

Krzysztof Habdas and Zbigniew Kisiel,
"Electric Dipole Moments from Stark Effect in Supersonic Expansion:
n-propanol, n-butanol, and n-butyl cyanide"
Molecules 2023, 28, 1962. <https://doi.org/10.3390/molecules28041962>

- 1/ Electric dipole moment fit for the Aa conformer of n-propanol
- 2/ Electric dipole moment fit for the GTg conformer of n-butanol
- 3/ Electric dipole moment fit for the GTg' conformer of n-butanol
- 4/ Electric dipole moment fit for the AA conformer of n-propyl cyanide
- 5/ Electric dipole moment fit for the GA conformer of n-propyl cyanide
- 6/ Example Stark electrode distance calibration using CH3CN in Ne expansion
- 7/ Example Stark electrode distance calibration using CH3I in Ne expansion

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Zbigniew KISIEL

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41 Lines read in
41 Lines fitted    --->    4 field free and    37 at non-zero field
 2 Constants fitted

```

```
! 202 <- 101
```

9.	2	0	2	1	0	1	4	0	2	0	0.0	14701.08390	0.00055	14701.0834	0.0000	0.00
!																
10.	2	0	2	1	0	1	4	2	2	2	2991.3	14701.09890	0.00111	14701.0978	110.9944	12319.76
11.	2	0	2	1	0	1	4	2	2	2	4390.5	14701.11460	0.00014	14701.1145	162.9128	26540.58
12.	2	0	2	1	0	1	4	2	2	2	6232.3	14701.14510	-0.00094	14701.1460	231.2542	53478.49
13.	2	0	2	1	0	1	4	2	2	2	7641.1	14701.17630	-0.00128	14701.1776	283.5288	80388.56
14.	2	0	2	1	0	1	4	2	2	2	8778.3	14701.20630	-0.00142	14701.2077	325.7254	106097.05
15.	2	0	2	1	0	1	4	2	2	2	10003.9	14701.24360	-0.00127	14701.2449	371.2022	137791.09
16.	2	0	2	1	0	1	4	2	2	2	11349.8	14701.29470	0.00344	14701.2913	421.1429	177361.31
17.	2	0	2	1	0	1	4	2	2	2	12393.4	14701.33590	0.00465	14701.3313	459.8664	211477.12

!																
18.	2	0	2	1	0	1	4	0	2	0	2994.2	14701.03580	-0.00276	14701.0386	111.1020	12343.66
19.	2	0	2	1	0	1	4	0	2	0	4395.3	14700.98350	-0.00334	14700.9868	163.0909	26598.64
20.	2	0	2	1	0	1	4	0	2	0	6239.3	14700.88660	-0.00227	14700.8889	231.5139	53598.69
21.	2	0	2	1	0	1	4	0	2	0	7641.1	14700.78710	-0.00458	14700.7917	283.5288	80388.56
22.	2	0	2	1	0	1	4	0	2	0	8783.8	14700.69510	-0.00284	14700.6979	325.9295	106230.04
23.	2	0	2	1	0	1	4	0	2	0	10014.6	14700.57950	-0.00289	14700.5824	371.5993	138086.01
24.	2	0	2	1	0	1	4	0	2	0	11349.8	14700.43950	-0.00044	14700.4399	421.1429	177361.31
25.	2	0	2	1	0	1	4	0	2	0	12393.4	14700.31770	0.00147	14700.3162	459.8664	211477.12

!-----
! 212 <- 111
!-----
!

26.	2	1	2	1	1	1	4	0	2	0	0.0	14450.47530	-0.00103	14450.4763	0.0000	0.00
!																
27.	2	1	2	1	1	1	4	0	2	0	1628.4	14450.90260	0.00216	14450.9004	60.4230	3650.94
28.	2	1	2	1	1	1	4	0	2	0	2027.9	14451.13190	-0.00160	14451.1335	75.2468	5662.07
29.	2	1	2	1	1	1	4	0	2	0	2423.6	14451.41220	-0.00182	14451.4140	89.9295	8087.31
30.	2	1	2	1	1	1	4	0	2	0	2736.4	14451.67130	0.00075	14451.6706	101.5362	10309.60
31.	2	1	2	1	1	1	4	0	2	0	3030.3	14451.93740	-0.00201	14451.9394	112.4416	12643.10

!-----
! 211 <- 110
!-----
!

32.	2	1	1	1	1	0	4	0	2	0	0.0	14955.90970	-0.00154	14955.9112	0.0000	0.00
!																
33.	2	1	1	1	1	0	4	0	2	0	2224.7	14955.91930	0.00203	14955.9173	82.5492	6814.36
34.	2	1	1	1	1	0	4	0	2	0	3045.1	14955.92650	0.00396	14955.9225	112.9907	12766.90
35.	2	1	1	1	1	0	4	0	2	0	3646.7	14955.92770	0.00026	14955.9274	135.3135	18309.76
36.	2	1	1	1	1	0	4	0	2	0	4147.8	14955.93460	0.00240	14955.9322	153.9072	23687.44
37.	2	1	1	1	1	0	4	0	2	0	4546.5	14955.93300	-0.00342	14955.9364	168.7013	28460.13

!																
38.	2	1	1	1	1	0	4	2	2	2	2224.7	14955.68150	0.00038	14955.6811	82.5492	6814.36
39.	2	1	1	1	1	0	4	2	2	2	3045.1	14955.48480	0.00435	14955.4804	112.9907	12766.90
40.	2	1	1	1	1	0	4	2	2	2	3646.7	14955.29630	0.00244	14955.2939	135.3135	18309.76
41.	2	1	1	1	1	0	4	2	2	2	4546.5	14954.95090	-0.00196	14954.9529	168.7013	28460.13

Standard deviation = 0.002291

ITERATION NO = 3 CONSTANTS, deviations and changes:

Mu.a	=	0.358858474 +- 0.000303856	0.000000000
Mu.b	=	1.281948710 +- 0.000593686	0.000000000

FINAL RESULTS OF LEAST SQUARES FITTING PROCEDURE
=====

FITTED CONSTANTS:

A	/MHz	26401.4764974393	1:Xab /MHz	0.
B	/MHz	3802.15317891442	1:XJ.a/kHz	0.
C	/MHz	3549.45832788319	1:XK.a/kHz	0.
DJ	/kHz	0.97882481121886	1:XJbc/kHz	0.
DJK	/kHz	-0.65770733393743	1:Ma /MHz	0.
DK	/kHz	151.280382690001	1:Mb-c/MHz	0.
dJ	/kHz	0.12547510773005	1:Tr /MHz	0.
dK	/kHz	-6.31899120921345	1:Xd /kHz	0.
HJ	/ Hz	-0.0273188744555	1:Xbc /MHz	0.
HJK	/ Hz	0.	1:Xac /MHz	0.
HKJ	/ Hz	-132.685651099522		
HK	/ Hz	0.		
hJ	/ Hz	-0.0075759732997		
hJK	/ Hz	0.	Mu.a /D	0.35885 (30)
hK	/ Hz	336.244125489832	Mu.b /D	1.28194 (59)
LKKJ	/mHz	0.	Mu.c /D	0.
1:Xa	/MHz	0.	d /cm	26.95
1:Xb-c	/MHz	0.	k /cm	0.

	Mu.a	Mu.b
Mu.a	1.0000	
Mu.b	-0.2953	1.0000

	J	K	K	<-	J	K	K	F	MF<-	F	MF	Volts	Obs	Obs-Calc	Calc	Field	Field**2
	-1	+1			-1	+1											
17.	2	0	2		1	0	1	4	2	2	2	12393.4	14701.33590	0.00465	14701.3313	459.8664	211477.12
21.	2	0	2		1	0	1	4	0	2	0	7641.1	14700.78710	-0.00458	14700.7917	283.5288	80388.56
39.	2	1	1		1	1	0	4	2	2	2	3045.1	14955.48480	0.00435	14955.4804	112.9907	12766.90
34.	2	1	1		1	1	0	4	0	2	0	3045.1	14955.92650	0.00396	14955.9225	112.9907	12766.90
16.	2	0	2		1	0	1	4	2	2	2	11349.8	14701.29470	0.00344	14701.2913	421.1429	177361.31

```

!
! 2006 measurements, Ar carrier d=26.950
! 2022 measurements, Ne carrier d=26.9727 and the actually applied voltages
! have been corrected to d=26.950 by
!  $V_{old} = V_{new} * (d_{old}/d_{new}) = V_{new} * 0.999158$ 
! where  $0.999158 = 26.950/26.9727$ 
!

```

```
! Rotational and cd constants are from the ASFIT fit of
! Dreizler+Scappini 1981 data and IFPA BF-FTMW + WG-FTMW + MMW
! lines (to average frequencies in cases of resolved A,E splitting)
```

```
! 101 <- 000
```

1.	1	0	1	0	0	0	2	0	0	0	0.0	7351.6088	0.00000	0.00000
2.	1	0	1	0	0	0	2	0	0	0	4391.3	7351.7336	0.06286	0.06337
3.	1	0	1	0	0	0	2	0	0	0	6244.8	7351.8647	0.12711	0.12815
4.	1	0	1	0	0	0	2	0	0	0	7645.7	7351.9905	0.19053	0.19209
5.	1	0	1	0	0	0	2	0	0	0	8777.4	7352.1148	0.25111	0.25316
6.	1	0	1	0	0	0	2	0	0	0	10005.6	7352.2622	0.32628	0.32896
7.	1	0	1	0	0	0	2	0	0	0	11349.8	7352.4499	0.41982	0.42326
8.	1	0	1	0	0	0	2	0	0	0	12400.3	7352.6134	0.50111	0.50522

```
! 202 <- 101
```

9.	2	0	2	1	0	1	4	0	2	0	0.0	14701.0839	0.00000	0.00000
10.	2	0	2	1	0	1	4	2	2	2	2991.3	14701.0989	0.00677	0.00767
11.	2	0	2	1	0	1	4	2	2	2	4390.5	14701.1146	0.01459	0.01652
12.	2	0	2	1	0	1	4	2	2	2	6232.3	14701.1451	0.02939	0.03329
13.	2	0	2	1	0	1	4	2	2	2	7641.1	14701.1763	0.04418	0.05005
14.	2	0	2	1	0	1	4	2	2	2	8778.3	14701.2063	0.05831	0.06606
15.	2	0	2	1	0	1	4	2	2	2	10003.9	14701.2436	0.07572	0.08580
16.	2	0	2	1	0	1	4	2	2	2	11349.8	14701.2947	0.09747	0.11045
17.	2	0	2	1	0	1	4	2	2	2	12393.4	14701.3359	0.11621	0.13171

18.	2	0	2	1	0	1	4	0	2	0	2994.2	14701.0358	-0.00835	-0.03644
19.	2	0	2	1	0	1	4	0	2	0	4395.3	14700.9835	-0.01799	-0.07852
20.	2	0	2	1	0	1	4	0	2	0	6239.3	14700.8866	-0.03625	-0.15821
21.	2	0	2	1	0	1	4	0	2	0	7641.1	14700.7871	-0.05437	-0.23726
22.	2	0	2	1	0	1	4	0	2	0	8783.8	14700.6951	-0.07184	-0.31350
23.	2	0	2	1	0	1	4	0	2	0	10014.6	14700.5795	-0.09338	-0.40747
24.	2	0	2	1	0	1	4	0	2	0	11349.8	14700.4395	-0.11993	-0.52329
25.	2	0	2	1	0	1	4	0	2	0	12393.4	14700.3177	-0.14299	-0.62387

```
! 212 <- 111
```

26.	2	1	2	1	1	1	4	0	2	0	0.0	14450.4753	0.00000	0.00000
!														
27.	2	1	2	1	1	1	4	0	2	0	1628.4	14450.9026	0.00204	0.42141
28.	2	1	2	1	1	1	4	0	2	0	2027.9	14451.1319	0.00317	0.65242

```

29.  2  1  2  1  1  1  4  0  2  0  2423.6  14451.4122  0.00452  0.92994
30.  2  1  2  1  1  1  4  0  2  0  2736.4  14451.6713  0.00576  1.18324
31.  2  1  2  1  1  1  4  0  2  0  3030.3  14451.9374  0.00707  1.44819
!
!-----
!  211 <- 110
!-----
!
32.  2  1  1  1  1  0  4  0  2  0  0.0  14955.9097  0.00000  0.00000
!
33.  2  1  1  1  1  0  4  0  2  0  2224.7  14955.9193  0.00368  0.00235
34.  2  1  1  1  1  0  4  0  2  0  3045.1  14955.9265  0.00690  0.00440
35.  2  1  1  1  1  0  4  0  2  0  3646.7  14955.9277  0.00989  0.00631
36.  2  1  1  1  1  0  4  0  2  0  4147.8  14955.9346  0.01280  0.00816
37.  2  1  1  1  1  0  4  0  2  0  4546.5  14955.9330  0.01538  0.00980
!
38.  2  1  1  1  1  0  4  2  2  2  2224.7  14955.6815  -0.20901  -0.02090
39.  2  1  1  1  1  0  4  2  2  2  3045.1  14955.4848  -0.39094  -0.03914
40.  2  1  1  1  1  0  4  2  2  2  3646.7  14955.2963  -0.55981  -0.05611
41.  2  1  1  1  1  0  4  2  2  2  4546.5  14954.9509  -0.86772  -0.08713

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QSTARK - Fully diagonalizing fit of Stark shifts in a rotor
with zero or one quadrupolar nuclei

version 14.XI.2022

Zbigniew KISIEL

n-butanol, Tgt conformer

Calculation for J and F exceeding the value in data by at least 2
The fit will be made to TRANSITION FREQUENCIES

74 Lines read in
74 Lines fitted ----> 6 field free and 68 at non-zero field
3 Constants fitted

TRANSITIONS (F and MF in units of 1/2):

J	K	K	<-	J	K	K	F	MF<-	F	MF	Volts	Obs	Obs-Calc	Calc	Field	Field**2
-1	+1			-1	+1											

! Zero field frequencies are AE averaged state frequencies from
! the Kawashima et al. JPCA 2022 paper. Assumed spectroscopic parameters are
! from refit of the AE-averaged subset from that paper limited to Ka=2.

