Table S1. Measured and predicted transitions and selected predicted transitions in band 3 spectral region (84–116 GHz) of DMSO.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| *J’* | *K*a’ | *K*c’ | *J’’* | *K*a’’ | *K*c’’ | Sym | Calc/MHz | Diff/MHz | Obs/MHz |
| 1 | 1 | 1 | 0 | 0 | 0 | /AA | 11255.3536a | -0.0049 | 11255.35 |
| 1 | 1 | 1 | 0 | 0 | 0 | /EE | 11255.3509 | -0.0022 | 11255.35 |
| 1 | 1 | 1 | 0 | 0 | 0 | /AE | 11255.3482 | 0.0005 | 11255.35 |
| 1 | 1 | 1 | 0 | 0 | 0 | /EA | 11255.3482 | 0.0005 | 11255.35 |
| 4 | 2 | 2 | 3 | 1 | 3 | /AA | 69504.4424 | -0.0024 | 69504.44 |
| 4 | 2 | 2 | 3 | 1 | 3 | /EE | 69504.4197 | 0.0203 | 69504.44 |
| 4 | 2 | 2 | 3 | 1 | 3 | /AE | 69504.397 | 0.043 | 69504.44 |
| 4 | 2 | 2 | 3 | 1 | 3 | /EA | 69504.397 | 0.043 | 69504.44 |
| 4 | 3 | 1 | 3 | 2 | 2 | /AA | 63435.4847 | -0.0047 | 63435.48 |
| 4 | 3 | 1 | 3 | 2 | 2 | /EE | 63435.4721 | 0.0079 | 63435.48 |
| 4 | 3 | 1 | 3 | 2 | 2 | /AE | 63435.4595 | 0.0205 | 63435.48 |
| 4 | 3 | 1 | 3 | 2 | 2 | /EA | 63435.4595 | 0.0205 | 63435.48 |
| 4 | 3 | 2 | 3 | 0 | 3 | /AA | 69568.964 | 0.026 | 69568.99 |
| 4 | 3 | 2 | 3 | 0 | 3 | /EE | 69568.9398 | 0.0502 | 69568.99 |
| 4 | 3 | 2 | 3 | 0 | 3 | /AE | 69568.9156 | 0.0744 | 69568.99 |
| 4 | 3 | 2 | 3 | 0 | 3 | /EA | 69568.9156 | 0.0744 | 69568.99 |
| 4 | 4 | 1 | 3 | 1 | 2 | /AA | 64714.0517 | -0.0217 | 64714.03 |
| 4 | 4 | 1 | 3 | 1 | 2 | /EE | 64714.0226 | 0.0074 | 64714.03 |
| 4 | 4 | 1 | 3 | 1 | 2 | /AE | 64713.9935 | 0.0365 | 64714.03 |
| 4 | 4 | 1 | 3 | 1 | 2 | /EA | 64713.9935 | 0.0365 | 64714.03 |
| 5 | 1 | 4 | 4 | 0 | 4 | /AA | 69725.898 | 0.002 | 69725.9 |
| 5 | 1 | 4 | 4 | 0 | 4 | /EE | 69725.8797 | 0.0203 | 69725.9 |
| 5 | 1 | 4 | 4 | 0 | 4 | /AE | 69725.8615 | 0.0385 | 69725.9 |
| 5 | 1 | 4 | 4 | 0 | 4 | /EA | 69725.8615 | 0.0385 | 69725.9 |
| 5 | 2 | 3 | 4 | 1 | 3 | /AA | 69719.0547 | 0.0453 | 69719.1 |
| 5 | 2 | 3 | 4 | 1 | 3 | /EE | 69719.0368 | 0.0632 | 69719.1 |
| 5 | 2 | 3 | 4 | 1 | 3 | /AE | 69719.0188 | 0.0812 | 69719.1 |
