | 29 | |
| 3 | 9 | 5 | 2 | 0 | 4-11 | 10 | 3 | 1 | 4-6 | 8 | 42 | 47 | 4-1 | 7 | 435 | 416 | 4 | 5 | 0 | 205 | 224 | |
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| 3 | 9 | 7 | 6 | 9 | 4-11 | 12 | 12 | 9 | 4-6 | 10 | -4 | 0 | 4-1 | 9 | 17 | 17 | 4 | 5 | 2 | 5 | 6 | |
| 3 | 10 | 0 | 1 | 0 | 4-11 | 13 | -2 | 0 | 4-6 | 11 | 0 | 0 | 4-1 | 10 | -1 | 2 | 4 | 5 | 3 | 7 | 5 | |
| 3 | 10 | 1 | -2 | 2 | 4-10 | 1 | -3 | 1 | 4-6 | 12 | 0 | 1 | 4-1 | 11 | 9 | 7 | 4 | 5 | 4 | 54 | 57 | |
| 3 | 10 | 2 | 8 | 8 | 4-10 | 2 | 14 | 10 | 4-6 | 13 | -4 | 1 | 4-1 | 12 | 8 | 6 | 4 | 5 | 5 | 0 | 8 | |
| 3 | 10 | 3 | 5 | 2 | 4-10 | 3 | 14 | 17 | 4-6 | 14 | 2 | 2 | 4 | 0 | 0 | 3 | 4 | 5 | 6 | -7 | 0 | |
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| 3 | 10 | 5 | 12 | 11 | 4-10 | 5 | 13 | 15 | 4-5 | 2 | 14 | 10 | 4 | 0 | 2 | 49 | 47 | 4 | 5 | 8 | 7 | 5 |
| 3 | 10 | 6 | 1 | 5 | 4-10 | 6 | 4 | 2 | 4-5 | 3 | 141 | 127 | 4 | 0 | 3 | 23 | 26 | 4 | 5 | 9 | 13 | 9 |
| 3 | 11 | 0 | 58 | 58 | 4-10 | 7 | 4 | 1 | 4-5 | 4 | 14 | 13 | 4 | 0 | 4 | -2 | 11 | 4 | 6 | 0 | 13 | 8 |
| 3 | 11 | 1 | 2 | 0 | 4-10 | 8 | 6 | 8 | 4-5 | 5 | 27 | 31 | 4 | 0 | 5 | 94 | 91 | 4 | 6 | 1 | 6 | 0 |
| 3 | 11 | 2 | 2 | 5 | 4-10 | 9 | 10 | 9 | 4-5 | 6 | -12 | 0 | 4 | 0 | 6 | 63 | 62 | 4 | 6 | 2 | 50 | 65 |
| 3 | 11 | 3 | 2 | 4 | 4-10 | 10 | 2 | 7 | 4-5 | 7 | 24 | 21 | 4 | 0 | 7 | 4 | 7 | 4 | 6 | 3 | 60 | 63 |
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| 3 | 12 | 2 | -9 | 0 | 4-9 | 1 | 17 | 13 | 4-5 | 11 | 38 | 32 | 4 | 0 | 11 | -1 | 0 | 4 | 6 | 7 | 10 | 10 |
| 3 | 12 | 3 | 0 | 2 | 4-9 | 2 | 13 | 13 | 4-5 | 12 | 2 | 2 | 4 | 0 | 12 | 0 | 0 | 4 | 6 | 8 | 1 | 0 |
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| 4-15 | 6 | 1 | 1 | 1 | 4-9 | 7 | 14 | 16 | 4-4 | 3 | 59 | 63 | 4 | 1 | 4 | 13 | 17 | 4 | 7 | 4 | 0 | 3 |
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| 4-14 | 5 | -2 | 0 | 0 | 4-9 | 12 | 0 | 0 | 4-4 | 8 | 2 | 0 | 4 | 1 | 9 | 2 | 1 | 4 | 8 | 1 | -6 | 1 |
