# Supplemental Data

# Fits and Analyses

11dfscp3ene Separate

| | obs | o-c | error | blends | Notes |
|---|---|---|---|---|---|
| | | | o-c | wt | |
| 1: 2 1 2 0 1 1 1 0 | 6917.0167 | 0.0086 | 0.010 | | |
| 2: 2 1 2 1 1 1 1 1 | 6917.0190 | -0.0174 | 0.010 | | |
| 3: 2 0 2 0 1 0 1 0 | 7005.3453 | -0.0010 | 0.010 | | |
| 4: 2 0 2 1 1 0 1 1 | 7005.3468 | -0.0140 | 0.010 | | |
| 5: 2 1 1 0 1 1 0 0 | 7100.6875 | -0.0067 | 0.010 | | |
| 6: 3 2 2 0 3 0 3 0 | 7186.1321 | -0.0037 | 0.010 | | |
| 7: 4 2 3 0 4 0 4 0 | 7218.1642 | -0.0057 | 0.010 | | |
| 8: 5 2 4 0 5 0 5 0 | 7279.1347 | 0.0066 | 0.010 | | |
| 9: 2 1 2 0 1 1 1 0 | 6917.0151 | 0.0070 | 0.010 | -0.0072 | 0.50 |
| 10: 2 1 2 1 1 1 1 1 | 6917.0151 | -0.0214 | 0.010 | -0.0072 | 0.50 |
| 11: 2 0 2 0 1 0 1 0 | 7005.3482 | 0.0018 | 0.010 | -0.0054 | 0.50 |
| 12: 2 0 2 1 1 0 1 1 | 7005.3482 | -0.0126 | 0.010 | -0.0054 | 0.50 |
| 13: 2 1 1 0 1 1 0 0 | 7100.6825 | -0.0117 | 0.010 | | |
| 14: 3 2 2 0 3 0 3 0 | 7186.1321 | -0.0037 | 0.010 | | |
| 15: 4 2 3 0 4 0 4 0 | 7218.1618 | -0.0082 | 0.010 | | |
| 16: 5 2 4 0 5 0 5 0 | 7279.1432 | 0.0151 | 0.010 | | |
| 17: 3 1 3 0 2 1 2 0 | 10373.3425 | 0.0075 | 0.010 | | |
| 18: 3 0 3 0 2 0 2 0 | 10499.2285 | 0.0081 | 0.010 | | |
| 19: 3 2 2 0 2 2 1 0 | 10513.1606 | 0.0051 | 0.010 | | |
| 20: 3 2 1 0 2 2 0 0 | 10527.2463 | 0.0080 | 0.010 | | |

/ instead of : below denotes (o-c)>3*err

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 21: | 3 | 1 | 2 | 0 | 2 | 1 | 1 | 0 | 10648.7744 | -0.0049 | 0.010 | | |
| 22: | 4 | 1 | 4 | 0 | 3 | 1 | 3 | 0 | 13827.1864 | 0.0204 | 0.010 | -0.0073 | 0.50 |
| 23: | 4 | 1 | 4 | 1 | 3 | 1 | 3 | 1 | 13827.1864 | -0.0351 | 0.010 | -0.0073 | 0.50 |
| 24: | 4 | 0 | 4 | 0 | 3 | 0 | 3 | 0 | 13982.7281 | -0.0056 | 0.010 | | |
| 25: | 4 | 2 | 3 | 0 | 3 | 2 | 2 | 0 | 14014.7855 | 0.0175 | 0.010 | | |
| 26: | 4 | 3 | 2 | 0 | 3 | 3 | 1 | 0 | 14024.1248 | -0.0011 | 0.010 | | |
| 27: | 4 | 3 | 1 | 0 | 3 | 3 | 0 | 0 | 14024.6266 | 0.0096 | 0.010 | | |
| 28: | 4 | 2 | 2 | 0 | 3 | 2 | 1 | 0 | 14049.7693 | 0.0187 | 0.010 | 0.0221 | 0.50 |
| 29: | 4 | 2 | 2 | 1 | 3 | 2 | 1 | 1 | 14049.7693 | 0.0256 | 0.010 | 0.0221 | 0.50 |
| 30: | 4 | 1 | 3 | 1 | 3 | 1 | 2 | 1 | 14194.0110 | 0.0127 | 0.010 | -0.0029 | 0.50 |
| 31: | 4 | 1 | 3 | 0 | 3 | 1 | 2 | 0 | 14194.0110 | -0.0184 | 0.010 | -0.0029 | 0.50 |
| 32: | 5 | 1 | 5 | 0 | 4 | 1 | 4 | 0 | 17277.9158 | 0.0568 | 0.010 | 0.0204 | 0.50 |
| 33: | 5 | 1 | 5 | 1 | 4 | 1 | 4 | 1 | 17277.9158 | -0.0160 | 0.010 | 0.0204 | 0.50 |
| 34: | 5 | 0 | 5 | 0 | 4 | 0 | 4 | 0 | 17453.0393 | -0.0097 | 0.010 | | |
| 35: | 5 | 0 | 5 | 1 | 4 | 0 | 4 | 1 | 17453.1552 | 0.0004 | 0.010 | | |
| 36: | 5 | 2 | 4 | 0 | 4 | 2 | 3 | 0 | 17513.9781 | -0.0290 | 0.010 | | |
| 37: | 5 | 2 | 4 | 1 | 4 | 2 | 3 | 1 | 17514.0783 | 0.0173 | 0.010 | | |
| 38: | 5 | 4 | 2 | 1 | 4 | 4 | 1 | 1 | 17529.0060 | -0.0176 | 0.010 | | |

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PARAMETERS IN FIT (values truncated and Nlines statistics):

| | | | |
|---|---|---|---|
| 10000 | A /MHz | 3544.4238(21) | 1 |
| 20000 | B /MHz | 1798.1419(16) | 2 |
| 30000 | C /MHz | 1706.2987(19) | 3 |
| 299 | DJ /kHz | 0.201(25) | 4 |
| 1199 | DJK /kHz | 5.873(92) | 5 |
| 10011 | A /MHz | 3545.23(46) | 6 |

| | | | |
|---|---|---|---|
| 20011 | B /MHz | 1798.1357(38) | 7 |
| 30011 | C /MHz | 1706.3101(26) | 8 |
| 210001 | Fbc /MHz | 0.68(11) | 9 |
| 11 | E1 /MHz | 13006.(510) | 10 |

MICROWAVE AVG = -0.000519 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.011774 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 1.17742 1.17742

distinct frequency lines in fit: 32

distinct parameters of fit: 10

| MICROWAVE | lines fitted | | lines | lines | RMS | RMS ERROR | J range | Ka range | freq. range |
|---|---|---|---|---|---|---|---|---|---|
| | total | dv=0 | dv.ne.0 | UNFITTD | e>900 | | | | |
| v"= 0 | 26 | 26 | 0 | 0 | 0 | 0.011266 | 1.12664 | 1 5 0 3 | 6917 17514 |
| v"= 1 | 6 | 6 | 0 | 0 | 0 | 0.013639 | 1.36387 | 1 5 0 4 | 6917 17529 |
| total: | 32 | 32 | 0 | 0 | 0 | 0.011748 | 1.17478 | | |

NOTE: the RMS values above are for Nlines statistics, but the 'total' values may differ slightly from those in the .FIT file since the o-c values for this evaluation are as rounded in the .FIT.

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

| | | | |
|---|---|---|---|
| 10000 | A /MHz | 3544.4239(30) | 1 |

| | | | |
|---|---|---|---|
| 20000 | B /MHz | 1798.1419(23) | 2 |
| 30000 | C /MHz | 1706.2988(27) | 3 |
| 299 | DJ /kHz | 0.201(36) | 4 |
| 1199 | DJK /kHz | 5.87(13) | 5 |
| 10011 | A /MHz | 3545.23(65) | 6 |
| 20011 | B /MHz | 1798.1357(53) | 7 |
| 30011 | C /MHz | 1706.3102(37) | 8 |
| 210001 | Fbc /MHz | 0.68(16) | 9 |
| 11 | E1 /MHz | 13006.(724) | 10 |

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Worst fitted constants, with greater than 20% uncertainty: %

| | | | | |
|---|---|---|---|---|
| 210001 | Fbc /MHz | 0.68(16) | 9 | 23.7 |

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CORRELATION COEFFICIENTS, C.ij:

| | A | B | C | -DJ | -DJK | A | B | C |
|---|---|---|---|---|---|---|---|---|
| A | 1.0000 | | | | | | | |
| B | 0.1035 | 1.0000 | | | | | | |
| C | 0.1674 | -0.6544 | 1.0000 | | | | | |
| -DJ | -0.0519 | 0.1311 | -0.7375 | 1.0000 | | | | |
| -DJK | -0.5554 | -0.2623 | 0.2744 | -0.2528 | 1.0000 | | | |
| A | -0.2469 | -0.3943 | 0.5300 | -0.4740 | 0.3138 | 1.0000 | | |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| B | 0.2506 | -0.3141 | 0.5264 | -0.4625 | -0.2849 | 0.4727 | 1.0000 | |
| C | -0.0181 | 0.4082 | -0.2389 | -0.0829 | 0.0232 | -0.4992 | -0.6754 | 1.0000 |
| Fbc | 0.2616 | 0.3453 | -0.3940 | 0.4112 | 0.1576 | -0.5005 | -0.4920 | 0.1760 |
| E1 | 0.0261 | -0.2312 | 0.2273 | -0.2420 | -0.4966 | 0.2740 | 0.5636 | -0.1893 |

| | Fbc | E1 |
|---|---|---|
| Fbc | 1.0000 | |
| E1 | -0.7338 | 1.0000 |

Mean value of |C.ij|, i.ne.j = 0.3362

Mean value of C.ij, i.ne.j = -0.0854

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

| | | | |
|---|---|---|---|
| 36: -2.9 | 28: 2.2 | 32: 2.0 | 38: -1.8 |
| 25: 1.8 | 2: -1.7 | 37: 1.7 | 16: 1.5 |
| 4: -1.4 | 13: -1.2 | 34: -1.0 | 27: 1.0 |
| 1: 0.9 | 15: -0.8 | 18: 0.8 | 20: 0.8 |
| 17: 0.8 | 22: -0.7 | 9: -0.7 | 5: -0.7 |
| 8: 0.7 | 7: -0.6 | 24: -0.6 | 11: -0.5 |
| 19: 0.5 | 21: -0.5 | 6: -0.4 | 14: -0.4 |
| 30: -0.3 | 26: -0.1 | 3: -0.1 | 35: 0.0 |
| 33: 0.0 | 31: 0.0 | 29: 0.0 | 23: 0.0 |
| 12: 0.0 | 10: 0.0 | | |

36: 5 2 4 0 4 2 3 0 17513.9781 -0.0290 0.010

28: 4 2 2 0 3 2 1 0 14049.7693 0.0187 0.010 0.0221 0.50

32: 5 1 5 0 4 1 4 0 17277.9158 0.0568 0.010 0.0204 0.50

38: 5 4 2 1 4 4 1 1 17529.0060 -0.0176 0.010

25: 4 2 3 0 3 2 2 0 14014.7855 0.0175 0.010

2: 2 1 2 1 1 1 1 1 6917.0190 -0.0174 0.010

37: 5 2 4 1 4 2 3 1 17514.0783 0.0173 0.010

16: 5 2 4 0 5 0 5 0 7279.1432 0.0151 0.010

4: 2 0 2 1 1 0 1 1 7005.3468 -0.0140 0.010

13: 2 1 1 0 1 1 0 0 7100.6825 -0.0117 0.010

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_____/ SPFIT output reformatted with PIFORM

11dfscp3ene Together

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obs o-c error blends Notes

o-c wt

/ instead of : below denotes (o-c)>3*err

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1: 2 1 2 0 1 1 1 0 6917.0167 0.0025 0.010

2: 2 1 2 1 1 1 1 1 6917.0190 0.0039 0.010

3: 2 0 2 0 1 0 1 0 7005.3453 -0.0020 0.010

4: 2 0 2 1 1 0 1 1 7005.3468 -0.0029 0.010

5: 2 1 1 0 1 1 0 0 7100.6875 -0.0022 0.010

6: 3 2 2 0 3 0 3 0 7186.1321 -0.0176 0.010

7: 4 2 3 0 4 0 4 0 7218.1642 -0.0095 0.010

8: 5 2 4 0 5 0 5 0 7279.1347 0.0244 0.010

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 9: | 2 | 1 | 2 | 0 | 1 | 1 | 1 | 0 | 6917.0151 | 0.0009 | 0.010 | 0.0004 | 0.50 |
| 10: | 2 | 1 | 2 | 1 | 1 | 1 | 1 | 1 | 6917.0151 | 0.0000 | 0.010 | 0.0004 | 0.50 |
| 11: | 2 | 0 | 2 | 0 | 1 | 0 | 1 | 0 | 7005.3482 | 0.0008 | 0.010 | -0.0004 | 0.50 |
| 12: | 2 | 0 | 2 | 1 | 1 | 0 | 1 | 1 | 7005.3482 | -0.0015 | 0.010 | -0.0004 | 0.50 |
| 13: | 2 | 1 | 1 | 0 | 1 | 1 | 0 | 0 | 7100.6825 | -0.0071 | 0.010 | | |
| 14: | 3 | 2 | 2 | 0 | 3 | 0 | 3 | 0 | 7186.1321 | -0.0176 | 0.010 | | |
| 15: | 4 | 2 | 3 | 0 | 4 | 0 | 4 | 0 | 7218.1618 | -0.0120 | 0.010 | | |
| 16/ | 5 | 2 | 4 | 0 | 5 | 0 | 5 | 0 | 7279.1432 | 0.0330 | 0.010 | | |
| 17: | 3 | 1 | 3 | 0 | 2 | 1 | 2 | 0 | 10373.3425 | -0.0036 | 0.010 | | |
| 18: | 3 | 0 | 3 | 0 | 2 | 0 | 2 | 0 | 10499.2285 | 0.0037 | 0.010 | | |
| 19: | 3 | 2 | 2 | 0 | 2 | 2 | 1 | 0 | 10513.1606 | 0.0041 | 0.010 | | |
| 20: | 3 | 2 | 1 | 0 | 2 | 2 | 0 | 0 | 10527.2463 | 0.0049 | 0.010 | | |
| 21: | 3 | 1 | 2 | 0 | 2 | 1 | 1 | 0 | 10648.7744 | 0.0000 | 0.010 | | |
| 22: | 4 | 1 | 4 | 0 | 3 | 1 | 3 | 0 | 13827.1864 | 0.0015 | 0.010 | 0.0022 | 0.50 |
| 23: | 4 | 1 | 4 | 1 | 3 | 1 | 3 | 1 | 13827.1864 | 0.0028 | 0.010 | 0.0022 | 0.50 |
| 24: | 4 | 0 | 4 | 0 | 3 | 0 | 3 | 0 | 13982.7281 | -0.0169 | 0.010 | | |
| 25: | 4 | 2 | 3 | 0 | 3 | 2 | 2 | 0 | 14014.7855 | 0.0163 | 0.010 | | |
| 26: | 4 | 3 | 2 | 0 | 3 | 3 | 1 | 0 | 14024.1248 | -0.0038 | 0.010 | | |
| 27: | 4 | 3 | 1 | 0 | 3 | 3 | 0 | 0 | 14024.6266 | -0.0022 | 0.010 | | |
| 28: | 4 | 2 | 2 | 0 | 3 | 2 | 1 | 0 | 14049.7693 | 0.0119 | 0.010 | 0.0126 | 0.50 |
| 29: | 4 | 2 | 2 | 1 | 3 | 2 | 1 | 1 | 14049.7693 | 0.0133 | 0.010 | 0.0126 | 0.50 |
| 30: | 4 | 1 | 3 | 1 | 3 | 1 | 2 | 1 | 14194.0110 | -0.0066 | 0.010 | -0.0112 | 0.50 |
| 31: | 4 | 1 | 3 | 0 | 3 | 1 | 2 | 0 | 14194.0110 | -0.0156 | 0.010 | -0.0112 | 0.50 |
| 32: | 5 | 1 | 5 | 0 | 4 | 1 | 4 | 0 | 17277.9158 | 0.0267 | 0.010 | 0.0273 | 0.50 |
| 33: | 5 | 1 | 5 | 1 | 4 | 1 | 4 | 1 | 17277.9158 | 0.0279 | 0.010 | 0.0273 | 0.50 |
| 34/ | 5 | 0 | 5 | 0 | 4 | 0 | 4 | 0 | 17453.0393 | -0.0325 | 0.010 | | |
| 35/ | 5 | 0 | 5 | 1 | 4 | 0 | 4 | 1 | 17453.1552 | 0.0354 | 0.010 | | |
| 36/ | 5 | 2 | 4 | 0 | 4 | 2 | 3 | 0 | 17513.9781 | -0.0301 | 0.010 | | |
| 37: | 5 | 2 | 4 | 1 | 4 | 2 | 3 | 1 | 17514.0783 | 0.0256 | 0.010 | | |
| 38: | 5 | 4 | 2 | 1 | 4 | 4 | 1 | 1 | 17529.0060 | -0.0255 | 0.010 | | |

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PARAMETERS IN FIT (values truncated and Nlines statistics):

| | | | |
|---|---|---|---|
| 10099 | A /MHz | 3544.4280(19) | 1 |
| 20099 | B /MHz | 1798.1391(12) | 2 |
| 30099 | C /MHz | 1706.3013(13) | 3 |
| 299 | DJ /kHz | 0.161(21) | 4 |
| 1199 | DJK /kHz | 5.818(79) | 5 |
| 210001 | Fbc /MHz | 0.861(72) | 6 |
| 11 | E1 /MHz | 11799.(749) | 7 |

MICROWAVE AVG = -0.000031 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.016637 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 1.66374 1.66374

distinct frequency lines in fit: 32

distinct parameters of fit: 7

| MICROWAVE | lines fitted | | lines | lines | RMS | RMS ERROR | J range | Ka range | freq. range |
|---|---|---|---|---|---|---|---|---|---|
| | total | dv=0 | dv.ne.0 | UNFITTD | e>900 | | | | |
| v"= 0 | 26 | 26 | 0 | 0 | 0 | 0.015337 | 1.53370 | 1 5 | 0 3 | 6917 | 17514 |
| v"= 1 | 6 | 6 | 0 | 0 | 0 | 0.021240 | 2.12396 | 1 5 | 0 4 | 6917 | 17529 |
| total: | 32 | 32 | 0 | 0 | 0 | 0.016604 | 1.66043 | | | | |

NOTE: the RMS values above are for Nlines statistics, but the 'total' values may differ slightly from

those in the .FIT file since the o-c values for this evaluation are as rounded in the .FIT.

