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New Investigation of Millimeter-Wave Rotational Spectrum of CF_3CN in the Excited Vibrational States $\nu_7 = 1$ and $\nu_8 = 1$

MOTAMEDI, MASOUD* and VAHABZADEH ZARGARI, BAHRAM

The University of Kurdistan,
Sanandaj, Iran

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Abstract: The millimeter-wave rotational spectra of the excited vibrational states $\nu_7 = 1$ and $\nu_8 = 1$ of the symmetric top molecule trifluoroacetonitrile, CF_3CN , have been analyzed again. The $\ell = \pm 1$ series have been assigned and the rotational parameters including $B_7 = 2944.9748(14)$ MHz, $q_t^+ = 1.4505(16)$ MHz for $\nu_7 = 1$ and $B_8 = 2950.4853(4)$ MHz, $q_t^+ = 3.6035(20)$ MHz for $\nu_8 = 1$ states were determined accurately.

Keywords: millimetre-wave rotational spectra, excited vibrational state, symmetric top molecules, CF_3CN

Introduction

Trifluoroacetonitrile, CF_3CN is a symmetric top molecule and belong to the C_{3v} point group. The symmetry species for this point group are A_1 , A_2 , and E. This compound has 8 different fundamental frequencies and $4 + 4 \times 2 = 12$ modes of vibration. The vibrational spectrum of CF_3CN was originally assigned by Edgell and Potter¹. Several authors²⁻⁹ have studied the rotational spectra of the ground state and some excited states. The nuclear quadrupole hyperfine structure observed in the ground vibrational state has been the subject of recent Fourier transform work by Cox et al¹⁰. The lowest doubly degenerate vibrational level, $\nu_8 = 1$, is approximately a $-\text{C}-\text{C} \equiv \text{N}$ bending mode and lies at 192 cm^{-1} and consequently has a population which is 25% of the ground state (ignoring degeneracy) at the temperature of 200 K. The next highest frequency is $\nu_7 = 1$ at 464 cm^{-1} (CF_3 rock), thus has population 3.5% so there is no doubt about the assignment of the series of lines which lie to high frequency of the ground state rotational transitions. Owing to the large dipole moment and the large thermal population, the spectra are intense. The aim of this study is determination of rotational parameters for mixing the low and high J values, which are more accurate and reliable.

Theory

Rotational frequencies for transitions $J \rightarrow J + 1$ in the excited degenerate vibrational state $v_t = 1$, $\ell_t = \pm 1$ of molecules with axial symmetry were calculated by Nielsen¹¹. Although this theory was fairly satisfactory for the rotation spectrum of these types of molecules, but some of the calculated frequencies by this method were different from the observed frequencies. This formula was extended to the case of higher J values by Gordy *et al.*¹². The frequency of transition $J \rightarrow J + 1$ for molecules belonging to the point group C_{3v} in singly excited vibrational state $v_t = 1$ is given by the approximate perturbation expression, Eq (1).

$$v = 2B(J + 1) - 4D_J(J + 1)^3 - 2D_{JK}(J + 1)k^2 + 2\eta_J(J + 1)k\ell + \Delta v \quad (1)$$

where Δv has the value $\pm q_t^+(J + 1)$ if $(k\ell - 1) = 0$ (ℓ - type doubling) or

$$\Delta v = -\frac{(q_t^+)^2(J + 1)^3}{4(B - A + A\zeta)(k\ell - 1)} \quad \text{if } (k\ell - 1) \neq 0 \quad (\ell \text{ - type resonance}) \quad (2)$$

Because of a degenerate vibrational state, additional parameters were involved in the calculation of the energy levels. The extra parameters, q_t^+ (ℓ -type coupling constant), $A\zeta$ and η_J which gives the J and k dependence of $A\zeta$, are necessary to determine the frequency of spectra. ℓ is the vibrational angular momentum quantum number and can accept the value $\ell = \pm 1$; therefore, there are two different series in the spectrum. Eq (1) shows a pattern for doubly degenerate states of a C_{3v} molecule that is predominately due to the splitting of the positive and negative series by ℓ -type resonance. As can be seen in Eq (2), this resonance is inversely proportional to $(k\ell - 1)$. Thus, one series goes from high frequency at low k to low frequency at high k , while the other is at low frequency.

