

The quasi-unchanged gas-phase molecular structures of the atmospheric aerosol precursor β -pinene and its oxidation product
nopinone

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Electronic Supplementary Information (ESI) available: [Fits: Spectroscopy and Structures]

- Fits of rotational lines of beta-pinene and its ^{13}C isotopologues (pp 2-16)
- Fits of rotational lines of nopinone and its ^{13}C and ^{18}O isotopologues (pp 17-39)
- rs structure. Coordinates for beta-pinene and nopinone (p 40)
- r0 structure of beta-pinene (pp 41-43)
- r(1)m structure of beta-pinene (pp 44-46)
- r0 structure of nopinone (pp 47-50)
- r(1)m structure of nopinone (pp 51-54)

							obs	o-c	error	blends	Notes
										o-c	wt
/ instead of : below denotes (o-c)>3*err											
1:	1	0	1	0	0	0	2444.4920	0.0003	0.002		
2:	1	1	1	0	0	0	3052.7207	0.0008	0.002		
3:	1	1	0	0	0	0	3195.5494	-0.0002	0.002		
4:	4	3	2	4	2	3	3467.4830	-0.0006	0.001		
5:	5	3	3	5	2	4	3573.3757	-0.0024	0.001		
6:	9	3	7	9	2	8	4713.6145	0.0010	0.001		
7:	8	2	7	8	1	8	4717.0256	-0.0007	0.001		
8:	6	4	3	6	3	4	4719.1267	-0.0008	0.001		
9:	2	1	2	1	1	1	4746.1524	0.0002	0.002		
10:	2	0	2	1	0	1	4866.6525	-0.0001	0.002		
11:	2	1	2	1	0	1	5354.3807	0.0002	0.002		
12:	2	1	1	1	0	1	5782.8678	-0.0011	0.002		
13:	6	5	1	6	4	2	6045.5670	-0.0046	0.002		
14:	3	0	3	2	1	2	6759.8186	-0.0002	0.002		
15:	2	2	1	1	1	0	6856.4951	-0.0005	0.002		
16:	2	2	0	1	1	1	7021.6521	-0.0021	0.002		
17:	3	1	3	2	1	2	7106.2106	-0.0008	0.002		
18:	3	0	3	2	0	2	7247.5459	-0.0007	0.002		
19:	3	2	1	2	2	0	7419.3841	-0.0053	0.002		
20:	3	1	2	2	1	1	7532.4824	-0.0007	0.002		
21:	3	1	3	2	0	2	7593.9395	0.0002	0.002		
22:	3	1	2	2	0	2	8448.7024	0.0028	0.002		
23:	4	0	4	3	1	3	9234.8930	-0.0008	0.002		
24:	5	2	3	4	3	2	9349.6406	-0.0015	0.001		
25:	4	1	4	3	1	3	9453.5101	0.0004	0.002		
26:	4	0	4	3	0	3	9581.2863	-0.0001	0.002		
27:	4	2	3	3	2	2	9760.4776	0.0004	0.002		
28:	4	1	4	3	0	3	9799.9021	-0.0001	0.002		
29:	4	2	2	3	2	1	9956.9572	-0.0002	0.002		
30:	4	1	3	3	1	2	10011.7539	-0.0005	0.002		
31:	3	3	1	2	2	0	10722.3649	-0.0010	0.002		
32:	3	3	0	2	2	0	10724.5806	0.0005	0.002		
33:	3	3	1	2	2	1	10744.6932	-0.0015	0.002		
34:	3	3	0	2	2	1	10746.9092	0.0004	0.002		
35:	5	1	4	4	2	2	10778.7121	0.0010	0.001		
36:	5	1	4	4	2	3	11083.4412	0.0001	0.002		
37:	4	1	3	3	0	3	11212.9088	0.0013	0.002		
38:	4	2	3	3	1	2	11386.1479	0.0008	0.002		
39:	5	0	5	4	1	4	11662.8820	0.0006	0.002		
40:	5	0	5	4	0	4	11881.4971	0.0000	0.002		
41:	5	1	5	4	0	4	12006.4335	0.0000	0.002		
42:	5	2	4	4	2	3	12172.9087	-0.0004	0.002		
43:	4	2	3	3	1	3	12240.9082	0.0008	0.002		
44:	5	4	1	4	4	0	12273.3763	-0.0027	0.001		
45:	5	3	3	4	3	2	12278.8031	-0.0004	0.001		
46:	5	3	2	4	3	1	12322.9060	0.0008	0.001		
47:	5	1	4	4	1	3	12457.8329	-0.0007	0.001		
48:	5	2	3	4	2	2	12512.3955	-0.0003	0.001		
49:	4	2	2	3	1	3	12545.6373	-0.0001	0.002		
50:	7	3	4	6	4	3	12858.2441	0.0044	0.002		
51:	7	2	6	6	3	3	13032.1273	-0.0001	0.002		
52:	4	3	2	3	2	1	13119.7110	0.0000	0.002		
53:	4	3	2	3	2	2	13227.9600	-0.0008	0.002		
54:	4	3	1	3	2	2	13243.2409	0.0005	0.002		
55:	5	2	4	4	1	3	13547.3018	0.0000	0.001		
56:	6	1	5	5	2	4	13768.4828	-0.0001	0.001		
57:	6	0	6	5	1	5	14044.5335	-0.0002	0.001		
58:	5	1	4	4	0	4	14089.4553	0.0006	0.001		
59:	5	2	3	4	1	3	14191.5179	-0.0005	0.001		
60:	6	1	6	5	1	5	14110.8665	-0.0002	0.001		
61:	6	0	6	5	0	5	14169.4699	-0.0001	0.001		
62:	5	2	3	4	1	3	14191.5179	-0.0005	0.001		
63:	6	1	6	5	0	5	14235.8032	0.0001	0.001		
64:	4	4	1	3	3	0	14537.6891	0.0003	0.001		
65:	4	4	0	3	3	1	14540.0857	0.0011	0.001		
66:	6	2	5	5	2	4	14568.0927	-0.0002	0.001		
67:	6	3	4	5	3	3	14738.0315	0.0001	0.001		
68:	6	4	3	5	4	2	14740.8553	0.0022	0.001		
69:	6	4	2	5	4	1	14747.1987	-0.0009	0.001		
70:	6	3	3	5	3	2	14847.7610	0.0001	0.001		
71:	6	1	5	5	1	4	14857.9509	-0.0001	0.001		
72:	5	2	4	4	1	4	14960.3110	0.0041	0.002		
73:	6	2	4	5	2	3	15059.1614	-0.0002	0.001		
74:	5	3	3	4	2	2	15441.5566	-0.0006	0.001		
75:	5	3	2	4	2	2	15500.9387	0.0004	0.001		
76:	6	2	5	5	1	4	15657.5614	0.0004	0.001		
77:	5	3	3	4	2	3	15746.2866	-0.0006	0.001		
78:	5	3	2	4	2	3	15805.6679	-0.0004	0.001		
79:	7	0	7	6	1	6	16391.9711	0.0001	0.001		
80:	7	1	7	6	1	6	16425.4128	-0.0003	0.001		
81:	7	0	7	6	0	6	16458.3037	-0.0002	0.001		
82:	7	1	7	6	0	6	16491.7460	-0.0001	0.001		
83:	6	2	4	5	1	4	16792.8463	-0.0001	0.002		
84:	7	2	6	6	2	5	16944.5542	-0.0004	0.001		
85:	5	4	2	4	3	1	16979.8270	-0.0028	0.002		
86:	5	4	1	4	3	1	16981.4482	-0.0013	0.001		

87:	5	4	2	4	3	2	16995.1121	0.0027	0.001
88:	5	4	1	4	3	2	16996.7301	0.0010	0.001
89:	6	1	5	5	0	5	17065.9090	0.0005	0.002
90:	7	3	5	6	3	4	17188.9350	-0.0001	0.002
91:	7	1	6	6	1	5	17205.1253	0.0001	0.001
92:	7	4	4	6	4	3	17214.9080	0.0001	0.001
93:	7	4	3	6	4	2	17235.3779	0.0002	0.001
94:	7	3	4	6	3	3	17408.2560	-0.0005	0.001
95:	7	2	5	6	2	4	17577.1090	-0.0005	0.001
96:	6	3	4	5	2	3	17667.1933	0.0005	0.001
97:	6	2	5	5	1	5	17740.5836	0.0014	0.002
98:	7	2	6	6	1	5	17744.1651	0.0004	0.001
99:	6	3	3	5	2	3	17836.3032	-0.0001	0.002
100:	6	3	4	5	2	4	18311.4096	0.0001	0.002
101:	5	5	1	4	4	0	18342.7018	-0.0008	0.001
102:	5	5	0	4	4	1	18342.8996	0.0018	0.001
103:	6	3	3	5	2	4	18480.5201	0.0000	0.001
104:	8	0	8	7	1	7	18718.0059	-0.0003	0.001
105:	8	1	8	7	1	7	18734.2577	0.0003	0.001
106:	8	0	8	7	0	7	18751.4484	0.0000	0.001
107:	8	1	8	7	0	7	18767.6999	0.0003	0.001
108:	6	2	4	5	1	5	18875.8697	0.0021	0.002
109:	8	1	7	7	2	6	18967.9853	-0.0002	0.001
110:	8	2	7	7	2	6	19302.4265	-0.0003	0.001
111:	6	4	2	5	3	2	19405.7440	0.0000	0.002
112:	6	4	3	5	3	2	19397.7770	-0.0007	0.001
113:	6	4	3	5	3	3	19457.1586	-0.0002	0.002
114:	6	4	2	5	3	3	19465.1254	0.0002	0.001
115:	8	1	7	7	1	6	19507.0252	0.0001	0.001
116:	8	3	6	7	3	5	19626.2163	-0.0003	0.001
117:	7	3	5	6	2	4	19796.9666	0.0003	0.001
118:	8	2	7	7	1	6	19841.4667	0.0003	0.001
119:	8	3	5	7	3	4	19993.1708	-0.0005	0.001

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1901.889134(96)	1
20000	B	/MHz	1293.660842(48)	2
30000	C	/MHz	1150.831081(50)	3
200	DelJ	/kHz	0.07551(46)	4
1100	DelJK	/kHz	-0.0323(24)	5
2000	DelK	/kHz	0.0760(31)	6
40100	delJ	/kHz	0.01876(25)	7
41000	delK	/kHz	-0.0503(38)	8

MICROWAVE AVG = -0.000063 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.001226 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 0.83004 0.83004

distinct frequency lines in fit: 119
distinct parameters of fit: 8

	upper state	lower state	overall
limits of quantum number 1:	1 9	0 9	0 9
limits of quantum number 2:	0 5	0 4	0 5
limits of quantum number 3:	0 8	0 8	0 8

frequency range: 2444 19993

Standard errors are obtained by multiplying the previous errors by: 0.859431

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

10000	A	/MHz	1901.889134(82)	1
20000	B	/MHz	1293.660842(41)	2
30000	C	/MHz	1150.831081(42)	3
200	DelJ	/kHz	0.07551(39)	4
1100	DelJK	/kHz	-0.0324(21)	5
2000	DelK	/kHz	0.0761(26)	6
40100	delJ	/kHz	0.01876(22)	7
41000	delK	/kHz	-0.0503(32)	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ	-DelJK	-DelK	-delJ	-delK
A	1.0000							
B	0.0840	1.0000						
C	0.1807	-0.0233	1.0000					
-DelJ	0.0453	-0.7790	-0.3268	1.0000				
-DelJK	-0.5851	0.2897	-0.2899	-0.4861	1.0000			
-DelK	-0.4160	-0.1627	0.1829	0.1902	-0.3736	1.0000		
-delJ	0.1625	-0.6645	0.6247	0.3584	-0.5153	0.2779	1.0000	
-delK	0.0673	-0.4251	0.2297	0.5534	-0.4377	0.1666	0.2899	1.0000

Mean value of |C.ij|, i.ne.j = 0.3282
Mean value of C.ij, i.ne.j = -0.0636

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

87:	2.7	44:	-2.7	19:	-2.6	5:	-2.4
13:	-2.3	68:	2.2	50:	2.2	72:	2.1
102:	1.8	24:	-1.5	85:	-1.4	22:	1.4
86:	-1.3	65:	1.1	16:	-1.0	108:	1.0
35:	1.0	6:	1.0	88:	1.0	69:	-0.9
46:	0.8	101:	-0.8	8:	-0.8	33:	-0.8
47:	-0.7	7:	-0.7	97:	0.7	112:	-0.7
37:	0.6	74:	-0.6	77:	-0.6	4:	-0.6
58:	0.6	12:	-0.6	119:	-0.5	95:	-0.5
94:	-0.5	62:	-0.5	59:	-0.5	31:	-0.5
96:	0.5	17:	-0.4	45:	-0.4	43:	0.4
53:	-0.4	98:	0.4	78:	-0.4	76:	0.4
75:	0.4	38:	0.4				

87:	5	4	2	4	3	2	16995.1121	0.0027	0.001
44:	5	4	1	4	4	0	12273.3763	-0.0027	0.001
19:	3	2	1	2	2	0	7419.3841	-0.0053	0.002
5:	5	3	3	5	2	4	3573.3757	-0.0024	0.001
13:	6	5	1	6	4	2	6045.5670	-0.0046	0.002
68:	6	4	3	5	4	2	14740.8553	0.0022	0.001
50:	7	3	4	6	4	3	12858.2441	0.0044	0.002
72:	5	2	4	4	1	4	14960.3110	0.0041	0.002
102:	5	5	0	4	4	1	18342.8996	0.0018	0.001
24:	5	2	3	4	3	2	9349.6406	-0.0015	0.001

/ SPFIT output reformatted with PIFORM

							obs	o-c	error	blends	Notes	
										o-c	wt	
/ instead of : below denotes (o-c)>3*err												
1:	3	0	3	2	0	2	7238.8889	-0.0014	0.002			
2:	4	0	4	3	0	3	9570.9004	-0.0003	0.002			
3:	5	1	5	4	0	4	11994.1788	0.0002	0.002			
4:	5	0	5	4	0	4	11869.7171	-0.0001	0.002			
5:	5	1	5	4	1	4	11776.7465	0.0000	0.002			
6:	4	1	4	3	1	3	9444.3208	-0.0003	0.002			
7:	3	1	3	2	0	2	7582.9030	0.0009	0.002			
8:	3	1	3	2	1	2	7099.0821	-0.0001	0.002			
9:	4	1	4	3	0	3	9788.3329	0.0000	0.002			
10:	4	0	4	3	1	3	9226.8899	0.0009	0.002			
11:	5	0	5	4	1	4	11652.2854	0.0002	0.002			
12:	6	0	6	5	1	5	14031.8620	0.0002	0.002			
13:	6	0	6	5	0	5	14156.3226	-0.0004	0.002			

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1894.0328 (42)	1
20000	B	/MHz	1291.1235 (11)	2
30000	C	/MHz	1150.04857 (58)	3
200	DelJ	/kHz	0.0756 (55)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

MICROWAVE AVG = -0.000009 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.000584 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.29202 0.29202

distinct frequency lines in fit: 13
 distinct parameters of fit: 4

		upper state	lower state	overall
limits of quantum number 1:	3	6	2	5
limits of quantum number 2:	0	1	0	1
limits of quantum number 3:	3	6	2	5

frequency range: 7099 14156

Standard errors are obtained by multiplying the previous errors by: 0.350964

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

10000	A	/MHz	1894.0328 (14)	1
20000	B	/MHz	1291.12357 (41)	2
30000	C	/MHz	1150.04857 (20)	3
200	DelJ	/kHz	0.0756 (19)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ
A	1.0000			
B	0.9420	1.0000		
C	-0.9249	-0.8801	1.0000	
-DelJ	0.7434	0.6492	-0.9162	1.0000

Mean value of |C.ij|, i.ne.j = 0.8426
 Mean value of C.ij, i.ne.j = -0.0644

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

1:	-0.7	7:	0.4	10:	0.4	13:	-0.2
6:	-0.1	2:	-0.1	12:	0.1	11:	0.1
3:	0.1	4:	-0.1	8:	-0.1	9:	0.0
5:	0.0						

1:	3	0	3	2	0	2		7238.8889	-0.0014	0.002
7:	3	1	3	2	0	2		7582.9030	0.0009	0.002
10:	4	0	4	3	1	3		9226.8899	0.0009	0.002
13:	6	0	6	5	0	5		14156.3226	-0.0004	0.002
6:	4	1	4	3	0	3		9444.3208	-0.0003	0.002
2:	4	0	4	3	0	3		9570.9004	-0.0003	0.002
12:	6	0	6	5	1	5		14031.8620	0.0002	0.002
11:	5	0	5	4	1	4		11652.2854	0.0002	0.002
3:	5	1	5	4	0	4		11994.1788	0.0002	0.002
4:	5	0	5	4	0	4		11869.7171	-0.0001	0.002

/ SPFIT output reformatted with PIFORM

						obs	o-c	error	blends	Notes
									o-c	wt
/ instead of : below denotes (o-c)>3*err										
1:	3	1	3	2	1	2	7071.9698	0.0000	0.002	
2:	4	1	4	3	1	3	9408.1814	0.0000	0.002	
3:	5	0	5	4	0	4	11826.2932	-0.0002	0.002	
4:	5	1	5	4	1	4	11731.5437	0.0002	0.002	
5:	4	1	4	3	0	3	9759.4406	-0.0002	0.002	
6:	5	1	5	4	0	4	11954.4233	0.0000	0.002	
7:	6	0	6	5	0	5	14103.4065	-0.0002	0.002	
8:	5	0	5	4	1	4	11603.4134	-0.0002	0.002	
9:	4	0	4	3	1	3	9185.3015	0.0000	0.002	
10:	4	0	4	3	0	3	9536.5614	0.0003	0.002	
11:	6	0	6	5	1	5	13975.2772	0.0002	0.002	
12:	6	1	6	5	0	5	14171.8463	0.0001	0.002	

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1899.8107(82)	1
20000	B	/MHz	1287.2707(21)	2
30000	C	/MHz	1145.30340(87)	3
200	DelJ	/kHz	0.0778(66)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

MICROWAVE AVG = 0.000001 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.000209 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.10434 0.10434

distinct frequency lines in fit: 12
 distinct parameters of fit: 4

	upper state	lower state	overall
limits of quantum number 1:	3 6	2 5	2 6
limits of quantum number 2:	0 1	0 1	0 1
limits of quantum number 3:	3 6	2 5	2 6

frequency range: 7071 14171

Standard errors are obtained by multiplying the previous errors by: 0.127790

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

10000	A	/MHz	1899.8107(10)	1
20000	B	/MHz	1287.27072(27)	2
30000	C	/MHz	1145.30340(11)	3
200	DelJ	/kHz	0.07780(84)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ
A	1.0000			
B	0.9840	1.0000		
C	-0.9577	-0.9476	1.0000	
-DelJ	0.8130	0.7894	-0.9360	1.0000

Mean value of |C.ij|, i.ne.j = 0.9046
 Mean value of C.ij, i.ne.j = -0.0425

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

10:	0.1	5:	-0.1	11:	0.1	4:	0.1
8:	-0.1	7:	-0.1	3:	-0.1	12:	0.1
9:	0.0	6:	0.0	2:	0.0	1:	0.0
10:	4 0 4	3 0 3					
5:	4 1 4	3 0 3					
11:	6 0 6	5 1 5					
4:	5 1 5	4 1 4					
8:	5 0 5	4 1 4					
7:	6 0 6	5 0 5					
3:	5 0 5	4 0 4					
12:	6 1 6	5 0 5					
9:	4 0 4	3 1 3					
6:	5 1 5	4 0 4					

/ SPFIT output reformatted with PIFORM

							obs	o-c	error	blends	Notes
										o-c	wt
/ instead of : below denotes (o-c)>3*err											
1:	5	1	5	4	1	4	11694.2443	0.0000	0.002		
2:	4	1	4	3	1	3	9378.4051	-0.0002	0.002		
3:	3	1	3	2	1	2	7049.6869	-0.0001	0.002		
4:	3	0	3	2	0	2	7191.0191	-0.0008	0.002		
5:	6	1	6	5	1	5	13998.8767	-0.0003	0.002		
6:	4	0	4	3	0	3	9506.7416	0.0000	0.002		
7:	6	1	6	5	0	5	14126.5118	-0.0001	0.002		
8:	5	0	5	4	1	4	11566.6099	0.0003	0.002		
9:	5	1	5	4	0	4	11916.4898	0.0007	0.002		
10:	3	1	3	2	0	2	7541.6017	0.0007	0.002		
11:	4	1	4	3	0	3	9728.9857	-0.0006	0.002		
12:	4	0	4	3	1	3	9156.1612	0.0005	0.002		

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1895.8035(45)	1
20000	B	/MHz	1283.7245(12)	2
30000	C	/MHz	1141.54329(66)	3
200	DelJ	/kHz	0.0755(66)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

MICROWAVE AVG = -0.000008 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.000498 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.24908 0.24908

distinct frequency lines in fit: 12
 distinct parameters of fit: 4

	upper state	lower state	overall
limits of quantum number 1:	3 6	2 5	2 6
limits of quantum number 2:	0 1	0 1	0 1
limits of quantum number 3:	3 6	2 5	2 6

frequency range: 7049 14126

Standard errors are obtained by multiplying the previous errors by: 0.305059

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

10000	A	/MHz	1895.8035(13)	1
20000	B	/MHz	1283.72456(38)	2
30000	C	/MHz	1141.54329(20)	3
200	DelJ	/kHz	0.0755(20)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ
A	1.0000			
B	0.9539	1.0000		
C	-0.9322	-0.9088	1.0000	
-DelJ	0.8083	0.7689	-0.9514	1.0000

Mean value of |C.ij|, i.ne.j = 0.8873
 Mean value of C.ij, i.ne.j = -0.0436

No correlations with absolute value greater than 0.9950
 Worst fitted lines (obs-calc/error):

4:	-0.4	10:	0.3	9:	0.3	11:	-0.3
12:	0.2	8:	0.1	5:	-0.1	2:	-0.1
7:	-0.1	3:	-0.1	6:	0.0	1:	0.0
4:	3 0 3	2 0 2	7191.0191	-0.0008	0.002		
10:	3 1 3	2 0 2	7541.6017	0.0007	0.002		
9:	5 1 5	4 0 4	11916.4898	0.0007	0.002		
11:	4 1 4	3 0 3	9728.9857	-0.0006	0.002		
12:	4 0 4	3 1 3	9156.1612	0.0005	0.002		
8:	5 0 5	4 1 4	11566.6099	0.0003	0.002		
5:	6 1 6	5 1 5	13998.8767	-0.0003	0.002		
2:	4 1 4	3 1 3	9378.4051	-0.0002	0.002		
7:	6 1 6	5 0 5	14126.5118	-0.0001	0.002		
3:	3 1 3	2 1 2	7049.6869	-0.0001	0.002		

/ SPFIT output reformatted with PIFORM

						obs	o-c	error	blends	Notes
									o-c	wt
/ instead of : below denotes (o-c)>3*err										
1:	6	0	6	5	1	5	13967.8360	0.0021	0.002	
2:	5	0	5	4	1	4	11608.0935	-0.0006	0.002	
3:	4	0	4	3	1	3	9201.6539	-0.0013	0.002	
4:	6	1	6	5	1	5	14023.8194	-0.0016	0.002	
5:	6	1	6	5	0	5	14132.8158	-0.0011	0.002	
6:	5	1	5	4	1	4	11717.0909	0.0008	0.002	
7:	5	1	5	4	0	4	11914.1496	0.0012	0.002	
8:	6	0	6	5	0	5	14076.8296	0.0000	0.002	
9:	5	0	5	4	0	4	11805.1527	0.0002	0.002	
10:	4	1	4	3	1	3	9398.7151	0.0015	0.002	
11:	4	1	4	3	0	3	9720.3998	-0.0011	0.002	
12:	4	0	4	3	0	3	9523.3426	0.0000	0.002	
13:	3	0	3	2	0	2	7208.5486	0.0001	0.002	
14:	3	1	3	2	1	2	7066.5439	-0.0005	0.002	

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1878.2029(64)	1
20000	B	/MHz	1291.1367(17)	2
30000	C	/MHz	1143.14149(75)	3
200	DelJ	/kHz	0.0665(61)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

