

Rotational Spectrum, Conformational Composition, and
Quantum Chemical Calculations of Cyanomethyl Formate
(HC(O)OCH₂C≡N), a Compound of Potential Astrochemical
Interest

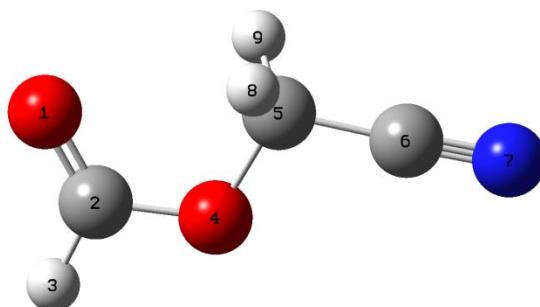
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Supporting Information

Table S1. MP2/cc-pVTZ and MP2/cc-pVQZ Results for Conformer I of Cyanomethyl Formate



MP2/cc-pVTZ Results

Principal axis orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-2.274844	0.577557	0.000000
2	6	-1.738548	-0.499439	0.000000
3	1	-2.242386	-1.467965	0.000000
4	8	-0.403990	-0.701827	0.000000
5	6	0.340747	0.523275	0.000000
6	6	1.756907	0.170404	0.000000
7	7	2.899223	-0.079130	0.000000
8	1	0.099394	1.113449	0.882028
9	1	0.099394	1.113449	-0.882028

Rotational constants (MHZ):

19312.8796218 1776.7145685 1643.6290360

! Optimized Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	!
! R1	R(1,2)	1.2031	-DE/DX = 0.0	!
! R2	R(2,3)	1.0917	-DE/DX = 0.0	!
! R3	R(2,4)	1.3498	-DE/DX = 0.0	!
! R4	R(4,5)	1.4337	-DE/DX = 0.0	!
! R5	R(5,6)	1.4595	-DE/DX = 0.0	!
! R6	R(5,8)	1.0884	-DE/DX = 0.0	!
! R7	R(5,9)	1.0884	-DE/DX = 0.0	!
! R8	R(6,7)	1.1693	-DE/DX = 0.0002	!

! A1	A(1,2,3)	126.0447	-DE/DX =	0.0	!
! A2	A(1,2,4)	125.0945	-DE/DX =	0.0	!
! A3	A(3,2,4)	108.8607	-DE/DX =	0.0	!
! A4	A(2,4,5)	112.6721	-DE/DX =	0.0001	!
! A5	A(4,5,6)	107.3036	-DE/DX =	0.0	!
! A6	A(4,5,8)	110.3754	-DE/DX =	0.0	!
! A7	A(4,5,9)	110.3754	-DE/DX =	0.0	!
! A8	A(6,5,8)	110.2604	-DE/DX =	0.0	!
! A9	A(6,5,9)	110.2604	-DE/DX =	0.0	!
! A10	A(8,5,9)	108.2737	-DE/DX =	0.0	!
! A11	L(5,6,7,3,-1)	181.6692	-DE/DX =	0.0	!
! A12	L(5,6,7,3,-2)	180.0	-DE/DX =	0.0	!
! D1	D(1,2,3,4)	180.0	-DE/DX =	0.0	!
! D2	D(1,2,4,5)	0.0	-DE/DX =	0.0	!
! D3	D(3,2,4,5)	180.0	-DE/DX =	0.0	!
! D4	D(2,4,5,6)	180.0	-DE/DX =	0.0	!
! D5	D(2,4,5,8)	59.8267	-DE/DX =	0.0	!
! D6	D(2,4,5,9)	-59.8267	-DE/DX =	0.0	!

Distance matrix (angstroms):

		1	2	3	4	5
1	O	0.000000				
2	C	1.203136	0.000000			
3	H	2.045780	1.091740	0.000000		
4	O	2.266477	1.349817	1.991650	0.000000	
5	C	2.616154	2.317199	3.261535	1.433704	0.000000
6	C	4.052258	3.559058	4.321875	2.330292	1.459462
7	N	5.215574	4.656777	5.325881	3.361393	2.628439
8	H	2.588853	2.599502	3.595220	2.080047	1.088361
9	H	2.588853	2.599502	3.595220	2.080047	1.088361
		6	7	8	9	
6	C	0.000000				
7	N	1.169253	0.000000			
8	H	2.101109	3.168479	0.000000		
9	H	2.101109	3.168479	1.764057	0.000000	