In order to obtain more accuracy in rotational energies for singly excited vibrational states than can be obtained from perturbation theory, it is necessary to set up a rotational Hamiltonian as a matrix (H) in equation $H\psi = E\psi$ and diagonalise to obtain the energy^{13,14}. The Hamiltonian was set up for a symmetric top molecule like CF_3CN . This rotation-vibrational Hamiltonian has two different blocks that belong to the different $\ell = +1$ and $\ell = -1$ series. k and ℓ are no longer good quantum numbers, but $(k - \ell)$ or $(k\ell - 1)$ may be used to distinguish between the symmetry species. Those levels with $(k\ell - 1) = 3n$, where n is an integer, are of species A_1 or A_2 . If $(k\ell - 1) \neq 3n$ the species are E . The q_t^+ produces a first order splitting of the $(k\ell - 1) = 0$, A_1A_2 pair, which are the familiar ℓ -doublets, as shown by Grenier-Besson and Amat¹⁵. The main difference from the ground state spectra is the splitting of the $|k - \ell| = 0$ into two widely separate ℓ -doublets and the splitting due to ℓ -resonance.

The diagonal matrix elements are given by :

$$\langle v_t, \ell_t, J, k | H/h | v_t, \ell_t, J, k \rangle = BJ(J + 1) + (A - B)k^2 - 2A\zeta k\ell - D_J J^2(J + 1)^2 - D_{JK} J(J + 1)k^2 - D_K k^4 + \eta_J J(J + 1)k\ell + \eta_K k^3\ell + H_J J^3(J + 1)^3 + H_{JK} J^2(J + 1)^2 k^2 + H_{KJ} J(J + 1)k^4 + H_K k^6 \quad (3)$$

In addition, there are off-diagonal terms that arise from the transformation. The major one of these gives rise to the ℓ doubling:

$$\langle v_t, \ell, J, k | H/h | v_t, \ell \pm 2, J, k \pm 2 \rangle = -\frac{1}{4} q_t^+ \{ (v_t \mp \ell)(v_t \pm \ell + 2)[J(J + 1) - k(k \pm 1)] [J(J + 1) - (k \pm 1)(k \pm 2)] \}^{1/2} \quad (4)$$

$$\text{and } \langle v_t, \ell, J, k | H/h | v_t, \ell \pm 2, J, k \mp 1 \rangle = -r_t [(v_t + 1)^2 - (\ell \pm 1)^2]^{1/2} [J(J + 1)$$

$$-k(k \mp 1)]^{1/2}(2k \mp 1) \quad (5)$$

and hence, the lines can be assigned. The results of refinement are listed in Table 2, and the values of the constants obtained are shown in Table 3.

Results and Discussion

$v_7 = 1$ State

Whittle et al.⁴ measured spectra at low- J where the ℓ -resonance effects are very small and nuclear quadrupole coupling effects are important and hence they were unable to determine a value for $A\zeta$. Carpenter and co-workers determined $A\zeta$ and other structural parameters at high J value precisely⁶. The B_7 in this state is only slightly smaller than the ground state value; consequently, the spectrum lies amongst the much stronger transitions due to the ground state (Fig 1).

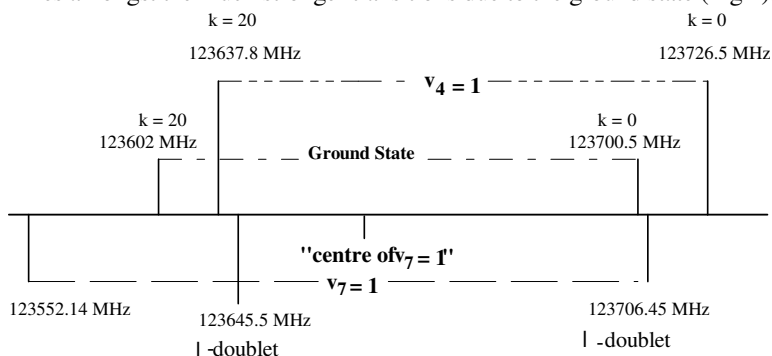


Figure 1. Relative position of ground, $v_4 = 1$ and $v_7 = 1$ states for $J = 20$ of CF_3CN