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

| | | | |
|---|---|---|---|
| 10099 | A /MHz | 3544.4280(35) | 1 |
| 20099 | B /MHz | 1798.1391(23) | 2 |
| 30099 | C /MHz | 1706.3013(25) | 3 |
| 299 | DJ /kHz | 0.162(40) | 4 |
| 1199 | DJK /kHz | 5.82(14) | 5 |
| 210001 | Fbc /MHz | 0.86(13) | 6 |
| 11 | E1 /MHz | 11799.(1409) | 7 |

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Worst fitted constants, with greater than 20% uncertainty: %

| | | | | |
|---|---|---|---|---|
| 299 | DJ /kHz | 0.162(40) | 4 | 24.9 |

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CORRELATION COEFFICIENTS, C.ij:

| | A | B | C | -DJ | -DJK | Fbc | E1 |
|---|---|---|---|---|---|---|---|
| A | 1.0000 | | | | | | |
| B | 0.2881 | 1.0000 | | | | | |
| C | 0.1957 | -0.3504 | 1.0000 | | | | |
| -DJ | -0.1510 | -0.2017 | -0.7392 | 1.0000 | | | |

| | | | | | | |
|---|---|---|---|---|---|---|
| -DJK | -0.5044 | -0.3132 | 0.3200 | -0.4272 | 1.0000 | |
| Fbc | 0.3335 | 0.1211 | -0.1794 | 0.2246 | -0.3261 | 1.0000 |
| E1 | 0.0971 | -0.0409 | -0.0668 | 0.2832 | -0.5499 | 0.6489 | 1.0000 |

Mean value of |C.ij|, i.ne.j = 0.3030

Mean value of C.ij, i.ne.j = -0.0637

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

| | | | |
|---|---|---|---|
| 35: 3.5 | 16: 3.3 | 34: -3.2 | 36: -3.0 |
| 32: 2.7 | 37: 2.6 | 38: -2.5 | 8: 2.4 |
| 6: -1.8 | 14: -1.8 | 24: -1.7 | 25: 1.6 |
| 28: 1.3 | 15: -1.2 | 30: -1.1 | 7: -0.9 |
| 13: -0.7 | 20: 0.5 | 19: 0.4 | 2: 0.4 |
| 26: -0.4 | 18: 0.4 | 17: -0.4 | 4: -0.3 |
| 1: 0.2 | 27: -0.2 | 5: -0.2 | 22: 0.2 |
| 3: -0.2 | 9: 0.0 | 11: 0.0 | 33: 0.0 |
| 31: 0.0 | 29: 0.0 | 23: 0.0 | 21: 0.0 |
| 12: 0.0 | 10: 0.0 | | |

| | | | | | |
|---|---|---|---|---|---|
| 35/ 5 0 5 1 4 0 4 1 | 17453.1552 | 0.0354 | 0.010 | | |
| 16/ 5 2 4 0 5 0 5 0 | 7279.1432 | 0.0330 | 0.010 | | |
| 34/ 5 0 5 0 4 0 4 0 | 17453.0393 | -0.0325 | 0.010 | | |
| 36/ 5 2 4 0 4 2 3 0 | 17513.9781 | -0.0301 | 0.010 | | |
| 32: 5 1 5 0 4 1 4 0 | 17277.9158 | 0.0267 | 0.010 | 0.0273 | 0.50 |
| 37: 5 2 4 1 4 2 3 1 | 17514.0783 | 0.0256 | 0.010 | | |

38: 5 4 2 1 4 4 1 1 17529.0060 -0.0255 0.010

8: 5 2 4 0 5 0 5 0 7279.1347 0.0244 0.010

6: 3 2 2 0 3 0 3 0 7186.1321 -0.0176 0.010

14: 3 2 2 0 3 0 3 0 7186.1321 -0.0176 0.010

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_____/ SPFIT output reformatted with PIFORM

Silicon 30 11dfscp3ene

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obs o-c error blends Notes

o-c wt

/ instead of : below denotes (o-c)>3*err

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1: 2 1 2 0 1 1 1 0 6903.7342 -0.0125 0.010

2: 2 0 2 0 1 0 1 0 6991.7507 -0.0024 0.010

3: 2 1 1 0 1 1 0 0 7086.6956 -0.0079 0.010

4: 3 1 3 0 2 1 2 0 10353.4645 0.0031 0.010

5: 3 0 3 0 2 0 2 0 10478.9132 -0.0005 0.010

6: 3 2 2 0 2 2 1 0 10492.7269 0.0110 0.010

7: 3 2 1 0 2 2 0 0 10506.6646 -0.0024 0.010

8: 3 1 2 0 2 1 1 0 10627.7917 -0.0212 0.010

9: 4 1 4 0 3 1 3 0 13800.7090 0.0081 0.010

10: 4 0 4 0 3 0 3 0 13955.8093 -0.0004 0.010

11: 4 2 3 0 3 2 2 0 13987.5399 0.0103 0.010

12: 4 3 2 0 3 3 1 0 13996.8145 0.0113 0.010

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 13: | 4 | 3 | 1 | 0 | 3 | 3 | 0 | 0 | 13997.3130 | 0.0101 | 0.010 |
| 14: | 4 | 2 | 2 | 0 | 3 | 2 | 1 | 0 | 14022.1986 | 0.0098 | 0.010 |
| 15: | 4 | 1 | 3 | 0 | 3 | 1 | 2 | 0 | 14166.1041 | -0.0092 | 0.010 |
| 16: | 5 | 1 | 5 | 0 | 4 | 1 | 4 | 0 | 17244.8050 | -0.0215 | 0.010 |
| 17: | 5 | 0 | 5 | 0 | 4 | 0 | 4 | 0 | 17419.6070 | -0.0157 | 0.010 |
| 18: | 5 | 0 | 5 | 1 | 4 | 0 | 4 | 1 | 17419.6936 | 0.0128 | 0.010 |
| 19: | 5 | 2 | 4 | 0 | 4 | 2 | 3 | 0 | 17479.9890 | 0.0095 | 0.010 |
| 20/ | 5 | 2 | 4 | 1 | 4 | 2 | 3 | 1 | 17480.0751 | 0.0381 | 0.010 |
| 21: | 5 | 4 | 1 | 0 | 4 | 4 | 1 | 0 | 17494.9301 | 0.0023 | 0.010 |
| 22: | 5 | 3 | 3 | 0 | 4 | 3 | 2 | 0 | 17498.6608 | -0.0277 | 0.010 |
| 23: | 5 | 3 | 2 | 0 | 4 | 3 | 1 | 0 | 17500.4135 | -0.0207 | 0.010 |
| 24/ | 5 | 2 | 3 | 0 | 4 | 2 | 2 | 0 | 17548.3730 | -0.0358 | 0.010 |
| 25/ | 5 | 2 | 3 | 1 | 4 | 2 | 2 | 1 | 17548.4450 | 0.0366 | 0.010 |
| 26/ | 5 | 1 | 4 | 0 | 4 | 1 | 3 | 0 | 17700.4308 | -0.0378 | 0.010 |
| 27/ | 5 | 1 | 4 | 1 | 4 | 1 | 3 | 1 | 17700.5151 | 0.0429 | 0.010 |

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PARAMETERS IN FIT (values truncated and Nlines statistics):

| | | | |
|---|---|---|---|
| 10099 | A /MHz | 3544.41(16) | 1 |
| 20099 | B /MHz | 1794.5529(11) | 2 |
| 30099 | C /MHz | 1703.0745(10) | 3 |
| 299 | DJ /kHz | 0.244(16) | 4 |
| 1199 | DJK /kHz | 5.417(68) | 5 |
| 210001 | Fbc /MHz | 0.49(14) | 6 |
| 11 | E1 /MHz | 8391.(624) | 7 |

MICROWAVE AVG = -0.000358 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.020135 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 2.01347 2.01347

distinct frequency lines in fit: 27

distinct parameters of fit: 7

| MICROWAVE | lines fitted | | lines | lines | RMS | RMS ERROR | J range | Ka range | freq. range |
|---|---|---|---|---|---|---|---|---|---|
| | total | dv=0 | dv.ne.0 | UNFITTD | e>900 | | | | |
| v"= 0 | 23 | 23 | 0 | 0 | 0 | 0.016290 | 1.62898 | 1 5 0 4 | 6904 17700 |
| v"= 1 | 4 | 4 | 0 | 0 | 0 | 0.034624 | 3.46245 | 4 5 0 2 | 17420 17701 |
| total: | 27 | 27 | 0 | 0 | 0 | 0.020091 | 2.00912 | | |

NOTE: the RMS values above are for Nlines statistics, but the 'total' values may differ slightly from those in the .FIT file since the o-c values for this evaluation are as rounded in the .FIT.

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

| | | | |
|---|---|---|---|
| 10099 | A /MHz | 3544.41(37) | 1 |
| 20099 | B /MHz | 1794.5529(25) | 2 |
| 30099 | C /MHz | 1703.0745(25) | 3 |
| 299 | DJ /kHz | 0.245(39) | 4 |
| 1199 | DJK /kHz | 5.42(15) | 5 |
| 210001 | Fbc /MHz | 0.50(32) | 6 |
| 11 | E1 /MHz | 8391.(1459) | 7 |

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Worst fitted constants, with greater than 20% uncertainty: %

210001 Fbc /MHz 0.50(32) 6 65.5

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CORRELATION COEFFICIENTS, C.ij:

| | A | B | C | -DJ | -DJK | Fbc | E1 |
|---|---|---|---|---|---|---|---|
| A | 1.0000 | | | | | | |
| B | 0.2455 | 1.0000 | | | | | |
| C | -0.3277 | -0.1203 | 1.0000 | | | | |
| -DJ | -0.1266 | -0.6108 | -0.5330 | 1.0000 | | | |
| -DJK | 0.3571 | -0.1005 | -0.1342 | -0.2341 | 1.0000 | | |
| Fbc | 0.0363 | 0.1487 | 0.0256 | 0.0616 | -0.4057 | 1.0000 | |
| E1 | 0.0821 | 0.1323 | 0.0155 | 0.0739 | -0.4053 | 0.9757 | 1.0000 |

Mean value of |C.ij|, i.ne.j = 0.2454

Mean value of C.ij, i.ne.j = -0.0402

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 27: | 4.3 | 20: | 3.8 | 26: | -3.8 | 25: | 3.7 |
| 24: | -3.6 | 22: | -2.8 | 16: | -2.1 | 8: | -2.1 |

23: -2.1 17: -1.6 18: 1.3 1: -1.2

12: 1.1 6: 1.1 11: 1.0 13: 1.0

14: 1.0 19: 0.9 15: -0.9 9: 0.8

3: -0.8 4: 0.3 7: -0.2 2: -0.2

21: 0.2 5: -0.1 10: 0.0

27/ 5 1 4 1 4 1 3 1 17700.5151 0.0429 0.010

20/ 5 2 4 1 4 2 3 1 17480.0751 0.0381 0.010

26/ 5 1 4 0 4 1 3 0 17700.4308 -0.0378 0.010

25/ 5 2 3 1 4 2 2 1 17548.4450 0.0366 0.010

24/ 5 2 3 0 4 2 2 0 17548.3730 -0.0358 0.010

22: 5 3 3 0 4 3 2 0 17498.6608 -0.0277 0.010

16: 5 1 5 0 4 1 4 0 17244.8050 -0.0215 0.010

8: 3 1 2 0 2 1 1 0 10627.7917 -0.0212 0.010

23: 5 3 2 0 4 3 1 0 17500.4135 -0.0207 0.010

17: 5 0 5 0 4 0 4 0 17419.6070 -0.0157 0.010

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_____/ SPFIT output reformatted with PIFORM

11dfscp3ene Silicon 29

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obs o-c error blends Notes

o-c wt

/ instead of : below denotes (o-c)>3*err

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1: 2 1 2 0 1 1 1 0 6910.3172 -0.0100 0.010

2: 2 0 2 0 1 0 1 0 6998.4765 -0.0080 0.010

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3: | 2 | 1 | 1 | 0 | 1 | 1 | 0 | 0 | 7093.6164 | -0.0028 | 0.010 | | |
| 4/ | 3 | 1 | 3 | 0 | 2 | 1 | 2 | 0 | 10363.2869 | -0.0349 | 0.010 | | |
| 5: | 3 | 0 | 3 | 0 | 2 | 0 | 2 | 0 | 10488.9676 | 0.0007 | 0.010 | | |
| 6: | 3 | 2 | 2 | 0 | 2 | 2 | 1 | 0 | 10502.8531 | 0.0172 | 0.010 | | |
| 7: | 3 | 2 | 1 | 1 | 2 | 2 | 0 | 1 | 10516.8477 | -0.0093 | 0.010 | | |
| 8: | 3 | 1 | 2 | 0 | 2 | 1 | 1 | 0 | 10638.1811 | 0.0055 | 0.010 | | |
| 9: | 4 | 1 | 4 | 0 | 3 | 1 | 3 | 0 | 13813.8359 | 0.0060 | 0.010 | | |
| 10: | 4 | 0 | 4 | 0 | 3 | 0 | 3 | 0 | 13969.1522 | 0.0183 | 0.010 | | |
| 11: | 4 | 2 | 3 | 0 | 3 | 2 | 2 | 0 | 14001.0318 | 0.0185 | 0.010 | | |
| 12: | 4 | 3 | 2 | 0 | 3 | 3 | 1 | 0 | 14010.3395 | 0.0073 | 0.010 | | |
| 13: | 4 | 3 | 1 | 0 | 3 | 3 | 0 | 0 | 14010.8423 | 0.0118 | 0.010 | | |
| 14: | 4 | 2 | 2 | 0 | 3 | 2 | 1 | 0 | 14035.8366 | -0.0078 | 0.010 | | |
| 15: | 4 | 1 | 3 | 0 | 3 | 1 | 2 | 0 | 14179.9058 | -0.0023 | 0.010 | | |
| 16: | 5 | 1 | 5 | 0 | 4 | 1 | 4 | 0 | 17261.2242 | 0.0137 | 0.010 | | |
| 17: | 5 | 0 | 5 | 0 | 4 | 0 | 4 | 0 | 17436.1286 | -0.0288 | 0.010 | | |
| 18: | 5 | 0 | 5 | 1 | 4 | 0 | 4 | 1 | 17436.2094 | 0.0006 | 0.010 | | |
| 19/ | 5 | 2 | 4 | 1 | 4 | 2 | 3 | 1 | 17496.9020 | 0.0328 | 0.010 | | |
| 20/ | 5 | 4 | 2 | 1 | 4 | 4 | 1 | 1 | 17511.7384 | -0.0484 | 0.010 | | |
| 21/ | 5 | 4 | 1 | 0 | 4 | 4 | 0 | 0 | 17511.8382 | 0.0339 | 0.010 | 0.0406 | 0.50 |
| 22: | 5 | 4 | 2 | 0 | 4 | 4 | 1 | 0 | 17511.8382 | 0.0472 | 0.010 | 0.0406 | 0.50 |
| 23: | 5 | 3 | 3 | 0 | 4 | 3 | 2 | 0 | 17515.6155 | -0.0182 | 0.010 | | |
| 24/ | 5 | 3 | 2 | 1 | 4 | 3 | 1 | 1 | 17517.3184 | -0.0384 | 0.010 | | |
| 25/ | 5 | 3 | 2 | 0 | 4 | 3 | 1 | 0 | 17517.4132 | 0.0395 | 0.010 | | |
| 26/ | 5 | 2 | 3 | 0 | 4 | 2 | 2 | 0 | 17565.5338 | -0.0474 | 0.010 | | |
| 27/ | 5 | 2 | 3 | 1 | 4 | 2 | 2 | 1 | 17565.6178 | 0.0399 | 0.010 | | |
| 28: | 5 | 1 | 4 | 0 | 4 | 1 | 3 | 0 | 17717.6676 | -0.0067 | 0.010 | | |

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PARAMETERS IN FIT (values truncated and Nlines statistics):

| | | | |
|---|---|---|---|
| 10099 | A /MHz | 3543.44(16) | 1 |
| 20099 | B /MHz | 1796.3239(12) | 2 |
| 30099 | C /MHz | 1704.6779(12) | 3 |
| 299 | DJ /kHz | 0.223(20) | 4 |
| 1199 | DJK /kHz | 5.728(58) | 5 |
| 210001 | Fbc /MHz | 0.863(68) | 6 |
| 11 | E1 /MHz | 11476.(475) | 7 |

MICROWAVE AVG = -0.000387 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.024462 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 2.44624 2.44624

distinct frequency lines in fit: 27

distinct parameters of fit: 7

| MICROWAVE | lines fitted | | | lines | lines | RMS | RMS ERROR | J range | Ka range | freq. range |
|---|---|---|---|---|---|---|---|---|---|---|
| | total | dv=0 | dv.ne.0 | UNFITTD | e>900 | | | | | |
| v"= 0 | 21 | 21 | 0 | 0 | 0 | 0.021309 | 2.13087 | 1 5 | 0 4 | 6910 17718 |
| v"= 1 | 6 | 6 | 0 | 0 | 0 | 0.033095 | 3.30954 | 2 5 | 0 4 | 10517 17566 |
| total: | 27 | 27 | 0 | 0 | 0 | 0.024425 | 2.44245 | | | |

NOTE: the RMS values above are for Nlines statistics, but the 'total' values may differ slightly from those in the .FIT file since the o-c values for this evaluation are as rounded in the .FIT.