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| 4-14 | 7 | 2 | 1 | 1 | 4-9 | 14 | 1 | 0 | 4-4 | 10 | 8 | 14 | 4 | 1 | 11 | 0 | 3 | 4 | 8 | 3 | -4 | 0 |
| 4-14 | 8 | 1 | 2 | 4 | 4-8 | 1 | 0 | 2 | 4-4 | 11 | 9 | 6 | 4 | 1 | 12 | 3 | 3 | 4 | 8 | 4 | 6 | 4 |
| 4-14 | 9 | 0 | 3 | 4 | 4-8 | 2 | 6 | 5 | 4-4 | 12 | -1 | 2 | 4 | 2 | 0 | 0 | 3 | 4 | 8 | 5 | -6 | 0 |
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| 4-13 | 3 | 1 | 5 | 4 | 4-8 | 6 | 1 | 2 | 4-3 | 3 | 0 | 5 | 4 | 2 | 4 | 225 | 242 | 4 | 9 | 2 | -3 | 0 |
| 4-13 | 4 | 4 | 2 | 2 | 4-8 | 7 | 0 | 2 | 4-3 | 4 | 117 | 112 | 4 | 2 | 5 | 2 | 12 | 4 | 9 | 3 | -2 | 1 |
| 4-13 | 5 | 0 | 1 | 1 | 4-8 | 8 | 37 | 44 | 4-3 | 5 | 17 | 19 | 4 | 2 | 6 | 27 | 25 | 4 | 9 | 4 | -8 | 0 |
| 4-13 | 6 | 2 | 0 | 0 | 4-8 | 9 | 4 | 1 | 4-3 | 6 | 20 | 21 | 4 | 2 | 7 | 2 | 4 | 4 | 9 | 5 | -8 | 1 |
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| 4-13 | 8 | 0 | 3 | 4 | 4-8 | 11 | 0 | 2 | 4-3 | 8 | 53 | 58 | 4 | 2 | 9 | 1 | 1 | 4 | 10 | 1 | 0 | 5 |
| 4-13 | 9 | -6 | 1 | 1 | 4-8 | 12 | 3 | 1 | 4-3 | 9 | 46 | 40 | 4 | 2 | 10 | -3 | 0 | 4 | 10 | 2 | 6 | 3 |
| 4-13 | 10 | -3 | 0 | 0 | 4-8 | 13 | 0 | 0 | 4-3 | 10 | 0 | 5 | 4 | 2 | 11 | 2 | 2 | 4 | 10 | 3 | 3 | 0 |
| 4-13 | 11 | 1 | 0 | 0 | 4-8 | 14 | -1 | 0 | 4-3 | 11 | 30 | 24 | 4 | 3 | 0 | 0 | 1 | 4 | 10 | 4 | -2 | 0 |
| 4-12 | 1 | 2 | 0 | 0 | 4-7 | 1 | 2 | 8 | 4-3 | 12 | 8 | 7 | 4 | 3 | 1 | 9 | 5 | 4 | 11 | 0 | 0 | 0 |
| 4-12 | 2 | 1 | 3 | 4 | 4-7 | 2 | -6 | 3 | 4-3 | 13 | 1 | 2 | 4 | 3 | 2 | 11 | 10 | 4 | 11 | 1 | -11 | 0 |
| 4-12 | 3 | 1 | 0 | 4 | 4-7 | 3 | -1 | 3 | 4-2 | 1 | 14 | 8 | 4 | 3 | 3 | 17 | 11 | 4 | 11 | 2 | 2 | 3 |
| 4-12 | 4 | 4 | 6 | 4 | 4-7 | 4 | 30 | 20 | 4-2 | 2 | -5 | 0 | 4 | 3 | 4 | 120 | 113 | 4 | 12 | 0 | -4 | 2 |
| 4-12 | 5 | 0 | 3 | 4 | 4-7 | 5 | 5 | 1 | 4-2 | 3 | 124 | 111 | 4 | 3 | 5 | -1 | 0 | 4 | 12 | 1 | 3 | 0 |
| 4-12 | 6 | -3 | 0 | 4 | 4-7 | 6 | -5 | 2 | 4-2 | 4 | 38 | 43 | 4 | 3 | 6 | 23 | 25 | 5-12 | 1 | 0 | 2 | 2 |
| 4-12 | 7 | 3 | 0 | 4 | 4-7 | 7 | 14 | 8 | 4-2 | 5 | 510 | 559 | 4 | 3 | 7 | 0 | 0 | 5-12 | 2 | 3 | 2 | 2 |