In this work, some of the frequencies selected from ref⁴ and all of the frequencies from ref⁶ have been mixed and refined them together by least square method¹⁶. If all the sextic constants were included in the fit, these were not only strongly correlated but also had standard deviations which were of about the same absolute magnitudes as the quantities themselves. This means that actual values are not significant, hence all were set to zero. Due to increasing of data from low and high J values our results are more reliable. A least-squares refinement of the 80 observations was carried out using the programme¹⁶. The results of fitting are given in Table 1 and obtained results are shown in Table 2. The Fortrat-like diagram in this state is shown in Fig. 2. This diagram shows that the ' ℓ ' doublet splitting is smaller than this term in the $v_8 = 1$ state (Fig 3).

In $v_7 = 1$ state the most important splitting for $(k\ell - 1) \neq 0$ is due to the centrifugal distortion η_J because the term $|B - A + A\zeta|$ has the very large value of 2952 MHz. This experiment gives $A\zeta = -197.8$ (58.8) MHz. The lack of precision is a consequence of the weak ℓ -resonance and that many of the lower $k\ell - 1$ lines are obscured by the ground state. The parameter η_J , which is to be regarded as a type of centrifugal distortion constant, has a negative value. As can be seen from Eq (6)

$$v = 2B(J+1) - 4D_J(J+1)^3 - 2D_{JK}(J+1)k^2 + 2\eta_J(J+1)k\ell + \Delta v \quad (6)$$

this results in the positive series being displaced to lower frequency and the negative series to higher frequency. The prediction list produced after final fitting shows that the microwave lines of $v_7 = 1$ state seen by Whittle et al.⁴ consisted of many overlapping lines for $J'' = 4$ and 5. According to this prediction list most of their assignment of the positive series is incorrect but based on our obtained constants, there is good agreement with negative series. Investigation in ground, $v_4 = 1$ and $v_7 = 1$ states show that they overlapped to each other (see Fig 1, the scale is arbitrary).

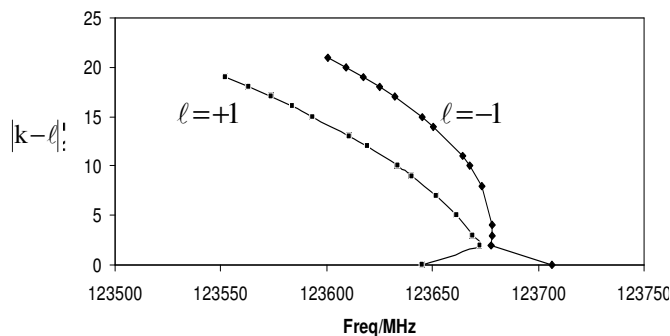


Figure 2 Fortrat - like diagram of CF_3CN in $v_7=1$ State. $J = 20 \rightarrow 21$

Table 1. Results of Refinement of Observed Frequencies for CF_3CN in $v_7 = 1$ State.