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

| | | | |
|---|---|---|---|
| 10099 | A /MHz | 3543.45(47) | 1 |
| 20099 | B /MHz | 1796.3240(36) | 2 |
| 30099 | C /MHz | 1704.6780(36) | 3 |
| 299 | DJ /kHz | 0.223(58) | 4 |
| 1199 | DJK /kHz | 5.73(16) | 5 |
| 210001 | Fbc /MHz | 0.86(19) | 6 |
| 11 | E1 /MHz | 11476.(1350) | 7 |

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Worst fitted constants, with greater than 20% uncertainty: %

| | | | | |
|---|---|---|---|---|
| 299 | DJ /kHz | 0.223(58) | 4 | 26.1 |
| 210001 | Fbc /MHz | 0.86(19) | 6 | 22.4 |

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CORRELATION COEFFICIENTS, C.ij:

| | A | B | C | -DJ | -DJK | Fbc | E1 |
|---|---|---|---|---|---|---|---|
| A | 1.0000 | | | | | | |
| B | 0.2727 | 1.0000 | | | | | |
| C | -0.3813 | -0.1257 | 1.0000 | | | | |
| -DJ | -0.0516 | -0.6035 | -0.5985 | 1.0000 | | | |
| -DJK | 0.3591 | -0.0279 | -0.0131 | -0.2852 | 1.0000 | | |
| Fbc | -0.2197 | 0.1838 | 0.1218 | -0.1778 | -0.2508 | 1.0000 | |
| E1 | 0.1701 | -0.1232 | -0.0865 | 0.1506 | -0.2006 | -0.1997 | 1.0000 |

Mean value of |C.ij|, i.ne.j = 0.2192

Mean value of C.ij, i.ne.j = -0.0994

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

| | | | |
|---|---|---|---|
| 20: -4.8 | 26: -4.7 | 21: 4.1 | 27: 4.0 |
| 25: 4.0 | 24: -3.8 | 4: -3.5 | 19: 3.3 |
| 17: -2.9 | 11: 1.8 | 10: 1.8 | 23: -1.8 |
| 6: 1.7 | 16: 1.4 | 13: 1.2 | 1: -1.0 |
| 7: -0.9 | 2: -0.8 | 14: -0.8 | 12: 0.7 |
| 28: -0.7 | 9: 0.6 | 8: 0.5 | 3: -0.3 |
| 15: -0.2 | 5: 0.1 | 18: 0.1 | 22: 0.0 |

| | | | | | |
|---|---|---|---|---|---|
| 20/ 5 4 2 1 | 4 4 1 1 | 17511.7384 | -0.0484 | 0.010 | |
| 26/ 5 2 3 0 | 4 2 2 0 | 17565.5338 | -0.0474 | 0.010 | |
| 21/ 5 4 1 0 | 4 4 0 0 | 17511.8382 | 0.0339 | 0.010 | 0.0406 0.50 |
| 27/ 5 2 3 1 | 4 2 2 1 | 17565.6178 | 0.0399 | 0.010 | |
| 25/ 5 3 2 0 | 4 3 1 0 | 17517.4132 | 0.0395 | 0.010 | |
| 24/ 5 3 2 1 | 4 3 1 1 | 17517.3184 | -0.0384 | 0.010 | |
| 4/ 3 1 3 0 | 2 1 2 0 | 10363.2869 | -0.0349 | 0.010 | |
| 19/ 5 2 4 1 | 4 2 3 1 | 17496.9020 | 0.0328 | 0.010 | |
| 17: 5 0 5 0 | 4 0 4 0 | 17436.1286 | -0.0288 | 0.010 | |
| 11: 4 2 3 0 | 3 2 2 0 | 14001.0318 | 0.0185 | 0.010 | |

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_____/ SPFIT output reformatted with PIFORM

11dfscp3ene 3&4 Carbon-13

| | | obs | o-c | error o-c | blends wt | Notes |
|---|---|---|---|---|---|---|
| / instead of : below denotes (o-c)>3*err | | | | | | |
| 1: | 2 1 2 1 1 1 | 6872.6291 | -0.0069 | 0.010 | | |
| 2: | 2 0 2 1 0 1 | 6970.9813 | -0.0081 | 0.010 | | |
| 3: | 2 1 1 1 1 0 | 7078.3533 | -0.0062 | 0.010 | | |
| 4: | 3 1 3 2 1 2 | 10306.1667 | -0.0005 | 0.010 | | |
| 5: | 3 0 3 2 0 2 | 10445.2035 | 0.0011 | 0.010 | | |
| 6: | 3 2 2 2 2 1 | 10463.1129 | -0.0225 | 0.010 | | |
| 7: | 3 2 1 2 2 0 | 10481.1953 | -0.0010 | 0.010 | | |
| 8: | 3 1 2 2 1 1 | 10614.6259 | -0.0018 | 0.010 | | |
| 9: | 4 1 4 3 1 3 | 13736.5388 | 0.0130 | 0.010 | | |
| 10/ | 4 0 4 3 0 3 | 13906.2416 | 0.0316 | 0.010 | | |
| 11: | 4 2 3 3 2 2 | 13947.2820 | -0.0114 | 0.010 | | |
| 12: | 4 3 2 3 3 1 | 13959.3061 | 0.0039 | 0.010 | | |
| 13: | 4 3 1 3 3 0 | 13960.0713 | 0.0210 | 0.010 | | |
| 14: | 4 2 2 3 2 1 | 13992.0602 | -0.0090 | 0.010 | | |
| 15: | 4 1 3 3 1 2 | 14147.2335 | 0.0086 | 0.010 | | |
| 16: | 5 1 5 4 1 4 | 17162.9131 | -0.0180 | 0.010 | | |
| 17: | 5 0 5 4 0 4 | 17350.6456 | 0.0150 | 0.010 | | |
| 18/ | 5 2 4 4 2 3 | 17428.3805 | -0.0308 | 0.010 | | |
| 19: | 5 3 3 4 3 2 | 17452.5122 | 0.0019 | 0.010 | | |
| 20: | 5 3 2 4 3 1 | 17455.1171 | -0.0044 | 0.010 | | |
| 21: | 5 2 3 4 2 2 | 17516.4748 | 0.0275 | 0.010 | | |
| 22: | 5 1 4 4 1 3 | 17674.6145 | -0.0141 | 0.010 | | |

PARAMETERS IN FIT (values truncated and Nlines statistics):

| | | | |
|---|---|---|---|
| 10000 | A /MHz | 3494.65(16) | 1 |
| 20000 | B /MHz | 1795.3127(12) | 2 |
| 30000 | C /MHz | 1692.4509(12) | 3 |
| 200 | DJ /kHz | 0.258(21) | 4 |
| 1100 | DJK /kHz | 5.32(10) | 5 |

MICROWAVE AVG = -0.000504 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.015180 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 1.51802 1.51802

distinct frequency lines in fit: 22

distinct parameters of fit: 5

| | upper state | | lower state | | overall | |
|---|---|---|---|---|---|---|
| limits of quantum number 1: | 2 | 5 | 1 | 4 | 1 | 5 |
| limits of quantum number 2: | 0 | 3 | 0 | 3 | 0 | 3 |
| limits of quantum number 3: | 1 | 5 | 0 | 4 | 0 | 5 |

frequency range: 6872 17674

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

| | | | |
|---|---|---|---|
| 10000 | A /MHz | 3494.65(29) | 1 |
| 20000 | B /MHz | 1795.3127(22) | 2 |
| 30000 | C /MHz | 1692.4510(22) | 3 |
| 200 | DJ /kHz | 0.258(37) | 4 |

1100 DJK /kHz 5.32(17) 5

CORRELATION COEFFICIENTS, C.ij:

| | A | B | C | -DJ | -DJK |
|---|---|---|---|---|---|
| A | 1.0000 | | | | |
| B | 0.2196 | 1.0000 | | | |
| C | -0.3381 | -0.1109 | 1.0000 | | |
| -DJ | -0.1561 | -0.5635 | -0.5699 | 1.0000 | |
| -DJK | 0.5035 | -0.1318 | -0.1142 | -0.2625 | 1.0000 |

Mean value of |C.ij|, i.ne.j = 0.2970

Mean value of C.ij, i.ne.j = -0.1524

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

| | | | |
|---|---|---|---|
| 10: 3.2 | 18: -3.1 | 21: 2.8 | 6: -2.2 |
| 13: 2.1 | 16: -1.8 | 17: 1.5 | 22: -1.4 |
| 9: 1.3 | 11: -1.1 | 14: -0.9 | 15: 0.9 |
| 2: -0.8 | 1: -0.7 | 3: -0.6 | 20: -0.4 |
| 12: 0.4 | 19: 0.2 | 8: -0.2 | 5: 0.1 |
| 7: -0.1 | 4: -0.1 | | |

10/ 4 0 4 3 0 3 13906.2416 0.0316 0.010

18/ 5 2 4 4 2 3 17428.3805 -0.0308 0.010

| | | | |
|---|---|---|---|
| 21: 5 2 3 | 4 2 2 | 17516.4748 | 0.0275 0.010 |
| 6: 3 2 2 | 2 2 1 | 10463.1129 | -0.0225 0.010 |
| 13: 4 3 1 | 3 3 0 | 13960.0713 | 0.0210 0.010 |
| 16: 5 1 5 | 4 1 4 | 17162.9131 | -0.0180 0.010 |
| 17: 5 0 5 | 4 0 4 | 17350.6456 | 0.0150 0.010 |
| 22: 5 1 4 | 4 1 3 | 17674.6145 | -0.0141 0.010 |
| 9: 4 1 4 | 3 1 3 | 13736.5388 | 0.0130 0.010 |
| 11: 4 2 3 | 3 2 2 | 13947.2820 | -0.0114 0.010 |

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_____/ SPFIT output reformatted with PIFORM

11dfscp3ene 1&2 Carbon-13

| | | obs | o-c | error o-c | blends wt | Notes |
|---|---|---|---|---|---|---|
| / instead of : below denotes (o-c)>3*err | | | | | | |
| 1: | 2 1 2 1 1 1 | 6817.4411 | -0.0080 | 0.010 | | |
| 2: | 2 0 2 1 0 1 | 6905.7642 | -0.0020 | 0.010 | | |
| 3: | 2 1 1 1 1 0 | 7001.0493 | 0.0115 | 0.010 | | |
| 4: | 3 1 3 2 1 2 | 10224.0152 | -0.0017 | 0.010 | | |
| 5: | 3 0 3 2 0 2 | 10349.9358 | 0.0078 | 0.010 | | |
| 6: | 3 2 2 2 2 1 | 10363.7596 | -0.0032 | 0.010 | | |
| 7: | 3 2 1 2 2 0 | 10377.7232 | 0.0034 | 0.010 | | |
| 8: | 4 1 4 3 1 3 | 13628.0931 | -0.0184 | 0.010 | | |
| 9: | 4 0 4 3 0 3 | 13783.8285 | 0.0108 | 0.010 | | |
| 10: | 4 2 3 3 2 2 | 13815.5901 | -0.0186 | 0.010 | | |
| 11: | 4 3 2 3 3 1 | 13824.8574 | -0.0214 | 0.010 | | |
| 12: | 4 3 1 3 3 0 | 13825.3949 | 0.0163 | 0.010 | | |
| 13: | 4 2 2 3 2 1 | 13850.2917 | 0.0095 | 0.010 | | |
| 14: | 4 1 3 3 1 2 | 13994.8006 | 0.0115 | 0.010 | | |
| 15: | 5 1 5 4 1 4 | 17029.1166 | 0.0217 | 0.010 | | |
| 16: | 5 0 5 4 0 4 | 17204.6058 | -0.0070 | 0.010 | | |
| 17: | 5 2 4 4 2 3 | 17265.0912 | -0.0168 | 0.010 | | |
| 18: | 5 4 1 4 4 0 | 17280.0412 | -0.0142 | 0.010 | | |
| 19: | 5 3 3 4 3 2 | 17283.8167 | 0.0203 | 0.010 | | |
| 20: | 5 3 2 4 3 1 | 17285.5681 | 0.0258 | 0.010 | | |
| 21: | 5 2 3 4 2 2 | 17333.5501 | -0.0152 | 0.010 | | |
| 22: | 5 1 4 4 1 3 | 17486.3099 | -0.0108 | 0.010 | | |

PARAMETERS IN FIT (values truncated and Nlines statistics):

| | | | |
|---|---|---|---|
| 10000 | A /MHz | 3533.34(20) | 1 |
| 20000 | B /MHz | 1773.2145(14) | 2 |
| 30000 | C /MHz | 1681.4202(12) | 3 |
| 200 | DJ /kHz | 0.181(22) | 4 |
| 1100 | DJK /kHz | 5.082(69) | 5 |

MICROWAVE AVG = 0.000063 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.014271 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 1.42713 1.42713

distinct frequency lines in fit: 22

distinct parameters of fit: 5

| | upper state | | lower state | | overall | |
|---|---|---|---|---|---|---|
| limits of quantum number 1: | 2 | 5 | 1 | 4 | 1 | 5 |
| limits of quantum number 2: | 0 | 4 | 0 | 4 | 0 | 4 |
| limits of quantum number 3: | 1 | 5 | 0 | 4 | 0 | 5 |

frequency range: 6817 17486

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

| | | | |
|---|---|---|---|
| 10000 | A /MHz | 3533.34(33) | 1 |
| 20000 | B /MHz | 1773.2146(22) | 2 |
| 30000 | C /MHz | 1681.4202(20) | 3 |

| | | | |
|---|---|---|---|
| 200 | DJ /kHz | 0.181(36) | 4 |
| 1100 | DJK /kHz | 5.08(11) | 5 |

CORRELATION COEFFICIENTS, C.ij:

| | A | B | C | -DJ | -DJK |
|---|---|---|---|---|---|
| A | 1.0000 | | | | |
| B | 0.2714 | 1.0000 | | | |
| C | -0.2826 | -0.1350 | 1.0000 | | |
| -DJ | -0.1734 | -0.6098 | -0.5574 | 1.0000 | |
| -DJK | 0.4238 | -0.0484 | -0.0161 | -0.3158 | 1.0000 |

Mean value of |C.ij|, i.ne.j = 0.2834

Mean value of C.ij, i.ne.j = -0.1443

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

| | | | |
|---|---|---|---|
| 20: 2.6 | 15: 2.2 | 11: -2.1 | 19: 2.0 |
| 10: -1.9 | 8: -1.8 | 17: -1.7 | 12: 1.6 |
| 21: -1.5 | 18: -1.4 | 14: 1.1 | 3: 1.1 |
| 22: -1.1 | 9: 1.1 | 13: 0.9 | 1: -0.8 |
| 5: 0.8 | 16: -0.7 | 7: 0.3 | 6: -0.3 |
| 2: -0.2 | 4: -0.2 | | |