MICROWAVE AVG = -0.000013 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.001122 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.56081 0.56081

distinct frequency lines in fit: 14
 distinct parameters of fit: 4

	upper state	lower state	overall
limits of quantum number 1:	3 6	2 5	2 6
limits of quantum number 2:	0 1	0 1	0 1
limits of quantum number 3:	3 6	2 5	2 6

frequency range: 7066 14132

Standard errors are obtained by multiplying the previous errors by: 0.663559

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

10000	A	/MHz	1878.2029(42)	1
20000	B	/MHz	1291.1367(11)	2
30000	C	/MHz	1143.14149(49)	3
200	DelJ	/kHz	0.0665(40)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ
A	1.0000			
B	0.9719	1.0000		
C	-0.9483	-0.9400	1.0000	
-DelJ	0.8244	0.8041	-0.9498	1.0000

Mean value of |C.ij|, i.ne.j = 0.9064
 Mean value of C.ij, i.ne.j = -0.0396

No correlations with absolute value greater than 0.9950
 Worst fitted lines (obs-calc/error):

1:	1.0	4:	-0.8	10:	0.8	3:	-0.6
7:	0.6	5:	-0.6	11:	-0.6	6:	0.4
2:	-0.3	14:	-0.2	9:	0.1	13:	0.1
12:	0.0	8:	0.0				

1:	6	0	6	5	1	5	13967.8360	0.0021	0.002
4:	6	1	6	5	1	5	14023.8194	-0.0016	0.002
10:	4	1	4	3	1	3	9398.7151	0.0015	0.002
3:	4	0	4	3	1	3	9201.6539	-0.0013	0.002
7:	5	1	5	4	0	4	11914.1496	0.0012	0.002
5:	6	1	6	5	0	5	14132.8158	-0.0011	0.002
11:	4	1	4	3	0	3	9720.3998	-0.0011	0.002
6:	5	1	5	4	1	4	11717.0909	0.0008	0.002
2:	5	0	5	4	1	4	11608.0935	-0.0006	0.002
14:	3	1	3	2	1	2	7066.5439	-0.0005	0.002

/ SPFIT output reformatted with PIFORM

						obs	o-c	error	blends	Notes
									o-c	wt
/ instead of : below denotes (o-c)>3*err										
1:	5	1	5	4	1	4	11738.6052	0.0002	0.002	
2:	4	1	4	3	1	3	9415.1564	0.0000	0.002	
3:	6	1	6	5	1	5	14050.5379	0.0004	0.002	
4:	3	0	3	2	0	2	7220.6242	-0.0006	0.002	
5:	4	0	4	3	0	3	9541.9672	-0.0001	0.002	
6:	3	1	3	2	1	2	7078.2446	-0.0004	0.002	
7:	5	0	5	4	0	4	11829.8553	-0.0001	0.002	
8:	6	0	6	5	0	5	14106.5142	-0.0001	0.002	
9:	6	0	6	5	1	5	13989.3876	0.0006	0.002	
10:	6	1	6	5	0	5	14167.6637	-0.0010	0.002	
11:	5	1	5	4	0	4	11946.9834	0.0006	0.002	
12:	5	0	5	4	1	4	11621.4774	-0.0002	0.002	
13:	4	1	4	3	0	3	9750.3452	0.0001	0.002	
14:	4	0	4	3	1	3	9206.7782	-0.0005	0.002	
15:	3	1	3	2	0	2	7555.8139	0.0004	0.002	
16:	3	0	3	2	1	2	6743.0572	0.0007	0.002	

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1891.7105(38)	1
20000	B	/MHz	1291.5946(11)	2
30000	C	/MHz	1145.46166(53)	3
200	DelJ	/kHz	0.0779(48)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

MICROWAVE AVG = 0.000000 MHz, IR AVG = 0.000000
 MICROWAVE RMS = 0.000502 MHz, IR RMS = 0.000000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.25079 0.25079

distinct frequency lines in fit: 16
 distinct parameters of fit: 4

	upper state	lower state	overall
limits of quantum number 1:	3 6	2 5	2 6
limits of quantum number 2:	0 1	0 1	0 1
limits of quantum number 3:	3 6	2 5	2 6

frequency range: 6743 14167

Standard errors are obtained by multiplying the previous errors by: 0.289587

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

10000	A	/MHz	1891.7105(11)	1
20000	B	/MHz	1291.59469(33)	2
30000	C	/MHz	1145.46166(15)	3
200	DelJ	/kHz	0.0779(13)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ
A	1.0000			
B	0.9580	1.0000		
C	-0.9148	-0.9034	1.0000	
-DelJ	0.7505	0.7223	-0.9347	1.0000

Mean value of |C.ij|, i.ne.j = 0.8639
 Mean value of C.ij, i.ne.j = -0.0537

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

10: -0.5	16: 0.3	4: -0.3	11: 0.3
9: 0.3	14: -0.2	15: 0.2	6: -0.2
3: 0.2	1: 0.1	12: -0.1	13: 0.1
8: -0.1	7: -0.1	5: -0.1	2: 0.0
10: 6 1 6	5 0 5	14167.6637	-0.0010 0.002
16: 3 0 3	2 1 2	6743.0572	0.0007 0.002
4: 3 0 3	2 0 2	7220.6242	-0.0006 0.002
11: 5 1 5	4 0 4	11946.9834	0.0006 0.002

9:	6	0	6	5	1	5	13989.3876	0.0006	0.002
14:	4	0	4	3	1	3	9206.7782	-0.0005	0.002
15:	3	1	3	2	0	2	7555.8139	0.0004	0.002
6:	3	1	3	2	1	2	7078.2446	-0.0004	0.002
3:	6	1	6	5	1	5	14050.5379	0.0004	0.002
1:	5	1	5	4	1	4	11738.6052	0.0002	0.002

/ SPFIT output reformatted with PIFORM

						obs	o-c	error	blends	Notes
									o-c	wt
/ instead of : below denotes (o-c)>3*err										
1:	3	0	3	2	0	2	7227.1927	0.0000	0.002	
2:	6	0	6	5	0	5	14130.7355	0.0003	0.002	
3:	5	1	5	4	1	4	11754.6477	0.0000	0.002	
4:	5	0	5	4	0	4	11849.0904	0.0008	0.002	
5:	3	1	3	2	1	2	7085.9492	-0.0009	0.002	
6:	5	0	5	4	1	4	11627.4090	0.0008	0.002	
7:	5	1	5	4	0	4	11976.3287	-0.0002	0.002	
8:	6	0	6	5	1	5	14003.4947	-0.0010	0.002	
9:	6	1	6	5	0	5	14198.5894	-0.0003	0.002	
10:	6	1	6	5	1	5	14071.3491	-0.0012	0.002	
11:	3	1	3	2	0	2	7577.0631	-0.0006	0.002	
12:	4	0	4	3	1	3	9205.0595	0.0002	0.002	
13:	4	1	4	3	1	3	9426.7409	0.0003	0.002	
14:	4	0	4	3	0	3	9554.9294	-0.0008	0.002	

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1900.9961 (41)	1
20000	B	/MHz	1289.7573 (11)	2
30000	C	/MHz	1147.59339 (57)	3
200	DelJ	/kHz	0.0710 (53)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

MICROWAVE AVG = -0.000191 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.000685 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.34264 0.30941

distinct frequency lines in fit: 14
 distinct parameters of fit: 4

	upper state	lower state	overall
limits of quantum number 1:	3 6	2 5	2 6
limits of quantum number 2:	0 1	0 1	0 1
limits of quantum number 3:	3 6	2 5	2 6

frequency range: 7085 14198

Standard errors are obtained by multiplying the previous errors by: 0.366099

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

10000	A	/MHz	1900.9961 (15)	1
20000	B	/MHz	1289.75731 (41)	2
30000	C	/MHz	1147.59339 (20)	3
200	DelJ	/kHz	0.0710 (19)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

Worst fitted lines (obs-calc/error):

10: -0.6	8: -0.5	5: -0.4	14: -0.4
4: 0.4	6: 0.4	11: -0.3	13: 0.1
2: 0.1	9: -0.1	12: 0.1	7: -0.1
3: 0.0	1: 0.0		

10:	6	1	6	5	1	5	14071.3491	-0.0012	0.002
8:	6	0	6	5	1	5	14003.4947	-0.0010	0.002
5:	3	1	3	2	1	2	7085.9492	-0.0009	0.002
14:	4	0	4	3	0	3	9554.9294	-0.0008	0.002
4:	5	0	5	4	0	4	11849.0904	0.0008	0.002
6:	5	0	5	4	1	4	11627.4090	0.0008	0.002
11:	3	1	3	2	0	2	7577.0631	-0.0006	0.002
13:	4	1	4	3	1	3	9426.7409	0.0003	0.002
2:	6	0	6	5	0	5	14130.7355	0.0003	0.002
9:	6	1	6	5	0	5	14198.5894	-0.0003	0.002

						obs	o-c	error	blends	Notes
									o-c	wt
/ instead of : below denotes (o-c)>3*err										
1:	3	0	3	2	0	2	7227.1927	0.0001	0.002	
2:	6	0	6	5	0	5	14130.7355	0.0007	0.002	
3:	5	1	5	4	1	4	11754.6477	0.0000	0.002	
4:	5	0	5	4	0	4	11849.0904	0.0010	0.002	
5:	3	1	3	2	1	2	7085.9492	-0.0011	0.002	
6:	5	0	5	4	1	4	11627.4090	0.0008	0.002	
7:	5	1	5	4	0	4	11976.3287	0.0000	0.002	
8:	6	0	6	5	1	5	14003.4947	-0.0006	0.002	

9:	6	1	6	5	0	5	14198.5894	0.0000	0.002
10:	6	1	6	5	1	5	14071.3491	-0.0008	0.002
11:	3	1	3	2	0	2	7577.0631	0.0000	0.002
12:	4	0	4	3	1	3	9205.0595	0.0000	0.002
13:	4	1	4	3	1	3	9426.7409	0.0002	0.002
14:	4	0	4	3	0	3	9554.9294	-0.0006	0.002

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1900.9961(41)	1
20000	B	/MHz	1289.7573(11)	2
30000	C	/MHz	1147.59339(57)	3
200	DelJ	/kHz	0.0710(53)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

MICROWAVE AVG = -0.000019 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.000619 MHz, IR RMS = 0.00000
END OF ITERATION 2 OLD, NEW RMS ERROR= 0.30941 0.30941

distinct frequency lines in fit: 14
distinct parameters of fit: 4

		upper state	lower state	overall
limits of quantum number 1:		3 6	2 5	2 6
limits of quantum number 2:		0 1	0 1	0 1
limits of quantum number 3:		3 6	2 5	2 6
frequency range:		7085	14198	

Standard errors are obtained by muliptyling the previous errors by: 0.366099

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

10000	A	/MHz	1900.9961(15)	1
20000	B	/MHz	1289.75731(41)	2
30000	C	/MHz	1147.59339(20)	3
200	DelJ	/kHz	0.0710(19)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ
A	1.0000			
B	0.9415	1.0000		
C	-0.9066	-0.8898	1.0000	
-DelJ	0.7602	0.7212	-0.9452	1.0000

Mean value of |C.ij|, i.ne.j = 0.8608
Mean value of C.ij, i.ne.j = -0.0531

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

5:	-0.6	4:	0.5	10:	-0.4	6:	0.4
2:	0.3	14:	-0.3	8:	-0.3	13:	0.1
1:	0.1	12:	0.0	11:	0.0	9:	0.0
7:	0.0	3:	0.0				
5:	3 1 3	2 1 2	7085.9492	-0.0011	0.002		
4:	5 0 5	4 0 4	11849.0904	0.0010	0.002		
10:	6 1 6	5 1 5	14071.3491	-0.0008	0.002		
6:	5 0 5	4 1 4	11627.4090	0.0008	0.002		
2:	6 0 6	5 0 5	14130.7355	0.0007	0.002		
14:	4 0 4	3 0 3	9554.9294	-0.0006	0.002		
8:	6 0 6	5 1 5	14003.4947	-0.0006	0.002		
13:	4 1 4	3 1 3	9426.7409	0.0002	0.002		
1:	3 0 3	2 0 2	7227.1927	0.0001	0.002		
12:	4 0 4	3 1 3	9205.0595	0.0000	0.002		

						obs	o-c	error	blends o-c	Notes wt
/ instead of : below denotes (o-c)>3*err										
1:	5	0	5	4	0	4	11848.5702	0.0007	0.002	
2:	5	1	5	4	1	4	11756.4265	0.0010	0.002	
3:	4	1	4	3	1	3	9427.3886	0.0000	0.002	
4:	4	0	4	3	0	3	9552.1358	-0.0010	0.002	
5:	3	0	3	2	0	2	7223.0587	-0.0003	0.002	
6:	3	1	3	2	1	2	7085.8899	0.0003	0.002	
7:	5	0	5	4	1	4	11631.6096	0.0002	0.002	
8:	5	1	5	4	0	4	11973.3850	-0.0005	0.002	
9:	6	0	6	5	0	5	14132.7022	-0.0004	0.002	
10:	4	0	4	3	1	3	9210.4281	-0.0003	0.002	
11:	4	1	4	3	0	3	9769.0967	-0.0002	0.002	
12:	3	1	3	2	0	2	7564.7681	0.0006	0.002	

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1881.7682(45)	1
20000	B	/MHz	1286.3789(12)	2
30000	C	/MHz	1148.60619(67)	3
200	DelJ	/kHz	0.0724(70)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

MICROWAVE AVG = -0.000001 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.000585 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.29232 0.29232

distinct frequency lines in fit: 12
 distinct parameters of fit: 4

	upper state	lower state	overall
limits of quantum number 1:	3 6	2 5	2 6
limits of quantum number 2:	0 1	0 1	0 1
limits of quantum number 3:	3 6	2 5	2 6

frequency range: 7085 14132

Standard errors are obtained by multiplying the previous errors by: 0.358017

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

10000	A	/MHz	1881.7682(16)	1
20000	B	/MHz	1286.37890(45)	2
30000	C	/MHz	1148.60619(23)	3
200	DelJ	/kHz	0.0724(25)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ
A	1.0000			
B	0.9501	1.0000		
C	-0.9277	-0.8946	1.0000	
-DelJ	0.7704	0.7077	-0.9340	1.0000

Mean value of |C.ij|, i.ne.j = 0.8641
 Mean value of C.ij, i.ne.j = -0.0547

No correlations with absolute value greater than 0.9950
 Worst fitted lines (obs-calc/error):

4:	-0.5	2:	0.5	1:	0.3	12:	0.3
8:	-0.2	9:	-0.2	6:	0.1	10:	-0.1
5:	-0.1	11:	-0.1	7:	0.1	3:	0.0
4:	4	0	4	3	0	3	9552.1358 -0.0010 0.002
2:	5	1	5	4	1	4	11756.4265 0.0010 0.002
1:	5	0	5	4	0	4	11848.5702 0.0007 0.002
12:	3	1	3	2	0	2	7564.7681 0.0006 0.002
8:	5	1	5	4	0	4	11973.3850 -0.0005 0.002
9:	6	0	6	5	0	5	14132.7022 -0.0004 0.002
6:	3	1	3	2	1	2	7085.8899 0.0003 0.002
10:	4	0	4	3	1	3	9210.4281 -0.0003 0.002
5:	3	0	3	2	0	2	7223.0587 -0.0003 0.002
11:	4	1	4	3	0	3	9769.0967 -0.0002 0.002

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						obs	o-c	error	blends	Notes
									o-c	wt
/ instead of : below denotes (o-c)>3*err										

1:	5	0	5	4	0	4	11826.8586	0.0008	0.002	
2:	4	0	4	3	0	3	9534.0399	0.0000	0.002	
3:	3	1	3	2	1	2	7072.2545	-0.0027	0.002	
4:	3	0	3	2	0	2	7208.6939	-0.0007	0.002	
5:	4	1	4	3	1	3	9409.5222	0.0005	0.002	
6:	5	1	5	4	1	4	11734.4773	0.0010	0.002	
7:	6	0	6	5	0	5	14107.1928	-0.0003	0.002	
8:	6	1	6	5	0	5	14174.9795	-0.0002	0.002	
9:	6	0	6	5	1	5	13980.8849	-0.0006	0.002	
10:	5	1	5	4	0	4	11953.1660	0.0006	0.002	
11:	5	0	5	4	1	4	11608.1681	-0.0005	0.002	
12:	4	1	4	3	0	3	9752.7281	-0.0008	0.002	
13:	4	0	4	3	1	3	9190.8341	0.0015	0.002	
14:	3	1	3	2	0	2	7551.9029	0.0009	0.002	

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1878.4290(41)	1
20000	B	/MHz	1283.1506(11)	2
30000	C	/MHz	1146.60842(57)	3
200	DelJ	/kHz	0.0719(54)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

MICROWAVE AVG = -0.000039 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.001048 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.52424 0.52424

distinct frequency lines in fit: 14
 distinct parameters of fit: 4

	upper state	lower state	overall
limits of quantum number 1:	3 6	2 5	2 6
limits of quantum number 2:	0 1	0 1	0 1
limits of quantum number 3:	3 6	2 5	2 6
frequency range:	7072	14174	

Standard errors are obtained by multiplying the previous errors by: 0.620289

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

10000	A	/MHz	1878.4290(25)	1
20000	B	/MHz	1283.15066(69)	2
30000	C	/MHz	1146.60842(35)	3
200	DelJ	/kHz	0.0719(33)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ
A	1.0000			
B	0.9468	1.0000		
C	-0.9233	-0.8881	1.0000	
-DelJ	0.7724	0.7089	-0.9390	1.0000

Mean value of |C.ij|, i.ne.j = 0.8631

Mean value of C.ij, i.ne.j = -0.0537

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

3:	-1.4	13:	0.8	6:	0.5	14:	0.4
12:	-0.4	1:	0.4	4:	-0.3	9:	-0.3
10:	0.3	11:	-0.2	5:	0.2	7:	-0.1
8:	-0.1	2:	0.0				

3:	3	1	3	2	1	2	7072.2545	-0.0027	0.002
13:	4	0	4	3	1	3	9190.8341	0.0015	0.002
6:	5	1	5	4	1	4	11734.4773	0.0010	0.002
14:	3	1	3	2	0	2	7551.9029	0.0009	0.002
12:	4	1	4	3	0	3	9752.7281	-0.0008	0.002
1:	5	0	5	4	0	4	11826.8586	0.0008	0.002
4:	3	0	3	2	0	2	7208.6939	-0.0007	0.002
9:	6	0	6	5	1	5	13980.8849	-0.0006	0.002
10:	5	1	5	4	0	4	11953.1660	0.0006	0.002
11:	5	0	5	4	1	4	11608.1681	-0.0005	0.002

/ SPFIT output reformatted with PIFORM

						obs	o-c	error	blends	Notes
									o-c	wt
/ instead of : below denotes (o-c)>3*err										
1:	5	1	5	4	0	4	11849.0689	-0.0004	0.002	
2:	3	1	3	2	0	2	7505.9970	0.0006	0.002	
3:	4	1	4	3	0	3	9678.2438	-0.0001	0.002	
4:	5	0	5	4	0	4	11712.0472	-0.0006	0.002	
5:	4	0	4	3	0	3	9443.6180	-0.0009	0.002	
6:	5	1	5	4	1	4	11614.4436	-0.0008	0.002	
7:	4	1	4	3	1	3	9313.6846	0.0000	0.002	
8:	5	0	5	4	1	4	11477.4229	0.0000	0.002	
9:	6	0	6	5	0	5	13966.8588	0.0010	0.002	
10:	6	0	6	5	1	5	13829.8363	0.0000	0.002	
11:	4	0	4	3	1	3	9079.0596	0.0000	0.002	
12:	3	0	3	2	0	2	7141.4367	-0.0004	0.002	
13:	3	1	3	2	1	2	7000.4546	0.0022	0.002	

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1897.8335(41)	1
20000	B	/MHz	1273.5367(11)	2
30000	C	/MHz	1133.86192(56)	3
200	DelJ	/kHz	0.0777(53)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

MICROWAVE AVG = 0.000039 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.000817 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.40856 0.40856

distinct frequency lines in fit: 13
 distinct parameters of fit: 4

	upper state	lower state	overall
limits of quantum number 1:	3 6	2 5	2 6
limits of quantum number 2:	0 1	0 1	0 1
limits of quantum number 3:	3 6	2 5	2 6

frequency range: 7000 13966

Standard errors are obtained by multiplying the previous errors by: 0.491028

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

10000	A	/MHz	1897.8335(20)	1
20000	B	/MHz	1273.53678(55)	2
30000	C	/MHz	1133.86192(27)	3
200	DelJ	/kHz	0.0777(26)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ
A	1.0000			
B	0.9408	1.0000		
C	-0.9214	-0.8723	1.0000	
-DelJ	0.7304	0.6283	-0.9115	1.0000

Mean value of |C.ij|, i.ne.j = 0.8341
 Mean value of C.ij, i.ne.j = -0.0676

No correlations with absolute value greater than 0.9950
 Worst fitted lines (obs-calc/error):

13:	1.1	9:	0.5	5:	-0.4	6:	-0.4
2:	0.3	4:	-0.3	12:	-0.2	1:	-0.2
3:	-0.1	11:	0.0	10:	0.0	8:	0.0
7:	0.0						

13:	3	1	3	2	1	2	7000.4546	0.0022	0.002
9:	6	0	6	5	0	5	13966.8588	0.0010	0.002
5:	4	0	4	3	0	3	9443.6180	-0.0009	0.002
6:	5	1	5	4	1	4	11614.4436	-0.0008	0.002
2:	3	1	3	2	0	2	7505.9970	0.0006	0.002
4:	5	0	5	4	0	4	11712.0472	-0.0006	0.002
12:	3	0	3	2	0	2	7141.4367	-0.0004	0.002
1:	5	1	5	4	0	4	11849.0689	-0.0004	0.002
3:	4	1	4	3	0	3	9678.2438	-0.0001	0.002
11:	4	0	4	3	1	3	9079.0596	0.0000	0.002

/ SPFIT output reformatted with PIFORM

					obs	o-c	error	blends	Notes
								o-c	wt
/ instead of : below denotes (o-c)>3*err									
1:	5	1	5	4	1	4	11603.6719	-0.0006	0.002
2:	5	0	5	4	0	4	11697.0072	-0.0008	0.002
3:	6	0	6	5	0	5	13947.1742	0.0007	0.002
4:	4	0	4	3	0	3	9434.9046	-0.0003	0.002
5:	4	1	4	3	1	3	9306.7110	-0.0006	0.002
6:	3	1	3	2	1	2	6996.5079	0.0022	0.002
7:	3	0	3	2	0	2	7139.0884	0.0003	0.002
8:	5	0	5	4	1	4	11480.9637	-0.0005	0.002
9:	5	1	5	4	0	4	11819.7162	-0.0002	0.002
10:	6	1	6	5	0	5	14011.9174	-0.0001	0.002
11:	6	1	6	5	1	5	13889.2099	0.0007	0.002
12:	6	0	6	5	1	5	13824.4650	-0.0001	0.002
13:	4	1	4	3	0	3	9650.9489	0.0000	0.002

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1885.8091(68)	1
20000	B	/MHz	1276.9992(16)	2
30000	C	/MHz	1132.08127(78)	3
200	DelJ	/kHz	0.0805(65)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

MICROWAVE AVG = 0.000042 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.000793 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.39627 0.39627

distinct frequency lines in fit: 13
 distinct parameters of fit: 4

	upper state	lower state	overall
limits of quantum number 1:	3 6	2 5	2 6
limits of quantum number 2:	0 1	0 1	0 1
limits of quantum number 3:	3 6	2 5	2 6

frequency range: 6996 14011

Standard errors are obtained by multiplying the previous errors by: 0.476257

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

10000	A	/MHz	1885.8091(32)	1
20000	B	/MHz	1276.99920(78)	2
30000	C	/MHz	1132.08127(37)	3
200	DelJ	/kHz	0.0805(30)	4
1100	DelJK	/kHz	[-0.038647301]	5
2000	DelK	/kHz	[0.089184483]	6
40100	delJ	/kHz	[0.019430668]	7
41000	delK	/kHz	[-0.044809258]	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ
A	1.0000			
B	0.9610	1.0000		
C	-0.9534	-0.9278	1.0000	
-DelJ	0.8420	0.7944	-0.9545	1.0000