	J	k	ℓ	Fobs / MHz	o-c / MHz	error / MHz
1	4	3	1	29448.420	0.226	0.4
2	4	2	1	29448.840	0.044	0.3
3	4	0	1	29449.800	0.228	0.4
4	5	4	1	35337.110	0.213	0.4
5	5	3	1	35337.850	0.093	0.3
6	5	2	1	35338.460	-0.025	0.3
7	5	5	-1	35339.500	0.139	0.3
8	5	0	-1	35339.400	0.007	0.3
9	5	4	-1	35339.620	-0.041	0.3
10	5	1	-1	35339.800	0.112	0.3
11	5	1	1	35347.600	-0.114	0.2
12	5	-1	-1	35330.300	-0.007	0.2
13	19	2	-1	117789.986	0.047	0.3
14	19	3	-1	117789.986	-0.030	0.3
15	19	6	-1	117787.097	-0.059	0.3
16	19	7	-1	117785.153	-0.062	0.2
17	19	9	-1	117779.820	-0.054	0.2
18	19	10	-1	117776.445	-0.032	0.2
19	19	11	-1	117772.638	0.041	0.2
20	19	12	-1	117768.305	0.071	0.3
21	19	13	-1	117763.417	0.028	0.2
22	19	14	-1	117758.126	0.065	0.3
23	19	2	1	117787.097	-0.108	0.3
24	19	4	1	117781.022	-0.024	0.2
25	19	6	1	117773.691	-0.033	0.2
26	19	7	1	117769.391	0.002	0.2
27	19	8	1	117764.579	-0.008	0.2
28	19	10	1	117753.590	0.028	0.2
29	20	-1	-1	123706.428	-0.004	0.2
30	20	1	-1	123677.565	-0.013	0.3
31	20	2	-1	123678.361	0.046	0.3
32	20	3	-1	123678.361	-0.047	0.3
33	20	7	-1	123673.353	-0.033	0.2

34	20	9	-1	123667.737	-0.045	0.2
35	20	10	-1	123664.133	-0.084	0.2
36	20	13	-1	123650.457	-0.020	0.2
37	20	14	-1	123644.922	0.038	0.2
38	20	16	-1	123632.172	-0.008	0.2
39	20	17	-1	123625.046	-0.024	0.2
40	20	18	-1	123617.459	0.006	0.2
41	20	19	-1	123609.300	-0.031	0.2
42	20	20	-1	123600.737	0.034	0.2
43	20	3	1	123672.340	-0.002	0.2
44	20	4	1	123669.073	-0.007	0.2
45	20	6	1	123661.378	0.007	0.2
46	20	8	1	123651.807	0.038	0.2
47	20	10	1	123640.210	0.023	0.2
48	20	11	1	123633.622	-0.025	0.2
49	20	13	1	123619.137	0.077	0.2
50	20	14	1	123610.942	-0.070	0.2
51	20	16	1	123593.410	0.005	0.2
52	20	17	1	123583.839	-0.007	0.2
53	20	18	1	123573.754	-0.028	0.2
54	20	19	1	123563.171	-0.043	0.2
55	20	20	1	123552.060	-0.081	0.2
56	21	1	1	129596.073	0.033	0.2
57	21	1	-1	129565.711	-0.016	0.3
58	21	2	-1	129566.562	0.036	0.3
59	21	3	-1	129566.562	-0.077	0.3
60	21	6	-1	129563.470	-0.058	0.3
61	21	7	-1	129561.391	-0.007	0.2
62	21	8	-1	129558.678	-0.054	0.3
63	21	9	-1	129555.532	0.000	0.2
64	21	10	-1	129551.726	-0.072	0.2
65	21	12	-1	129542.802	0.066	0.2
66	21	13	-1	129537.442	0.034	0.2
67	21	14	-1	129531.560	0.011	0.2
68	21	17	-1	129510.805	0.012	0.2
69	21	18	-1	129502.870	0.056	0.2
70	21	-2	-1	129563.876	-0.084	0.3
71	21	3	1	129560.433	0.022	0.2
72	21	4	1	129556.990	0.025	0.2
73	21	6	1	129548.972	0.105	0.2
74	21	7	1	129544.057	-0.030	0.2
75	21	8	1	129538.860	0.063	0.2
76	21	10	1	129526.696	0.037	0.2
77	21	11	1	129519.825	0.020	0.2
78	21	13	1	129504.583	0.062	0.2
79	21	14	1	129496.080	-0.009	0.2
80	21	19	1	129446.035	0.025	0.2
sum of squared defects					0.223083	
standard deviation					0.064878	

Table 2 Comparison of rotation-vibration parameters for CF₃CN in $v_7 = 1$ and $v_8 = 1,2,3,4$ states

