

III. Observed and fitted positions of the **nu_3** excited state, assuming gnd state fitted to combination differences from JILA data (nu_3 and nu_4 bands) plus Miller's LIF data

Residual std
 dev: 0.0029

| Excited state (v=1): | | | Gnd State (v=0): | | | Observed [cm ⁻¹] | Calculated [cm ⁻¹] | Obs-Calc [cm ⁻¹] | Weighting factors |
|----------------------|-----|-----|------------------|------|------|---------------------------------|-----------------------------------|---------------------------------|----------------------|
| J' | Ka' | Kc' | J'' | Ka'' | Kc'' | | | | |
| P | | | | | | | | | |
| Branch | | | | | | | | | |
| 4 | 1 | 4 | 5 | 0 | 5 | 3072.5845 | 3072.5849 | -0.0004 | 1 |
| 4 | 0 | 4 | 5 | 1 | 5 | 3072.5475 | 3072.5503 | -0.0028 | 1 |
| 5 | 1 | 5 | 6 | 0 | 6 | 3072.4538 | 3072.4542 | -0.0004 | 1 |
| 5 | 0 | 5 | 6 | 1 | 6 | 3072.4364 | 3072.4377 | -0.0013 | 1 |
| 6 | 1 | 6 | 7 | 0 | 7 | 3072.3273 | 3072.3281 | -0.0008 | 1 |
| 6 | 2 | 5 | 7 | 1 | 6 | 3072.2664 | 3072.268 | -0.0017 | 1 |
| 6 | 0 | 6 | 7 | 1 | 7 | 3072.3197 | 3072.3208 | -0.0011 | 1 |
| 7 | 1 | 7 | 8 | 0 | 8 | 3072.2033 | 3072.2045 | -0.0011 | 1 |
| 7 | 2 | 6 | 8 | 1 | 7 | 3072.1171 | 3072.1145 | 0.0027 | 1 |
| 7 | 0 | 7 | 8 | 1 | 8 | 3072.1992 | 3072.2013 | -0.0021 | 1 |
| 7 | 1 | 6 | 8 | 2 | 7 | 3072.0427 | 3072.0408 | 0.0019 | 1 |
| 8 | 1 | 8 | 9 | 0 | 9 | 3072.0801 | 3072.0819 | -0.0018 | 0.5 |
| 8 | 2 | 7 | 9 | 1 | 8 | 3071.9739 | 3071.9742 | -0.0003 | 0.5 |
| 8 | 0 | 8 | 9 | 1 | 9 | 3072.0801 | 3072.0807 | -0.0005 | 0.5 |
| 8 | 1 | 7 | 9 | 2 | 8 | 3071.9347 | 3071.9368 | -0.0021 | 0.5 |
| 9 | 1 | 9 | 10 | 0 | 10 | 3071.9579 | 3071.9599 | -0.002 | 0.5 |
| 9 | 2 | 8 | 10 | 1 | 9 | 3071.8399 | 3071.8425 | -0.0026 | 1 |
| 9 | 0 | 9 | 10 | 1 | 10 | 3071.9579 | 3071.9594 | -0.0015 | 0.5 |
| 9 | 1 | 8 | 10 | 2 | 9 | 3071.8206 | 3071.8247 | -0.0041 | 1 |
| 10 | 1 | 10 | 11 | 0 | 11 | 3071.8367 | 3071.838 | -0.0013 | 0.5 |
| 10 | 2 | 9 | 11 | 1 | 10 | 3071.7131 | 3071.7156 | -0.0024 | 1 |
| 10 | 0 | 10 | 11 | 1 | 11 | 3071.8367 | 3071.8378 | -0.0011 | 0.5 |
| 10 | 1 | 9 | 11 | 2 | 10 | 3071.7072 | 3071.7075 | -0.0002 | 1 |
| 11 | 1 | 11 | 12 | 0 | 12 | 3071.7146 | 3071.7162 | -0.0017 | 0.5 |
| 11 | 2 | 10 | 12 | 1 | 11 | 3071.5867 | 3071.5911 | -0.0043 | 1 |
| 11 | 0 | 11 | 12 | 1 | 12 | 3071.7146 | 3071.7161 | -0.0016 | 0.5 |
| 11 | 1 | 10 | 12 | 2 | 11 | 3071.5834 | 3071.5875 | -0.0041 | 1 |
| 12 | 1 | 12 | 13 | 0 | 13 | 3071.5921 | 3071.5944 | -0.0024 | 0.5 |