Mean value of |C.ij|, i.ne.j = 0.9055
 Mean value of C.ij, i.ne.j = -0.0397

No correlations with absolute value greater than 0.9950
 Worst fitted lines (obs-calc/error):

6:	1.1	2:	-0.4	11:	0.3	3:	0.3
5:	-0.3	1:	-0.3	8:	-0.2	7:	0.1
4:	-0.1	9:	-0.1	10:	-0.1	12:	-0.1
13:	0.0						

6:	3	1	3	2	1	2	6996.5079	0.0022	0.002
2:	5	0	5	4	0	4	11697.0072	-0.0008	0.002
11:	6	1	6	5	1	5	13889.2099	0.0007	0.002
3:	6	0	6	5	0	5	13947.1742	0.0007	0.002
5:	4	1	4	3	1	3	9306.7110	-0.0006	0.002
1:	5	1	5	4	1	4	11603.6719	-0.0006	0.002
8:	5	0	5	4	1	4	11480.9637	-0.0005	0.002
7:	3	0	3	2	0	2	7139.0884	0.0003	0.002
4:	4	0	4	3	0	3	9434.9046	-0.0003	0.002
9:	5	1	5	4	0	4	11819.7162	-0.0002	0.002

/ SPFIT output reformatted with PIFORM

						obs	o-c	error	blends o-c	wt	Notes
/ instead of : below denotes (o-c)>3*err											
1:	5	1	4	5	0	5	2102.1763	-0.0027	0.002		
2:	1	0	1	0	0	0	2461.5890	0.0000	0.002		
3:	1	1	1	0	0	0	3087.0963	-0.0003	0.002		
4:	7	3	5	7	2	6	3979.3024	0.0006	0.002		
5:	2	0	2	1	1	1	4278.4779	0.0008	0.002		
6:	2	1	2	1	1	1	4789.6226	0.0003	0.002		
7:	4	4	0	4	3	1	4804.1075	0.0011	0.002		
8:	6	4	3	6	3	4	4808.6678	0.0000	0.002		
9:	5	4	2	5	3	3	4808.9195	-0.0022	0.002		
10:	2	0	2	1	0	1	4903.9849	0.0001	0.002		
11:	2	1	1	1	1	0	5056.7289	-0.0003	0.002		
12:	2	1	2	1	0	1	5415.1308	0.0008	0.002		
13:	7	5	3	7	4	4	6154.3798	-0.0028	0.002		
14:	3	0	3	2	1	2	6799.3393	-0.0003	0.002		
15:	2	2	1	1	1	0	6933.2532	0.0006	0.002		
16:	2	2	0	1	1	0	6952.4435	0.0003	0.002		
17:	2	2	1	1	1	1	7066.8060	-0.0007	0.002		
18:	2	2	0	1	1	1	7085.9955	-0.0019	0.002		
19:	3	1	3	2	1	2	7173.1887	0.0008	0.002		
20:	3	0	3	2	0	2	7310.4855	0.0005	0.002		
21:	3	2	2	2	2	1	7384.7587	-0.0004	0.002		
22:	3	1	2	2	1	1	7572.0991	-0.0004	0.002		
23:	3	1	3	2	0	2	7684.3333	0.0001	0.002		
24:	3	1	2	2	0	2	8483.9067	0.0007	0.002		
25:	3	2	2	2	1	1	9261.2827	0.0002	0.002		
26:	4	0	4	3	1	3	9300.4905	0.0002	0.002		
27:	3	2	1	2	1	1	9354.7448	-0.0002	0.002		
28:	4	0	4	3	0	3	9674.3392	0.0007	0.002		
29:	3	2	1	2	1	2	9755.4063	0.0000	0.002		
30:	4	2	3	3	2	2	9831.3318	0.0001	0.002		
31:	4	3	2	3	3	1	9880.0355	-0.0013	0.002		
32:	4	3	1	3	3	0	9890.3585	-0.0035	0.002		
33:	4	1	4	3	0	3	9919.3799	0.0001	0.002		
34:	4	2	2	3	2	1	10003.1919	-0.0008	0.002		
35:	4	1	3	3	1	2	10069.4078	-0.0005	0.002		
36:	3	3	1	2	2	0	10838.2292	-0.0011	0.002		
37:	3	3	0	2	2	1	10859.1664	0.0002	0.002		
38:	6	2	5	5	3	2	11023.5578	0.0004	0.002		
39:	5	1	4	4	2	3	11087.7365	-0.0007	0.002		
40:	4	1	3	3	0	3	11242.8293	-0.0001	0.002		
41:	4	2	3	3	1	2	11520.5127	-0.0018	0.002		
42:	5	0	5	4	1	4	11760.1142	0.0001	0.002		
43:	5	1	5	4	1	4	11906.1723	0.0006	0.002		
44:	5	0	5	4	0	4	12005.1553	0.0000	0.002		
45:	6	2	4	5	3	3	12081.1110	0.0005	0.002		
46:	5	1	5	4	0	4	12151.2137	0.0007	0.002		
47:	5	2	4	4	2	3	12265.3305	-0.0002	0.002		
48:	5	4	2	4	4	1	12350.4814	0.0032	0.002		
49:	5	3	3	4	3	2	12357.6015	0.0000	0.002		
50:	5	3	2	4	3	1	12392.6611	-0.0012	0.002		
51:	7	3	5	6	4	2	12488.7895	0.0007	0.002		
52:	5	1	4	4	1	3	12538.8431	-0.0002	0.002		
53:	5	2	3	4	2	2	12567.0291	0.0000	0.002		
54:	4	3	2	3	2	1	13259.2358	-0.0003	0.002		
55:	4	3	1	3	2	2	13364.7684	-0.0005	0.002		
56:	5	2	4	4	1	3	13716.4381	0.0012	0.002		
57:	6	1	5	5	2	4	13791.6685	-0.0004	0.002		
58:	5	1	4	4	0	4	14107.3345	0.0001	0.002		
59:	6	0	6	5	1	5	14175.3776	0.0002	0.002		
60:	6	1	6	5	1	5	14256.3305	0.0001	0.002		
61:	5	2	3	4	1	3	14283.4586	-0.0002	0.002		
62:	6	0	6	5	0	5	14321.4356	0.0006	0.002		
63:	6	1	6	5	0	5	14402.3885	0.0005	0.002		
64:	6	2	5	5	2	4	14684.3256	-0.0005	0.002		
65:	6	4	3	5	4	2	14833.2846	0.0011	0.002		
66:	6	3	4	5	3	3	14833.5373	0.0000	0.002		
67:	6	4	2	5	4	1	14837.8940	-0.0003	0.002		
68:	7	2	5	6	3	4	14913.7741	0.0022	0.002		
69:	6	3	3	5	3	2	14921.7905	0.0008	0.002		
70:	6	1	5	5	1	4	14969.2625	0.0000	0.002		
71:	6	2	4	5	2	3	15127.7270	0.0005	0.002		
72:	5	3	3	4	2	2	15613.6437	-0.0012	0.002		
73:	6	2	5	5	1	4	15861.9197	0.0000	0.002		
74:	5	3	2	4	2	3	15926.0995	-0.0001	0.002		
75:	7	1	6	6	2	5	16460.0968	0.0007	0.002		
76:	7	0	7	6	1	6	16555.6600	0.0001	0.002		
77:	7	1	7	6	1	6	16598.2487	0.0002	0.002		
78:	7	0	7	6	0	6	16636.6128	0.0000	0.002		
79:	7	1	7	6	0	6	16679.2018	0.0004	0.002		
80:	7	2	6	6	2	5	17086.7872	-0.0005	0.002		
81:	5	4	2	4	3	1	17154.4522	-0.0009	0.002		
82:	5	4	1	4	3	2	17167.6973	0.0011	0.002		
83:	7	1	6	6	1	5	17352.7537	0.0004	0.002		
84:	7	3	4	6	3	3	17483.0496	0.0005	0.002		

85:	6	3	4	5	2	3	17880.1531	-0.0001	0.002
86:	7	2	6	6	1	5	17979.4442	-0.0007	0.002
87:	6	3	3	5	2	4	18582.5590	0.0005	0.002
88:	6	2	4	5	1	5	18828.4661	0.0027	0.002
89:	8	0	8	7	0	7	18955.3849	-0.0006	0.002
90:	8	1	8	7	0	7	18976.9698	-0.0004	0.002
91:	6	4	3	5	3	2	19595.0739	-0.0003	0.002
92:	6	4	2	5	3	3	19647.9890	0.0000	0.002
93:	8	1	7	7	1	6	19692.0746	-0.0001	0.002
94:	8	3	6	7	3	5	19762.0422	-0.0002	0.002
95:	8	5	4	7	5	3	19786.7177	0.0003	0.002
96:	8	5	3	7	5	2	19788.6119	-0.0018	0.002
97:	8	4	5	7	4	4	19811.8313	0.0010	0.002
98:	8	4	4	7	4	3	19851.1782	0.0010	0.002
99:	3	2	1	2	2	0	7459.0257	-0.0054	0.002
100/	3	1	2	2	2	1	5695.5696	-0.0066	0.002
101:	8	6	3	7	6	2	19765.6462	-0.0043	0.002
102:	8	6	2	7	6	1	19765.6983	0.0039	0.002
103/	6	3	3	5	4	2	10160.0058	0.0069	0.002
104:	4	2	2	3	0	3	12959.2628	0.0034	0.002
105:	8	3	5	7	4	4	15559.5564	-0.0056	0.002
106:	7	2	6	6	3	3	13188.5544	-0.0010	0.002
107:	5	4	1	4	4	0	12351.5164	-0.0032	0.002
108:	4	2	2	3	1	3	12585.4095	-0.0016	0.002
109:	5	3	3	4	2	3	15878.9677	-0.0009	0.002
110:	5	3	2	4	2	2	15660.7755	-0.0003	0.002
111:	4	3	2	3	2	2	13352.6982	-0.0005	0.002
112:	4	2	2	3	1	2	11785.8371	-0.0011	0.002
113:	3	3	1	2	2	1	10857.4208	-0.0002	0.002
114:	4	4	0	3	3	0	14694.4737	0.0053	0.002
115:	4	4	1	3	3	0	14694.3335	-0.0034	0.002
116:	4	4	0	3	3	1	14696.2187	0.0052	0.002
117:	4	4	1	3	3	1	14696.0787	-0.0033	0.002
118:	5	5	0	4	4	1	18541.6158	0.0039	0.002
119:	5	5	1	4	4	0	18541.4709	-0.0006	0.002

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1923.07939(12)	1
20000	B	/MHz	1297.571854(78)	2
30000	C	/MHz	1164.017499(85)	3
200	DelJ	/kHz	0.10346(79)	4
1100	DelJK	/kHz	-0.0942(37)	5
2000	DelK	/kHz	0.1311(56)	6
40100	delJ	/kHz	0.03110(47)	7
41000	delK	/kHz	-0.032(11)	8

MICROWAVE AVG = -0.000098 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.001863 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.93138 0.93138

distinct frequency lines in fit: 119
 distinct parameters of fit: 8

	upper state	lower state	overall
limits of quantum number 1:	1 8	0 7	0 8
limits of quantum number 2:	0 6	0 6	0 6
limits of quantum number 3:	0 8	0 7	0 8

frequency range: 2102 19851

Standard errors are obtained by multiplying the previous errors by: 0.964359

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

10000	A	/MHz	1923.07939(11)	1
20000	B	/MHz	1297.571854(75)	2
30000	C	/MHz	1164.017499(81)	3
200	DelJ	/kHz	0.10346(76)	4
1100	DelJK	/kHz	-0.0942(35)	5
2000	DelK	/kHz	0.1311(54)	6
40100	delJ	/kHz	0.03110(45)	7
41000	delK	/kHz	-0.032(10)	8

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

41000	delK	/kHz	-0.032(10)	8	32.7
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CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ	-DelJK	-DelK	-delJ	-delK
A	1.0000							
B	-0.0513	1.0000						
C	0.0167	-0.2128	1.0000					
-DelJ	0.1017	-0.7610	-0.1333	1.0000				
-DelJK	-0.2115	0.4930	-0.3763	-0.6897	1.0000			
-DelK	-0.6176	-0.1698	0.3011	0.2535	-0.5048	1.0000		
-delJ	0.1302	-0.6488	0.5568	0.1958	-0.2397	0.0871	1.0000	

-delK -0.0135 -0.4418 0.5199 0.5527 -0.7789 0.4436 0.1233 1.0000

Mean value of |C.ij|, i.ne.j = 0.3438
Mean value of C.ij, i.ne.j = -0.0741

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

103:	3.4	100:	-3.3	105:	-2.8	99:	-2.7
114:	2.6	116:	2.6	101:	-2.1	102:	1.9
118:	1.9	32:	-1.8	115:	-1.7	104:	1.7
117:	-1.6	48:	1.6	107:	-1.6	13:	-1.4
88:	1.4	1:	-1.4	9:	-1.1	68:	1.1
18:	-0.9	96:	-0.9	41:	-0.9	108:	-0.8
31:	-0.6	50:	-0.6	72:	-0.6	56:	0.6
82:	0.6	36:	-0.6	112:	-0.6	7:	0.6
65:	0.6	98:	0.5	97:	0.5	106:	-0.5
109:	-0.4	81:	-0.4	34:	-0.4	69:	0.4
19:	0.4	12:	0.4	5:	0.4	28:	0.3
17:	-0.3	46:	0.3	24:	0.3	86:	-0.3
39:	-0.3	75:	0.3				

103/	6	3	3	5	4	2	10160.0058	0.0069	0.002
100/	3	1	2	2	2	1	5695.5696	-0.0066	0.002
105:	8	3	5	7	4	4	15559.5564	-0.0056	0.002
99:	3	2	1	2	2	0	7459.0257	-0.0054	0.002
114:	4	4	0	3	3	0	14694.4737	0.0053	0.002
116:	4	4	0	3	3	1	14696.2187	0.0052	0.002
101:	8	6	3	7	6	2	19765.6462	-0.0043	0.002
102:	8	6	2	7	6	1	19765.6983	0.0039	0.002
118:	5	5	0	4	4	1	18541.6158	0.0039	0.002
32:	4	3	1	3	3	0	9890.3585	-0.0035	0.002

/ SPFIT output reformatted with PIFORM

							obs	o-c	error	blends	Notes
										o-c	wt
/ instead of : below denotes (o-c)>3*err											
1:	5	0	5	4	0	4	11992.7960	0.0003	0.002		
2:	3	0	3	2	0	2	7301.4950	-0.0003	0.002		
3:	3	1	3	2	1	2	7165.7800	-0.0003	0.002		
4:	3	3	1	2	2	0	10795.7420	-0.0003	0.002		
5:	5	1	5	4	0	4	12138.3350	0.0002	0.002		
6:	3	3	0	2	2	1	10816.3200	-0.0002	0.002		
7:	2	2	0	1	1	1	7058.5464	0.0008	0.002		
8:	2	2	1	1	1	0	6907.8731	0.0002	0.002		
9:	3	1	2	2	1	1	7559.4757	-0.0021	0.002		
10:	4	0	4	3	1	3	9292.2263	0.0009	0.002		
11:	4	1	4	3	1	3	9535.9575	0.0007	0.002		
12:	4	0	4	3	0	3	9663.4784	0.0003	0.002		
13:	4	2	3	3	2	2	9817.9590	-0.0002	0.002		
14:	4	1	4	3	0	3	9907.2093	-0.0002	0.002		
15:	4	2	2	3	2	1	9987.0594	0.0000	0.002		
16:	4	1	3	3	1	2	10053.0448	-0.0002	0.002		
17:	4	2	3	3	1	2	11492.7276	-0.0004	0.002		
18:	5	0	5	4	1	4	11749.0646	0.0004	0.002		
19:	5	1	5	4	1	4	11894.6036	0.0002	0.002		
20:	5	2	4	4	2	3	12249.0133	-0.0010	0.002		
21:	5	3	3	4	3	2	12339.7904	0.0006	0.002		
22:	5	3	2	4	3	1	12374.1430	0.0004	0.002		
23:	5	1	4	4	1	3	12519.2346	0.0001	0.002		
24:	5	2	3	4	2	2	12546.0675	0.0000	0.002		
25:	4	3	2	3	2	1	13214.0221	0.0009	0.002		
26:	5	2	4	4	1	3	13688.6972	-0.0001	0.002		
27:	6	0	6	5	1	5	14162.0950	0.0005	0.002		
28:	6	1	6	5	1	5	14242.9094	-0.0001	0.002		
29:	6	0	6	5	0	5	14307.6335	-0.0001	0.002		
30:	6	1	6	5	0	5	14388.4488	0.0000	0.002		
31:	6	3	3	5	3	2	14898.6628	0.0003	0.002		
32:	6	1	5	5	1	4	14947.0876	-0.0007	0.002		
33:	6	2	4	5	2	3	15102.1893	0.0008	0.002		
34:	4	3	1	3	2	2	13317.7556	-0.0004	0.002		
35:	6	2	5	5	2	4	14665.3090	-0.0015	0.002		

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1914.89569 (65)	1
20000	B	/MHz	1294.99356 (26)	2
30000	C	/MHz	1163.18936 (21)	3
200	DelJ	/kHz	0.0990 (25)	4
1100	DelJK	/kHz	-0.088 (15)	5
2000	DelK	/kHz	0.163 (54)	6
40100	delJ	/kHz	0.0290 (20)	7
41000	delK	/kHz	[-0.032378873]	8

MICROWAVE AVG = -0.000005 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.000649 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.32464 0.32464

distinct frequency lines in fit: 35
 distinct parameters of fit: 7

		upper state	lower state	overall
limits of quantum number 1:	2	6	1	5
limits of quantum number 2:	0	3	0	3
limits of quantum number 3:	0	6	0	5

frequency range: 6907 15102

Standard errors are obtained by multiplying the previous errors by: 0.362959

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

10000	A	/MHz	1914.89569 (23)	1
20000	B	/MHz	1294.993562 (96)	2
30000	C	/MHz	1163.189369 (78)	3
200	DelJ	/kHz	0.09900 (91)	4
1100	DelJK	/kHz	-0.0882 (57)	5
2000	DelK	/kHz	0.163 (19)	6
40100	delJ	/kHz	0.02902 (73)	7
41000	delK	/kHz	[-0.032378873]	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ	-DelJK	-DelK	-delJ
A	1.0000						
B	0.4207	1.0000					
C	-0.3893	-0.3635	1.0000				
-DelJ	0.0433	-0.5921	-0.3873	1.0000			
-DelJK	-0.2823	0.0405	-0.1187	-0.3288	1.0000		
-DelK	-0.8582	-0.3895	0.4369	0.0511	-0.1664	1.0000	

-delJ -0.3156 -0.7956 0.6976 0.3094 -0.2788 0.4016 1.0000

Mean value of |C.ij|, i.ne.j = 0.3651
Mean value of C.ij, i.ne.j = -0.1364

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

9: -1.0	35: -0.8	20: -0.5	10: 0.4
25: 0.4	7: 0.4	33: 0.4	11: 0.3
32: -0.3	21: 0.3	27: 0.2	34: -0.2
18: 0.2	22: 0.2	17: -0.2	31: 0.1
4: -0.1	12: 0.1	3: -0.1	2: -0.1
1: 0.1	16: -0.1	5: 0.1	14: -0.1
13: -0.1	8: 0.1	6: -0.1	19: 0.1
23: 0.1	29: -0.1	28: -0.1	26: -0.1
30: 0.0	24: 0.0	15: 0.0	

9: 3 1 2	2 1 1	7559.4757	-0.0021	0.002
35: 6 2 5	5 2 4	14665.3090	-0.0015	0.002
20: 5 2 4	4 2 3	12249.0133	-0.0010	0.002
10: 4 0 4	3 1 3	9292.2263	0.0009	0.002
25: 4 3 2	3 2 1	13214.0221	0.0009	0.002
7: 2 2 0	1 1 1	7058.5464	0.0008	0.002
33: 6 2 4	5 2 3	15102.1893	0.0008	0.002
11: 4 1 4	3 1 3	9535.9575	0.0007	0.002
32: 6 1 5	5 1 4	14947.0876	-0.0007	0.002
21: 5 3 3	4 3 2	12339.7904	0.0006	0.002

/ SPFIT output reformatted with PIFORM

						obs	o-c	error	blends	Notes
									o-c	wt
/ instead of : below denotes (o-c)>3*err										
1:	3	0	3	2	0	2	7276.7471	0.0000	0.002	
2:	5	0	5	4	0	4	11950.6180	0.0008	0.002	
3:	6	1	6	5	0	5	14339.3307	-0.0002	0.002	
4:	5	1	5	4	0	4	12099.8354	-0.0002	0.002	
5:	2	0	2	1	0	1	4881.0601	0.0003	0.002	
6:	3	1	2	2	1	1	7536.4556	-0.0004	0.002	
7:	5	0	5	4	1	4	11701.5137	0.0000	0.002	
8:	3	1	3	2	0	2	7655.1163	0.0007	0.002	
9:	6	1	6	5	1	5	14190.1123	-0.0002	0.002	
10:	5	1	5	4	1	4	11850.7331	0.0009	0.002	
11:	4	2	3	3	1	2	11487.2137	0.0008	0.002	
12:	6	1	5	5	1	4	14901.0195	0.0000	0.002	
13:	3	0	3	2	1	2	6761.1827	0.0005	0.002	
14:	2	2	1	1	1	0	6921.4389	-0.0005	0.002	
15:	4	0	4	3	1	3	9251.8314	0.0000	0.002	
16:	3	1	3	2	1	2	7139.5453	-0.0053	0.002	
17:	4	2	3	3	2	2	9785.1262	0.0009	0.002	
18:	4	0	4	3	0	3	9630.2001	0.0001	0.002	
19:	4	1	4	3	1	3	9500.9355	0.0005	0.002	
20:	3	2	2	2	1	1	9238.5418	-0.0018	0.002	
21:	4	1	4	3	0	3	9879.3040	0.0005	0.002	
22:	4	2	2	3	2	1	9954.6932	0.0011	0.002	
23:	4	1	3	3	1	2	10022.3378	-0.0012	0.002	
24:	3	3	1	2	2	0	10821.9700	0.0001	0.002	
25:	3	3	0	2	2	1	10842.5673	0.0004	0.002	
26:	5	1	5	4	0	4	12099.8366	0.0009	0.002	
27:	5	3	3	4	3	2	12298.9399	0.0018	0.002	
28:	5	3	2	4	3	1	12333.1312	-0.0004	0.002	
29:	5	2	3	4	2	2	12506.1611	-0.0002	0.002	
30:	4	3	2	3	2	1	13231.9826	-0.0004	0.002	
31:	4	3	1	3	2	2	13335.8247	0.0000	0.002	
32:	5	2	4	4	1	3	13672.8093	0.0010	0.002	
33:	6	0	6	5	1	5	14106.9838	-0.0005	0.002	
34:	6	2	5	5	2	4	14615.9497	-0.0006	0.004	
35:	6	4	3	5	4	2	14762.6787	0.0008	0.002	
36:	6	3	4	5	3	3	14763.2412	-0.0030	0.002	
37:	6	4	2	5	4	1	14767.1251	-0.0006	0.002	
38:	6	3	3	5	3	2	14849.4253	0.0012	0.004	
39:	6	2	4	5	2	3	15055.0913	0.0009	0.002	
40:	5	3	3	4	2	2	15576.2277	-0.0012	0.002	
41:	5	3	2	4	2	3	15883.8322	0.0011	0.002	
42:	5	1	4	4	1	3	12480.8531	0.0001	0.002	

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1920.96273 (70)	1
20000	B	/MHz	1291.42523 (26)	2
30000	C	/MHz	1158.55459 (21)	3
200	DelJ	/kHz	0.1015 (24)	4
1100	DelJK	/kHz	-0.0907 (94)	5
2000	DelK	/kHz	0.143 (56)	6
40100	delJ	/kHz	0.0307 (21)	7
41000	delK	/kHz	[-0.032378873]	8