| 5 | 2 | 3 | 4 | 1 | 3 | /EA | 69719.0188 | 0.0812 | 69719.1 |
| 5 | 2 | 4 | 4 | 1 | 4 | /AA | 69725.9115 | -0.0115 | 69725.9 |
| 5 | 2 | 4 | 4 | 1 | 4 | /EE | 69725.8932 | 0.0068 | 69725.9 |
| 5 | 2 | 4 | 4 | 1 | 4 | /AE | 69725.8749 | 0.0251 | 69725.9 |
| 5 | 2 | 4 | 4 | 1 | 4 | /EA | 69725.8749 | 0.0251 | 69725.9 |
| 5 | 3 | 2 | 4 | 4 | 1 | /AA | 60694.1188 | 0.0112 | 60694.13 |
| 5 | 3 | 2 | 4 | 4 | 1 | /EE | 60694.1175 | 0.0125 | 60694.13 |
| 5 | 3 | 2 | 4 | 4 | 1 | /AE | 60694.1163 | 0.0137 | 60694.13 |
| 5 | 3 | 2 | 4 | 4 | 1 | /EA | 60694.1163 | 0.0137 | 60694.13 |
| 5 | 3 | 2 | 4 | 2 | 2 | /AA | 69659.2322 | -0.0522 | 69659.18 |
| 5 | 3 | 2 | 4 | 2 | 2 | /EE | 69659.2157 | -0.0357 | 69659.18 |
| 5 | 3 | 2 | 4 | 2 | 2 | /AE | 69659.1992 | -0.0192 | 69659.18 |
| 5 | 3 | 2 | 4 | 2 | 2 | /EA | 69659.1992 | -0.0192 | 69659.18 |
| 5 | 3 | 3 | 4 | 2 | 3 | /AA | 69721.0093 | 0.0207 | 69721.03 |
| 5 | 3 | 3 | 4 | 2 | 3 | /EE | 69720.9913 | 0.0387 | 69721.03 |
| 5 | 3 | 3 | 4 | 2 | 3 | /AE | 69720.9732 | 0.0568 | 69721.03 |
| 5 | 3 | 3 | 4 | 2 | 3 | /EA | 69720.9732 | 0.0568 | 69721.03 |
| 5 | 4 | 1 | 4 | 3 | 2 | /AA | 77083.1787 | 0.0113 | 77083.19 |
| 5 | 4 | 1 | 4 | 3 | 2 | /EE | 77083.1661 | 0.0239 | 77083.19 |
| 5 | 4 | 1 | 4 | 3 | 2 | /AE | 77083.1536 | 0.0364 | 77083.19 |
| 5 | 4 | 1 | 4 | 3 | 2 | /EA | 77083.1536 | 0.0364 | 77083.19 |
| 5 | 4 | 1 | 4 | 3 | 1 | /AA | 69439.5082 | -0.0082 | 69439.5 |
| 5 | 4 | 1 | 4 | 3 | 1 | /EE | 69439.4934 | 0.0066 | 69439.5 |
| 5 | 4 | 1 | 4 | 3 | 1 | /AE | 69439.4786 | 0.0214 | 69439.5 |
| 5 | 4 | 1 | 4 | 3 | 1 | /EA | 69439.4786 | 0.0214 | 69439.5 |
| 5 | 4 | 2 | 4 | 3 | 1 | /AA | 62100.4323 | -0.0323 | 62100.4 |
| 5 | 4 | 2 | 4 | 3 | 1 | /EE | 62100.4115 | -0.0115 | 62100.4 |
| 5 | 4 | 2 | 4 | 3 | 1 | /AE | 62100.3908 | 0.0092 | 62100.4 |
| 5 | 4 | 2 | 4 | 3 | 1 | /EA | 62100.3908 | 0.0092 | 62100.4 |
| 5 | 4 | 2 | 4 | 3 | 2 | /AA | 69744.1028 | 0.0372 | 69744.14 |
| 5 | 4 | 2 | 4 | 3 | 2 | /EE | 69744.0843 | 0.0557 | 69744.14 |