! 1_11 <- 0_00 bR

1.	1	1	1	0	0	0	2	0	0	0	0.0	14657.17380	-0.00087	14657.1747	0.0000	0.00
2.	1	1	1	0	0	0	2	0	0	0	3031.1	14657.58000	0.00077	14657.5792	112.3562	12623.91
3.	1	1	1	0	0	0	2	0	0	0	4053.0	14657.89930	0.00170	14657.8976	150.2358	22570.78
4.	1	1	1	0	0	0	2	0	0	0	5056.4	14658.30090	0.00184	14658.2991	187.4296	35129.84
5.	1	1	1	0	0	0	2	0	0	0	6068.8	14658.79610	0.00313	14658.7930	224.9570	50605.65
6.	1	1	1	0	0	0	2	0	0	0	7081.5	14659.37390	-0.00194	14659.3758	262.4956	68903.91
7.	1	1	1	0	0	0	2	0	0	0	8085.2	14660.03800	-0.00262	14660.0406	299.7005	89820.39

! 1_10 <- 0_00 cR

8.	1	1	0	0	0	0	2	0	0	0	0.0	14839.20240	-0.00133	14839.2037	0.0000	0.00
9.	1	1	0	0	0	0	2	0	0	0	3027.5	14839.53140	-0.00123	14839.5326	112.2227	12593.94
10.	1	1	0	0	0	0	2	0	0	0	4041.6	14839.79080	0.00068	14839.7901	149.8132	22443.99
11.	1	1	0	0	0	0	2	0	0	0	5054.9	14840.12180	0.00031	14840.1215	187.3740	35109.00
12.	1	1	0	0	0	0	2	0	0	0	6079.3	14840.53150	-0.00051	14840.5320	225.3462	50780.92
13.	1	1	0	0	0	0	2	0	0	0	7067.6	14841.00210	0.00180	14841.0003	261.9803	68633.68
14.	1	1	0	0	0	0	2	0	0	0	8086.1	14841.55600	-0.00144	14841.5574	299.7339	89840.38

```

! 2_11<-2_02 bQ
!-----
15. 2 1 1 2 0 2 4 0 4 0 0.0 10462.69900 -0.00047 10462.6995 0.0000 0.00

16. 2 1 1 2 0 2 4 4 4 4 2023.2 10462.94000 0.00404 10462.9360 74.9956 5624.33
17. 2 1 1 2 0 2 4 4 4 4 3031.3 10463.23270 0.00247 10463.2302 112.3636 12625.58
18. 2 1 1 2 0 2 4 4 4 4 4046.1 10463.65350 0.00870 10463.6448 149.9800 22494.00
19. 2 1 1 2 0 2 4 4 4 4 5054.2 10464.17790 0.00393 10464.1740 187.3480 35099.28

!-----
! 3_03 <- 2_02 aR
!-----
20. 3 0 3 2 0 2 6 0 4 0 0.0 13673.15690 0.00006 13673.1568 0.0000 0.00

21. 3 0 3 2 0 2 6 0 4 0 3038.4 13673.57420 0.00443 13673.5698 112.6268 12684.79
22. 3 0 3 2 0 2 6 0 4 0 4048.6 13673.89240 0.00256 13673.8898 150.0727 22521.80
23. 3 0 3 2 0 2 6 0 4 0 5060.5 13674.30500 0.00327 13674.3017 187.5815 35186.84
24. 3 0 3 2 0 2 6 0 4 0 6066.6 13674.80290 0.00121 13674.8017 224.8755 50568.97
25. 3 0 3 2 0 2 6 0 4 0 8076.8 13676.06620 -0.00371 13676.0699 299.3891 89633.85

26. 3 0 3 2 0 2 6 2 4 2 3038.4 13673.51020 0.00435 13673.5058 112.6268 12684.79
27. 3 0 3 2 0 2 6 2 4 2 4048.6 13673.77590 -0.00062 13673.7765 150.0727 22521.80
28. 3 0 3 2 0 2 6 2 4 2 5060.5 13674.12420 -0.00081 13674.1250 187.5815 35186.84
29. 3 0 3 2 0 2 6 2 4 2 6076.2 13674.55290 0.00020 13674.5527 225.2313 50729.14
30. 3 0 3 2 0 2 6 2 4 2 7077.1 13675.05290 0.00239 13675.0505 262.3325 68818.32
31. 3 0 3 2 0 2 6 2 4 2 8076.8 13675.62570 0.00231 13675.6234 299.3891 89633.85

32. 3 0 3 2 0 2 6 4 4 4 3038.4 13673.31930 0.00559 13673.3137 112.6268 12684.79
33. 3 0 3 2 0 2 6 4 4 4 4048.6 13673.43590 0.00054 13673.4354 150.0727 22521.80
34. 3 0 3 2 0 2 6 4 4 4 5060.5 13673.59220 0.00021 13673.5920 187.5815 35186.84
35. 3 0 3 2 0 2 6 4 4 4 6076.2 13673.78430 0.00011 13673.7842 225.2313 50729.14
36. 3 0 3 2 0 2 6 4 4 4 7076.8 13674.01080 0.00299 13674.0078 262.3213 68812.48
37. 3 0 3 2 0 2 6 4 4 4 8076.8 13674.25940 -0.00589 13674.2653 299.3891 89633.85

! Delta M = +1
38. 3 0 3 2 0 2 6 4 4 2 5060.5 13673.85510 -0.00153 13673.8566 187.5815 35186.84
39. 3 0 3 2 0 2 6 4 4 2 6076.2 13674.16390 -0.00188 13674.1658 225.2313 50729.14
40. 3 0 3 2 0 2 6 4 4 2 7076.8 13674.52610 0.00058 13674.5255 262.3213 68812.48
41. 3 0 3 2 0 2 6 4 4 2 8076.8 13674.93510 -0.00469 13674.9398 299.3891 89633.85

42. 3 0 3 2 0 2 6 6 4 4 3038.4 13673.15220 -0.00025 13673.1524 112.6268 12684.79
43. 3 0 3 2 0 2 6 6 4 4 4048.6 13673.14400 -0.00504 13673.1490 150.0727 22521.80
44. 3 0 3 2 0 2 6 6 4 4 6066.2 13673.13890 -0.00044 13673.1393 224.8606 50562.30
45. 3 0 3 2 0 2 6 6 4 4 7074.9 13673.13620 0.00317 13673.1330 262.2509 68775.54
46. 3 0 3 2 0 2 6 6 4 4 8076.8 13673.13020 0.00438 13673.1258 299.3891 89633.85

!-----
! 3_12 <- 2_11 aR
!-----
47. 3 1 2 2 1 1 6 0 4 0 0.0 13954.44580 0.00179 13954.4440 0.0000 0.00

48. 3 1 2 2 1 1 6 0 4 0 4043.2 13954.47500 -0.00197 13954.4770 149.8725 22461.76
49. 3 1 2 2 1 1 6 0 4 0 5060.8 13954.49240 -0.00324 13954.4956 187.5927 35191.01
50. 3 1 2 2 1 1 6 0 4 0 6057.1 13954.52400 0.00605 13954.5180 224.5233 50410.72
51. 3 1 2 2 1 1 6 0 4 0 7071.1 13954.54380 -0.00096 13954.5448 262.1100 68701.68
52. 3 1 2 2 1 1 6 0 4 0 8085.6 13954.58060 0.00490 13954.5757 299.7153 89829.27

53. 3 1 2 2 1 1 6 2 4 2 4043.2 13954.33530 -0.00188 13954.3372 149.8725 22461.76
54. 3 1 2 2 1 1 6 2 4 2 5060.8 13954.27590 -0.00077 13954.2767 187.5927 35191.01
55. 3 1 2 2 1 1 6 2 4 2 6057.1 13954.20150 -0.00286 13954.2044 224.5233 50410.72
56. 3 1 2 2 1 1 6 2 4 2 7071.1 13954.11820 0.00070 13954.1175 262.1100 68701.68
57. 3 1 2 2 1 1 6 2 4 2 8085.6 13954.01610 -0.00113 13954.0172 299.7153 89829.27

58. 3 1 2 2 1 1 6 4 4 4 2020.0 13954.31470 0.00203 13954.3127 74.8769 5606.56
59. 3 1 2 2 1 1 6 4 4 4 4043.2 13953.91440 -0.00388 13953.9183 149.8725 22461.76
60. 3 1 2 2 1 1 6 4 4 4 5060.8 13953.61880 -0.00211 13953.6209 187.5927 35191.01
61. 3 1 2 2 1 1 6 4 4 4 6057.1 13953.27370 0.00779 13953.2659 224.5233 50410.72
62. 3 1 2 2 1 1 6 4 4 4 7075.6 13952.83780 -0.00020 13952.8380 262.2769 68789.15

! Delta M = +1
63. 3 1 2 2 1 1 6 6 4 4 4043.2 13954.06350 -0.00472 13954.0682 149.8725 22461.76
64. 3 1 2 2 1 1 6 6 4 4 5060.8 13953.86270 0.00688 13953.8558 187.5927 35191.01
65. 3 1 2 2 1 1 6 6 4 4 6064.7 13953.60510 0.00481 13953.6003 224.8050 50537.30

!-----
! 3_13<-2_12 aR
!-----
66. 3 1 3 2 1 2 6 0 4 0 0.0 13408.40100 -0.00023 13408.4012 0.0000 0.00

67. 3 1 3 2 1 2 6 0 4 0 3038.8 13408.42560 0.00388 13408.4217 112.6416 12688.13

68. 3 1 3 2 1 2 6 2 4 2 3038.8 13408.49490 0.00369 13408.4912 112.6416 12688.13
69. 3 1 3 2 1 2 6 2 4 2 4043.7 13408.56290 0.00235 13408.5606 149.8910 22467.32

```

70.	3	1	3	2	1	2	6	2	4	2	5054.9	13408.64900	-0.00116	13408.6502	187.3740	35109.00
71.	3	1	3	2	1	2	6	4	4	4	2028.4	13408.53570	0.00150	13408.5342	75.1883	5653.28
72.	3	1	3	2	1	2	6	4	4	4	3038.8	13408.70180	0.00224	13408.6996	112.6416	12688.13
73.	3	1	3	2	1	2	6	4	4	4	4043.7	13408.92900	-0.00022	13408.9292	149.8910	22467.32
74.	3	1	3	2	1	2	6	4	4	4	5054.9	13409.22540	-0.00034	13409.2257	187.3740	35109.00

Standard deviation = 0.003153

ITERATION NO = 3 CONSTANTS, deviations and changes:

Mu.a	=	0.713680449	+-	0.000365989	0.000000001
Mu.b	=	0.898876976	+-	0.000442430	0.000000000
Mu.c	=	0.807144715	+-	0.000547181	0.000000000

FINAL RESULTS OF LEAST SQUARES FITTING PROCEDURE

=====

FITTED CONSTANTS:

A	/MHz	12467.7415597117	1:Xab	/MHz	0.
B	/MHz	2371.5177110614	1:XJ.a	/kHz	0.
C	/MHz	2189.4793994294	1:XK.a	/kHz	0.
DJ	/kHz	0.756259417	1:XJbc	/kHz	0.
DJK	/kHz	-6.180283871	1:Ma	/MHz	0.
DK	/kHz	60.254623227	1:Mb-c	/MHz	0.
dJ	/kHz	0.124839613	1:Tr	/MHz	0.
dK	/kHz	2.063149976	1:Xd	/kHz	0.
HJ	/ Hz	0.	1:Xbc	/MHz	0.
HJK	/ Hz	0.	1:Xac	/MHz	0.
HKJ	/ Hz	0.			
HK	/ Hz	0.			
hJ	/ Hz	0.			
hJK	/ Hz	0.	Mu.a	/D	0.71368 (36)
hK	/ Hz	0.	Mu.b	/D	0.89887 (44)
LKKJ	/mHz	0.	Mu.c	/D	0.80714 (54)
1:Xa	/MHz	0.	d	/cm	26.9776
1:Xb-c	/MHz	0.	k	/cm	0.

CORRELATION COEFFICIENTS:

	Mu.a	Mu.b	Mu.c
Mu.a	1.0000		
Mu.b	-0.2588	1.0000	
Mu.c	-0.0867	0.7003	1.0000

WORST FITTED LINES:

	J	K	K	<-	J	K	K	F	MF<-	F	MF	Volts	Obs	Obs-Calc	Calc	Field	Field**2
	-1	+1			-1	+1											
18.	2	1	1	2	0	2	4	4	4	4		4046.1	10463.65350	0.00870	10463.6448	149.9800	22494.00
61.	3	1	2	2	1	1	6	4	4	4		6057.1	13953.27370	0.00779	13953.2659	224.5233	50410.72
64.	3	1	2	2	1	1	6	6	4	4		5060.8	13953.86270	0.00688	13953.8558	187.5927	35191.01
50.	3	1	2	2	1	1	6	0	4	0		6057.1	13954.52400	0.00605	13954.5180	224.5233	50410.72
37.	3	0	3	2	0	2	6	4	4	4		8076.8	13674.25940	-0.00589	13674.2653	299.3891	89633.85

CONTRIBUTIONS (from gradients) OF INDIVIDUAL CONSTANTS TO FREQUENCY:

	Mu.a	Mu.b	Mu.c
--	------	------	------

!
! Zero field frequencies are AE averaged state frequencies from
! the Kawashima et al. JPCA 2022 paper. Assumed spectroscopic parameters are
! from refit of the AE-averaged subset from that paper limited to Ka=2.
!

!-----
! 1_11 <- 0_00 bR
!-----

1.	1	1	1	0	0	0	2	0	0	0	0.0	14657.1738	0.00000	0.00000	0.00000
2.	1	1	1	0	0	0	2	0	0	0	3031.1	14657.5800	0.08264	0.28555	-0.03609
3.	1	1	1	0	0	0	2	0	0	0	4053.0	14657.8993	0.14775	0.51008	-0.06418
4.	1	1	1	0	0	0	2	0	0	0	5056.4	14658.3009	0.22996	0.79298	-0.09921
5.	1	1	1	0	0	0	2	0	0	0	6068.8	14658.7961	0.33127	1.14067	-0.14171
6.	1	1	1	0	0	0	2	0	0	0	7081.5	14659.3739	0.45106	1.55048	-0.19102

```

7.  1  1  1  0  0  0  2  0  0  0  8085.2  14660.0380  0.58800  2.01721 -0.24613
!-----
!  1_10 <- 0_00  cR
!-----
8.  1  1  0  0  0  0  2  0  0  0  0.0  14839.2024  0.00000  0.00000  0.00000

9.  1  1  0  0  0  0  2  0  0  0  3027.5  14839.5314  0.08386  0.04581 -0.19942
10.  1  1  0  0  0  0  2  0  0  0  4041.6  14839.7908  0.14944  0.08189 -0.35560
11.  1  1  0  0  0  0  2  0  0  0  5054.9  14840.1218  0.23376  0.12862 -0.55669
12.  1  1  0  0  0  0  2  0  0  0  6079.3  14840.5315  0.33809  0.18698 -0.80596
13.  1  1  0  0  0  0  2  0  0  0  7067.6  14841.0021  0.45693  0.25417 -1.09050
14.  1  1  0  0  0  0  2  0  0  0  8086.1  14841.5560  0.59808  0.33496 -1.42928
!-----
!  2_11<-2_02  bQ
!-----
15.  2  1  1  2  0  2  4  0  4  0  0.0  10462.6990  0.00000  0.00000  0.00000

16.  2  1  1  2  0  2  4  4  4  4  2023.2  10462.9400  0.14861  0.07102 -0.01682
17.  2  1  1  2  0  2  4  4  4  4  3031.3  10463.2327  0.33336  0.15939 -0.03781
18.  2  1  1  2  0  2  4  4  4  4  4046.1  10463.6535  0.59334  0.28388 -0.06746
19.  2  1  1  2  0  2  4  4  4  4  5054.2  10464.1779  0.92465  0.44280 -0.10546
!-----
!  3_03 <- 2_02  aR
!-----
20.  3  0  3  2  0  2  6  0  4  0  0.0  13673.1569  0.00000  0.00000  0.00000

21.  3  0  3  2  0  2  6  0  4  0  3038.4  13673.5742 -0.00911  0.24784 -0.17408
22.  3  0  3  2  0  2  6  0  4  0  4048.6  13673.8924 -0.01615  0.43984 -0.30896
23.  3  0  3  2  0  2  6  0  4  0  5060.5  13674.3050 -0.02520  0.68678 -0.48245
24.  3  0  3  2  0  2  6  0  4  0  6066.6  13674.8029 -0.03616  0.98631 -0.69292
25.  3  0  3  2  0  2  6  0  4  0  8076.8  13676.0662 -0.06385  1.74511 -1.22625

26.  3  0  3  2  0  2  6  2  4  2  3038.4  13673.5102 -0.00249  0.20503 -0.14648
27.  3  0  3  2  0  2  6  2  4  2  4048.6  13673.7759 -0.00433  0.36398 -0.26005
28.  3  0  3  2  0  2  6  2  4  2  5060.5  13674.1242 -0.00656  0.56858 -0.40623
29.  3  0  3  2  0  2  6  2  4  2  6076.2  13674.5529 -0.00911  0.81956 -0.58556
30.  3  0  3  2  0  2  6  2  4  2  7077.1  13675.0529 -0.01181  1.11154 -0.79419
31.  3  0  3  2  0  2  6  2  4  2  8076.8  13675.6257 -0.01455  1.44736 -1.03416

32.  3  0  3  2  0  2  6  4  4  4  3038.4  13673.3193  0.01710  0.07629 -0.06349
33.  3  0  3  2  0  2  6  4  4  4  4048.6  13673.4359  0.03035  0.13545 -0.11272
34.  3  0  3  2  0  2  6  4  4  4  5060.5  13673.5922  0.04743  0.21161 -0.17610
35.  3  0  3  2  0  2  6  4  4  4  6076.2  13673.7843  0.06838  0.30507 -0.25388
36.  3  0  3  2  0  2  6  4  4  4  7076.8  13674.0108  0.09277  0.41381 -0.34437
37.  3  0  3  2  0  2  6  4  4  4  8076.8  13674.2594  0.12085  0.53900 -0.44855
! Delta M = +1
38.  3  0  3  2  0  2  6  4  4  2  5060.5  13673.8551 -0.02316  0.43729 -0.28574
39.  3  0  3  2  0  2  6  4  4  2  6076.2  13674.1639 -0.03304  0.63029 -0.41187
40.  3  0  3  2  0  2  6  4  4  2  7076.8  13674.5261 -0.04425  0.85472 -0.55854
41.  3  0  3  2  0  2  6  4  4  2  8076.8  13674.9351 -0.05681  1.11298 -0.72731

42.  3  0  3  2  0  2  6  6  4  4  3038.4  13673.1522  0.00712 -0.00260  0.00891
43.  3  0  3  2  0  2  6  6  4  4  4048.6  13673.1440  0.01264 -0.00462  0.01582
44.  3  0  3  2  0  2  6  6  4  4  6066.2  13673.1389  0.02838 -0.01037  0.03551
45.  3  0  3  2  0  2  6  6  4  4  7074.9  13673.1362  0.03860 -0.01410  0.04829
46.  3  0  3  2  0  2  6  6  4  4  8076.8  13673.1302  0.05031 -0.01838  0.06293
!-----
!  3_12 <- 2_11  aR
!-----
47.  3  1  2  2  1  1  6  0  4  0  0.0  13954.4458  0.00000  0.00000  0.00000

48.  3  1  2  2  1  1  6  0  4  0  4043.2  13954.4750 -0.00445 -0.00060 -0.03799
49.  3  1  2  2  1  1  6  0  4  0  5060.8  13954.4924 -0.00697 -0.00094 -0.05952
50.  3  1  2  2  1  1  6  0  4  0  6057.1  13954.5240 -0.00999 -0.00136 -0.08524
51.  3  1  2  2  1  1  6  0  4  0  7071.1  13954.5438 -0.01361 -0.00187 -0.11614
52.  3  1  2  2  1  1  6  0  4  0  8085.6  13954.5806 -0.01780 -0.00247 -0.15181

53.  3  1  2  2  1  1  6  2  4  2  4043.2  13954.3353 -0.12606 -0.01838 -0.03764
54.  3  1  2  2  1  1  6  2  4  2  5060.8  13954.2759 -0.19741 -0.02878 -0.05894
55.  3  1  2  2  1  1  6  2  4  2  6057.1  13954.2015 -0.28265 -0.04119 -0.08438
56.  3  1  2  2  1  1  6  2  4  2  7071.1  13954.1182 -0.38498 -0.05609 -0.11492
57.  3  1  2  2  1  1  6  2  4  2  8085.6  13954.0161 -0.50303 -0.07328 -0.15013

58.  3  1  2  2  1  1  6  4  4  4  2020.0  13954.3147 -0.12253 -0.01791 -0.00914
59.  3  1  2  2  1  1  6  4  4  4  4043.2  13953.9144 -0.48991 -0.07164 -0.03645
60.  3  1  2  2  1  1  6  4  4  4  5060.8  13953.6188 -0.76636 -0.11207 -0.05691
61.  3  1  2  2  1  1  6  4  4  4  6057.1  13953.2737 -1.09579 -0.16027 -0.08118
62.  3  1  2  2  1  1  6  4  4  4  7075.6  13952.8378 -1.49199 -0.21824 -0.11021