MICROWAVE AVG = -0.000021 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.001228 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.60675 0.60675

distinct frequency lines in fit: 42
 distinct parameters of fit: 7

	upper state	lower state	overall
limits of quantum number 1:	2 6	1 5	1 6
limits of quantum number 2:	0 4	0 4	0 4
limits of quantum number 3:	0 6	0 5	0 6

frequency range: 4881 15883

Standard errors are obtained by muliptying the previous errors by: 0.664661

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

10000	A	/MHz	1920.96273 (46)	1
20000	B	/MHz	1291.42523 (17)	2
30000	C	/MHz	1158.55460 (13)	3
200	DelJ	/kHz	0.1015 (16)	4
1100	DelJK	/kHz	-0.0907 (62)	5
2000	DelK	/kHz	0.143 (37)	6
40100	delJ	/kHz	0.0308 (13)	7
41000	delK	/kHz	[-0.032378873]	8

Worst fitted constants, with greater than 20% uncertainty:

%

2000	DelK /kHz	0.143(37)	6	26.0
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CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ	-DelJK	-DelK	-delJ
A	1.0000						
B	0.5706	1.0000					
C	-0.5854	-0.4694	1.0000				
-DelJ	-0.0076	-0.5622	-0.3461	1.0000			
-DelJK	-0.1827	0.0980	0.0889	-0.5117	1.0000		
-DelK	-0.9360	-0.5400	0.5602	0.0773	-0.0821	1.0000	
-delJ	-0.5086	-0.8292	0.7295	0.2993	-0.2087	0.5216	1.0000

Mean value of |C.ij|, i.ne.j = 0.4150

Mean value of C.ij, i.ne.j = -0.1345

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

16:	-2.6	36:	-1.5	27:	0.9	20:	-0.9
40:	-0.6	23:	-0.6	22:	0.6	41:	0.6
32:	0.5	17:	0.4	39:	0.4	26:	0.4
10:	0.4	35:	0.4	2:	0.4	11:	0.4
8:	0.3	37:	-0.3	38:	0.3	21:	0.2
19:	0.2	33:	-0.2	14:	-0.2	13:	0.2
6:	-0.2	28:	-0.2	25:	0.2	30:	-0.2
5:	0.1	34:	-0.1	9:	-0.1	3:	-0.1
29:	-0.1	4:	-0.1	42:	0.1	18:	0.1
24:	0.1	31:	0.0	15:	0.0	12:	0.0
7:	0.0	1:	0.0				

16:	3	1	3	2	1	2	7139.5453	-0.0053	0.002
36:	6	3	4	5	3	3	14763.2412	-0.0030	0.002
27:	5	3	3	4	3	2	12298.9399	0.0018	0.002
20:	3	2	2	2	1	1	9238.5418	-0.0018	0.002
40:	5	3	3	4	2	2	15576.2277	-0.0012	0.002
23:	4	1	3	3	1	2	10022.3378	-0.0012	0.002
22:	4	2	2	3	2	1	9954.6932	0.0011	0.002
41:	5	3	2	4	2	3	15883.8322	0.0011	0.002
32:	5	2	4	4	1	3	13672.8093	0.0010	0.002
17:	4	2	3	3	2	2	9785.1262	0.0009	0.002

/ SPFIT output reformatted with PIFORM

						obs	o-c	error	blends	Notes
									o-c	wt
/ instead of : below denotes (o-c)>3*err										

1:	3	0	3	2	0	2	7254.8930	0.0006	0.002	
2:	5	0	5	4	0	4	11914.0520	0.0017	0.002	
3:	5	0	5	4	1	4	11665.5040	0.0003	0.002	
4:	5	1	5	4	0	4	12062.8480	-0.0002	0.002	
5:	4	0	4	3	1	3	9223.2660	-0.0002	0.002	
6:	6	0	6	5	1	5	14063.5250	0.0001	0.002	
7:	5	1	5	4	1	4	11814.3010	-0.0005	0.002	
8:	4	2	3	3	1	2	11456.1370	-0.0005	0.002	
9:	2	1	2	1	0	1	5381.4150	0.0004	0.002	
10:	3	1	3	2	1	2	7117.7270	0.0001	0.002	
11:	5	2	4	4	2	3	12171.6209	-0.0001	0.002	
12:	5	3	3	4	3	2	12262.7429	0.0000	0.002	
13:	5	3	2	4	3	1	12297.0279	0.0013	0.002	
14:	5	1	4	4	1	3	12444.5251	-0.0005	0.002	
15:	5	2	3	4	2	2	12470.1610	-0.0002	0.002	
16:	4	3	2	3	2	1	13199.6445	-0.0002	0.002	
17:	5	2	4	4	1	3	13634.4131	-0.0024	0.004	
18:	6	1	6	5	1	5	14146.3694	0.0005	0.002	
19:	6	1	6	5	0	5	14295.1664	-0.0003	0.002	
20:	6	2	5	5	2	4	14572.3265	-0.0009	0.002	
21:	4	4	1	3	3	0	14640.1194	0.0000	0.004	
22:	6	3	4	5	3	3	14719.7993	0.0007	0.002	
23:	6	4	2	5	4	1	14723.7324	0.0007	0.004	
24:	6	3	3	5	3	2	14806.1936	0.0005	0.002	
25:	6	1	5	5	1	4	14857.2933	-0.0018	0.002	
26:	6	2	4	5	2	3	15011.8320	0.0003	0.002	
27:	5	3	2	4	2	3	15844.5770	0.0017	0.002	
28:	3	3	0	2	2	1	10817.5706	-0.0008	0.002	
29:	3	3	1	2	2	0	10796.9409	-0.0007	0.002	
30:	4	1	3	3	1	2	9993.3424	-0.0006	0.002	
31:	4	2	2	3	2	1	9925.8836	0.0006	0.002	
32:	4	3	1	3	3	0	9814.2536	-0.0046	0.002	
33:	4	1	4	3	0	3	9849.5308	-0.0002	0.002	
34:	4	3	2	3	3	1	9804.1670	-0.0008	0.002	
35:	4	2	3	3	2	2	9756.1024	0.0006	0.002	
36:	4	0	4	3	0	3	9600.9847	0.0002	0.002	
37:	4	1	4	3	1	3	9471.8134	0.0005	0.002	
38:	3	2	2	2	1	1	9214.7812	0.0036	0.002	
39:	3	1	3	2	0	2	7632.6097	-0.0009	0.002	
40:	3	1	2	2	1	1	7514.7426	0.0008	0.002	
41:	3	1	3	2	1	2	7117.7283	0.0014	0.002	
42:	2	2	0	1	1	1	7056.7938	-0.0012	0.002	
43:	2	2	1	1	1	0	6904.9597	-0.0021	0.004	

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1916.68508(48)	1
20000	B	/MHz	1287.81886(25)	2
30000	C	/MHz	1154.91051(18)	3
200	DelJ	/kHz	0.0963(22)	4
1100	DelJK	/kHz	-0.065(12)	5
2000	DelK	/kHz	0.155(35)	6
40100	delJ	/kHz	0.0260(18)	7
41000	delK	/kHz	[-0.032378873]	8

MICROWAVE AVG = -0.000068 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.001274 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.59728 0.59728

distinct frequency lines in fit: 43
 distinct parameters of fit: 7

	upper state	lower state	overall
limits of quantum number 1:	2 6	1 5	1 6
limits of quantum number 2:	0 4	0 4	0 4
limits of quantum number 3:	0 6	0 5	0 6

frequency range: 5381 15844

Standard errors are obtained by multiplying the previous errors by: 0.652771

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

10000	A	/MHz	1916.68508(31)	1
20000	B	/MHz	1287.81886(16)	2
30000	C	/MHz	1154.91052(12)	3
200	DelJ	/kHz	0.0963(14)	4
1100	DelJK	/kHz	-0.0656(78)	5
2000	DelK	/kHz	0.155(22)	6
40100	delJ	/kHz	0.0260(12)	7
41000	delK	/kHz	[-0.032378873]	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ	-DelJK	-DelK	-delJ
A	1.0000						
B	0.3651	1.0000					
C	-0.3989	-0.3891	1.0000				
-DelJ	0.0694	-0.5775	-0.3678	1.0000			
-DelJK	-0.3173	-0.1558	0.0388	-0.2875	1.0000		
-DelK	-0.7901	-0.2108	0.3798	-0.0107	-0.2052	1.0000	
-delJ	-0.2978	-0.7826	0.7015	0.2949	-0.0992	0.2947	1.0000

Mean value of |C.ij|, i.ne.j = 0.3350
Mean value of C.ij, i.ne.j = -0.1308

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

32: -2.3	38: 1.8	25: -0.9	27: 0.8
2: 0.8	41: 0.7	13: 0.6	17: -0.6
42: -0.6	43: -0.5	20: -0.4	39: -0.4
40: 0.4	28: -0.4	34: -0.4	29: -0.3
22: 0.3	31: 0.3	30: -0.3	35: 0.3
1: 0.3	37: 0.2	7: -0.2	14: -0.2
18: 0.2	24: 0.2	8: -0.2	9: 0.2
23: 0.2	3: 0.1	19: -0.1	26: 0.1
36: 0.1	33: -0.1	4: -0.1	16: -0.1
15: -0.1	5: -0.1	10: 0.1	6: 0.1
11: -0.1	21: 0.0	12: 0.0	
32: 4 3 1	3 3 0	9814.2536	-0.0046 0.002
38: 3 2 2	2 1 1	9214.7812	0.0036 0.002
25: 6 1 5	5 1 4	14857.2933	-0.0018 0.002
27: 5 3 2	4 2 3	15844.5770	0.0017 0.002
2: 5 0 5	4 0 4	11914.0520	0.0017 0.002
41: 3 1 3	2 1 2	7117.7283	0.0014 0.002
13: 5 3 2	4 3 1	12297.0279	0.0013 0.002
17: 5 2 4	4 1 3	13634.4131	-0.0024 0.004
42: 2 2 0	1 1 1	7056.7938	-0.0012 0.002
43: 2 2 1	1 1 0	6904.9597	-0.0021 0.004

/ SPFIT output reformatted with PIFORM

							obs	o-c	error	blends	Notes
										o-c	wt
/ instead of : below denotes (o-c)>3*err											
1:	5	1	5	4	1	4	11832.6000	-0.0006	0.002		
2:	3	1	3	2	1	2	7131.9230	0.0002	0.002		
3:	5	0	5	4	0	4	11925.9960	0.0016	0.002		
4:	3	0	3	2	0	2	7270.7350	-0.0007	0.002		
5:	5	0	5	4	1	4	11705.8580	0.0005	0.002		
6:	3	1	2	2	1	1	7547.7945	0.0002	0.002		
7:	3	0	3	2	1	2	6785.4550	-0.0007	0.002		
8:	7	0	7	6	0	6	16523.7328	0.0010	0.002		
9:	7	1	7	6	1	6	16490.3686	-0.0002	0.002		
10:	5	3	2	4	2	3	15797.1310	0.0008	0.002		
11:	5	3	3	4	2	2	15447.1513	0.0009	0.002		
12:	6	2	4	5	2	3	15088.0377	0.0019	0.002		
13:	6	1	5	5	1	4	14897.1156	-0.0011	0.002		
14:	6	3	3	5	3	2	14880.0983	0.0005	0.002		
15:	6	4	2	5	4	1	14783.8976	0.0000	0.002		
16:	6	4	3	5	4	2	14777.9688	-0.0009	0.002		
17:	6	3	4	5	3	3	14775.7754	-0.0004	0.002		
18:	6	1	6	5	0	5	14292.4036	-0.0005	0.002		
19:	4	4	1	3	3	0	14516.3280	-0.0004	0.002		
20:	4	4	0	3	3	1	14518.5951	0.0000	0.002		
21:	6	2	5	5	2	4	14611.7709	-0.0018	0.002		
22:	4	1	4	3	0	3	9835.0252	-0.0011	0.002		
23:	6	0	6	5	1	5	14097.8590	0.0005	0.002		
24:	4	3	1	3	2	2	13232.9206	0.0002	0.002		
25:	5	2	3	4	2	2	12536.4280	0.0003	0.002		
26:	5	1	4	4	1	3	12487.3450	-0.0009	0.002		
27:	5	3	2	4	3	1	12351.9781	-0.0006	0.002		
28:	5	3	3	4	3	2	12310.1391	-0.0010	0.002		
29:	5	2	4	4	2	3	12208.0809	-0.0004	0.002		
30:	5	1	5	4	0	4	12052.7374	-0.0001	0.002		
31:	4	2	3	3	1	2	11402.8175	0.0020	0.002		
32:	3	3	0	2	2	1	10732.0420	-0.0007	0.002		
33:	4	1	3	3	1	2	10033.4631	-0.0001	0.002		
34:	4	2	2	3	2	1	9977.2706	-0.0002	0.002		
35:	4	2	3	3	2	2	9787.7705	0.0014	0.002		
36:	4	0	4	3	0	3	9614.8888	-0.0006	0.002		
37:	4	1	4	3	1	3	9488.5594	0.0000	0.002		
38:	4	0	4	3	1	3	9268.4223	-0.0001	0.002		
39:	3	1	3	2	0	2	7617.2027	0.0000	0.002		
40:	3	2	2	2	2	1	7353.4350	0.0035	0.002		
41:	2	2	0	1	1	1	7011.8140	-0.0019	0.002		
42:	2	2	1	1	1	0	6851.0230	-0.0007	0.002		

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1898.37181(37)	1
20000	B	/MHz	1295.23572(23)	2
30000	C	/MHz	1155.91088(14)	3
200	DelJ	/kHz	0.1000(22)	4
1100	DelJK	/kHz	-0.0991(95)	5
2000	DelK	/kHz	0.104(19)	6
40100	delJ	/kHz	0.0285(15)	7
41000	delK	/kHz	[-0.032378873]	8

MICROWAVE AVG = -0.000016 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.001059 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.52970 0.52970

distinct frequency lines in fit: 42
 distinct parameters of fit: 7

	upper state	lower state	overall
limits of quantum number 1:	2 7	1 6	1 7
limits of quantum number 2:	0 4	0 4	0 4
limits of quantum number 3:	0 7	0 6	0 7

frequency range: 6785 16523

Standard errors are obtained by multiplying the previous errors by: 0.580257

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

10000	A	/MHz	1898.37181(21)	1
20000	B	/MHz	1295.23573(13)	2
30000	C	/MHz	1155.910888(85)	3
200	DelJ	/kHz	0.1000(12)	4
1100	DelJK	/kHz	-0.0991(55)	5
2000	DelK	/kHz	0.105(11)	6
40100	delJ	/kHz	0.02855(89)	7
41000	delK	/kHz	[-0.032378873]	8

CORRELATION COEFFICIENTS, C.ij:

A B C -DelJ -DelJK -DelK -delJ

A	1.0000										
B	0.2152	1.0000									
C	-0.2217	-0.3091	1.0000								
-DelJ	0.0392	-0.7171	-0.2560	1.0000							
-DelJK	-0.3259	0.0881	0.0305	-0.4849	1.0000						
-DelK	-0.7285	-0.1556	0.2196	0.1298	-0.2873	1.0000					
-delJ	-0.1100	-0.8382	0.5132	0.6290	-0.3409	0.2276	1.0000				

Mean value of |C.ij|, i.ne.j = 0.3270
Mean value of C.ij, i.ne.j = -0.1277

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

40:	1.8	31:	1.0	12:	0.9	41:	-0.9
21:	-0.9	3:	0.8	35:	0.7	22:	-0.6
13:	-0.6	28:	-0.5	8:	0.5	11:	0.4
16:	-0.4	26:	-0.4	10:	0.4	42:	-0.3
32:	-0.3	4:	-0.3	7:	-0.3	36:	-0.3
27:	-0.3	1:	-0.3	18:	-0.2	23:	0.2
14:	0.2	5:	0.2	29:	-0.2	17:	-0.2
19:	-0.2	25:	0.1	9:	-0.1	24:	0.1
6:	0.1	34:	-0.1	2:	0.1	33:	-0.1
38:	-0.1	30:	-0.1	39:	0.0	37:	0.0
20:	0.0	15:	0.0				

40:	3	2	2	2	2	1	7353.4350	0.0035	0.002
31:	4	2	3	3	1	2	11402.8175	0.0020	0.002
12:	6	2	4	5	2	3	15088.0377	0.0019	0.002
41:	2	2	0	1	1	1	7011.8140	-0.0019	0.002
21:	6	2	5	5	2	4	14611.7709	-0.0018	0.002
3:	5	0	5	4	0	4	11925.9960	0.0016	0.002
35:	4	2	3	3	2	2	9787.7705	0.0014	0.002
22:	4	1	4	3	0	3	9835.0252	-0.0011	0.002
13:	6	1	5	5	1	4	14897.1156	-0.0011	0.002
28:	5	3	3	4	3	2	12310.1391	-0.0010	0.002

/ SPFIT output reformatted with PIFORM

						obs	o-c	error	blends	Notes
									o-c	wt
/ instead of : below denotes (o-c)>3*err										
1:	3	0	3	2	0	2	7282.6648	0.0001	0.002	
2:	5	0	5	4	0	4	11951.5830	0.0000	0.002	
3:	3	0	3	2	1	2	6782.1440	-0.0002	0.002	
4:	3	3	0	2	2	1	10803.3500	0.0000	0.002	
5:	3	1	2	2	1	1	7553.0115	0.0007	0.002	
6:	5	2	4	4	2	3	12223.6970	-0.0012	0.002	
7:	5	1	5	4	0	4	12088.4688	0.0002	0.002	
8:	3	1	3	2	1	2	7143.9532	0.0004	0.002	
9:	3	3	1	2	2	0	10781.0514	-0.0007	0.002	
10:	7	1	7	6	1	6	16523.7282	0.0016	0.002	
11:	3	2	2	2	1	1	9212.7668	0.0031	0.002	
12:	4	0	4	3	1	3	9271.9381	0.0001	0.002	
13:	4	1	4	3	1	3	9505.5181	-0.0002	0.002	
14:	4	2	3	3	2	2	9799.1936	0.0002	0.002	
15:	4	1	4	3	0	3	9867.3273	0.0004	0.002	
16:	4	2	2	3	2	1	9980.4244	0.0003	0.002	
17:	4	1	3	3	1	2	10042.1334	-0.0005	0.002	
18:	3	3	0	2	2	1	10803.3499	0.0000	0.002	
19:	4	2	3	3	1	2	11458.9465	0.0002	0.002	
20:	5	0	5	4	1	4	11718.0028	0.0001	0.002	
21:	5	3	2	4	3	1	12359.5840	0.0002	0.002	
22:	5	1	4	4	1	3	12501.3758	0.0000	0.002	
23:	5	2	3	4	2	2	12539.8197	0.0001	0.002	
24:	4	3	2	3	2	1	13191.7672	-0.0007	0.002	
25:	4	3	1	3	2	2	13304.1015	-0.0013	0.002	
26:	5	2	4	4	1	3	13640.5105	0.0000	0.002	
27:	6	0	6	5	1	5	14118.9141	-0.0006	0.002	
28:	6	1	6	5	1	5	14193.4766	-0.0007	0.002	
29:	6	1	6	5	0	5	14330.3617	-0.0012	0.002	
30:	4	4	1	3	3	0	14616.6535	-0.0024	0.002	
31:	4	4	0	3	3	1	14618.7290	0.0033	0.002	
32:	6	3	4	5	3	3	14789.4335	-0.0001	0.002	
33:	6	4	3	5	4	2	14790.3211	0.0015	0.002	
34:	6	3	3	5	3	2	14885.7699	0.0000	0.002	
35:	6	4	2	5	4	1	14795.5642	-0.0009	0.002	
36:	6	1	5	5	1	4	14918.9517	-0.0004	0.002	
37:	6	2	4	5	2	3	15093.9420	0.0005	0.002	
38:	5	3	3	4	2	2	15532.4819	-0.0004	0.002	
39:	4	0	4	3	0	3	9633.7462	-0.0002	0.002	

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1912.52742 (38)	1
20000	B	/MHz	1295.39144 (24)	2
30000	C	/MHz	1158.39667 (17)	3
200	DelJ	/kHz	0.0999 (24)	4
1100	DelJK	/kHz	-0.0841 (98)	5
2000	DelK	/kHz	0.149 (20)	6
40100	delJ	/kHz	0.0310 (16)	7
41000	delK	/kHz	[-0.032378873]	8

MICROWAVE AVG = 0.000025 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.001047 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.52360 0.52360

distinct frequency lines in fit: 39
 distinct parameters of fit: 7

		upper state	lower state	overall
limits of quantum number 1:	3	7	2	6
limits of quantum number 2:	0	4	0	4
limits of quantum number 3:	0	7	0	6

frequency range: 6782 16523

Standard errors are obtained by multiplying the previous errors by: 0.578039

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

10000	A	/MHz	1912.52742 (21)	1
20000	B	/MHz	1295.39145 (14)	2
30000	C	/MHz	1158.396672 (98)	3
200	DelJ	/kHz	0.0999 (13)	4
1100	DelJK	/kHz	-0.0841 (56)	5
2000	DelK	/kHz	0.150 (11)	6
40100	delJ	/kHz	0.03104 (97)	7
41000	delK	/kHz	[-0.032378873]	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ	-DelJK	-DelK	-delJ
A	1.0000						
B	0.3544	1.0000					

C	-0.3702	-0.3075	1.0000					
-DelJ	0.0099	-0.7036	-0.3044	1.0000				
-DelJK	-0.2957	0.1915	-0.0053	-0.5191	1.0000			
-DelK	-0.7679	-0.3413	0.3729	0.1682	-0.2764	1.0000		
-delJ	-0.2631	-0.8328	0.5591	0.5420	-0.3805	0.3892	1.0000	

Mean value of |C.ij|, i.ne.j = 0.3788
Mean value of C.ij, i.ne.j = -0.1324

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

31: 1.6	11: 1.5	30: -1.2	10: 0.8
33: 0.8	25: -0.6	6: -0.6	29: -0.6
35: -0.4	5: 0.3	24: -0.3	28: -0.3
9: -0.3	27: -0.3	37: 0.2	17: -0.2
8: 0.2	38: -0.2	36: -0.2	15: 0.2
16: 0.1	39: -0.1	3: -0.1	19: 0.1
7: 0.1	14: 0.1	13: -0.1	21: 0.1
20: 0.1	32: -0.1	1: 0.1	23: 0.1
12: 0.1	34: 0.0	26: 0.0	22: 0.0
18: 0.0	4: 0.0	2: 0.0	

31: 4 4 0	3 3 1	14618.7290	0.0033	0.002
11: 3 2 2	2 1 1	9212.7668	0.0031	0.002
30: 4 4 1	3 3 0	14616.6535	-0.0024	0.002
10: 7 1 7	6 1 6	16523.7282	0.0016	0.002
33: 6 4 3	5 4 2	14790.3211	0.0015	0.002
25: 4 3 1	3 2 2	13304.1015	-0.0013	0.002
6: 5 2 4	4 2 3	12223.6970	-0.0012	0.002
29: 6 1 6	5 0 5	14330.3617	-0.0012	0.002
35: 6 4 2	5 4 1	14795.5642	-0.0009	0.002
5: 3 1 2	2 1 1	7553.0115	0.0007	0.002

