A microwave spectroscopic and quantum chemical study of propa-1,2-dienyl selenocyanate (H_2=C=CHSeC≡N) and cyclopropyl selenocyanate (C_3H_5SeC≡N)†

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Electronic supplementary information (ESI)

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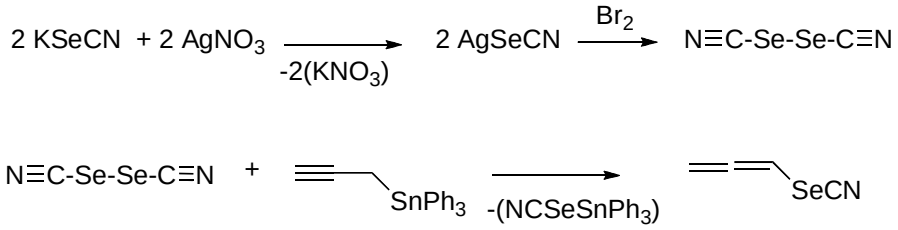
Preparation of the Compounds

Selenocyanic Acid, Propa-1,2-diene Ester (Allenyl Selenocyanate)[1]

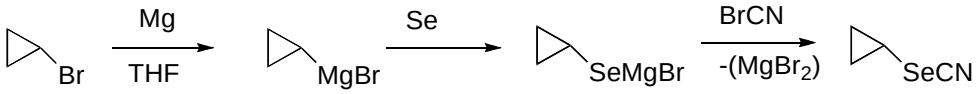


In a 250 mL three necked flask were introduced, under nitrogen, potassium selenocyanate (2.5 g, 17.5 mmol) and water (60 mL). Silver nitrate (3g, 17.5 mmol) was slowly added at room temperature by portions. After 30 min of stirring, the solution was filtrated and silver selenocyanate, dried under vacuum, was obtained as a white solid in a 92 % yield (3.41 g, 16.0 mmol).[2]

Silver selenocyanate (3.41 g, 16.0 mmol) dissolved in benzene (20 mL) was introduced in a 100 mL three necked flask equipped with a stirring bar, a dropping funnel and a nitrogen inlet. The flask was cooled at 10 °C and dibromine (1.28 g, 8 mmol) was then added dropwise. The mixture was stirred for 30 min, filtrated and introduced dropwise in another flask containing prop-2-ynyltriphenylstannane[3] (2.73 g, 7 mmol) in benzene (20 mL) at 10 °C. The mixture was stirred for 1 h and water was added. The reaction mixture was taken up in diethyl ether/water (3 x 50 mL). The organic phases were combined and dried over $MgSO_4$. After filtration, the solvent was removed under vacuum. Selenocyanic acid, 1,2-propadiene ester was purified by distillation using a vacuum line and selective trapping at −30 °C. The presence of small amounts of

selenocyanic, 2-propynyl ester (≈ 3 – 5 %) cannot be avoided. This ratio increased on standing at room temperature and the sample should be kept at a low temperature (−30 °C). Yield: 55 %; bp ≈ 40 °C (0.1 mbar). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.17 (d, $^{4}J_{HH}$ = 6.1 Hz, 2H, CH_2); 6.03 (t, $^{4}J_{HH}$ = 6.1 Hz, $^{2}J_{SeH}$ = 26.2 Hz, 1H, CH-Se). ^{13}C NMR (100 MHz, $CDCl_3$): δ 71.2 (d, $^{1}J_{CH}$ = 202.4 Hz, $^{1}J_{CSe}$ = 89.2 Hz, CH); 80.5 (t, $^{1}J_{CH}$ = 170.9 Hz, CH_2); 100.7 (s, CN), 208.5 (s, C=C=C). ^{77}Se NMR (57.2 MHz, $CDCl_3$): δ 277.4.

Selenocyanic acid, Cyclopropane Ester (Cyclopropyl Selenocyanate).



Cyclopropylmagnesium bromide was prepared by slow addition of cyclopropyl bromide (6.05 g, 50 mmol) in THF (30 mL) to Mg (1.2 g, 50 mmol) in THF (20mL) at 0 °C. The solution was then warmed to 50 °C for 20 min and then cooled to 0°C, at which time selenium powder (3.95 g, 50 mmol) was added by portions in 10 min and then stirred at room temperature for 30 min. The solution was introduced into a dropping funnel and poured into a 250 mL flask containing a cooled (−40 °C) solution of cyanogen bromide (5.1 g, 48 mmol) in THF (20 mL). The solution was then allowed to warm to room temperature and stirred for 20 min. Water (20 mL) was added and the organic phase was separated, the aqueous layer was extracted with diethyl ether (2 × 30 mL). The organic phases were combined and dried with $MgSO_4$. The solvent was removed in vacuo and purification was performed by distillation in vacuo. Bp: 40 °C (0.1 mmHg). Yield:

3.31 g, 22.5 mmol, 45 %. ^{1}H NMR ($CDCl_3$) δ 0.93 (td, $^{3}J_{HH}$ = 6.6 Hz, $^{3}J_{HH}$ = 4.3 Hz, 2H cycle); 1.16 (td, $^{3}J_{HH}$ = 7.4 Hz, $^{3}J_{HH}$ = 6.6 Hz, 2H cycle); 2.53 (tt, $^{3}J_{HH}$ = 7.4 Hz, $^{3}J_{HH}$ = 4.3 Hz, 1H, CH). ^{13}C NMR ($CDCl_3$) δ 8.55 (d, $^{1}J_{CH}$ = 187.9 Hz, CH); 9.13 (t, $^{1}J_{CH}$ = 164.6 Hz, CH_2); 101.6 (s, CN). ^{77}Se NMR ($CDCl_3$) δ 322.4.

Comments for Spectroscopic Tables:

Hamiltonian: Watson's A-reduction I^r representation[4]

Transition labels: $J''\ K_{-1}''\ K_{+1}''\ \ J'\ K_{-1}'\ J\ K_{+1}'$

obs. – calc.: the observed – the calculated residuals

weight: the estimated uncertainties of the observed frequencies. Each transition is weighted according to the inverse square of its estimated uncertainty

t: Student's t-test[5]

distortion correction: centrifugal distortion correction

total: correction from quartic and sextic (if included) centrifugal distortion constants

higher: contribution from sextic centrifugal distortion constants

fixed: contribution from fixed quartic and/or fixed sextic centrifugal distortion constants. The values of fixed constants are also displayed.

rms deviation: root-mean-square deviation. Defined dimensionless in a weighted least-squares fit[5]

κ: Ray's asymmetry parameter[6] defined by $\kappa = (2B - A - C)/(A - C)$

Inertial defect: defined by $\Delta = I_c - I_a - I_b$

Significant digits: the number of significant digits of each fitted constant are listed on the diagonal of the correlation matrix.

Units: the observed frequencies, the residuals, the distortion corrections, and the rotational constants are in MHz, the quartic centrifugal distortion constants are in kHz, the sextic centrifugal distortion constants are in Hz, and the principal axis inertial constants and the inertial defect are in u $Å^2$.

Table 1S Microwave spectrum of the ground vibrational state of the *anticlinal* conformer of $H_2C{=}C{=}CH^{80}SeCN$

Total number of transitions: 156

Transition	obs. frequency	obs.- calc.	weight	t	distortion corrections total	higher	fixed
19 5 14 20 5 15	49518.900	-0.012	0.10	-0.2	-11.594	-0.178	-0.676
19 7 13 20 7 14	49313.360	-0.173	0.10	-1.1	6.187	-0.362	-0.718
19 7 12 20 7 13	49313.360	-0.267	0.10	-1.7	6.186	-0.362	-0.717
19 8 12 20 8 13	49278.560	0.239	0.10	1.6	16.315	-0.475	-0.605
19 8 11 20 8 12	49278.560	0.237	0.10	1.6	16.315	-0.475	-0.605
19 9 11 20 9 12	49258.870	-0.063	0.10	-0.4	27.602	-0.603	-0.469
19 9 10 20 9 11	49258.870	-0.063	0.10	-0.4	27.602	-0.603	-0.469
19 14 6 20 14 7	49267.610	0.325	0.10	2.2	102.681	-1.464	0.532
19 14 5 20 14 6	49267.610	0.325	0.10	2.2	102.681	-1.464	0.532
20 7 14 21 7 15	51796.750	-0.053	0.10	-0.3	3.496	-0.419	-0.874
20 7 13 21 7 14	51796.750	-0.232	0.10	-1.5	3.494	-0.419	-0.871
20 8 13 21 8 14	51754.720	-0.182	0.10	-1.2	14.215	-0.550	-0.759
20 8 12 21 8 13	51754.720	-0.187	0.10	-1.2	14.215	-0.550	-0.759
21 5 16 22 5 17	54589.300	-0.119	0.20	-0.5	-20.942	-0.230	-0.755
21 6 16 22 6 17	54365.510	-0.044	0.20	-0.1	-9.941	-0.349	-1.158
21 10 12 22 10 13	54189.640	-0.058	0.10	-0.4	38.004	-0.991	-0.620
21 10 11 22 10 12	54189.640	-0.058	0.10	-0.4	38.004	-0.991	-0.620
22 5 18 23 5 19	56981.800	-0.163	0.20	-0.6	-23.476	-0.270	-1.719
22 6 17 23 6 18	56866.100	0.085	0.10	0.6	-14.273	-0.396	-1.360
22 6 16 23 6 17	56878.770	0.314	0.15	1.4	-14.550	-0.395	-1.221
22 8 15 23 8 16	56713.550	-0.188	0.10	-1.2	8.606	-0.720	-1.119
22 8 14 23 8 15	56713.550	-0.207	0.10	-1.3	8.605	-0.720	-1.119
22 9 14 23 9 15	56680.130	0.147	0.10	0.9	21.784	-0.915	-0.974
22 9 13 23 9 14	56680.130	0.146	0.10	0.9	21.784	-0.915	-0.974
22 10 13 23 10 14	56661.430	0.155	0.10	1.0	36.276	-1.132	-0.803
22 10 12 23 10 13	56661.430	0.155	0.10	1.0	36.276	-1.132	-0.803
23 8 16 24 8 17	59196.230	0.048	0.10	0.3	5.035	-0.816	-1.326
23 8 15 24 8 16	59196.230	0.010	0.10	0.1	5.034	-0.816	-1.325
23 9 15 24 9 16	59156.660	0.096	0.10	0.6	18.881	-1.038	-1.180
23 9 14 24 9 15	59156.660	0.095	0.10	0.6	18.881	-1.038	-1.180
23 10 14 24 10 15	59134.120	0.159	0.10	1.0	34.061	-1.285	-1.005
23 10 13 24 10 14	59134.120	0.159	0.10	1.0	34.061	-1.285	-1.005
24 8 17 25 8 18	61680.800	0.026	0.10	0.2	0.910	-0.921	-1.552
24 8 16 25 8 17	61680.800	-0.044	0.10	-0.3	0.908	-0.921	-1.550
24 9 16 25 9 17	61634.540	-0.166	0.10	-1.0	15.447	-1.172	-1.406
24 9 15 25 9 16	61634.540	-0.168	0.10	-1.0	15.447	-1.172	-1.406
24 10 15 25 10 16	61607.910	0.107	0.10	0.7	31.331	-1.451	-1.228
24 10 14 25 10 15	61607.910	0.107	0.10	0.7	31.331	-1.451	-1.228
24 11 14 25 11 15	61593.800	0.060	0.10	0.4	48.657	-1.759	-1.022
24 11 13 25 11 14	61593.800	0.060	0.10	0.4	48.657	-1.759	-1.022
24 12 13 25 12 14	61589.070	0.244	0.10	1.5	67.481	-2.096	-0.789
24 12 12 25 12 13	61589.070	0.244	0.10	1.5	67.481	-2.096	-0.789
25 6 20 26 6 21	64387.180	0.284	0.10	2.3	-30.824	-0.563	-2.128
25 6 20 26 6 21	64387.180	0.284	0.10	2.3	-30.824	-0.563	-2.128
25 6 19 26 6 20	64432.830	-0.053	0.10	-0.6	-32.240	-0.555	-1.621
25 8 18 26 8 19	64167.480	-0.134	0.15	-0.5	-3.802	-1.033	-1.796
25 8 17 26 8 18	64167.480	-0.260	0.15	-1.1	-3.806	-1.033	-1.792
25 9 17 26 9 18	64114.400	-0.075	0.10	-0.5	11.454	-1.316	-1.651
25 9 16 26 9 17	64114.400	-0.079	0.10	-0.5	11.454	-1.316	-1.651
25 10 16 26 10 17	64082.620	-0.229	0.10	-1.4	28.059	-1.630	-1.472
25 10 15 26 10 16	64082.620	-0.230	0.10	-1.4	28.059	-1.630	-1.472
25 11 15 26 11 16	64065.470	-0.095	0.15	-0.4	46.130	-1.977	-1.262