| 5 | 4 | 2 | 4 | 3 | 2 | /AE | 69744.0658 | 0.0742 | 69744.14 |
| 5 | 4 | 2 | 4 | 3 | 2 | /EA | 69744.0658 | 0.0742 | 69744.14 |
| 5 | 5 | 0 | 4 | 4 | 1 | /AA | 71997.8481 | 0.0019 | 71997.85 |
| 5 | 5 | 0 | 4 | 4 | 1 | /EE | 71997.8327 | 0.0173 | 71997.85 |
| 5 | 5 | 0 | 4 | 4 | 1 | /AE | 71997.8173 | 0.0327 | 71997.85 |
| 5 | 5 | 0 | 4 | 4 | 1 | /EA | 71997.8174 | 0.0326 | 71997.85 |
| 5 | 5 | 0 | 4 | 4 | 0 | /AA | 69818.6721 | -0.0321 | 69818.64 |
| 5 | 5 | 0 | 4 | 4 | 0 | /EE | 69818.6518 | -0.0118 | 69818.64 |
| 5 | 5 | 0 | 4 | 4 | 0 | /AE | 69818.6316 | 0.0084 | 69818.64 |
| 5 | 5 | 0 | 4 | 4 | 0 | /EA | 69818.6316 | 0.0084 | 69818.64 |
| 5 | 5 | 1 | 4 | 2 | 2 | /AA | 79031.5989 | -0.0389 | 79031.56 |
| 5 | 5 | 1 | 4 | 2 | 2 | /EE | 79031.561 | -0.001 | 79031.56 |
| 5 | 5 | 1 | 4 | 2 | 2 | /AE | 79031.5232 | 0.0368 | 79031.56 |
| 5 | 5 | 1 | 4 | 2 | 2 | /EA | 79031.5231 | 0.0369 | 79031.56 |
| 5 | 5 | 1 | 4 | 4 | 0 | /AA | 67887.3094 | -0.0394 | 67887.27 |
| 5 | 5 | 1 | 4 | 4 | 0 | /EE | 67887.282 | -0.012 | 67887.27 |
| 5 | 5 | 1 | 4 | 4 | 0 | /AE | 67887.2545 | 0.0155 | 67887.27 |
| 5 | 5 | 1 | 4 | 4 | 0 | /EA | 67887.2545 | 0.0155 | 67887.27 |
| 5 | 5 | 1 | 4 | 4 | 1 | /AA | 70066.4855 | -0.0355 | 70066.45 |
| 5 | 5 | 1 | 4 | 4 | 1 | /EE | 70066.4629 | -0.0129 | 70066.45 |
| 5 | 5 | 1 | 4 | 4 | 1 | /AE | 70066.4403 | 0.0097 | 70066.45 |
| 5 | 5 | 1 | 4 | 4 | 1 | /EA | 70066.4403 | 0.0097 | 70066.45 |
| 6 | 2 | 4 | 5 | 3 | 3 | /AA | 64394.8377 | 0.0123 | 64394.85 |
| 6 | 2 | 4 | 5 | 3 | 3 | /EE | 64394.8287 | 0.0213 | 64394.85 |
| 6 | 2 | 4 | 5 | 3 | 3 | /AE | 64394.8196 | 0.0304 | 64394.85 |
| 6 | 2 | 4 | 5 | 3 | 3 | /EA | 64394.8196 | 0.0304 | 64394.85 |
| 6 | 3 | 3 | 5 | 4 | 2 | /AA | 69839.7205 | -0.0205 | 69839.7 |
| 6 | 3 | 3 | 5 | 4 | 2 | /EE | 69839.7094 | -0.0094 | 69839.7 |
| 6 | 3 | 3 | 5 | 4 | 2 | /AE | 69839.6983 | 0.0017 | 69839.7 |
| 6 | 3 | 3 | 5 | 4 | 2 | /EA | 69839.6983 | 0.0017 | 69839.7 |
| 6 | 3 | 4 | 5 | 2 | 3 | /AA | 64397.5206 | -0.0006 | 64397.52 |