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|----|---|----|----|---|----|-----------|-----------|---------|-----|
| 12 | 2 | 11 | 13 | 1 | 12 | 3071.4635 | 3071.4677 | -0.0042 | 0.5 |
| 12 | 0 | 12 | 13 | 1 | 13 | 3071.5921 | 3071.5944 | -0.0023 | 0.5 |
| 12 | 1 | 11 | 13 | 2 | 12 | 3071.4635 | 3071.4662 | -0.0027 | 0.5 |
| 13 | 1 | 13 | 14 | 0 | 14 | 3071.4673 | 3071.4726 | -0.0053 | 0.5 |
| 13 | 2 | 12 | 14 | 1 | 13 | 3071.3393 | 3071.3449 | -0.0056 | 0.5 |
| 13 | 0 | 13 | 14 | 1 | 14 | 3071.4673 | 3071.4726 | -0.0053 | 0.5 |
| 13 | 1 | 12 | 14 | 2 | 13 | 3071.3393 | 3071.3442 | -0.0049 | 0.5 |
| 14 | 1 | 14 | 15 | 0 | 15 | 3071.3471 | 3071.3507 | -0.0036 | 0.5 |
| 14 | 2 | 13 | 15 | 1 | 14 | 3071.2204 | 3071.2222 | -0.0018 | 0.5 |
| 14 | 0 | 14 | 15 | 1 | 15 | 3071.3471 | 3071.3507 | -0.0036 | 0.5 |
| 14 | 1 | 13 | 15 | 2 | 14 | 3071.2204 | 3071.2219 | -0.0015 | 0.5 |
| 15 | 1 | 15 | 16 | 0 | 16 | 3071.2285 | 3071.2289 | -0.0003 | 0.5 |
| 15 | 0 | 15 | 16 | 1 | 16 | 3071.2285 | 3071.2289 | -0.0003 | 0.5 |
| 16 | 1 | 16 | 17 | 0 | 17 | 3071.1026 | 3071.1069 | -0.0043 | 0.5 |
| 16 | 0 | 16 | 17 | 1 | 17 | 3071.1026 | 3071.1069 | -0.0043 | 0.5 |
| 17 | 1 | 17 | 18 | 0 | 18 | 3070.9809 | 3070.985 | -0.0041 | 0.5 |
| 17 | 0 | 17 | 18 | 1 | 18 | 3070.9809 | 3070.985 | -0.0041 | 0.5 |
| 18 | 1 | 18 | 19 | 0 | 19 | 3070.8578 | 3070.863 | -0.0052 | 0.5 |
| 18 | 0 | 18 | 19 | 1 | 19 | 3070.8578 | 3070.863 | -0.0052 | 0.5 |
| 19 | 1 | 19 | 20 | 0 | 20 | 3070.7369 | 3070.741 | -0.0041 | 0.5 |
| 19 | 0 | 19 | 20 | 1 | 20 | 3070.7369 | 3070.741 | -0.0041 | 0.5 |
| 20 | 1 | 20 | 21 | 0 | 21 | 3070.6149 | 3070.619 | -0.004 | 0.5 |
| 20 | 0 | 20 | 21 | 1 | 21 | 3070.6149 | 3070.619 | -0.004 | 0.5 |

R Branch:

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| 5 | 1 | 5 | 4 | 0 | 4 | 3073.9187 | 3073.9173 | 0.0014 | 1 |
| 5 | 0 | 5 | 4 | 1 | 4 | 3073.8827 | 3073.8818 | 0.001 | 1 |
| 6 | 1 | 6 | 5 | 0 | 5 | 3074.0302 | 3074.0287 | 0.0014 | 1 |
| 6 | 0 | 6 | 5 | 1 | 5 | 3074.0123 | 3074.0116 | 0.0007 | 1 |
| 7 | 1 | 7 | 6 | 0 | 6 | 3074.146 | 3074.1443 | 0.0017 | 1 |
| 7 | 2 | 6 | 6 | 1 | 5 | 3074.3294 | 3074.3291 | 0.0003 | 1 |
| 7 | 0 | 7 | 6 | 1 | 6 | 3074.1382 | 3074.1366 | 0.0016 | 1 |
| 7 | 1 | 6 | 6 | 2 | 5 | 3074.1964 | 3074.1931 | 0.0034 | 1 |
| 8 | 1 | 8 | 7 | 0 | 7 | 3074.264 | 3074.2625 | 0.0016 | 1 |
| 8 | 2 | 7 | 7 | 1 | 6 | 3074.4236 | 3074.4205 | 0.0031 | 1 |
| 8 | 0 | 8 | 7 | 1 | 7 | 3074.26 | 3074.2591 | 0.0008 | 1 |
| 8 | 1 | 7 | 7 | 2 | 6 | 3074.3453 | 3074.3444 | 0.0008 | 1 |
| 9 | 1 | 9 | 8 | 0 | 8 | 3074.3851 | 3074.3818 | 0.0033 | 1 |
| 9 | 2 | 8 | 8 | 1 | 7 | 3074.5227 | 3074.5213 | 0.0014 | 1 |
| 9 | 0 | 9 | 8 | 1 | 8 | 3074.3825 | 3074.3804 | 0.002 | 1 |
| 9 | 1 | 8 | 8 | 2 | 7 | 3074.482 | 3074.4822 | -0.0002 | 1 |