25	11	14	26	11	15	64065.470	-0.095	0.15	-0.4	46.130	-1.977	-1.262
25	12	14	26	12	15	64058.820	0.374	0.15	1.5	65.736	-2.356	-1.024
25	12	13	26	12	14	64058.820	0.374	0.15	1.5	65.736	-2.356	-1.024
25	15	11	26	15	12	64076.590	0.039	0.10	0.2	134.124	-3.689	-0.139
25	15	10	26	15	11	64076.590	0.039	0.10	0.2	134.124	-3.689	-0.139
25	16	10	26	16	11	64091.890	0.063	0.10	0.4	160.177	-4.198	0.214
25	16	9	26	16	10	64091.890	0.063	0.10	0.4	160.177	-4.198	0.214
25	17	9	26	17	10	64110.230	-0.375	0.10	-2.5	187.879	-4.741	0.599
25	17	8	26	17	9	64110.230	-0.375	0.10	-2.5	187.879	-4.741	0.599
26	6	21	27	6	22	66899.010	-0.418	0.25	-1.1	-37.595	-0.626	-2.454
26	7	20	27	7	21	66755.670	0.322	0.20	1.0	-24.025	-0.872	-2.177
26	7	19	27	7	20	66760.300	0.217	0.25	0.5	-24.190	-0.871	-2.090
26	8	19	27	8	20	66656.780	-0.023	0.12	-0.1	-9.138	-1.154	-2.059
26	8	18	27	8	19	66656.780	-0.247	0.12	-1.3	-9.145	-1.154	-2.053
26	9	18	27	9	19	66595.630	-0.313	0.10	-1.9	6.869	-1.471	-1.917
26	9	17	27	9	18	66595.630	-0.321	0.10	-2.0	6.869	-1.471	-1.916
26	10	17	27	10	18	66558.980	-0.167	0.12	-0.9	24.216	-1.824	-1.737
26	10	16	27	10	17	66558.980	-0.168	0.12	-0.9	24.216	-1.824	-1.737
26	11	16	27	11	17	66538.090	-0.233	0.10	-1.4	43.046	-2.212	-1.524
26	11	15	27	11	16	66538.090	-0.233	0.10	-1.4	43.046	-2.212	-1.524
26	14	13	27	14	14	66533.120	0.236	0.10	1.5	109.130	-3.596	-0.708
26	14	12	27	14	13	66533.120	0.236	0.10	1.5	109.130	-3.596	-0.708
26	15	12	27	15	13	66543.550	0.093	0.10	0.6	134.475	-4.130	-0.377
26	15	11	27	15	12	66543.550	0.093	0.10	0.6	134.475	-4.130	-0.377
26	17	10	27	17	11	66577.220	0.048	0.10	0.3	190.252	-5.308	0.380
26	17	9	27	17	10	66577.220	0.048	0.10	0.3	190.252	-5.308	0.380
26	18	9	27	18	10	66598.970	-0.288	0.10	-2.0	220.707	-5.953	0.808
26	18	8	27	18	9	66598.970	-0.288	0.10	-2.0	220.707	-5.953	0.808
27	6	22	28	6	23	69413.990	0.057	0.10	9.9	-45.008	-0.693	-2.826
27	6	21	28	6	22	69513.230	0.137	0.20	0.7	-48.644	-0.673	-1.746
27	7	21	28	7	22	69259.510	0.260	0.20	0.8	-30.847	-0.967	-2.464
27	7	20	28	7	21	69267.120	0.345	0.15	1.5	-31.138	-0.965	-2.326
27	9	19	28	9	20	69079.120	-0.061	0.10	-0.4	1.661	-1.638	-2.203
27	9	18	28	9	19	69079.120	-0.076	0.10	-0.5	1.660	-1.638	-2.203
27	10	18	28	10	19	69036.910	0.164	0.10	1.0	19.772	-2.032	-2.024
27	10	17	28	10	18	69036.910	0.164	0.10	1.0	19.772	-2.032	-2.024
27	16	12	28	16	13	69025.320	0.142	0.10	0.9	162.284	-5.242	-0.270
27	16	11	28	16	12	69025.320	0.142	0.10	0.9	162.284	-5.242	-0.270
27	17	11	28	17	12	69043.670	-0.145	0.10	-0.9	192.063	-5.919	0.134
27	17	10	28	17	11	69043.670	-0.145	0.10	-0.9	192.063	-5.919	0.134
28	7	22	29	7	23	71766.450	0.055	0.25	0.1	-38.407	-1.069	-2.774
28	7	21	29	7	22	71778.220	0.097	0.15	0.4	-38.905	-1.065	-2.560
28	9	20	29	9	21	71564.250	-0.013	0.10	-0.1	-4.206	-1.816	-2.510
28	9	19	29	9	20	71564.250	-0.039	0.10	-0.2	-4.207	-1.816	-2.509
28	10	19	29	10	20	71515.690	-0.005	0.10	-0.0	14.698	-2.254	-2.334
28	10	18	29	10	19	71515.690	-0.006	0.10	-0.0	14.698	-2.254	-2.334
28	12	17	29	12	18	71471.370	-0.207	0.15	-0.8	57.108	-3.264	-1.869
28	12	16	29	12	17	71471.370	-0.207	0.15	-0.8	57.108	-3.264	-1.869
28	13	16	29	13	17	71466.380	-0.097	0.12	-0.5	80.811	-3.835	-1.587
28	13	15	29	13	16	71466.380	-0.097	0.12	-0.5	80.811	-3.835	-1.587
28	14	15	29	14	16	71469.100	-0.051	0.12	-0.3	106.253	-4.452	-1.274
28	14	14	29	14	15	71469.100	-0.051	0.12	-0.3	106.253	-4.452	-1.274
28	16	13	29	16	14	71492.310	0.215	0.12	1.1	162.471	-5.822	-0.552
28	16	12	29	16	13	71492.310	0.215	0.12	1.1	162.471	-5.822	-0.552
28	17	12	29	17	13	71510.410	-0.121	0.10	-0.8	193.289	-6.575	-0.140
28	17	11	29	17	12	71510.410	-0.121	0.10	-0.8	193.289	-6.575	-0.140
29	7	22	30	7	23	74294.970	0.274	0.10	4.0	-47.569	-1.170	-2.785
29	10	20	30	10	21	73995.990	-0.055	0.10	-0.3	8.961	-2.492	-2.666
29	10	19	30	10	20	73995.990	-0.057	0.10	-0.4	8.961	-2.492	-2.666
29	14	16	30	14	17	73938.100	0.218	0.10	1.4	103.906	-4.927	-1.597
29	14	15	30	14	16	73938.100	0.218	0.10	1.4	103.906	-4.927	-1.597
29	16	14	30	16	15	73959.230	0.055	0.10	0.3	162.050	-6.444	-0.861

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29 16 13 30 16 14   73959.230    0.055 0.10    0.3   162.050  -6.444   -0.861
29 17 13 30 17 14   73977.300   -0.023 0.10   -0.1   193.904  -7.278   -0.442
29 17 12 30 17 13   73977.300   -0.023 0.10   -0.1   193.904  -7.278   -0.442
29 18 12 30 18 13   73999.700    0.119 0.10    0.8   227.636  -8.162    0.015
29 18 11 30 18 12   73999.700    0.119 0.10    0.8   227.636  -8.162    0.015
30  9 22 31  9 23   76540.060   -0.202 0.10   -1.3   -18.053  -2.207   -3.188
30  9 21 31  9 22   76540.060   -0.285 0.10   -1.9   -18.057  -2.207   -3.184
30 10 21 31 10 22   76477.920    0.072 0.10    0.5     2.530  -2.745   -3.021
30 10 20 31 10 21   76477.920    0.069 0.10    0.4     2.530  -2.745   -3.021
30 11 20 31 11 21   76439.340   -0.035 0.10   -0.2    24.575  -3.336   -2.808
30 11 19 31 11 20   76439.340   -0.035 0.10   -0.2    24.575  -3.336   -2.808
30 12 19 31 12 20   76417.320   -0.145 0.10   -0.9    48.257  -3.980   -2.555
30 12 18 31 12 19   76417.320   -0.145 0.10   -0.9    48.257  -3.980   -2.555
30 16 15 31 16 16   76426.480    0.057 0.10    0.4   160.994  -7.108   -1.199
30 16 14 31 16 15   76426.480    0.057 0.10    0.4   160.994  -7.108   -1.199
30 17 14 31 17 15   76444.250    0.059 0.10    0.4   193.887  -8.028   -0.772
30 17 13 31 17 14   76444.250    0.059 0.10    0.4   193.887  -8.028   -0.772
30 18 13 31 18 14   76466.410    0.058 0.10    0.4   228.707  -9.004   -0.308
30 18 12 31 18 13   76466.410    0.058 0.10    0.4   228.707  -9.004   -0.308
30 19 12 31 19 13   76492.180   -0.229 0.10   -1.6   265.470 -10.035    0.195
30 19 11 31 19 12   76492.180   -0.229 0.10   -1.6   265.470 -10.035    0.195
31  8 24 32  8 25   79141.700    0.135 0.20    0.5   -46.490  -1.886   -3.667
31  9 23 32  9 24   79031.030   -0.309 0.15   -1.3   -26.107  -2.421   -3.558
31  9 22 32  9 23   79031.030   -0.450 0.15   -2.0   -26.115  -2.421   -3.552
31 10 22 32 10 23   78961.090   -0.067 0.10   -0.4    -4.629  -3.014   -3.400
31 10 21 32 10 22   78961.090   -0.072 0.10   -0.5    -4.629  -3.014   -3.399
31 11 21 32 11 22   78917.230   -0.087 0.10   -0.6    18.277  -3.664   -3.190
31 11 20 32 11 21   78917.230   -0.088 0.10   -0.6    18.277  -3.664   -3.190
31 12 20 32 12 21   78891.840    0.219 0.10    1.4    42.819  -4.374   -2.937
31 12 19 32 12 20   78891.840    0.219 0.10    1.4    42.819  -4.374   -2.937
31 14 18 32 14 19   78876.800    0.210 0.10    1.3    97.269  -5.974   -2.322
31 14 17 32 14 18   78876.800    0.210 0.10    1.3    97.269  -5.974   -2.322
31 15 17 32 15 18   78882.200    0.214 0.10    1.4   127.309  -6.865   -1.962
31 15 16 32 15 17   78882.200    0.214 0.10    1.4   127.309  -6.865   -1.962
31 16 16 32 16 17   78893.810   -0.032 0.10   -0.2   159.281  -7.816   -1.566
31 16 15 32 16 16   78893.810   -0.032 0.10   -0.2   159.281  -7.816   -1.566
31 17 15 32 17 16   78911.220    0.087 0.10    0.6   193.212  -8.829   -1.133
31 17 14 32 17 15   78911.220    0.087 0.10    0.6   193.212  -8.829   -1.133
31 18 14 32 18 15   78933.130    0.013 0.10    0.1   229.121  -9.902   -0.662
31 18 13 32 18 14   78933.130    0.013 0.10    0.1   229.121  -9.902   -0.662
31 19 13 32 19 14   78959.030   -0.217 0.12   -1.3   267.024 -11.036   -0.151
31 19 12 32 19 13   78959.030   -0.217 0.12   -1.3   267.024 -11.036   -0.151

rms deviation:  1.6350

Rotational constants (MHz)  and  kappa:
           5487.38       1325.4530       1129.3318    -0.91000
+-            5.6           0.081           0.089      0.00006

Inertial constants and defect (uÅ**2):
           92.0985       381.28781       447.50272       -25.9
+-          0.093           0.023           0.035         0.1

Quartic distortion constants:
      0.697001    -16.1413         190     0.29906      -0.993
+-    0.0041        0.021       fixed     0.017         fixed
```

```
Sextic distortion constants:
          0 -0.23357        0        0        0        0        0
+-     fixed  0.013      fixed    fixed    fixed    fixed    fixed


Significant Digits and Correlation Matrix:

   6       0.928  -0.890  -0.212  -0.242   0.278  -0.202
           8      -0.994  -0.515  -0.438   0.604  -0.431
                   8       0.598   0.511  -0.672   0.511
                           6       0.738  -0.937   0.862
                                   6      -0.601   0.960
                                           5      -0.717
                                                   5
```

Table 2S Microwave spectrum of the first excited state of the C-Se torsion of the *anticlinal* conformer of $H_2C{=}C{=}CH^{80}SeCN$

Total number of transitions: 173

Transition	obs. frequency	obs.- calc.	weight	t	distortion corrections total	higher	fixed
19 7 13 20 7 14	49534.090	0.190	0.10	1.7	5.197	-0.229	-0.732
19 7 12 20 7 13	49534.090	0.085	0.10	0.8	5.197	-0.229	-0.730
19 8 12 20 8 13	49497.320	0.045	0.10	0.4	16.235	-0.301	-0.616
19 8 11 20 8 12	49497.320	0.042	0.10	0.4	16.235	-0.301	-0.616
19 9 11 20 9 12	49477.330	-0.083	0.10	-0.8	28.616	-0.381	-0.477
19 9 10 20 9 11	49477.330	-0.083	0.10	-0.8	28.616	-0.381	-0.477
19 14 6 20 14 7	49490.070	-0.122	0.10	-1.1	111.528	-0.926	0.544
19 14 5 20 14 6	49490.070	-0.122	0.10	-1.1	111.528	-0.926	0.544
19 15 5 20 15 6	49504.820	0.084	0.10	0.7	132.380	-1.063	0.815
19 15 4 20 15 5	49504.820	0.084	0.10	0.7	132.380	-1.063	0.815
19 16 4 20 16 5	49521.980	0.118	0.12	0.9	154.667	-1.210	1.112
19 16 3 20 16 4	49521.980	0.118	0.12	0.9	154.667	-1.210	1.112
19 18 2 20 18 3	49562.700	-0.183	0.20	-0.8	203.554	-1.532	1.782
19 18 1 20 18 2	49562.700	-0.183	0.20	-0.8	203.554	-1.532	1.782
20 8 13 21 8 14	51984.930	-0.253	0.15	-1.4	13.711	-0.348	-0.774
20 8 12 21 8 13	51984.930	-0.259	0.15	-1.5	13.711	-0.348	-0.773
20 11 10 21 11 11	51945.530	0.277	0.20	1.2	57.143	-0.661	-0.275
20 11 9 21 11 10	51945.530	0.277	0.20	1.2	57.143	-0.661	-0.275
20 12 9 21 12 10	51947.960	0.054	0.20	0.2	74.550	-0.787	-0.063
20 12 8 21 12 9	51947.960	0.054	0.20	0.2	74.550	-0.787	-0.063
20 14 7 21 14 8	51966.670	-0.005	0.15	-0.0	113.830	-1.072	0.429
20 14 6 21 14 7	51966.670	-0.005	0.15	-0.0	113.830	-1.072	0.429
20 15 6 21 15 7	51981.400	0.141	0.15	0.8	135.716	-1.231	0.712
20 15 5 21 15 6	51981.400	0.141	0.15	0.8	135.716	-1.231	0.712
20 16 5 21 16 6	51998.800	0.124	0.20	0.5	159.105	-1.401	1.020
20 16 4 21 16 5	51998.800	0.124	0.20	0.5	159.105	-1.401	1.020
21 9 13 22 9 14	54445.270	-0.369	0.25	-1.2	24.374	-0.507	-0.802
21 9 12 22 9 13	54445.270	-0.369	0.25	-1.2	24.374	-0.507	-0.802
22 8 15 23 8 16	56966.770	-0.117	0.10	-1.0	7.103	-0.455	-1.141
22 8 14 23 8 15	56966.770	-0.139	0.10	-1.2	7.103	-0.455	-1.141
22 9 14 23 9 15	56931.870	-0.050	0.10	-0.4	21.475	-0.579	-0.993
22 9 13 23 9 14	56931.870	-0.051	0.10	-0.4	21.475	-0.579	-0.993
22 10 13 23 10 14	56912.770	-0.156	0.10	-1.3	37.380	-0.716	-0.817
22 10 12 23 10 13	56912.770	-0.156	0.10	-1.3	37.380	-0.716	-0.817
22 13 10 23 13 11	56910.280	0.188	0.15	1.1	94.631	-1.213	-0.139
22 13 9 23 13 10	56910.280	0.188	0.15	1.1	94.631	-1.213	-0.139
22 14 9 23 14 10	56920.680	0.179	0.25	0.6	116.951	-1.408	0.138
22 14 8 23 14 9	56920.680	0.179	0.25	0.6	116.951	-1.408	0.138
22 15 8 23 15 9	56934.970	0.110	0.15	0.6	140.904	-1.617	0.442
22 15 7 23 15 8	56934.970	0.110	0.15	0.6	140.904	-1.617	0.442
22 17 6 23 17 7	56973.370	0.023	0.10	0.2	193.731	-2.077	1.132
22 17 5 23 17 6	56973.370	0.023	0.10	0.2	193.731	-2.077	1.132
23 8 16 24 8 17	59460.870	-0.017	0.10	-0.1	2.957	-0.516	-1.353
23 8 15 24 8 16	59460.870	-0.060	0.10	-0.5	2.957	-0.516	-1.352
23 9 15 24 9 16	59419.760	0.019	0.10	0.2	18.018	-0.657	-1.203
23 9 14 24 9 15	59419.760	0.018	0.10	0.2	18.018	-0.657	-1.203
23 10 14 24 10 15	59396.656	-0.002	0.20	-0.0	34.654	-0.813	-1.024
23 10 13 24 10 14	59396.656	-0.002	0.20	-0.0	34.654	-0.813	-1.024
23 11 13 24 11 14	59385.540	-0.224	0.25	-0.8	52.916	-0.985	-0.817
23 11 12 24 11 13	59385.540	-0.224	0.25	-0.8	52.916	-0.985	-0.817
23 15 9 24 15 10	59411.940	-0.014	0.12	-0.1	142.707	-1.836	0.273
23 15 8 24 15 9	59411.940	-0.014	0.12	-0.1	142.707	-1.836	0.273

23	16	8	24	16	9	59429.880	0.144	0.12	1.0	169.399	-2.090	0.614
23	16	7	24	16	8	59429.880	0.144	0.12	1.0	169.399	-2.090	0.614
23	17	7	24	17	8	59450.640	-0.119	0.25	-0.4	197.802	-2.360	0.986
23	17	6	24	17	7	59450.640	-0.119	0.25	-0.4	197.802	-2.360	0.986
23	18	6	24	18	7	59474.450	-0.244	0.25	-0.8	227.922	-2.646	1.389
23	18	5	24	18	6	59474.450	-0.244	0.25	-0.8	227.922	-2.646	1.389
24	8	17	25	8	18	61957.150	0.022	0.10	0.2	-1.791	-0.582	-1.583
24	8	16	25	8	17	61957.150	-0.057	0.10	-0.5	-1.792	-0.582	-1.581
24	10	15	25	10	16	61881.600	0.029	0.12	0.2	31.352	-0.918	-1.251
24	10	14	25	10	15	61881.600	0.029	0.12	0.2	31.352	-0.918	-1.251
24	12	13	25	12	14	61863.630	0.188	0.25	0.6	71.170	-1.326	-0.801
24	12	12	25	12	13	61863.630	0.188	0.25	0.6	71.170	-1.326	-0.801
24	14	11	25	14	12	61875.400	-0.154	0.25	-0.5	117.929	-1.807	-0.242
24	14	10	25	14	11	61875.400	-0.154	0.25	-0.5	117.929	-1.807	-0.242
24	15	10	25	15	11	61889.290	0.038	0.10	0.3	143.949	-2.075	0.081
24	15	9	25	15	10	61889.290	0.038	0.10	0.3	143.949	-2.075	0.081
24	16	9	25	16	10	61907.270	0.297	0.15	1.7	171.741	-2.362	0.432
24	16	8	25	16	9	61907.270	0.297	0.15	1.7	171.741	-2.362	0.432
25	6	20	26	6	21	64685.720	0.120	0.15	0.8	-35.607	-0.355	-2.181
25	8	18	26	8	19	64455.930	0.213	0.20	0.9	-7.174	-0.653	-1.833
25	8	17	26	8	18	64455.930	0.069	0.20	0.3	-7.175	-0.653	-1.829
25	10	16	26	10	17	64367.360	-0.356	0.20	-1.5	27.446	-1.031	-1.500
25	10	15	26	10	16	64367.360	-0.357	0.20	-1.5	27.446	-1.031	-1.500
25	11	15	26	11	16	64350.370	-0.031	0.10	-0.3	47.296	-1.251	-1.285
25	11	14	26	11	15	64350.370	-0.031	0.10	-0.3	47.296	-1.251	-1.285
25	12	14	26	12	15	64344.290	0.366	0.20	1.5	68.913	-1.491	-1.041
25	12	13	26	12	14	64344.290	0.366	0.20	1.5	68.913	-1.491	-1.041
25	13	13	26	13	14	64345.460	-0.106	0.20	-0.4	92.325	-1.751	-0.768
25	13	12	26	13	13	64345.460	-0.106	0.20	-0.4	92.325	-1.751	-0.768
25	14	12	26	14	13	64353.820	0.249	0.12	1.7	117.552	-2.032	-0.467
25	14	11	26	14	12	64353.820	0.249	0.12	1.7	117.552	-2.032	-0.467
25	17	9	26	17	10	64405.800	0.118	0.10	1.0	204.234	-3.000	0.619
25	17	8	26	17	9	64405.800	0.118	0.10	1.0	204.234	-3.000	0.619
25	18	8	26	18	9	64430.000	-0.412	0.15	-2.4	236.821	-3.363	1.045
25	18	7	26	18	8	64430.000	-0.412	0.15	-2.4	236.821	-3.363	1.045
26	6	21	27	6	22	67210.960	-0.076	0.10	-1.5	-43.013	-0.395	-2.518
26	7	20	27	7	21	67060.800	0.529	0.20	2.3	-28.947	-0.551	-2.224
26	7	19	27	7	20	67065.760	0.170	0.20	0.7	-29.052	-0.550	-2.129
26	8	19	27	8	20	66956.880	0.113	0.10	1.0	-13.225	-0.730	-2.102
26	8	18	27	8	19	66956.880	-0.142	0.10	-1.2	-13.229	-0.730	-2.095
26	9	18	27	9	19	66893.170	-0.003	0.10	-0.0	4.010	-0.931	-1.956
26	9	17	27	9	18	66893.170	-0.012	0.10	-0.1	4.010	-0.931	-1.956
26	10	17	27	10	18	66855.320	0.174	0.10	1.5	22.907	-1.154	-1.772
26	10	16	27	10	17	66855.320	0.173	0.10	1.5	22.907	-1.154	-1.772
26	12	15	27	12	16	66825.050	-0.047	0.15	-0.3	66.038	-1.668	-1.304
26	12	14	27	12	15	66825.050	-0.047	0.15	-0.3	66.038	-1.668	-1.304
26	13	14	27	13	15	66825.050	0.024	0.15	0.1	90.363	-1.960	-1.026
26	13	13	27	13	14	66825.050	0.024	0.15	0.1	90.363	-1.960	-1.026
26	16	11	27	16	12	66861.950	0.154	0.20	0.6	174.643	-2.974	-7.2E-3
26	16	10	27	16	11	66861.950	0.154	0.20	0.6	174.643	-2.974	-7.2E-3
26	18	9	27	18	10	66907.920	-0.296	0.10	-2.6	240.363	-3.766	0.834
26	18	8	27	18	9	66907.920	-0.296	0.10	-2.6	240.363	-3.766	0.834
27	7	21	28	7	22	69577.170	0.318	0.20	1.4	-36.470	-0.611	-2.518
27	9	19	28	9	20	69387.840	-0.056	0.15	-0.3	-1.975	-1.036	-2.249
27	9	18	28	9	19	69387.840	-0.072	0.15	-0.4	-1.975	-1.036	-2.248
27	10	18	28	10	19	69344.020	0.106	0.10	0.9	17.705	-1.285	-2.065
27	10	17	28	10	18	69344.020	0.105	0.10	0.9	17.705	-1.285	-2.065
27	11	17	28	11	18	69318.550	-0.263	0.12	-1.9	39.180	-1.560	-1.845
27	11	16	28	11	17	69318.550	-0.263	0.12	-1.9	39.180	-1.560	-1.845
27	14	14	28	14	15	69310.630	-0.016	0.10	-0.1	114.935	-2.536	-0.993
27	14	13	28	14	14	69310.630	-0.016	0.10	-0.1	114.935	-2.536	-0.993
27	15	13	28	15	14	69322.630	0.182	0.10	1.5	144.062	-2.913	-0.646

27	15	12	28	15	13	69322.630	0.182	0.10	1.5	144.062	-2.913	-0.646
27	16	12	28	16	13	69339.230	-0.157	0.10	-1.3	175.153	-3.316	-0.267
27	16	11	28	16	12	69339.230	-0.157	0.10	-1.3	175.153	-3.316	-0.267
27	17	11	28	17	12	69360.880	0.141	0.12	1.0	208.218	-3.745	0.146
27	17	10	28	17	11	69360.880	0.141	0.12	1.0	208.218	-3.745	0.146
28	7	22	29	7	23	72096.790	-0.045	0.15	-0.3	-44.756	-0.675	-2.837
28	7	21	29	7	22	72110.420	0.388	0.25	1.4	-45.088	-0.673	-2.603
28	9	20	29	9	21	71884.500	-0.041	0.10	-0.3	-8.671	-1.148	-2.563
28	9	19	29	9	20	71884.500	-0.071	0.10	-0.6	-8.671	-1.148	-2.562
28	10	19	29	10	20	71833.980	-0.094	0.10	-0.8	11.811	-1.426	-2.382
28	10	18	29	10	19	71833.980	-0.095	0.10	-0.8	11.811	-1.426	-2.382
28	12	17	29	12	18	71789.640	0.022	0.20	0.1	58.325	-2.065	-1.905
28	12	16	29	12	17	71789.640	0.022	0.20	0.1	58.325	-2.065	-1.905
28	13	16	29	13	17	71785.300	-0.205	0.10	-1.7	84.490	-2.426	-1.616
28	13	15	29	13	16	71785.300	-0.205	0.10	-1.7	84.490	-2.426	-1.616
28	14	15	29	14	16	71789.640	-0.086	0.20	-0.4	112.644	-2.817	-1.294
28	14	14	29	14	15	71789.640	-0.086	0.20	-0.4	112.644	-2.817	-1.294
28	16	13	29	16	14	71817.020	-0.082	0.10	-0.7	175.000	-3.684	-0.553
28	16	12	29	16	13	71817.020	-0.082	0.10	-0.7	175.000	-3.684	-0.553
28	17	12	29	17	13	71838.150	-0.167	0.10	-1.5	209.231	-4.160	-0.132
28	17	11	29	17	12	71838.150	-0.167	0.10	-1.5	209.231	-4.160	-0.132
29	7	23	30	7	24	74620.380	0.201	0.15	1.2	-53.839	-0.743	-3.186
29	9	21	30	9	22	74383.300	0.108	0.10	0.9	-16.110	-1.268	-2.899
29	9	20	30	9	21	74383.300	0.053	0.10	0.5	-16.111	-1.268	-2.897
29	11	19	30	11	20	74291.380	0.079	0.10	0.7	28.340	-1.914	-2.501
29	11	18	30	11	19	74291.380	0.079	0.10	0.7	28.340	-1.914	-2.501
29	12	18	30	12	19	74273.090	0.070	0.10	0.6	53.431	-2.284	-2.243
29	12	17	30	12	18	74273.090	0.070	0.10	0.6	53.431	-2.284	-2.243
29	13	17	30	13	18	74266.900	0.340	0.20	1.4	80.526	-2.685	-1.950
29	13	16	30	13	17	74266.900	0.340	0.20	1.4	80.526	-2.685	-1.950
29	15	15	30	15	16	74279.090	0.025	0.20	0.1	140.868	-3.581	-1.263
29	15	14	30	15	15	74279.090	0.025	0.20	0.1	140.868	-3.581	-1.263
29	16	14	30	16	15	74294.970	0.026	0.10	0.2	174.161	-4.077	-0.869
29	16	13	30	16	14	74294.970	0.026	0.10	0.2	174.161	-4.077	-0.869
29	17	13	30	17	14	74315.960	0.032	0.20	0.1	209.555	-4.605	-0.439
29	17	12	30	17	13	74315.960	0.032	0.20	0.1	209.555	-4.605	-0.439
30	7	23	31	7	24	77177.090	-0.080	0.10	9.9	-64.677	-0.807	-3.033
30	9	22	31	9	23	76884.070	0.134	0.10	1.2	-24.328	-1.396	-3.257
30	9	21	31	9	22	76884.070	0.038	0.10	0.3	-24.330	-1.396	-3.253
30	11	20	31	11	21	76779.020	-0.148	0.10	-1.3	21.826	-2.110	-2.867
30	11	19	31	11	20	76779.020	-0.148	0.10	-1.3	21.826	-2.110	-2.867
30	16	15	31	16	16	76772.910	-0.005	0.12	-0.0	172.609	-4.497	-1.213
30	16	14	31	16	15	76772.910	-0.005	0.12	-0.0	172.609	-4.497	-1.213
30	17	14	31	17	15	76793.650	0.078	0.15	0.5	209.167	-5.079	-0.775
30	17	13	31	17	14	76793.650	0.078	0.15	0.5	209.167	-5.079	-0.775
31	8	24	32	8	25	79502.670	-0.177	0.20	-0.8	-54.741	-1.192	-3.748
31	8	23	32	8	24	79506.340	0.283	0.15	1.7	-54.845	-1.191	-3.661
31	9	23	32	9	24	79386.870	0.006	0.10	0.1	-33.359	-1.531	-3.636
31	9	22	32	9	23	79386.870	-0.159	0.10	-1.5	-33.364	-1.531	-3.630
31	10	22	32	10	23	79313.280	-0.196	0.10	-1.7	-10.339	-1.906	-3.474
31	10	21	32	10	22	79313.280	-0.202	0.10	-1.8	-10.339	-1.906	-3.473
31	11	21	32	11	22	79268.270	0.099	0.10	0.9	14.543	-2.318	-3.258
31	11	20	32	11	21	79268.270	0.099	0.10	0.9	14.543	-2.318	-3.258
31	12	20	32	12	21	79242.190	-0.045	0.10	-0.4	41.429	-2.767	-2.998
31	12	19	32	12	20	79242.190	-0.045	0.10	-0.4	41.429	-2.767	-2.998
31	15	17	32	15	18	79236.840	0.173	0.10	1.5	134.817	-4.343	-1.994
31	15	16	32	15	17	79236.840	0.173	0.10	1.5	134.817	-4.343	-1.994
31	16	16	32	16	17	79251.160	0.142	0.12	1.1	170.317	-4.945	-1.587
31	16	15	32	16	16	79251.160	0.142	0.12	1.1	170.317	-4.945	-1.587

rms deviation: 1.1929

```
Rotational constants (MHz)  and  kappa:
          5614.39       1334.6089       1130.7037    -0.90905
+-           8.1           0.086           0.087      0.00010


Inertial constants and defect (uÅ**2):
          90.0150       378.67205       446.95978       -21.7
+-         0.13           0.024           0.035           0.2