| 4-12 | 8 | 1 | 0 | 4 | 4-7 | 8 | 2 | 1 | 4-2 | 6 | 1 | 5 | 4 | 3 | 8 | 4 | 7 | 5-12 | 3 | 2 | 2 | 2 |
| 4-12 | 9 | 0 | 1 | 4 | 4-7 | 9 | -5 | 5 | 4-2 | 7 | 53 | 49 | 4 | 3 | 9 | 2 | 0 | 5-12 | 4 | 2 | 0 | 0 |
| 4-12 | 10 | -1 | 1 | 4 | 4-7 | 10 | 3 | 0 | 4-2 | 8 | 4 | 3 | 4 | 3 | 10 | 2 | 4 | 5-12 | 5 | -2 | 1 | 1 |
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| 4-12 | 12 | -1 | 0 | 4 | 4-7 | 12 | 1 | 4 | 4-2 | 10 | 39 | 37 | 4 | 4 | 1 | 0 | 0 | 5-12 | 7 | 1 | 1 | 1 |
| 4-11 | 1 | -5 | 3 | 4 | 4-7 | 13 | 0 | 0 | 4-2 | 11 | 3 | 0 | 4 | 4 | 2 | 35 | 31 | 5-12 | 8 | 0 | 2 | 2 |
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| 4-11 | 3 | -1 | 1 | 4 | 4-6 | 1 | 14 | 7 | 4-2 | 13 | 10 | 8 | 4 | 4 | 4 | 4 | 8 | 5-11 | 1 | 5 | 9 | 9 |
| 4-11 | 4 | 1 | 6 | 4 | 4-6 | 2 | 1 | 0 | 4-1 | 1 | 22 | 17 | 4 | 4 | 5 | 95 | 104 | 5-11 | 2 | -4 | 3 | 3 |

Reflections flagged with an asterisk were considered unobserved.

Obs & Calc for C₂₁H₂₀N₂

| H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc | H | K | L | Obs | Calc |
|------|----|---|-----|------|-----|----|---|-----|------|------|---|---|-----|------|------|---|---|-----|------|
| 5-11 | 3 | | -2 | 2 | 5-5 | 2 | | 9 | 8 | 5 1 | 2 | | -1 | 7 | 5 10 | 1 | | 1 | 0 |
| 5-11 | 4 | | -2 | 0 | 5-5 | 3 | | 3 | 8 | 5 1 | 3 | | 261 | 250 | 6-9 | 1 | | 2 | 3 |
| 5-11 | 5 | | 0 | 2 | 5-5 | 4 | | 7 | 6 | 5 1 | 4 | | 38 | 38 | 6-9 | 2 | | 0 | 5 |
| 5-11 | 6 | | 0 | 0 | 5-5 | 5 | | 9 | 11 | 5 1 | 5 | | 93 | 97 | 6-9 | 3 | | 0 | 4 |
| 5-11 | 7 | | 0 | 1 | 5-5 | 6 | | 20 | 23 | 5 1 | 6 | | 4 | 1 | 6-9 | 4 | | 0 | 1 |
| 5-11 | 8 | | -1 | 3 | 5-5 | 7 | | -1 | 0 | 5 1 | 7 | | 2 | 3 | 6-9 | 5 | | 2 | 1 |
| 5-11 | 9 | | -5 | 0 | 5-5 | 8 | | 12 | 14 | 5 1 | 8 | | 9 | 12 | 6-9 | 6 | | -1 | 1 |
| 5-11 | 10 | | 0 | 0 | 5-5 | 9 | | 6 | 2 | 5 1 | 9 | | -1 | 1 | 6-8 | 1 | | 4 | 4 |
| 5-10 | 1 | | -1 | 1 | 5-5 | 10 | | 2 | 2 | 5 2 | 0 | | 42 | 31 | 6-8 | 2 | | 5 | 9 |
| 5-10 | 2 | | 0 | 2 | 5-5 | 11 | | 1 | 2 | 5 2 | 1 | | 87 | 80 | 6-8 | 3 | | -4 | 2 |