```

```
! Delta M = +1
63.  3  1  2  2  1  1  6  6  4  4  4043.2  13954.0635  -0.41255  0.00748 -0.02991
64.  3  1  2  2  1  1  6  6  4  4  5060.8  13953.8627  -0.64521  0.01188 -0.04670
65.  3  1  2  2  1  1  6  6  4  4  6064.7  13953.6051  -0.92462  0.01732 -0.06677
```

```
!-----
!   3_13<-2_12  aR
!-----
66.  3  1  3  2  1  2  6  0  4  0  0.0  13408.4010  0.00000  0.00000  0.00000
67.  3  1  3  2  1  2  6  0  4  0  3038.8  13408.4256  -0.00262  0.02309 -0.00002
68.  3  1  3  2  1  2  6  2  4  2  3038.8  13408.4949  0.07457  0.02342  0.00801
69.  3  1  3  2  1  2  6  2  4  2  4043.7  13408.5629  0.13200  0.04146  0.01417
70.  3  1  3  2  1  2  6  2  4  2  5054.9  13408.6490  0.20619  0.06477  0.02212
71.  3  1  3  2  1  2  6  4  4  4  2028.4  13408.5357  0.13636  0.01088  0.01431
72.  3  1  3  2  1  2  6  4  4  4  3038.8  13408.7018  0.30581  0.02439  0.03207
73.  3  1  3  2  1  2  6  4  4  4  4043.7  13408.9290  0.54093  0.04311  0.05668
74.  3  1  3  2  1  2  6  4  4  4  5054.9  13409.2254  0.84413  0.06721  0.08837
-----
```

```
////////////////////////////////////
//////// cut here - please display and print using a fixed width font //////////
////////////////////////////////////
```

QSTARK - Fully diagonalizing fit of Stark shifts in a rotor
with zero or one quadrupolar nuclei

version 14.XI.2022

Zbigniew KISIEL

```
-----
GTgp final fit, Ne carrier
-----
```

Calculation for J and F exceeding the value in data by at least 2
The fit will be made to TRANSITION FREQUENCIES

```
36 Lines read in
36 Lines fitted  --->   5 field free and   31 at non-zero field
 3 Constants fitted
```

TRANSITIONS (F and MF in units of 1/2):

	J	K	K	<-	J	K	K	F	MF<-	F	MF	Volts	Obs	Obs-Calc	Calc	Field	Field**2
	-1	+1			-1	+1											
! Zero field frequencies are frequencies from the Kawashima et al.																	
! JPCA 2022 paper, assumed spectroscopic parameters are from refit of																	
! the AE-state averaged frequencies from that paper																	
!-----																	
! 1_10 <- 0_00 c.R																	
!-----																	
1.	1	1	0		0	0	0	2	0	0	0	0.0	14635.50060	0.00011	14635.5005	0.0000	0.00
2.	1	1	0		0	0	0	2	0	0	0	2025.7	14635.68520	0.00296	14635.6822	75.1019	5640.29
3.	1	1	0		0	0	0	2	0	0	0	3025.5	14635.91110	0.00509	14635.9060	112.1690	12581.88
4.	1	1	0		0	0	0	2	0	0	0	4038.1	14636.22250	-0.00060	14636.2231	149.7106	22413.27
5.	1	1	0		0	0	0	2	0	0	0	5063.5	14636.63230	-0.00481	14636.6371	187.7268	35241.37
6.	1	1	0		0	0	0	2	0	0	0	6068.2	14637.13520	0.00153	14637.1337	224.9756	50614.03
!-----																	
! 1_11 <- 0_00 b.R																	
!-----																	
7.	1	1	1		0	0	0	2	0	0	0	0.0	14451.16880	-0.00048	14451.1693	0.0000	0.00
8.	1	1	1		0	0	0	2	0	0	0	1512.4	14451.31920	0.00295	14451.3162	56.0715	3144.01
9.	1	1	1		0	0	0	2	0	0	0	2031.5	14451.43920	0.00478	14451.4344	75.3169	5672.63
10.	1	1	1		0	0	0	2	0	0	0	2530.7	14451.58670	0.00602	14451.5807	93.8245	8803.04
11.	1	1	1		0	0	0	2	0	0	0	3025.8	14451.75620	-0.00111	14451.7573	112.1801	12584.37
12.	1	1	1		0	0	0	2	0	0	0	3529.5	14451.97380	0.00456	14451.9692	130.8545	17122.91
13.	1	1	1		0	0	0	2	0	0	0	4044.7	14452.21990	0.00030	14452.2196	149.9553	22486.60

14.	1	1	1	0	0	0	2	0	0	0	4548.8	14452.49460	-0.00281	14452.4974	168.6446	28441.00
15.	1	1	1	0	0	0	2	0	0	0	5048.9	14452.80220	-0.00286	14452.8051	187.1856	35038.43

!-----
! 1_10 <- 1_01 b.Q
!-----

16.	1	1	0	1	0	1	2	0	2	0	0.0	10158.69090	-0.00126	10158.6922	0.0000	0.00
17.	1	1	0	1	0	1	2	2	2	2	1010.0	10159.30100	0.00535	10159.2957	37.4453	1402.15
18.	1	1	0	1	0	1	2	2	2	2	1523.1	10160.06030	0.00071	10160.0596	56.4682	3188.66
19.	1	1	0	1	0	1	2	2	2	2	2025.8	10161.09830	-0.00100	10161.0993	75.1056	5640.85

!-----
! 3_03 <- 2_02 a.R
!-----

20.	3	0	3	2	0	2	6	0	4	0	0.0	13420.23590	0.00001	13420.2359	0.0000	0.00
21.	3	0	3	2	0	2	6	0	4	0	3044.0	13420.66420	0.00172	13420.6625	112.8548	12736.22
22.	3	0	3	2	0	2	6	0	4	0	4034.5	13420.98680	0.00167	13420.9851	149.5772	22373.33
23.	3	0	3	2	0	2	6	0	4	0	5057.7	13421.41490	0.00185	13421.4131	187.5118	35160.68
24.	3	0	3	2	0	2	6	2	4	2	3044.0	13420.60870	0.00456	13420.6041	112.8548	12736.22
25.	3	0	3	2	0	2	6	2	4	2	4034.5	13420.88040	-0.00251	13420.8829	149.5772	22373.33
26.	3	0	3	2	0	2	6	2	4	2	5057.7	13421.24820	-0.00477	13421.2530	187.5118	35160.68
27.	3	0	3	2	0	2	6	4	4	4	3044.0	13420.43360	0.00517	13420.4284	112.8548	12736.22
28.	3	0	3	2	0	2	6	4	4	4	4034.5	13420.57670	0.00257	13420.5741	149.5772	22373.33
29.	3	0	3	2	0	2	6	4	4	4	5057.7	13420.76700	-0.00045	13420.7674	187.5118	35160.68

!-----
! 3_13 <- 2_12 a.R
!-----

30.	3	1	3	2	1	2	6	0	4	0	0.0	13152.31780	0.00037	13152.3174	0.0000	0.00
31.	3	1	3	2	1	2	6	0	4	0	2032.9	13152.32820	-0.00084	13152.3290	75.3688	5680.46
32.	3	1	3	2	1	2	6	0	4	0	3035.8	13152.34580	0.00247	13152.3433	112.5508	12667.69
33.	3	1	3	2	1	2	6	2	4	2	2032.9	13152.40940	0.00347	13152.4059	75.3688	5680.46
34.	3	1	3	2	1	2	6	2	4	2	3035.8	13152.51680	0.00206	13152.5147	112.5508	12667.69
35.	3	1	3	2	1	2	6	4	4	4	2032.9	13152.63650	0.00009	13152.6364	75.3688	5680.46
36.	3	1	3	2	1	2	6	4	4	4	3035.8	13153.02550	-0.00264	13153.0281	112.5508	12667.69

Standard deviation = 0.003120

ITERATION NO = 3 CONSTANTS, deviations and changes:

Mu.a	=	1.088135266 +- 0.000587385	0.000000000
Mu.b	=	1.030426294 +- 0.000920619	0.000000000
Mu.c	=	0.697987849 +- 0.001407785	0.000000000

FINAL RESULTS OF LEAST SQUARES FITTING PROCEDURE
=====

FITTED CONSTANTS:

A	/MHz	12305.00007	1:Xab /MHz	0.
B	/MHz	2330.57664	1:XJ.a/kHz	0.
C	/MHz	2146.23454	1:XK.a/kHz	0.
DJ	/kHz	0.7131	1:XJbc/kHz	0.
DJK	/kHz	-2.543	1:Ma /MHz	0.
DK	/kHz	73.01	1:Mb-c/MHz	0.
dJ	/kHz	0.13705	1:Tr /MHz	0.
dK	/kHz	2.45	1:Xd /kHz	0.
HJ	/ Hz	0.	1:Xbc /MHz	0.
HJK	/ Hz	0.	1:Xac /MHz	0.
HKJ	/ Hz	0.		
HK	/ Hz	0.		
hJ	/ Hz	0.		
hJK	/ Hz	0.	Mu.a /D	1.08813 (58)
hK	/ Hz	0.	Mu.b /D	1.03042 (92)
LKKJ	/mHz	0.	Mu.c /D	0.6979 (14)
1:Xa /MHz	0.		d /cm	26.9727
1:Xb-c/MHz	0.		k /cm	0.

CORRELATION COEFFICIENTS:

	Mu.a	Mu.b	Mu.c
Mu.a	1.0000		

Mu.b -0.1140 1.0000
Mu.c 0.2136 0.5636 1.0000

WORST FITTED LINES:

	J	K	K	<-	J	K	K	F	MF<-	F	MF	Volts	Obs	Obs-Calc	Calc	Field	Field**2
	-1	+1			-1	+1											
10.	1	1	1	0	0	0		2	0	0	0	2530.7	14451.58670	0.00602	14451.5807	93.8245	8803.04
17.	1	1	0	1	0	1		2	2	2	2	1010.0	10159.30100	0.00535	10159.2957	37.4453	1402.15
27.	3	0	3	2	0	2		6	4	4	4	3044.0	13420.43360	0.00517	13420.4284	112.8548	12736.22
3.	1	1	0	0	0	0		2	0	0	0	3025.5	14635.91110	0.00509	14635.9060	112.1690	12581.88
5.	1	1	0	0	0	0		2	0	0	0	5063.5	14636.63230	-0.00481	14636.6371	187.7268	35241.37

CONTRIBUTIONS (from gradients) OF INDIVIDUAL CONSTANTS TO FREQUENCY:

														Mu.a	Mu.b	Mu.c
! Zero field frequencies are frequencies from the Kawashima et al.																
! JPCA 2022 paper, assumed spectroscopic parameters are from refit of																
! the AE-state subset from that paper																
! -----																
! 1_10 <- 0_00 c.R																
! -----																
1.	1	1	0	0	0	0		2	0	0	0	0.0	14635.5006	0.00000	0.00000	0.00000
2.	1	1	0	0	0	0		2	0	0	0	2025.7	14635.6852	0.08897	0.02727	-0.06555
3.	1	1	0	0	0	0		2	0	0	0	3025.5	14635.9111	0.19845	0.06092	-0.14631
4.	1	1	0	0	0	0		2	0	0	0	4038.1	14636.2225	0.35348	0.10876	-0.26085
5.	1	1	0	0	0	0		2	0	0	0	5063.5	14636.6323	0.55572	0.17150	-0.41060
6.	1	1	0	0	0	0		2	0	0	0	6068.2	14637.1352	0.79801	0.24714	-0.59049
! -----																
! 1_11 <- 0_00 b.R																
! -----																
7.	1	1	1	0	0	0		2	0	0	0	0.0	14451.1688	0.00000	0.00000	0.00000
8.	1	1	1	0	0	0		2	0	0	0	1512.4	14451.3192	0.04873	0.09137	-0.00685
9.	1	1	1	0	0	0		2	0	0	0	2031.5	14451.4392	0.08792	0.16482	-0.01234
10.	1	1	1	0	0	0		2	0	0	0	2530.7	14451.5867	0.13643	0.25572	-0.01910
11.	1	1	1	0	0	0		2	0	0	0	3025.8	14451.7562	0.19503	0.36546	-0.02724
12.	1	1	1	0	0	0		2	0	0	0	3529.5	14451.9738	0.26536	0.49709	-0.03696
13.	1	1	1	0	0	0		2	0	0	0	4044.7	14452.2199	0.34848	0.65254	-0.04836
14.	1	1	1	0	0	0		2	0	0	0	4548.8	14452.4946	0.44075	0.82496	-0.06093
15.	1	1	1	0	0	0		2	0	0	0	5048.9	14452.8022	0.54297	1.01581	-0.07474
! -----																
! 1_10 <- 1_01 b.Q																
! -----																
16.	1	1	0	1	0	1		2	0	2	0	0.0	10158.6909	0.00000	0.00000	0.00000
17.	1	1	0	1	0	1		2	2	2	2	1010.0	10159.3010	0.56962	0.02016	-0.01197
18.	1	1	0	1	0	1		2	2	2	2	1523.1	10160.0603	1.28548	0.04592	-0.02720
19.	1	1	0	1	0	1		2	2	2	2	2025.8	10161.0983	2.25064	0.08138	-0.04805
! -----																
! 3_03 <- 2_02 a.R																
! -----																
20.	3	0	3	2	0	2		6	0	4	0	0.0	13420.2359	0.00000	0.00000	0.00000
21.	3	0	3	2	0	2		6	0	4	0	3044.0	13420.6642	-0.02165	0.31929	-0.12885
22.	3	0	3	2	0	2		6	0	4	0	4034.5	13420.9868	-0.03800	0.56065	-0.22626
23.	3	0	3	2	0	2		6	0	4	0	5057.7	13421.4149	-0.05965	0.88060	-0.35540
24.	3	0	3	2	0	2		6	2	4	2	3044.0	13420.6087	-0.00594	0.26536	-0.10892
25.	3	0	3	2	0	2		6	2	4	2	4034.5	13420.8804	-0.01021	0.46618	-0.19135
26.	3	0	3	2	0	2		6	2	4	2	5057.7	13421.2482	-0.01560	0.73267	-0.30073
27.	3	0	3	2	0	2		6	4	4	4	3044.0	13420.4336	0.04065	0.10297	-0.04893
28.	3	0	3	2	0	2		6	4	4	4	4034.5	13420.5767	0.07142	0.18088	-0.08595
29.	3	0	3	2	0	2		6	4	4	4	5057.7	13420.7670	0.11225	0.28425	-0.13506
! -----																
! 3_13 <- 2_12 a.R																
! -----																
30.	3	1	3	2	1	2		6	0	4	0	0.0	13152.3178	0.00000	0.00000	0.00000
31.	3	1	3	2	1	2		6	0	4	0	2032.9	13152.3282	-0.00278	0.01438	-0.00001