Quartic distortion constants:
      0.855065    -17.8190         190     0.15964      -0.993
+-    0.0043        0.020        fixed     0.018         fixed


Sextic distortion constants:
          0 -0.14778        0        0        0        0        0
+-    fixed  0.014      fixed    fixed    fixed    fixed    fixed


Significant Digits and Correlation Matrix:

   6       0.909  -0.845   0.411   0.258  -0.445   0.308
           8      -0.990   0.056  -0.073  -0.043   0.001
                   8       0.084   0.205  -0.093   0.130
                           6       0.905  -0.942   0.942
                                   6      -0.816   0.969
                                           5      -0.821
                                                   5
```

Table 3S Microwave spectrum of the first excited state of the lowest bending vibration of the *anticlinal* conformer of H2C=C=CH^{80}SeCN

Total number of transitions: 139

Transition	obs. frequency	obs.- calc.	weight	t	distortion corrections total	higher	fixed
19 5 14 20 5 15	49211.850	0.072	0.15	9.9	-8.431	-0.102	-0.642
19 7 13 20 7 14	49028.020	-0.279	0.10	-1.7	7.770	-0.207	-0.650
19 7 12 20 7 13	49028.020	-0.343	0.10	-2.0	7.770	-0.207	-0.649
19 8 12 20 8 13	48996.700	0.236	0.10	1.5	17.431	-0.271	-0.547
19 8 11 20 8 12	48996.700	0.234	0.10	1.5	17.431	-0.271	-0.546
19 9 11 20 9 12	48979.280	0.051	0.25	0.1	28.281	-0.344	-0.423
19 9 10 20 9 11	48979.280	0.051	0.25	0.1	28.281	-0.344	-0.423
19 10 10 20 10 11	48971.270	-0.104	0.20	-0.3	40.349	-0.425	-0.280
19 10 9 20 10 10	48971.270	-0.104	0.20	-0.3	40.349	-0.425	-0.280
22 5 18 23 5 19	56639.690	0.014	0.20	9.9	-18.837	-0.155	-1.516
22 6 17 23 6 18	56526.190	0.341	0.12	2.0	-10.225	-0.227	-1.227
22 6 16 23 6 17	56535.200	0.246	0.12	1.7	-10.315	-0.226	-1.128
22 8 15 23 8 16	56386.190	-0.068	0.10	-0.4	11.111	-0.411	-1.014
22 8 15 23 8 16	56386.190	-0.068	0.10	-0.4	11.111	-0.411	-1.014
22 8 14 23 8 15	56386.190	-0.081	0.10	-0.4	11.111	-0.411	-1.014
22 8 14 23 8 15	56386.190	-0.081	0.10	-0.4	11.111	-0.411	-1.014
22 9 14 23 9 15	56356.070	0.179	0.10	1.0	23.688	-0.522	-0.881
22 9 14 23 9 15	56356.070	0.179	0.10	1.0	23.688	-0.522	-0.881
22 9 13 23 9 14	56356.070	0.179	0.10	1.0	23.688	-0.522	-0.881
22 9 13 23 9 14	56356.070	0.179	0.10	1.0	23.688	-0.522	-0.881
22 10 13 23 10 14	56339.170	-0.258	0.12	-1.1	37.622	-0.646	-0.725
22 10 12 23 10 13	56339.170	-0.258	0.12	-1.1	37.622	-0.646	-0.725
22 14 9 23 14 10	56346.320	-0.161	0.10	-0.9	107.425	-1.269	0.123
22 14 8 23 14 9	56346.320	-0.161	0.10	-0.9	107.425	-1.269	0.123
22 15 8 23 15 9	56359.230	0.090	0.10	0.5	128.448	-1.457	0.392
22 15 7 23 15 8	56359.230	0.090	0.10	0.5	128.448	-1.457	0.392
22 16 7 23 16 8	56374.750	-0.014	0.10	-0.1	150.911	-1.658	0.685
22 16 6 23 16 7	56374.750	-0.014	0.10	-0.1	150.911	-1.658	0.685
23 6 18 24 6 19	59013.170	0.270	0.15	1.2	-14.295	-0.256	-1.429
23 6 17 24 6 18	59027.450	0.112	0.20	0.3	-14.464	-0.255	-1.273
23 8 16 24 8 17	58853.050	-0.162	0.10	-0.9	8.154	-0.466	-1.202
23 8 15 24 8 16	58853.050	-0.186	0.10	-1.0	8.154	-0.466	-1.202
23 9 15 24 9 16	58817.690	0.213	0.10	1.1	21.325	-0.592	-1.068
23 9 14 24 9 15	58817.690	0.212	0.10	1.1	21.325	-0.592	-1.068
24 8 17 25 8 18	61322.220	0.055	0.10	0.3	4.731	-0.526	-1.408
24 8 16 25 8 17	61322.220	0.010	0.10	0.1	4.731	-0.526	-1.407
24 9 16 25 9 17	61280.480	-0.040	0.10	-0.2	18.509	-0.669	-1.273
24 9 15 25 9 16	61280.480	-0.041	0.10	-0.2	18.509	-0.669	-1.273
24 10 15 25 10 16	61256.250	-0.324	0.10	-1.7	33.720	-0.828	-1.110
24 10 14 25 10 15	61256.250	-0.324	0.10	-1.7	33.720	-0.828	-1.110
24 11 14 25 11 15	61244.550	0.023	0.15	0.1	50.414	-1.003	-0.922
24 11 13 25 11 14	61244.550	0.023	0.15	0.1	50.414	-1.003	-0.922
24 12 13 25 12 14	61241.360	0.370	0.15	1.3	68.621	-1.195	-0.710
24 12 12 25 12 13	61241.360	0.370	0.15	1.3	68.621	-1.195	-0.710
24 14 11 25 14 12	61251.970	0.161	0.10	0.9	109.640	-1.629	-0.213
24 14 10 25 14 11	61251.970	0.161	0.10	0.9	109.640	-1.629	-0.213
24 15 10 25 15 11	61263.870	-0.029	0.10	-0.2	132.472	-1.871	0.072
24 15 9 25 15 10	61263.870	-0.029	0.10	-0.2	132.472	-1.871	0.072
25 8 18 26 8 19	63792.900	-0.313	0.10	-1.7	0.819	-0.590	-1.631
25 8 17 26 8 18	63792.900	-0.395	0.10	-2.1	0.818	-0.590	-1.628
25 9 17 26 9 18	63744.970	-0.115	0.10	-0.6	15.217	-0.751	-1.496
25 9 16 26 9 17	63744.970	-0.118	0.10	-0.6	15.217	-0.751	-1.496

25	10	16	26	10	17	63716.600	-0.218	0.10	-1.1	31.079	-0.930	-1.332
25	10	15	26	10	16	63716.600	-0.218	0.10	-1.1	31.079	-0.930	-1.332
25	11	15	26	11	16	63702.200	0.364	0.10	1.9	48.466	-1.128	-1.140
25	11	14	26	11	15	63702.200	0.364	0.10	1.9	48.466	-1.128	-1.140
25	12	14	26	12	15	63696.630	0.323	0.20	0.8	67.415	-1.344	-0.923
25	12	13	26	12	14	63696.630	0.323	0.20	0.8	67.415	-1.344	-0.923
25	13	13	26	13	14	63697.710	-0.155	0.20	-0.4	87.946	-1.579	-0.681
25	13	12	26	13	13	63697.710	-0.155	0.20	-0.4	87.946	-1.579	-0.681
25	14	12	26	14	13	63705.040	0.057	0.12	0.2	110.075	-1.832	-0.413
25	14	11	26	14	12	63705.040	0.057	0.12	0.2	110.075	-1.832	-0.413
25	16	10	26	16	11	63731.920	-0.192	0.10	-1.1	159.166	-2.395	0.201
25	16	9	26	16	10	63731.920	-0.192	0.10	-1.1	159.166	-2.395	0.201
26	7	19	27	7	20	66359.840	-0.090	0.20	-0.2	-17.328	-0.499	-1.919
26	8	19	27	8	20	66266.400	-0.053	0.15	-0.2	-3.610	-0.660	-1.871
26	8	18	27	8	19	66266.400	-0.199	0.15	-0.7	-3.611	-0.660	-1.867
26	9	18	27	9	19	66211.350	0.110	0.10	0.6	11.425	-0.840	-1.739
26	9	17	27	9	18	66211.350	0.105	0.10	0.5	11.424	-0.840	-1.739
26	10	17	27	10	18	66178.350	0.112	0.25	0.2	27.948	-1.041	-1.573
26	10	16	27	10	17	66178.350	0.111	0.25	0.2	27.948	-1.041	-1.573
26	12	15	27	12	16	66152.500	0.215	0.15	0.7	65.729	-1.505	-1.157
26	12	14	27	12	15	66152.500	0.215	0.15	0.7	65.729	-1.505	-1.157
26	13	14	27	13	15	66152.500	0.147	0.15	0.5	87.057	-1.767	-0.909
26	13	13	27	13	14	66152.500	0.147	0.15	0.5	87.057	-1.767	-0.909
26	16	11	27	16	12	66184.840	-0.036	0.10	-0.2	160.994	-2.681	-5.2E-3
26	16	10	27	16	11	66184.840	-0.036	0.10	-0.2	160.994	-2.681	-5.2E-3
27	7	21	28	7	22	68843.850	0.226	0.15	0.8	-22.901	-0.554	-2.238
27	7	20	28	7	21	68848.720	-0.139	0.15	-0.5	-22.994	-0.553	-2.144
27	9	19	28	9	20	68678.750	-0.304	0.10	-1.6	7.108	-0.935	-2.000
27	9	18	28	9	19	68678.750	-0.313	0.10	-1.6	7.108	-0.935	-2.000
27	10	18	28	10	19	68641.220	0.336	0.12	1.4	24.305	-1.160	-1.835
27	10	17	28	10	18	68641.220	0.336	0.12	1.4	24.305	-1.160	-1.835
27	14	14	28	14	15	68612.590	0.173	0.10	0.9	109.502	-2.287	-0.879
27	14	13	28	14	14	68612.590	0.173	0.10	0.9	109.502	-2.287	-0.879
27	15	13	28	15	14	68623.020	0.155	0.10	0.8	135.051	-2.627	-0.571
27	15	12	28	15	13	68623.020	0.155	0.10	0.8	135.051	-2.627	-0.571
27	16	12	28	16	13	68637.600	-0.206	0.12	-0.9	162.329	-2.990	-0.235
27	16	11	28	16	12	68637.600	-0.206	0.12	-0.9	162.329	-2.990	-0.235
28	7	22	29	7	23	71333.830	0.100	0.20	0.3	-29.119	-0.612	-2.519
28	7	21	29	7	22	71342.050	0.131	0.20	0.4	-29.285	-0.611	-2.373
28	9	20	29	9	21	71148.570	-0.028	0.10	-0.1	2.243	-1.037	-2.281
28	9	19	29	9	20	71148.570	-0.044	0.10	-0.2	2.243	-1.037	-2.281
28	10	19	29	10	20	71105.020	0.217	0.12	0.9	20.126	-1.287	-2.117
28	10	18	29	10	19	71105.020	0.216	0.12	0.9	20.126	-1.287	-2.117
28	11	18	29	11	19	71079.240	0.049	0.10	0.3	39.637	-1.562	-1.918
28	11	17	29	11	18	71079.240	0.049	0.10	0.3	39.637	-1.562	-1.918
28	12	17	29	12	18	71066.410	0.087	0.12	0.4	60.839	-1.862	-1.690
28	12	16	29	12	17	71066.410	0.087	0.12	0.4	60.839	-1.862	-1.690
28	13	16	29	13	17	71062.690	-0.184	0.10	-1.0	83.769	-2.188	-1.433
28	13	15	29	13	16	71062.690	-0.184	0.10	-1.0	83.769	-2.188	-1.433
28	15	14	29	15	15	71076.380	0.005	0.12	0.0	134.909	-2.918	-0.833
28	15	13	29	15	14	71076.380	0.005	0.12	0.0	134.909	-2.918	-0.833
28	16	13	29	16	14	71090.770	-0.136	0.10	-0.8	163.149	-3.321	-0.489
28	16	12	29	16	13	71090.770	-0.136	0.10	-0.8	163.149	-3.321	-0.489
29	7	23	30	7	24	73827.140	0.158	0.15	0.8	-35.957	-0.674	-2.824
29	7	22	30	7	23	73839.450	-0.110	0.10	9.9	-36.243	-0.672	-2.600
29	9	21	30	9	22	73619.850	-0.096	0.10	-0.5	-3.197	-1.146	-2.582
29	9	20	30	9	21	73619.850	-0.125	0.10	-0.7	-3.197	-1.146	-2.581
29	10	20	30	10	21	73570.160	0.113	0.10	0.6	15.389	-1.423	-2.420
29	10	19	30	10	20	73570.160	0.112	0.10	0.6	15.389	-1.423	-2.420
29	11	19	30	11	20	73540.190	-0.043	0.10	-0.2	35.626	-1.727	-2.222
29	11	18	30	11	19	73540.190	-0.043	0.10	-0.2	35.626	-1.727	-2.222
29	12	18	30	12	19	73524.420	-0.014	0.10	-0.1	57.591	-2.060	-1.990

```
29 12 18 30 12 19   73524.420   -0.014 0.10   -0.1    57.591  -2.060   -1.990
29 12 17 30 12 18   73524.420   -0.014 0.10   -0.1    57.591  -2.060   -1.990
29 12 17 30 12 18   73524.420   -0.014 0.10   -0.1    57.591  -2.060   -1.990
29 13 17 30 13 18   73519.050    0.107 0.15    0.4    81.329  -2.421   -1.729
29 13 16 30 13 17   73519.050    0.107 0.15    0.4    81.329  -2.421   -1.729
29 15 15 30 15 16   73530.400    0.240 0.10    1.3   134.234  -3.229   -1.119
29 15 14 30 15 15   73530.400    0.240 0.10    1.3   134.234  -3.229   -1.119
29 16 14 30 16 15   73544.050   -0.132 0.10   -0.8   163.436  -3.676   -0.769
29 16 13 30 16 14   73544.050   -0.132 0.10   -0.8   163.436  -3.676   -0.769
30  7 24 31  7 25   76323.460    0.113 0.20    0.4   -43.440  -0.739   -3.155
30  7 23 31  7 24   76342.470    0.131 0.15    9.9   -43.921  -0.736   -2.818
30  9 22 31  9 23   76093.450    0.276 0.15    1.0    -9.237  -1.262   -2.903
30  9 21 31  9 22   76093.450    0.225 0.15    0.8    -9.238  -1.262   -2.901
30 10 21 31 10 22   76036.530   -0.136 0.10   -0.7    10.068  -1.568   -2.745
30 10 20 31 10 21   76036.530   -0.137 0.10   -0.8    10.068  -1.568   -2.745
30 11 20 31 11 21   76002.160   -0.137 0.10   -0.7    31.043  -1.904   -2.547
30 11 19 31 11 20   76002.160   -0.137 0.10   -0.7    31.043  -1.904   -2.547
31  9 23 32  9 24   78568.490    0.131 0.10    0.9   -15.906  -1.385   -3.244
31  9 22 32  9 23   78568.490    0.043 0.10    0.3   -15.908  -1.384   -3.240
31 11 21 32 11 22   78465.270   -0.149 0.10   -0.8    25.865  -2.092   -2.896
31 11 20 32 11 21   78465.270   -0.149 0.10   -0.8    25.865  -2.092   -2.896
31 12 20 32 12 21   78443.040    0.075 0.10    0.4    49.380  -2.497   -2.663
31 12 19 32 12 20   78443.040    0.075 0.10    0.4    49.380  -2.497   -2.663
31 16 16 32 16 17   78451.310    0.029 0.10    0.4   162.328  -4.459   -1.406
31 16 15 32 16 16   78451.310    0.029 0.10    0.4   162.328  -4.459   -1.406


rms deviation:  1.6092  time (sec):