20: 5 3 2 4 3 1 17285.5681 0.0258 0.010

| | | | |
|---|---|---|---|
| 15: 5 1 5 | 4 1 4 | 17029.1166 | 0.0217 0.010 |
| 11: 4 3 2 | 3 3 1 | 13824.8574 | -0.0214 0.010 |
| 19: 5 3 3 | 4 3 2 | 17283.8167 | 0.0203 0.010 |
| 10: 4 2 3 | 3 2 2 | 13815.5901 | -0.0186 0.010 |
| 8: 4 1 4 | 3 1 3 | 13628.0931 | -0.0184 0.010 |
| 17: 5 2 4 | 4 2 3 | 17265.0912 | -0.0168 0.010 |
| 12: 4 3 1 | 3 3 0 | 13825.3949 | 0.0163 0.010 |
| 21: 5 2 3 | 4 2 2 | 17333.5501 | -0.0152 0.010 |
| 18: 5 4 1 | 4 4 0 | 17280.0412 | -0.0142 0.010 |

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_____/ SPFIT output reformatted with PIFORM

3SiCP Parent

| | | obs | o-c | error o-c | blends wt | Notes |
|---|---|---|---|---|---|---|
| / instead of : below denotes (o-c)>3*err | | | | | | |
| 1: | 1 0 1 0 0 0 0 0 | 7286.7327 | -0.0038 | 0.010 | | |
| 2: | 7 4 3 0 7 4 4 0 | 8010.9727 | 0.0095 | 0.010 | | |
| 3: | 4 2 2 0 4 2 3 0 | 8294.1383 | 0.0047 | 0.010 | | |
| 4: | 2 2 1 0 2 0 2 0 | 10164.4008 | 0.0147 | 0.010 | | |
| 5/ | 3 1 2 0 3 1 3 0 | 10370.5351 | -0.0781 | 0.010 | | |
| 6: | 3 1 2 1 3 1 3 1 | 10370.6312 | 0.0090 | 0.010 | | |
| 7: | 6 3 3 1 6 3 4 1 | 11284.8654 | -0.0026 | 0.010 | | |
| 8: | 6 3 3 0 6 3 4 0 | 11285.1515 | 0.0250 | 0.010 | | |
| 9: | 2 1 2 0 1 1 1 0 | 12783.6925 | 0.0086 | 0.010 | | |
| 10: | 3 2 2 0 3 0 3 0 | 12933.9109 | 0.0049 | 0.010 | | |
| 11: | 11 6 5 1 11 6 6 1 | 12958.0310 | 0.0000 | 0.010 | | |
| 12: | 11 6 5 0 11 6 6 0 | 12960.3195 | 0.0038 | 0.010 | | |
| 13: | 2 0 2 0 1 0 1 0 | 13627.9828 | -0.0257 | 0.010 | | |
| 14: | 2 0 2 1 1 0 1 1 | 13628.0354 | 0.0206 | 0.010 | | |
| 15: | 5 2 3 0 5 2 4 0 | 14043.8868 | 0.0272 | 0.010 | | |
| 16: | 8 4 4 1 8 4 5 1 | 14370.0898 | 0.0013 | 0.010 | | |
| 17/ | 8 4 4 0 8 4 5 0 | 14370.7425 | -0.0334 | 0.010 | | |
| 18: | 3 3 1 0 3 1 2 0 | 14425.1058 | -0.0089 | 0.010 | | |
| 19: | 4 3 2 0 4 1 3 0 | 15018.8384 | 0.0035 | 0.010 | | |
| 20: | 4 1 3 0 4 1 4 0 | 15832.9268 | 0.0204 | 0.010 | | |
| 21/ | 2 1 1 0 1 1 0 0 | 16363.1866 | -0.0370 | 0.010 | | |
| 22/ | 2 1 1 1 1 1 0 1 | 16363.2638 | 0.0356 | 0.010 | | |
| 23: | 4 2 3 0 4 0 4 0 | 16842.6227 | 0.0050 | 0.010 | -0.0177 | 0.50 |

```
 24:  4  2  3  1    4  0  4  1            16842.6227  -0.0404  0.010  -0.0177 0.50
 25:  5  3  3  0    5  1  4  0            17475.7920   0.0097  0.010
 26:  7  3  4  0    7  3  5  0            17703.8579   0.0031  0.010
 27:  5  1  4  0    4  3  1  0            17981.2284  -0.0001  0.010
-------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated and Nlines statistics):

      10099        A  /  /MHz        5948.1093(16)                  1
      20099        B  /  /MHz        4538.2601(14)                  2
      30099        C  /  /MHz        2748.4792(14)                  3
        299       DJ /  /kHz          0.712(39)                    4
       2099       DK /  /kHz           1.182(90)                   5
      40199       d1 /  /kHz          -0.340(13)                   6
      50099       d2 /  /kHz          -0.1114(77)                  7

         11       E1  /  /MHz      131812.(134)                    8

     210001       Fbc  /  /MHz          6.060(53)                   9

 MICROWAVE AVG =       -0.000206 MHz, IR AVG =       0.00000
 MICROWAVE RMS =        0.023051 MHz, IR RMS =       0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=       2.30512        2.30512

  distinct frequency lines in fit:    26
      distinct parameters of fit:     9

MICROWAVE      lines fitted      lines    lines     RMS      RMS ERROR    J range  Ka range    freq.
range
          total   dv=0 dv.ne.0   UNFITTD  e>900
```

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| v"= 0 | 20 | 20 | 0 | 0 | 0 | 0.024484 | 2.44841 | 0 | 11 | 0 | 6 | 7287 | 17981 |
| v"= 1 | 6 | 6 | 0 | 0 | 0 | 0.017230 | 1.72297 | 1 | 11 | 0 | 6 | 10371 | 16363 |

---

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| total: | 26 | 26 | 0 | 0 | 0 | 0.023014 | 2.30139 |

NOTE: the RMS values above are for Nlines statistics, but the 'total' values may differ slightly from those in the .FIT file since the o-c values for this evaluation are as rounded in the .FIT.

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

| | | | |
|---|---|---|---|
| 10099 | A / /MHz | 5948.1093(47) | 1 |
| 20099 | B / /MHz | 4538.2601(39) | 2 |
| 30099 | C / /MHz | 2748.4793(41) | 3 |
| 299 | DJ / /kHz | 0.71(11) | 4 |
| 2099 | DK / /kHz | 1.18(25) | 5 |
| 40199 | d1 / /kHz | -0.340(38) | 6 |
| 50099 | d2 / /kHz | -0.111(21) | 7 |
| 11 | E1 / /MHz | 131812.(381) | 8 |
| 210001 | Fbc / /MHz | 6.06(15) | 9 |

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Worst fitted constants, with greater than 20% uncertainty: %

| | | | | |
|---|---|---|---|---|
| 2099 | DK / /kHz | 1.18(25) | 5 | 21.7 |

---

CORRELATION COEFFICIENTS, C.ij:

| | A | B | C | -DJ | -DK | d1 | d2 | E1 |
|---|---|---|---|---|---|---|---|---|
| A | 1.0000 | | | | | | | |
| B | 0.8145 | 1.0000 | | | | | | |
| C | 0.5750 | 0.6865 | 1.0000 | | | | | |
| -DJ | -0.4719 | -0.5909 | -0.8317 | 1.0000 | | | | |
| -DK | -0.4090 | -0.1983 | 0.1696 | 0.0120 | 1.0000 | | | |
| d1 | -0.1765 | -0.2867 | 0.3925 | -0.3586 | 0.1613 | 1.0000 | | |
| d2 | 0.1028 | 0.2035 | -0.3216 | 0.3508 | 0.1276 | -0.9395 | 1.0000 | |
| E1 | -0.2297 | 0.0075 | -0.0447 | 0.1271 | 0.3824 | -0.0880 | 0.0557 | 1.0000 |
| Fbc | -0.2090 | 0.0017 | -0.0414 | 0.1295 | 0.3358 | -0.0765 | 0.0401 | 0.9420 |

| | Fbc |
|---|---|
| Fbc | 1.0000 |

Mean value of |C.ij|, i.ne.j = 0.3025

Mean value of C.ij, i.ne.j = 0.0095

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 5: | -7.8 | 21: | -3.7 | 22: | 3.6 | 17: | -3.3 |
| 15: | 2.7 | 13: | -2.6 | 8: | 2.5 | 14: | 2.1 |
| 20: | 2.0 | 23: | -1.8 | 4: | 1.5 | 25: | 1.0 |

```
 2:    0.9        6:    0.9       18:   -0.9        9:    0.9
10:    0.5        3:    0.5        1:   -0.4       12:    0.4
19:    0.3       26:    0.3        7:   -0.3       16:    0.1
27:    0.0       24:    0.0       11:    0.0

 5/  3  1  2  0    3  1  3  0          10370.5351  -0.0781  0.010
21/  2  1  1  0    1  1  0  0          16363.1866  -0.0370  0.010
22/  2  1  1  1    1  1  0  1          16363.2638   0.0356  0.010
17/  8  4  4  0    8  4  5  0          14370.7425  -0.0334  0.010
15:  5  2  3  0    5  2  4  0          14043.8868   0.0272  0.010
13:  2  0  2  0    1  0  1  0          13627.9828  -0.0257  0.010
 8:  6  3  3  0    6  3  4  0          11285.1515   0.0250  0.010
14:  2  0  2  1    1  0  1  1          13628.0354   0.0206  0.010
20:  4  1  3  0    4  1  4  0          15832.9268   0.0204  0.010
23:  4  2  3  0    4  0  4  0          16842.6227   0.0050  0.010  -0.0177 0.50
```

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_____/ SPFIT output reformatted with PIFORM

3SiCP 29Si

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| | | obs | o-c | error o-c | blends wt | Notes |
|---|---|---|---|---|---|---|
| / instead of : below denotes (o-c)>3*err | | | | | | |
| 1: | 1 0 1 0 0 0 | 7226.5573 | -0.0098 | 0.010 | | |
| 2: | 2 1 2 1 1 1 | 12660.6888 | 0.0024 | 0.010 | | |
| 3: | 2 0 2 1 0 1 | 13515.1930 | 0.0000 | 0.010 | | |
| 4: | 2 1 1 1 1 0 | 16245.5505 | 0.0024 | 0.010 | | |

---

PARAMETERS IN FIT (values truncated and Nlines statistics):

| | | | |
|---|---|---|---|
| 10000 | A / /MHz | 5947.901(40) | 1 |
| 20000 | B / /MHz | 4509.5060(39) | 2 |
| 30000 | C / /MHz | 2717.0640(39) | 3 |
| 200 | DJ / /kHz | [ 0.707924819] | 4 |
| 2000 | DK / /kHz | [ 1.136789663] | 5 |
| 40100 | d1 / /kHz | [-0.348099707] | 6 |
| 50000 | d2 / /kHz | [-0.105283752] | 7 |

MICROWAVE AVG = -0.001225 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.005198 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 0.51975 0.51975

distinct frequency lines in fit: 4

distinct parameters of fit: 3

| | upper state | | lower state | | overall | |
|---|---|---|---|---|---|---|
| limits of quantum number 1: | 1 | 2 | 0 | 1 | 0 | 2 |
| limits of quantum number 2: | 0 | 1 | 0 | 1 | 0 | 1 |
| limits of quantum number 3: | 1 | 2 | 0 | 1 | 0 | 2 |

frequency range: 7226 16245

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

| | | | |
|---|---|---|---|
| 10000 | A / /MHz | 5947.901(41) | 1 |
| 20000 | B / /MHz | 4509.5060(40) | 2 |
| 30000 | C / /MHz | 2717.0640(40) | 3 |
| 200 | DJ / /kHz | [ 0.707924819] | 4 |
| 2000 | DK / /kHz | [ 1.136789663] | 5 |
| 40100 | d1 / /kHz | [-0.348099707] | 6 |
| 50000 | d2 / /kHz | [-0.105283752] | 7 |

CORRELATION COEFFICIENTS, C.ij:

| | A / | B / | C / |
|---|---|---|---|
| A / | 1.0000 | | |
| B / | 0.2606 | 1.0000 | |
| C / | -0.6454 | -0.6364 | 1.0000 |

Mean value of |C.ij|, i.ne.j = 0.5142

Mean value of C.ij, i.ne.j = -0.3404

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

1: -1.0 4: 0.2 2: 0.2 3: 0.0

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1: | 1 | 0 | 1 | 0 | 0 | 0 | | 7226.5573 | -0.0098 | 0.010 | |
| 4: | 2 | 1 | 1 | 1 | 1 | 0 | | 16245.5505 | 0.0024 | 0.010 | |
| 2: | 2 | 1 | 2 | 1 | 1 | 1 | | 12660.6888 | 0.0024 | 0.010 | |
| 3: | 2 | 0 | 2 | 1 | 0 | 1 | | 13515.1930 | 0.0000 | 0.010 | |

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_____/ SPFIT output reformatted with PIFORM

3SiCP 30Si

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| | | | | | | | | obs | o-c | error | blends | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | | o-c | wt | |

/ instead of : below denotes (o-c)>3*err

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| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1: | 1 | 0 | 1 | 0 | 0 | 0 | | 7155.0931 | 0.0206 | 0.010 | | |
| 2: | 2 | 1 | 2 | 1 | 1 | 1 | | 12543.2359 | -0.0079 | 0.010 | | |
| 3: | 2 | 0 | 2 | 1 | 0 | 1 | | 13408.4800 | -0.0206 | 0.010 | | |
| 4: | 3 | 0 | 3 | 2 | 0 | 2 | | 18783.6626 | 0.0122 | 0.010 | | |

---

PARAMETERS IN FIT (values truncated and Nlines statistics):

| | | | |
|---|---|---|---|
| 10000 | A / /MHz | 5949.015(41) | 1 |
| 20000 | B / /MHz | 4460.985(11) | 2 |
| 30000 | C / /MHz | 2694.0901(55) | 3 |
| 200 | DJ / /kHz | [ 0.707924819] | 4 |
| 2000 | DK / /kHz | [ 1.136789663] | 5 |
| 40100 | d1 / /kHz | [-0.348099707] | 6 |
| 50000 | d2 / /kHz | [-0.105283752] | 7 |

MICROWAVE AVG = 0.001061 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.016347 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 1.63472 1.63472

distinct frequency lines in fit: 4

distinct parameters of fit: 3

| | upper state | | lower state | | overall | |
|---|---|---|---|---|---|---|
| limits of quantum number 1: | 1 | 3 | 0 | 2 | 0 | 3 |
| limits of quantum number 2: | 0 | 1 | 0 | 1 | 0 | 1 |
| limits of quantum number 3: | 1 | 3 | 0 | 2 | 0 | 3 |

frequency range: 7155 18783

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

| | | | |
|---|---|---|---|
| 10000 | A / /MHz | 5949.02(13) | 1 |
| 20000 | B / /MHz | 4460.985(37) | 2 |
| 30000 | C / /MHz | 2694.090(17) | 3 |
| 200 | DJ / /kHz | [ 0.707924819] | 4 |

| | | | |
|---|---|---|---|
| 2000 | DK / /kHz | [ 1.136789663] | 5 |
| 40100 | d1 / /kHz | [-0.348099707] | 6 |
| 50000 | d2 / /kHz | [-0.105283752] | 7 |

CORRELATION COEFFICIENTS, C.ij:

| | A / | B / | C / |
|---|---|---|---|
| A / | 1.0000 | | |
| B / | 0.6085 | 1.0000 | |
| C / | -0.8952 | -0.8220 | 1.0000 |

Mean value of |C.ij|, i.ne.j = 0.7752

Mean value of C.ij, i.ne.j = -0.3696

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

1: 2.1 3: -2.1 4: 1.2 2: -0.8

| | | | |
|---|---|---|---|
| 1: | 1 0 1 0 0 0 | 7155.0931 | 0.0206 0.010 |
| 3: | 2 0 2 1 0 1 | 13408.4800 | -0.0206 0.010 |
| 4: | 3 0 3 2 0 2 | 18783.6626 | 0.0122 0.010 |
| 2: | 2 1 2 1 1 1 | 12543.2359 | -0.0079 0.010 |