32.	3	1	3	2	1	2	6	0	4	0	3035.8	13152.3458	-0.00619	0.03207	-0.00003
33.	3	1	3	2	1	2	6	2	4	2	2032.9	13152.4094	0.07669	0.01450	0.00271
34.	3	1	3	2	1	2	6	2	4	2	3035.8	13152.5168	0.17095	0.03232	0.00604
35.	3	1	3	2	1	2	6	4	4	4	2032.9	13152.6365	0.31477	0.01484	0.01086
36.	3	1	3	2	1	2	6	4	4	4	3035.8	13153.0255	0.70073	0.03299	0.02416

//////////////////////////////////////
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 //////////////////////////////////////

QSTARK - Fully diagonalizing fit of Stark shifts in a rotor
 with zero or one quadrupolar nuclei

version 14.XI.2022

Zbigniew KISIEL

 AA conformer of valeronitrile

Calculation for J and F exceeding the value in data by at least 2
 The fit will be made to TRANSITION FREQUENCIES

77 Lines read in
 77 Lines fitted ----> 7 field free and 70 at non-zero field
 2 Constants fitted

TRANSITIONS (F and MF in units of 1/2):

	J	K	K	<-	J	K	K	F	MF	<-	F	MF	Volts	Obs	Obs-Calc	Calc	Field	Field**2
	-1	+1			-1	+1												
!	! Rotational and centrifugal parameters are fixed at values from																	
!	! A-reduction refit of data from Ordu et al., A&A 541 (2012) A121:1-8																	
!	!-----																	
!	! 4_14 <- 3_13 (a.R)																	
!	!-----																	
1.	4	1	4	3	1	3	8	0	6	0	0.0	10250.78160	-0.00003	10250.7816	0.0000	0.00		
2.	4	1	4	3	1	3	6	0	4	0	0.0	10250.84060	0.00002	10250.8406	0.0000	0.00		
3.	4	1	4	3	1	3	10	0	8	0	0.0	10250.89590	0.00003	10250.8959	0.0000	0.00		
4.	4	1	4	3	1	3	6	0	4	0	1014.0	10251.09260	0.00411	10251.0885	37.5867	1412.76		
5.	4	1	4	3	1	3	6	0	4	0	1525.0	10251.38160	-0.00037	10251.3820	56.5284	3195.46		
6.	4	1	4	3	1	3	6	0	4	0	1715.0	10251.51390	-0.00177	10251.5157	63.5713	4041.30		
7.	4	1	4	3	1	3	6	2	4	2	1014.0	10251.19740	0.00167	10251.1957	37.5867	1412.76		
8.	4	1	4	3	1	3	6	2	4	2	1515.4	10251.58520	0.00365	10251.5816	56.1725	3155.35		
9.	4	1	4	3	1	3	6	4	4	4	1316.9	10251.92790	-0.00307	10251.9310	48.8146	2382.86		
10.	4	1	4	3	1	3	6	4	4	4	1525.0	10252.23410	0.00285	10252.2312	56.5284	3195.46		
11.	4	1	4	3	1	3	6	4	4	4	1715.0	10252.52560	-0.00069	10252.5263	63.5713	4041.30		
12.	4	1	4	3	1	3	8	0	6	0	1014.0	10251.06940	0.00377	10251.0656	37.5867	1412.76		
13.	4	1	4	3	1	3	8	2	6	2	1525.0	10251.68010	-0.00312	10251.6832	56.5284	3195.46		
14.	4	1	4	3	1	3	8	2	6	2	1715.0	10251.95680	-0.00261	10251.9594	63.5713	4041.30		
15.	4	1	4	3	1	3	8	4	6	4	1009.1	10251.34120	-0.00277	10251.3440	37.4051	1399.14		
16.	4	1	4	3	1	3	10	4	8	4	1014.0	10251.24780	0.00316	10251.2446	37.5867	1412.76		
17.	4	1	4	3	1	3	10	4	8	4	1515.4	10251.61680	0.00227	10251.6145	56.1725	3155.35		
18.	4	1	4	3	1	3	10	4	8	4	1715.0	10251.79620	0.00578	10251.7904	63.5713	4041.30		
19.	4	1	4	3	1	3	10	6	8	6	1009.1	10251.40530	-0.00246	10251.4078	37.4051	1399.14		
20.	4	1	4	3	1	3	10	6	8	6	1315.0	10251.74540	0.00116	10251.7442	48.7441	2375.99		
21.	4	1	4	3	1	3	10	6	8	6	1525.0	10252.02070	-0.00112	10252.0218	56.5284	3195.46		
22.	4	1	4	3	1	3	10	6	8	6	1715.0	10252.30940	0.00278	10252.3066	63.5713	4041.30		
23.	4	1	4	3	1	3	10	8	8	8	1009.1	10251.68270	0.00034	10251.6824	37.4051	1399.14		
24.	4	1	4	3	1	3	10	8	8	8	1316.9	10252.23840	-0.00231	10252.2407	48.8146	2382.86		

```

!-----
!  4_04 <- 3_03 (a.R)
!-----
25.  4 0 4 3 0 3 6 0 4 0 0.0 10389.06600 -0.00001 10389.0660 0.0000 0.00
26.  4 0 4 3 0 3 8 0 6 0 0.0 10389.12170 0.00004 10389.1217 0.0000 0.00
27.  4 0 4 3 0 3 10 0 8 0 0.0 10389.14480 0.00003 10389.1448 0.0000 0.00
28.  4 0 4 3 0 3 6 0 6 0 0.0 10390.29700 -0.00002 10390.2970 0.0000 0.00

29.  4 0 4 3 0 3 6 0 4 0 3033.8 10388.79360 -0.00032 10388.7939 112.4563 12646.41
30.  4 0 4 3 0 3 6 0 4 0 4043.3 10388.57440 0.00290 10388.5715 149.8762 22462.87
31.  4 0 4 3 0 3 6 0 4 0 5050.5 10388.27720 0.00122 10388.2760 187.2109 35047.91
32.  4 0 4 3 0 3 6 0 4 0 5565.9 10388.09760 0.00171 10388.0959 206.3156 42566.13
33.  4 0 4 3 0 3 6 0 4 0 6055.8 10387.89870 -0.00810 10387.9068 224.4751 50389.08
34.  4 0 4 3 0 3 6 0 4 0 6576.5 10387.69360 0.00659 10387.6870 243.7763 59426.89

35.  4 0 4 3 0 3 6 2 4 2 3033.8 10388.91940 0.00364 10388.9158 112.4563 12646.41
36.  4 0 4 3 0 3 6 2 4 2 4043.3 10388.76770 0.00098 10388.7667 149.8762 22462.87
37.  4 0 4 3 0 3 6 2 4 2 5062.4 10388.55130 0.00136 10388.5499 187.6520 35213.26
38.  4 0 4 3 0 3 6 2 4 2 5565.0 10388.42390 0.00469 10388.4192 206.2822 42552.37

39.  4 0 4 3 0 3 6 4 4 4 3033.8 10389.30040 0.00245 10389.2979 112.4563 12646.41
40.  4 0 4 3 0 3 6 4 4 4 4043.3 10389.37540 0.00229 10389.3731 149.8762 22462.87
41.  4 0 4 3 0 3 6 4 4 4 5062.4 10389.40180 0.00504 10389.3968 187.6520 35213.26
! same Stark lobe but QSTARK labelling switch
42.  4 0 4 3 0 3 6 4 6 4 5565.0 10389.39680 0.00012 10389.3967 206.2822 42552.37
43.  4 0 4 3 0 3 6 4 6 4 6055.8 10389.39080 -0.00282 10389.3936 224.4751 50389.08
44.  4 0 4 3 0 3 6 4 6 4 6567.3 10389.38430 -0.00531 10389.3896 243.4353 59260.74
45.  4 0 4 3 0 3 6 4 6 4 7066.9 10389.38360 -0.00271 10389.3863 261.9544 68620.09

46.  4 0 4 3 0 3 8 0 6 0 5062.4 10388.48530 0.00295 10388.4823 187.6520 35213.26

47.  4 0 4 3 0 3 8 2 6 2 2019.1 10389.05500 0.00260 10389.0524 74.8436 5601.56
48.  4 0 4 3 0 3 8 2 6 2 4043.3 10388.92890 -0.00074 10388.9296 149.8762 22462.87
49.  4 0 4 3 0 3 8 2 6 2 5062.4 10388.89630 -0.00237 10388.8987 187.6520 35213.26
50.  4 0 4 3 0 3 8 2 6 2 5565.0 10388.89580 0.00127 10388.8945 206.2822 42552.37
51.  4 0 4 3 0 3 8 2 6 2 6055.8 10388.89780 0.00112 10388.8967 224.4751 50389.08
52.  4 0 4 3 0 3 8 2 6 2 6567.3 10388.90700 0.00271 10388.9043 243.4353 59260.74
53.  4 0 4 3 0 3 8 2 6 2 7069.8 10388.91700 0.00111 10388.9159 262.0619 68676.42

54.  4 0 4 3 0 3 8 4 6 4 3033.8 10389.23300 0.00336 10389.2296 112.4563 12646.41
55.  4 0 4 3 0 3 8 4 6 4 4038.8 10389.45660 0.00145 10389.4552 149.7094 22412.90
56.  4 0 4 3 0 3 8 4 6 4 5062.4 10389.84590 -0.00288 10389.8488 187.6520 35213.26

57.  4 0 4 3 0 3 8 6 6 6 2019.1 10389.25170 -0.00014 10389.2518 74.8436 5601.56
58.  4 0 4 3 0 3 8 6 6 6 3033.8 10389.42970 0.00261 10389.4271 112.4563 12646.41
59.  4 0 4 3 0 3 8 6 6 6 4038.8 10389.66930 -0.00168 10389.6710 149.7094 22412.90
60.  4 0 4 3 0 3 8 6 6 6 5062.4 10389.96870 -0.00145 10389.9701 187.6520 35213.26
61.  4 0 4 3 0 3 8 6 6 6 6055.8 10390.28730 0.00329 10390.2840 224.4751 50389.08

62.  4 0 4 3 0 3 10 4 8 4 2019.1 10389.08090 -0.00433 10389.0852 74.8436 5601.56
63.  4 0 4 3 0 3 10 4 8 4 4043.3 10388.83110 -0.00161 10388.8327 149.8762 22462.87
64.  4 0 4 3 0 3 10 4 8 4 5062.4 10388.60630 0.00198 10388.6043 187.6520 35213.26
65.  4 0 4 3 0 3 10 4 8 4 5565.0 10388.46910 0.00155 10388.4675 206.2822 42552.37

66.  4 0 4 3 0 3 10 6 8 6 3033.8 10389.19460 0.00723 10389.1874 112.4563 12646.41
67.  4 0 4 3 0 3 10 6 8 6 4043.3 10389.19800 0.00456 10389.1934 149.8762 22462.87
68.  4 0 4 3 0 3 10 6 8 6 5062.4 10389.18920 -0.00300 10389.1922 187.6520 35213.26
69.  4 0 4 3 0 3 10 6 8 6 5565.0 10389.19190 0.00138 10389.1905 206.2822 42552.37
70.  4 0 4 3 0 3 10 6 8 6 6044.8 10389.18740 -0.00157 10389.1890 224.0674 50206.19
71.  4 0 4 3 0 3 10 6 8 6 6567.3 10389.18540 -0.00238 10389.1878 243.4353 59260.74
72.  4 0 4 3 0 3 10 6 8 6 7069.8 10389.18400 -0.00344 10389.1874 262.0619 68676.42

73.  4 0 4 3 0 3 10 8 8 8 2019.1 10389.30670 0.00064 10389.3061 74.8436 5601.56
74.  4 0 4 3 0 3 10 8 8 8 3033.8 10389.51780 0.00481 10389.5130 112.4563 12646.41
75.  4 0 4 3 0 3 10 8 8 8 4043.3 10389.80600 -0.00109 10389.8071 149.8762 22462.87
76.  4 0 4 3 0 3 10 8 8 8 5062.4 10390.19580 -0.00036 10390.1962 187.6520 35213.26
77.  4 0 4 3 0 3 10 8 8 8 5565.0 10390.42960 0.00694 10390.4227 206.2822 42552.37

```

Standard deviation = 0.003023

ITERATION NO = 3 CONSTANTS, deviations and changes:

```

Mu.a      =      3.904682673 +-      0.001377092      0.000000000
Mu.b      =      1.666240438 +-      0.000944196      0.000000000

```

FINAL RESULTS OF LEAST SQUARES FITTING PROCEDURE
=====

FITTED CONSTANTS:

A /MHz 15028.68713 1:Xab /MHz 0.
B /MHz 1334.10731 1:XJ.a/kHz 0.
C /MHz 1263.856699 1:XK.a/kHz 0.
DJ /kHz 0.1458342 1:XJbc/kHz 0.
DJK /kHz -7.54678 1:Ma /MHz 0.
DK /kHz 214.3805 1:Mb-c/MHz 0.
dJ /kHz 0.0220207 1:Tr /MHz 0.
dK /kHz 0.4816 1:Xd /kHz 0.
HJ / Hz 0.00009962 1:Xbc /MHz 0.
HJK / Hz -0.006464 1:Xac /MHz 0.
HKJ / Hz -0.05301
HK / Hz 4.77
hJ / Hz 0.00003144
hJK / Hz 0.
hK / Hz 0.
LKKJ /mHz -0.02051
1:Xa /MHz -2.72667
1:Xb-c/MHz -1.37612
Mu.a /D 3.9046 (13)
Mu.b /D 1.66624 (94)
Mu.c /D 0.
d /cm 26.9776
k /cm 0.
1:X.bb /MHz 0.675275000000
1:X.cc /MHz 2.051395000000

CORRELATION COEFFICIENTS:

Mu.a Mu.b
Mu.a 1.0000
Mu.b -0.2177 1.0000

WORST FITTED LINES:

	J	K	K	<-	J	K	K	F	MF	<-	F	MF	Volts	Obs	Obs-Calc	Calc	Field	Field**2
	-1	+1			-1	+1												
33.	4	0	4		3	0	3	6	0		4	0	6055.8	10387.89870	-0.00810	10387.9068	224.4751	50389.08
66.	4	0	4		3	0	3	10	6		8	6	3033.8	10389.19460	0.00723	10389.1874	112.4563	12646.41
77.	4	0	4		3	0	3	10	8		8	8	5565.0	10390.42960	0.00694	10390.4227	206.2822	42552.37
34.	4	0	4		3	0	3	6	0		4	0	6576.5	10387.69360	0.00659	10387.6870	243.7763	59426.89
18.	4	1	4		3	1	3	10	4		8	4	1715.0	10251.79620	0.00578	10251.7904	63.5713	4041.30

CONTRIBUTIONS (from gradients) OF INDIVIDUAL CONSTANTS TO FREQUENCY:

Mu.a Mu.b
!
!-----
! 4_14 <- 3_13 (a.R)
!-----
1. 4 1 4 3 1 3 8 0 6 0 0.0 10250.7816 0.00000 0.00000
2. 4 1 4 3 1 3 6 0 4 0 0.0 10250.8406 0.00000 0.00000
3. 4 1 4 3 1 3 10 0 8 0 0.0 10250.8959 0.00000 0.00000
4. 4 1 4 3 1 3 6 0 4 0 1014.0 10251.0926 0.01773 0.22282
5. 4 1 4 3 1 3 6 0 4 0 1525.0 10251.3816 0.00672 0.50387
6. 4 1 4 3 1 3 6 0 4 0 1715.0 10251.5139 -0.00473 0.63732
7. 4 1 4 3 1 3 6 2 4 2 1014.0 10251.1974 0.12087 0.21161
8. 4 1 4 3 1 3 6 2 4 2 1515.4 10251.5852 0.19104 0.47401
9. 4 1 4 3 1 3 6 4 4 4 1316.9 10251.9279 0.61603 0.30109
10. 4 1 4 3 1 3 6 4 4 4 1525.0 10252.2341 0.73411 0.40668
11. 4 1 4 3 1 3 6 4 4 4 1715.0 10252.5256 0.86488 0.51922
12. 4 1 4 3 1 3 8 0 6 0 1014.0 10251.0694 0.06467 0.21916
13. 4 1 4 3 1 3 8 2 6 2 1525.0 10251.6801 0.54723 0.47614
14. 4 1 4 3 1 3 8 2 6 2 1715.0 10251.9568 0.74231 0.59968
15. 4 1 4 3 1 3 8 4 6 4 1009.1 10251.3412 0.46668 0.18747
16. 4 1 4 3 1 3 10 4 8 4 1014.0 10251.2478 0.11739 0.20374
17. 4 1 4 3 1 3 10 4 8 4 1515.4 10251.6168 0.17679 0.45911
18. 4 1 4 3 1 3 10 4 8 4 1715.0 10251.7962 0.20133 0.59115
19. 4 1 4 3 1 3 10 6 8 6 1009.1 10251.4053 0.31126 0.17817
20. 4 1 4 3 1 3 10 6 8 6 1315.0 10251.7454 0.50293 0.30615
21. 4 1 4 3 1 3 10 6 8 6 1525.0 10252.0207 0.66273 0.41543
22. 4 1 4 3 1 3 10 6 8 6 1715.0 10252.3094 0.82920 0.52958
23. 4 1 4 3 1 3 10 8 8 8 1009.1 10251.6827 0.64759 0.14399
24. 4 1 4 3 1 3 10 8 8 8 1316.9 10252.2384 1.10741 0.24884

```

!-----
!  4_04 <- 3_03 (a.R)
!-----
25.  4 0 4 3 0 3 6 0 4 0 0.0 10389.0660 0.00000 0.00000
26.  4 0 4 3 0 3 8 0 6 0 0.0 10389.1217 0.00000 0.00000
27.  4 0 4 3 0 3 10 0 8 0 0.0 10389.1448 0.00000 0.00000
28.  4 0 4 3 0 3 6 0 6 0 0.0 10390.2970 0.00000 0.00000

29.  4 0 4 3 0 3 6 0 4 0 3033.8 10388.7936 -0.15012 -0.13056
30.  4 0 4 3 0 3 6 0 4 0 4043.3 10388.5744 -0.28464 -0.23376
31.  4 0 4 3 0 3 6 0 4 0 5050.5 10388.2772 -0.46726 -0.36738
32.  4 0 4 3 0 3 6 0 4 0 5565.9 10388.0976 -0.57730 -0.44752
33.  4 0 4 3 0 3 6 0 4 0 6055.8 10387.8987 -0.69106 -0.53100
34.  4 0 4 3 0 3 6 0 4 0 6576.5 10387.6936 -0.82105 -0.62745

35.  4 0 4 3 0 3 6 2 4 2 3033.8 10388.9194 -0.06207 -0.11475
36.  4 0 4 3 0 3 6 2 4 2 4043.3 10388.7677 -0.15493 -0.20871
37.  4 0 4 3 0 3 6 2 4 2 5062.4 10388.5513 -0.28684 -0.33310
38.  4 0 4 3 0 3 6 2 4 2 5565.0 10388.4239 -0.36012 -0.40506

39.  4 0 4 3 0 3 6 4 4 4 3033.8 10389.3004 0.21623 -0.06578
40.  4 0 4 3 0 3 6 4 4 4 4043.3 10389.3754 0.22763 -0.13320
41.  4 0 4 3 0 3 6 4 4 4 5062.4 10389.4018 0.23839 -0.22584
! same Stark lobe but QSTARK labelling switch
42.  4 0 4 3 0 3 6 4 6 4 5565.0 10389.3968 0.26762 -0.27916
43.  4 0 4 3 0 3 6 4 6 4 6055.8 10389.3908 0.31285 -0.33591
44.  4 0 4 3 0 3 6 4 6 4 6567.3 10389.3843 0.37514 -0.39995
45.  4 0 4 3 0 3 6 4 6 4 7066.9 10389.3836 0.44810 -0.46727

46.  4 0 4 3 0 3 8 0 6 0 5062.4 10388.4853 -0.29431 -0.34444

47.  4 0 4 3 0 3 8 2 6 2 2019.1 10389.0550 -0.01216 -0.04949
48.  4 0 4 3 0 3 8 2 6 2 4043.3 10388.9289 0.09258 -0.18394
49.  4 0 4 3 0 3 8 2 6 2 5062.4 10388.8963 0.23837 -0.27706
50.  4 0 4 3 0 3 8 2 6 2 5565.0 10388.8958 0.32507 -0.32926
51.  4 0 4 3 0 3 8 2 6 2 6055.8 10388.8978 0.41444 -0.38441
52.  4 0 4 3 0 3 8 2 6 2 6567.3 10388.9070 0.51011 -0.44637
53.  4 0 4 3 0 3 8 2 6 2 7069.8 10388.9170 0.60521 -0.51178

54.  4 0 4 3 0 3 8 4 6 4 3033.8 10389.2330 0.28849 -0.06655
55.  4 0 4 3 0 3 8 4 6 4 4038.8 10389.4566 0.71391 -0.09552
56.  4 0 4 3 0 3 8 4 6 4 5062.4 10389.8459 1.28077 -0.12504

57.  4 0 4 3 0 3 8 6 6 6 2019.1 10389.2517 0.15207 -0.01617
58.  4 0 4 3 0 3 8 6 6 6 3033.8 10389.4297 0.35013 -0.03144
59.  4 0 4 3 0 3 8 6 6 6 4038.8 10389.6693 0.59449 -0.04583
60.  4 0 4 3 0 3 8 6 6 6 5062.4 10389.9687 0.83496 -0.05517
61.  4 0 4 3 0 3 8 6 6 6 6055.8 10390.2873 1.03076 -0.05717

62.  4 0 4 3 0 3 10 4 8 4 2019.1 10389.0809 -0.01949 -0.04759
63.  4 0 4 3 0 3 10 4 8 4 4043.3 10388.8311 -0.18183 -0.20300
64.  4 0 4 3 0 3 10 4 8 4 5062.4 10388.6063 -0.32444 -0.32577
65.  4 0 4 3 0 3 10 4 8 4 5565.0 10388.4691 -0.40156 -0.39715

66.  4 0 4 3 0 3 10 6 8 6 3033.8 10389.1946 0.09550 -0.07892
67.  4 0 4 3 0 3 10 6 8 6 4043.3 10389.1980 0.14852 -0.14530
68.  4 0 4 3 0 3 10 6 8 6 5062.4 10389.1892 0.22595 -0.23374
69.  4 0 4 3 0 3 10 6 8 6 5565.0 10389.1919 0.27559 -0.28518
70.  4 0 4 3 0 3 10 6 8 6 6044.8 10389.1874 0.33030 -0.33902
71.  4 0 4 3 0 3 10 6 8 6 6567.3 10389.1854 0.39778 -0.40285
72.  4 0 4 3 0 3 10 6 8 6 7069.8 10389.1840 0.47008 -0.46928

73.  4 0 4 3 0 3 10 8 8 8 2019.1 10389.3067 0.17443 -0.01158
74.  4 0 4 3 0 3 10 8 8 8 3033.8 10389.5178 0.40190 -0.02696
75.  4 0 4 3 0 3 10 8 8 8 4043.3 10389.8060 0.72865 -0.04941
76.  4 0 4 3 0 3 10 8 8 8 5062.4 10390.1958 1.16247 -0.07956
77.  4 0 4 3 0 3 10 8 8 8 5565.0 10390.4296 1.41475 -0.09719