/ SPFIT output reformatted with PIFORM

						obs	o-c	error	blends	Notes
									o-c	wt
/ instead of : below denotes (o-c)>3*err										
1:	3	0	3	2	0	2	7289.1890	0.0015	0.002	
2:	5	0	5	4	0	4	11971.2310	0.0007	0.002	
3:	5	1	5	4	1	4	11871.5110	0.0001	0.002	
4:	3	1	3	2	1	2	7152.0500	0.0001	0.002	
5:	5	1	5	4	0	4	12119.9690	0.0000	0.002	
6:	3	1	3	2	0	2	7666.7860	0.0000	0.002	
7:	5	2	4	4	2	3	12228.7733	0.0000	0.002	
8:	5	3	3	4	3	2	12319.8887	0.0000	0.002	
9:	5	3	2	4	3	1	12354.1720	-0.0007	0.002	
10:	5	1	4	4	1	3	12501.6253	0.0005	0.002	
11:	5	2	3	4	2	2	12527.2820	0.0008	0.002	
12:	4	3	2	3	2	1	13244.4830	0.0030	0.002	
13:	4	3	1	3	2	2	13348.4790	-0.0001	0.002	
14:	5	2	4	4	1	3	13691.1392	-0.0005	0.002	
15:	6	0	6	5	1	5	14132.2160	0.0000	0.002	
16:	6	0	6	5	0	5	14280.9555	0.0006	0.002	
17:	6	3	4	5	3	3	14788.3693	-0.0007	0.002	
18:	6	3	3	5	3	2	14874.7632	-0.0008	0.002	
19:	6	1	5	5	1	4	14925.8164	-0.0003	0.002	
20:	6	2	4	5	2	3	15080.3608	0.0012	0.002	
21:	5	3	2	4	2	3	15900.8295	0.0003	0.002	
22:	4	2	3	3	1	2	11501.3885	0.0005	0.002	
23:	3	3	0	2	2	1	10850.9719	0.0000	0.002	
24:	3	3	1	2	2	0	10830.3430	-0.0002	0.002	
25:	4	1	3	3	1	2	10039.0213	-0.0001	0.002	
26:	4	2	2	3	2	1	9971.5882	-0.0008	0.002	
27:	4	1	4	3	0	3	9895.1775	0.0007	0.002	
28:	4	2	3	3	2	2	9801.8229	0.0001	0.002	
29:	4	0	4	3	0	3	9646.7181	-0.0003	0.002	
30:	4	1	4	3	1	3	9517.5781	-0.0001	0.002	
31:	4	0	4	3	1	3	9269.1204	0.0004	0.002	
32:	3	2	2	2	1	1	9248.5602	-0.0051	0.002	
33:	6	1	6	5	1	5	14215.0236	0.0000	0.002	
34:	6	1	6	5	0	5	14363.7623	-0.0001	0.002	
35:	6	2	5	5	2	4	14640.9108	-0.0009	0.002	
36:	3	1	2	2	1	1	7548.9999	-0.0002	0.002	
37:	2	2	0	1	1	1	7079.1077	-0.0008	0.002	
38:	2	2	1	1	1	0	6927.2985	0.0005	0.002	

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1922.22158 (30)	1
20000	B	/MHz	1293.52329 (24)	2
30000	C	/MHz	1160.63617 (17)	3
200	DelJ	/kHz	0.1016 (25)	4
1100	DelJK	/kHz	-0.097 (13)	5
2000	DelK	/kHz	[0.131145949]	6
40100	delJ	/kHz	0.0296 (17)	7
41000	delK	/kHz	[-0.032378873]	8

MICROWAVE AVG = -0.000022 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.001127 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.56370 0.56370

distinct frequency lines in fit: 38
 distinct parameters of fit: 6

		upper state	lower state	overall
limits of quantum number 1:	2	6	1	5
limits of quantum number 2:	0	3	0	3
limits of quantum number 3:	0	6	0	5

frequency range: 6927 15900

Standard errors are obtained by multiplying the previous errors by: 0.614278

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

10000	A	/MHz	1922.22159 (18)	1
20000	B	/MHz	1293.52330 (14)	2
30000	C	/MHz	1160.63618 (10)	3
200	DelJ	/kHz	0.1016 (15)	4
1100	DelJK	/kHz	-0.0973 (84)	5
2000	DelK	/kHz	[0.131145949]	6
40100	delJ	/kHz	0.0297 (10)	7
41000	delK	/kHz	[-0.032378873]	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ	-DelJK	-delJ
A	1.0000					
B	0.1986	1.0000				
C	-0.1488	-0.1856	1.0000			

-DelJ	0.2250	-0.6419	-0.4722	1.0000		
-DelJK	-0.8471	-0.0630	0.1138	-0.4026	1.0000	
-delJ	0.0079	-0.7624	0.5707	0.3655	-0.1613	1.0000

Mean value of |C.ij|, i.ne.j = 0.3444
Mean value of C.ij, i.ne.j = -0.1469

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

32:	-2.6	12:	1.5	1:	0.8	20:	0.6
35:	-0.4	26:	-0.4	37:	-0.4	18:	-0.4
11:	0.4	27:	0.3	17:	-0.3	2:	0.3
9:	-0.3	16:	0.3	38:	0.2	14:	-0.2
22:	0.2	10:	0.2	31:	0.2	19:	-0.1
29:	-0.1	21:	0.1	36:	-0.1	24:	-0.1
34:	-0.1	13:	-0.1	30:	-0.1	28:	0.1
25:	-0.1	4:	0.1	3:	0.1	33:	0.0
23:	0.0	15:	0.0	8:	0.0	7:	0.0
6:	0.0	5:	0.0				

32:	3	2	2	2	1	1	9248.5602	-0.0051	0.002
12:	4	3	2	3	2	1	13244.4830	0.0030	0.002
1:	3	0	3	2	0	2	7289.1890	0.0015	0.002
20:	6	2	4	5	2	3	15080.3608	0.0012	0.002
35:	6	2	5	5	2	4	14640.9108	-0.0009	0.002
26:	4	2	2	3	2	1	9971.5882	-0.0008	0.002
37:	2	2	0	1	1	1	7079.1077	-0.0008	0.002
18:	6	3	3	5	3	2	14874.7632	-0.0008	0.002
11:	5	2	3	4	2	2	12527.2820	0.0008	0.002
27:	4	1	4	3	0	3	9895.1775	0.0007	0.002

/ SPFIT output reformatted with PIFORM

						obs	o-c	error	blends	Notes
									o-c	wt
/ instead of : below denotes (o-c)>3*err										
=====										
1:	2	0	2	1	0	1	4885.6610	0.0022	0.002	
2:	3	0	3	2	0	2	7285.3910	0.0000	0.002	
3:	5	0	5	4	0	4	11971.4550	0.0004	0.002	
4:	3	1	3	2	1	2	7152.5090	-0.0008	0.002	
5:	5	1	5	4	1	4	11874.1750	0.0001	0.002	
6:	5	0	5	4	1	4	11727.8250	-0.0002	0.002	
7:	5	1	5	4	0	4	12117.8040	-0.0001	0.002	
8:	6	2	4	5	2	3	15053.9828	0.0002	0.002	
9:	6	1	5	5	1	4	14907.0920	-0.0001	0.002	
10:	6	3	4	5	3	3	14772.4833	-0.0004	0.002	
11:	6	3	3	5	3	2	14854.8681	0.0009	0.002	
12:	6	0	6	5	0	5	14283.9512	0.0003	0.002	
13:	6	1	6	5	0	5	14365.7165	-0.0002	0.002	
14:	6	2	5	5	2	4	14630.8066	-0.0003	0.002	
15:	6	1	6	5	1	5	14219.3672	0.0001	0.002	
16:	6	0	6	5	1	5	14137.6013	0.0000	0.002	
17:	5	2	4	4	1	3	13646.2555	0.0008	0.002	
18:	4	3	1	3	2	2	13243.5142	0.0000	0.002	
19:	5	2	3	4	2	2	12506.2929	-0.0004	0.002	
20:	5	1	4	4	1	3	12483.3391	-0.0001	0.002	
21:	5	3	2	4	3	1	12339.3729	-0.0007	0.002	
22:	5	3	3	4	3	2	12306.7098	0.0002	0.002	
23:	5	2	4	4	2	3	12219.2210	0.0001	0.002	
24:	3	3	0	2	2	1	10750.0734	0.0001	0.002	
25:	4	2	3	3	1	2	11449.8249	-0.0012	0.002	
26:	3	3	1	2	2	0	10730.2995	0.0000	0.002	
27:	4	1	3	3	1	2	10022.7914	-0.0010	0.002	
28:	4	2	2	3	2	1	9956.4687	0.0014	0.002	
29:	4	1	4	3	0	3	9888.0554	0.0000	0.002	
30:	4	2	3	3	2	2	9793.4144	-0.0004	0.002	
31:	4	0	4	3	0	3	9644.4259	-0.0002	0.002	
32:	4	1	4	3	1	3	9518.9240	-0.0004	0.002	
33:	4	0	4	3	1	3	9275.2950	-0.0001	0.002	
34:	3	1	3	2	0	2	7654.5230	0.0010	0.002	
35:	3	1	2	2	1	1	7535.9995	0.0000	0.002	

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1902.3729(13)	1
20000	B	/MHz	1290.13956(36)	2
30000	C	/MHz	1161.76661(26)	3
200	DelJ	/kHz	0.1011(24)	4
1100	DelJK	/kHz	-0.085(16)	5
2000	DelK	/kHz	0.094(96)	6
40100	delJ	/kHz	0.0289(24)	7
41000	delK	/kHz	[-0.032378873]	8

MICROWAVE AVG = 0.000027 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.000665 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.33241 0.33241

distinct frequency lines in fit: 35
 distinct parameters of fit: 7

		upper state	lower state	overall
limits of quantum number 1:	2	6	1	5
limits of quantum number 2:	0	3	0	3
limits of quantum number 3:	0	6	0	5

frequency range: 4885 15053

Standard errors are obtained by multiplying the previous errors by: 0.371646

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

10000	A	/MHz	1902.37298(48)	1
20000	B	/MHz	1290.13956(13)	2
30000	C	/MHz	1161.766614(98)	3
200	DelJ	/kHz	0.10113(91)	4
1100	DelJK	/kHz	-0.0853(62)	5
2000	DelK	/kHz	0.094(35)	6
40100	delJ	/kHz	0.02897(90)	7
41000	delK	/kHz	[-0.032378873]	8

Worst fitted constants, with greater than 20% uncertainty:

2000	DelK	/kHz	0.094(35)	6	38.0
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CORRELATION COEFFICIENTS, C.ij:

A	B	C	-DelJ	-DelJK	-DelK	-delJ
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A	1.0000							
B	0.7440	1.0000						
C	-0.7166	-0.6491	1.0000					
-DelJ	0.0219	-0.4469	-0.2636	1.0000				
-DelJK	-0.5024	-0.2564	0.2269	-0.3615	1.0000			
-DelK	-0.9584	-0.7276	0.7211	0.0400	0.2952	1.0000		
-delJ	-0.6372	-0.8748	0.8039	0.2908	0.0448	0.6674	1.0000	

Mean value of |C.ij|, i.ne.j = 0.4881
Mean value of C.ij, i.ne.j = -0.1209

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

1:	1.1	28:	0.7	25:	-0.6	27:	-0.5
34:	0.5	11:	0.4	17:	0.4	4:	-0.4
21:	-0.3	19:	-0.2	10:	-0.2	32:	-0.2
3:	0.2	30:	-0.2	14:	-0.1	12:	0.1
13:	-0.1	6:	-0.1	31:	-0.1	22:	0.1
8:	0.1	5:	0.1	33:	-0.1	15:	0.1
9:	-0.1	24:	0.1	23:	0.1	20:	-0.1
7:	-0.1	35:	0.0	29:	0.0	26:	0.0
18:	0.0	16:	0.0	2:	0.0		

1:	2	0	2	1	0	1	4885.6610	0.0022	0.002
28:	4	2	2	3	2	1	9956.4687	0.0014	0.002
25:	4	2	3	3	1	2	11449.8249	-0.0012	0.002
27:	4	1	3	3	1	2	10022.7914	-0.0010	0.002
34:	3	1	3	2	0	2	7654.5230	0.0010	0.002
11:	6	3	3	5	3	2	14854.8681	0.0009	0.002
17:	5	2	4	4	1	3	13646.2555	0.0008	0.002
4:	3	1	3	2	1	2	7152.5090	-0.0008	0.002
21:	5	3	2	4	3	1	12339.3729	-0.0007	0.002
19:	5	2	3	4	2	2	12506.2929	-0.0004	0.002

/ SPFIT output reformatted with PIFORM

							obs	o-c	error	blends	Notes
										o-c	wt
/ instead of : below denotes (o-c)>3*err											

1:	3	1	3	2	0	2	7642.0610	0.0000	0.002		
2:	3	0	3	2	0	2	7271.1180	0.0004	0.002		
3:	5	1	5	4	1	4	11852.4960	0.0001	0.002		
4:	3	1	3	2	1	2	7139.0461	0.0007	0.002		
5:	5	0	5	4	0	4	11949.9940	0.0003	0.002		
6:	3	1	2	2	1	1	7518.8080	-0.0002	0.002		
7:	5	1	5	4	0	4	12098.2470	0.0002	0.002		
8:	2	2	1	1	1	0	6857.5160	0.0007	0.002		
9:	3	3	1	2	2	0	10712.1780	-0.0003	0.002		
10:	3	3	0	2	2	1	10731.5710	0.0008	0.002		
11:	4	0	4	3	1	3	9255.5231	-0.0003	0.002		
12:	4	0	4	3	0	3	9626.4664	-0.0004	0.002		
13:	4	1	4	3	1	3	9501.2746	0.0002	0.002		
14:	4	2	3	3	2	2	9772.9568	0.0007	0.002		
15:	4	1	4	3	0	3	9872.2172	-0.0005	0.002		
16:	4	2	2	3	2	1	9933.2473	-0.0011	0.002		
17:	4	1	3	3	1	2	10000.3753	-0.0003	0.002		
18:	4	2	3	3	1	2	11431.2660	-0.0013	0.002		
19:	5	0	5	4	1	4	11704.2426	-0.0001	0.002		
20:	5	2	4	4	2	3	12194.0632	0.0000	0.002		
21:	5	3	3	4	3	2	12280.0446	0.0004	0.002		
22:	5	3	2	4	3	1	12311.8350	0.0000	0.002		
23:	5	1	4	4	1	3	12456.2473	0.0000	0.002		
24:	5	2	3	4	2	2	12476.7274	0.0011	0.002		
25:	4	3	1	3	2	2	13219.0087	-0.0004	0.002		
26:	6	0	6	5	1	5	14110.5740	-0.0012	0.002		
27:	6	1	6	5	1	5	14193.7684	0.0003	0.002		
28:	6	0	6	5	0	5	14258.8282	0.0000	0.002		
29:	6	1	6	5	0	5	14342.0218	0.0007	0.002		
30:	6	2	5	5	2	4	14601.1989	-0.0002	0.002		
31:	6	3	4	5	3	3	14740.5403	0.0000	0.002		
32:	6	1	5	5	1	4	14876.0690	0.0000	0.002		

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1899.23767 (90)	1
20000	B	/MHz	1286.92061 (33)	2
30000	C	/MHz	1159.80470 (23)	3
200	DelJ	/kHz	0.1021 (29)	4
1100	DelJK	/kHz	-0.088 (17)	5
2000	DelK	/kHz	0.081 (72)	6
40100	delJ	/kHz	0.0301 (25)	7
41000	delK	/kHz	[-0.032378873]	8

MICROWAVE AVG = 0.000014 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.000585 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.29265 0.29265

distinct frequency lines in fit: 32
 distinct parameters of fit: 7

		upper state	lower state	overall
limits of quantum number 1:	2	6	1	5
limits of quantum number 2:	0	3	0	3
limits of quantum number 3:	0	6	0	5

frequency range: 6857 14876

Standard errors are obtained by multiplying the previous errors by: 0.331096

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

10000	A	/MHz	1899.23767 (29)	1
20000	B	/MHz	1286.92061 (10)	2
30000	C	/MHz	1159.804706 (77)	3
200	DelJ	/kHz	0.10215 (98)	4
1100	DelJK	/kHz	-0.0882 (58)	5
2000	DelK	/kHz	0.081 (23)	6
40100	delJ	/kHz	0.03010 (82)	7
41000	delK	/kHz	[-0.032378873]	8

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

2000 DelK /kHz 0.081 (23) 6 29.4

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ	-DelJK	-DelK	-delJ
A	1.0000						
B	0.5424	1.0000					
C	-0.5687	-0.5026	1.0000				

-DelJ	0.0218	-0.5826	-0.2474	1.0000			
-DelJK	-0.2943	-0.0457	0.0492	-0.4159	1.0000		
-DelK	-0.9127	-0.5096	0.5662	0.0769	-0.0394	1.0000	
-delJ	-0.4364	-0.8481	0.6757	0.4891	-0.2119	0.4905	1.0000

Mean value of |C.ij|, i.ne.j = 0.4060
Mean value of C.ij, i.ne.j = -0.1287

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

18: -0.6	26: -0.6	16: -0.6	24: 0.6
10: 0.4	4: 0.3	14: 0.3	8: 0.3
29: 0.3	15: -0.2	21: 0.2	25: -0.2
12: -0.2	2: 0.2	17: -0.1	5: 0.1
11: -0.1	9: -0.1	27: 0.1	6: -0.1
13: 0.1	30: -0.1	7: 0.1	19: -0.1
3: 0.1	32: 0.0	31: 0.0	28: 0.0
23: 0.0	22: 0.0	20: 0.0	1: 0.0

18: 4 2 3	3 1 2	11431.2660	-0.0013	0.002
26: 6 0 6	5 1 5	14110.5740	-0.0012	0.002
16: 4 2 2	3 2 1	9933.2473	-0.0011	0.002
24: 5 2 3	4 2 2	12476.7274	0.0011	0.002
10: 3 3 0	2 2 1	10731.5710	0.0008	0.002
4: 3 1 3	2 1 2	7139.0461	0.0007	0.002
14: 4 2 3	3 2 2	9772.9568	0.0007	0.002
8: 2 2 1	1 1 0	6857.5160	0.0007	0.002
29: 6 1 6	5 0 5	14342.0218	0.0007	0.002
15: 4 1 4	3 0 3	9872.2172	-0.0005	0.002

/ SPFIT output reformatted with PIFORM

						obs	o-c	error	blends	Notes
									o-c	wt
/ instead of : below denotes (o-c)>3*err										

1:	5	0	5	4	0	4	11829.7090	0.0000	0.002	
2:	3	0	3	2	0	2	7200.9280	-0.0008	0.002	
3:	5	1	5	4	1	4	11727.1020	-0.0002	0.002	
4:	3	1	2	2	1	1	7454.5410	-0.0006	0.002	
5:	5	0	5	4	1	4	11567.7250	-0.0003	0.002	
6:	3	0	3	2	1	2	6671.6800	0.0009	0.002	
7:	3	3	0	2	2	1	10818.9420	0.0011	0.002	
8:	5	1	5	4	0	4	11989.0855	-0.0003	0.002	
9:	5	2	4	4	2	3	12077.9286	0.0001	0.002	
10:	5	3	3	4	3	2	12164.9701	0.0003	0.002	
11:	5	3	2	4	3	1	12196.5356	-0.0006	0.002	
12:	5	1	4	4	1	3	12348.6891	-0.0003	0.002	
13:	5	2	3	4	2	2	12365.1476	0.0000	0.002	
14:	4	3	2	3	2	1	13184.9174	-0.0005	0.002	
15:	4	3	1	3	2	2	13283.5225	-0.0002	0.002	
16:	6	0	6	5	1	5	13952.5333	0.0003	0.002	
17:	6	1	6	5	1	5	14042.7453	0.0000	0.002	
18:	6	0	6	5	0	5	14111.9100	0.0001	0.002	
19:	6	1	6	5	0	5	14202.1223	0.0001	0.002	
20:	6	2	5	5	2	4	14461.4993	-0.0002	0.002	
21:	6	1	5	5	1	4	14746.5848	-0.0001	0.002	
22:	6	2	4	5	2	3	14886.9841	0.0005	0.002	
23:	4	2	3	3	1	2	11422.1018	0.0000	0.002	
24:	3	3	1	2	2	0	10799.3913	-0.0003	0.002	
25:	4	1	3	3	1	2	9914.5228	-0.0008	0.002	
26:	4	2	2	3	2	1	9842.5881	0.0008	0.002	
27:	4	1	4	3	0	3	9793.7783	0.0000	0.002	
28:	4	2	3	3	2	2	9680.2233	0.0012	0.002	
29:	4	0	4	3	0	3	9531.7947	0.0000	0.002	
30:	4	1	4	3	1	3	9401.2584	0.0002	0.002	
31:	4	0	4	3	1	3	9139.2736	-0.0009	0.002	
32:	3	1	3	2	0	2	7593.4498	0.0008	0.002	

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1919.0084(13)	1
20000	B	/MHz	1277.10613(37)	2
30000	C	/MHz	1146.46835(26)	3
200	DelJ	/kHz	0.0988(25)	4
1100	DelJK	/kHz	-0.079(19)	5
2000	DelK	/kHz	0.151(92)	6
40100	delJ	/kHz	0.0284(25)	7
41000	delK	/kHz	[-0.032378873]	8

MICROWAVE AVG = 0.000009 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.000556 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.27792 0.27792

distinct frequency lines in fit: 32
 distinct parameters of fit: 7

		upper state	lower state	overall
limits of quantum number 1:	3	6	2	5
limits of quantum number 2:	0	3	0	3
limits of quantum number 3:	0	6	0	5

frequency range: 6671 14886

Standard errors are obtained by multiplying the previous errors by: 0.314431

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

10000	A	/MHz	1919.00840(40)	1
20000	B	/MHz	1277.10613(11)	2
30000	C	/MHz	1146.468358(82)	3
200	DelJ	/kHz	0.09883(79)	4
1100	DelJK	/kHz	-0.0796(60)	5
2000	DelK	/kHz	0.151(28)	6
40100	delJ	/kHz	0.02842(79)	7
41000	delK	/kHz	[-0.032378873]	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ	-DelJK	-DelK	-delJ
A	1.0000						
B	0.7398	1.0000					
C	-0.6386	-0.6226	1.0000				
-DelJ	-0.1048	-0.5085	-0.2332	1.0000			
-DelJK	-0.4908	-0.3482	0.1777	-0.1420	1.0000		
-DelK	-0.9436	-0.6854	0.6502	0.1261	0.2169	1.0000	
-delJ	-0.6297	-0.8771	0.7944	0.3373	0.1348	0.6346	1.0000

Mean value of |C.ij|, i.ne.j = 0.4779

Mean value of C.ij, i.ne.j = -0.1149

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

28:	0.6	7:	0.6	6:	0.4	31:	-0.4
32:	0.4	26:	0.4	25:	-0.4	2:	-0.4
11:	-0.3	4:	-0.3	14:	-0.2	22:	0.2
5:	-0.1	8:	-0.1	12:	-0.1	24:	-0.1
10:	0.1	16:	0.1	30:	0.1	15:	-0.1
20:	-0.1	3:	-0.1	19:	0.1	18:	0.1
9:	0.1	21:	-0.1	29:	0.0	27:	0.0
23:	0.0	17:	0.0	13:	0.0	1:	0.0

28:	4	2	3	3	2	2	9680.2233	0.0012	0.002
7:	3	3	0	2	2	1	10818.9420	0.0011	0.002
6:	3	0	3	2	1	2	6671.6800	0.0009	0.002
31:	4	0	4	3	1	3	9139.2736	-0.0009	0.002
32:	3	1	3	2	0	2	7593.4498	0.0008	0.002
26:	4	2	2	3	2	1	9842.5881	0.0008	0.002
25:	4	1	3	3	1	2	9914.5228	-0.0008	0.002
2:	3	0	3	2	0	2	7200.9280	-0.0008	0.002
11:	5	3	2	4	3	1	12196.5356	-0.0006	0.002
4:	3	1	2	2	1	1	7454.5410	-0.0006	0.002

/ SPFIT output reformatted with PIFORM

						obs	o-c	error	blends	Notes
									o-c	wt
/ instead of : below denotes (o-c)>3*err										
1:	3	0	3	2	0	2	7113.7206	0.0015	0.004	
2:	5	0	5	4	0	4	11671.4818	0.0007	0.004	
3:	5	0	5	4	1	4	11429.2608	0.0001	0.004	
4:	5	1	5	4	0	4	11814.6616	0.0008	0.004	
5:	6	1	6	5	0	5	13998.0090	0.0011	0.004	
6:	4	1	3	3	1	2	9815.7819	0.0007	0.004	
7:	4	1	4	3	0	3	9651.5946	-0.0008	0.004	
8:	4	0	4	3	0	3	9409.3756	0.0005	0.004	
9:	4	1	4	3	1	3	9279.2970	0.0019	0.004	
10:	4	0	4	3	1	3	9037.0744	-0.0002	0.004	
11:	5	2	3	4	2	2	12253.1533	0.0011	0.004	
12:	4	3	2	3	2	1	13023.7118	-0.0002	0.004	
13:	6	2	5	5	2	4	14293.3582	0.0000	0.004	
14:	5	2	4	4	2	3	11940.6855	-0.0092	0.004	
15:	3	3	0	2	2	1	10690.8416	0.0008	0.004	
16:	3	3	1	2	2	0	10668.9841	-0.0005	0.004	
17:	3	1	2	2	1	1	7382.7910	0.0005	0.004	
18:	3	1	3	2	0	2	7486.0194	0.0000	0.004	
19:	6	1	5	5	1	4	14582.5863	0.0000	0.004	
20:	6	2	4	5	2	3	14751.1092	0.0016	0.004	
21:	4	2	2	3	2	1	9750.9746	0.0003	0.004	