_____

_____/ SPFIT output reformatted with PIFORM

3SiCPF2 Durig and Laane v0

| | obs | o-c | error o-c | blends wt | Notes |
|---|---|---|---|---|---|
| / instead of : below denotes (o-c)>3*err | | | | | |
| 1/ 8 0 8 7 0 7 | 27774.3400 | 0.2597 | 0.050 | | |
| 2/ 8 1 8 7 1 7 | 27607.1200 | 0.3499 | 0.050 | | |
| 3: 8 2 7 7 2 6 | 27991.7800 | 0.1023 | 0.050 | | |
| 4/ 8 2 6 7 2 5 | 28252.1000 | 0.5245 | 0.050 | | |
| 5/ 8 1 7 7 1 6 | 28320.8900 | 0.3860 | 0.050 | | |
| 6/ 9 1 9 8 1 8 | 31042.2200 | 0.3534 | 0.050 | | |
| 7/ 9 0 9 8 0 8 | 31189.5700 | 0.2126 | 0.050 | | |
| 8: 9 2 8 8 2 7 | 31475.9300 | -0.0194 | 0.050 | | |
| 9/ 9 3 7 8 3 6 | 31579.2200 | -0.4290 | 0.050 | | |
| 10/ 9 3 6 8 3 5 | 31617.1400 | -0.1922 | 0.050 | | |
| 11/ 9 2 7 8 2 6 | 31824.8200 | 0.7012 | 0.050 | | |
| 12/ 9 1 8 8 1 7 | 31830.9600 | 0.3897 | 0.050 | | |
| 13: 10 1 10 9 1 9 | 34473.2900 | 0.1354 | 0.050 | | |
| 14: 10 0 10 9 0 9 | 34597.3700 | -0.0332 | 0.050 | | |
| 15/ 10 2 9 9 2 8 | 34954.9600 | -0.2884 | 0.050 | | |
| 16/ 10 3 8 9 3 7 | 35091.9200 | -0.4296 | 0.050 | | |
| 17/ 10 3 7 9 3 6 | 35155.3700 | -0.2941 | 0.050 | | |
| 18: 11 1 11 10 1 10 | 37900.9800 | 0.0311 | 0.050 | | |
| 19/ 11 0 11 10 0 10 | 38001.4400 | -0.2007 | 0.050 | | |
| 20/ 11 2 10 10 2 9 | 38428.6800 | -0.5193 | 0.050 | | |
| 21/ 11 3 8 10 3 7 | 38703.8600 | -0.3313 | 0.050 | | |
| 22/ 11 1 10 10 1 9 | 38810.6400 | -0.1632 | 0.050 | | |

PARAMETERS IN FIT (values truncated):

| | | | |
|---|---|---|---|
| 10000 | A /MHz | 3546.08(19) | 1 |
| 20000 | B /MHz | 1798.0697(20) | 2 |
| 30000 | C /MHz | 1706.2465(18) | 3 |

MICROWAVE AVG = 0.024792 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.335823 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 6.71645 6.71645

distinct frequency lines in fit: 22

distinct parameters of fit: 3

| | upper state | lower state | overall |
|---|---|---|---|
| limits of quantum number 1: | 8 11 | 7 10 | 7 11 |
| limits of quantum number 2: | 0 3 | 0 3 | 0 3 |
| limits of quantum number 3: | 6 11 | 5 10 | 5 11 |

frequency range: 27607 38810

Standard errors are obtained by muliplying the previous errors by: 7.227271

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

| | | | |
|---|---|---|---|
| 10000 | A /MHz | 3546.1(14) | 1 |
| 20000 | B /MHz | 1798.070(14) | 2 |
| 30000 | C /MHz | 1706.247(13) | 3 |

CORRELATION COEFFICIENTS, C.ij:

| | A | B | C |
|---|---|---|---|
| A | 1.0000 | | |
| B | 0.6185 | 1.0000 | |
| C | -0.7793 | -0.7991 | 1.0000 |

Mean value of |C.ij|, i.ne.j = 0.7323

Mean value of C.ij, i.ne.j = -0.3199

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

| | | | |
|---|---|---|---|
| 11: 14.0 | 4: 10.5 | 20: -10.4 | 16: -8.6 |
| 9: -8.6 | 12: 7.8 | 5: 7.7 | 6: 7.1 |
| 2: 7.0 | 21: -6.6 | 17: -5.9 | 15: -5.8 |
| 1: 5.2 | 7: 4.3 | 19: -4.0 | 10: -3.8 |
| 22: -3.3 | 13: 2.7 | 3: 2.0 | 14: -0.7 |
| 18: 0.6 | 8: -0.4 | | |

| | | | |
|---|---|---|---|
| 11/ 9 2 7 | 8 2 6 | 31824.8200 | 0.7012 0.050 |
| 4/ 8 2 6 | 7 2 5 | 28252.1000 | 0.5245 0.050 |
| 20/ 11 2 10 | 10 2 9 | 38428.6800 | -0.5193 0.050 |
| 16/ 10 3 8 | 9 3 7 | 35091.9200 | -0.4296 0.050 |
| 9/ 9 3 7 | 8 3 6 | 31579.2200 | -0.4290 0.050 |
| 12/ 9 1 8 | 8 1 7 | 31830.9600 | 0.3897 0.050 |
| 5/ 8 1 7 | 7 1 6 | 28320.8900 | 0.3860 0.050 |
| 6/ 9 1 9 | 8 1 8 | 31042.2200 | 0.3534 0.050 |
| 2/ 8 1 8 | 7 1 7 | 27607.1200 | 0.3499 0.050 |
| 21/ 11 3 8 | 10 3 7 | 38703.8600 | -0.3313 0.050 |

_____/ SPFIT output reformatted with PIFORM

3SiCPF2 Durig and Laane v1

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| | obs | o-c | error o-c | blends wt | Notes |
|---|---|---|---|---|---|
| / instead of : below denotes (o-c)>3*err | | | | | |
| 1/ 8 0 8 7 0 7 | 27885.8900 | 0.3057 | 0.050 | | |
| 2/ 8 1 8 7 1 7 | 27720.1000 | 0.2804 | 0.050 | | |
| 3: 9 1 9 8 1 8 | 31170.2400 | 0.1346 | 0.050 | | |
| 4/ 9 0 9 8 0 8 | 31317.9600 | 0.1927 | 0.050 | | |
| 5: 10 0 10 9 0 9 | 34742.4700 | -0.0914 | 0.050 | | |
| 6: 10 1 10 9 1 9 | 34616.7900 | 0.0113 | 0.050 | | |
| 7/ 10 2 9 9 2 8 | 35077.9000 | -0.1539 | 0.050 | | |
| 8/ 11 0 11 10 0 10 | 38162.9600 | -0.2503 | 0.050 | | |
| 9/ 11 1 11 10 1 10 | 38059.8800 | -0.2310 | 0.050 | | |

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PARAMETERS IN FIT (values truncated):

| | | | |
|---|---|---|---|
| 10000 | A /MHz | 3543.57(40) | 1 |
| 20000 | B /MHz | 1801.8784(81) | 2 |
| 30000 | C /MHz | 1714.0210(30) | 3 |

MICROWAVE AVG = 0.022026 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.204300 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 4.08599 4.08599

distinct frequency lines in fit: 9

distinct parameters of fit: 3

| | upper state | lower state | overall |
|---|---|---|---|
| limits of quantum number 1: | 8 11 | 7 10 | 7 11 |
| limits of quantum number 2: | 0 2 | 0 2 | 0 2 |
| limits of quantum number 3: | 8 11 | 7 10 | 7 11 |

frequency range: 27720 38162

Standard errors are obtained by muliplying the previous errors by: 5.004295

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

| | | | |
|---|---|---|---|
| 10000 | A /MHz | 3543.6(20) | 1 |
| 20000 | B /MHz | 1801.878(40) | 2 |
| 30000 | C /MHz | 1714.021(15) | 3 |

CORRELATION COEFFICIENTS, C.ij:

| | A | B | C |
|---|---|---|---|
| A | 1.0000 | | |
| B | 0.2360 | 1.0000 | |
| C | -0.7995 | -0.6690 | 1.0000 |

Mean value of |C.ij|, i.ne.j = 0.5682

Mean value of C.ij, i.ne.j = -0.4108

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

1: 6.1 2: 5.6 8: -5.0 9: -4.6

4: 3.9 7: -3.1 3: 2.7 5: -1.8

6: 0.2

1/ 8 0 8 7 0 7 27885.8900 0.3057 0.050

2/ 8 1 8 7 1 7 27720.1000 0.2804 0.050

8/ 11 0 11 10 0 10 38162.9600 -0.2503 0.050

9/ 11 1 11 10 1 10 38059.8800 -0.2310 0.050

4/ 9 0 9 8 0 8 31317.9600 0.1927 0.050

7/ 10 2 9 9 2 8 35077.9000 -0.1539 0.050

3: 9 1 9 8 1 8 31170.2400 0.1346 0.050

5: 10 0 10 9 0 9 34742.4700 -0.0914 0.050

6: 10 1 10 9 1 9 34616.7900 0.0113 0.050

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_____/ SPFIT output reformatted with PIFORM

3SiCPF2 Durig and Laane v2

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obs o-c error blends Notes

o-c wt

/ instead of : below denotes (o-c)>3*err

---

1/ 8 1 8 7 1 7 27814.1100 0.1774 0.050

2: 9 1 9 8 1 8 31276.9100 0.1004 0.050

3/ 9 0 9 8 0 8 31424.2100 -0.2435 0.050

4/ 10 0 10 9 0 9 34863.3500 0.2116 0.050

5: 10 1 10 9 1 9 34736.2100 -0.0216 0.050

6: 11 0 11 10 0 10 38297.4600 0.0332 0.050

7/ 11 1 11 10 1 10 38192.2200 -0.2179 0.050

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PARAMETERS IN FIT (values truncated):

| | | | |
|---|---|---|---|
| 10000 | A /MHz | 3542.20(54) | 1 |
| 20000 | B /MHz | 1805.187(43) | 2 |
| 30000 | C /MHz | 1720.4696(89) | 3 |

MICROWAVE AVG = 0.005666 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.166795 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 3.33590 3.33590

distinct frequency lines in fit: 7

distinct parameters of fit: 3

| | upper state | lower state | overall |
|---|---|---|---|
| limits of quantum number 1: | 8 11 | 7 10 | 7 11 |
| limits of quantum number 2: | 0 1 | 0 1 | 0 1 |
| limits of quantum number 3: | 8 11 | 7 10 | 7 11 |

frequency range: 27814 38297

Standard errors are obtained by muliplying the previous errors by: 4.412981

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

| | | | |
|---|---|---|---|
| 10000 | A /MHz | 3542.2(23) | 1 |
| 20000 | B /MHz | 1805.19(18) | 2 |
| 30000 | C /MHz | 1720.470(39) | 3 |

CORRELATION COEFFICIENTS, C.ij:

| | A | B | C |
|---|---|---|---|
| A | 1.0000 | | |
| B | 0.6421 | 1.0000 | |
| C | -0.7967 | -0.9646 | 1.0000 |

Mean value of |C.ij|, i.ne.j = 0.8011

Mean value of C.ij, i.ne.j = -0.3731

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

| | | | |
|---|---|---|---|
| 3: -4.9 | 7: -4.4 | 4: 4.2 | 1: 3.5 |
| 2: 2.0 | 6: 0.7 | 5: -0.4 | |

| | | | |
|---|---|---|---|
| 3/ 9 0 9 | 8 0 8 | 31424.2100 | -0.2435 0.050 |
| 7/ 11 1 11 | 10 1 10 | 38192.2200 | -0.2179 0.050 |
| 4/ 10 0 10 | 9 0 9 | 34863.3500 | 0.2116 0.050 |
| 1/ 8 1 8 | 7 1 7 | 27814.1100 | 0.1774 0.050 |
| 2: 9 1 9 | 8 1 8 | 31276.9100 | 0.1004 0.050 |
| 6: 11 0 11 | 10 0 10 | 38297.4600 | 0.0332 0.050 |
| 5: 10 1 10 | 9 1 9 | 34736.2100 | -0.0216 0.050 |

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_____/ SPFIT output reformatted with PIFORM

3SiCPF2 Durig and Laane v3

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| | obs | o-c | error o-c | blends wt | Notes |
|---|---|---|---|---|---|
| / instead of : below denotes (o-c)>3*err | | | | | |
| 1: 8 1 8 7 1 7 | 27896.8500 | -0.0098 | 0.050 | | |
| 2: 9 1 9 8 1 8 | 31370.9200 | 0.0250 | 0.050 | | |
| 3: 10 1 10 9 1 9 | 34841.5000 | -0.0215 | 0.050 | | |
| 4: 11 1 11 10 1 10 | 38308.9100 | 0.0063 | 0.050 | | |

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PARAMETERS IN FIT (values truncated):

| | | | |
|---|---|---|---|
| 10000 | A /MHz | 3830.(147) | 1 |
| 20000 | B /MHz | 1811.7(17) | 2 |
| 30000 | C /MHz | 1724.87(62) | 3 |

MICROWAVE AVG = -0.000012 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.017535 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 0.35071 0.35071

distinct frequency lines in fit: 4

distinct parameters of fit: 3

| | upper state | lower state | overall |
|---|---|---|---|
| limits of quantum number 1: | 8 11 | 7 10 | 7 11 |
| limits of quantum number 2: | 1 1 | 1 1 | 1 1 |
| limits of quantum number 3: | 8 11 | 7 10 | 7 11 |

frequency range: 27896 38308

Standard errors are obtained by muliplying the previous errors by: 0.701420

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

| | | | |
|---|---|---|---|
| 10000 | A /MHz | 3830.(103) | 1 |
| 20000 | B /MHz | 1811.7(12) | 2 |
| 30000 | C /MHz | 1724.87(43) | 3 |

CORRELATION COEFFICIENTS, C.ij:

| | A | B | C |
|---|---|---|---|
| A | 1.0000 | | |
| B | 0.9991 | 1.0000 | |
| C | -0.9998 | -0.9998 | 1.0000 |

Mean value of |C.ij|, i.ne.j = 0.9996

Mean value of C.ij, i.ne.j = -0.3335

Worst correlations, with absolute value greater than 0.9950:

| | | | | |
|---|---|---|---|---|
| 20000 | B | <-> | 10000 A | 0.999124 |
| 30000 | C | <-> | 10000 A | -0.999756 |
| 30000 | C | <-> | 20000 B | -0.999799 |

Worst fitted lines (obs-calc/error):

2: 0.5 3: -0.4 1: -0.2 4: 0.1

2: 9 1 9 8 1 8 31370.9200 0.0250 0.050

3: 10 1 10 9 1 9 34841.5000 -0.0215 0.050

1: 8 1 8 7 1 7 27896.8500 -0.0098 0.050

4: 11 1 11 10 1 10 38308.9100 0.0063 0.050

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_____/ SPFIT output reformatted with PIFORM