Vibro-Rot alpha Matrix (MHz)

	a	b	c
Q(1)	-9.32954	0.88825	0.63404
Q(2)	17.91197	1.11608	1.04215
Q(3)	2.06877	0.99976	0.62835
Q(4)	1.09578	5.73135	4.90378
Q(5)	80.03270	0.47898	0.95520
Q(6)	26.29131	-0.40327	-1.88926
Q(7)	10.85703	-0.87908	0.93990
Q(8)	10.99928	-0.60545	1.09542
Q(9)	33.46756	0.12554	-0.77875
Q(10)	82.00267	3.11806	3.57281
Q(11)	37.77008	1.15554	0.07844
Q(12)	-218.14660	-0.45988	1.51426
Q(13)	65.08592	4.83155	-0.62587
Q(14)	200.93738	2.41188	6.47556
Q(15)	-12.72754	1.92976	2.16929
Q(16)	-172.91488	1.39050	1.56425
Q(17)	43.20536	-1.20781	-1.73667
Q(18)	-11.60320	1.98161	1.00046
Q(19)	-12.63245	2.02450	1.63147
Q(20)	-380.43598	-2.10901	-0.31598
Q(21)	572.56427	-2.45109	-6.15949

Rotational Constants (MHz)

equilibrium (e), ground vibr.state (00), and 00 + centr. dist.(0)

Ae=	19312.878	A00=	19129.628	A0=	19129.628
Be=	1776.715	B00=	1766.681	B0=	1766.682
Ce=	1643.629	C00=	1635.279	C0=	1635.278

Vibrational Energies and Rotational Constants (cm-1)

Mode(Quanta) E(harm) E(anharm)

Fundamental Bands (DE w.r.t. Ground State)

1(1)	3167.308	3024.841
2(1)	3132.601	2985.553
3(1)	3112.722	3023.514
4(1)	2215.850	2176.386
5(1)	1791.748	1763.584
6(1)	1504.501	1482.910
7(1)	1405.028	1373.205
8(1)	1396.295	1366.395
9(1)	1272.380	1243.979
10(1)	1208.406	1167.924
11(1)	1049.616	1027.550
12(1)	1027.201	1012.289
13(1)	1011.333	983.926
14(1)	979.016	959.858
15(1)	774.385	766.182
16(1)	521.506	516.527
17(1)	342.429	341.563
18(1)	339.848	332.279
19(1)	272.902	269.769
20(1)	159.457	159.613
21(1)	49.771	47.654

Quartic Centrifugal Distortion Constants (MHz)

(Asymmetrically reduced)	(Symmetrically reduced)
DELTA N = 0.000195780	D N = 0.000193224
DELTA K = 0.056725521	D K = 0.056712740
DELTA NK = -0.001344526	D NK = -0.001329189
delta N = 0.000021795	d 1 = -0.000021795
delta K = 0.001352383	d 2 = -0.000001278

Sextic Centrifugal Distortion Constants (MHz)

(Asymmetrically reduced)	(Symmetrically reduced)
PHI N = 0.1776922954D-10	H N = 0.1923751884D-10
PHI K = 0.4595724352D-06	H K = 0.4548115907D-06
PHI NK = -0.4838720482D-08	H NK = -0.6887892115D-08
PHI KN = -0.2797347229D-06	H KN = -0.2729261751D-06
phi N = -0.4949700470D-12	h 1 = -0.9770384689D-12
phi K = 0.3410618375D-06	h 2 = -0.7341446472D-12
phi NK = -0.1770073041D-08	h 3 = 0.4820684219D-12

Nuclear quadrupole coupling constants [Chi] (MHz):

7 N(14)			
aa=	-3.8010	ba=	1.3623
ab=	1.3623	bb=	1.9433
ac=	-0.0063	bc=	0.0010
		cc=	1.8576

Zero-point correction=	0.060905 (Hartree/Particle)
Thermal correction to Energy=	0.066881
Thermal correction to Enthalpy=	0.067825
Thermal correction to Gibbs Free Energy=	0.030735
Sum of electronic and zero-point Energies=	-320.686980
Sum of electronic and thermal Energies=	-320.681004
Sum of electronic and thermal Enthalpies=	-320.680059
Sum of electronic and thermal Free Energies=	-320.717150

MP2/cc-pVQZ Results

Principal axis orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-2.271490	0.575013	0.000000
2	6	-1.735718	-0.499481	0.000000
3	1	-2.238944	-1.467445	0.000000
4	8	-0.403593	-0.698046	0.000000

5	6	0.341367	0.524202	0.000000
6	6	1.754796	0.169905	0.000000
7	7	2.893500	-0.080910	0.000000
8	1	0.099700	1.113437	0.881555
9	1	0.099700	1.113437	-0.881555