PARAMETERS IN FIT (values truncated):

10000	A	/MHz	1895.75670 (47)	1
20000	B	/MHz	1266.94249 (62)	2
30000	C	/MHz	1130.08034 (51)	3
200	DelJ	/kHz	0.1035 (56)	4
1100	DelJK	/kHz	[-0.094170351]	5
2000	DelK	/kHz	[0.131145949]	6
40100	delJ	/kHz	0.0297 (52)	7
41000	delK	/kHz	[-0.032378873]	8

MICROWAVE AVG = 0.000036 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.002201 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 0.55014 0.55014

distinct frequency lines in fit: 21
distinct parameters of fit: 5

	upper state	lower state	overall
limits of quantum number 1:	3 6	2 5	2 6
limits of quantum number 2:	0 3	0 2	0 3
limits of quantum number 3:	0 6	0 5	0 6

frequency range: 7113 14751

Standard errors are obtained by multiplying the previous errors by: 0.630265

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

10000	A	/MHz	1895.75670 (29)	1
20000	B	/MHz	1266.94249 (39)	2
30000	C	/MHz	1130.08034 (32)	3
200	DelJ	/kHz	0.1035 (35)	4
1100	DelJK	/kHz	[-0.094170351]	5
2000	DelK	/kHz	[0.131145949]	6
40100	delJ	/kHz	0.0297 (32)	7
41000	delK	/kHz	[-0.032378873]	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DelJ	-delJ
A	1.0000				
B	0.2491	1.0000			
C	-0.0883	-0.3881	1.0000		
-DelJ	-0.2018	-0.5633	-0.4732	1.0000	
-delJ	-0.1704	-0.7946	0.7500	0.1234	1.0000

Mean value of |C.ij|, i.ne.j = 0.3802
Mean value of C.ij, i.ne.j = -0.1557

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

14:	-2.3	9:	0.5	20:	0.4	1:	0.4
11:	0.3	5:	0.3	7:	-0.2	4:	0.2
15:	0.2	2:	0.2	6:	0.2	17:	0.1
16:	-0.1	8:	0.1	21:	0.1	10:	-0.1
12:	-0.1	3:	0.0	19:	0.0	18:	0.0

13: 0.0

14:	5	2	4	4	2	3	11940.6855	-0.0092	0.004
9:	4	1	4	3	1	3	9279.2970	0.0019	0.004
20:	6	2	4	5	2	3	14751.1092	0.0016	0.004
1:	3	0	3	2	0	2	7113.7206	0.0015	0.004
11:	5	2	3	4	2	2	12253.1533	0.0011	0.004
5:	6	1	6	5	0	5	13998.0090	0.0011	0.004
7:	4	1	4	3	0	3	9651.5946	-0.0008	0.004
4:	5	1	5	4	0	4	11814.6616	0.0008	0.004
15:	3	3	0	2	2	1	10690.8416	0.0008	0.004
2:	5	0	5	4	0	4	11671.4818	0.0007	0.004

/ SPFIT output reformatted with PIFORM

Substitution (r_s) coordinates ($\text{\AA}$) for the carbon atoms of the β -pinene molecule, in the principal axis frame.

	a_s	b_s	c_s
C ₁	-0.1334(112)*i	-0.5592(27)	-0.8909(17)
C ₂	1.3738(11)	-0.4896(31)	-0.2374(63)
C ₃	1.6925(9)	0.8472(18)	0.3966(38)
C ₄	0.4235(36)	1.6591(9)	0.7853(19)
C ₅	-0.7888(19)	1.2019(13)	0.0444(338)*i
C ₆	1.0732(14)	0.3031(50)	0.1859(81)
C ₇	-0.3299(46)	0.8436(18)	-1.4639(10)
C ₈	-0.8581(18)	-0.9124(17)	1.5860(10)
C ₉	-2.4671(6)	-0.7129(21)	-0.2976(51)
C ₁₀	2.2318(7)	-1.5225(10)	-0.2202(68)

Substitution (r_s) coordinates ($\text{\AA}$) for the carbon atoms of the nopinone molecule, in the principal axis frame.

	a_s	b_s	c_s
C ₁	-0.1386(108)*i	-0.5690(26)	-0.8964(17)
C ₂	1.3449(11)	-0.4956(30)	-0.2214(68)
C ₃	1.6556(9)	0.8304(18)	0.4566(33)
C ₄	0.3999(38)	1.6916(9)	0.7593(20)
C ₅	-0.8070(19)	1.2099(12)	0.0249(603)*i
C ₆	-1.0895(14)	-0.2874(52)	0.1902(79)
C ₇	-0.3326(45)	0.8352(18)	-1.4752(10)
C ₈	-0.8591(18)	-0.8878(17)	1.5935(9)
C ₉	-2.4825(6)	-0.7110(21)	-0.2837(53)
O	2.1410(7)	-1.4177(11)	-0.2185(69)

B-pinene - r0

26								
1	0	0	0	0.000000	0.000000	0.000000	12.0000000	C2
2	1	0	0	1.525312	0.000000	0.000000	12.0000000	C3
3	2	1	0	1.548338	113.399623	0.000000	12.0000000	C4
4	3	2	1	1.540526	111.286429	-21.561477	12.0000000	C5
5	4	3	2	1.556118	110.784586	58.618319	12.0000000	C6
6	5	4	3	1.578251	85.688128	-82.715355	12.0000000	C1
7	1	6	5	1.340419	123.281985	118.818727	12.0000000	C10
8	4	3	2	1.555506	108.868128	-36.617617	12.0000000	C7
9	5	6	1	1.523637	118.016528	-38.628750	12.0000000	C8
10	5	6	1	1.536716	111.343446	-165.287629	12.0000000	C9
11	6	1	2	1.096000	112.465000	165.399000	1.0078250	
12	7	1	2	1.087000	121.363000	2.154000	1.0078250	
13	7	1	2	1.086000	120.935000	-177.440000	1.0078250	
14	2	1	6	1.097000	107.360000	-93.173000	1.0078250	
15	2	1	6	1.095000	110.311000	151.326000	1.0078250	
16	3	2	1	1.096000	109.189000	-144.470000	1.0078250	
17	3	2	1	1.095000	110.964000	98.082000	1.0078250	
18	4	3	2	1.097000	111.693000	-168.367000	1.0078250	
19	8	4	3	1.091000	112.810000	-163.048000	1.0078250	
20	8	4	3	1.094000	117.648000	-34.731000	1.0078250	
21	9	5	4	1.097000	110.177000	68.814000	1.0078250	
22	9	5	4	1.097000	109.894000	-172.427000	1.0078250	
23	9	5	4	1.092000	112.964000	-52.601000	1.0078250	
24	10	5	4	1.096000	110.129000	166.806000	1.0078250	
25	10	5	4	1.096000	109.933000	-74.373000	1.0078250	
26	10	5	4	1.093000	112.797000	46.078000	1.0078250	

|
|

|__ Generated by STRFIT from a run resulting in:

R(2, 1) =	1.525312 +	0.007504
R(3, 2) =	1.548338 +	0.006175
R(4, 3) =	1.540526 +	0.008055
R(5, 4) =	1.556118 +	0.008878
R(6, 5) =	1.578251 +	0.010469
R(7, 1) =	1.340419 +	0.005161
R(8, 4) =	1.555506 +	0.011980
R(9, 5) =	1.523637 +	0.012245
R(10, 5) =	1.536716 +	0.007444
A(3, 2, 1) =	113.399623 +	0.168232
A(4, 3, 2) =	111.286429 +	0.303109
A(5, 4, 3) =	110.784586 +	0.598261
A(6, 5, 4) =	85.688128 +	0.496775
A(7, 1, 6) =	123.281985 +	0.637301
A(8, 4, 3) =	108.868128 +	0.519362
A(9, 5, 6) =	118.016528 +	0.482016
A(10, 5, 6) =	111.343446 +	1.014873
D(4, 3, 2, 1) =	-21.561477 +	0.933595
D(5, 4, 3, 2) =	58.618319 +	0.880369
D(6, 5, 4, 3) =	-82.715355 +	0.769784
D(7, 1, 6, 5) =	118.818727 +	1.160437
D(8, 4, 3, 2) =	-36.617617 +	0.505926
D(9, 5, 6, 1) =	-38.628750 +	0.907390
D(10, 5, 6, 1) =	-165.287629 +	0.638968

Chi-squared = 0.0005695175
Deviation of fit = 0.007955

Ni	Axis	Iobs	Icalc	Io-c	Bobs	Bcalc	Bo-c
1	a	265.72476	265.71740	0.00736	1901.8890	1901.9417	-0.0526
1	b	390.65804	390.64602	0.01202	1293.6608	1293.7006	-0.0398
1	c	439.14263	439.13089	0.01174	1150.8311	1150.8619	-0.0308
2	a	266.01546	266.01624	-0.00078	1899.8107	1899.8051	0.0056
2	b	392.59731	392.59805	-0.00074	1287.2707	1287.2683	0.0024
2	c	441.26212	441.26256	-0.00044	1145.3034	1145.3023	0.0011
3	a	266.57774	266.57902	-0.00128	1895.8035	1895.7944	0.0091
3	b	393.68183	393.68304	-0.00121	1283.7245	1283.7205	0.0040
3	c	442.71562	442.71570	-0.00007	1141.5432	1141.5430	0.0002
4	a	269.07583	269.07698	-0.00115	1878.2029	1878.1949	0.0080
4	b	391.42177	391.42360	-0.00183	1291.1367	1291.1307	0.0060
4	c	442.09667	442.09683	-0.00016	1143.1414	1143.1410	0.0004
5	a	267.15452	267.15425	0.00027	1891.7105	1891.7124	-0.0019
5	b	391.28300	391.28203	0.00097	1291.5946	1291.5978	-0.0032
5	c	441.20118	441.20278	-0.00160	1145.4616	1145.4574	0.0042
6	a	265.84958	265.85388	-0.00431	1900.9961	1900.9653	0.0308
6	b	391.84040	391.84273	-0.00233	1289.7573	1289.7496	0.0077
6	c	440.38163	440.38003	0.00160	1147.5933	1147.5975	-0.0042
7	a	266.82696	266.82113	0.00583	1894.0328	1894.0742	-0.0414
7	b	391.42577	391.43392	-0.00815	1291.1235	1291.0966	0.0269
7	c	439.44148	439.44846	-0.00698	1150.0485	1150.0302	0.0183
8	a	267.99055	267.99026	0.00028	1885.8091	1885.8111	-0.0020
8	b	395.75515	395.75454	0.00061	1276.9992	1277.0012	-0.0020
8	c	446.41587	446.41768	-0.00181	1132.0812	1132.0766	0.0046
9	a	268.56603	268.56957	-0.00354	1881.7682	1881.7434	0.0248
9	b	392.86948	392.86930	0.00018	1286.3789	1286.3795	-0.0006
9	c	439.99332	439.99216	0.00116	1148.6061	1148.6091	-0.0030
10	a	269.04345	269.04660	-0.00315	1878.4290	1878.4070	0.0220
10	b	393.85791	393.85937	-0.00146	1283.1506	1283.1458	0.0048
10	c	440.75991	440.76017	-0.00027	1146.6084	1146.6077	0.0007
11	a	266.29260	266.29199	0.00061	1897.8335	1897.8378	-0.0043

11	b	396.83113	396.82908	0.00205	1273.5367	1273.5433	-0.0066
11	c	445.71478	445.71797	-0.00319	1133.8619	1133.8538	0.0081

Correlation coefficients:

		1	2	3	4	5	6	7	8
1:	R(2, 1)	1.000							
2:	R(3, 2)	-0.478	1.000						
3:	R(4, 3)	0.100	-0.521	1.000					
4:	R(5, 4)	-0.115	0.095	-0.176	1.000				
5:	R(6, 5)	-0.017	-0.178	0.216	-0.131	1.000			
6:	R(7, 1)	-0.318	0.169	-0.232	0.090	0.043	1.000		
7:	R(8, 4)	0.022	0.262	-0.725	-0.099	-0.342	0.196	1.000	
8:	R(9, 5)	0.074	0.110	-0.198	-0.270	-0.658	0.091	0.257	1.000
9:	R(10, 5)	-0.106	-0.057	0.191	-0.213	0.616	-0.144	-0.177	-0.814
10:	A(3, 2, 1)	0.003	-0.456	0.320	-0.099	-0.002	-0.203	-0.040	-0.080
11:	A(4, 3, 2)	0.329	-0.367	-0.354	-0.012	-0.122	0.141	0.520	0.112
12:	A(5, 4, 3)	0.086	0.272	-0.750	-0.085	-0.484	0.244	0.792	0.653
13:	A(6, 5, 4)	0.066	0.128	-0.335	-0.492	-0.569	0.226	0.633	0.724
14:	A(7, 1, 6)	0.791	-0.097	-0.304	-0.104	-0.163	-0.189	0.464	0.133
15:	A(8, 4, 3)	-0.126	0.042	0.202	0.244	0.316	-0.005	-0.719	-0.118
16:	A(9, 5, 6)	-0.082	0.084	-0.163	0.706	-0.118	-0.122	0.102	-0.502
17:	A(10, 5, 6)	0.129	0.068	-0.195	0.259	-0.558	0.219	0.130	0.795
18:	D(4, 3, 2, 1)	0.329	-0.206	-0.296	-0.059	-0.099	0.447	0.368	0.148
19:	D(5, 4, 3, 2)	-0.150	0.017	0.540	-0.045	0.508	-0.259	-0.744	-0.493
20:	D(6, 5, 4, 3)	0.187	-0.002	-0.505	-0.010	-0.386	0.346	0.702	0.640
21:	D(7, 1, 6, 5)	-0.351	-0.095	0.486	-0.239	0.128	-0.531	-0.531	-0.082
22:	D(8, 4, 3, 2)	-0.148	0.174	0.307	0.119	0.129	-0.143	-0.425	-0.096
23:	D(9, 5, 6, 1)	0.130	0.094	-0.250	0.621	-0.363	-0.183	0.170	0.262
24:	D(10, 5, 6, 1)	0.257	-0.089	0.163	-0.564	-0.071	-0.484	-0.117	0.496
		9	10	11	12	13	14	15	16
9:	R(10, 5)	1.000							
10:	A(3, 2, 1)	0.091	1.000						
11:	A(4, 3, 2)	-0.126	-0.140	1.000					
12:	A(5, 4, 3)	-0.601	-0.094	0.416	1.000				
13:	A(6, 5, 4)	-0.405	0.000	0.322	0.682	1.000			
14:	A(7, 1, 6)	-0.106	0.074	0.332	0.431	0.275	1.000		
15:	A(8, 4, 3)	0.030	-0.064	-0.603	-0.428	-0.526	-0.350	1.000	
16:	A(9, 5, 6)	0.214	0.021	0.077	-0.127	-0.420	0.057	-0.125	1.000
17:	A(10, 5, 6)	-0.915	-0.147	0.114	0.562	0.371	0.107	0.074	-0.146
18:	D(4, 3, 2, 1)	-0.183	0.019	0.726	0.456	0.338	0.390	-0.412	-0.073
19:	D(5, 4, 3, 2)	0.496	-0.006	-0.741	-0.819	-0.612	-0.407	0.646	-0.108
20:	D(6, 5, 4, 3)	-0.630	-0.047	0.572	0.853	0.658	0.409	-0.462	-0.149
21:	D(7, 1, 6, 5)	0.231	0.001	-0.385	-0.529	-0.284	-0.611	0.266	-0.162
22:	D(8, 4, 3, 2)	0.098	-0.069	-0.701	-0.497	-0.272	-0.251	0.564	-0.085
23:	D(9, 5, 6, 1)	-0.572	-0.107	0.113	0.366	-0.162	0.231	-0.034	0.477
24:	D(10, 5, 6, 1)	-0.212	0.033	-0.077	0.109	0.176	0.223	0.080	-0.474
		17	18	19	20	21	22	23	24
17:	A(10, 5, 6)	1.000							
18:	D(4, 3, 2, 1)	0.202	1.000						
19:	D(5, 4, 3, 2)	-0.505	-0.716	1.000					
20:	D(6, 5, 4, 3)	0.682	0.537	-0.867	1.000				
21:	D(7, 1, 6, 5)	-0.302	-0.655	0.559	-0.603	1.000			
22:	D(8, 4, 3, 2)	-0.077	-0.813	0.751	-0.470	0.319	1.000		
23:	D(9, 5, 6, 1)	0.628	-0.062	-0.385	0.423	-0.203	-0.075	1.000	
24:	D(10, 5, 6, 1)	0.201	-0.200	0.034	0.065	0.385	0.076	0.109	1.000

ISOTOPIC SPECIES 2, changes from parent species:
atom no.,parameter no.,value 1 4 13.0033548

ISOTOPIC SPECIES 3, changes from parent species:
atom no.,parameter no.,value 2 4 13.0033548

ISOTOPIC SPECIES 4, changes from parent species:
atom no.,parameter no.,value 3 4 13.0033548

ISOTOPIC SPECIES 5, changes from parent species:
atom no.,parameter no.,value 4 4 13.0033548

ISOTOPIC SPECIES 6, changes from parent species:
atom no.,parameter no.,value 5 4 13.0033548

ISOTOPIC SPECIES 7, changes from parent species:
atom no.,parameter no.,value 6 4 13.0033548

ISOTOPIC SPECIES 8, changes from parent species:
atom no.,parameter no.,value 7 4 13.0033548

ISOTOPIC SPECIES 9, changes from parent species:
atom no.,parameter no.,value 8 4 13.0033548

ISOTOPIC SPECIES 10, changes from parent species:
atom no.,parameter no.,value 9 4 13.0033548

ISOTOPIC SPECIES 11, changes from parent species:
atom no.,parameter no.,value 10 4 13.0033548

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.

!
! B-pinene, r_0 coordinates
!

INPUT CARTESIANS:

2-C(1)	-1.37685	0.00236	-0.49349	0.00607	0.24655	0.01256
3-C(2)	-1.69491	0.00188	0.84940	0.00344	-0.40310	0.00740
4-C(3)	-0.43338	0.00526	1.66002	0.00183	-0.78885	0.00413
5-C(4)	0.79419	0.00378	1.20392	0.00247	0.02250	0.01134
6-C(5)	1.07617	0.00297	-0.30923	0.00905	-0.20629	0.01298
1-C(6)	-0.02949	0.00963	-0.55929	0.00521	0.89182	0.00342
10-C(7)	-2.23374	0.00138	-1.52405	0.00206	0.22609	0.00810
7-c(8)	0.33846	0.00792	0.84629	0.00331	1.46611	0.00213
8-C(9)	0.86241	0.00359	-0.91471	0.00336	-1.58802	0.00199
9-C(10)	2.46885	0.00124	-0.71717	0.00403	0.29922	0.00634

CALCULATED INTERNALS:

!
! Bond lengths
!

C(1)	C(2)	=	1.52531 + 0.00876
C(2)	C(3)	=	1.54834 + 0.00542
C(3)	C(4)	=	1.54053 + 0.00824
C(4)	C(5)	=	1.55611 + 0.00951
C(5)	C(6)	=	1.57825 + 0.01182
C(1)	C(7)	=	1.34042 + 0.00523
C(4)	c(8)	=	1.55551 + 0.01105
C(5)	C(9)	=	1.52364 + 0.01253
C(10)	C(5)	=	1.53672 + 0.00616
C(6)	C(10)	=	2.57251 + 0.00958
C(1)	C(6)	=	1.49535 + 0.01056
c(8)	C(6)	=	1.56232 + 0.00645

!
! Bond angles
!

C(3)	C(2)	C(1)	=	113.39975 + 0.22645	
C(4)	C(3)	C(2)	=	111.28609 + 0.35415	! comments can also be placed here
C(5)	C(4)	C(3)	=	110.78446 + 0.54198	
C(6)	C(5)	C(4)	=	85.68853 + 0.58032	
C(7)	C(1)	C(2)	=	122.48523 + 0.49383	
c(8)	C(4)	C(3)	=	108.86819 + 0.45474	
C(9)	C(5)	C(6)	=	118.01651 + 0.46167	
C(10)	C(5)	C(4)	=	111.96193 + 0.56883	
C(9)	C(5)	C(10)	=	108.66104 + 0.57240	
C(9)	C(5)	C(4)	=	119.62557 + 0.82906	
C(10)	C(5)	C(6)	=	111.34345 + 0.82146	
C(6)	c(8)	C(4)	=	86.25604 + 0.26029	
C(5)	C(4)	c(8)	=	88.05017 + 0.57648	
C(5)	C(6)	c(8)	=	87.03195 + 0.54952	
C(1)	C(6)	c(8)	=	109.34393 + 0.55729	
C(6)	C(1)	C(2)	=	114.23087 + 0.38983	
C(6)	C(1)	C(7)	=	123.28175 + 0.60889	
C(1)	C(6)	C(5)	=	108.90601 + 0.59176	

!
! dihedral angles
!