Rotational constants (MHz)  and  kappa:
           5637.51       1316.2496       1125.0842    -0.91527
+-           14             0.16            0.17       0.00014


Inertial constants and defect (uÅ**2):
           89.6457       383.95383       449.19223       -24.4
+-          0.23           0.048           0.068           0.3


Quartic distortion constants:
      0.654873    -15.6476         190     0.13438      -0.993
+-    0.0056        0.031        fixed     0.022         fixed


Sextic distortion constants:
          0 -0.13320        0        0        0        0        0
+-    fixed  0.021      fixed    fixed    fixed    fixed    fixed


Significant Digits and Correlation Matrix:

   6       0.961  -0.934   0.107  -0.091  -0.056   0.025
           8      -0.996  -0.131  -0.286   0.213  -0.167
                   8       0.217   0.363  -0.294   0.247
                           6       0.841  -0.936   0.911
                                   6      -0.738   0.959
                                           5      -0.773
                                                   5
```

Table 4S Microwave spectrum of the ground vibrational state of the *anticlinal* conformer of H2C=C=CH^{78}SeCN

Total number of transitions: 62

Transition	obs. frequency	obs.- calc.	weight	t	distortion corrections total	higher	fixed
19 7 13 20 7 14	49383.190	0.126	0.10	1.1	6.865	-0.422	-1.878
19 7 12 20 7 13	49383.190	0.044	0.10	0.4	6.865	-0.422	-1.877
19 8 12 20 8 13	49349.470	-0.001	0.10	-0.0	17.209	-0.554	-1.514
19 8 11 20 8 12	49349.470	-0.003	0.10	-0.0	17.209	-0.554	-1.514
19 10 10 20 10 11	49323.120	0.054	0.10	0.5	41.615	-0.868	-0.933
19 10 9 20 10 10	49323.120	0.054	0.10	0.5	41.615	-0.868	-0.933
20 7 14 21 7 15	51868.950	-0.223	0.10	-2.0	4.212	-0.488	-2.341
20 7 13 21 7 14	51868.950	-0.381	0.10	-3.4	4.210	-0.488	-2.341
20 8 13 21 8 14	51829.110	-0.001	0.15	-0.0	15.136	-0.640	-1.905
20 8 12 21 8 13	51829.110	-0.005	0.15	-0.0	15.136	-0.640	-1.905
20 9 12 21 9 13	51806.900	0.078	0.15	0.4	27.318	-0.812	-1.550
20 9 11 21 9 12	51806.900	0.078	0.15	0.4	27.318	-0.812	-1.550
20 14 7 21 14 8	51812.800	-0.203	0.15	-1.4	108.420	-1.973	-0.048
20 14 6 21 14 7	51812.800	-0.203	0.15	-1.4	108.420	-1.973	-0.048
22 8 15 23 8 16	56794.060	0.208	0.10	1.7	9.593	-0.839	-2.891
22 8 14 23 8 15	56794.060	0.191	0.10	1.6	9.592	-0.839	-2.890
22 9 14 23 9 15	56761.840	0.018	0.10	0.1	23.038	-1.065	-2.403
22 9 13 23 9 14	56761.840	0.017	0.10	0.1	23.038	-1.065	-2.403
22 10 13 23 10 14	56744.700	0.216	0.15	1.1	37.876	-1.318	-1.991
22 10 13 23 10 14	56744.700	0.216	0.15	1.1	37.876	-1.318	-1.991
22 13 10 23 13 11	56742.400	0.053	0.15	0.3	91.151	-2.233	-0.915
22 13 9 23 13 10	56742.400	0.053	0.15	0.3	91.151	-2.233	-0.915
23 9 15 24 9 16	59241.390	-0.050	0.20	-0.2	20.165	-1.209	-2.930
23 9 14 24 9 15	59241.390	-0.051	0.20	-0.2	20.165	-1.209	-2.930
24 8 17 25 8 18	61766.720	0.223	0.12	1.5	1.995	-1.073	-4.201
24 8 16 25 8 17	61766.720	0.163	0.12	1.1	1.994	-1.073	-4.201
24 9 16 25 9 17	61722.520	-0.036	0.15	-0.2	16.766	-1.365	-3.531
24 9 15 25 9 16	61722.520	-0.038	0.15	-0.2	16.766	-1.365	-3.531
24 12 13 25 12 14	61680.800	-0.132	0.15	-0.7	70.034	-2.440	-2.076
24 12 12 25 12 13	61680.800	-0.132	0.15	-0.7	70.034	-2.440	-2.076
24 13 12 25 13 13	61684.090	0.091	0.20	0.4	90.940	-2.866	-1.659
24 13 11 25 13 12	61684.090	0.091	0.20	0.4	90.940	-2.866	-1.659
25 9 17 26 9 18	64205.000	-0.238	0.10	-1.9	12.814	-1.533	-4.217
25 9 16 26 9 17	64205.000	-0.241	0.10	-1.9	12.814	-1.533	-4.216
25 10 16 26 10 17	64175.400	-0.032	0.10	-0.3	29.741	-1.899	-3.589
25 10 15 26 10 16	64175.400	-0.032	0.10	-0.3	29.741	-1.899	-3.589
26 9 18 27 9 19	66689.750	0.197	0.20	0.8	8.278	-1.714	-4.993
26 9 17 27 9 18	66689.750	0.190	0.20	0.7	8.278	-1.714	-4.993
26 11 16 27 11 17	66635.660	0.106	0.15	0.6	45.164	-2.577	-3.661
26 11 15 27 11 16	66635.660	0.106	0.15	0.6	45.164	-2.577	-3.661
26 12 15 27 12 16	66627.570	0.168	0.15	0.9	66.050	-3.071	-3.120
26 12 14 27 12 15	66627.570	0.168	0.15	0.9	66.050	-3.071	-3.120
26 13 14 27 13 15	66627.570	0.086	0.15	0.5	88.628	-3.608	-2.618
26 13 13 27 13 14	66627.570	0.086	0.15	0.5	88.628	-3.608	-2.618
26 15 12 27 15 13	66645.870	0.167	0.12	1.4	138.962	-4.810	-1.658
26 15 11 27 15 12	66645.870	0.167	0.12	1.4	138.962	-4.810	-1.658
26 16 11 27 16 12	66661.620	-0.170	0.20	-0.8	166.750	-5.474	-1.178
26 16 10 27 16 11	66661.620	-0.170	0.20	-0.8	166.750	-5.474	-1.178
27 10 18 28 10 19	69135.190	-0.120	0.12	-0.8	21.522	-2.367	-5.038
27 10 17 28 10 18	69135.190	-0.121	0.12	-0.8	21.522	-2.367	-5.038
27 12 16 28 12 17	69101.350	-0.292	0.12	-2.1	63.204	-3.423	-3.742
27 12 15 28 12 16	69101.350	-0.292	0.12	-2.1	63.204	-3.423	-3.742

```
28  9 20 29  9 21   71663.270   -0.097 0.15   -0.5    -2.664  -2.116   -6.859
28  9 19 29  9 20   71663.270   -0.119 0.15   -0.6    -2.665  -2.116   -6.859
28 10 19 29 10 20   71617.280    0.114 0.10    0.9    16.490  -2.626   -5.899
28 10 18 29 10 19   71617.280    0.113 0.10    0.9    16.490  -2.626   -5.899
29  9 21 30  9 22   74153.020    0.009 0.12    0.1    -9.135  -2.337   -7.968
29  9 20 30  9 21   74153.020   -0.031 0.12   -0.2    -9.136  -2.337   -7.968
31  9 23 32  9 24   79138.300    0.141 0.10    1.4   -24.240  -2.822  -10.594
31  9 22 32  9 23   79138.300    0.021 0.10    0.2   -24.245  -2.822  -10.595
31 10 22 32 10 23   79070.940   -0.063 0.12   -0.5    -2.647  -3.512   -9.134
31 10 21 32 10 22   79070.940   -0.068 0.12   -0.5    -2.647  -3.512   -9.134


rms deviation:  1.2503


Rotational constants (MHz)  and  kappa:
            5536.2       1326.3581       1132.1943    -0.91182
+-           fixed          0.038           0.044      0.00004


Inertial constants and defect (uÅ**2):
            91.286       381.02762       446.37133      -25.94
+-           fixed         0.011           0.017          0.03


Quartic distortion constants:
      0.720042     -16.679         190       0.229      -0.993
+-    0.0040         0.054       fixed       fixed       fixed


Sextic and higher distortion constants:
          0 -0.27198        0        0        0        0        0
+-    fixed  0.037      fixed    fixed    fixed    fixed    fixed


Significant Digits and Correlation Matrix:

   8      -0.977   0.640  -0.288   0.121
           8      -0.466   0.476   0.079
                   6       0.502   0.803
                           5       0.901
                                   5
```

Table 5S Microwave spectrum of the ground vibrational state of *synclinal* conformer of $C_3H_5{}^{80}SeCN$

Total number of transitions: 161

Transition	obs. frequency	obs.- calc.	weight	t	distortion corrections total	distortion corrections fixed
11 8 4 12 8 5	38248.560	-0.138	0.15	-0.5	5.134	-0.532
11 8 3 12 8 4	38248.560	-0.157	0.15	-0.6	5.134	-0.532
11 9 3 12 9 4	38189.244	0.201	0.30	0.4	9.300	-0.337
11 9 2 12 9 3	38189.244	0.200	0.30	0.4	9.300	-0.337
11 10 2 12 10 3	38148.600	0.137	0.15	0.5	13.897	-0.157
11 10 1 12 10 2	38148.600	0.137	0.15	0.5	13.897	-0.157
12 6 7 13 6 8	41780.650	-0.172	0.20	-0.5	-4.398	-1.529
12 6 6 13 6 7	41823.390	-0.080	0.30	-0.2	-4.623	-1.607
12 8 5 13 8 6	41490.950	0.066	0.10	0.4	3.528	-0.846
12 8 4 13 8 5	41490.950	-0.008	0.10	-0.0	3.528	-0.846
12 9 4 13 9 5	41413.950	0.040	0.10	0.2	8.101	-0.597
12 9 3 13 9 4	41413.950	0.038	0.10	0.2	8.101	-0.597
12 10 3 13 10 4	41361.370	0.045	0.10	0.3	13.123	-0.375
12 10 2 13 10 3	41361.370	0.045	0.10	0.3	13.123	-0.375
12 11 2 13 11 3	41324.700	0.173	0.20	0.5	18.618	-0.166
12 11 1 13 11 2	41324.935	0.408	0.20	1.2	18.618	-0.166
13 9 5 14 9 6	44649.380	0.238	0.10	1.4	6.386	-0.940
13 9 4 14 9 5	44649.380	0.231	0.10	1.4	6.386	-0.940
13 11 3 14 11 4	44535.590	0.203	0.10	1.2	17.811	-0.412
13 11 2 14 11 3	44535.590	0.203	0.10	1.2	17.811	-0.412
13 12 2 14 12 3	44501.720	-0.107	0.15	-0.4	24.283	-0.171
13 12 1 14 12 2	44501.720	-0.107	0.15	-0.4	24.283	-0.171
14 9 6 15 9 7	47895.550	-0.116	0.10	-0.7	4.098	-1.383
14 9 5 15 9 6	47895.550	-0.142	0.10	-0.8	4.098	-1.383
14 11 4 15 11 5	47753.280	-0.135	0.10	-0.8	16.471	-0.733
14 11 3 15 11 4	47753.280	-0.135	0.10	-0.8	16.471	-0.733
14 13 2 15 13 3	47680.280	-0.095	0.20	-0.3	30.976	-0.171
14 13 1 15 13 2	47680.280	-0.095	0.20	-0.3	30.976	-0.171
14 14 1 15 14 2	47658.090	-0.154	0.15	-0.6	39.070	0.104
14 14 0 15 14 1	47658.090	-0.154	0.15	-0.6	39.070	0.104
15 7 8 16 7 9	51557.340	-0.228	0.20	-0.7	-10.728	-3.278
15 9 7 16 9 8	51154.030	-0.436	0.10	-2.6	1.176	-1.945
15 9 6 16 9 7	51154.030	-0.523	0.10	-3.1	1.175	-1.945
15 12 4 16 12 5	50926.720	0.083	0.10	0.5	22.045	-0.802
15 12 3 16 12 4	50926.720	0.083	0.10	0.5	22.045	-0.802
16 8 9 17 8 10	54608.000	0.175	0.20	0.5	-8.995	-3.336
16 8 8 17 8 9	54613.600	0.165	0.20	0.5	-9.058	-3.354
16 9 8 17 9 9	54426.340	-0.252	0.10	-1.5	-2.447	-2.650
16 9 7 17 9 8	54426.340	-0.519	0.10	-3.1	-2.450	-2.650
16 12 5 17 12 6	54148.970	-0.040	0.10	-0.2	20.026	-1.247
16 12 4 17 12 5	54148.970	-0.040	0.10	-0.2	20.026	-1.247
16 13 4 17 13 5	54101.610	-0.198	0.10	-1.2	28.657	-0.871
16 13 3 17 13 4	54101.610	-0.198	0.10	-1.2	28.657	-0.871
16 14 3 17 14 4	54067.280	0.326	0.25	0.8	37.907	-0.510
16 14 2 17 14 3	54067.280	0.326	0.25	0.8	37.907	-0.510
16 16 1 17 16 2	54022.850	-0.074	0.15	-0.3	58.315	0.198
16 16 0 17 16 1	54022.850	-0.074	0.15	-0.3	58.315	0.198
17 10 8 18 10 9	57562.420	-0.306	0.10	-1.8	0.708	-2.842
17 10 7 18 10 8	57562.420	-0.336	0.10	-2.0	0.707	-2.842
17 11 7 18 11 8	57456.020	-0.109	0.10	-0.6	8.741	-2.282
17 11 6 18 11 7	57456.020	-0.110	0.10	-0.6	8.741	-2.282
17 12 6 18 12 7	57378.620	-0.023	0.10	-0.1	17.338	-1.796

17	12	5	18	12	6	57378.620	-0.023	0.10	-0.1	17.338	-1.796
17	13	5	18	13	6	57321.410	0.013	0.15	0.0	26.546	-1.354
17	13	4	18	13	5	57321.410	0.013	0.15	0.0	26.546	-1.354
17	14	4	18	14	5	57278.890	0.092	0.10	0.5	36.393	-0.938
17	14	3	18	14	4	57278.890	0.092	0.10	0.5	36.393	-0.938
18	7	11	19	7	12	61884.160	-0.124	0.20	9.9	-30.728	-8.478
18	8	11	19	8	12	61270.650	0.017	0.20	0.1	-19.894	-5.694
18	10	9	19	10	10	60835.770	-0.016	0.10	-0.1	-3.898	-3.739
18	10	8	19	10	9	60835.770	-0.106	0.10	-0.6	-3.899	-3.739
18	11	8	19	11	9	60708.650	0.077	0.10	0.5	4.738	-3.050
18	11	7	19	11	8	60708.650	0.074	0.10	0.4	4.738	-3.050
18	12	7	19	12	8	60616.010	-0.005	0.10	-0.0	13.927	-2.465
18	12	6	19	12	7	60616.010	-0.005	0.10	-0.0	13.927	-2.465
18	13	6	19	13	7	60547.670	0.261	0.10	1.5	23.733	-1.944
18	13	5	19	13	6	60547.670	0.261	0.10	1.5	23.733	-1.944
18	14	5	19	14	6	60496.090	0.039	0.10	0.2	34.194	-1.462
18	14	4	19	14	5	60496.090	0.039	0.10	0.2	34.194	-1.462
18	15	4	19	15	5	60457.830	0.290	0.10	1.7	45.338	-1.003
18	15	3	19	15	4	60457.830	0.290	0.10	1.7	45.338	-1.003
18	17	2	19	17	3	60408.270	0.352	0.10	2.1	69.736	-0.115
18	17	1	19	17	2	60408.270	0.352	0.10	2.1	69.736	-0.115
18	18	1	19	18	2	60393.350	0.189	0.15	0.7	83.012	0.329
18	18	0	19	18	1	60393.350	0.189	0.15	0.7	83.012	0.329
19	7	13	20	7	14	64928.310	0.152	0.30	2.3	-33.150	-8.206
19	8	12	20	8	13	64628.710	-0.173	0.20	-0.6	-26.716	-7.242
19	8	11	20	8	12	64693.370	0.065	0.20	0.2	-27.808	-7.643
19	9	11	20	9	12	64334.210	0.029	0.20	0.1	-18.263	-5.899
19	9	10	20	9	11	64339.240	0.251	0.20	0.7	-18.349	-5.925
19	11	9	20	11	10	63971.340	0.136	0.10	0.8	-0.081	-3.978
19	11	8	20	11	9	63971.340	0.126	0.10	0.7	-0.082	-3.978
19	12	8	20	12	9	63861.600	-0.029	0.10	-0.2	9.734	-3.273
19	12	7	20	12	8	63861.600	-0.030	0.10	-0.2	9.734	-3.273
19	13	7	20	13	8	63780.150	-0.085	0.10	-0.5	20.164	-2.656
19	13	6	20	13	7	63780.150	-0.085	0.10	-0.5	20.164	-2.656
19	14	6	20	14	7	63719.090	0.059	0.10	0.3	31.260	-2.095
19	14	5	20	14	6	63719.090	0.059	0.10	0.3	31.260	-2.095
19	15	5	20	15	6	63672.680	-0.123	0.10	-0.7	43.057	-1.570
19	15	4	20	15	5	63672.680	-0.123	0.10	-0.7	43.057	-1.570
19	18	2	20	18	3	63593.700	0.255	0.10	1.5	82.847	-0.083
19	18	1	20	18	2	63593.700	0.255	0.10	1.5	82.847	-0.083
19	19	1	20	19	2	63580.550	-0.015	0.10	-0.1	97.618	0.410
19	19	0	20	19	1	63580.550	-0.015	0.10	-0.1	97.618	0.410
20	8	13	21	8	14	68002.130	0.075	0.20	0.3	-34.462	-9.044
20	9	12	21	9	13	67671.000	0.294	0.20	0.9	-25.451	-7.470
20	9	11	21	9	12	67682.200	0.373	0.30	0.7	-25.676	-7.542
20	10	10	21	10	11	67422.160	-0.304	0.10	-1.9	-15.802	-6.137
20	12	9	21	12	10	67116.000	-0.014	0.10	-0.1	4.698	-4.238
20	12	8	21	12	9	67116.000	-0.015	0.10	-0.1	4.698	-4.238
20	13	8	21	13	9	67020.610	0.324	0.10	1.9	15.783	-3.506
20	13	7	21	13	8	67020.610	0.324	0.10	1.9	15.783	-3.506
20	14	7	21	14	8	66948.090	0.024	0.10	0.1	27.537	-2.853
20	14	6	21	14	7	66948.090	0.024	0.10	0.1	27.537	-2.853
20	16	5	21	16	6	66851.350	-0.204	0.10	-1.2	53.217	-1.679
20	16	4	21	16	5	66851.350	-0.204	0.10	-1.2	53.217	-1.679
20	17	4	21	17	5	66820.370	0.172	0.10	1.0	67.194	-1.126
20	17	3	21	17	4	66820.370	0.172	0.10	1.0	67.194	-1.126
20	18	3	21	18	4	66796.850	-0.199	0.10	-1.2	81.949	-0.583
20	18	2	21	18	3	66796.850	-0.199	0.10	-1.2	81.949	-0.583
21	9	13	22	9	14	71026.200	0.792	0.20	2.5	-33.725	-9.340
21	9	12	22	9	13	71049.840	0.052	0.20	0.2	-34.278	-9.531
21	12	10	22	12	11	70379.800	0.069	0.10	0.4	-1.246	-5.384
21	12	9	22	12	10	70379.800	0.066	0.10	0.4	-1.246	-5.384

21	14	8	22	14	9	70183.580	0.086	0.10	0.5	22.971	-3.750
21	14	7	22	14	8	70183.580	0.086	0.10	0.5	22.971	-3.750
21	16	6	22	16	7	70069.490	-0.253	0.10	-1.5	50.054	-2.406
21	16	5	22	16	6	70069.490	-0.253	0.10	-1.5	50.054	-2.406
21	17	5	22	17	6	70032.220	-0.034	0.15	-0.1	64.761	-1.786
21	17	4	22	17	5	70032.220	-0.034	0.15	-0.1	64.761	-1.786
21	19	3	22	19	4	69983.640	0.019	0.10	0.1	96.606	-0.587
21	19	2	22	19	3	69983.640	0.019	0.10	0.1	96.606	-0.587
22	9	13	23	9	14	74449.220	0.405	0.30	0.8	-44.409	-11.999
22	10	13	23	10	14	74067.800	-0.074	0.20	-0.2	-31.809	-9.553
22	10	12	23	10	13	74071.700	-0.143	0.20	-0.4	-31.914	-9.585
22	12	11	23	12	12	73653.350	-0.030	0.15	-0.1	-8.168	-6.735
22	12	10	23	12	11	73653.350	-0.040	0.15	-0.2	-8.168	-6.735
22	13	10	23	13	11	73523.780	-0.008	0.10	-0.0	4.346	-5.700
22	13	9	23	13	10	73523.780	-0.008	0.10	-0.0	4.346	-5.700
22	14	9	23	14	10	73425.900	0.236	0.10	1.4	17.505	-4.805
22	14	8	23	14	9	73425.900	0.236	0.10	1.4	17.505	-4.805
22	16	7	23	16	8	73292.700	-0.106	0.15	-0.4	46.036	-3.262
22	16	6	23	16	7	73292.700	-0.106	0.15	-0.4	46.036	-3.262
22	17	6	23	17	7	73248.500	-0.015	0.10	-0.1	61.490	-2.563
22	17	5	23	17	6	73248.500	-0.015	0.10	-0.1	61.490	-2.563
22	19	4	23	19	5	73189.760	-0.107	0.10	-0.6	94.902	-1.233
22	19	3	23	19	4	73189.760	-0.107	0.10	-0.6	94.902	-1.233
22	22	1	23	22	2	73153.190	0.286	0.10	2.1	151.483	0.725
22	22	0	23	22	1	73153.190	0.286	0.10	2.1	151.483	0.725
23	10	13	24	10	14	77425.490	0.556	0.20	1.7	-41.855	-11.828
23	11	13	24	11	14	77139.039	0.145	0.10	1.0	-28.990	-9.823
23	12	12	24	12	13	76937.760	0.148	0.15	0.6	-16.142	-8.318
23	12	11	24	12	12	76937.760	0.120	0.15	0.5	-16.143	-8.318
23	13	11	24	13	12	76788.280	0.118	0.10	0.7	-2.839	-7.087
23	13	10	24	13	11	76788.280	0.117	0.10	0.7	-2.839	-7.087
23	14	10	24	14	11	76674.730	-0.212	0.20	-0.6	11.078	-6.036
23	14	9	24	14	10	76674.730	-0.212	0.20	-0.6	11.078	-6.036
23	15	9	24	15	10	76588.150	0.086	0.15	0.3	25.706	-5.107
23	15	8	24	15	9	76588.150	0.086	0.15	0.3	25.706	-5.107
23	16	8	24	16	9	76520.650	-0.331	0.10	-2.1	41.110	-4.261
23	16	7	24	16	8	76520.650	-0.331	0.10	-2.1	41.110	-4.261
23	18	6	24	18	7	76429.400	-0.053	0.10	-0.3	74.400	-2.721
23	18	5	24	18	6	76429.400	-0.053	0.10	-0.3	74.400	-2.721
23	19	5	24	19	6	76399.530	0.079	0.10	0.5	92.339	-1.993
23	19	4	24	19	5	76399.530	0.079	0.10	0.5	92.339	-1.993
23	20	4	24	20	5	76377.330	-0.095	0.10	-0.6	111.164	-1.279
23	20	3	24	20	4	76377.330	-0.095	0.10	-0.6	111.164	-1.279
23	21	3	24	21	4	76361.670	-0.375	0.10	-2.4	130.888	-0.570
23	21	2	24	21	3	76361.670	-0.375	0.10	-2.4	130.888	-0.570
23	22	2	24	22	3	76352.250	-0.033	0.15	-0.1	151.521	0.140
23	22	1	24	22	2	76352.250	-0.033	0.15	-0.1	151.521	0.140

rms deviation: 1.6787

Rotational constants (MHz) and kappa:

	4176.37	1812.9645	1338.2711	-0.66549
+-	1.9	0.096	0.099	0.00010

Inertial constants and defect (uÅ**2):

	121.009	278.75840	377.63581	-22.13
+-	0.055	0.015	0.028	0.10

```
Quartic distortion constants:
        1.2605     -9.5769        30.7       0.407       0.696
+-      0.0029      0.0087       fixed       fixed       fixed


Significant Digits and Correlation Matrix:

   6       0.993  -0.988   0.381  -0.451
           8      -0.999   0.459  -0.535
                   8      -0.461   0.559
                           5      -0.817
                                   5
```

Table 6S Microwave spectrum of the first excited state of the torsion about the C–Se bond of the *synclinal* conformer of $C_3H_5{}^{80}SeCN$

Total number of transitions: 85

Transition	obs. frequency	obs.- calc.	weight	t	distortion corrections total	higher	fixed
11 8 4 12 8 5	38239.000	0.297	0.20	0.7	5.020	-0.530	
11 8 3 12 8 4	38239.000	0.280	0.20	0.6	5.019	-0.530	
11 9 3 12 9 4	38179.420	-0.318	0.20	-0.7	8.936	-0.337	
11 9 2 12 9 3	38179.420	-0.318	0.20	-0.7	8.936	-0.337	
11 11 1 12 11 2	38111.370	-0.189	0.20	-0.4	17.996	0.014	
11 11 0 12 11 1	38111.370	-0.189	0.20	-0.4	17.996	0.014	
12 12 1 13 12 2	41289.000	0.138	0.14	0.5	23.366	0.034	
12 12 0 13 12 1	41289.000	0.138	0.14	0.5	23.366	0.034	
13 8 6 14 8 7	44733.530	0.106	0.20	0.2	1.598	-1.252	
13 8 5 14 8 6	44733.530	-0.134	0.20	-0.3	1.597	-1.252	
13 9 5 14 9 6	44637.440	0.276	0.15	0.9	6.310	-0.935	
13 9 4 14 9 5	44637.440	0.270	0.15	0.8	6.310	-0.935	
13 10 4 14 10 5	44571.000	-0.136	0.10	-0.7	11.449	-0.663	
13 10 3 14 10 4	44571.000	-0.136	0.10	-0.7	11.449	-0.663	
13 11 3 14 11 4	44525.000	0.432	0.15	1.3	17.051	-0.414	
13 11 2 14 11 3	44525.000	0.432	0.15	1.3	17.051	-0.414	
13 12 2 14 12 3	44490.860	-0.344	0.20	-0.8	23.133	-0.175	
13 12 2 14 12 3	44490.850	-0.354	0.10	-1.8	23.133	-0.175	
13 12 1 14 12 2	44490.860	-0.344	0.20	-0.8	23.133	-0.175	
13 12 1 14 12 2	44490.850	-0.354	0.10	-1.8	23.133	-0.175	
13 13 1 14 13 2	44466.900	-0.301	0.20	-0.7	29.707	0.061	
13 13 0 14 13 1	44466.900	-0.301	0.20	-0.7	29.707	0.061	
14 11 4 15 11 5	47741.780	0.331	0.20	0.8	15.863	-0.732	
14 11 3 15 11 4	47741.780	0.331	0.20	0.8	15.863	-0.732	
15 9 7 16 9 8	51139.550	0.286	0.10	1.5	1.554	-1.933	
15 9 6 16 9 7	51139.550	0.203	0.10	1.0	1.553	-1.933	
15 12 4 16 12 5	50914.200	0.322	0.15	1.0	21.183	-0.802	
15 12 3 16 12 4	50914.200	0.322	0.15	1.0	21.183	-0.802	
15 14 2 16 14 3	50847.330	-0.326	0.10	-1.7	36.914	-0.174	
15 14 1 16 14 2	50847.330	-0.326	0.10	-1.7	36.914	-0.174	
16 13 4 17 13 5	54088.220	0.029	0.10	0.1	27.491	-0.871	
16 13 3 17 13 4	54088.220	0.029	0.10	0.1	27.491	-0.871	
17 9 9 18 9 10	57694.540	0.478	0.10	3.2	-5.812	-3.499	
17 9 8 18 9 9	57694.540	-0.230	0.10	-1.5	-5.821	-3.501	
17 10 8 18 10 9	57545.640	0.065	0.10	0.3	1.302	-2.823	
17 10 7 18 10 8	57545.640	0.037	0.10	0.2	1.302	-2.823	
17 15 3 18 15 4	57232.390	-0.202	0.15	-0.6	44.740	-0.543	
17 15 2 18 15 3	57232.390	-0.202	0.15	-0.6	44.740	-0.543	
18 10 9 19 10 10	60816.930	0.102	0.10	0.5	-2.924	-3.713	
18 10 8 19 10 9	60816.930	0.017	0.10	0.1	-2.926	-3.713	
18 11 8 19 11 9	60691.390	0.238	0.15	0.7	5.209	-3.031	
18 11 7 19 11 8	60691.390	0.235	0.15	0.7	5.209	-3.031	
18 12 7 19 12 8	60600.000	0.436	0.15	1.3	13.856	-2.452	
18 12 6 19 12 7	60600.000	0.436	0.15	1.3	13.856	-2.452	
18 14 5 19 14 6	60480.800	0.342	0.10	1.6	32.915	-1.460	