```

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////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////
//////////////////////////////////////////////////////////////// cut here - please display and print using a fixed width font //
////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////

```

QSTARK - Fully diagonalizing fit of Stark shifts in a rotor
with zero or one quadrupolar nuclei

GA conformer of valeronitrile

Calculation for J and F exceeding the value in data by at least 2
The fit will be made to TRANSITION FREQUENCIES

99 Lines read in
99 Lines fitted ----> 14 field free and 85 at non-zero field
3 Constants fitted

TRANSITIONS (F and MF in units of 1/2):

	J	K	K	<-	J	K	K	F	MF	<-	F	MF	Volts	Obs	Obs-Calc	Calc	Field	Field**2
	-1	+1			-1	+1												
! Rotational and centrifugal parameters are fixed at values from																		
! A-reduction refit of data from Ordu et al., A&A 541 (2012) A121:1-8																		
! -----																		
! 110 <- 000 cR																		
! -----																		
1.	1	1	0		0	0	0	0	0	2	0		0.0	9423.23330	0.00015	9423.2331	0.0000	0.00
2.	1	1	0		0	0	0	4	0	2	0		0.0	9424.12270	0.00017	9424.1225	0.0000	0.00
3.	1	1	0		0	0	0	2	0	2	0		0.0	9424.71560	0.00016	9424.7154	0.0000	0.00
4.	1	1	0		0	0	0	0	0	2	0		515.6	9423.64480	0.00094	9423.6439	19.1122	365.27
5.	1	1	0		0	0	0	0	0	2	0		619.9	9423.74270	0.00018	9423.7425	22.9783	528.00
6.	1	1	0		0	0	0	0	0	2	0		718.0	9423.82150	-0.00003	9423.8215	26.6147	708.34
7.	1	1	0		0	0	0	0	0	2	0		807.7	9423.88740	0.00158	9423.8858	29.9397	896.38
8.	1	1	0		0	0	0	0	0	2	0		911.6	9423.95510	-0.00031	9423.9554	33.7910	1141.83
9.	1	1	0		0	0	0	2	2	2	2		412.9	9425.07960	-0.00306	9425.0827	15.3053	234.25
10.	1	1	0		0	0	0	2	2	2	2		500.8	9425.29360	-0.00092	9425.2945	18.5635	344.61
11.	1	1	0		0	0	0	4	0	2	0		403.6	9424.37780	0.00251	9424.3753	14.9606	223.82
12.	1	1	0		0	0	0	4	0	2	0		515.6	9424.59760	0.00279	9424.5948	19.1122	365.27
13.	1	1	0		0	0	0	4	0	2	0		617.7	9424.88840	0.00754	9424.8809	22.8968	524.26
14.	1	1	0		0	0	0	4	2	2	2		403.6	9424.31620	0.00115	9424.3151	14.9606	223.82
15.	1	1	0		0	0	0	4	2	2	2		515.6	9424.38410	0.00051	9424.3836	19.1122	365.27
16.	1	1	0		0	0	0	4	2	2	2		619.9	9424.44110	0.00002	9424.4411	22.9783	528.00
17.	1	1	0		0	0	0	4	2	2	2		709.3	9424.48750	-0.00026	9424.4878	26.2922	691.28
18.	1	1	0		0	0	0	4	2	2	2		807.7	9424.53880	0.00008	9424.5387	29.9397	896.38
19.	1	1	0		0	0	0	4	2	2	2		915.4	9424.59420	-0.00185	9424.5961	33.9319	1151.37
! -----																		
! 312 <- 211 aR																		
! -----																		
20.	3	1	2		2	1	1	8	0	6	0		0.0	10375.72220	0.00065	10375.7216	0.0000	0.00
21.	3	1	2		2	1	1	6	0	4	0		0.0	10375.73360	0.00064	10375.7330	0.0000	0.00
22.	3	1	2		2	1	1	4	0	2	0		0.0	10375.84600	0.00060	10375.8454	0.0000	0.00
23.	3	1	2		2	1	1	4	0	2	0		1621.7	10375.73370	-0.00187	10375.7356	60.1128	3613.55
24.	3	1	2		2	1	1	4	0	2	0		2730.2	10375.68100	-0.00216	10375.6832	101.2025	10241.94
25.	3	1	2		2	1	1	4	2	2	2		1621.7	10375.36600	-0.00220	10375.3682	60.1128	3613.55
26.	3	1	2		2	1	1	4	2	2	2		2219.5	10375.12400	-0.00027	10375.1243	82.2720	6768.68
! same Stark lobe but label switch																		
27.	3	1	2		2	1	1	4	2	4	2		2730.5	10374.87380	0.00169	10374.8721	101.2136	10244.19
28.	3	1	2		2	1	1	6	0	4	0		1621.7	10375.45850	-0.00065	10375.4591	60.1128	3613.55
29.	3	1	2		2	1	1	6	0	4	0		2219.5	10375.22000	-0.00032	10375.2203	82.2720	6768.68
30.	3	1	2		2	1	1	6	0	4	0		2730.5	10374.95170	-0.00581	10374.9575	101.2136	10244.19
31.	3	1	2		2	1	1	6	2	4	2		1621.7	10375.00840	0.00215	10375.0062	60.1128	3613.55
32.	3	1	2		2	1	1	6	2	4	2		2219.5	10374.11350	-0.00359	10374.1171	82.2720	6768.68
33.	3	1	2		2	1	1	6	4	4	4		1621.7	10374.89570	0.00302	10374.8927	60.1128	3613.55
34.	3	1	2		2	1	1	6	4	4	4		2219.5	10374.16840	0.00769	10374.1607	82.2720	6768.68
35.	3	1	2		2	1	1	8	0	6	0		2219.5	10375.31300	-0.00141	10375.3144	82.2720	6768.68
36.	3	1	2		2	1	1	8	0	6	0		2730.5	10375.05140	-0.00066	10375.0521	101.2136	10244.19
37.	3	1	2		2	1	1	8	2	6	2		1621.7	10375.59540	-0.00152	10375.5969	60.1128	3613.55
38.	3	1	2		2	1	1	8	2	6	2		2730.2	10375.57260	0.00444	10375.5682	101.2025	10241.94
39.	3	1	2		2	1	1	8	4	6	4		1621.7	10375.39260	0.00297	10375.3896	60.1128	3613.55
40.	3	1	2		2	1	1	8	4	6	4		2219.5	10375.16310	-0.00337	10375.1665	82.2720	6768.68

41.	3	1	2	2	1	1	8	4	6	4	2730.5	10374.92130	0.00031	10374.9210	101.2136	10244.19
42.	3	1	2	2	1	1	8	6	6	6	1621.7	10374.74450	0.00191	10374.7426	60.1128	3613.55
43.	3	1	2	2	1	1	8	6	6	6	2219.5	10373.87230	0.00346	10373.8688	82.2720	6768.68

!-----
! 212 <- 101 bR
!-----

44.	2	1	2	1	0	1	4	0	4	0	0.0	12297.78200	-0.00003	12297.7820	0.0000	0.00
45.	2	1	2	1	0	1	4	0	2	0	0.0	12297.79480	0.00034	12297.7945	0.0000	0.00
46.	2	1	2	1	0	1	6	0	4	0	0.0	12298.41770	0.00039	12298.4173	0.0000	0.00
47.	2	1	2	1	0	1	2	0	0	0	0.0	12298.75200	0.00034	12298.7517	0.0000	0.00
48.	2	1	2	1	0	1	2	0	2	0	0.0	12298.78270	-0.00004	12298.7827	0.0000	0.00

49.	2	1	2	1	0	1	2	0	0	0	1006.5	12298.91290	-0.00507	12298.9180	37.3087	1391.94
50.	2	1	2	1	0	1	2	0	0	0	1621.8	12299.20630	-0.00593	12299.2122	60.1165	3614.00

51.	2	1	2	1	0	1	2	2	2	2	1006.5	12298.71670	-0.00064	12298.7173	37.3087	1391.94
52.	2	1	2	1	0	1	2	2	2	2	1621.8	12298.76590	-0.00250	12298.7684	60.1165	3614.00
53.	2	1	2	1	0	1	2	2	2	2	2121.5	12298.91610	-0.00028	12298.9164	78.6393	6184.14
54.	2	1	2	1	0	1	2	2	2	2	2533.4	12299.09110	-0.00244	12299.0935	93.9075	8818.63

! same Stark lobe but label switch

55.	2	1	2	1	0	1	4	2	2	2	2932.6	12299.29950	-0.00497	12299.3045	108.7050	11816.78
56.	2	1	2	1	0	1	4	2	2	2	3331.2	12299.54560	-0.00484	12299.5504	123.4802	15247.36

57.	2	1	2	1	0	1	4	0	2	0	1621.8	12298.06100	0.00296	12298.0580	60.1165	3614.00
58.	2	1	2	1	0	1	4	0	2	0	2121.5	12298.24840	0.00275	12298.2457	78.6393	6184.14
59.	2	1	2	1	0	1	4	0	2	0	2533.4	12298.43750	-0.00061	12298.4381	93.9075	8818.63
60.	2	1	2	1	0	1	4	0	2	0	2932.6	12298.65580	-0.00151	12298.6573	108.7050	11816.78
61.	2	1	2	1	0	1	4	0	2	0	3331.2	12298.90490	-0.00346	12298.9084	123.4802	15247.36

62.	2	1	2	1	0	1	4	2	2	2	1006.5	12297.77760	0.00508	12297.7725	37.3087	1391.94
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63.	2	1	2	1	0	1	4	2	4	2	1006.5	12297.43390	-0.00174	12297.4356	37.3087	1391.94
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64.	2	1	2	1	0	1	4	4	4	4	1006.5	12297.60510	-0.00158	12297.6067	37.3087	1391.94
65.	2	1	2	1	0	1	4	4	4	4	1621.8	12297.25320	0.00426	12297.2489	60.1165	3614.00
66.	2	1	2	1	0	1	4	4	4	4	2121.5	12296.79940	0.00003	12296.7994	78.6393	6184.14

67.	2	1	2	1	0	1	6	0	4	0	2121.5	12297.52550	0.00406	12297.5214	78.6393	6184.14
-----	---	---	---	---	---	---	---	---	---	---	--------	-------------	---------	------------	---------	---------

68.	2	1	2	1	0	1	6	2	4	2	2533.4	12297.47170	-0.00003	12297.4717	93.9075	8818.63
69.	2	1	2	1	0	1	6	2	4	2	2932.6	12297.21090	-0.00061	12297.2115	108.7050	11816.78
70.	2	1	2	1	0	1	6	2	4	2	3335.6	12296.91310	-0.00387	12296.9170	123.6433	15287.67

71.	2	1	2	1	0	1	6	4	4	4	1006.5	12298.43990	0.00497	12298.4349	37.3087	1391.94
72.	2	1	2	1	0	1	6	4	4	4	1621.8	12298.54210	-0.00027	12298.5424	60.1165	3614.00
73.	2	1	2	1	0	1	6	4	4	4	2121.5	12298.71180	0.00708	12298.7047	78.6393	6184.14
74.	2	1	2	1	0	1	6	4	4	4	2533.4	12298.88220	-0.00223	12298.8844	93.9075	8818.63
75.	2	1	2	1	0	1	6	4	4	4	2932.6	12299.09100	-0.00437	12299.0954	108.7050	11816.78
76.	2	1	2	1	0	1	6	4	4	4	3331.2	12299.33860	-0.00206	12299.3407	123.4802	15247.36

!-----
! 313 <- 202 bR
!-----

77.	3	1	3	2	0	2	6	0	4	0	0.0	15291.71500	0.00056	15291.7144	0.0000	0.00
78.	3	1	3	2	0	2	8	0	6	0	0.0	15292.34710	0.00058	15292.3465	0.0000	0.00
79.	3	1	3	2	0	2	4	0	2	0	0.0	15292.56050	0.00052	15292.5600	0.0000	0.00

80.	3	1	3	2	0	2	4	0	2	0	1510.1	15292.21330	-0.00416	15292.2175	55.9761	3133.32
81.	3	1	3	2	0	2	4	0	2	0	2524.2	15291.59180	0.00224	15291.5896	93.5665	8754.69

82.	3	1	3	2	0	2	6	0	4	0	1510.1	15291.34250	-0.00132	15291.3438	55.9761	3133.32
83.	3	1	3	2	0	2	6	0	4	0	2028.4	15291.04050	-0.00341	15291.0439	75.1883	5653.28
84.	3	1	3	2	0	2	6	0	4	0	3035.4	15290.19590	-0.00549	15290.2014	112.5156	12659.75

85.	3	1	3	2	0	2	6	2	4	2	1510.1	15291.02300	-0.00317	15291.0262	55.9761	3133.32
86.	3	1	3	2	0	2	6	2	4	2	2028.4	15290.47050	-0.00904	15290.4795	75.1883	5653.28
87.	3	1	3	2	0	2	6	2	4	2	2524.2	15289.78480	-0.00957	15289.7944	93.5665	8754.69

88.	3	1	3	2	0	2	6	4	4	4	2524.2	15292.30170	0.00252	15292.2992	93.5665	8754.69
89.	3	1	3	2	0	2	6	4	4	4	3036.6	15292.46670	0.00001	15292.4667	112.5600	12669.76

90.	3	1	3	2	0	2	8	0	6	0	1510.1	15291.73500	0.00277	15291.7322	55.9761	3133.32
91.	3	1	3	2	0	2	8	0	6	0	3035.4	15289.87780	0.00227	15289.8755	112.5156	12659.75

92.	3	1	3	2	0	2	8	4	6	4	2028.4	15291.59610	0.00069	15291.5954	75.1883	5653.28
93.	3	1	3	2	0	2	8	4	6	4	2524.6	15291.19760	0.00656	15291.1910	93.5813	8757.47
94.	3	1	3	2	0	2	8	4	6	4	3035.4	15290.69640	0.00528	15290.6911	112.5156	12659.75

95.	3	1	3	2	0	2	8	6	6	6	1510.1	15292.58870	0.00494	15292.5838	55.9761	3133.32
96.	3	1	3	2	0	2	8	6	6	6	2028.4	15292.78980	0.00402	15292.7858	75.1883	5653.28
97.	3	1	3	2	0	2	8	6	6	6	2524.2	15293.05000	0.00721	15293.0428	93.5665	8754.69

98.	3	1	3	2	0	2	8	6	6	6	2524.2	15293.05000	0.00721	15293.0428	93.5665	8754.69
99.	3	1	3	2	0	2	8	6	6	6	3036.6	15293.36860	-0.00657	15293.3752	112.5600	12669.76

Standard deviation = 0.003466

ITERATION NO = 3 CONSTANTS, deviations and changes:

Mu.a	=	2.685545733	+-	0.001276761	0.000000000
Mu.b	=	2.852087694	+-	0.003165046	0.000000000
Mu.c	=	0.389738395	+-	0.015466209	-0.000000001

FINAL RESULTS OF LEAST SQUARES FITTING PROCEDURE
=====

FITTED CONSTANTS:

A	/MHz	7635.62481	1:Xab	/MHz	0.
B	/MHz	1788.636927	1:XJ.a	/kHz	0.
C	/MHz	1554.218399	1:XK.a	/kHz	0.
DJ	/kHz	0.878123	1:XJbc	/kHz	0.
DJK	/kHz	-10.00176	1:Ma	/MHz	0.
DK	/kHz	52.4857	1:Mb-c	/MHz	0.
dJ	/kHz	0.2333427	1:Tr	/MHz	0.
dK	/kHz	1.72956	1:Xd	/kHz	0.
HJ	/ Hz	0.00058741	1:Xbc	/MHz	0.
HJK	/ Hz	0.01675	1:Xac	/MHz	0.
HKJ	/ Hz	-0.36068			
HK	/ Hz	1.4593			
hJ	/ Hz	0.0002657			
hJK	/ Hz	-0.0047	Mu.a	/D	2.6855(12)
hK	/ Hz	0.1004	Mu.b	/D	2.8520(31)
LKKJ	/mHz	0.01863	Mu.c	/D	0.389(15)
1:Xa	/MHz	-0.0414	d	/cm	26.9776
1:Xb-c	/MHz	-3.91148	k	/cm	0.
1:X.bb	/MHz	-1.935040000000			
1:X.cc	/MHz	1.976440000000			

CORRELATION COEFFICIENTS:

	Mu.a	Mu.b	Mu.c
Mu.a	1.0000		
Mu.b	-0.6375	1.0000	
Mu.c	-0.6625	0.9596	1.0000

WORST FITTED LINES:

	J	K	K	<-	J	K	K	F	MF<-	F	MF	Volts	Obs	Obs-Calc	Calc	Field	Field**2
	-1	+1			-1	+1											
87.	3	1	3	2	0	2	6	2	4	2		2524.2	15289.78480	-0.00957	15289.7944	93.5665	8754.69
86.	3	1	3	2	0	2	6	2	4	2		2028.4	15290.47050	-0.00904	15290.4795	75.1883	5653.28
34.	3	1	2	2	1	1	6	4	4	4		2219.5	10374.16840	0.00769	10374.1607	82.2720	6768.68
13.	1	1	0	0	0	0	4	0	2	0		617.7	9424.88840	0.00754	9424.8809	22.8968	524.26
97.	3	1	3	2	0	2	8	6	6	6		2524.2	15293.05000	0.00721	15293.0428	93.5665	8754.69

CONTRIBUTIONS (from gradients) OF INDIVIDUAL CONSTANTS TO FREQUENCY:

														Mu.a	Mu.b	Mu.c
!																
!																
!	110	<-	000	cR												
!																
1.	1	1	0	0	0	0	0	0	2	0		0.0	9423.2333	0.00000	0.00000	0.00000
2.	1	1	0	0	0	0	4	0	2	0		0.0	9424.1227	0.00000	0.00000	0.00000
3.	1	1	0	0	0	0	2	0	2	0		0.0	9424.7156	0.00000	0.00000	0.00000
4.	1	1	0	0	0	0	0	0	2	0		515.6	9423.6448	0.23524	0.02962	0.00062
5.	1	1	0	0	0	0	0	0	2	0		619.9	9423.7427	0.23187	0.03792	0.00089
6.	1	1	0	0	0	0	0	0	2	0		718.0	9423.8215	0.22399	0.04695	0.00118
7.	1	1	0	0	0	0	0	0	2	0		807.7	9423.8874	0.22286	0.05668	0.00148
8.	1	1	0	0	0	0	0	0	2	0		911.6	9423.9551	0.23153	0.06985	0.00188
9.	1	1	0	0	0	0	2	2	2	2		412.9	9425.0796	0.40228	0.03043	0.00044
10.	1	1	0	0	0	0	2	2	2	2		500.8	9425.2936	0.63661	0.04677	0.00065
11.	1	1	0	0	0	0	4	0	2	0		403.6	9424.3778	0.28909	0.02474	0.00040
12.	1	1	0	0	0	0	4	0	2	0		515.6	9424.5976	0.57210	0.04488	0.00067

13.	1	1	0	0	0	0	4	0	2	0	617.7	9424.8884	0.92383	0.06899	0.00097
14.	1	1	0	0	0	0	4	2	2	2	403.6	9424.3162	0.11409	0.01681	0.00038
15.	1	1	0	0	0	0	4	2	2	2	515.6	9424.3841	0.12465	0.02465	0.00061
16.	1	1	0	0	0	0	4	2	2	2	619.9	9424.4411	0.13203	0.03345	0.00088
17.	1	1	0	0	0	0	4	2	2	2	709.3	9424.4875	0.14203	0.04240	0.00114
18.	1	1	0	0	0	0	4	2	2	2	807.7	9424.5388	0.15852	0.05382	0.00148
19.	1	1	0	0	0	0	4	2	2	2	915.4	9424.5942	0.18306	0.06820	0.00189

```

!-----
! 312 <- 211 aR
!-----
20.  3  1  2  2  1  1  8  0  6  0      0.0  10375.7222  0.00000  0.00000  0.00000
21.  3  1  2  2  1  1  6  0  4  0      0.0  10375.7336  0.00000  0.00000  0.00000
22.  3  1  2  2  1  1  4  0  2  0      0.0  10375.8460  0.00000  0.00000  0.00000

23.  3  1  2  2  1  1  4  0  2  0  1621.7  10375.7337 -0.05040 -0.00763 -0.00038
24.  3  1  2  2  1  1  4  0  2  0  2730.2  10375.6810 -0.04780 -0.00297 -0.00097

25.  3  1  2  2  1  1  4  2  2  2  1621.7  10375.3660 -0.26507 -0.04767 -0.00058
26.  3  1  2  2  1  1  4  2  2  2  2219.5  10375.1240 -0.41925 -0.07668 -0.00101
! same Stark lobe but label switch
27.  3  1  2  2  1  1  4  2  4  2  2730.5  10374.8738 -0.61761 -0.12737 -0.00155

28.  3  1  2  2  1  1  6  0  4  0  1621.7  10375.4585 -0.21911 -0.05514 -0.00058
29.  3  1  2  2  1  1  6  0  4  0  2219.5  10375.2200 -0.41004 -0.10315 -0.00109
30.  3  1  2  2  1  1  6  0  4  0  2730.5  10374.9517 -0.61997 -0.15590 -0.00164

31.  3  1  2  2  1  1  6  2  4  2  1621.7  10375.0084 -0.74622 -0.21704 -0.00125
32.  3  1  2  2  1  1  6  2  4  2  2219.5  10374.1135 -1.53034 -0.43254 -0.00244

33.  3  1  2  2  1  1  6  4  4  4  1621.7  10374.8957 -0.75233 -0.11492 -0.00095
34.  3  1  2  2  1  1  6  4  4  4  2219.5  10374.1684 -1.38602 -0.12985 -0.00151

35.  3  1  2  2  1  1  8  0  6  0  2219.5  10375.3130 -0.38983 -0.11342 -0.00111
36.  3  1  2  2  1  1  8  0  6  0  2730.5  10375.0514 -0.61085 -0.17152 -0.00168

37.  3  1  2  2  1  1  8  2  6  2  1621.7  10375.5954 -0.05484  0.00259 -0.00035
38.  3  1  2  2  1  1  8  2  6  2  2730.2  10375.5726 -0.03729  0.02507 -0.00089

39.  3  1  2  2  1  1  8  4  6  4  1621.7  10375.3926 -0.23314 -0.03078 -0.00052
40.  3  1  2  2  1  1  8  4  6  4  2219.5  10375.1631 -0.40866 -0.06689 -0.00098
41.  3  1  2  2  1  1  8  4  6  4  2730.5  10374.9213 -0.61272 -0.11881 -0.00153

42.  3  1  2  2  1  1  8  6  6  6  1621.7  10374.7445 -0.81877 -0.17628 -0.00116
43.  3  1  2  2  1  1  8  6  6  6  2219.5  10373.8723 -1.53854 -0.34743 -0.00219

```

```

!-----
! 212 <- 101 bR
!-----
44.  2  1  2  1  0  1  4  0  4  0      0.0  12297.7820  0.00000  0.00000  0.00000
45.  2  1  2  1  0  1  4  0  2  0      0.0  12297.7948  0.00000  0.00000  0.00000
46.  2  1  2  1  0  1  6  0  4  0      0.0  12298.4177  0.00000  0.00000  0.00000
47.  2  1  2  1  0  1  2  0  0  0      0.0  12298.7520  0.00000  0.00000  0.00000
48.  2  1  2  1  0  1  2  0  2  0      0.0  12298.7827  0.00000  0.00000  0.00000

49.  2  1  2  1  0  1  2  0  0  0  1006.5  12298.9129  0.04610  0.12093 -0.00296
50.  2  1  2  1  0  1  2  0  0  0  1621.8  12299.2063  0.18353  0.31843 -0.00727

51.  2  1  2  1  0  1  2  2  2  2  1006.5  12298.7167 -0.12935  0.10918 -0.00414
52.  2  1  2  1  0  1  2  2  2  2  1621.8  12298.7659 -0.13773  0.29691 -0.00943
53.  2  1  2  1  0  1  2  2  2  2  2121.5  12298.9161 -0.13247  0.51502 -0.01544
54.  2  1  2  1  0  1  2  2  2  2  2533.4  12299.0911 -0.14842  0.73718 -0.02175
! same Stark lobe but label switch
55.  2  1  2  1  0  1  4  2  2  2  2932.6  12299.2995 -0.17727  0.98933 -0.02900
56.  2  1  2  1  0  1  4  2  2  2  3331.2  12299.5456 -0.21550  1.27753 -0.03733