! Optimized Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	!
! R1	R(1,2)	1.2007	-DE/DX = 0.0001	!
! R2	R(2,3)	1.091	-DE/DX = 0.0001	!
! R3	R(2,4)	1.3468	-DE/DX = -0.0002	!
! R4	R(4,5)	1.4314	-DE/DX = -0.0001	!
! R5	R(5,6)	1.4572	-DE/DX = 0.0	!
! R6	R(5,8)	1.0875	-DE/DX = 0.0001	!
! R7	R(5,9)	1.0875	-DE/DX = 0.0001	!
! R8	R(6,7)	1.166	-DE/DX = 0.0002	!
! A1	A(1,2,3)	126.0288	-DE/DX = 0.0001	!
! A2	A(1,2,4)	124.9801	-DE/DX = -0.0001	!
! A3	A(3,2,4)	108.991	-DE/DX = 0.0	!
! A4	A(2,4,5)	112.8843	-DE/DX = -0.0001	!
! A5	A(4,5,6)	107.2902	-DE/DX = 0.0	!
! A6	A(4,5,8)	110.3035	-DE/DX = 0.0	!
! A7	A(4,5,9)	110.3035	-DE/DX = 0.0	!
! A8	A(6,5,8)	110.3212	-DE/DX = 0.0	!
! A9	A(6,5,9)	110.3212	-DE/DX = 0.0	!
! A10	A(8,5,9)	108.3085	-DE/DX = 0.0	!
! A11	L(5,6,7,3,-1)	181.6503	-DE/DX = 0.0	!
! A12	L(5,6,7,3,-2)	180.0	-DE/DX = 0.0	!
! D1	D(1,2,3,4)	-180.0	-DE/DX = 0.0	!
! D2	D(1,2,4,5)	0.0	-DE/DX = 0.0	!
! D3	D(3,2,4,5)	-180.0	-DE/DX = 0.0	!
! D4	D(2,4,5,6)	180.0	-DE/DX = 0.0	!
! D5	D(2,4,5,8)	59.8026	-DE/DX = 0.0	!
! D6	D(2,4,5,9)	-59.8026	-DE/DX = 0.0	!

Distance matrix (angstroms):

	1	2	3	4	5
1 O	0.000000				
2 C	1.200662	0.000000			
3 H	2.042717	1.090958	0.000000		
4 O	2.260469	1.346842	1.990097	0.000000	
5 C	2.613351	2.315645	3.259550	1.431383	0.000000
6 C	4.046615	3.554120	4.316350	2.326367	1.457157
7 N	5.206473	4.648103	5.316433	3.354353	2.622888
8 H	2.586423	2.597577	3.592680	2.076516	1.087539
9 H	2.586423	2.597577	3.592680	2.076516	1.087539
	6	7	8	9	
6 C	0.000000				
7 N	1.166000	0.000000			
8 H	2.099222	3.163688	0.000000		
9 H	2.099222	3.163688	1.763111	0.000000	

Rotational constants (MHZ):

19402.3768537 1782.5564564 1649.2586088

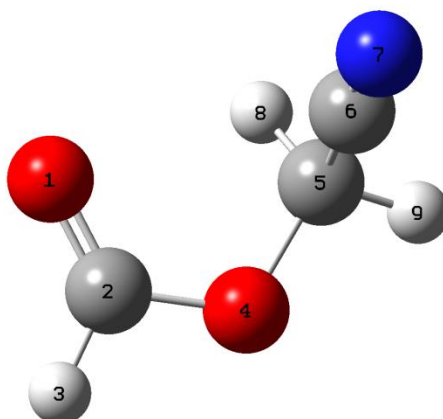
Nuclear quadrupole coupling constants [Chi] (MHZ):

7 N(14)

aa=	-3.8787	ba=	1.4015	ca=	0.0000
ab=	1.4015	bb=	1.9865	cb=	0.0000
ac=	0.0000	bc=	0.0000	cc=	1.8922

MP2/cc-pvQZ electronic energy: -320.8494894

Table S2. MP2/cc-pVTZ and MP2/cc-pVQZ Results for Conformer II of Cyanomethyl Formate



MP2/cc-pVTZ Results

Principal axis orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-1.389902	-1.096600	0.344671
2	6	-1.526811	-0.135380	-0.362992
3	1	-2.314166	0.010692	-1.105015
4	8	-0.722200	0.954304	-0.363408
5	6	0.353335	0.873793	0.577106
6	6	1.431463	0.013384	0.083504
7	7	2.306304	-0.653825	-0.314075
8	1	-0.001931	0.492069	1.531658
9	1	0.720285	1.888544	0.690915

Rotational constants (MHZ):

7416.6359521 2676.2664956 2229.1287255

! Optimized Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	!
! R1	R(1,2)	1.2014	-DE/DX = 0.0	!
! R2	R(2,3)	1.0917	-DE/DX = 0.0	!
! R3	R(2,4)	1.3546	-DE/DX = 0.0	!
! R4	R(4,5)	1.431	-DE/DX = 0.0	!