Parameter	$v_7 = 1$ (Ref 6)	$v_7 = 1$ (this work)	$v_8 = 1$ (Ref 6)	$v_8 = 1$ (this work)	$v_8 = 2$	$v_8 = 3$	$v_8 = 4$
A/MHz	5700.0*	5700.0*	5700.0*	5700.0*	5700.0*	5700.0*	5700.0*
B/MHz	2944.9711 (18)	2944.9748 (14)	2950.4839 (3)	2950.4853 (4)	2955.46351 (49)	2960.4506 (7)	2965.1734(81)
A ζ /MHz	-197.6 (48.3)	-197.8 (58.8)	2991.63 (13)	2991.70 (25)	2964.1 (27)	2985.19 (6)	2978.99 (17)
q _t ⁺ /MHz	1.4512 (14)	1.4505 (16)	3.6028 (11)	3.6035 (20)	3.4673 (20)	3.5982 (3)	3.5806 (6)
r _t	-	-	-	-	-	0.050 (19)	0.0*
D _J /kHz	0.3065 (20)	0.3106 (16)	0.31392 (25)	0.31463 (42)	0.31707 (34)	0.3241 (8)	0.3070 (92)
D _{JK} /kHz	6.01319 (11)	6.0132 (13)	5.7989 (25)	5.8035 (26)	5.8015 (27)	5.7333 (68)	5.7052 (21)
η_J /kHz	-28.916 (11)	-28.915 (13)	22.996 (8)	23.003 (14)	16.790 (23)	22.965 (4)	22.9178 (7)
η_K /kHz	-	-	-19.1916*	-	0.0*	0.0*	0.0*
H _J /mHz	0.0*	0.0*	0.0*	0.0	0.0*	0.0*	0.0*
H _{JK} /mHz	0.0*	0.0*	15.10 (12)	17.1 (2.1)	27.6 (24)	0.0*	0.0*
H _{KJ} /mHz	0.0*	0.0*	-21.0 (32)	-20.0 (5.9)	-21.0*	0.0*	0.0*
q _J /Hz	0.0*	0.0*	3.5(6)	3.51(1.13)	0.0*	0.0*	0.0*
g _{II} /kHz	-	-	-	-	-23.85 (11)	-32.100 (6)	-31.791 (24)
x _{II} /MHz	-	-	-	-	8783.6(78)	9312.1(94)	9224.11*
η_{JJ} /Hz	-	-	-	-	0.188(23)	0.0*	0.0*
η_{JK} /Hz	-	-	-	-	0.0*	-	-

*constrained at this value.

$\nu_8 = 1$ State

The microwave and millimeter wave spectra of this state have been recorded by Whittle *et al*⁴. The highest J'' spectrum do not fit the perturbation formulae¹⁵ and hence Cox and co-workers¹⁰ tried setting up the Hamiltonian as a matrix and diagonalising. To aim to obtain more accurate parameters, we have mixed all of the transitions from Ref⁶ and some of the from Ref⁴. A least-squares refinement of the (201) observations was carried out using the programme¹⁵. The result of the fitting is shown in Table 3 and obtained results are in Table 2 where a comparison is made with the results of Carpenter *et al*⁶ for this state and other vibrational excited states $\nu_8 = 2,3,4$ ^{7,9}. Our B value is slightly larger but difference between other parameters is negligible. Table 2 shows a linear relationship between B values in different vibrational excited states for this molecule. The refinement to two sextics (H_{JK} and H_{KJ} parameters), while constraining H_J to zero, gave a good fit between observed and calculated frequencies, and reasonable standard deviations in the sextic terms H_{JK} and H_{KJ} .