```
18 14  4 19 14  5   60480.800    0.342 0.10    1.6    32.915  -1.460
18 15  4 19 15  5   60441.750   -0.255 0.15   -0.8    43.389  -1.007
18 15  3 19 15  4   60441.750   -0.255 0.15   -0.8    43.389  -1.007
18 17  2 19 17  3   60392.370    0.375 0.15    1.2    66.316  -0.130
18 17  1 19 17  2   60392.370    0.375 0.15    1.2    66.316  -0.130
19  9 11 20  9 12   64310.000   -0.404 0.10    9.9   -16.351  -5.857
19 12  8 20 12  9   63843.850    0.054 0.10    0.3    10.036  -3.253
19 12  7 20 12  8   63843.850    0.053 0.10    0.3    10.036  -3.253
19 15  5 20 15  6   63656.020   -0.243 0.15   -0.7    41.374  -1.569
19 15  4 20 15  5   63656.020   -0.243 0.15   -0.7    41.374  -1.569
20 13  8 21 13  9   67002.000    0.079 0.10    0.4    15.866  -3.487
20 13  7 21 13  8   67002.000    0.079 0.10    0.4    15.866  -3.487
20 14  7 21 14  8   66929.970   -0.275 0.10   -1.3    26.923  -2.840
20 14  6 21 14  7   66929.970   -0.275 0.10   -1.3    26.923  -2.840
20 17  4 21 17  5   66802.450   -0.011 0.10   -0.1    64.202  -1.134
20 17  3 21 17  4   66802.450   -0.011 0.10   -0.1    64.202  -1.134
21 11 11 22 11 12   70507.040   -0.257 0.10   -1.7   -10.573  -6.370
21 11 10 22 11 11   70507.040   -0.337 0.10   -2.2   -10.575  -6.370
21 13  9 22 13 10   70248.490    0.208 0.10    1.1    11.076  -4.487
21 13  8 22 13  9   70248.490    0.208 0.10    1.1    11.076  -4.487
21 14  8 22 14  9   70164.020   -0.471 0.10   -2.4    22.781  -3.730
21 14  7 22 14  8   70164.020   -0.471 0.10   -2.4    22.781  -3.730
21 17  5 22 17  6   70013.100   -0.494 0.15   -1.5    62.073  -1.788
21 17  4 22 17  5   70013.100   -0.494 0.15   -1.5    62.073  -1.788
22 14  9 23 14 10   73405.790    0.360 0.10    2.0    17.805  -4.776
22 14  8 23 14  9   73405.790    0.360 0.10    2.0    17.805  -4.776
22 16  7 23 16  8   73273.290    0.030 0.10    0.2    44.640  -3.250
22 16  6 23 16  7   73273.290    0.030 0.10    0.2    44.640  -3.250
22 19  4 23 19  5   73169.650    0.037 0.15    0.1    90.573  -1.246
22 19  3 23 19  4   73169.650    0.037 0.15    0.1    90.573  -1.246
23 13 11 24 13 12   76765.450   -0.103 0.15   -0.4    -1.167  -7.039
23 13 10 24 13 11   76765.450   -0.104 0.15   -0.4    -1.167  -7.039
23 17  7 24 17  8   76448.600   -0.043 0.10   -0.2    55.445  -3.461
23 17  6 24 17  7   76448.600   -0.043 0.10   -0.2    55.445  -3.461
23 18  6 24 18  7   76408.960    0.234 0.10    1.3    71.492  -2.719
23 18  5 24 18  6   76408.960    0.234 0.10    1.3    71.492  -2.719
23 21  3 24 21  4   76339.440   -0.290 0.15   -1.2   124.578  -0.596
23 21  2 24 21  3   76339.440   -0.290 0.15   -1.2   124.578  -0.596
23 23  1 24 23  2   76323.570    0.266 0.15    9.9   164.212   0.812
23 23  0 24 23  1   76323.570    0.266 0.15    9.9   164.212   0.812


rms deviation:  2.2360


Rotational constants (MHz)  and  kappa:
           4171.62        1810.869        1340.066    -0.66746
+-           fixed           0.031           0.042     0.00005


Inertial constants and defect (uÅ**2):
           121.147        279.0810        377.1301      -23.10
+-           fixed          0.0048          0.012         0.02
```

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Quartic distortion constants:
        1.1490       -8.983         30.7        0.407        0.696
+-      0.0060        0.020        fixed        fixed        fixed


Significant Digits and Correlation Matrix:
   7      -0.988    0.778   -0.867
           7       -0.696    0.863
                    5       -0.851
                             4
```

Table 7S Microwave spectrum of the first excited state of the lowest bending vibration of the *synclinal* conformer of $C_3H_5{}^{80}SeCN$

Total number of transitions: 89

Transition	obs. frequency	obs.- calc.	weight	t	distortion corrections total	fixed
11 7 5 12 7 6	38318.380	0.266	0.20	0.6	1.276	-0.758
11 7 4 12 7 5	38318.380	-0.443	0.20	-1.0	1.273	-0.758
11 8 4 12 8 5	38228.300	0.076	0.15	0.2	5.069	-0.532
11 8 3 12 8 4	38228.300	0.057	0.15	0.2	5.069	-0.532
12 8 5 13 8 6	41468.210	0.039	0.10	0.2	3.421	-0.845
12 8 4 13 8 5	41468.210	-0.033	0.10	-0.2	3.421	-0.845
12 9 4 13 9 5	41391.580	-0.366	0.10	-1.9	8.032	-0.597
12 9 3 13 9 4	41391.580	-0.368	0.10	-1.9	8.032	-0.597
13 9 5 14 9 6	44624.800	-0.193	0.10	-1.0	6.269	-0.939
13 9 4 14 9 5	44624.800	-0.200	0.10	-1.0	6.269	-0.939
13 11 3 14 11 4	44512.790	0.365	0.15	1.2	17.790	-0.413
13 11 2 14 11 3	44512.790	0.365	0.15	1.2	17.790	-0.413
14 9 6 15 9 7	47869.290	0.072	0.15	0.2	3.922	-1.381
14 9 5 15 9 6	47869.290	0.047	0.15	0.1	3.922	-1.381
14 10 5 15 10 6	47786.830	0.149	0.15	0.5	9.905	-1.038
14 10 4 15 10 5	47786.830	0.149	0.15	0.5	9.905	-1.038
14 14 1 15 14 2	47634.340	-0.127	0.15	-0.4	39.194	0.101
14 14 0 15 14 1	47634.340	-0.127	0.15	-0.4	39.194	0.101
15 9 7 16 9 8	51125.480	-0.114	0.15	-0.4	0.931	-1.942
15 9 6 16 9 7	51125.480	-0.199	0.15	-0.6	0.931	-1.942
15 10 6 16 10 7	51023.880	-0.075	0.15	-0.2	7.415	-1.512
15 10 5 16 10 6	51023.880	-0.077	0.15	-0.2	7.415	-1.512
15 11 5 16 11 6	50951.930	-0.121	0.15	-0.4	14.416	-1.140
15 11 4 16 11 5	50951.930	-0.121	0.15	-0.4	14.416	-1.140
15 12 4 16 12 5	50899.750	-0.361	0.15	-1.1	21.976	-0.802
15 12 3 16 12 4	50899.750	-0.361	0.15	-1.1	21.976	-0.802
15 15 1 16 15 2	50814.900	0.293	0.20	0.7	48.209	0.144
15 15 0 16 15 1	50814.900	0.293	0.20	0.7	48.209	0.144
16 9 8 17 9 9	54395.110	-0.051	0.10	-0.3	-2.771	-2.646
16 9 7 17 9 8	54395.110	-0.312	0.10	-1.7	-2.774	-2.646
16 10 7 17 10 8	54271.800	0.326	0.10	1.6	4.252	-2.105
16 10 6 17 10 7	54271.800	0.317	0.10	1.5	4.252	-2.105
16 11 6 17 11 7	54183.720	-0.164	0.15	-0.5	11.786	-1.650
16 11 5 17 11 6	54183.720	-0.164	0.15	-0.5	11.786	-1.650
16 14 3 17 14 4	54039.260	-0.096	0.10	-0.5	37.923	-0.511
16 14 2 17 14 3	54039.260	-0.096	0.10	-0.5	37.923	-0.511
17 9 9 18 9 10	57679.180	0.160	0.10	1.0	-7.259	-3.518
17 10 8 18 10 9	57530.390	0.354	0.10	1.7	0.351	-2.837
17 10 7 18 10 8	57530.390	0.325	0.10	1.6	0.351	-2.837
17 11 7 18 11 8	57424.720	0.211	0.10	1.0	8.451	-2.279
17 11 6 18 11 7	57424.730	0.221	0.10	1.1	8.451	-2.279
17 12 6 18 12 7	57348.000	0.154	0.10	0.7	17.120	-1.794
17 12 5 18 12 6	57348.000	0.154	0.10	0.7	17.120	-1.794
17 13 5 18 13 6	57291.500	0.243	0.10	1.2	26.406	-1.353
17 13 4 18 13 5	57291.500	0.243	0.10	1.2	26.406	-1.353
17 14 4 18 14 5	57249.000	-0.199	0.10	-1.0	36.338	-0.938
17 14 3 18 14 4	57249.000	-0.199	0.10	-1.0	36.338	-0.938
18 10 9 19 10 10	60800.790	0.292	0.10	1.5	-4.355	-3.733
18 10 8 19 10 9	60800.790	0.203	0.10	1.0	-4.357	-3.733
18 11 8 19 11 9	60674.500	-0.048	0.10	-0.2	4.351	-3.046
18 11 7 19 11 8	60674.500	-0.051	0.10	-0.2	4.351	-3.046
18 12 7 19 12 8	60582.970	0.015	0.10	0.1	13.616	-2.462

```
18 12  6 19 12  7   60582.970    0.015 0.10    0.1    13.616  -2.462
18 13  6 19 13  7   60515.000   -0.115 0.10   -0.6    23.505  -1.942
18 13  5 19 13  6   60515.000   -0.115 0.10   -0.6    23.505  -1.942
19 10 10 20 10 11   64084.220    0.436 0.10    2.5    -9.942  -4.818
19 10  9 20 10 10   64084.220    0.187 0.10    1.1    -9.946  -4.819
19 11  9 20 11 10   63934.340   -0.323 0.10   -1.6    -0.579  -3.972
19 11  8 20 11  9   63934.340   -0.332 0.10   -1.6    -0.579  -3.972
19 12  8 20 12  9   63825.860   -0.354 0.10   -1.7     9.317  -3.268
19 12  7 20 12  8   63825.860   -0.354 0.10   -1.7     9.317  -3.268
19 13  7 20 13  8   63745.860    0.151 0.10    0.7    19.834  -2.653
19 13  6 20 13  7   63745.860    0.151 0.10    0.7    19.834  -2.653
20 12  9 21 12 10   67077.760   -0.384 0.10   -1.9     4.162  -4.232
20 12  8 21 12  9   67077.760   -0.385 0.10   -1.9     4.162  -4.232
20 14  7 21 14  8   66912.500    0.447 0.10    2.2    27.191  -2.850
20 14  6 21 14  7   66912.500    0.447 0.10    2.2    27.191  -2.850
21 11 11 22 11 12   70487.850   -0.170 0.10   -1.0   -13.213  -6.404
21 11 10 22 11 11   70487.850   -0.254 0.10   -1.5   -13.215  -6.404
21 12 10 22 12 11   70339.320    0.020 0.10    0.1    -1.917  -5.376
21 12  9 22 12 10   70339.320    0.016 0.10    0.1    -1.917  -5.376
21 13  9 22 13 10   70229.150    0.414 0.10    2.2     9.956  -4.508
21 13  8 22 13  9   70229.150    0.414 0.10    2.2     9.956  -4.508
21 14  8 22 14  9   70145.150   -0.043 0.10   -0.2    22.500  -3.745
21 14  7 22 14  8   70145.150   -0.043 0.10   -0.2    22.500  -3.745
21 15  7 22 15  8   70081.210   -0.306 0.10   -1.6    35.772  -3.052
21 15  6 22 15  7   70081.210   -0.306 0.10   -1.6    35.772  -3.052
22 11 12 23 11 13   73782.790   -0.075 0.10   -0.6   -21.072  -7.967
22 11 11 23 11 12   73782.790   -0.298 0.10   -2.4   -21.078  -7.968
22 14  9 23 14 10   73385.020    0.028 0.10    0.2    16.893  -4.798
22 14  8 23 14  9   73385.020    0.028 0.10    0.2    16.893  -4.798
22 18  5 23 18  6   73177.420    0.334 0.20    0.8    77.674  -1.892
22 18  4 23 18  5   73177.420    0.334 0.20    0.8    77.674  -1.892
22 20  3 23 20  4   73135.170    0.057 0.20    0.2   113.095  -0.588
22 20  2 23 20  3   73135.170    0.057 0.20    0.2   113.095  -0.588
23 14 10 24 14 11   76631.890    0.078 0.15    0.3    10.310  -6.027
23 14  9 24 14 10   76631.890    0.078 0.15    0.3    10.310  -6.027
23 21  3 24 21  4   76323.570   -0.137 0.15    9.9   131.143  -0.576
23 21  2 24 21  3   76323.570   -0.137 0.15    9.9   131.143  -0.576


rms deviation:  2.1992


Rotational constants (MHz)  and  kappa:
            4160.7       1810.5563        1339.289    -0.66593
+-           fixed          0.038            0.051     0.00006


Inertial constants and defect (uÅ**2):
            121.46       279.12918        377.3488      -23.25
+-           fixed         0.0059           0.014        0.02


Quartic distortion constants:
        1.2890      -9.664        30.7       0.407       0.696
+-      0.0073       0.028       fixed       fixed       fixed


Significant Digits and Correlation Matrix:
   8      -0.992   0.870  -0.898
            7      -0.819   0.902
                     5      -0.885
                              4
```