! R5	R(5,6)	1.465	-DE/DX =	0.0	!
! R6	R(5,8)	1.0877	-DE/DX =	0.0	!
! R7	R(5,9)	1.085	-DE/DX =	0.0	!
! R8	R(6,7)	1.1699	-DE/DX =	0.0	!
! A1	A(1,2,3)	126.1263	-DE/DX =	0.0	!
! A2	A(1,2,4)	125.1769	-DE/DX =	0.0	!
! A3	A(3,2,4)	108.6964	-DE/DX =	0.0	!
! A4	A(2,4,5)	113.6397	-DE/DX =	0.0	!
! A5	A(4,5,6)	111.3894	-DE/DX =	0.0	!
! A6	A(4,5,8)	110.5509	-DE/DX =	0.0	!
! A7	A(4,5,9)	105.6939	-DE/DX =	0.0	!
! A8	A(6,5,8)	109.2647	-DE/DX =	0.0	!
! A9	A(6,5,9)	109.616	-DE/DX =	0.0	!
! A10	A(8,5,9)	110.2806	-DE/DX =	0.0	!
! A11	L(5,6,7,1,-1)	181.1608	-DE/DX =	0.0	!
! A12	L(5,6,7,1,-2)	179.65	-DE/DX =	0.0	!
! D1	D(1,2,3,4)	179.7712	-DE/DX =	0.0	!
! D2	D(1,2,4,5)	0.2326	-DE/DX =	0.0	!
! D3	D(3,2,4,5)	-179.9936	-DE/DX =	0.0	!
! D4	D(2,4,5,6)	77.7173	-DE/DX =	0.0	!
! D5	D(2,4,5,8)	-43.9686	-DE/DX =	0.0	!
! D6	D(2,4,5,9)	-163.2991	-DE/DX =	0.0	!

Distance matrix (angstroms):

		1	2	3	4	5
1	O	0.000000				
2	C	1.201447	0.000000			
3	H	2.044981	1.091725	0.000000		
4	O	2.270113	1.354552	1.993675	0.000000	
5	C	2.641089	2.331773	3.269562	1.431022	0.000000
6	C	3.043086	2.995476	3.929671	2.392347	1.465027
7	N	3.780468	3.868327	4.734545	3.429337	2.634750
8	H	2.420594	2.511703	3.539803	2.079357	1.087703
9	H	3.672038	3.202567	3.994946	2.016226	1.085046
		6	7	8	9	
6	C	0.000000				
7	N	1.169865	0.000000			
8	H	2.093061	3.169819	0.000000		
9	H	2.095459	3.160554	1.782859	0.000000	

Vibro-Rot alpha Matrix (MHz)

	a	b	c
Q(1)	-4.20489	3.36151	2.66389
Q(2)	5.77002	1.51522	1.61891
Q(3)	10.95884	-2.68891	0.49563
Q(4)	12.85974	8.84333	6.61976
Q(5)	23.49793	-2.90231	-0.58392
Q(6)	-14.67429	-0.82088	0.01968
Q(7)	12.36789	3.88198	0.36812
Q(8)	7.10334	-3.92929	-2.79793
Q(9)	25.63677	-8.37472	-3.89372
Q(10)	24.87463	2.54515	2.29974
Q(11)	18.46467	-3.51847	-1.16080
Q(12)	-9.78574	1.86118	1.50715
Q(13)	24.17957	-1.22965	1.01792
Q(14)	16.13428	12.43226	6.30885
Q(15)	-29.30683	19.10249	8.37556
Q(16)	-2.96325	-2.44555	2.90028
Q(17)	5.92209	-5.79209	-1.22793
Q(18)	-25.23492	5.73653	5.05952
Q(19)	42.67035	-6.15273	-1.26879
Q(20)	-3.44844	-1.97068	-2.48777
Q(21)	-158.64745	46.44196	21.64665

Rotational Constants (MHz)

equilibrium (e), ground vibr.state (00), and 00 + centr. dist.(0)

Ae=	7416.636	A00=	7425.549	A0=	7425.546
Be=	2676.267	B00=	2643.319	B0=	2643.352
Ce=	2229.129	C00=	2205.389	C0=	2205.358

Vibrational Energies and Rotational Constants (cm-1)