C(4)	C(3)	C(2)	C(1)	=	-21.56132 + 0.78260
C(7)	C(1)	C(2)	C(3)	=	-155.82564 + 0.77586
C(7)	C(1)	C(2)	C(6)	=	-179.48208 + 1.54790
c(8)	C(6)	C(5)	C(4)	=	-26.64258 + 0.54166
C(9)	C(5)	C(4)	C(3)	=	37.22016 + 0.74371

B-pinene r(l)m

26									
1	0	0	0	0.000000	0.000000	0.000000	12.0000000	C2	
2	1	0	0	1.513164	0.000000	0.000000	12.0000000	C3	
3	2	1	0	1.545948	113.381709	0.000000	12.0000000	C4	
4	3	2	1	1.530242	111.510167	-21.469623	12.0000000	C5	
5	4	3	2	1.546006	111.910288	57.131062	12.0000000	C6	
6	5	4	3	1.560767	86.553501	-81.019273	12.0000000	C1	
7	1	6	5	1.339495	123.201133	119.154197	12.0000000	C10	
8	4	3	2	1.563486	108.515655	-36.987628	12.0000000	C7	
9	5	6	1	1.537912	117.675486	-38.139736	12.0000000	C8	
10	5	6	1	1.526112	112.902156	-164.832388	12.0000000	C9	
11	6	1	2	1.092000	112.512000	166.091000	1.0078250		
12	7	1	2	1.082000	121.274000	2.256000	1.0078250		
13	7	1	2	1.082000	120.913000	-177.344000	1.0078250		
14	2	1	6	1.092000	107.200000	-92.222000	1.0078250		
15	2	1	6	1.091000	110.363000	152.423000	1.0078250		
16	3	2	1	1.092000	109.228000	-145.513000	1.0078250		
17	3	2	1	1.091000	110.851000	97.158000	1.0078250		
18	4	3	2	1.092000	111.842000	-168.059000	1.0078250		
19	8	4	3	1.086000	112.707000	-163.390000	1.0078250		
20	8	4	3	1.090000	117.672000	-35.075000	1.0078250		
21	9	5	4	1.093000	110.239000	68.702000	1.0078250		
22	9	5	4	1.092000	109.877000	-172.562000	1.0078250		
23	9	5	4	1.088000	112.955000	-52.800000	1.0078250		
24	10	5	4	1.092000	110.159000	166.756000	1.0078250		
25	10	5	4	1.092000	109.953000	-74.441000	1.0078250		
26	10	5	4	1.088000	112.760000	46.005000	1.0078250		

|
|

|__ Generated by STRFIT from a run resulting in:

R(2, 1) =	1.513164 +	0.009892
R(3, 2) =	1.545948 +	0.007217
R(4, 3) =	1.530242 +	0.012338
R(5, 4) =	1.546006 +	0.009627
R(6, 5) =	1.560767 +	0.015250
R(7, 1) =	1.339495 +	0.004885
R(8, 4) =	1.563486 +	0.012989
R(9, 5) =	1.537912 +	0.016302
R(10, 5) =	1.526112 +	0.009456
A(3, 2, 1) =	113.381709 +	0.189602
A(4, 3, 2) =	111.510167 +	0.357183
A(5, 4, 3) =	111.910288 +	0.908489
A(6, 5, 4) =	86.553501 +	0.755226
A(7, 1, 6) =	123.201133 +	0.619112
A(8, 4, 3) =	108.515655 +	0.544366
A(9, 5, 6) =	117.675486 +	0.570464
A(10, 5, 6) =	112.902156 +	1.482989
D(4, 3, 2, 1) =	-21.469623 +	0.927842
D(5, 4, 3, 2) =	57.131062 +	1.309901
D(6, 5, 4, 3) =	-81.019273 +	1.527345
D(7, 1, 6, 5) =	119.154197 +	1.133099
D(8, 4, 3, 2) =	-36.987628 +	0.537554
D(9, 5, 6, 1) =	-38.139736 +	0.916929
D(10, 5, 6, 1) =	-164.832388 +	0.707072
c_a =	0.137356 +	0.063172
c_b =	0.091508 +	0.056046
c_c =	0.081503 +	0.057913

Chi-squared = 0.0003340576
Deviation of fit = 0.007462

Ni	Axis	Iobs	Icalc	Io-c	Bobs	Bcalc	Bo-c
1	a	265.72476	265.72352	0.00124	1901.8890	1901.8979	-0.0089
1	b	390.65804	390.65065	0.00739	1293.6608	1293.6853	-0.0245
1	c	439.14263	439.13590	0.00674	1150.8311	1150.8488	-0.0177
2	a	266.01546	266.01754	-0.00208	1899.8107	1899.7959	0.0148
2	b	392.59731	392.59716	0.00015	1287.2707	1287.2712	-0.0005
2	c	441.26212	441.26245	-0.00033	1145.3034	1145.3025	0.0009
3	a	266.57774	266.57611	0.00163	1895.8035	1895.8151	-0.0116
3	b	393.68183	393.68214	-0.00031	1283.7245	1283.7235	0.0010
3	c	442.71562	442.71553	0.00009	1141.5432	1141.5434	-0.0002
4	a	269.07583	269.07517	0.00067	1878.2029	1878.2076	-0.0047
4	b	391.42177	391.42244	-0.00067	1291.1367	1291.1345	0.0022
4	c	442.09667	442.09650	0.00017	1143.1414	1143.1418	-0.0004
5	a	267.15452	267.15579	-0.00127	1891.7105	1891.7015	0.0090
5	b	391.28300	391.28491	-0.00191	1291.5946	1291.5883	0.0063
5	c	441.20118	441.19879	0.00239	1145.4616	1145.4678	-0.0062
6	a	265.84958	265.85134	-0.00176	1900.9961	1900.9835	0.0126
6	b	391.84040	391.83829	0.00211	1289.7573	1289.7642	-0.0069
6	c	440.38163	440.38348	-0.00185	1147.5933	1147.5885	0.0048
7	a	266.82696	266.82046	0.00650	1894.0328	1894.0789	-0.0461
7	b	391.42577	391.43282	-0.00705	1291.1235	1291.1002	0.0233
7	c	439.44148	439.45062	-0.00914	1150.0485	1150.0246	0.0239
8	a	267.99055	267.99332	-0.00277	1885.8091	1885.7896	0.0195
8	b	395.75515	395.75712	-0.00197	1276.9992	1276.9929	0.0063
8	c	446.41587	446.41406	0.00180	1132.0812	1132.0858	-0.0046
9	a	268.56603	268.56619	-0.00016	1881.7682	1881.7671	0.0011
9	b	392.86948	392.86955	-0.00007	1286.3789	1286.3787	0.0002
9	c	439.99332	439.99115	0.00217	1148.6061	1148.6118	-0.0057
10	a	269.04345	269.04420	-0.00075	1878.4290	1878.4237	0.0053

10	b	393.85791	393.85708	0.00083	1283.1506	1283.1533	-0.0027
10	c	440.75991	440.76065	-0.00075	1146.6084	1146.6065	0.0019
11	a	266.29260	266.29383	-0.00124	1897.8335	1897.8247	0.0088
11	b	396.83113	396.82963	0.00150	1273.5367	1273.5415	-0.0048
11	c	445.71478	445.71608	-0.00130	1133.8619	1133.8586	0.0033

Correlation coefficients:

		1	2	3	4	5	6	7	8
1:	R(2, 1)	1.000							
2:	R(3, 2)	-0.034	1.000						
3:	R(4, 3)	0.026	-0.597	1.000					
4:	R(5, 4)	0.266	0.225	-0.049	1.000				
5:	R(6, 5)	0.216	-0.272	0.611	0.125	1.000			
6:	R(7, 1)	-0.237	0.081	-0.035	0.089	0.106	1.000		
7:	R(8, 4)	-0.066	0.187	-0.628	-0.175	-0.435	0.125	1.000	
8:	R(9, 5)	-0.154	0.006	-0.370	-0.358	-0.658	0.020	0.489	1.000
9:	R(10, 5)	0.251	0.110	0.285	0.125	0.618	-0.072	-0.408	-0.884
10:	A(3, 2, 1)	-0.095	-0.619	0.517	-0.138	0.257	-0.106	-0.044	-0.031
11:	A(4, 3, 2)	-0.022	-0.504	-0.089	-0.186	-0.085	0.119	0.553	0.367
12:	A(5, 4, 3)	-0.221	0.067	-0.623	-0.302	-0.609	0.088	0.798	0.830
13:	A(6, 5, 4)	-0.213	-0.027	-0.431	-0.515	-0.611	0.081	0.714	0.858
14:	A(7, 1, 6)	0.640	0.025	-0.257	-0.017	-0.130	-0.179	0.389	0.060
15:	A(8, 4, 3)	0.093	0.156	0.190	0.339	0.326	0.008	-0.753	-0.352
16:	A(9, 5, 6)	0.074	0.194	0.026	0.624	0.088	-0.078	-0.204	-0.678
17:	A(10, 5, 6)	-0.263	-0.180	-0.204	-0.127	-0.516	0.122	0.383	0.866
18:	D(4, 3, 2, 1)	0.124	-0.279	-0.029	-0.097	0.000	0.457	0.264	0.074
19:	D(5, 4, 3, 2)	0.259	0.224	0.355	0.262	0.496	-0.142	-0.743	-0.723
20:	D(6, 5, 4, 3)	-0.279	-0.303	-0.206	-0.306	-0.334	0.154	0.647	0.757
21:	D(7, 1, 6, 5)	-0.327	-0.126	0.245	-0.289	0.013	-0.523	-0.373	0.054
22:	D(8, 4, 3, 2)	0.118	0.296	0.189	0.264	0.192	-0.123	-0.497	-0.323
23:	D(9, 5, 6, 1)	-0.067	-0.009	-0.231	0.377	-0.377	-0.189	0.285	0.417
24:	D(10, 5, 6, 1)	0.011	-0.128	-0.088	-0.578	-0.273	-0.437	0.144	0.661
25:	c_a	-0.696	-0.298	-0.055	-0.485	-0.387	0.001	0.143	0.306
26:	c_b	-0.158	0.384	-0.719	-0.153	-0.695	-0.115	0.190	0.231
27:	c_c	-0.278	0.278	-0.438	-0.171	-0.529	-0.054	-0.034	-0.032
		9	10	11	12	13	14	15	16
9:	R(10, 5)	1.000							
10:	A(3, 2, 1)	-0.019	1.000						
11:	A(4, 3, 2)	-0.407	0.151	1.000					
12:	A(5, 4, 3)	-0.791	-0.036	0.544	1.000				
13:	A(6, 5, 4)	-0.698	0.041	0.519	0.873	1.000			
14:	A(7, 1, 6)	-0.016	-0.010	0.180	0.218	0.121	1.000		
15:	A(8, 4, 3)	0.309	-0.143	-0.678	-0.559	-0.621	-0.266	1.000	
16:	A(9, 5, 6)	0.506	-0.115	-0.288	-0.503	-0.654	0.094	0.163	1.000
17:	A(10, 5, 6)	-0.947	0.068	0.464	0.776	0.700	-0.008	-0.279	-0.509
18:	D(4, 3, 2, 1)	-0.140	0.126	0.603	0.234	0.170	0.363	-0.371	-0.047
19:	D(5, 4, 3, 2)	0.748	-0.153	-0.794	-0.889	-0.812	-0.187	0.712	0.383
20:	D(6, 5, 4, 3)	-0.785	0.224	0.730	0.860	0.815	0.097	-0.586	-0.569
21:	D(7, 1, 6, 5)	0.041	0.019	-0.201	-0.175	-0.027	-0.629	0.158	-0.224
22:	D(8, 4, 3, 2)	0.353	-0.185	-0.757	-0.576	-0.458	-0.169	0.649	0.186
23:	D(9, 5, 6, 1)	-0.630	-0.040	0.259	0.471	0.164	0.172	-0.177	0.146
24:	D(10, 5, 6, 1)	-0.474	0.055	0.182	0.452	0.489	0.143	-0.138	-0.619
25:	c_a	-0.455	0.103	0.284	0.408	0.380	-0.111	-0.254	-0.180
26:	c_b	-0.194	-0.465	-0.187	0.313	0.256	0.074	-0.037	0.027
27:	c_c	-0.010	-0.397	-0.304	0.019	-0.041	0.063	0.088	0.266
		17	18	19	20	21	22	23	24
17:	A(10, 5, 6)	1.000							
18:	D(4, 3, 2, 1)	0.159	1.000						
19:	D(5, 4, 3, 2)	-0.784	-0.476	1.000					
20:	D(6, 5, 4, 3)	0.860	0.298	-0.928	1.000				
21:	D(7, 1, 6, 5)	-0.061	-0.630	0.220	-0.134	1.000			
22:	D(8, 4, 3, 2)	-0.373	-0.734	0.771	-0.595	0.202	1.000		
23:	D(9, 5, 6, 1)	0.652	-0.054	-0.496	0.484	-0.117	-0.211	1.000	
24:	D(10, 5, 6, 1)	0.481	-0.179	-0.347	0.428	0.410	-0.136	0.265	1.000
25:	c_a	0.473	0.136	-0.484	0.491	0.118	-0.305	0.226	0.229
26:	c_b	0.081	-0.121	-0.098	-0.049	0.039	0.005	0.079	0.130
27:	c_c	-0.106	-0.009	0.099	-0.266	-0.028	0.091	-0.016	-0.056
		25	26	27					
25:	c_a	1.000							
26:	c_b	0.321	1.000						
27:	c_c	0.461	0.842	1.000					

ISOTOPIC SPECIES 2, changes from parent species:
atom no.,parameter no.,value 1 4 13.0033544

ISOTOPIC SPECIES 3, changes from parent species:
atom no.,parameter no.,value 2 4 13.0033544

ISOTOPIC SPECIES 4, changes from parent species:
atom no.,parameter no.,value 3 4 13.0033544

ISOTOPIC SPECIES 5, changes from parent species:
atom no.,parameter no.,value 4 4 13.0033544

ISOTOPIC SPECIES 6, changes from parent species:
atom no.,parameter no.,value 5 4 13.0033544

ISOTOPIC SPECIES 7, changes from parent species:
atom no.,parameter no.,value 6 4 13.0033544

ISOTOPIC SPECIES 8, changes from parent species:
atom no.,parameter no.,value 7 4 13.0033544

ISOTOPIC SPECIES 9, changes from parent species:
atom no.,parameter no.,value 8 4 13.0033544

ISOTOPIC SPECIES 10, changes from parent species:
atom no.,parameter no.,value 9 4 13.0033544

ISOTOPIC SPECIES 11, changes from parent species:
atom no.,parameter no.,value 10 4 13.0033544

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.

!
! B-pinene, r_m^1 coordinates
!

INPUT CARTESIANS:

2-C(1)	-1.37448	0.00328	-0.49076	0.00632	0.23935	0.01274
3-C(2)	-1.69323	0.00308	0.84573	0.00487	-0.39458	0.00897
4-C(3)	-0.43531	0.00940	1.65639	0.00293	-0.78244	0.00522
5-C(4)	0.79248	0.00504	1.19963	0.00354	0.00846	0.01419
6-C(5)	1.07466	0.00395	-0.30815	0.00850	-0.18418	0.01914
1-C(6)	-0.03270	0.01277	-0.55610	0.00539	0.88738	0.00386
10-C(7)	-2.23127	0.00287	-1.52024	0.00314	0.22140	0.00843
7-c(8)	0.34157	0.01233	0.84086	0.00507	1.46189	0.00275
8-C(9)	0.86263	0.00577	-0.91074	0.00419	-1.58314	0.00286
9-C(10)	2.46575	0.00284	-0.71416	0.00429	0.29440	0.00721

CALCULATED INTERNALS:

!
! Bond lengths
!

C(1)	C(2)	=	1.51317 + 0.00965
C(2)	C(3)	=	1.54595 + 0.00897
C(3)	C(4)	=	1.53024 + 0.01167
C(4)	C(5)	=	1.54601 + 0.00953
C(5)	C(6)	=	1.56076 + 0.01650
C(1)	C(7)	=	1.33949 + 0.00610
C(4)	c(8)	=	1.56349 + 0.01405
C(5)	C(9)	=	1.53791 + 0.01802
C(10)	C(5)	=	1.52611 + 0.00820
C(6)	C(10)	=	2.57271 + 0.01285
C(1)	C(6)	=	1.49150 + 0.01320
c(8)	C(6)	=	1.55616 + 0.00809

!
! Bond angles
!

C(3)	C(2)	C(1)	=	113.38163 + 0.34619	
C(4)	C(3)	C(2)	=	111.51054 + 0.45628	! comments can also be placed here
C(5)	C(4)	C(3)	=	111.91031 + 0.71743	
C(6)	C(5)	C(4)	=	86.55377 + 0.74396	
C(7)	C(1)	C(2)	=	122.57944 + 0.53476	
c(8)	C(4)	C(3)	=	108.51550 + 0.65110	
C(9)	C(5)	C(6)	=	117.67580 + 0.55732	
C(10)	C(5)	C(4)	=	112.75318 + 0.67994	
C(9)	C(5)	C(10)	=	107.85993 + 0.74571	
C(9)	C(5)	C(4)	=	118.05502 + 1.11711	
C(10)	C(5)	C(6)	=	112.90234 + 1.17219	
C(6)	c(8)	C(4)	=	86.10999 + 0.33371	
C(5)	C(4)	c(8)	=	86.82872 + 0.81953	
C(5)	C(6)	c(8)	=	86.57251 + 0.69583	
C(1)	C(6)	c(8)	=	109.72111 + 0.70763	
C(6)	C(1)	C(2)	=	114.21867 + 0.43376	
C(6)	C(1)	C(7)	=	123.20121 + 0.64035	
C(1)	C(6)	C(5)	=	109.45217 + 0.71912	

!
! dihedral angles
!

C(4)	C(3)	C(2)	C(1)	=	-21.46915 + 0.92725
C(7)	C(1)	C(2)	C(3)	=	-155.97132 + 0.82839
C(7)	C(1)	C(2)	C(6)	=	179.71076 + 1.60943
c(8)	C(6)	C(5)	C(4)	=	-27.82516 + 0.75790
C(9)	C(5)	C(4)	C(3)	=	38.66213 + 1.00245

NOPINONE r0

24									
1	0	0	0	0.000000	0.000000	0.000000	12.0000000	C2	
2	1	0	0	1.534537	0.000000	0.000000	12.0000000	C3	
3	2	1	0	1.546399	114.067535	0.000000	12.0000000	C4	
4	3	2	1	1.542437	111.337059	-16.104284	12.0000000	C5	
5	4	3	2	1.553474	111.068969	55.468082	12.0000000	C6	
6	1	2	3	1.501171	114.934004	18.845337	12.0000000	C1	
7	4	3	2	1.551058	108.651479	-40.124462	12.0000000	C7	
8	5	6	1	1.527915	117.620100	-38.655914	12.0000000	C8	
9	5	4	3	1.534558	112.139832	165.336741	12.0000000	C9	
10	6	1	2	1.094200	111.205100	168.514800	1.0078250		
11	2	1	6	1.097700	105.297900	-98.940700	1.0078250		
12	2	1	6	1.093800	108.035300	147.751500	1.0078250		
13	3	2	1	1.096000	109.657700	-138.975900	1.0078250		
14	3	2	1	1.095500	110.422200	103.495300	1.0078250		
15	4	3	2	1.096510	111.611600	-171.885200	1.0078250		
16	7	4	3	1.090800	113.131300	-162.141500	1.0078250		
17	7	4	3	1.095100	117.409300	-33.804600	1.0078250		
18	8	5	4	1.096900	110.072500	70.069800	1.0078250		
19	8	5	4	1.096400	109.906800	-171.182100	1.0078250		
20	8	5	4	1.093400	113.320100	-50.942000	1.0078250		
21	9	5	4	1.096100	110.196600	166.693900	1.0078250		
22	9	5	4	1.096700	109.716600	-74.430100	1.0078250		
23	9	5	4	1.093300	112.685200	45.878100	1.0078250		
24	1	2	3	1.214172	121.433562	-160.657410	15.9949140	O	

|
|
|__ Generated by STRFIT from a run resulting in:

```

R( 2, 1) =      1.534537 +    0.007382
R( 3, 2) =      1.546399 +    0.005921
R( 4, 3) =      1.542437 +    0.007310
R( 5, 4) =      1.553474 +    0.009056
R( 6, 1) =      1.501171 +    0.010641
R( 7, 4) =      1.551058 +    0.010432
R( 8, 5) =      1.527915 +    0.012165
R( 9, 5) =      1.534558 +    0.007249
R(24, 1) =      1.214172 +    0.004479
A( 3, 2, 1) =    114.067535 +    0.177188
A( 4, 3, 2) =    111.337059 +    0.278871
A( 5, 4, 3) =    111.068969 +    0.534416
A( 6, 1, 2) =    114.934004 +    0.382291
A( 7, 4, 3) =    108.651479 +    0.501082
A( 8, 5, 6) =    117.620100 +    0.480104
A( 9, 5, 4) =    112.139832 +    0.613535
A(24, 1, 2) =    121.433562 +    0.613314
D( 4, 3, 2, 1) =   -16.104284 +    0.916398
D( 5, 4, 3, 2) =    55.468082 +    0.836784
D( 6, 1, 2, 3) =    18.845337 +    1.086951
D( 7, 4, 3, 2) =   -40.124462 +    0.521272
D( 8, 5, 6, 1) =   -38.655914 +    0.892399
D( 9, 5, 4, 3) =    165.336741 +    0.818521
D(24, 1, 2, 3) =  -160.657410 +    0.909246

```

Chi-squared = 0.0005672109
Deviation of fit = 0.007939

Ni	Axis	Iobs	Icalc	Io-c	Bobs	Bcalc	Bo-c
1	a	262.79675	262.78940	0.00735	1923.0794	1923.1332	-0.0538
1	b	389.48056	389.46850	0.01206	1297.5719	1297.6120	-0.0402
1	c	434.16788	434.15596	0.01192	1164.0175	1164.0495	-0.0320
2	a	263.08632	263.08848	-0.00216	1920.9627	1920.9470	0.0158
2	b	391.33432	391.33510	-0.00078	1291.4252	1291.4227	0.0026
2	c	436.21510	436.21508	0.00002	1158.5546	1158.5547	-0.0001
3	a	263.67347	263.67413	-0.00065	1916.6851	1916.6803	0.0048
3	b	392.43020	392.43082	-0.00062	1287.8189	1287.8168	0.0021
3	c	437.59149	437.59164	-0.00016	1154.9105	1154.9101	0.0004
4	a	266.21709	266.21890	-0.00182	1898.3718	1898.3589	0.0129
4	b	390.18304	390.18356	-0.00052	1295.2357	1295.2340	0.0017
4	c	437.21278	437.21210	0.00068	1155.9109	1155.9127	-0.0018
5	a	264.24667	264.24628	0.00040	1912.5274	1912.5303	-0.0029
5	b	390.13613	390.13593	0.00020	1295.3915	1295.3921	-0.0007
5	c	436.27457	436.27602	-0.00144	1158.3967	1158.3928	0.0038
6	a	262.91402	262.91766	-0.00364	1922.2216	1922.1950	0.0266
6	b	390.69958	390.70103	-0.00145	1293.5233	1293.5185	0.0048
6	c	435.43276	435.43236	0.00039	1160.6362	1160.6372	-0.0010
7	a	263.91986	263.91399	0.00588	1914.8957	1914.9383	-0.0426
7	b	390.25600	390.26417	-0.00817	1294.9936	1294.9665	0.0271
7	c	434.47698	434.48489	-0.00791	1163.1894	1163.1682	0.0212
8	a	265.65716	265.65942	-0.00226	1902.3730	1902.3568	0.0162
8	b	391.72430	391.72495	-0.00065	1290.1396	1290.1374	0.0022
8	c	435.00907	435.00836	0.00071	1161.7666	1161.7685	-0.0019
9	a	266.09572	266.09798	-0.00226	1899.2377	1899.2215	0.0161
9	b	392.70411	392.70556	-0.00146	1286.9206	1286.9158	0.0048
9	c	435.74492	435.74592	-0.00100	1159.8047	1159.8020	0.0027
10	a	263.35425	263.35363	0.00062	1919.0084	1919.0129	-0.0045
10	b	395.72201	395.71978	0.00223	1277.1061	1277.1133	-0.0072
10	c	440.81374	440.81719	-0.00345	1146.4684	1146.4594	0.0090
11	a	266.58432	266.58565	-0.00133	1895.7567	1895.7472	0.0095
11	b	398.89657	398.89733	-0.00076	1266.9425	1266.9401	0.0024
11	c	447.20627	447.20603	0.00024	1130.0803	1130.0809	-0.0006

Correlation coefficients:

		1	2	3	4	5	6	7	8
1:	R(2, 1)	1.000							
2:	R(3, 2)	-0.548	1.000						
3:	R(4, 3)	0.186	-0.503	1.000					
4:	R(5, 4)	-0.130	0.106	-0.213	1.000				
5:	R(6, 1)	-0.419	0.194	-0.016	-0.089	1.000			
6:	R(7, 4)	-0.019	0.203	-0.672	-0.081	0.132	1.000		
7:	R(8, 5)	0.026	0.095	-0.139	-0.291	0.019	0.202	1.000	
8:	R(9, 5)	-0.047	-0.058	0.153	-0.228	0.067	-0.128	-0.796	1.000
9:	R(24, 1)	-0.301	0.231	-0.211	0.158	-0.491	0.084	0.023	-0.086
10:	A(3, 2, 1)	-0.058	-0.417	0.374	-0.094	0.279	-0.073	-0.083	0.109
11:	A(4, 3, 2)	0.336	-0.373	-0.340	0.000	-0.110	0.519	0.057	-0.067
12:	A(5, 4, 3)	0.025	0.231	-0.701	-0.072	-0.037	0.737	0.654	-0.607
13:	A(6, 1, 2)	-0.341	0.221	-0.057	0.057	-0.346	-0.149	-0.008	-0.017
14:	A(7, 4, 3)	-0.119	0.064	0.146	0.229	-0.274	-0.722	-0.073	-0.013
15:	A(8, 5, 6)	-0.069	0.104	-0.218	0.738	0.182	0.153	-0.496	0.162
16:	A(9, 5, 4)	0.080	0.078	-0.136	-0.641	-0.037	0.102	0.791	-0.447
17:	A(24, 1, 2)	-0.649	0.087	0.203	0.085	0.577	-0.300	-0.047	0.029
18:	D(4, 3, 2, 1)	0.354	-0.193	-0.279	-0.053	-0.367	0.358	0.061	-0.077
19:	D(5, 4, 3, 2)	-0.132	0.062	0.486	-0.058	0.055	-0.716	-0.441	0.451
20:	D(6, 1, 2, 3)	-0.380	0.160	0.091	0.029	0.390	-0.079	-0.017	0.033
21:	D(7, 4, 3, 2)	-0.167	0.165	0.317	0.119	0.065	-0.463	-0.053	0.046
22:	D(8, 5, 6, 1)	0.078	0.075	-0.246	0.624	-0.076	0.167	0.251	-0.595
23:	D(9, 5, 4, 3)	0.028	-0.169	-0.093	-0.184	0.042	0.309	-0.714	0.787
24:	D(24, 1, 2, 3)	0.292	0.124	-0.268	0.021	-0.549	0.307	0.035	-0.039