| 6 | 3 | 4 | 5 | 2 | 3 | /EE | 64397.5115 | 0.0085 | 64397.52 |
| 6 | 3 | 4 | 5 | 2 | 3 | /AE | 64397.5023 | 0.0177 | 64397.52 |
| 6 | 3 | 4 | 5 | 2 | 3 | /EA | 64397.5023 | 0.0177 | 64397.52 |
| 6 | 4 | 3 | 5 | 3 | 2 | /AA | 69996.8253 | -0.0253 | 69996.8 |
| 6 | 4 | 3 | 5 | 3 | 2 | /EE | 69996.8105 | -0.0105 | 69996.8 |
| 6 | 4 | 3 | 5 | 3 | 2 | /AE | 69996.7957 | 0.0043 | 69996.8 |
| 6 | 4 | 3 | 5 | 3 | 2 | /EA | 69996.7957 | 0.0043 | 69996.8 |
| 6 | 5 | 2 | 5 | 4 | 1 | /AA | 76360.197 | -0.017 | 76360.18 |
| 6 | 5 | 2 | 5 | 4 | 1 | /EE | 76360.169 | 0.011 | 76360.18 |
| 6 | 5 | 2 | 5 | 4 | 1 | /AE | 76360.141 | 0.039 | 76360.18 |
| 6 | 5 | 2 | 5 | 4 | 1 | /EA | 76360.1409 | 0.0391 | 76360.18 |
| 7 | 0 | 7 | 6 | 1 | 6 | /AA | 61815.3559 | 0.0241 | 61815.38 |
| 7 | 0 | 7 | 6 | 1 | 6 | /EE | 61815.3541 | 0.0259 | 61815.38 |
| 7 | 0 | 7 | 6 | 1 | 6 | /AE | 61815.3523 | 0.0277 | 61815.38 |
| 7 | 0 | 7 | 6 | 1 | 6 | /EA | 61815.3523 | 0.0277 | 61815.38 |
| 7 | 1 | 7 | 6 | 0 | 6 | /AA | 61815.3559 | 0.0241 | 61815.38 |
| 7 | 1 | 7 | 6 | 0 | 6 | /EE | 61815.3541 | 0.0259 | 61815.38 |
| 7 | 1 | 7 | 6 | 0 | 6 | /AE | 61815.3523 | 0.0277 | 61815.38 |
| 7 | 1 | 7 | 6 | 0 | 6 | /EA | 61815.3523 | 0.0277 | 61815.38 |
| 7 | 1 | 6 | 6 | 2 | 5 | /AA | 67323.2908 | -0.0208 | 67323.27 |
| 7 | 1 | 6 | 6 | 2 | 5 | /EE | 67323.2854 | -0.0154 | 67323.27 |
| 7 | 1 | 6 | 6 | 2 | 5 | /AE | 67323.28 | -0.01 | 67323.27 |
| 7 | 1 | 6 | 6 | 2 | 5 | /EA | 67323.28 | -0.01 | 67323.27 |
| 7 | 2 | 6 | 6 | 1 | 5 | /AA | 67323.2912 | -0.0212 | 67323.27 |
| 7 | 2 | 6 | 6 | 1 | 5 | /EE | 67323.2857 | -0.0157 | 67323.27 |
| 7 | 2 | 6 | 6 | 1 | 5 | /AE | 67323.2803 | -0.0103 | 67323.27 |
| 7 | 2 | 6 | 6 | 1 | 5 | /EA | 67323.2803 | -0.0103 | 67323.27 |
| 7 | 3 | 4 | 6 | 4 | 3 | /AA | 78339.7837 | -0.0937 | 78339.69 |
| 7 | 3 | 4 | 6 | 4 | 3 | /EE | 78339.7712 | -0.0812 | 78339.69 |
| 7 | 3 | 4 | 6 | 4 | 3 | /AE | 78339.7588 | -0.0688 | 78339.69 |
| 7 | 3 | 4 | 6 | 4 | 3 | /EA | 78339.7588 | -0.0688 | 78339.69 |