Mode(Quanta)	E(harm)	E(anharm)
Fundamental Bands (DE w.r.t. Ground State)		
1(1)	3199.440	3057.749
2(1)	3132.783	2986.402
3(1)	3128.287	3003.269
4(1)	2205.882	2166.304
5(1)	1798.461	1768.065
6(1)	1484.229	1444.219
7(1)	1409.168	1377.578
8(1)	1398.503	1366.575
9(1)	1316.971	1283.013
10(1)	1182.851	1143.316
11(1)	1049.085	1027.578
12(1)	1043.514	1022.781
13(1)	990.261	966.958
14(1)	928.991	917.707
15(1)	768.992	757.378
16(1)	569.546	558.960
17(1)	349.394	342.606
18(1)	336.913	329.223
19(1)	299.428	296.490
20(1)	173.916	172.638
21(1)	66.730	62.193

Quartic Centrifugal Distortion Constants (MHz)

(Asymmetrically reduced)		(Symmetrically reduced)	
DELTA N =	0.005295512	D N =	0.005002197
DELTA K =	0.060808901	D K =	0.059342323
DELTA NK =	-0.024584340	D NK =	-0.022824447
delta N =	0.001738543	d 1 =	-0.001738543
delta K =	0.013025074	d 2 =	-0.000146658

Sextic Centrifugal Distortion Constants (MHz)

(Asymmetrically reduced)		(Symmetrically reduced)	
PHI N =	-0.4606138089D-07	H N =	-0.4182552090D-07
PHI K =	0.4377939163D-05	H K =	0.4378259783D-05
PHI NK =	0.3711940720D-06	H NK =	0.3459163206D-06
PHI KN =	-0.1730503290D-05	H KN =	-0.1709782018D-05
phi N =	-0.1912256977D-07	h 1 =	-0.1912218294D-07
phi K =	-0.4463756420D-06	h 2 =	-0.2117929994D-08
phi NK =	-0.4520987437D-06	h 3 =	-0.3868334297D-12

Nuclear quadrupole coupling constants [Chi] (MHz):

7 N(14)			
aa=	-1.3468	ba=	2.5839
ab=	2.5839	bb=	-0.0932
ac=	1.6817	bc=	-1.0912
		cc=	1.4399

Zero-point correction=	0.061131 (Hartree/Particle)
Thermal correction to Energy=	0.066989
Thermal correction to Enthalpy=	0.067933
Thermal correction to Gibbs Free Energy=	0.031198
Sum of electronic and zero-point Energies=	-320.687048
Sum of electronic and thermal Energies=	-320.681190
Sum of electronic and thermal Enthalpies=	-320.680246
Sum of electronic and thermal Free Energies=	-320.716981

MP2/cc-pVQZ Results

Principal axis orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-1.389990	-1.091741	0.346339
2	6	-1.523754	-0.135038	-0.363944

3	1	-2.308175	0.008361	-1.108499
4	8	-0.719080	0.950732	-0.363490
5	6	0.354643	0.873808	0.575781
6	6	1.429551	0.012313	0.083902
7	7	2.300168	-0.654747	-0.313600
8	1	-0.000874	0.495627	1.530713
9	1	0.721162	1.888202	0.685936

! Optimized Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	!
! R1	R(1,2)	1.199	-DE/DX = 0.0	!
! R2	R(2,3)	1.091	-DE/DX = 0.0	!
! R3	R(2,4)	1.3514	-DE/DX = -0.0001	!
! R4	R(4,5)	1.4286	-DE/DX = 0.0	!
! R5	R(5,6)	1.4627	-DE/DX = 0.0	!
! R6	R(5,8)	1.0869	-DE/DX = 0.0	!
! R7	R(5,9)	1.0842	-DE/DX = 0.0	!
! R8	R(6,7)	1.1666	-DE/DX = 0.0	!
! A1	A(1,2,3)	126.112	-DE/DX = 0.0	!
! A2	A(1,2,4)	125.0589	-DE/DX = 0.0	!
! A3	A(3,2,4)	108.8285	-DE/DX = 0.0	!
! A4	A(2,4,5)	113.8572	-DE/DX = 0.0	!
! A5	A(4,5,6)	111.2801	-DE/DX = 0.0	!
! A6	A(4,5,8)	110.5202	-DE/DX = 0.0	!
! A7	A(4,5,9)	105.6937	-DE/DX = 0.0	!
! A8	A(6,5,8)	109.3232	-DE/DX = 0.0	!
! A9	A(6,5,9)	109.6815	-DE/DX = 0.0	!
! A10	A(8,5,9)	110.2956	-DE/DX = 0.0	!
! A11	L(5,6,7,1,-1)	181.1431	-DE/DX = 0.0	!
! A12	L(5,6,7,1,-2)	179.5446	-DE/DX = 0.0	!
! D1	D(1,2,3,4)	179.749	-DE/DX = 0.0	!
! D2	D(1,2,4,5)	0.4294	-DE/DX = 0.0	!
! D3	D(3,2,4,5)	-179.8183	-DE/DX = 0.0	!
! D4	D(2,4,5,6)	77.6319	-DE/DX = 0.0	!
! D5	D(2,4,5,8)	-44.0328	-DE/DX = 0.0	!
! D6	D(2,4,5,9)	-163.3646	-DE/DX = 0.0	!