Holding Coriolis 3SiCPF2

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obs o-c error blends Notes

o-c wt

/ instead of : below denotes (o-c)>3*err

---

1: 2 1 2 0 1 1 1 0 6917.0167 -0.0021 0.010

2: 2 1 2 1 1 1 1 1 6917.0190 -0.0007 0.010

3: 2 0 2 0 1 0 1 0 7005.3453 -0.0046 0.010

4: 2 0 2 1 1 0 1 1 7005.3468 -0.0055 0.010

5: 2 1 1 0 1 1 0 0 7100.6875 -0.0030 0.010

6: 3 2 2 0 3 0 3 0 7186.1321 -0.0171 0.010

7: 4 2 3 0 4 0 4 0 7218.1642 -0.0099 0.010

8: 5 2 4 0 5 0 5 0 7279.1347 0.0239 0.010

9: 2 1 2 0 1 1 1 0 6917.0151 -0.0037 0.010 -0.0042 0.50

10: 2 1 2 1 1 1 1 1 6917.0151 -0.0047 0.010 -0.0042 0.50

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 11: | 2 | 0 | 2 | 0 | 1 | 0 | 1 | 0 | 7005.3482 | -0.0017 | 0.010 | -0.0030 | 0.50 |
| 12: | 2 | 0 | 2 | 1 | 1 | 0 | 1 | 1 | 7005.3482 | -0.0041 | 0.010 | -0.0030 | 0.50 |
| 13: | 2 | 1 | 1 | 0 | 1 | 1 | 0 | 0 | 7100.6825 | -0.0080 | 0.010 | | |
| 14: | 3 | 2 | 2 | 0 | 3 | 0 | 3 | 0 | 7186.1321 | -0.0171 | 0.010 | | |
| 15: | 4 | 2 | 3 | 0 | 4 | 0 | 4 | 0 | 7218.1618 | -0.0123 | 0.010 | | |
| 16/ | 5 | 2 | 4 | 0 | 5 | 0 | 5 | 0 | 7279.1432 | 0.0325 | 0.010 | | |
| 17: | 3 | 1 | 3 | 0 | 2 | 1 | 2 | 0 | 10373.3425 | -0.0089 | 0.010 | | |
| 18: | 3 | 0 | 3 | 0 | 2 | 0 | 2 | 0 | 10499.2285 | 0.0011 | 0.010 | | |
| 19: | 3 | 2 | 2 | 0 | 2 | 2 | 1 | 0 | 10513.1606 | 0.0005 | 0.010 | | |
| 20: | 3 | 2 | 1 | 0 | 2 | 2 | 0 | 0 | 10527.2463 | 0.0019 | 0.010 | | |
| 21: | 3 | 1 | 2 | 0 | 2 | 1 | 1 | 0 | 10648.7744 | 0.0003 | 0.010 | | |
| 22: | 4 | 1 | 4 | 0 | 3 | 1 | 3 | 0 | 13827.1864 | -0.0025 | 0.010 | -0.0018 | 0.50 |
| 23: | 4 | 1 | 4 | 1 | 3 | 1 | 3 | 1 | 13827.1864 | -0.0011 | 0.010 | -0.0018 | 0.50 |
| 24: | 4 | 0 | 4 | 0 | 3 | 0 | 3 | 0 | 13982.7281 | -0.0178 | 0.010 | | |
| 25: | 4 | 2 | 3 | 0 | 3 | 2 | 2 | 0 | 14014.7855 | 0.0146 | 0.010 | | |
| 26: | 4 | 3 | 2 | 0 | 3 | 3 | 1 | 0 | 14024.1248 | -0.0077 | 0.010 | | |
| 27: | 4 | 3 | 1 | 0 | 3 | 3 | 0 | 0 | 14024.6266 | -0.0061 | 0.010 | | |
| 28: | 4 | 2 | 2 | 0 | 3 | 2 | 1 | 0 | 14049.7693 | 0.0117 | 0.010 | 0.0124 | 0.50 |
| 29: | 4 | 2 | 2 | 1 | 3 | 2 | 1 | 1 | 14049.7693 | 0.0131 | 0.010 | 0.0124 | 0.50 |
| 30: | 4 | 1 | 3 | 1 | 3 | 1 | 2 | 1 | 14194.0110 | -0.0030 | 0.010 | -0.0076 | 0.50 |
| 31: | 4 | 1 | 3 | 0 | 3 | 1 | 2 | 0 | 14194.0110 | -0.0120 | 0.010 | -0.0076 | 0.50 |
| 32: | 5 | 1 | 5 | 0 | 4 | 1 | 4 | 0 | 17277.9158 | 0.0266 | 0.010 | 0.0273 | 0.50 |
| 33: | 5 | 1 | 5 | 1 | 4 | 1 | 4 | 1 | 17277.9158 | 0.0279 | 0.010 | 0.0273 | 0.50 |
| 34: | 5 | 0 | 5 | 0 | 4 | 0 | 4 | 0 | 17453.0393 | -0.0294 | 0.010 | | |
| 35/ | 5 | 0 | 5 | 1 | 4 | 0 | 4 | 1 | 17453.1552 | 0.0385 | 0.010 | | |
| 36: | 5 | 2 | 4 | 0 | 4 | 2 | 3 | 0 | 17513.9781 | -0.0272 | 0.010 | | |
| 37: | 5 | 2 | 4 | 1 | 4 | 2 | 3 | 1 | 17514.0783 | 0.0286 | 0.010 | | |
| 38/ | 5 | 4 | 2 | 1 | 4 | 4 | 1 | 1 | 17529.0060 | -0.0301 | 0.010 | | |
| 39/ | 5 | 4 | 2 | 0 | 4 | 4 | 1 | 0 | 17529.1118 | 0.0712 | 0.010 | | |
| 40/ | 5 | 3 | 3 | 1 | 4 | 3 | 2 | 1 | 17532.8218 | -0.0374 | 0.010 | | |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 41: | 5 | 3 | 3 | 0 | 4 | 3 | 2 | 0 | 17532.9140 | 0.0086 | 0.010 | | |
| 42/ | 5 | 3 | 2 | 1 | 4 | 3 | 1 | 1 | 17534.5832 | -0.0503 | 0.010 | | |
| 43: | 5 | 3 | 2 | 0 | 4 | 3 | 1 | 0 | 17534.6821 | 0.0300 | 0.010 | | |
| 44: | 5 | 2 | 3 | 0 | 4 | 2 | 2 | 0 | 17583.0556 | -0.0125 | 0.010 | | |
| 45: | 5 | 1 | 4 | 1 | 4 | 1 | 3 | 1 | 17735.2402 | -0.0208 | 0.010 | | |
| 46/ | 5 | 1 | 4 | 0 | 4 | 1 | 3 | 0 | 17735.3261 | 0.0361 | 0.010 | | |
| 47: | 8 | 0 | 8 | 0 | 7 | 0 | 7 | 0 | 27774.3400 | 0.0013 | 0.050 | | |
| 48: | 8 | 1 | 8 | 0 | 7 | 1 | 7 | 0 | 27607.1200 | -0.0104 | 0.050 | | |
| 49: | 8 | 2 | 7 | 0 | 7 | 2 | 6 | 0 | 27991.7800 | 0.1116 | 0.050 | | |
| 50: | 8 | 2 | 6 | 0 | 7 | 2 | 5 | 0 | 28252.1000 | 0.0368 | 0.050 | | |
| 51: | 8 | 1 | 7 | 0 | 7 | 1 | 6 | 0 | 28320.8900 | 0.0204 | 0.050 | | |
| 52: | 9 | 1 | 9 | 0 | 8 | 1 | 8 | 0 | 31042.2200 | 0.0934 | 0.050 | | |
| 53: | 9 | 0 | 9 | 0 | 8 | 0 | 8 | 0 | 31189.5700 | 0.0957 | 0.050 | | |
| 54/ | 9 | 2 | 8 | 0 | 8 | 2 | 7 | 0 | 31475.9300 | 0.2142 | 0.050 | | |
| 55/ | 9 | 3 | 7 | 0 | 8 | 3 | 6 | 0 | 31579.2200 | -1.1108 | 0.050 | | |
| 56: | 9 | 3 | 6 | 0 | 8 | 3 | 5 | 0 | 31617.1400 | -0.0262 | 0.050 | | |
| 57/ | 9 | 2 | 7 | 0 | 8 | 2 | 6 | 0 | 31824.8200 | 0.2603 | 0.050 | | |
| 58/ | 9 | 1 | 8 | 0 | 8 | 1 | 7 | 0 | 31830.9600 | 0.1968 | 0.050 | | |
| 59: | 10 | 1 | 10 | 0 | 9 | 1 | 9 | 0 | 34473.2900 | 0.0237 | 0.050 | | |
| 60: | 10 | 0 | 10 | 0 | 9 | 0 | 9 | 0 | 34597.3700 | 0.0269 | 0.050 | | |

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PARAMETERS IN FIT (values truncated):

| | | | |
|---|---|---|---|
| 10099 | A /MHz | 3544.4281(15) | 1 |
| 20099 | B /MHz | 1798.13899(81) | 2 |
| 30099 | C /MHz | 1706.30313(80) | 3 |
| 299 | DJ /kHz | 0.1905(62) | 4 |
| 1199 | DJK /kHz | 5.750(43) | 5 |

210001 Fbc /MHz [ 0.861530104] 6

11 E1 /MHz [11805.724020849] 7

MICROWAVE AVG = -0.001555 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.163393 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 3.79668 3.79668

distinct frequency lines in fit: 54

distinct parameters of fit: 5

| MICROWAVE | lines fitted total | dv=0 | dv.ne.0 | lines UNFITTD | lines e>900 | RMS | RMS ERROR | J range | Ka range | freq. range |
|---|---|---|---|---|---|---|---|---|---|---|
| v"= 0 | 45 | 45 | 0 | 0 | 0 | 0.178496 | 3.94752 | 1 10 | 0 4 | 6917 34597 |
| v"= 1 | 9 | 9 | 0 | 0 | 0 | 0.029165 | 2.91654 | 1 5 | 0 4 | 6917 17735 |
| total: | 54 | 54 | 0 | 0 | 0 | 0.163378 | 3.79519 | | | |

Standard errors are obtained by muliplying the previous errors by: 3.985684

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded)

| | | | |
|---|---|---|---|
| 10099 | A /MHz | 3544.4281(60) | 1 |
| 20099 | B /MHz | 1798.1390(32) | 2 |
| 30099 | C /MHz | 1706.3031(31) | 3 |
| 299 | DJ /kHz | 0.191(24) | 4 |
| 1199 | DJK /kHz | 5.75(17) | 5 |

210001 Fbc /MHz [ 0.861530104] 6

11 E1 /MHz [11805.724020849] 7

CORRELATION COEFFICIENTS, C.ij:

| | A | B | C | -DJ | -DJK |
|---|---|---|---|---|---|
| A | 1.0000 | | | | |
| B | 0.1589 | 1.0000 | | | |
| C | 0.3843 | -0.4718 | 1.0000 | | |
| -DJ | -0.2038 | -0.2016 | -0.5254 | 1.0000 | |
| -DJK | -0.6255 | -0.4547 | -0.0023 | -0.0729 | 1.0000 |

Mean value of |C.ij|, i.ne.j = 0.3101

Mean value of C.ij, i.ne.j = -0.2015

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 55: | -22.2 | 39: | 7.1 | 57: | 5.2 | 42: | -5.0 |
| 54: | 4.3 | 58: | 3.9 | 35: | 3.9 | 40: | -3.7 |
| 46: | 3.6 | 16: | 3.2 | 38: | -3.0 | 43: | 3.0 |
| 34: | -2.9 | 37: | 2.9 | 32: | 2.7 | 36: | -2.7 |
| 8: | 2.4 | 49: | 2.2 | 45: | -2.1 | 53: | 1.9 |
| 52: | 1.9 | 24: | -1.8 | 6: | -1.7 | 14: | -1.7 |
| 25: | 1.5 | 44: | -1.2 | 28: | 1.2 | 15: | -1.2 |

7: -1.0 17: -0.9 41: 0.9 13: -0.8

26: -0.8 30: -0.8 50: 0.7 27: -0.6

4: -0.5 60: 0.5 56: -0.5 59: 0.5

3: -0.5 9: -0.4 51: 0.4 5: -0.3

11: -0.3 1: -0.2 48: -0.2 20: 0.2

22: -0.2 18: 0.1

| | | | |
|---|---|---|---|
| 55/ 9 3 7 0 | 8 3 6 0 | 31579.2200 | -1.1108 0.050 |
| 39/ 5 4 2 0 | 4 4 1 0 | 17529.1118 | 0.0712 0.010 |
| 57/ 9 2 7 0 | 8 2 6 0 | 31824.8200 | 0.2603 0.050 |
| 42/ 5 3 2 1 | 4 3 1 1 | 17534.5832 | -0.0503 0.010 |
| 54/ 9 2 8 0 | 8 2 7 0 | 31475.9300 | 0.2142 0.050 |
| 58/ 9 1 8 0 | 8 1 7 0 | 31830.9600 | 0.1968 0.050 |
| 35/ 5 0 5 1 | 4 0 4 1 | 17453.1552 | 0.0385 0.010 |
| 40/ 5 3 3 1 | 4 3 2 1 | 17532.8218 | -0.0374 0.010 |
| 46/ 5 1 4 0 | 4 1 3 0 | 17735.3261 | 0.0361 0.010 |
| 16/ 5 2 4 0 | 5 0 5 0 | 7279.1432 | 0.0325 0.010 |

_____

_____/ SPFIT output reformatted with PIFORM

Adjusted Transitions

| | | obs | o-c | error o-c | blends wt | Notes |
|---|---|---|---|---|---|---|
| / instead of : below denotes (o-c)>3*err | | | | | | |
| 1: | 2 1 2 0 1 1 1 0 | 6917.0167 | 0.0000 | 0.010 | | |
| 2: | 2 1 2 1 1 1 1 1 | 6917.0190 | 0.0012 | 0.010 | | |
| 3: | 2 0 2 0 1 0 1 0 | 7005.3453 | -0.0003 | 0.010 | | |
| 4: | 2 0 2 1 1 0 1 1 | 7005.3468 | -0.0013 | 0.010 | | |
| 5: | 2 1 1 0 1 1 0 0 | 7100.6875 | 0.0025 | 0.010 | | |
| 6: | 3 2 2 0 3 0 3 0 | 7186.1321 | -0.0059 | 0.010 | | |
| 7: | 4 2 3 0 4 0 4 0 | 7218.1642 | -0.0069 | 0.010 | | |
| 8: | 5 2 4 0 5 0 5 0 | 7279.1347 | 0.0097 | 0.010 | | |
| 9: | 2 1 2 0 1 1 1 0 | 6917.0151 | -0.0017 | 0.010 | -0.0022 | 0.50 |
| 10: | 2 1 2 1 1 1 1 1 | 6917.0151 | -0.0027 | 0.010 | -0.0022 | 0.50 |
| 11: | 2 0 2 0 1 0 1 0 | 7005.3482 | 0.0024 | 0.010 | 0.0013 | 0.50 |
| 12: | 2 0 2 1 1 0 1 1 | 7005.3482 | 0.0000 | 0.010 | 0.0013 | 0.50 |
| 13: | 2 1 1 0 1 1 0 0 | 7100.6825 | -0.0024 | 0.010 | | |
| 14: | 3 2 2 0 3 0 3 0 | 7186.1321 | -0.0059 | 0.010 | | |
| 15: | 4 2 3 0 4 0 4 0 | 7218.1618 | -0.0093 | 0.010 | | |
| 16: | 5 2 4 0 5 0 5 0 | 7279.1432 | 0.0182 | 0.010 | | |
| 17: | 3 1 3 0 2 1 2 0 | 10373.3425 | -0.0077 | 0.010 | | |
| 18: | 3 0 3 0 2 0 2 0 | 10499.2285 | 0.0069 | 0.010 | | |
| 19: | 3 2 2 0 2 2 1 0 | 10513.1606 | 0.0034 | 0.010 | | |
| 20: | 3 2 1 0 2 2 0 0 | 10527.2463 | 0.0053 | 0.010 | | |
| 21: | 3 1 2 0 2 1 1 0 | 10648.7744 | 0.0068 | 0.010 | | |
| 22: | 4 1 4 0 3 1 3 0 | 13827.1864 | -0.0040 | 0.010 | -0.0034 | 0.50 |
| 23: | 4 1 4 1 3 1 3 1 | 13827.1864 | -0.0027 | 0.010 | -0.0034 | 0.50 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 24: | 4 | 0 | 4 | 0 | 3 | 0 | 3 | 0 | 13982.7281 | -0.0113 | 0.010 | |
| 25: | 4 | 2 | 3 | 0 | 3 | 2 | 2 | 0 | 14014.7855 | 0.0129 | 0.010 | |
| 26: | 4 | 3 | 2 | 0 | 3 | 3 | 1 | 0 | 14024.1248 | -0.0055 | 0.010 | |
| 27: | 4 | 3 | 1 | 0 | 3 | 3 | 0 | 0 | 14024.6266 | -0.0032 | 0.010 | |
| 28: | 4 | 2 | 2 | 0 | 3 | 2 | 1 | 0 | 14049.7693 | 0.0113 | 0.010 | 0.0120 0.50 |
| 29: | 4 | 2 | 2 | 1 | 3 | 2 | 1 | 1 | 14049.7693 | 0.0126 | 0.010 | 0.0120 0.50 |
| 30: | 4 | 1 | 3 | 1 | 3 | 1 | 2 | 1 | 14194.0110 | 0.0017 | 0.010 | -0.0027 0.50 |
| 31: | 4 | 1 | 3 | 0 | 3 | 1 | 2 | 0 | 14194.0110 | -0.0071 | 0.010 | -0.0027 0.50 |
| 32: | 5 | 1 | 5 | 0 | 4 | 1 | 4 | 0 | 17277.9158 | 0.0199 | 0.010 | 0.0205 0.50 |
| 33: | 5 | 1 | 5 | 1 | 4 | 1 | 4 | 1 | 17277.9158 | 0.0211 | 0.010 | 0.0205 0.50 |
| 34: | 5 | 0 | 5 | 0 | 4 | 0 | 4 | 0 | 17453.0393 | -0.0233 | 0.010 | |
| 35/ | 5 | 0 | 5 | 1 | 4 | 0 | 4 | 1 | 17453.1552 | 0.0446 | 0.010 | |
| 36/ | 5 | 2 | 4 | 0 | 4 | 2 | 3 | 0 | 17513.9781 | -0.0383 | 0.010 | |
| 37: | 5 | 2 | 4 | 1 | 4 | 2 | 3 | 1 | 17514.0783 | 0.0175 | 0.010 | |
| 38: | 5 | 4 | 2 | 1 | 4 | 4 | 1 | 1 | 17529.0060 | -0.0298 | 0.010 | |
| 39/ | 5 | 4 | 2 | 0 | 4 | 4 | 1 | 0 | 17529.1118 | 0.0715 | 0.010 | |
| 40/ | 5 | 3 | 3 | 1 | 4 | 3 | 2 | 1 | 17532.8218 | -0.0428 | 0.010 | |
| 41: | 5 | 3 | 3 | 0 | 4 | 3 | 2 | 0 | 17532.9140 | 0.0034 | 0.010 | |
| 42/ | 5 | 3 | 2 | 1 | 4 | 3 | 1 | 1 | 17534.5832 | -0.0533 | 0.010 | |
| 43: | 5 | 3 | 2 | 0 | 4 | 3 | 1 | 0 | 17534.6821 | 0.0271 | 0.010 | |
| 44: | 5 | 2 | 3 | 0 | 4 | 2 | 2 | 0 | 17583.0556 | -0.0208 | 0.010 | |
| 45: | 5 | 1 | 4 | 1 | 4 | 1 | 3 | 1 | 17735.2402 | -0.0213 | 0.010 | |
| 46/ | 5 | 1 | 4 | 0 | 4 | 1 | 3 | 0 | 17735.3261 | 0.0358 | 0.010 | |
| 47: | 8 | 0 | 8 | 0 | 7 | 0 | 7 | 0 | 27774.3400 | -0.0052 | 0.050 | |
| 48: | 8 | 1 | 8 | 0 | 7 | 1 | 7 | 0 | 27607.1200 | -0.0488 | 0.050 | |
| 49: | 8 | 2 | 7 | 0 | 7 | 2 | 6 | 0 | 27991.7800 | 0.0329 | 0.050 | |
| 50: | 8 | 2 | 6 | 0 | 7 | 2 | 5 | 0 | 28252.1000 | -0.0296 | 0.050 | |
| 51: | 8 | 1 | 7 | 0 | 7 | 1 | 6 | 0 | 28320.8900 | -0.0327 | 0.050 | |
| 52: | 9 | 1 | 9 | 0 | 8 | 1 | 8 | 0 | 31042.2200 | 0.0394 | 0.050 | |
| 53: | 9 | 0 | 9 | 0 | 8 | 0 | 8 | 0 | 31189.5700 | 0.0790 | 0.050 | |

```
 54:  9  2  8  0    8  2  7  0          31475.9300   0.0965  0.050
 55/  9  3  7  1    8  3  6  1          31579.2200  -0.2349  0.050
 56:  9  3  6  0    8  3  5  0          31617.1400  -0.0868  0.050
 57/  9  2  7  0    8  2  6  0          31824.8200   0.1590  0.050
 58:  9  1  8  0    8  1  7  0          31830.9600   0.1063  0.050
 59: 10  1 10  0    9  1  9  0          34473.2900  -0.0481  0.050
 60: 10  0 10  0    9  0  9  0          34597.3700  -0.0034  0.050
```