Table 8S Microwave spectrum of the third excited state of the *synclinal* conformer of $C_3H_5{}^{80}SeCN$

Total number of transitions: 32

Transition	obs. frequency	obs.- calc.	weight	t	distortion corrections total	distortion corrections fixed
14 11 4 15 11 5	47843.400	-0.271	0.20	-0.5	19.471	-0.737
14 11 3 15 11 4	47843.400	-0.271	0.20	-0.5	19.471	-0.737
15 11 5 16 11 6	51078.280	0.621	0.20	1.2	18.033	-1.156
15 11 4 16 11 5	51078.280	0.621	0.20	1.2	18.033	-1.156
16 13 4 17 13 5	54203.870	-0.101	0.10	9.9	33.159	-0.868
16 13 3 17 13 4	54203.870	-0.101	0.10	9.9	33.159	-0.868
17 12 6 18 12 7	57490.940	-0.576	0.10	-4.3	22.200	-1.823
17 12 5 18 12 6	57490.940	-0.576	0.10	-4.3	22.200	-1.823
17 14 4 18 14 5	57387.620	0.496	0.10	6.2	41.805	-0.931
17 14 3 18 14 4	57387.620	0.496	0.10	6.2	41.805	-0.931
17 15 3 18 15 4	57354.320	0.342	0.12	2.2	52.614	-0.511
17 15 2 18 15 3	57354.320	0.342	0.12	2.2	52.614	-0.511
18 14 5 19 14 6	60612.800	0.319	0.10	1.9	40.311	-1.469
18 14 4 19 14 5	60612.800	0.319	0.10	1.9	40.311	-1.469
19 9 11 20 9 12	64487.480	0.652	0.15	9.9	-12.841	-6.042
19 9 10 20 9 11	64492.140	-0.459	0.15	9.9	-12.944	-6.070
19 13 7 20 13 8	63907.560	-0.341	0.10	9.9	26.727	-2.701
19 13 6 20 13 7	63907.560	-0.341	0.10	9.9	26.727	-2.701
19 16 4 20 16 5	63758.400	-0.676	0.15	-1.7	63.163	-1.048
19 16 3 20 16 4	63758.400	-0.676	0.15	-1.7	63.163	-1.048
20 13 8 21 13 9	67157.260	0.001	0.15	0.0	23.161	-3.574
20 13 7 21 13 8	67157.260	0.001	0.15	0.0	23.161	-3.574
22 12 11 23 12 12	73816.750	0.510	0.20	9.9	0.672	-6.891
22 12 10 23 12 11	73816.750	0.497	0.20	9.9	0.672	-6.891
22 17 6 23 17 7	73392.800	0.030	0.15	9.9	72.365	-2.575
22 17 5 23 17 6	73392.800	0.030	0.15	9.9	72.365	-2.575
22 20 3 23 20 4	73312.180	-0.019	0.15	9.9	125.244	-0.507
22 20 2 23 20 3	73312.180	-0.019	0.15	9.9	125.244	-0.507
23 20 4 24 20 5	76526.030	0.272	0.15	9.9	124.709	-1.222
23 20 3 24 20 4	76526.030	0.272	0.15	9.9	124.709	-1.222
23 22 2 24 22 3	76498.740	-0.244	0.15	9.9	166.225	0.263
23 22 1 24 22 2	76498.740	-0.244	0.15	9.9	166.225	0.263

rms deviation: 3.2402

Rotational constants (MHz) and kappa:

	4176.4	1820.090	1335.633	-0.65893
+-	fixed	0.084	0.10	0.00012

Inertial constants and defect (uÅ**2):

	121.01	277.6671	378.3816	-20.29
+-	fixed	0.013	0.029	0.04

Quartic distortion constants:

	1.106	-9.842	30.7	0.407	0.696
+-	0.023	0.054	fixed	fixed	fixed

```
Significant Digits and Correlation Matrix:
   7      -0.984   0.825  -0.885
           7      -0.728   0.855
                   4      -0.911
                           4
```

Table 9S Microwave spectrum of the ground vibrational state of the *synclinal* conformer of $C_3H_5Se^{78}CN$

Total number of transitions: 99

Transition	obs. frequency	obs.- calc.	weight	t	distortion corrections total	distortion corrections fixed
11 7 4 12 7 5	38392.140	-0.081	0.10	-0.4	1.527	-0.745
11 8 4 12 8 5	38303.290	0.146	0.15	0.5	5.335	-0.525
11 8 3 12 8 4	38303.290	0.129	0.15	0.4	5.335	-0.525
11 10 2 12 10 3	38205.520	-0.091	0.10	-0.5	14.208	-0.163
11 10 1 12 10 2	38205.520	-0.091	0.10	-0.5	14.208	-0.163
12 8 5 13 8 6	41548.810	0.308	0.20	0.7	3.748	-0.832
12 8 4 13 8 5	41548.810	0.244	0.20	0.6	3.748	-0.832
12 9 4 13 9 5	41473.750	0.208	0.15	0.7	8.375	-0.591
12 9 3 13 9 4	41473.750	0.207	0.15	0.6	8.375	-0.591
12 11 2 13 11 3	41386.940	0.278	0.10	1.4	19.026	-0.175
12 11 1 13 11 2	41386.940	0.278	0.10	1.4	19.026	-0.175
12 12 1 13 12 2	41361.370	-0.099	0.10	-0.5	25.084	0.022
12 12 0 13 12 1	41361.370	-0.099	0.10	-0.5	25.084	0.022
13 9 5 14 9 6	44712.120	0.001	0.10	0.0	6.684	-0.925
13 9 4 14 9 5	44712.120	-0.005	0.10	-0.0	6.684	-0.925
13 11 3 14 11 4	44601.140	-0.352	0.10	-1.8	18.250	-0.416
13 11 2 14 11 3	44601.140	-0.352	0.10	-1.8	18.250	-0.416
13 12 2 14 12 3	44569.150	0.189	0.15	0.6	24.805	-0.184
13 12 1 14 12 2	44569.150	0.189	0.15	0.6	24.805	-0.184
14 8 7 15 8 8	48080.000	-0.064	0.20	-0.1	-1.113	-1.759
14 8 6 15 8 7	48080.000	-0.741	0.20	-1.7	-1.118	-1.760
14 10 5 15 10 6	47880.110	-0.442	0.15	-1.4	10.424	-1.025
14 10 4 15 10 5	47880.110	-0.442	0.15	-1.4	10.424	-1.025
15 10 6 16 10 7	51123.310	0.010	0.20	0.0	8.029	-1.488
15 10 5 16 10 6	51123.310	0.008	0.20	0.0	8.029	-1.488
15 12 4 16 12 5	51001.310	-0.323	0.20	-0.7	22.643	-0.800
15 12 3 16 12 4	51001.310	-0.323	0.20	-0.7	22.643	-0.800
16 10 7 17 10 8	54376.470	0.345	0.10	1.7	4.974	-2.068
16 10 6 17 10 7	54376.470	0.338	0.10	1.7	4.974	-2.068
16 15 2 17 15 3	54123.280	-0.314	0.15	-1.0	48.781	-0.186
16 15 1 17 15 2	54123.280	-0.314	0.15	-1.0	48.781	-0.186
17 14 4 18 14 5	57363.730	-0.281	0.10	-1.4	37.309	-0.943
17 14 3 18 14 4	57363.730	-0.281	0.10	-1.4	37.309	-0.943
18 8 11 19 8 12	61339.130	-0.117	0.20	-0.4	-19.507	-5.572
18 8 10 19 8 11	61365.110	-0.701	0.20	-2.5	-19.912	-5.715
18 10 9 19 10 10	60915.200	0.022	0.10	0.1	-3.372	-3.661
18 10 8 19 10 9	60915.200	-0.053	0.10	-0.3	-3.373	-3.661
18 11 8 19 11 9	60791.750	0.335	0.10	1.6	5.355	-2.991
18 11 7 19 11 8	60791.750	0.333	0.10	1.6	5.355	-2.991
18 12 7 19 12 8	60701.700	0.269	0.10	1.3	14.648	-2.424
18 12 6 19 12 7	60701.700	0.269	0.10	1.3	14.648	-2.424
18 13 6 19 13 7	60634.570	-0.253	0.10	-1.2	24.571	-1.920
18 13 5 19 13 6	60634.570	-0.253	0.10	-1.2	24.571	-1.920
18 15 4 19 15 5	60547.670	-0.203	0.15	-0.6	46.447	-1.013
18 15 3 19 15 4	60547.670	-0.203	0.15	-0.6	46.447	-1.013
18 16 3 19 16 4	60520.280	-0.031	0.10	-0.2	58.443	-0.584
18 16 2 19 16 3	60520.280	-0.031	0.10	-0.2	58.443	-0.584
19 8 12 20 8 13	64697.550	-0.882	0.20	9.9	-26.299	-7.092
19 9 11 20 9 12	64409.460	-0.411	0.20	-1.0	-17.765	-5.770
19 10 10 20 10 11	64203.080	-0.060	0.15	-0.2	-8.801	-4.723
19 10 9 20 10 10	64203.080	-0.273	0.15	-0.9	-8.805	-4.724
19 11 9 20 11 10	64056.390	-0.243	0.15	-0.8	0.578	-3.898

```
19 11  8 20 11  9   64056.390   -0.252 0.15   -0.8     0.577  -3.898
19 12  8 20 12  9   63950.070   -0.021 0.15   -0.1    10.500  -3.212
19 12  7 20 12  8   63950.070   -0.021 0.15   -0.1    10.500  -3.212
19 14  6 20 14  7   63812.020    0.325 0.10    1.6    32.282  -2.073
19 14  5 20 14  6   63812.020    0.325 0.10    1.6    32.282  -2.073
19 15  5 20 15  6   63766.730   -0.264 0.10   -1.3    44.226  -1.567
19 15  4 20 15  5   63766.730   -0.264 0.10   -1.3    44.226  -1.567
19 18  2 20 18  3   63691.270    0.307 0.10    1.7    84.528  -0.138
19 18  1 20 18  2   63691.270    0.307 0.10    1.7    84.528  -0.138
20  9 12 21  9 13   67746.900   -0.157 0.20   -0.4   -24.905  -7.306
20  9 11 21  9 12   67756.750    0.149 0.20    0.4   -25.101  -7.371
20 11 10 21 11 11   67332.510    0.063 0.10    0.3    -5.081  -4.984
20 11  9 21 11 10   67332.510    0.038 0.10    0.2    -5.082  -4.984
20 14  7 21 14  8   67044.050   -0.163 0.15   -0.5    28.615  -2.812
20 14  6 21 14  7   67044.050   -0.163 0.15   -0.5    28.615  -2.812
20 15  6 21 15  7   66991.260    0.146 0.10    0.7    41.236  -2.230
20 15  5 21 15  6   66991.260    0.146 0.10    0.7    41.236  -2.230
21  9 13 22  9 14   71102.190    0.100 0.25    0.2   -33.128  -9.137
21 12 10 22 12 11   70473.840    0.306 0.10    1.6    -0.380  -5.274
21 12  9 22 12 10   70473.840    0.303 0.10    1.6    -0.381  -5.274
21 16  6 22 16  7   70173.080    0.188 0.10    0.9    51.519  -2.389
21 16  5 22 16  6   70173.080    0.188 0.10    0.9    51.519  -2.389
21 19  3 22 19  4   70090.500   -0.004 0.10   -0.0    98.666  -0.640
21 19  2 22 19  3   70090.500   -0.004 0.10   -0.0    98.666  -0.640
22 11 12 23 11 13   73919.020    0.113 0.10    0.7   -19.342  -7.807
22 11 11 23 11 12   73919.020   -0.074 0.10   -0.5   -19.347  -7.808
22 12 11 23 12 12   73749.520    0.085 0.15    0.3    -7.246  -6.593
22 12 10 23 12 11   73749.520    0.077 0.15    0.3    -7.247  -6.593
22 13 10 23 13 11   73623.280   -0.218 0.20   -0.5     5.395  -5.587
22 13  9 23 13 10   73623.280   -0.218 0.20   -0.5     5.395  -5.587
22 14  9 23 14 10   73528.550    0.316 0.10    1.8    18.700  -4.718
22 14  8 23 14  9   73528.550    0.316 0.10    1.8    18.700  -4.718
22 15  8 23 15  9   73455.090   -0.338 0.10   -1.9    32.743  -3.940
22 15  7 23 15  8   73455.090   -0.338 0.10   -1.9    32.743  -3.940
22 19  4 23 19  5   73300.810   -0.061 0.15   -0.2    97.056  -1.272
22 19  3 23 19  4   73300.810   -0.061 0.15   -0.2    97.056  -1.272
22 20  3 23 20  4   73284.290    0.276 0.10    2.0   115.277  -0.648
22 20  2 23 20  3   73284.290    0.276 0.10    2.0   115.277  -0.648
22 21  2 23 21  3   73273.290    0.323 0.15    1.3   134.380  -0.024
22 21  1 23 21  2   73273.290    0.323 0.15    1.3   134.380  -0.024
23  9 14 24  9 15   77951.700    0.203 0.25    9.9   -55.431 -14.709
23 17  7 24 17  8   76580.970   -0.310 0.10   -1.8    59.139  -3.438
23 17  6 24 17  7   76580.970   -0.310 0.10   -1.8    59.139  -3.438
23 18  6 24 18  7   76543.300    0.185 0.20    0.4    76.421  -2.714
23 18  5 24 18  6   76543.300    0.185 0.20    0.4    76.421  -2.714
23 19  5 24 19  6   76514.020   -0.456 0.10   -2.7    94.588  -2.014
23 19  4 24 19  5   76514.020   -0.456 0.10   -2.7    94.588  -2.014


rms deviation:  2.2214


Rotational constants (MHz)  and  kappa:
           4219.67       1814.6722        1341.927     -0.6714
+-            6.9            0.33             0.34       0.0004


Inertial constants and defect (uÅ**2):
           119.767       278.49607        376.6071       -21.7
+-           0.19           0.051            0.095          0.3
```

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Quartic distortion constants:
        1.2662       -9.723         30.7        0.407       0.696
+-      0.0063        0.021        fixed        fixed       fixed


Significant Digits and Correlation Matrix:

   6        0.997  -0.995    0.425  -0.485
            8      -1.000    0.481  -0.543
                    7       -0.488   0.559
                             5      -0.881
                              4
```

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