Distance matrix (angstroms):

		1	2	3	4	5
1	O	0.000000				
2	C	1.199031	0.000000			
3	H	2.042019	1.090982	0.000000		
4	O	2.263995	1.351443	1.992066	0.000000	
5	C	2.638138	2.330071	3.267476	1.428646	0.000000
6	C	3.039345	2.990700	3.923319	2.386924	1.462719
7	N	3.774089	3.859405	4.723177	3.419928	2.629172
8	H	2.419116	2.511300	3.539281	2.076282	1.086880
9	H	3.667744	3.199281	3.991326	2.013565	1.084189
		6	7	8	9	
6	C	0.000000				
7	N	1.166598	0.000000			
8	H	2.091166	3.165383	0.000000		
9	H	2.093614	3.155775	1.781642	0.000000	

Rotational constants (MHZ):

7444.7154122 2685.5526941 2238.1904391

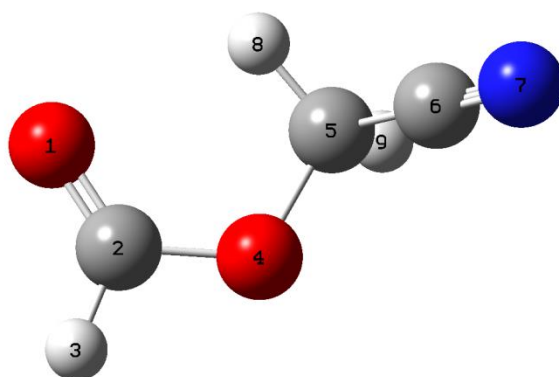
Nuclear quadrupole coupling constants [Chi] (MHZ):

7 N(14)

aa= -1.3583 ba= 2.6411 ca= 1.7204
ab= 2.6411 bb= -0.1141 cb= -1.1133
ac= 1.7204 bc= -1.1133 cc= 1.4723

MP2/cc-pvQZ electronic energy: -320.8497034

Table S3. MP2/cc-pVTZ Results for the Transition State for the Conversion of Conformers I and II of Cyanomethyl Formate



----- ! Optimized Parameters ! ! (Angstroms and Degrees) ! -----				
! Name	Definition	Value	Derivative Info.	!

! R1	R(1,2)	1.2016	-DE/DX = 0.0	!
! R2	R(2,3)	1.0916	-DE/DX = 0.0	!
! R3	R(2,4)	1.3546	-DE/DX = 0.0	!
! R4	R(4,5)	1.4328	-DE/DX = 0.0	!
! R5	R(5,6)	1.4613	-DE/DX = 0.0	!
! R6	R(5,8)	1.0877	-DE/DX = 0.0	!
! R7	R(5,9)	1.0875	-DE/DX = 0.0	!
! R8	R(6,7)	1.1697	-DE/DX = 0.0	!
! A1	A(1,2,3)	125.7259	-DE/DX = 0.0	!
! A2	A(1,2,4)	126.184	-DE/DX = 0.0	!
! A3	A(3,2,4)	108.0899	-DE/DX = 0.0	!
! A4	A(2,4,5)	115.1291	-DE/DX = 0.0	!
! A5	A(4,5,6)	108.703	-DE/DX = 0.0	!
! A6	A(4,5,8)	110.0533	-DE/DX = 0.0	!
! A7	A(4,5,9)	108.5274	-DE/DX = 0.0	!
! A8	A(6,5,8)	110.3156	-DE/DX = 0.0	!
! A9	A(6,5,9)	109.7756	-DE/DX = 0.0	!
! A10	A(8,5,9)	109.4371	-DE/DX = 0.0	!
! A11	L(5,6,7,3,-1)	180.9506	-DE/DX = 0.0	!
! A12	L(5,6,7,3,-2)	180.2796	-DE/DX = 0.0	!
! D1	D(1,2,3,4)	179.8597	-DE/DX = 0.0	!
! D2	D(1,2,4,5)	0.7836	-DE/DX = 0.0	!
! D3	D(3,2,4,5)	-179.3576	-DE/DX = 0.0	!
! D4	D(2,4,5,6)	129.7133	-DE/DX = 0.0	!

```

! D5      D(2,4,5,8)          8.7975      -DE/DX =    0.0      !
! D6      D(2,4,5,9)        -110.9344     -DE/DX =    0.0      !
-----