| 5-10 | 3 | | 7 | 7 | 5-4 | 1 | | 29 | 22 | 5 2 | 2 | | 38 | 37 | 6-8 | 4 | | 0 | 0 |
| 5-10 | 4 | | -9 | 2 | 5-4 | 2 | | 14 | 12 | 5 2 | 3 | | 2 | 2 | 6-8 | 5 | | 2 | 0 |
| 5-10 | 5 | | 0 | 0 | 5-4 | 3 | | 19 | 22 | 5 2 | 4 | | -6 | 0 | 6-8 | 6 | | 0 | 0 |
| 5-10 | 6 | | 3 | 0 | 5-4 | 4 | | 3 | 2 | 5 2 | 5 | | 16 | 14 | 6-8 | 7 | | 2 | 3 |
| 5-10 | 7 | | 0 | 0 | 5-4 | 5 | | 15 | 14 | 5 2 | 6 | | 6 | 7 | 6-7 | 1 | | 1 | 4 |
| 5-10 | 8 | | 2 | 2 | 5-4 | 6 | | -12 | 0 | 5 2 | 7 | | 1 | 0 | 6-7 | 2 | | 2 | 2 |
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| 5-10 | 10 | | -1 | 4 | 5-4 | 8 | | 35 | 38 | 5 2 | 9 | | 6 | 4 | 6-7 | 4 | | 2 | 3 |
| 5-10 | 11 | | -1 | 1 | 5-4 | 9 | | 3 | 2 | 5 3 | 0 | | 74 | 74 | 6-7 | 5 | | 1 | 0 |
| 5-9 | 1 | | 11 | 8 | 5-4 | 10 | | 15 | 13 | 5 3 | 1 | | 18 | 16 | 6-7 | 6 | | 8 | 8 |
| 5-9 | 2 | | -3 | 1 | 5-4 | 11 | | 4 | 4 | 5 3 | 2 | | 18 | 20 | 6-7 | 7 | | -3 | 1 |
| 5-9 | 3 | | 0 | 3 | 5-3 | 1 | | -2 | 4 | 5 3 | 3 | | 69 | 71 | 6-7 | 8 | | 7 | 9 |
| 5-9 | 4 | | 1 | 1 | 5-3 | 2 | | 41 | 45 | 5 3 | 4 | | 16 | 19 | 6-6 | 1 | | 3 | 0 |
| 5-9 | 5 | | 3 | 0 | 5-3 | 3 | | -16 | 1 | 5 3 | 5 | | -7 | 6 | 6-6 | 2 | | -4 | 0 |
| 5-9 | 6 | | -3 | 0 | 5-3 | 4 | | 7 | 4 | 5 3 | 6 | | -1 | 1 | 6-6 | 3 | | -4 | 0 |
| 5-9 | 7 | | 1 | 1 | 5-3 | 5 | | 5 | 6 | 5 3 | 7 | | -2 | 1 | 6-6 | 4 | | -1 | 0 |
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| 5-9 | 9 | | 4 | 1 | 5-3 | 7 | | 21 | 16 | 5 4 | 0 | | 0 | 1 | 6-6 | 6 | | 1 | 1 |
| 5-9 | 10 | | 0 | 2 | 5-3 | 8 | | 0 | 0 | 5 4 | 1 | | 24 | 16 | 6-6 | 7 | | -2 | 3 |
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| 5-8 | 3 | | 2 | 1 | 5-2 | 1 | | 34 | 26 | 5 4 | 5 | | -4 | 1 | 6-5 | 3 | | 2 | 5 |
| 5-8 | 4 | | 4 | 2 | 5-2 | 2 | | -8 | 0 | 5 4 | 6 | | -8 | 0 | 6-5 | 4 | | -3 | 1 |
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| 5-8 | 6 | | 15 | 14 | 5-2 | 4 | | -1 | 1 | 5 4 | 8 | | 0 | 0 | 6-5 | 6 | | -1 | 2 |
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| 5-8 | 8 | | 2 | 3 | 5-2 | 6 | | 0 | 6 | 5 5 | 1 | | 2 | 3 | 6-5 | 8 | | 0 | 0 |