| 7 | 4 | 4 | 6 | 3 | 3 | /AA | 78347.8675 | -0.0875 | 78347.78 |
| 7 | 4 | 4 | 6 | 3 | 3 | /EE | 78347.8547 | -0.0747 | 78347.78 |
| 7 | 4 | 4 | 6 | 3 | 3 | /AE | 78347.842 | -0.062 | 78347.78 |
| 7 | 4 | 4 | 6 | 3 | 3 | /EA | 78347.842 | -0.062 | 78347.78 |
| 8 | 0 | 8 | 7 | 1 | 7 | /AA | 70252.0827 | -0.0027 | 70252.08 |
| 8 | 0 | 8 | 7 | 1 | 7 | /EE | 70252.0809 | -0.0009 | 70252.08 |
| 8 | 0 | 8 | 7 | 1 | 7 | /AE | 70252.0791 | 0.0009 | 70252.08 |
| 8 | 0 | 8 | 7 | 1 | 7 | /EA | 70252.0791 | 0.0009 | 70252.08 |
| 8 | 1 | 8 | 7 | 0 | 7 | /AA | 70252.0827 | -0.0027 | 70252.08 |
| 8 | 1 | 8 | 7 | 0 | 7 | /EE | 70252.0809 | -0.0009 | 70252.08 |
| 8 | 1 | 8 | 7 | 0 | 7 | /AE | 70252.0791 | 0.0009 | 70252.08 |
| 8 | 1 | 8 | 7 | 0 | 7 | /EA | 70252.0791 | 0.0009 | 70252.08 |
| 8 | 1 | 7 | 7 | 2 | 6 | /AA | 75759.823 | -0.003 | 75759.82 |
| 8 | 1 | 7 | 7 | 2 | 6 | /EE | 75759.8176 | 0.0024 | 75759.82 |
| 8 | 1 | 7 | 7 | 2 | 6 | /AE | 75759.8122 | 0.0078 | 75759.82 |
| 8 | 1 | 7 | 7 | 2 | 6 | /EA | 75759.8122 | 0.0078 | 75759.82 |
| 8 | 2 | 7 | 7 | 1 | 6 | /AA | 75759.823 | -0.003 | 75759.82 |
| 8 | 2 | 7 | 7 | 1 | 6 | /EE | 75759.8176 | 0.0024 | 75759.82 |
| 8 | 2 | 7 | 7 | 1 | 6 | /AE | 75759.8122 | 0.0078 | 75759.82 |
| 8 | 2 | 7 | 7 | 1 | 6 | /EA | 75759.8122 | 0.0078 | 75759.82 |
| 9 | 0 | 9 | 8 | 1 | 8 | /AA | 78688.5846 | -0.0046 | 78688.58 |
| 9 | 0 | 9 | 8 | 1 | 8 | /EE | 78688.5829 | -0.0029 | 78688.58 |
| 9 | 0 | 9 | 8 | 1 | 8 | /AE | 78688.5811 | -0.0011 | 78688.58 |
| 9 | 0 | 9 | 8 | 1 | 8 | /EA | 78688.5811 | -0.0011 | 78688.58 |
| 9 | 1 | 9 | 8 | 0 | 8 | /AA | 78688.5846 | -0.0046 | 78688.58 |
| 9 | 1 | 9 | 8 | 0 | 8 | /EE | 78688.5829 | -0.0029 | 78688.58 |
| 9 | 1 | 9 | 8 | 0 | 8 | /AE | 78688.5811 | -0.0011 | 78688.58 |
| 9 | 1 | 9 | 8 | 0 | 8 | /EA | 78688.5811 | -0.0011 | 78688.58 |
| 11 | 11 | 0 | 11 | 10 | 1 | /AA | 8591.5954 | -0.0014 | 8591.594 |
| 11 | 11 | 0 | 11 | 10 | 1 | /EE | 8591.515 | 0 | 8591.515 |
| 11 | 11 | 0 | 11 | 10 | 1 | /AE | 8591.4341 | 0.0069 | 8591.441 |