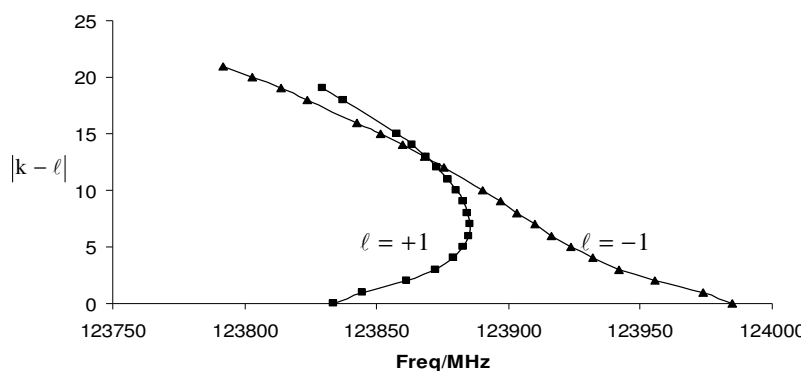


Figure 3 Fortrat - like diagram of CF_3CN in $\nu_8=1$ State. $J = 20 \rightarrow 21$

Table 3. Results of Refinement of Observed Frequencies for CF_3CN in $\nu_8 = 1$ State.

	J	k	ℓ	Fobs/ MHz	o-c /MHz	error / MHz
1	16	-1	-1	100372.090	-0.040	0.2
2	16	0	-1	100355.260	-0.057	0.2
3	16	1	-1	100338.250	0.006	0.2
4	16	2	-1	100328.240	0.013	0.2
5	16	3	-1	100321.400	-0.006	0.2
6	16	4	-1	100315.950	0.000	0.2
7	16	5	-1	100311.050	-0.011	0.2
8	16	6	-1	100306.356	0.003	0.2
9	16	7	-1	100301.550	-0.070	0.2
10	16	8	-1	100296.740	-0.005	0.2
11	16	10	-1	100286.250	-0.046	0.2
12	16	11	-1	100280.560	-0.084	0.2
13	16	12	-1	100274.686	0.014	0.2
14	16	13	-1	100268.374	0.008	0.2
15	16	14	-1	100261.730	0.016	0.2

Table 3 contd..

16	16	15	-1	100254.684	-0.021	0.2
17	16	2	1	100266.120	0.021	0.2
18	16	3	1	100282.000	0.010	0.2
19	16	4	1	100290.050	0.013	0.2
20	16	5	1	100294.060	-0.040	0.2
21	16	6	1	100295.990	-0.020	0.2
22	16	10	1	100293.150	0.006	0.2
23	16	11	1	100290.770	0.024	0.2
24	16	12	1	100287.850	0.028	0.2
25	16	13	1	100284.416	0.011	0.2
26	16	14	1	100280.560	0.044	0.4
27	16	15	1	100276.236	0.065	0.2
28	16	16	1	100271.464	0.083	0.2
29	17-16	-1		106168.350	0.002	0.2
30	17-15	-1		106173.150	-0.226	0.2
31	17-13	-1		106182.030	0.039	0.2
32	17-11	-1		106188.570	0.006	0.2
33	17-10	-1		106191.100	0.089	0.2
34	17	-8	-1	106193.840	-0.099	0.4
35	17	-7	-1	106193.840	-0.357	0.4
36	17	-5	-1	106191.100	0.072	0.2
37	17	-3	-1	106177.430	0.128	0.2
38	17	-2	-1	106160.860	0.007	0.2
39	17	1	-1	106242.630	0.093	0.2
40	17	2	-1	106231.550	0.091	0.2
41	17	3	-1	106223.850	0.044	0.2
42	17	4	-1	106217.810	0.102	0.2
43	17	5	-1	106212.330	0.036	0.2
44	17	6	-1	106207.150	0.021	0.2
45	17	7	-1	106201.910	-0.068	0.2
46	17	8	-1	106196.810	0.106	0.2
47	17	9	-1	106191.100	-0.122	0.2
48	17	10	-1	106185.850	0.374	0.4
49	17	11	-1	106179.370	-0.058	0.2
50	17	12	-1	106173.150	0.098	0.2
51	17	13	-1	106166.250	-0.079	0.4
52	17	14	-1	106159.210	-0.035	0.2
53	18-16	-1		112065.150	0.069	0.2
54	18-14	-1		112075.290	0.196	0.2
55	18-13	-1		112079.250	-0.071	0.2
56	18-11	-1		112086.390	0.288	0.2
57	18-10	-1		112088.790	0.207	0.2
58	18	-9	-1	112090.530	0.149	0.2
59	18	-6	-1	112090.530	0.181	0.2
60	18	-4	-1	112082.400	0.275	0.2
61	18	-3	-1	112071.900	-0.358	0.4
62	18	0	-1	112164.880	-0.070	0.2

Table 3 contd..