		9	10	11	12	13	14	15	16
9:	R(24, 1)	1.000							
10:	A(3, 2, 1)	-0.393	1.000						
11:	A(4, 3, 2)	0.068	-0.290	1.000					
12:	A(5, 4, 3)	0.133	-0.159	0.374	1.000				
13:	A(6, 1, 2)	0.860	-0.435	0.005	-0.052	1.000			
14:	A(7, 4, 3)	0.111	-0.016	-0.584	-0.380	0.189	1.000		
15:	A(8, 5, 6)	-0.103	0.034	0.109	-0.088	-0.229	-0.148	1.000	
16:	A(9, 5, 4)	-0.049	-0.049	-0.008	0.496	-0.016	0.072	-0.770	1.000
17:	A(24, 1, 2)	-0.319	0.256	-0.329	-0.290	-0.213	0.209	0.071	-0.135
18:	D(4, 3, 2, 1)	0.393	-0.216	0.699	0.404	0.351	-0.401	-0.015	0.070
19:	D(5, 4, 3, 2)	-0.156	0.117	-0.729	-0.792	-0.003	0.630	-0.165	-0.181
20:	D(6, 1, 2, 3)	-0.467	0.212	-0.449	-0.138	-0.507	0.157	0.133	-0.048
21:	D(7, 4, 3, 2)	-0.096	0.095	-0.688	-0.511	-0.093	0.576	-0.110	-0.040
22:	D(8, 5, 6, 1)	-0.192	-0.048	0.104	0.396	-0.425	-0.033	0.503	-0.127
23:	D(9, 5, 4, 3)	-0.047	0.129	0.326	-0.219	-0.088	-0.407	0.191	-0.410
24:	D(24, 1, 2, 3)	0.534	-0.102	0.013	0.249	0.303	-0.018	-0.055	0.046

		17	18	19	20	21	22	23	24
17:	A(24, 1, 2)	1.000							
18:	D(4, 3, 2, 1)	-0.668	1.000						
19:	D(5, 4, 3, 2)	0.353	-0.700	1.000					
20:	D(6, 1, 2, 3)	0.708	-0.881	0.389	1.000				
21:	D(7, 4, 3, 2)	0.333	-0.827	0.779	0.531	1.000			
22:	D(8, 5, 6, 1)	0.112	-0.094	-0.390	0.308	-0.062	1.000		
23:	D(9, 5, 4, 3)	-0.146	0.215	0.027	-0.078	-0.313	-0.410	1.000	
24:	D(24, 1, 2, 3)	-0.747	0.340	-0.125	-0.469	0.049	-0.121	0.060	1.000

ISOTOPIC SPECIES 2, changes from parent species:
atom no.,parameter no.,value 1 4 13.0033548

ISOTOPIC SPECIES 3, changes from parent species:
atom no.,parameter no.,value 2 4 13.0033548

ISOTOPIC SPECIES 4, changes from parent species:
atom no.,parameter no.,value 3 4 13.0033548

ISOTOPIC SPECIES 5, changes from parent species:
atom no.,parameter no.,value 4 4 13.0033548

ISOTOPIC SPECIES 6, changes from parent species:
atom no.,parameter no.,value 5 4 13.0033548

ISOTOPIC SPECIES 7, changes from parent species:
atom no.,parameter no.,value 6 4 13.0033548

ISOTOPIC SPECIES 8, changes from parent species:
atom no.,parameter no.,value 7 4 13.0033548

ISOTOPIC SPECIES 9, changes from parent species:
atom no.,parameter no.,value 8 4 13.0033548

ISOTOPIC SPECIES 10, changes from parent species:
atom no.,parameter no.,value 9 4 13.0033548

ISOTOPIC SPECIES 11, changes from parent species:
atom no.,parameter no.,value 24 4 17.9991604

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.

!
! Nopinone, r_0 coordinates
!

INPUT CARTESIANS:

2-C(1)	-1.34770	0.00234	-0.49999	0.00578	0.23312	0.01145
3-C(2)	-1.65809	0.00191	0.83266	0.00351	-0.46151	0.00654
4-C(3)	-0.40875	0.00520	1.69267	0.00177	-0.76301	0.00423
5-C(4)	0.81254	0.00368	1.21162	0.00244	0.04702	0.00959
6-C(5)	1.09264	0.00290	-0.29518	0.00927	-0.20672	0.01269
1-C(6)	-0.00311	0.00904	-0.56950	0.00505	0.89702	0.00339
7-C(7)	0.34307	0.00779	0.83744	0.00329	1.47718	0.00210
8-C(8)	0.86385	0.00354	-0.89020	0.00340	-1.59529	0.00196
9-C(9)	2.48427	0.00121	-0.71549	0.00402	0.28479	0.00616
O	-2.14188	0.00079	-1.41837	0.00127	0.22491	0.00659

CALCULATED INTERNALS:

!
! Bond lengths
!

C(1)	C(2)	=	1.53454 + 0.00840
C(2)	C(3)	=	1.54641 + 0.00521
C(3)	C(4)	=	1.54244 + 0.00753
C(4)	C(5)	=	1.55348 + 0.00969
C(5)	C(6)	=	1.57929 + 0.01144
C(6)	C(7)	=	1.56074 + 0.00622
C(6)	C(5)	=	1.57929 + 0.01144

!
! Bond angles
!

C(7)	C(4)	C(5)	=	88.34887 + 0.53947
C(4)	C(5)	C(6)	=	85.94153 + 0.55923
C(5)	C(6)	C(7)	=	87.09469 + 0.53589
C(5)	C(6)	C(1)	=	107.71765 + 0.55339
O	C(1)	C(2)	=	121.43350 + 0.48653
O	C(1)	C(6)	=	123.63039 + 0.60538
C(1)	C(6)	C(7)	=	108.74301 + 0.53210
C(8)	C(5)	C(4)	=	119.94537 + 0.78959
C(9)	C(5)	C(6)	=	110.96375 + 0.79869
C(4)	C(7)	C(6)	=	86.66678 + 0.24968
C(8)	C(5)	C(9)	=	108.67576 + 0.57317

! comments can also be placed here

!
! dihedral angles
!

O	C(1)	C(6)	C(5)	=	121.29047 + 0.94277
O	C(1)	C(2)	C(3)	=	-160.65782 + 0.72658
C(8)	C(5)	C(4)	C(3)	=	36.03907 + 0.68935
C(8)	C(5)	C(4)	C(7)	=	145.41462 + 0.46351
C(9)	C(5)	C(4)	C(7)	=	-85.28798 + 0.75106
C(3)	C(4)	C(7)	C(6)	=	85.68913 + 0.45238
O	C(1)	C(2)	C(6)	=	-179.50374 + 1.43525
C(8)	C(5)	C(6)	C(1)	=	-38.65597 + 0.76000

NOPINONE r(1)m

24										
1	0	0	0	0.000000	0.000000	0.000000	12.0000000	C2		
2	1	0	0	1.525052	0.000000	0.000000	12.0000000	C3		
3	2	1	0	1.544211	114.061028	0.000000	12.0000000	C4		
4	3	2	1	1.533442	111.516406	-15.771708	12.0000000	C5		
5	4	3	2	1.545037	112.020746	54.179826	12.0000000	C6		
6	1	2	3	1.497910	114.977589	19.058257	12.0000000	C1		
7	4	3	2	1.558886	108.315310	-40.483960	12.0000000	C7		
8	5	4	3	1.538746	118.638265	37.286906	12.0000000	C8		
9	5	4	3	1.526050	112.767242	165.006965	12.0000000	C9		
10	6	1	2	1.089500	111.340500	168.185500	1.0078250			
11	2	1	6	1.093400	105.146300	-97.537000	1.0078250			
12	2	1	6	1.089200	108.112000	149.174100	1.0078250			
13	3	2	1	1.091400	109.693600	-140.188000	1.0078250			
14	3	2	1	1.091000	110.278600	102.441000	1.0078250			
15	4	3	2	1.091800	111.751000	-171.619400	1.0078250			
16	7	4	3	1.086400	112.995800	-162.471200	1.0078250			
17	7	4	3	1.090500	117.454200	-34.145700	1.0078250			
18	8	5	4	1.092400	110.119300	70.235400	1.0078250			
19	8	5	4	1.091900	109.875200	-171.026000	1.0078250			
20	8	5	4	1.089400	113.342000	-50.873000	1.0078250			
21	9	5	4	1.091500	110.209600	166.753400	1.0078250			
22	9	5	4	1.092200	109.719100	-74.397300	1.0078250			
23	9	5	4	1.089000	112.663000	45.908500	1.0078250			
24	1	6	7	1.215030	123.686162	-145.802779	15.9949140	O		

|
|
|__ Generated by STRFIT from a run resulting in:

```

R( 2, 1) =      1.525052 +    0.010567
R( 3, 2) =      1.544211 +    0.007684
R( 4, 3) =      1.533442 +    0.013226
R( 5, 4) =      1.545037 +    0.010903
R( 6, 1) =      1.497910 +    0.013135
R( 7, 4) =      1.558886 +    0.013359
R( 8, 5) =      1.538746 +    0.017667
R( 9, 5) =      1.526050 +    0.010231
R(24, 1) =      1.215030 +    0.004785
A( 3, 2, 1) =    114.061028 +    0.216448
A( 4, 3, 2) =    111.516406 +    0.367881
A( 5, 4, 3) =    112.020746 +    0.991179
A( 6, 1, 2) =    114.977589 +    0.434255
A( 7, 4, 3) =    108.315310 +    0.597915
A( 8, 5, 4) =    118.638265 +    1.513527
A( 9, 5, 4) =    112.767242 +    0.868558
A(24, 1, 6) =    123.686162 +    0.681233
D( 4, 3, 2, 1) =   -15.771708 +    1.034233
D( 5, 4, 3, 2) =    54.179826 +    1.446595
D( 6, 1, 2, 3) =    19.058257 +    1.197257
D( 7, 4, 3, 2) =   -40.483960 +    0.629165
D( 8, 5, 4, 3) =    37.286906 +    1.408316
D( 9, 5, 4, 3) =    165.006965 +    0.970989
D(24, 1, 6, 7) =  -145.802779 +    1.245668
c_a =      0.115058 +    0.068392
c_b =      0.075951 +    0.058243
c_c =      0.072790 +    0.059418

```

Chi-squared = 0.0004063310
Deviation of fit = 0.008229

Ni	Axis	Iobs	Icalc	Io-c	Bobs	Bcalc	Bo-c
1	a	262.79675	262.79455	0.00220	1923.0794	1923.0955	-0.0161
1	b	389.48056	389.47253	0.00803	1297.5719	1297.5986	-0.0268
1	c	434.16788	434.16052	0.00736	1164.0175	1164.0372	-0.0197
2	a	263.08632	263.09044	-0.00412	1920.9627	1920.9326	0.0301
2	b	391.33432	391.33528	-0.00096	1291.4252	1291.4221	0.0032
2	c	436.21510	436.21386	0.00124	1158.5546	1158.5579	-0.0033
3	a	263.67347	263.67138	0.00209	1916.6851	1916.7003	-0.0152
3	b	392.43020	392.42996	0.00024	1287.8189	1287.8196	-0.0008
3	c	437.59149	437.59148	0.00000	1154.9105	1154.9105	0.0000
4	a	266.21709	266.21715	-0.00006	1898.3718	1898.3714	0.0004
4	b	390.18304	390.18288	0.00016	1295.2357	1295.2363	-0.0005
4	c	437.21278	437.21160	0.00118	1155.9109	1155.9140	-0.0031
5	a	264.24667	264.24671	-0.00004	1912.5274	1912.5271	0.0003
5	b	390.13613	390.13784	-0.00170	1295.3915	1295.3858	0.0057
5	c	436.27457	436.27294	0.00163	1158.3967	1158.4010	-0.0043
6	a	262.91402	262.91625	-0.00223	1922.2216	1922.2053	0.0163
6	b	390.69958	390.69706	0.00252	1293.5233	1293.5317	-0.0084
6	c	435.43276	435.43554	-0.00278	1160.6362	1160.6288	0.0074
7	a	263.91986	263.91345	0.00641	1914.8957	1914.9422	-0.0465
7	b	390.25600	390.26355	-0.00754	1294.9936	1294.9685	0.0250
7	c	434.47698	434.48656	-0.00958	1163.1894	1163.1637	0.0256
8	a	265.65716	265.65689	0.00027	1902.3730	1902.3749	-0.0020
8	b	391.72430	391.72523	-0.00094	1290.1396	1290.1365	0.0031
8	c	435.00907	435.00662	0.00245	1161.7666	1161.7731	-0.0065
9	a	266.09572	266.09608	-0.00036	1899.2377	1899.2351	0.0026
9	b	392.70411	392.70391	0.00020	1286.9206	1286.9213	-0.0006
9	c	435.74492	435.74648	-0.00156	1159.8047	1159.8006	0.0042
10	a	263.35425	263.35529	-0.00104	1919.0084	1919.0008	0.0076
10	b	395.72201	395.71965	0.00236	1277.1061	1277.1138	-0.0076
10	c	440.81374	440.81615	-0.00240	1146.4684	1146.4621	0.0062

11	a	266.58432	266.58743	-0.00311	1895.7567	1895.7346	0.0221
11	b	398.89657	398.89891	-0.00234	1266.9425	1266.9350	0.0074
11	c	447.20627	447.20382	0.00245	1130.0803	1130.0865	-0.0062

Correlation coefficients:

		1	2	3	4	5	6	7	8
1:	R(2, 1)	1.000							
2:	R(3, 2)	-0.080	1.000						
3:	R(4, 3)	0.051	-0.562	1.000					
4:	R(5, 4)	0.238	0.250	-0.044	1.000				
5:	R(6, 1)	-0.161	0.377	-0.112	0.075	1.000			
6:	R(7, 4)	-0.085	0.117	-0.625	-0.211	-0.091	1.000		
7:	R(8, 5)	-0.130	-0.006	-0.379	-0.389	-0.211	0.506	1.000	
8:	R(9, 5)	0.239	0.118	0.301	0.137	0.288	-0.435	-0.874	1.000
9:	R(24, 1)	-0.348	0.079	-0.081	0.035	-0.472	0.101	0.075	-0.155
10:	A(3, 2, 1)	-0.129	-0.581	0.489	-0.159	-0.039	-0.030	-0.004	-0.033
11:	A(4, 3, 2)	0.022	-0.507	-0.109	-0.204	-0.398	0.581	0.346	-0.386
12:	A(5, 4, 3)	-0.208	0.021	-0.627	-0.328	-0.285	0.805	0.828	-0.798
13:	A(6, 1, 2)	-0.398	-0.053	0.213	-0.054	-0.372	-0.170	-0.039	-0.046
14:	A(7, 4, 3)	0.094	0.195	0.183	0.363	0.018	-0.764	-0.348	0.316
15:	A(8, 5, 4)	0.231	0.004	0.515	0.077	0.303	-0.685	-0.837	0.908
16:	A(9, 5, 4)	-0.117	-0.029	-0.371	-0.641	-0.251	0.446	0.875	-0.679
17:	A(24, 1, 6)	0.627	-0.094	-0.222	-0.083	-0.274	0.373	0.107	-0.057
18:	D(4, 3, 2, 1)	0.050	-0.348	-0.022	-0.183	-0.438	0.324	0.133	-0.200
19:	D(5, 4, 3, 2)	0.235	0.267	0.353	0.294	0.364	-0.760	-0.699	0.735
20:	D(6, 1, 2, 3)	-0.256	0.122	-0.097	-0.031	0.221	0.108	0.173	-0.139
21:	D(7, 4, 3, 2)	0.101	0.315	0.193	0.295	0.281	-0.548	-0.312	0.346
22:	D(8, 5, 4, 3)	-0.281	-0.319	-0.254	-0.225	-0.421	0.729	0.612	-0.683
23:	D(9, 5, 4, 3)	0.106	-0.210	0.236	-0.038	0.010	0.069	-0.687	0.705
24:	D(24, 1, 6, 7)	-0.181	0.218	-0.004	0.040	0.769	-0.245	-0.161	0.201
25:	c_a	-0.677	-0.317	-0.078	-0.488	-0.173	0.204	0.308	-0.465
26:	c_b	-0.177	0.357	-0.740	-0.160	0.230	0.251	0.265	-0.233
27:	c_c	-0.347	0.238	-0.423	-0.174	0.332	-0.018	-0.007	-0.045

		9	10	11	12	13	14	15	16
9:	R(24, 1)	1.000							
10:	A(3, 2, 1)	-0.265	1.000						
11:	A(4, 3, 2)	0.137	0.054	1.000					
12:	A(5, 4, 3)	0.152	-0.021	0.542	1.000				
13:	A(6, 1, 2)	0.841	-0.183	0.110	-0.058	1.000			
14:	A(7, 4, 3)	0.024	-0.132	-0.682	-0.563	0.107	1.000		
15:	A(8, 5, 4)	-0.184	0.011	-0.493	-0.920	0.027	0.477	1.000	
16:	A(9, 5, 4)	0.024	0.027	0.315	0.764	-0.037	-0.263	-0.627	1.000
17:	A(24, 1, 6)	-0.219	-0.035	0.239	0.252	-0.417	-0.292	-0.180	0.167
18:	D(4, 3, 2, 1)	0.434	-0.017	0.685	0.328	0.428	-0.449	-0.252	0.143
19:	D(5, 4, 3, 2)	-0.208	-0.121	-0.794	-0.884	-0.075	0.725	0.859	-0.582
20:	D(6, 1, 2, 3)	-0.434	0.187	-0.206	0.151	-0.492	0.013	-0.175	0.153
21:	D(7, 4, 3, 2)	-0.165	-0.088	-0.763	-0.595	-0.158	0.678	0.467	-0.310
22:	D(8, 5, 4, 3)	0.199	0.216	0.753	0.816	0.060	-0.699	-0.843	0.469
23:	D(9, 5, 4, 3)	-0.054	0.209	0.204	-0.356	-0.005	-0.235	0.540	-0.468
24:	D(24, 1, 6, 7)	-0.617	-0.064	-0.400	-0.294	-0.499	0.132	0.283	-0.190
25:	c_a	0.199	0.121	0.295	0.441	0.214	-0.303	-0.436	0.333
26:	c_b	0.000	-0.407	-0.146	0.368	-0.212	-0.073	-0.300	0.269
27:	c_c	0.044	-0.363	-0.278	0.051	-0.063	0.064	-0.032	0.001

		17	18	19	20	21	22	23	24
17:	A(24, 1, 6)	1.000							
18:	D(4, 3, 2, 1)	0.349	1.000						
19:	D(5, 4, 3, 2)	-0.239	-0.597	1.000					
20:	D(6, 1, 2, 3)	-0.296	-0.770	0.042	1.000				
21:	D(7, 4, 3, 2)	-0.227	-0.815	0.799	0.338	1.000			
22:	D(8, 5, 4, 3)	0.208	0.462	-0.950	0.104	-0.676	1.000		
23:	D(9, 5, 4, 3)	0.119	0.190	0.180	-0.128	-0.180	-0.120	1.000	
24:	D(24, 1, 6, 7)	-0.384	-0.621	0.378	0.523	0.330	-0.404	-0.095	1.000
25:	c_a	-0.040	0.272	-0.516	0.036	-0.343	0.545	-0.177	-0.073
26:	c_b	0.114	-0.113	-0.142	0.082	-0.009	0.048	-0.350	0.249
27:	c_c	0.023	-0.054	0.063	-0.078	0.081	-0.137	-0.247	0.339

		25	26	27
25:	c_a	1.000		
26:	c_b	0.352	1.000	
27:	c_c	0.506	0.830	1.000

ISOTOPIC SPECIES 2, changes from parent species:
atom no.,parameter no.,value 1 4 13.0033548

ISOTOPIC SPECIES 3, changes from parent species:
atom no.,parameter no.,value 2 4 13.0033548

ISOTOPIC SPECIES 4, changes from parent species:
atom no.,parameter no.,value 3 4 13.0033548

ISOTOPIC SPECIES 5, changes from parent species:
atom no.,parameter no.,value 4 4 13.0033548

ISOTOPIC SPECIES 6, changes from parent species:
atom no.,parameter no.,value 5 4 13.0033548

ISOTOPIC SPECIES 7, changes from parent species:
atom no.,parameter no.,value 6 4 13.0033548

ISOTOPIC SPECIES 8, changes from parent species:
atom no.,parameter no.,value 7 4 13.0033548

ISOTOPIC SPECIES 9, changes from parent species:
atom no.,parameter no.,value 8 4 13.0033548

ISOTOPIC SPECIES 10, changes from parent species:
atom no.,parameter no.,value 9 4 13.0033548

ISOTOPIC SPECIES 11, changes from parent species:
atom no.,parameter no.,value 24 4 17.9991604

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.

!
! Nopinone, r_m coordinates
!

INPUT CARTESIANS:

2-C(1)	-1.34539	0.00352	-0.49683	0.00679	0.23057	0.01215
3-C(2)	-1.65662	0.00333	0.82925	0.00548	-0.45531	0.00885
4-C(3)	-0.41032	0.01026	1.68941	0.00318	-0.75770	0.00588
5-C(4)	0.81109	0.00536	1.20791	0.00388	0.03461	0.01475
6-C(5)	1.09106	0.00420	-0.29499	0.00962	-0.18915	0.02073
1-C(6)	-0.00396	0.01334	-0.56654	0.00588	0.89349	0.00418
7-C(7)	0.34451	0.01291	0.83255	0.00561	1.47389	0.00293
8-C(8)	0.86395	0.00610	-0.88671	0.00470	-1.59130	0.00313
9-C(9)	2.48153	0.00301	-0.71303	0.00477	0.28061	0.00778
O	-2.14021	0.00218	-1.41576	0.00250	0.21952	0.00865

CALCULATED INTERNALS:

!
! Bond lengths
!

C(1)	C(2)	=	1.52505 + 0.01021
C(2)	C(3)	=	1.54421 + 0.00962
C(3)	C(4)	=	1.53344 + 0.01244
C(4)	C(5)	=	1.54504 + 0.01081
C(5)	C(6)	=	1.56362 + 0.01772
C(6)	C(7)	=	1.55427 + 0.00863
C(6)	C(5)	=	1.56362 + 0.01772

!
! Bond angles
!

C(7)	C(4)	C(5)	=	87.34789 + 0.87274
C(4)	C(5)	C(6)	=	86.66093 + 0.81511
C(5)	C(6)	C(7)	=	86.85955 + 0.73943
C(5)	C(6)	C(1)	=	108.21841 + 0.73690
O	C(1)	C(2)	=	121.33492 + 0.57388
O	C(1)	C(6)	=	123.68633 + 0.69560
C(1)	C(6)	C(7)	=	108.91413 + 0.74583
C(8)	C(5)	C(4)	=	118.63848 + 1.19593
C(9)	C(5)	C(6)	=	112.17146 + 1.25495
C(4)	C(7)	C(6)	=	86.50733 + 0.36210
C(8)	C(5)	C(9)	=	108.03759 + 0.81947
C(8)	C(5)	C(6)	=	117.43765 + 0.60135

! comments can also be placed here

!
! dihedral angles
!

O	C(1)	C(6)	C(5)	=	121.22717 + 1.05074
O	C(1)	C(2)	C(3)	=	-160.55259 + 0.84928
C(8)	C(5)	C(4)	C(3)	=	37.28717 + 1.07297
C(8)	C(5)	C(4)	C(7)	=	145.98701 + 0.70852
C(9)	C(5)	C(4)	C(7)	=	-86.29313 + 1.22283
C(3)	C(4)	C(7)	C(6)	=	85.77997 + 0.70313
O	C(1)	C(2)	C(6)	=	-179.61125 + 1.58187
C(8)	C(5)	C(6)	C(1)	=	-38.29688 + 0.87838
C(6)	C(5)	C(4)	C(3)	=	-82.31958 + 1.09583