| 11 | 11 | 0 | 11 | 10 | 1 | /EA | 8591.435 | 0.006 | 8591.441 |
| 12 | 12 | 0 | 12 | 11 | 1 | /AA | 9797.2421 | -0.0001 | 9797.242 |
| 12 | 12 | 0 | 12 | 11 | 1 | /EE | 9797.1491 | 0.0019 | 9797.151 |
| 12 | 12 | 0 | 12 | 11 | 1 | /AE | 9797.0555 | 0.0055 | 9797.061 |
| 12 | 12 | 0 | 12 | 11 | 1 | /EA | 9797.0567 | 0.0043 | 9797.061 |
| 13 | 13 | 0 | 13 | 12 | 1 | /AA | 11081.9353 | -0.0063 | 11081.93 |
| 13 | 13 | 0 | 13 | 12 | 1 | /EE | 11081.8307 | -0.0007 | 11081.83 |
| 13 | 13 | 0 | 13 | 12 | 1 | /AE | 11081.7251 | 0.0039 | 11081.73 |
| 13 | 13 | 0 | 13 | 12 | 1 | /EA | 11081.7271 | 0.0019 | 11081.73 |
| 14 | 14 | 0 | 14 | 13 | 1 | /AA | 12422.3675 | 0.0005 | 12422.37 |
| 14 | 14 | 0 | 14 | 13 | 1 | /EE | 12422.2526 | -0.0016 | 12422.25 |
| 14 | 14 | 0 | 14 | 13 | 1 | /AE | 12422.1363 | -0.0023 | 12422.13 |
| 14 | 14 | 0 | 14 | 13 | 1 | /EA | 12422.1393 | -0.0053 | 12422.13 |
| 15 | 15 | 0 | 15 | 14 | 1 | /AA | 13795.4662 | -0.0012 | 13795.47 |
| 15 | 15 | 0 | 15 | 14 | 1 | /EE | 13795.3427 | 0.0023 | 13795.35 |
| 15 | 15 | 0 | 15 | 14 | 1 | /AE | 13795.217 | 0.008 | 13795.23 |
| 15 | 15 | 0 | 15 | 14 | 1 | /EA | 13795.2214 | 0.0036 | 13795.23 |
| 16 | 16 | 0 | 16 | 15 | 1 | /AA | 15180.6562 | -0.0012 | 15180.66 |
| 16 | 16 | 0 | 16 | 15 | 1 | /EE | 15180.5257 | 0.0033 | 15180.53 |
| 16 | 16 | 0 | 16 | 15 | 1 | /AE | 15180.3919 | 0.0111 | 15180.4 |
| 16 | 16 | 0 | 16 | 15 | 1 | /EA | 15180.3984 | 0.0046 | 15180.4 |
| 17 | 17 | 0 | 17 | 16 | 1 | /AA | 16561.547 | 0.002 | 16561.55 |
| 17 | 17 | 0 | 17 | 16 | 1 | /EE | 16561.4109 | 0.0001 | 16561.41 |
| 17 | 17 | 0 | 17 | 16 | 1 | /AE | 16561.27 | 0.002 | 16561.27 |
| 17 | 17 | 0 | 17 | 16 | 1 | /EA | 16561.2795 | -0.0075 | 16561.27 |
| 18 | 18 | 0 | 18 | 17 | 1 | /AA | 17926.7329 | 0.0021 | 17926.74 |
| 18 | 18 | 0 | 18 | 17 | 1 | /EE | 17926.5924 | 0.0016 | 17926.59 |
| 18 | 18 | 0 | 18 | 17 | 1 | /AE | 17926.445 | 0.001 | 17926.45 |
| 18 | 18 | 0 | 18 | 17 | 1 | /EA | 17926.4589 | -0.0129 | 17926.45 |
| 19 | 19 | 0 | 19 | 18 | 1 | /AA | 19269.6478 | -0.0128 | 19269.64 |