63	18	1	-1	112147.050	0.136	0.2
64	18	2	-1	112134.870	0.024	0.2
65	18	3	-1	112126.380	0.032	0.2
66	18	4	-1	112119.660	0.080	0.2
67	18	5	-1	112113.650	0.038	0.2
68	18	6	-1	112107.980	0.014	0.2
69	18	7	-1	112102.420	0.043	0.2
70	18	8	-1	112096.790	0.102	0.2
71	18	9	-1	112090.530	-0.271	0.2
72	18	10	-1	112084.890	0.237	0.2
73	18	12	-1	112071.900	0.490	0.4
74	20	-1	-1	123985.036	-0.026	0.2
75	20	1	1	123833.833	-0.012	0.2
76	20	0	-1	123973.622	-0.019	0.2
77	20	1	-1	123955.695	-0.006	0.2
78	20	2	-1	123941.967	-0.004	0.2
79	20	3	-1	123931.788	-0.022	0.2
80	20	4	-1	123923.624	-0.019	0.2
81	20	5	-1	123916.487	-0.009	0.2
82	20	6	-1	123909.792	-0.028	0.2
83	20	7	-1	123903.279	-0.015	0.2
84	20	8	-1	123896.714	-0.010	0.2
85	20	9	-1	123889.980	-0.006	0.2
86	20	11	-1	123875.641	-0.059	0.2
87	20	12	-1	123867.993	-0.063	0.2
88	20	13	-1	123859.976	-0.060	0.2
89	20	14	-1	123851.580	-0.037	0.2
90	20	15	-1	123842.751	-0.033	0.2
91	20	17	-1	123823.849	0.026	0.2
92	20	18	-1	123813.670	-0.008	0.2
93	20	19	-1	123803.071	-0.009	0.2
94	20	20	-1	123792.073	0.049	0.2
95	20	2	1	123844.766	-0.014	0.2
96	20	3	1	123861.224	-0.037	0.2
97	20	4	1	123872.495	-0.065	0.2
98	20	5	1	123879.307	-0.011	0.2
99	20	6	1	123883.064	-0.044	0.2
100	20	7	1	123884.884	-0.021	0.2
101	20	8	1	123885.248	-0.010	0.2
102	20	9	1	123884.455	-0.032	0.2
103	20	10	1	123882.765	-0.022	0.2
104	20	11	1	123880.295	0.014	0.2
105	20	12	1	123877.045	-0.006	0.2
106	20	13	1	123873.145	-0.009	0.2
107	20	14	1	123868.610	-0.018	0.2
108	20	15	1	123863.478	-0.025	0.2

Table 3 contd..