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PARAMETERS IN FIT (values truncated):

| | | | |
|---|---|---|---|
| 10099 | A /MHz | 3543.62(20) | 1 |
| 20099 | B /MHz | 1798.13696(88) | 2 |
| 30099 | C /MHz | 1706.30289(92) | 3 |
| 299 | DJ /kHz | 0.1857(88) | 4 |
| 1199 | DJK /kHz | 5.607(51) | 5 |
| 2099 | DK /kHz | -200.(50) | 6 |
| 210001 | Fbc /MHz | [ 0.861530104] | 7 |
| 11 | E1 /MHz | [11805.724020849] | 8 |

MICROWAVE AVG = 0.000486 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.051632 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 2.13760 2.13760

distinct frequency lines in fit: 54
distinct parameters of fit: 6

| MICROWAVE | lines fitted | | lines | lines | RMS | RMS ERROR | J range | | Ka range | | freq. range | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | total | dv=0 | dv.ne.0 | UNFITTD | e>900 | | | | | | | |
| v"= 0 | 44 | 44 | 0 | 0 | 0 | 0.042724 | 1.78971 | 1 | 10 | 0 | 4 | 6917 34597 |
| v"= 1 | 10 | 10 | 0 | 0 | 0 | 0.079686 | 3.24460 | 1 | 9 | 0 | 4 | 6917 31579 |
| total: | 54 | 54 | 0 | 0 | 0 | 0.051607 | 2.13528 | | | | | |

Standard errors are obtained by muliplying the previous errors by: 2.267267

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded)

| | | | |
|---|---|---|---|
| 10099 | A /MHz | 3543.62(45) | 1 |
| 20099 | B /MHz | 1798.1370(19) | 2 |
| 30099 | C /MHz | 1706.3029(20) | 3 |
| 299 | DJ /kHz | 0.186(19) | 4 |
| 1199 | DJK /kHz | 5.61(11) | 5 |
| 2099 | DK /kHz | -200.(113) | 6 |
| 210001 | Fbc /MHz | [ 0.861530104] | 7 |
| 11 | E1 /MHz | [11805.724020849] | 8 |

Worst fitted constants, with greater than 20% uncertainty: %

| | | | | |
|---|---|---|---|---|
| 2099 | DK /kHz | -200.(113) | 6 | 56.7 |

CORRELATION COEFFICIENTS, C.ij:

| | A | B | C | -DJ | -DJK | -DK |
|---|---|---|---|---|---|---|
| A | 1.0000 | | | | | |
| B | 0.3951 | 1.0000 | | | | |
| C | -0.4945 | -0.5722 | 1.0000 | | | |
| -DJ | 0.7150 | 0.1528 | -0.6742 | 1.0000 | | |
| -DJK | -0.5391 | -0.5638 | 0.2643 | -0.4262 | 1.0000 | |
| -DK | -1.0000 | -0.3940 | 0.4970 | -0.7161 | 0.5351 | 1.0000 |

Mean value of |C.ij|, i.ne.j = 0.5293

Mean value of C.ij, i.ne.j = -0.1880

Worst correlations, with absolute value greater than 0.9950:

2099 -DK <-> 10099 A -0.999971

Worst fitted lines (obs-calc/error):

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 39: | 7.1 | 42: | -5.3 | 55: | -4.7 | 35: | 4.5 |
| 40: | -4.3 | 36: | -3.8 | 46: | 3.6 | 57: | 3.2 |
| 38: | -3.0 | 43: | 2.7 | 34: | -2.3 | 45: | -2.1 |
| 58: | 2.1 | 44: | -2.1 | 32: | 2.1 | 54: | 1.9 |
| 16: | 1.8 | 37: | 1.8 | 56: | -1.7 | 53: | 1.6 |
| 25: | 1.3 | 28: | 1.2 | 24: | -1.1 | 48: | -1.0 |
| 8: | 1.0 | 59: | -1.0 | 15: | -0.9 | 52: | 0.8 |
| 17: | -0.8 | 7: | -0.7 | 18: | 0.7 | 21: | 0.7 |

49: 0.7 51: -0.7 50: -0.6 6: -0.6

14: -0.6 26: -0.5 20: 0.5 41: 0.3

19: 0.3 22: -0.3 27: -0.3 30: -0.3

5: 0.2 13: -0.2 9: -0.2 4: -0.1

11: 0.1 2: 0.1

39/ 5 4 2 0 4 4 1 0 17529.1118 0.0715 0.010

42/ 5 3 2 1 4 3 1 1 17534.5832 -0.0533 0.010

55/ 9 3 7 1 8 3 6 1 31579.2200 -0.2349 0.050

35/ 5 0 5 1 4 0 4 1 17453.1552 0.0446 0.010

40/ 5 3 3 1 4 3 2 1 17532.8218 -0.0428 0.010

36/ 5 2 4 0 4 2 3 0 17513.9781 -0.0383 0.010

46/ 5 1 4 0 4 1 3 0 17735.3261 0.0358 0.010

57/ 9 2 7 0 8 2 6 0 31824.8200 0.1590 0.050

38: 5 4 2 1 4 4 1 1 17529.0060 -0.0298 0.010

43: 5 3 2 0 4 3 1 0 17534.6821 0.0271 0.010

_____

_____/ SPFIT output reformatted with PIFORM

Fit Coriolis

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obs o-c error blends Notes

o-c wt

/ instead of : below denotes (o-c)>3*err

---

1: 2 1 2 0 1 1 1 0 6917.0167 0.0029 0.010

2: 2 1 2 1 1 1 1 1 6917.0190 0.0044 0.010

3: 2 0 2 0 1 0 1 0 7005.3453 -0.0012 0.010

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 4: | 2 | 0 | 2 | 1 | 1 | 0 | 1 | 1 | 7005.3468 | -0.0017 | 0.010 | |
| 5: | 2 | 1 | 1 | 0 | 1 | 1 | 0 | 0 | 7100.6875 | -0.0014 | 0.010 | |
| 6: | 3 | 2 | 2 | 0 | 3 | 0 | 3 | 0 | 7186.1321 | -0.0106 | 0.010 | |
| 7: | 4 | 2 | 3 | 0 | 4 | 0 | 4 | 0 | 7218.1642 | -0.0082 | 0.010 | |
| 8: | 5 | 2 | 4 | 0 | 5 | 0 | 5 | 0 | 7279.1347 | 0.0158 | 0.010 | |
| 9: | 2 | 1 | 2 | 0 | 1 | 1 | 1 | 0 | 6917.0151 | 0.0012 | 0.010 | 0.0008 0.50 |
| 10: | 2 | 1 | 2 | 1 | 1 | 1 | 1 | 1 | 6917.0151 | 0.0004 | 0.010 | 0.0008 0.50 |
| 11: | 2 | 0 | 2 | 0 | 1 | 0 | 1 | 0 | 7005.3482 | 0.0016 | 0.010 | 0.0007 0.50 |
| 12: | 2 | 0 | 2 | 1 | 1 | 0 | 1 | 1 | 7005.3482 | -0.0002 | 0.010 | 0.0007 0.50 |
| 13: | 2 | 1 | 1 | 0 | 1 | 1 | 0 | 0 | 7100.6825 | -0.0064 | 0.010 | |
| 14: | 3 | 2 | 2 | 0 | 3 | 0 | 3 | 0 | 7186.1321 | -0.0106 | 0.010 | |
| 15: | 4 | 2 | 3 | 0 | 4 | 0 | 4 | 0 | 7218.1618 | -0.0106 | 0.010 | |
| 16: | 5 | 2 | 4 | 0 | 5 | 0 | 5 | 0 | 7279.1432 | 0.0244 | 0.010 | |
| 17: | 3 | 1 | 3 | 0 | 2 | 1 | 2 | 0 | 10373.3425 | -0.0031 | 0.010 | |
| 18: | 3 | 0 | 3 | 0 | 2 | 0 | 2 | 0 | 10499.2285 | 0.0048 | 0.010 | |
| 19: | 3 | 2 | 2 | 0 | 2 | 2 | 1 | 0 | 10513.1606 | 0.0024 | 0.010 | |
| 20: | 3 | 2 | 1 | 0 | 2 | 2 | 0 | 0 | 10527.2463 | 0.0050 | 0.010 | |
| 21: | 3 | 1 | 2 | 0 | 2 | 1 | 1 | 0 | 10648.7744 | 0.0009 | 0.010 | |
| 22: | 4 | 1 | 4 | 0 | 3 | 1 | 3 | 0 | 13827.1864 | 0.0021 | 0.010 | 0.0041 0.50 |
| 23: | 4 | 1 | 4 | 1 | 3 | 1 | 3 | 1 | 13827.1864 | 0.0061 | 0.010 | 0.0041 0.50 |
| 24: | 4 | 0 | 4 | 0 | 3 | 0 | 3 | 0 | 13982.7281 | -0.0155 | 0.010 | |
| 25: | 4 | 2 | 3 | 0 | 3 | 2 | 2 | 0 | 14014.7855 | 0.0122 | 0.010 | |
| 26: | 4 | 3 | 2 | 0 | 3 | 3 | 1 | 0 | 14024.1248 | -0.0106 | 0.010 | |
| 27: | 4 | 3 | 1 | 0 | 3 | 3 | 0 | 0 | 14024.6266 | -0.0052 | 0.010 | |
| 28: | 4 | 2 | 2 | 0 | 3 | 2 | 1 | 0 | 14049.7693 | 0.0123 | 0.010 | 0.0130 0.50 |
| 29: | 4 | 2 | 2 | 1 | 3 | 2 | 1 | 1 | 14049.7693 | 0.0136 | 0.010 | 0.0130 0.50 |
| 30: | 4 | 1 | 3 | 1 | 3 | 1 | 2 | 1 | 14194.0110 | 0.0010 | 0.010 | -0.0067 0.50 |
| 31: | 4 | 1 | 3 | 0 | 3 | 1 | 2 | 0 | 14194.0110 | -0.0145 | 0.010 | -0.0067 0.50 |
| 32/ | 5 | 1 | 5 | 0 | 4 | 1 | 4 | 0 | 17277.9158 | 0.0274 | 0.010 | 0.0303 0.50 |
| 33: | 5 | 1 | 5 | 1 | 4 | 1 | 4 | 1 | 17277.9158 | 0.0331 | 0.010 | 0.0303 0.50 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 34/ | 5 | 0 | 5 | 0 | 4 | 0 | 4 | 0 | 17453.0393 | -0.0308 | 0.010 |
| 35/ | 5 | 0 | 5 | 1 | 4 | 0 | 4 | 1 | 17453.1552 | 0.0474 | 0.010 |
| 36/ | 5 | 2 | 4 | 0 | 4 | 2 | 3 | 0 | 17513.9781 | -0.0384 | 0.010 |
| 37: | 5 | 2 | 4 | 1 | 4 | 2 | 3 | 1 | 17514.0783 | 0.0277 | 0.010 |
| 38/ | 5 | 4 | 2 | 1 | 4 | 4 | 1 | 1 | 17529.0060 | -0.0313 | 0.010 |
| 39/ | 5 | 4 | 2 | 0 | 4 | 4 | 1 | 0 | 17529.1118 | 0.0702 | 0.010 |
| 40/ | 5 | 3 | 3 | 1 | 4 | 3 | 2 | 1 | 17532.8218 | -0.0393 | 0.010 |
| 41: | 5 | 3 | 3 | 0 | 4 | 3 | 2 | 0 | 17532.9140 | -0.0102 | 0.010 |
| 42/ | 5 | 3 | 2 | 1 | 4 | 3 | 1 | 1 | 17534.5832 | -0.0524 | 0.010 |
| 43: | 5 | 3 | 2 | 0 | 4 | 3 | 1 | 0 | 17534.6821 | 0.0262 | 0.010 |
| 44: | 5 | 2 | 3 | 0 | 4 | 2 | 2 | 0 | 17583.0556 | -0.0174 | 0.010 |
| 45: | 5 | 1 | 4 | 1 | 4 | 1 | 3 | 1 | 17735.2402 | -0.0094 | 0.010 |
| 46: | 5 | 1 | 4 | 0 | 4 | 1 | 3 | 0 | 17735.3261 | 0.0278 | 0.010 |
| 47: | 8 | 0 | 8 | 0 | 7 | 0 | 7 | 0 | 27774.3400 | -0.0313 | 0.050 |
| 48: | 8 | 1 | 8 | 0 | 7 | 1 | 7 | 0 | 27607.1200 | -0.0429 | 0.050 |
| 49: | 8 | 2 | 7 | 0 | 7 | 2 | 6 | 0 | 27991.7800 | 0.0311 | 0.050 |
| 50: | 8 | 2 | 6 | 0 | 7 | 2 | 5 | 0 | 28252.1000 | -0.0094 | 0.050 |
| 51: | 8 | 1 | 7 | 0 | 7 | 1 | 6 | 0 | 28320.8900 | -0.0319 | 0.050 |
| 52: | 9 | 1 | 9 | 0 | 8 | 1 | 8 | 0 | 31042.2200 | 0.0405 | 0.050 |
| 53: | 9 | 0 | 9 | 0 | 8 | 0 | 8 | 0 | 31189.5700 | 0.0433 | 0.050 |
| 54: | 9 | 2 | 8 | 0 | 8 | 2 | 7 | 0 | 31475.9300 | 0.0860 | 0.050 |
| 55/ | 9 | 3 | 7 | 1 | 8 | 3 | 6 | 1 | 31579.2200 | -0.1770 | 0.050 |
| 56: | 9 | 3 | 6 | 0 | 8 | 3 | 5 | 0 | 31617.1400 | -0.0843 | 0.050 |
| 57/ | 9 | 2 | 7 | 0 | 8 | 2 | 6 | 0 | 31824.8200 | 0.1897 | 0.050 |
| 58: | 9 | 1 | 8 | 0 | 8 | 1 | 7 | 0 | 31830.9600 | 0.1162 | 0.050 |
| 59: | 10 | 1 | 10 | 0 | 9 | 1 | 9 | 0 | 34473.2900 | -0.0552 | 0.050 |
| 60: | 10 | 0 | 10 | 0 | 9 | 0 | 9 | 0 | 34597.3700 | -0.0509 | 0.050 |

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PARAMETERS IN FIT (values truncated):

| | | | |
|---|---|---|---|
| 10099 | A /MHz | 3544.4249(16) | 1 |
| 20099 | B /MHz | 1798.13881(85) | 2 |
| 30099 | C /MHz | 1706.30123(83) | 3 |
| 299 | DJ /kHz | 0.1645(67) | 4 |
| 1199 | DJK /kHz | 5.760(47) | 5 |
| 210001 | Fbc /MHz | 0.807(42) | 6 |
| 11 | E1 /MHz | 12431.(159) | 7 |

MICROWAVE AVG = 0.000437 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.049092 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 2.15515 2.15515

distinct frequency lines in fit: 54

distinct parameters of fit: 7

| MICROWAVE | lines fitted | | lines | lines | RMS | RMS ERROR | J range | Ka range | freq. range |
|---|---|---|---|---|---|---|---|---|---|
| | total | dv=0 | dv.ne.0 | UNFITTD | e>900 | | | | |
| v"= 0 | 44 | 44 | 0 | 0 | 0 | 0.045291 | 1.86718 | 1 10 0 4 | 6917 34597 |
| v"= 1 | 10 | 10 | 0 | 0 | 0 | 0.063063 | 3.11339 | 1 9 0 4 | 6917 31579 |
| total: | 54 | 54 | 0 | 0 | 0 | 0.049070 | 2.15309 | | |