| 19 | 19 | 0 | 19 | 18 | 1 | /EE | 19269.5041 | 0.0029 | 19269.51 |
| 19 | 19 | 0 | 19 | 18 | 1 | /AE | 19269.3503 | 0.0307 | 19269.38 |
| 19 | 19 | 0 | 19 | 18 | 1 | /EA | 19269.3705 | 0.0105 | 19269.38 |
| 2 | 1 | 1 | 2 | 0 | 2 | /AA | 8080.3662 | -0.0042 | 8080.362 |
| 2 | 1 | 1 | 2 | 0 | 2 | /EE | 8080.3629 | -0.0009 | 8080.362 |
| 2 | 1 | 1 | 2 | 0 | 2 | /AE | 8080.3596 | 0.0024 | 8080.362 |
| 2 | 1 | 1 | 2 | 0 | 2 | /EA | 8080.3596 | 0.0024 | 8080.362 |
| 2 | 2 | 1 | 2 | 1 | 2 | /AA | 8453.3219 | -0.0074 | 8453.315 |
| 2 | 2 | 1 | 2 | 1 | 2 | /EE | 8453.3139 | 0.0006 | 8453.315 |
| 2 | 2 | 1 | 2 | 1 | 2 | /AE | 8453.3058 | -0.0006 | 8453.305 |
| 2 | 2 | 1 | 2 | 1 | 2 | /EA | 8453.3058 | -0.0006 | 8453.305 |
| 3 | 2 | 1 | 3 | 1 | 2 | /AA | 7911.5052 | -0.0028 | 7911.502 |
| 3 | 2 | 1 | 3 | 1 | 2 | /EE | 7911.5038 | -0.0014 | 7911.502 |
| 3 | 2 | 1 | 3 | 1 | 2 | /AE | 7911.5025 | -0.0001 | 7911.502 |
| 3 | 2 | 1 | 3 | 1 | 2 | /EA | 7911.5025 | -0.0001 | 7911.502 |
| 3 | 3 | 1 | 3 | 2 | 2 | /AA | 8644.4281 | 0 | 8644.428 |
| 3 | 3 | 1 | 3 | 2 | 2 | /EE | 8644.4176 | 0.0003 | 8644.418 |
| 3 | 3 | 1 | 3 | 2 | 2 | /AE | 8644.4071 | -0.0003 | 8644.407 |
| 3 | 3 | 1 | 3 | 2 | 2 | /EA | 8644.4071 | -0.0003 | 8644.407 |
| 4 | 3 | 1 | 4 | 2 | 2 | /AA | 7708.0989 | 0.0035 | 7708.102 |
| 4 | 3 | 1 | 4 | 2 | 2 | /EE | 7708.0996 | 0.0028 | 7708.102 |
| 4 | 3 | 1 | 4 | 2 | 2 | /AE | 7708.1003 | 0.0021 | 7708.102 |
| 4 | 3 | 1 | 4 | 2 | 2 | /EA | 7708.1004 | 0.002 | 7708.102 |
| 4 | 4 | 1 | 4 | 3 | 2 | /AA | 8900.6851 | -0.0039 | 8900.681 |
| 4 | 4 | 1 | 4 | 3 | 2 | /EE | 8900.6713 | 0.0027 | 8900.674 |
| 4 | 4 | 1 | 4 | 3 | 2 | /AE | 8900.6576 | -0.0001 | 8900.658 |
| 4 | 4 | 1 | 4 | 3 | 2 | /EA | 8900.6575 | 0 | 8900.658 |
| 5 | 5 | 1 | 5 | 4 | 2 | /AA | 9223.0678 | -0.0017 | 9223.066 |
| 5 | 5 | 1 | 5 | 4 | 2 | /EE | 9223.0499 | -0.0007 | 9223.049 |
| 5 | 5 | 1 | 5 | 4 | 2 | /AE | 9223.032 | -0.0014 | 9223.031 |
| 5 | 5 | 1 | 5 | 4 | 2 | /EA | 9223.032 | -0.0014 | 9223.031 |