```

```

          Distance matrix (angstroms):
          1          2          3          4          5
1  O      0.000000
2  C      1.201589    0.000000
3  H      2.041392    1.091628    0.000000
4  O      2.280468    1.354571    1.986153    0.000000
5  C      2.692449    2.352923    3.278818    1.432820    0.000000
6  C      3.845502    3.423840    4.206068    2.351841    1.461298
7  N      4.892952    4.451983    5.141301    3.383111    2.630901
8  H      2.213347    2.395962    3.468376    2.074836    1.087730
9  H      3.328022    3.001691    3.859677    2.055660    1.087451
          6          7          8          9
6  C      0.000000
7  N      1.169695    0.000000
8  H      2.102918    3.174145    0.000000
9  H      2.096005    3.164948    1.775653    0.000000

```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-2.080664	-0.723949	-0.297316
2	6	0	-1.668077	0.401976	-0.220630
3	1	0	-2.215597	1.302280	-0.505808
4	8	0	-0.449153	0.777709	0.235342
5	6	0	0.406872	-0.297473	0.640532
6	6	0	1.707329	-0.129614	-0.004471
7	7	0	2.755298	-0.010412	-0.510177
8	1	0	-0.033825	-1.251348	0.359346
9	1	0	0.524122	-0.257464	1.720903

Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

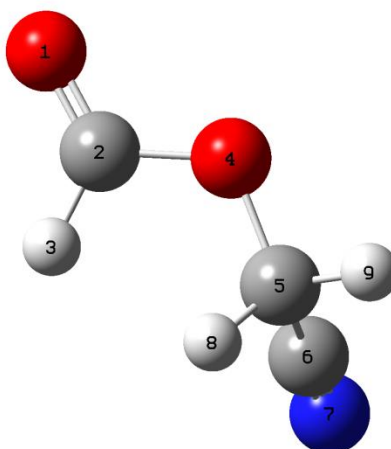
1			2			3				
A			A			A				
Frequencies --	-42.1127		177.2639		304.3902					
Red. masses --	6.0955		5.3634		4.6148					
Frc consts --	0.0064		0.0993		0.2519					
IR Inten --	7.1351		7.2314		12.8213					
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	8	-0.21	0.06	0.24	-0.08	0.09	0.08	0.32	-0.06	0.11
2	6	-0.07	0.02	0.05	0.17	0.02	-0.19	0.07	0.05	0.03
3	1	-0.02	0.06	0.05	0.43	0.06	-0.58	-0.12	-0.08	0.02
4	8	0.06	-0.08	-0.22	0.14	-0.12	-0.04	0.04	0.16	-0.05
5	6	-0.02	-0.15	-0.27	-0.01	-0.16	0.17	-0.18	-0.08	-0.15
6	6	0.10	0.02	0.01	-0.03	-0.14	0.14	-0.12	-0.07	0.06
7	7	0.18	0.14	0.22	-0.21	0.28	-0.13	-0.16	0.01	0.02
8	1	0.06	-0.10	-0.57	-0.05	-0.16	0.23	-0.28	0.08	-0.52
9	1	-0.22	-0.41	-0.24	-0.07	-0.05	0.17	-0.40	-0.43	-0.11

```

Zero-point correction=          0.060874 (Hartree/Particle)
Thermal correction to Energy=    0.065965
Thermal correction to Enthalpy=   0.066909
Thermal correction to Gibbs Free Energy= 0.032132
Sum of electronic and zero-point Energies= -320.685951
Sum of electronic and thermal Energies=    -320.680861
Sum of electronic and thermal Enthalpies=  -320.679917
Sum of electronic and thermal Free Energies= -320.714694

```

Table S4. MP2/cc-pVTZ Results for Conformer III of Cyanomethyl Formate



Principal axis orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-2.389366	-0.607253	-0.082994
2	6	-1.333343	-0.216991	0.314837
3	1	-0.872500	-0.505614	1.270928
4	8	-0.571687	0.662790	-0.395318
5	6	0.667389	1.007872	0.214212
6	6	1.674471	-0.043859	0.033674
7	7	2.469440	-0.892304	-0.099829
8	1	0.545301	1.208586	1.279254
9	1	1.001746	1.918939	-0.272200

Rotational constants (MHZ):

10077.8335799 2003.9277755 1763.1636856

! Optimized Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	!
! R1	R(1,2)	1.1941	-DE/DX = 0.0	!
! R2	R(2,3)	1.0999	-DE/DX = 0.0	!
! R3	R(2,4)	1.3633	-DE/DX = 0.0	!
! R4	R(4,5)	1.4233	-DE/DX = 0.0	!
! R5	R(5,6)	1.4673	-DE/DX = 0.0	!
! R6	R(5,8)	1.0906	-DE/DX = 0.0	!
! R7	R(5,9)	1.0856	-DE/DX = 0.0	!
! R8	R(6,7)	1.1703	-DE/DX = 0.0	!
! A1	A(1,2,3)	125.0577	-DE/DX = 0.0	!
! A2	A(1,2,4)	122.1059	-DE/DX = 0.0	!
! A3	A(3,2,4)	112.8346	-DE/DX = 0.0	!
! A4	A(2,4,5)	114.8191	-DE/DX = 0.0	!