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| 5-8 | 10 | | 2 | 2 | 5-2 | 8 | | 5 | 5 | 5 5 | 3 | | 21 | 15 | 6-4 | 2 | | 0 | 2 |
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| 5-7 | 4 | | -1 | 2 | 5-1 | 2 | | 33 | 34 | 5 6 | 0 | | 12 | 11 | 6-4 | 7 | | 0 | 1 |
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| 5-7 | 6 | | -5 | 1 | 5-1 | 4 | | 9 | 13 | 5 6 | 2 | | 19 | 23 | 6-3 | 1 | | 3 | 5 |
| 5-7 | 7 | | 2 | 3 | 5-1 | 5 | | 14 | 16 | 5 6 | 3 | | -5 | 0 | 6-3 | 2 | | 4 | 6 |
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| 5-7 | 10 | | 1 | 3 | 5-1 | 8 | | 24 | 13 | 5 6 | 6 | | 4 | 4 | 6-3 | 5 | | -1 | 6 |
| 5-7 | 11 | | -1 | 2 | 5-1 | 9 | | 5 | 7 | 5 7 | 0 | | -4 | 1 | 6-3 | 6 | | 0 | 0 |
| 5-7 | 12 | | 5 | 6 | 5-1 | 10 | | -3 | 0 | 5 7 | 1 | | 14 | 11 | 6-3 | 7 | | -6 | 0 |
| 5-6 | 1 | | 20 | 22 | 5 0 | 0 | | 0 | 0 | 5 7 | 2 | | 0 | 0 | 6-3 | 8 | | 3 | 1 |
| 5-6 | 2 | | -1 | 0 | 5 0 | 1 | | 42 | 34 | 5 7 | 3 | | 6 | 6 | 6-2 | 1 | | 11 | 15 |
| 5-6 | 3 | | 2 | 3 | 5 0 | 2 | | -1 | 3 | 5 7 | 4 | | -3 | 1 | 6-2 | 2 | | 0 | 0 |
| 5-6 | 4 | | -4 | 1 | 5 0 | 3 | | 191 | 181 | 5 7 | 5 | | 0 | 0 | 6-2 | 3 | | 1 | 0 |
| 5-6 | 5 | | -4 | 0 | 5 0 | 4 | | -1 | 4 | 5 8 | 0 | | 1 | 4 | 6-2 | 4 | | -1 | 3 |
| 5-6 | 6 | | 3 | 3 | 5 0 | 5 | | 0 | 9 | 5 8 | 1 | | 12 | 15 | 6-2 | 5 | | 14 | 10 |
| 5-6 | 7 | | -5 | 11 | 5 0 | 6 | | 30 | 29 | 5 8 | 2 | | 0 | 2 | 6-2 | 6 | | 1 | 1 |
| 5-6 | 8 | | -3 | 0 | 5 0 | 7 | | 3 | 1 | 5 8 | 3 | | 2 | 2 | 6-2 | 7 | | 5 | 4 |
| 5-6 | 9 | | 3 | 3 | 5 0 | 8 | | -3 | 1 | 5 8 | 4 | | 0 | 1 | 6-2 | 8 | | 8 | 6 |
| 5-6 | 10 | | 7 | 2 | 5 0 | 9 | | 1 | 1 | 5 9 | 0 | | 1 | 1 | 6-1 | 1 | | 4 | 0 |
| 5-6 | 11 | | 1 | 6 | 5 0 | 10 | | 12 | 8 | 5 9 | 1 | | 1 | 0 | 6-1 | 2 | | 10 | 9 |
| 5-6 | 12 | | 2 | 3 | 5 1 | 0 | | 23 | 27 | 5 9 | 2 | | 20 | 18 | 6-1 | 3 | | 5 | 3 |
| 5-5 | 1 | | 1 | 0 | 5 1 | 1 | | 21 | 27 | 5 10 | 0 | | 7 | 6 | 6-1 | 4 | | -2 | 5 |

an asterisk were considered unobserved.

Reflections flagged with