57.  2  1  2  1  0  1  4  0  2  0  1621.8  12298.0610 -0.04805  0.30293 -0.00883
58.  2  1  2  1  0  1  4  0  2  0  2121.5  12298.2484 -0.08194  0.51842 -0.01511
59.  2  1  2  1  0  1  4  0  2  0  2533.4  12298.4375 -0.11643  0.73936 -0.02154
60.  2  1  2  1  0  1  4  0  2  0  2932.6  12298.6558 -0.15539  0.99085 -0.02886
61.  2  1  2  1  0  1  4  0  2  0  3331.2  12298.9049 -0.19958  1.27869 -0.03723

62.  2  1  2  1  0  1  4  2  2  2  1006.5  12297.7776 -0.18312  0.10554 -0.00451

63.  2  1  2  1  0  1  4  2  4  2  1006.5  12297.4339 -0.41122 -0.00066 -0.00242

64.  2  1  2  1  0  1  4  4  4  4  1006.5  12297.6051 -0.30570  0.09729 -0.00534
65.  2  1  2  1  0  1  4  4  4  4  1621.8  12297.2532 -0.87785  0.24722 -0.01442
66.  2  1  2  1  0  1  4  4  4  4  2121.5  12296.7994 -1.54504  0.42073 -0.02497

67.  2  1  2  1  0  1  6  0  4  0  2121.5  12297.5255 -1.04541  0.04979 -0.00552

```

68.	2	1	2	1	0	1	6	2	4	2	2533.4	12297.4717	-0.89343	0.11130	-0.00385
69.	2	1	2	1	0	1	6	2	4	2	2932.6	12297.2109	-1.16849	0.15122	-0.00497
70.	2	1	2	1	0	1	6	2	4	2	3335.6	12296.9131	-1.49101	0.19726	-0.00631
71.	2	1	2	1	0	1	6	4	4	4	1006.5	12298.4399	-0.07116	0.11311	-0.00375
72.	2	1	2	1	0	1	6	4	4	4	1621.8	12298.5421	-0.09810	0.29955	-0.00917
73.	2	1	2	1	0	1	6	4	4	4	2121.5	12298.7118	-0.12001	0.51584	-0.01536
74.	2	1	2	1	0	1	6	4	4	4	2533.4	12298.8822	-0.14614	0.73731	-0.02174
75.	2	1	2	1	0	1	6	4	4	4	2932.6	12299.0910	-0.17895	0.98919	-0.02902
76.	2	1	2	1	0	1	6	4	4	4	3331.2	12299.3386	-0.21855	1.27731	-0.03736

```

!-----
! 313 <- 202 bR
!-----
77.  3  1  3  2  0  2  6  0  4  0      0.0  15291.7150      0.00000  0.00000  0.00000
78.  3  1  3  2  0  2  8  0  6  0      0.0  15292.3471      0.00000  0.00000  0.00000
79.  3  1  3  2  0  2  4  0  2  0      0.0  15292.5605      0.00000  0.00000  0.00000

80.  3  1  3  2  0  2  4  0  2  0  1510.1  15292.2133  -0.03028 -0.31416  0.00679
81.  3  1  3  2  0  2  4  0  2  0  2524.2  15291.5918  -0.07622 -0.87978  0.01945

82.  3  1  3  2  0  2  6  0  4  0  1510.1  15291.3425  -0.04922 -0.31635  0.00631
83.  3  1  3  2  0  2  6  0  4  0  2028.4  15291.0405  -0.09090 -0.57234  0.01142
84.  3  1  3  2  0  2  6  0  4  0  3035.4  15290.1959  -0.21669 -1.29142  0.02576

85.  3  1  3  2  0  2  6  2  4  2  1510.1  15291.0230  -0.12983 -0.53360  0.01004
86.  3  1  3  2  0  2  6  2  4  2  2028.4  15290.4705  -0.25370 -0.96570  0.01760
87.  3  1  3  2  0  2  6  2  4  2  2524.2  15289.7848  -0.42566 -1.49949  0.02636

88.  3  1  3  2  0  2  6  4  4  4  2524.2  15292.3017  -0.40938  0.79649 -0.03902
89.  3  1  3  2  0  2  6  4  4  4  3036.6  15292.4667  -0.71229  1.13302 -0.05955

90.  3  1  3  2  0  2  8  0  6  0  1510.1  15291.7350  -0.07061 -0.52426  0.01156
91.  3  1  3  2  0  2  8  0  6  0  3035.4  15289.8778  -0.31764 -2.11746  0.04560

92.  3  1  3  2  0  2  8  4  6  4  2028.4  15291.5961  -0.15142 -0.58273  0.00984
93.  3  1  3  2  0  2  8  4  6  4  2524.6  15291.1976  -0.21306 -0.90162  0.01596
94.  3  1  3  2  0  2  8  4  6  4  3035.4  15290.6964  -0.28420 -1.30374  0.02398

95.  3  1  3  2  0  2  8  6  6  6  1510.1  15292.5887  -0.06450  0.29871 -0.01186
96.  3  1  3  2  0  2  8  6  6  6  2028.4  15292.7898  -0.10119  0.54143 -0.02100
97.  3  1  3  2  0  2  8  6  6  6  2524.2  15293.0500  -0.13856  0.84142 -0.03206
98.  3  1  3  2  0  2  8  6  6  6  2524.2  15293.0500  -0.13856  0.84142 -0.03206
99.  3  1  3  2  0  2  8  6  6  6  3036.6  15293.3686  -0.18110  1.22081 -0.04589

```

```

////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////
//////////////////////////////////////////////////////////////// cut here - please display and print using a fixed width font //
////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////

```

QSTARK - Fully diagonalizing fit of Stark shifts in a rotor
with zero or one quadrupolar nuclei

version 26.VIII.2022

Zbigniew KISIEL

```

-----
Stark electrode calibration
methyl cyanide, ground state, 20.X.2022 Ne carrier
-----

```

Calculation for J and F exceeding the value in data by at least 1
The fit will be made to TRANSITION FREQUENCIES