109	20	16	1	123857.779	-0.020	0.2
110	20	19	1	123837.391	0.029	0.2
111	20	20	1	123829.556	0.083	0.2
112	21	2	-1	129845.648	0.008	0.2
113	21	3	-1	129834.618	-0.075	0.2
114	21	4	-1	129825.749	-0.067	0.2
115	21	5	-1	129818.000	-0.053	0.2
116	21	6	-1	129810.764	-0.068	0.2
117	21	7	-1	129803.730	-0.081	0.2
118	21	8	-1	129796.710	-0.065	0.2
119	21	9	-1	129789.542	-0.047	0.2
120	21	10	-1	129782.130	-0.031	0.2
121	21	12	-1	129766.270	-0.071	0.2
122	21	13	-1	129757.757	-0.115	0.2
123	21	14	-1	129748.916	-0.078	0.2
124	21	15	-1	129739.602	-0.086	0.2
125	21	16	-1	129729.923	-0.018	0.2
126	21	17	-1	129719.706	-0.033	0.2
127	21	18	-1	129709.050	-0.025	0.2
128	21	19	-1	129697.958	0.018	0.2
129	21	20	-1	129686.330	0.002	0.2
130	21	21	-1	129674.265	0.030	0.2
131	21	-1	-1	129729.467	-0.044	0.2
132	21	2	1	129739.254	-0.077	0.2
133	21	3	1	129755.373	-0.014	0.2
134	21	4	1	129767.159	-0.044	0.2
135	21	5	1	129774.476	-0.109	0.2
136	21	6	1	129778.823	-0.055	0.2
137	21	8	1	129781.590	-0.046	0.2
138	21	9	1	129780.983	-0.033	0.2
139	21	10	1	129779.349	-0.041	0.2
140	21	11	1	129776.852	-0.041	0.2
141	21	12	1	129773.612	-0.007	0.2
142	21	13	1	129769.602	-0.027	0.2
143	21	14	1	129764.906	-0.063	0.2
144	21	15	1	129759.645	-0.025	0.2
145	21	16	1	129753.699	-0.059	0.2
146	21	17	1	129747.251	0.002	0.2
147	21	18	1	129740.136	-0.023	0.2
148	21	19	1	129732.495	-0.002	0.2
149	21	20	1	129724.283	0.010	0.3
150	21	21	1	129715.508	0.015	0.3
151	26	2	-1	159363.470	-0.007	0.2
152	26	3	-1	159349.780	0.151	0.2
153	26	4	-1	159337.460	-0.042	0.2
154	26	5	-1	159326.640	0.014	0.2

Table 3 contd..

155	26	6	-1	159316.480	-0.041	0.2
156	26	7	-1	159306.900	0.083	0.2
157	26	8	-1	159297.170	-0.080	0.2
158	32	-1	-1	194806.540	-0.068	0.4
159	32	0	-1	194802.700	-0.045	0.4
160	32	1	-1	194792.560	-0.035	0.4
161	32	2	-1	194779.160	0.068	0.4
162	32	3	-1	194764.600	0.011	0.4
163	32	4	-1	194750.320	0.058	0.4
164	32	6	-1	194723.020	-0.161	0.4
165	32	7	-1	194710.200	-0.040	0.4
166	32	8	-1	194697.500	0.040	0.4
167	32	9	-1	194684.760	0.085	0.4
168	32	10	-1	194671.720	-0.025	0.4
169	32	11	-1	194658.520	-0.038	0.4
170	32	12	-1	194645.020	-0.003	0.4
171	32	14	-1	194616.900	0.263	0.4
172	32	15	-1	194601.778	0.095	0.4
173	32	16	-1	194586.175	0.005	0.4
174	32	17	-1	194570.090	0.025	0.4
175	32	19	-1	194536.070	0.080	0.4
176	32	20	-1	194518.090	0.110	0.4
177	32	21	-1	194499.320	0.018	0.4
178	32	22	-1	194479.953	0.010	0.4
179	32	23	-1	194459.970	0.078	0.4
180	32	24	-1	194439.340	0.199	0.4
181	32	25	-1	194417.840	0.160	0.4
182	32	26	-1	194395.553	0.050	0.4
183	32	1	1	194569.240	-0.041	0.4
184	32	3	1	194580.200	-0.050	0.4
185	32	4	1	194590.040	0.092	0.4
186	32	5	1	194599.240	0.118	0.4
187	32	6	1	194606.740	0.142	0.4
188	32	8	1	194615.400	-0.006	0.4
189	32	12	1	194612.148	0.143	0.4
190	32	13	1	194607.760	0.090	0.4
191	32	14	1	194602.160	0.005	0.4
192	32	15	1	194595.698	0.167	0.4
193	32	16	1	194587.875	0.019	0.4
194	32	17	1	194579.175	0.002	0.4
195	32	21	1	194534.860	-0.143	0.4
196	32	22	1	194521.353	-0.359	0.4
197	32	24	1	194492.485	-0.050	0.4
198	32	25	1	194476.440	-0.230	0.4
199	32	27	1	194442.430	0.004	0.4
200	32	28	1	194423.923	-0.136	0.4
201	32	29	1	194404.923	0.055	0.4

sum of squared defects	=	1.445583
standard deviation	=	0.091148

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