Standard errors are obtained by muliplying the previous errors by: 2.310072

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded)

| | | | |
|---|---|---|---|
| 10099 | A /MHz | 3544.4249(38) | 1 |
| 20099 | B /MHz | 1798.1388(19) | 2 |
| 30099 | C /MHz | 1706.3012(19) | 3 |
| 299 | DJ /kHz | 0.165(15) | 4 |
| 1199 | DJK /kHz | 5.76(10) | 5 |
| 210001 | Fbc /MHz | 0.807(97) | 6 |
| 11 | E1 /MHz | 12431.(367) | 7 |

CORRELATION COEFFICIENTS, C.ij:

| | A | B | C | -DJ | -DJK | Fbc | E1 |
|---|---|---|---|---|---|---|---|
| A | 1.0000 | | | | | | |
| B | 0.2086 | 1.0000 | | | | | |
| C | 0.2316 | -0.4895 | 1.0000 | | | | |
| -DJ | -0.0268 | -0.1370 | -0.5632 | 1.0000 | | | |
| -DJK | -0.6158 | -0.5149 | 0.0703 | -0.1141 | 1.0000 | | |
| Fbc | 0.3874 | 0.1073 | -0.2497 | 0.3759 | -0.1335 | 1.0000 | |
| E1 | -0.1294 | 0.1653 | 0.0525 | -0.2046 | -0.2388 | -0.5549 | 1.0000 |

Mean value of |C.ij|, i.ne.j = 0.2653

Mean value of C.ij, i.ne.j = -0.1130

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

| | | | |
|---|---|---|---|
| 39: 7.0 | 42: -5.2 | 35: 4.7 | 40: -3.9 |
| 36: -3.8 | 57: 3.8 | 55: -3.5 | 38: -3.1 |
| 34: -3.1 | 32: 3.0 | 46: 2.8 | 37: 2.8 |
| 43: 2.6 | 16: 2.4 | 58: 2.3 | 44: -1.7 |
| 54: 1.7 | 56: -1.7 | 8: 1.6 | 24: -1.6 |
| 28: 1.3 | 25: 1.2 | 59: -1.1 | 6: -1.1 |
| 15: -1.1 | 14: -1.1 | 26: -1.1 | 41: -1.0 |
| 60: -1.0 | 45: -0.9 | 53: 0.9 | 48: -0.9 |
| 7: -0.8 | 52: 0.8 | 30: -0.7 | 13: -0.6 |
| 51: -0.6 | 47: -0.6 | 49: 0.6 | 27: -0.5 |
| 20: 0.5 | 18: 0.5 | 2: 0.4 | 22: 0.4 |
| 17: -0.3 | 1: 0.3 | 19: 0.2 | 50: -0.2 |
| 4: -0.2 | 5: -0.1 | | |

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 39/ | 5 | 4 | 2 | 0 | 4 | 4 | 1 | 0 | 17529.1118 | 0.0702 | 0.010 | | | | |
| 42/ | 5 | 3 | 2 | 1 | 4 | 3 | 1 | 1 | 17534.5832 | -0.0524 | 0.010 | | | | |
| 35/ | 5 | 0 | 5 | 1 | 4 | 0 | 4 | 1 | 17453.1552 | 0.0474 | 0.010 | | | | |
| 40/ | 5 | 3 | 3 | 1 | 4 | 3 | 2 | 1 | 17532.8218 | -0.0393 | 0.010 | | | | |
| 36/ | 5 | 2 | 4 | 0 | 4 | 2 | 3 | 0 | 17513.9781 | -0.0384 | 0.010 | | | | |
| 57/ | 9 | 2 | 7 | 0 | 8 | 2 | 6 | 0 | 31824.8200 | 0.1897 | 0.050 | | | | |
| 55/ | 9 | 3 | 7 | 1 | 8 | 3 | 6 | 1 | 31579.2200 | -0.1770 | 0.050 | | | | |
| 38/ | 5 | 4 | 2 | 1 | 4 | 4 | 1 | 1 | 17529.0060 | -0.0313 | 0.010 | | | | |
| 34/ | 5 | 0 | 5 | 0 | 4 | 0 | 4 | 0 | 17453.0393 | -0.0308 | 0.010 | | | | |
| 32/ | 5 | 1 | 5 | 0 | 4 | 1 | 4 | 0 | 17277.9158 | 0.0274 | 0.010 | 0.0303 | 0.50 | | |

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_____/ SPFIT output reformatted with PIFORM

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 ____________________________________________________________________________
|                                                                            |
|   KRA  -  SINGLE ISOTOPIC SUBSTITUTION - Various permutations              |
|           of Kraitchman's equations for symmetric/asymmetric tops          |
|____________________________________________________________________________|
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version 27.XI.2013 Zbigniew KISIEL

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11dfscp3ene

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parent species

Planar calculation will be made from I.a and I.b

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Si-29

---

The parent species:

| | | | |
|---|---|---|---|
| X, Y, Z = | 3544.42800000 | 1798.13910000 | 1706.30130000 |
| eX, eY, eZ = | 0.00350000 | 0.00230000 | 0.00250000 |
| IX, IY, IZ = | 142.58407986 | 281.05667965 | 296.18391840 |
| eIX,eIY,eIZ = | 0.00014080 | 0.00035950 | 0.00043396 |
| PX, PY, PZ = | 217.32825910 | 78.85565930 | 63.72842056 |

Mass = 120.02068630

The isotopic species:

X, Y, Z = 3543.45000000 1796.32400000 1704.67800000

eX, eY, eZ = 0.47000000 0.00360000 0.00360000

IX, IY, IZ = 142.62343338 281.34067407 296.46596307

eIX,eIY,eIZ = 0.01891744 0.00056383 0.00062609

PX, PY, PZ = 217.59160188 78.87436119 63.74907218

Mass change = 0.99956780

Total mass = 121.02025410

M DM/(M+DM) = 0.99131186

KRAITCHMAN RESULTS:

a b

PLANAR: 0.53517 +- 0.00063 0.19945 +- 0.04794

+Costain err. 0.53517 +- 0.00287 0.19945 +- 0.04853

a b c

NONPLANAR: 0.51534 +- 0.00927 0.13739 +- 0.03479 0.14455 +- 0.03315

+Costain err. 0.51534 +- 0.00971 0.13739 +- 0.03647 0.14455 +- 0.03474

R= 0.55258 +- 0.01571

DIX,DIY,DIZ = 0.03935352 0.28399441 0.28204468

DPX,DPY,DPZ = 0.26334278 0.01870189 0.02065163

IXY,IXZ,IYZ = -138.47259980 -153.59983854 -15.12723874

---

Si-30

---

The parent species:

| | | | |
|---|---|---|---|
| X, Y, Z = | 3544.42800000 | 1798.13910000 | 1706.30130000 |
| eX, eY, eZ = | 0.00350000 | 0.00230000 | 0.00250000 |
| IX, IY, IZ = | 142.58407986 | 281.05667965 | 296.18391840 |
| eIX,eIY,eIZ = | 0.00014080 | 0.00035950 | 0.00043396 |
| PX, PY, PZ = | 217.32825910 | 78.85565930 | 63.72842056 |

Mass = 120.02068630

The isotopic species:

| | | | |
|---|---|---|---|
| X, Y, Z = | 3544.41000000 | 1794.55290000 | 1703.07450000 |
| eX, eY, eZ = | 0.37000000 | 0.00250000 | 0.00240000 |
| IX, IY, IZ = | 142.58480396 | 281.61833792 | 296.74509541 |
| eIX,eIY,eIZ = | 0.01488439 | 0.00039232 | 0.00041818 |
| PX, PY, PZ = | 217.88931469 | 78.85578073 | 63.72902323 |

Mass change = 1.99684360

Total mass = 122.01752990

M DM/(M+DM) = 1.96416482

KRAITCHMAN RESULTS:

| | a | b |
|---|---|---|
| PLANAR: | 0.53474 +- 0.00025 | 0.01924 +- 0.19775 |

+Costain err.  0.53474 +- 0.00282  0.01924 +- 0.21256

a  b  c

NONPLANAR:  0.53446 +- 0.00355  0.00788 +- 0.24179  0.01755 +- 0.10851

+Costain err.  0.53446 +- 0.00453  0.00788 +- 0.30776  0.01755 +- 0.13814

R= 0.53480 +- 0.00785

| | | | |
|---|---|---|---|
| DIX,DIY,DIZ = | 0.00072410 | 0.56165826 | 0.56117702 |
| DPX,DPY,DPZ = | 0.56105559 | 0.00012143 | 0.00060267 |
| IXY,IXZ,IYZ = | -138.47259980 | -153.59983854 | -15.12723874 |

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C-13 1/4

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The parent species:

| | | | |
|---|---|---|---|
| X, Y, Z = | 3544.42800000 | 1798.13910000 | 1706.30130000 |
| eX, eY, eZ = | 0.00350000 | 0.00230000 | 0.00250000 |
| IX, IY, IZ = | 142.58407986 | 281.05667965 | 296.18391840 |
| eIX,eIY,eIZ = | 0.00014080 | 0.00035950 | 0.00043396 |
| PX, PY, PZ = | 217.32825910 | 78.85565930 | 63.72842056 |

Mass = 120.02068630

The isotopic species:

| | | | |
|---|---|---|---|
| X, Y, Z = | 3494.65000000 | 1795.31270000 | 1692.45100000 |

eX, eY, eZ = 0.29000000 0.00220000 0.00220000

IX, IY, IZ = 144.61505587 281.49915332 298.60776176

eIX,eIY,eIZ = 0.01200073 0.00034495 0.00038816

PX, PY, PZ = 217.74592961 80.86183215 63.75322372

Mass change = 1.00335484

Total mass = 121.02404114

M DM/(M+DM) = 0.99503648

KRAITCHMAN RESULTS:

a b

PLANAR: 0.66194 +- 0.00037 1.43095 +- 0.00423

+Costain err. 0.66194 +- 0.00230 1.43095 +- 0.00436

a b c

NONPLANAR: 0.64312 +- 0.00463 1.42090 +- 0.00215 0.16825 +- 0.02039

+Costain err. 0.64312 +- 0.00518 1.42090 +- 0.00239 0.16825 +- 0.02226

R= 1.56871 +- 0.00386

DIX,DIY,DIZ = 2.03097601 0.44247367 2.42384336

DPX,DPY,DPZ = 0.41767051 2.00617285 0.02480316

IXY,IXZ,IYZ = -138.47259980 -153.59983854 -15.12723874

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C-13 2/3

---

The parent species:

| | | | |
|---|---|---|---|
| X, Y, Z = | 3544.42800000 | 1798.13910000 | 1706.30130000 |
| eX, eY, eZ = | 0.00350000 | 0.00230000 | 0.00250000 |
| IX, IY, IZ = | 142.58407986 | 281.05667965 | 296.18391840 |
| eIX,eIY,eIZ = | 0.00014080 | 0.00035950 | 0.00043396 |
| PX, PY, PZ = | 217.32825910 | 78.85565930 | 63.72842056 |

Mass = 120.02068630

The isotopic species:

| | | | |
|---|---|---|---|
| X, Y, Z = | 3533.34000000 | 1773.21460000 | 1681.42020000 |
| eX, eY, eZ = | 0.33000000 | 0.00220000 | 0.00200000 |
| IX, IY, IZ = | 143.03152400 | 285.00724334 | 300.56675006 |
| eIX,eIY,eIZ = | 0.01335858 | 0.00035360 | 0.00035752 |
| PX, PY, PZ = | 221.27123470 | 79.29551536 | 63.73600864 |

Mass change = 1.00335484

Total mass = 121.02404114

M DM/(M+DM) = 0.99503648

KRAITCHMAN RESULTS:

| | a | b |
|---|---|---|
| PLANAR: | 1.98933 +- 0.00016 | 0.68008 +- 0.01015 |
| +Costain err. | 1.98933 +- 0.00077 | 0.68008 +- 0.01039 |

a b c

NONPLANAR: 1.98743 +- 0.00169 0.67410 +- 0.00513 0.08972 +- 0.03955

+Costain err. 1.98743 +- 0.00185 0.67410 +- 0.00559 0.08972 +- 0.04294

R= 2.10055 +- 0.00311

DIX,DIY,DIZ = 0.44744414 3.95056369 4.38283166

DPX,DPY,DPZ = 3.94297561 0.43985606 0.00758808

IXY,IXZ,IYZ = -138.47259980 -153.59983854 -15.12723874

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|                                                                           |
|    E V A L  -  Internals and their errors from Cartesians                 |
|___________________________________________________________________________|
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version 19.VI.2017 Zbigniew KISIEL

WARNING:

The EVAL uncertainties are evaluated by assuming that
the correlation matrix is a unit matrix.

The EVAL uncertainties may thus differ significantly
(but typically by not more than 30% either way)
from uncertainties in explicitly fitted internals
corresponding to the input Cartesians.

! 11dfscp3ene Si-29

!

INPUT CARTESIANS:

| | | | | | | |
|---|---|---|---|---|---|---|
| Si-29 | 0.51534 | 0.00971 | 0.13739 | 0.03647 | 0.14455 | 0.03474 |
| C(1) | -1.98743 | 0.00185 | 0.67410 | 0.00559 | -0.08972 | 0.04294 |
| C(2) | -1.98743 | 0.00185 | -0.67410 | 0.00559 | -0.08972 | 0.04294 |
| C(3) | -0.64312 | 0.00518 | -1.42090 | 0.00239 | 0.16825 | 0.02226 |
| C(4) | -0.64312 | 0.00518 | 1.42090 | 0.00239 | 0.16825 | 0.02226 |

CALCULATED INTERNALS:

!

! Bond Lengths

!

Si-29 C(3) = 1.94187 +- 0.03006

Si-29 C(4) = 1.72916 +- 0.02811

C(1) C(4) = 1.55930 +- 0.00974

C(1) C(2) = 1.34820 +- 0.00791

C(2) C(3) = 1.55930 +- 0.00974

!

! Bond Angles

!

C(3) Si-29 C(4) = 101.29202 +- 0.53388

Si-29 C(4) C(1) = 102.69831 +- 0.90228

C(4) C(1) C(2) = 118.61565 +- 0.65041

C(1) C(2) C(3) = 118.61565 +- 0.65038

C(2) C(3) Si-29 = 97.35222 +- 0.74091

!

! Dihedral Angles

!

Si-29 C(4) C(1) C(2) = 8.23438 +- 4.22980

C(4) C(1) C(2) C(3) = 0.00000 +- 5.41973

C(1) C(2) C(3) Si-29 = -7.20653 +- 4.02348

C(2) C(3) Si-29 C(4) = 10.63523 +- 2.52151

C(3) Si-29 C(4) C(1) = -10.81436 +- 2.57351

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|                                                                            |
|     E V A L  -  Internals and their errors from Cartesians                 |
|____________________________________________________________________________|
 version 19.VI.2017                          Zbigniew KISIEL
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WARNING:

The EVAL uncertainties are evaluated by assuming that
the correlation matrix is a unit matrix.

The EVAL uncertainties may thus differ significantly
(but typically by not more than 30% either way)
from uncertainties in explicitly fitted internals
corresponding to the input Cartesians.

! 11dfscp3ene Si-30

!

INPUT CARTESIANS:

| | | | | | | |
|---|---|---|---|---|---|---|
| Si-30 | 0.53446 | 0.00453 | 0.00788 | 0.30776 | 0.01755 | 0.13814 |
| C(1) | -1.98743 | 0.00185 | 0.67410 | 0.00559 | -0.08972 | 0.04294 |
| C(2) | -1.98743 | 0.00185 | -0.67410 | 0.00559 | -0.08972 | 0.04294 |
| C(3) | -0.64312 | 0.00518 | -1.42090 | 0.00239 | 0.16825 | 0.02226 |
| C(4) | -0.64312 | 0.00518 | 1.42090 | 0.00239 | 0.16825 | 0.02226 |

CALCULATED INTERNALS:

!

! Bond Lengths

!

Si-30 C(3) = 1.85764 +- 0.23706

Si-30 C(4) = 1.84554 +- 0.23592

C(1) C(4) = 1.55930 +- 0.00974

C(1) C(2) = 1.34820 +- 0.00791

C(2) C(3) = 1.55930 +- 0.00974

!

! Bond Angles

!

C(3) Si-30 C(4) = 100.24043 +- 0.88606

Si-30 C(4) C(1) = 99.78163 +- 5.96991

C(4) C(1) C(2) = 118.61565 +- 0.65041

C(1) C(2) C(3) = 118.61565 +- 0.65038

C(2) C(3) Si-30 = 99.48121 +- 5.88851

!

! Dihedral Angles

!

Si-30 C(4) C(1) C(2) = 11.73582 +- 6.07476

C(4) C(1) C(2) C(3) = 0.00000 +- 5.41973

C(1) C(2) C(3) Si-30 = -11.64782 +- 6.03921

C(2) C(3) Si-30 C(4) = 16.10069 +- 6.13063

C(3) Si-30 C(4) C(1) = -16.11541 +- 6.13581

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