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|----|---|----|----|---|----|-----------|-----------|---------|-----|
| 10 | 1 | 10 | 9 | 0 | 9 | 3074.5038 | 3074.5017 | 0.0021 | 0.5 |
| 10 | 2 | 9 | 9 | 1 | 8 | 3074.6323 | 3074.6301 | 0.0022 | 1 |
| 10 | 0 | 10 | 9 | 1 | 9 | 3074.5038 | 3074.5012 | 0.0026 | 0.5 |
| 10 | 1 | 9 | 9 | 2 | 8 | 3074.6115 | 3074.6112 | 0.0003 | 1 |
| 11 | 1 | 11 | 10 | 0 | 10 | 3074.6252 | 3074.6219 | 0.0033 | 0.5 |
| 11 | 2 | 10 | 10 | 1 | 9 | 3074.7475 | 3074.744 | 0.0035 | 1 |
| 11 | 0 | 11 | 10 | 1 | 10 | 3074.6252 | 3074.6216 | 0.0035 | 0.5 |
| 11 | 1 | 10 | 10 | 2 | 9 | 3074.7383 | 3074.7353 | 0.003 | 1 |
| 12 | 1 | 12 | 11 | 0 | 11 | 3074.7443 | 3074.7421 | 0.0022 | 0.5 |
| 12 | 2 | 11 | 11 | 1 | 10 | 3074.8608 | 3074.8608 | 0 | 1 |
| 12 | 0 | 12 | 11 | 1 | 11 | 3074.7443 | 3074.742 | 0.0023 | 0.5 |
| 12 | 1 | 11 | 11 | 2 | 10 | 3074.8577 | 3074.8569 | 0.0008 | 1 |
| 13 | 1 | 13 | 12 | 0 | 12 | 3074.8618 | 3074.8623 | -0.0005 | 0.5 |
| 13 | 2 | 12 | 12 | 1 | 11 | 3074.9785 | 3074.979 | -0.0005 | 1 |
| 13 | 0 | 13 | 12 | 1 | 12 | 3074.8618 | 3074.8623 | -0.0004 | 0.5 |
| 13 | 1 | 12 | 12 | 2 | 11 | 3074.9767 | 3074.9773 | -0.0006 | 1 |
| 14 | 1 | 14 | 13 | 0 | 13 | 3074.9845 | 3074.9825 | 0.0019 | 0.5 |
| 14 | 2 | 13 | 13 | 1 | 12 | 3075.0998 | 3075.0978 | 0.002 | 0.5 |
| 14 | 0 | 14 | 13 | 1 | 13 | 3074.9845 | 3074.9825 | 0.0019 | 0.5 |
| 14 | 1 | 13 | 13 | 2 | 12 | 3075.0998 | 3075.0971 | 0.0028 | 0.5 |
| 16 | 1 | 16 | 15 | 0 | 15 | 3075.2248 | 3075.2229 | 0.0019 | 0.5 |
| 16 | 2 | 15 | 15 | 1 | 14 | 3075.3348 | 3075.3362 | -0.0014 | 0.5 |
| 16 | 0 | 16 | 15 | 1 | 15 | 3075.2248 | 3075.2229 | 0.0019 | 0.5 |
| 16 | 1 | 15 | 15 | 2 | 14 | 3075.3348 | 3075.3361 | -0.0013 | 0.5 |
| 17 | 1 | 17 | 16 | 0 | 16 | 3075.3457 | 3075.3431 | 0.0027 | 0.5 |
| 17 | 2 | 16 | 16 | 1 | 15 | 3075.4534 | 3075.4555 | -0.0021 | 0.5 |
| 17 | 0 | 17 | 16 | 1 | 16 | 3075.3457 | 3075.3431 | 0.0027 | 0.5 |
| 17 | 1 | 16 | 16 | 2 | 15 | 3075.4534 | 3075.4555 | -0.002 | 0.5 |
| 18 | 1 | 18 | 17 | 0 | 17 | 3075.4647 | 3075.4632 | 0.0015 | 0.5 |
| 18 | 2 | 17 | 17 | 1 | 16 | 3075.5816 | 3075.5748 | 0.0068 | 0.5 |
| 18 | 0 | 18 | 17 | 1 | 17 | 3075.4647 | 3075.4632 | 0.0015 | 0.5 |
| 18 | 1 | 17 | 17 | 2 | 16 | 3075.5816 | 3075.5748 | 0.0068 | 0.5 |
| 19 | 1 | 19 | 18 | 0 | 18 | 3075.5856 | 3075.5833 | 0.0024 | 0.5 |
| 19 | 2 | 18 | 18 | 1 | 17 | 3075.6974 | 3075.6941 | 0.0032 | 0.5 |
| 19 | 0 | 19 | 18 | 1 | 18 | 3075.5856 | 3075.5833 | 0.0024 | 0.5 |
| 19 | 1 | 18 | 18 | 2 | 17 | 3075.6974 | 3075.6941 | 0.0033 | 0.5 |
| 20 | 1 | 20 | 19 | 0 | 19 | 3075.7061 | 3075.7033 | 0.0027 | 0.5 |
| 20 | 2 | 19 | 19 | 1 | 18 | 3075.8143 | 3075.8134 | 0.0009 | 0.5 |
| 20 | 0 | 20 | 19 | 1 | 19 | 3075.7061 | 3075.7033 | 0.0027 | 0.5 |
| 20 | 1 | 19 | 19 | 2 | 18 | 3075.8143 | 3075.8134 | 0.0009 | 0.5 |
| 21 | 1 | 21 | 20 | 0 | 20 | 3075.8256 | 3075.8233 | 0.0022 | 0.5 |

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|----|---|----|----|---|----|-----------|-----------|--------|-----|
| 21 | 2 | 20 | 20 | 1 | 19 | 3075.9346 | 3075.9327 | 0.0019 | 0.5 |
| 21 | 0 | 21 | 20 | 1 | 20 | 3075.8256 | 3075.8233 | 0.0022 | 0.5 |
| 21 | 1 | 20 | 20 | 2 | 19 | 3075.9346 | 3075.9327 | 0.0019 | 0.5 |
| 22 | 1 | 22 | 21 | 0 | 21 | 3075.9437 | 3075.9433 | 0.0004 | 0.5 |
| 22 | 0 | 22 | 21 | 1 | 21 | 3075.9437 | 3075.9433 | 0.0004 | 0.5 |