```

28 Lines read in
28 Lines fitted  --->   3 field free and   25 at non-zero field
 1 Constants fitted

```

TRANSITIONS (F and MF in units of 1/2):

	J	K	K	<-	J	K	K	F	MF	<-	F	MF	Volts	Obs	Obs-Calc	Calc	Field	Field**2
	-1	+1			-1	+1												
1.	1	0	1		0	0	0	2	2		2	2	0.0	18396.72280	-0.00243	18396.7252	0.0000	0.00
2.	1	0	1		0	0	0	2	0		2	0	3855.1	18397.74070	0.00508	18397.7356	142.9721	20441.02
3.	1	0	1		0	0	0	2	2		2	2	3855.1	18398.11100	-0.00123	18398.1122	142.9721	20441.02

4.	1	0	1	0	0	0	2	0	2	0	5465.2	18398.75410	-0.00158	18398.7557	202.6851	41081.23
5.	1	0	1	0	0	0	2	2	2	2	5465.2	18399.23890	-0.00631	18399.2452	202.6851	41081.23
6.	1	0	1	0	0	0	2	0	2	0	6677.1	18399.74830	-0.00748	18399.7558	247.6302	61320.70
7.	1	0	1	0	0	0	2	2	2	2	6677.1	18400.28450	-0.00647	18400.2910	247.6302	61320.70
8.	1	0	1	0	0	0	2	0	2	0	7686.2	18400.74200	0.00131	18400.7407	285.0541	81255.87
9.	1	0	1	0	0	0	2	2	2	2	7686.2	18401.29420	-0.00582	18401.3000	285.0541	81255.87
10.	1	0	1	0	0	0	2	0	2	0	8487.6	18401.61790	-0.00345	18401.6213	314.7753	99083.46
11.	1	0	1	0	0	0	2	2	2	2	8487.6	18402.18900	-0.00541	18402.1944	314.7753	99083.46

23.	1	0	1	0	0	0	0	0	2	0	0.0	18399.89170	-0.00069	18399.8924	0.0000	0.00
24.	1	0	1	0	0	0	0	0	2	0	3855.1	18401.55770	-0.00055	18401.5583	142.9721	20441.02
25.	1	0	1	0	0	0	0	0	2	0	5465.2	18403.61480	0.00141	18403.6134	202.6851	41081.23
26.	1	0	1	0	0	0	0	0	2	0	6677.1	18405.78340	-0.00078	18405.7842	247.6302	61320.70
27.	1	0	1	0	0	0	0	0	2	0	7686.2	18407.97260	-0.00419	18407.9768	285.0541	81255.87
28.	1	0	1	0	0	0	4	0	2	0	8487.6	18409.94610	-0.01155	18409.9576	314.7753	99083.46

ITERATION NO = 1 CONSTANTS, deviations and changes:

TRANSITIONS (F and MF in units of 1/2):

12.	1	0	1	0	0	0	4	0	2	0	0.0	18397.99550	-0.00101	18397.9965	0.0000	0.00
13.	1	0	1	0	0	0	4	0	2	0	3855.1	18399.65030	0.00081	18399.6495	142.9218	20426.63
14.	1	0	1	0	0	0	4	2	2	2	3855.1	18399.93240	0.00398	18399.9284	142.9218	20426.63
15.	1	0	1	0	0	0	4	0	2	0	5465.2	18400.94270	-0.00269	18400.9454	202.6137	41052.31
16.	1	0	1	0	0	0	4	2	2	2	5465.2	18402.14970	0.00369	18402.1460	202.6137	41052.31
17.	1	0	1	0	0	0	4	0	2	0	6677.1	18402.05450	-0.00561	18402.0601	247.5430	61277.53
18.	1	0	1	0	0	0	4	2	2	2	6677.1	18404.38920	0.00390	18404.3853	247.5430	61277.53
19.	1	0	1	0	0	0	4	0	2	0	7686.2	18403.10580	0.00270	18403.1031	284.9538	81198.65
20.	1	0	1	0	0	0	4	2	2	2	7686.2	18406.61250	0.00106	18406.6114	284.9538	81198.65
21.	1	0	1	0	0	0	0	0	2	0	8487.6	18404.01710	0.00172	18404.0154	314.6644	99013.69
22.	1	0	1	0	0	0	4	2	2	2	8487.6	18408.60600	-0.00384	18408.6098	314.6644	99013.69

Standard deviation = 0.003361

TRANSITIONS (F and MF in units of 1/2):

1.	1	0	1	0	0	0	2	2	2	2	0.0	18396.72280	-0.00243	18396.7252	0.0000	0.00
2.	1	0	1	0	0	0	2	0	2	0	3855.1	18397.74070	0.00580	18397.7349	142.9217	20426.62
3.	1	0	1	0	0	0	2	2	2	2	3855.1	18398.11100	-0.00039	18398.1114	142.9217	20426.62
4.	1	0	1	0	0	0	2	0	2	0	5465.2	18398.75410	-0.00015	18398.7543	202.6137	41052.29
5.	1	0	1	0	0	0	2	2	2	2	5465.2	18399.23890	-0.00479	18399.2437	202.6137	41052.29
6.	1	0	1	0	0	0	2	0	2	0	6677.1	18399.74830	-0.00535	18399.7536	247.5429	61277.50
7.	1	0	1	0	0	0	2	2	2	2	6677.1	18400.28450	-0.00426	18400.2888	247.5429	61277.50
8.	1	0	1	0	0	0	2	0	2	0	7686.2	18400.74200	0.00413	18400.7379	284.9537	81198.62
9.	1	0	1	0	0	0	2	2	2	2	7686.2	18401.29420	-0.00294	18401.2971	284.9537	81198.62
10.	1	0	1	0	0	0	2	0	2	0	8487.6	18401.61790	0.00000	18401.6179	314.6644	99013.66
11.	1	0	1	0	0	0	2	2	2	2	8487.6	18402.18900	-0.00192	18402.1909	314.6644	99013.66

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12.	1	0	1	0	0	0	4	0	2	0	0.0	18397.99550	-0.00101	18397.9965	0.0000	0.00
13.	1	0	1	0	0	0	4	0	2	0	3855.1	18399.65030	0.00081	18399.6495	142.9217	20426.62
14.	1	0	1	0	0	0	4	2	2	2	3855.1	18399.93240	0.00398	18399.9284	142.9217	20426.62
15.	1	0	1	0	0	0	4	0	2	0	5465.2	18400.94270	-0.00269	18400.9454	202.6137	41052.29
16.	1	0	1	0	0	0	4	2	2	2	5465.2	18402.14970	0.00369	18402.1460	202.6137	41052.29
17.	1	0	1	0	0	0	4	0	2	0	6677.1	18402.05450	-0.00561	18402.0601	247.5429	61277.50
18.	1	0	1	0	0	0	4	2	2	2	6677.1	18404.38920	0.00390	18404.3853	247.5429	61277.50
19.	1	0	1	0	0	0	4	0	2	0	7686.2	18403.10580	0.00270	18403.1031	284.9537	81198.62
20.	1	0	1	0	0	0	4	2	2	2	7686.2	18406.61250	0.00106	18406.6114	284.9537	81198.62
21.	1	0	1	0	0	0	0	0	2	0	8487.6	18404.01710	0.00172	18404.0154	314.6644	99013.66
22.	1	0	1	0	0	0	4	2	2	2	8487.6	18408.60600	-0.00383	18408.6098	314.6644	99013.66

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23.	1	0	1	0	0	0	0	0	2	0	0.0	18399.89170	-0.00069	18399.8924	0.0000	0.00
24.	1	0	1	0	0	0	0	0	2	0	3855.1	18401.55770	0.00078	18401.5569	142.9217	20426.62
25.	1	0	1	0	0	0	0	0	2	0	5465.2	18403.61480	0.00445	18403.6104	202.6137	41052.29
26.	1	0	1	0	0	0	0	0	2	0	6677.1	18405.78340	0.00393	18405.7795	247.5429	61277.50
27.	1	0	1	0	0	0	0	0	2	0	7686.2	18407.97260	0.00214	18407.9705	284.9537	81198.62
28.	1	0	1	0	0	0	4	0	2	0	8487.6	18409.94610	-0.00377	18409.9499	314.6644	99013.66

Standard deviation = 0.003361

ITERATION NO = 3 CONSTANTS, deviations and changes:

d = 26.973503266 +- 0.001689792 0.000000000

FINAL RESULTS OF LEAST SQUARES FITTING PROCEDURE

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FITTED CONSTANTS:

A	/MHz	148900.1236	1:Xab /MHz	0.
B	/MHz	9198.899299	1:XJ.a/kHz	0.
C	/MHz	9198.899299	1:XK.a/kHz	0.
DJ	/kHz	3.804801256	1:XJbc/kHz	0.
DJK	/kHz	177.417	1:Ma /MHz	-0.0007
DK	/kHz	2830.04	1:Mb-c/MHz	0.
dJ	/kHz	0.	1:Tr /MHz	-0.0044
dK	/kHz	0.	1:Xd /kHz	0.
HJ	/ Hz	-0.014	1:Xbc /MHz	0.
HJK	/ Hz	0.	1:Xac /MHz	0.
HKJ	/ Hz	0.		
HK	/ Hz	0.		
hJ	/ Hz	0.		
hJK	/ Hz	0.	Mu.a /D	3.92197
hK	/ Hz	0.	Mu.b /D	0.
LKKJ	/mHz	0.	Mu.c /D	0.
1:Xa /MHz	-4.22534		d /cm	26.9735(16)
1:Xb-c/MHz	0.		k /cm	0.
1:X.bb /MHz	2.112670000000			
1:X.cc /MHz	2.112670000000			

WORST FITTED LINES:

	J	K	K	<-	J	K	K	F	MF	<-	F	MF	Volts	Obs	Obs-Calc	Calc	Field	Field**2
	-1	+1			-1	+1												
2.	1	0	1	0	0	0	2	0	2	0	3855.1	18397.74070	0.00580	18397.7349	142.9217	20426.62		
17.	1	0	1	0	0	0	4	0	2	0	6677.1	18402.05450	-0.00561	18402.0601	247.5429	61277.50		
6.	1	0	1	0	0	0	2	0	2	0	6677.1	18399.74830	-0.00535	18399.7536	247.5429	61277.50		
5.	1	0	1	0	0	0	2	2	2	2	5465.2	18399.23890	-0.00479	18399.2437	202.6137	41052.29		
25.	1	0	1	0	0	0	0	0	2	0	5465.2	18403.61480	0.00445	18403.6104	202.6137	41052.29		

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QSTARK - Fully diagonalizing fit of Stark shifts in a rotor
with zero or one quadrupolar nuclei

version 26.VIII.2022

Zbigniew KISIEL

Stark electrode calibration
methyl iodide, ground state, 20.X.2022, Ne carrier

Calculation for J and F exceeding the value in data by at least 1
The fit will be made to TRANSITION FREQUENCIES

31 Lines read in
30 Lines fitted ----> 3 field free and 27 at non-zero field
1 Constants fitted

TRANSITIONS (F and MF in units of 1/2):

	J	K	K	<-	J	K	K	F	MF	<-	F	MF	Volts	Obs	Obs-Calc	Calc	Field	Field**2
	-1	+1			-1	+1												
1.	1	0	1	0	0	0		5	1	5	1		0.0	14694.92870	-0.00108	14694.9298	0.0000	0.00
2.	1	0	1	0	0	0		5	3	5	3		6269.7	14695.70170	0.00220	14695.6995	232.4694	54042.03
3.	1	0	1	0	0	0		5	5	5	5		6269.7	14696.07190	-0.00007	14696.0720	232.4694	54042.03
4.	1	0	1	0	0	0		5	3	5	3		8695.4	14696.41330	0.00347	14696.4098	322.4101	103948.26
5.	1	0	1	0	0	0		5	5	5	5		8695.4	14697.12490	-0.00124	14697.1261	322.4101	103948.26
6.	1	0	1	0	0	0		5	3	5	3		10920.8	14697.26250	-0.00092	14697.2634	404.9240	163963.44
7.	1	0	1	0	0	0		5	5	5	5		10920.8	14698.39000	-0.00306	14698.3931	404.9240	163963.44
8.	1	0	1	0	0	0		5	3	5	3		12324.2	0.00000	-14697.90086--	14697.9009	456.9596	208812.06
9.	1	0	1	0	0	0		5	5	5	5		12324.2	14699.33230	-0.00697	14699.3393	456.9596	208812.06
10.	1	0	1	0	0	0		7	1	5	1		0.0	15100.74080	-0.00561	15100.7464	0.0000	0.00
11.	1	0	1	0	0	0		7	1	5	1		6269.7	15101.72590	0.00472	15101.7212	232.4694	54042.03
12.	1	0	1	0	0	0		7	3	5	3		6269.7	15101.66660	0.00409	15101.6625	232.4694	54042.03
13.	1	0	1	0	0	0		7	5	5	5		6269.7	15101.54880	0.00404	15101.5448	232.4694	54042.03
14.	1	0	1	0	0	0		7	1	5	1		8695.4	15102.62450	0.00438	15102.6201	322.4101	103948.26
15.	1	0	1	0	0	0		7	3	5	3		8695.4	15102.51060	0.00255	15102.5081	322.4101	103948.26
16.	1	0	1	0	0	0		7	5	5	5		8695.4	15102.28560	0.00316	15102.2824	322.4101	103948.26
17.	1	0	1	0	0	0		7	1	5	1		10920.8	15103.69970	0.00015	15103.6996	404.9240	163963.44
18.	1	0	1	0	0	0		7	3	5	3		10920.8	15103.52500	0.00071	15103.5243	404.9240	163963.44
19.	1	0	1	0	0	0		7	5	5	5		10920.8	15103.17040	0.00032	15103.1701	404.9240	163963.44
20.	1	0	1	0	0	0		7	1	5	1		12324.2	15104.50190	-0.00317	15104.5051	456.9596	208812.06
21.	1	0	1	0	0	0		7	3	5	3		12324.2	15104.28100	-0.00229	15104.2833	456.9596	208812.06
22.	1	0	1	0	0	0		7	5	5	5		12324.2	15103.83220	-0.00158	15103.8338	456.9596	208812.06
23.	1	0	1	0	0	0		3	1	5	1		0.0	15275.89340	0.00020	15275.8932	0.0000	0.00
24.	1	0	1	0	0	0		3	1	5	1		6269.7	15276.73940	0.00326	15276.7361	232.4694	54042.03
25.	1	0	1	0	0	0		3	3	5	3		6269.7	15276.65350	0.00356	15276.6499	232.4694	54042.03
26.	1	0	1	0	0	0		3	1	5	1		8695.4	15277.51940	0.00369	15277.5157	322.4101	103948.26
27.	1	0	1	0	0	0		3	3	5	3		8695.4	15277.35310	0.00362	15277.3495	322.4101	103948.26
28.	1	0	1	0	0	0		3	1	5	1		10920.8	15278.45450	-0.00014	15278.4546	404.9240	163963.44
29.	1	0	1	0	0	0		3	3	5	3		10920.8	15278.19200	0.00037	15278.1916	404.9240	163963.44
30.	1	0	1	0	0	0		3	1	5	1		12324.2	15279.15630	-0.00103	15279.1573	456.9596	208812.06
31.	1	0	1	0	0	0		3	3	5	3		12324.2	15278.82040	-0.00120	15278.8216	456.9596	208812.06

Standard deviation = 0.003062

ITERATION NO = 1 CONSTANTS, deviations and changes:

d = 26.971915388 +- 0.003341456 0.001915388

TRANSITIONS (F and MF in units of 1/2):

	J	K	K	<-	J	K	K	F	MF	<-	F	MF	Volts	Obs	Obs-Calc	Calc	Field	Field**2
	-1	+1			-1	+1												
1.	1	0	1	0	0	0		5	1	5	1		0.0	14694.92870	-0.00108	14694.9298	0.0000	0.00
2.	1	0	1	0	0	0		5	3	5	3		6269.7	14695.70170	0.00231	14695.6994	232.4529	54034.35
3.	1	0	1	0	0	0		5	5	5	5		6269.7	14696.07190	0.00009	14696.0718	232.4529	54034.35
4.	1	0	1	0	0	0		5	3	5	3		8695.4	14696.41330	0.00368	14696.4096	322.3872	103933.50
5.	1	0	1	0	0	0		5	5	5	5		8695.4	14697.12490	-0.00092	14697.1258	322.3872	103933.50
6.	1	0	1	0	0	0		5	3	5	3		10920.8	14697.26250	-0.00059	14697.2631	404.8952	163940.15
7.	1	0	1	0	0	0		5	5	5	5		10920.8	14698.39000	-0.00257	14698.3926	404.8952	163940.15
8.	1	0	1	0	0	0		5	3	5	3		12324.2	0.00000	-14697.90044--	14697.9004	456.9271	208782.41
9.	1	0	1	0	0	0		5	5	5	5		12324.2	14699.33230	-0.00635	14699.3386	456.9271	208782.41

10.	1	0	1	0	0	0	7	1	5	1	0.0	15100.74080	-0.00561	15100.7464	0.0000	0.00
11.	1	0	1	0	0	0	7	1	5	1	6269.7	15101.72590	0.00485	15101.7210	232.4529	54034.35
12.	1	0	1	0	0	0	7	3	5	3	6269.7	15101.66660	0.00422	15101.6624	232.4529	54034.35
13.	1	0	1	0	0	0	7	5	5	5	6269.7	15101.54880	0.00415	15101.5446	232.4529	54034.35
14.	1	0	1	0	0	0	7	1	5	1	8695.4	15102.62450	0.00465	15102.6199	322.3872	103933.50
15.	1	0	1	0	0	0	7	3	5	3	8695.4	15102.51060	0.00280	15102.5078	322.3872	103933.50
16.	1	0	1	0	0	0	7	5	5	5	8695.4	15102.28560	0.00338	15102.2822	322.3872	103933.50
17.	1	0	1	0	0	0	7	1	5	1	10920.8	15103.69970	0.00056	15103.6991	404.8952	163940.15
18.	1	0	1	0	0	0	7	3	5	3	10920.8	15103.52500	0.00111	15103.5239	404.8952	163940.15
19.	1	0	1	0	0	0	7	5	5	5	10920.8	15103.17040	0.00067	15103.1697	404.8952	163940.15
20.	1	0	1	0	0	0	7	1	5	1	12324.2	15104.50190	-0.00264	15104.5045	456.9271	208782.41
21.	1	0	1	0	0	0	7	3	5	3	12324.2	15104.28100	-0.00179	15104.2828	456.9271	208782.41
22.	1	0	1	0	0	0	7	5	5	5	12324.2	15103.83220	-0.00114	15103.8333	456.9271	208782.41

23.	1	0	1	0	0	0	3	1	5	1	0.0	15275.89340	0.00020	15275.8932	0.0000	0.00
24.	1	0	1	0	0	0	3	1	5	1	6269.7	15276.73940	0.00338	15276.7360	232.4529	54034.35
25.	1	0	1	0	0	0	3	3	5	3	6269.7	15276.65350	0.00366	15276.6498	232.4529	54034.35
26.	1	0	1	0	0	0	3	1	5	1	8695.4	15277.51940	0.00392	15277.5155	322.3872	103933.50
27.	1	0	1	0	0	0	3	3	5	3	8695.4	15277.35310	0.00382	15277.3493	322.3872	103933.50
28.	1	0	1	0	0	0	3	1	5	1	10920.8	15278.45450	0.00022	15278.4543	404.8952	163940.15
29.	1	0	1	0	0	0	3	3	5	3	10920.8	15278.19200	0.00070	15278.1913	404.8952	163940.15
30.	1	0	1	0	0	0	3	1	5	1	12324.2	15279.15630	-0.00057	15279.1569	456.9271	208782.41
31.	1	0	1	0	0	0	3	3	5	3	12324.2	15278.82040	-0.00079	15278.8212	456.9271	208782.41

Standard deviation = 0.003045

ITERATION NO = 2 CONSTANTS, deviations and changes:

d = 26.971915593 +- 0.003323180 0.000000205

TRANSITIONS (F and MF in units of 1/2):

	J	K	K	<-	J	K	K	F	MF	<-	F	MF	Volts	Obs	Obs-Calc	Calc	Field	Field**2
	-1	+1			-1	+1												
1.	1	0	1	0	0	0		5	1	5	1		0.0	14694.92870	-0.00108	14694.9298	0.0000	0.00
2.	1	0	1	0	0	0		5	3	5	3		6269.7	14695.70170	0.00231	14695.6994	232.4529	54034.35
3.	1	0	1	0	0	0		5	5	5	5		6269.7	14696.07190	0.00009	14696.0718	232.4529	54034.35
4.	1	0	1	0	0	0		5	3	5	3		8695.4	14696.41330	0.00368	14696.4096	322.3872	103933.50
5.	1	0	1	0	0	0		5	5	5	5		8695.4	14697.12490	-0.00092	14697.1258	322.3872	103933.50
6.	1	0	1	0	0	0		5	3	5	3		10920.8	14697.26250	-0.00059	14697.2631	404.8952	163940.15
7.	1	0	1	0	0	0		5	5	5	5		10920.8	14698.39000	-0.00257	14698.3926	404.8952	163940.15
8.	1	0	1	0	0	0		5	3	5	3		12324.2	0.00000	-14697.90044--	14697.9004	456.9271	208782.40
9.	1	0	1	0	0	0		5	5	5	5		12324.2	14699.33230	-0.00635	14699.3386	456.9271	208782.40

10.	1	0	1	0	0	0	7	1	5	1	0.0	15100.74080	-0.00561	15100.7464	0.0000	0.00
11.	1	0	1	0	0	0	7	1	5	1	6269.7	15101.72590	0.00485	15101.7210	232.4529	54034.35
12.	1	0	1	0	0	0	7	3	5	3	6269.7	15101.66660	0.00422	15101.6624	232.4529	54034.35
13.	1	0	1	0	0	0	7	5	5	5	6269.7	15101.54880	0.00415	15101.5446	232.4529	54034.35
14.	1	0	1	0	0	0	7	1	5	1	8695.4	15102.62450	0.00465	15102.6199	322.3872	103933.50
15.	1	0	1	0	0	0	7	3	5	3	8695.4	15102.51060	0.00280	15102.5078	322.3872	103933.50
16.	1	0	1	0	0	0	7	5	5	5	8695.4	15102.28560	0.00338	15102.2822	322.3872	103933.50
17.	1	0	1	0	0	0	7	1	5	1	10920.8	15103.69970	0.00056	15103.6991	404.8952	163940.15
18.	1	0	1	0	0	0	7	3	5	3	10920.8	15103.52500	0.00111	15103.5239	404.8952	163940.15
19.	1	0	1	0	0	0	7	5	5	5	10920.8	15103.17040	0.00067	15103.1697	404.8952	163940.15
20.	1	0	1	0	0	0	7	1	5	1	12324.2	15104.50190	-0.00264	15104.5045	456.9271	208782.40
21.	1	0	1	0	0	0	7	3	5	3	12324.2	15104.28100	-0.00179	15104.2828	456.9271	208782.40
22.	1	0	1	0	0	0	7	5	5	5	12324.2	15103.83220	-0.00114	15103.8333	456.9271	208782.40

23.	1	0	1	0	0	0	3	1	5	1	0.0	15275.89340	0.00020	15275.8932	0.0000	0.00
24.	1	0	1	0	0	0	3	1	5	1	6269.7	15276.73940	0.00338	15276.7360	232.4529	54034.35
25.	1	0	1	0	0	0	3	3	5	3	6269.7	15276.65350	0.00366	15276.6498	232.4529	54034.35
26.	1	0	1	0	0	0	3	1	5	1	8695.4	15277.51940	0.00392	15277.5155	322.3872	103933.50
27.	1	0	1	0	0	0	3	3	5	3	8695.4	15277.35310	0.00382	15277.3493	322.3872	103933.50
28.	1	0	1	0	0	0	3	1	5	1	10920.8	15278.45450	0.00022	15278.4543	404.8952	163940.15
29.	1	0	1	0	0	0	3	3	5	3	10920.8	15278.19200	0.00070	15278.1913	404.8952	163940.15
30.	1	0	1	0	0	0	3	1	5	1	12324.2	15279.15630	-0.00057	15279.1569	456.9271	208782.40
31.	1	0	1	0	0	0	3	3	5	3	12324.2	15278.82040	-0.00079	15278.8212	456.9271	208782.40

Standard deviation = 0.003045

ITERATION NO = 3 CONSTANTS, deviations and changes:

d = 26.971915593 +- 0.003323180 0.000000000

FINAL RESULTS OF LEAST SQUARES FITTING PROCEDURE
=====

FITTED CONSTANTS:

A

/MHz

155094.63

B

/MHz

7501.275744

C

/MHz

7501.275744

DJ

/kHz

6.307543

DJK

/kHz

98.7688

DK

/kHz

2689.14

dJ

/kHz

0.

dK

/kHz

0.

HJ

/ Hz

-0.003452

HJK

/ Hz

0.05847

HKJ

/ Hz

4.617

HK

/ Hz

0.

hJ

/ Hz

0.

hJK

/ Hz

0.

hK

/ Hz

0.

LKKJ

/mHz

0.

1:Xa

/MHz

-1934.1395

1:Xb-c

/MHz

0.

1:X.bb

/MHz

967.069750000000

1:X.cc

/MHz

967.069750000000

1:Xab

/MHz

0.

1:XJ.a

/kHz

0.

1:XK.a

/kHz

0.

1:XJbc

/kHz

0.

1:Ma

/MHz

-0.017383

1:Mb-c

/MHz

0.

1:Tr

/MHz

-0.052223

1:Xd

/kHz

0.

1:Xbc

/MHz

0.

1:Xac

/MHz

0.

Mu.a

/D

1.6406

Mu.b

/D

0.

Mu.c

/D

0.

d

/cm

26.9719 (33)

k

/cm

0.

WORST FITTED LINES:

	J	K	K	<-	J	K	K	F	MF<-	F	MF	Volts	Obs	Obs-Calc	Calc	Field	Field**2
	-1	+1			-1	+1											
9.	1	0	1	0	0	0	0	5	5	5	5	12324.2	14699.33230	-0.00635	14699.3386	456.9271	208782.40
10.	1	0	1	0	0	0	0	7	1	5	1	0.0	15100.74080	-0.00561	15100.7464	0.0000	0.00
11.	1	0	1	0	0	0	0	7	1	5	1	6269.7	15101.72590	0.00485	15101.7210	232.4529	54034.35
14.	1	0	1	0	0	0	0	7	1	5	1	8695.4	15102.62450	0.00465	15102.6199	322.3872	103933.50
12.	1	0	1	0	0	0	0	7	3	5	3	6269.7	15101.66660	0.00422	15101.6624	232.4529	54034.35

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