| 9 | 9 | 1 | 9 | 8 | 2 | /AA | 11186.9977 | 0.0053 | 11187 |
| 9 | 9 | 1 | 9 | 8 | 2 | /EE | 11186.9554 | 0.0036 | 11186.96 |
| 9 | 9 | 1 | 9 | 8 | 2 | /AE | 11186.9132 | 0.0028 | 11186.92 |
| 9 | 9 | 1 | 9 | 8 | 2 | /EA | 11186.9129 | 0.0031 | 11186.92 |
| 14 | 13 | 1 | 14 | 12 | 2 | /AA | 8356.373 | 0 | 8356.373 |
| 14 | 13 | 1 | 14 | 12 | 2 | /EE | 8356.3241 | -0.0011 | 8356.323 |
| 14 | 13 | 1 | 14 | 12 | 2 | /AE | 8356.2751 | -0.0031 | 8356.272 |
| 14 | 13 | 1 | 14 | 12 | 2 | /EA | 8356.2752 | -0.0032 | 8356.272 |
| 14 | 14 | 1 | 14 | 13 | 2 | /AA | 15091.9647 | 0.0093 | 15091.97 |
| 14 | 14 | 1 | 14 | 13 | 2 | /EE | 15091.8788 | -0.0008 | 15091.88 |
| 14 | 14 | 1 | 14 | 13 | 2 | /AE | 15091.7943 | -0.0083 | 15091.79 |
| 14 | 14 | 1 | 14 | 13 | 2 | /EA | 15091.7914 | -0.0054 | 15091.79 |
| 15 | 14 | 1 | 15 | 13 | 2 | /AA | 9077.6499 | -0.0029 | 9077.647 |
| 15 | 14 | 1 | 15 | 13 | 2 | /EE | 9077.5871 | -0.0011 | 9077.586 |
| 15 | 14 | 1 | 15 | 13 | 2 | /AE | 9077.5242 | -0.0012 | 9077.523 |
| 15 | 14 | 1 | 15 | 13 | 2 | /EA | 9077.5244 | -0.0014 | 9077.523 |
| 15 | 15 | 1 | 15 | 14 | 2 | /AA | 16036.3692 | 0.0098 | 16036.38 |
| 15 | 15 | 1 | 15 | 14 | 2 | /EE | 16036.2738 | -0.0008 | 16036.27 |
| 15 | 15 | 1 | 15 | 14 | 2 | /AE | 16036.1806 | -0.0066 | 16036.17 |
| 15 | 15 | 1 | 15 | 14 | 2 | /EA | 16036.1762 | -0.0022 | 16036.17 |
| 16 | 15 | 1 | 16 | 14 | 2 | /AA | 9953.8952 | -0.0022 | 9953.893 |
| 16 | 15 | 1 | 16 | 14 | 2 | /EE | 9953.8179 | -0.0009 | 9953.817 |
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| 10 | 6 | 5 | 9 | 5 | 4 | /AE | 114670.9527 |  |  |
| 10 | 6 | 5 | 9 | 5 | 4 | /EA | 114670.9527 |  |  |
| 11 | 0 | 11 | 10 | 1 | 10 | /AA | 95560.8020 |  |  |
| 11 | 0 | 11 | 10 | 1 | 10 | /EE | 95560.8002 |  |  |
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| 11 | 4 | 8 | 10 | 3 | 7 | /EA | 112081.5418 |  |  |

a The frequency predictions include the methyl internal rotation effect and are based on the global fit parameters reported in Table 4