! A5	A(4,5,6)	111.7789	-DE/DX =	0.0	!
! A6	A(4,5,8)	111.4293	-DE/DX =	0.0	!
! A7	A(4,5,9)	106.2435	-DE/DX =	0.0	!
! A8	A(6,5,8)	109.2018	-DE/DX =	0.0	!
! A9	A(6,5,9)	109.5748	-DE/DX =	0.0	!
! A10	A(8,5,9)	108.5169	-DE/DX =	0.0	!
! A11	L(5,6,7,1,-1)	179.4487	-DE/DX =	0.0	!
! A12	L(5,6,7,1,-2)	180.7167	-DE/DX =	0.0	!
! D1	D(1,2,3,4)	-179.5268	-DE/DX =	0.0	!
! D2	D(1,2,4,5)	-179.0794	-DE/DX =	0.0	!
! D3	D(3,2,4,5)	1.3778	-DE/DX =	0.0	!
! D4	D(2,4,5,6)	78.3115	-DE/DX =	0.0	!
! D5	D(2,4,5,8)	-44.1882	-DE/DX =	0.0	!
! D6	D(2,4,5,9)	-162.2033	-DE/DX =	0.0	!

Distance matrix (angstroms):

	1	2	3	4	5
1 O	0.000000				
2 C	1.194052	0.000000			
3 H	2.035760	1.099904	0.000000		
4 O	2.239311	1.363252	2.057190	0.000000	
5 C	3.469973	2.348051	2.403861	1.423348	0.000000
6 C	4.104363	3.025884	2.868985	2.393452	1.467292
7 N	4.867189	3.884476	3.632776	3.428423	2.637551
8 H	3.710156	2.547876	2.224569	2.085604	1.090645
9 H	4.232858	3.218609	3.431107	2.017116	1.085557
	6	7	8	9	
6 C	0.000000				
7 N	1.170323	0.000000			
8 H	2.096453	3.165110	0.000000		
9 H	2.097306	3.175992	1.766339	0.000000	

Vibro-Rot alpha Matrix (MHz)

	a	b	c
Q(1)	-69.31240	9.52591	4.39487
Q(2)	-19.01400	3.92103	1.65089
Q(3)	-34.18162	5.78491	2.31845
Q(4)	50.86941	2.45132	3.57648
Q(5)	13.46880	2.93624	2.82019
Q(6)	-10.18326	1.09068	-0.67852
Q(7)	-48.70019	7.16957	3.05481
Q(8)	21.55013	0.57772	1.94452
Q(9)	120.05631	-12.95815	-6.03202
Q(10)	102.78471	-7.66334	-1.58303
Q(11)	9.00100	3.22721	1.90991
Q(12)	21.88516	-0.17273	0.49017
Q(13)	-36.60602	7.39720	3.87523
Q(14)	80.11544	-2.17266	1.30546
Q(15)	16.79455	0.47920	1.01443
Q(16)	-162.03361	18.12700	9.46320
Q(17)	153.89603	-24.20364	-8.32243
Q(18)	-51.80954	-0.38586	-1.98025
Q(19)	101.34662	-8.86708	-4.94788
Q(20)	84.27027	-14.50915	-5.59275
Q(21)	-391.56123	29.86579	15.59194

Rotational Constants (MHz)

equilibrium (e), ground vibr.state (00), and 00 + centr. dist.(0)

Ae= 10077.833	A00= 10101.515	A0= 10101.514
Be= 2003.928	B00= 1993.117	B0= 1993.161
Ce= 1763.164	C00= 1751.027	C0= 1750.984

Vibrational Energies and Rotational Constants (cm-1)

Mode(Quanta)	E(harm)	E(anharm)
--------------	---------	-----------

Fundamental Bands (DE w.r.t. Ground State)

1(1)	3185.204	3043.017
2(1)	3101.745	3004.466
3(1)	3031.530	2948.545
4(1)	2198.713	2158.792

5(1)	1839.942	1807.458
6(1)	1499.832	1474.671
7(1)	1433.241	1425.522
8(1)	1401.085	1365.538
9(1)	1317.526	1283.390
10(1)	1153.078	1111.462
11(1)	1079.223	1053.693
12(1)	1033.713	1012.936
13(1)	994.602	973.468
14(1)	930.331	923.248
15(1)	687.060	678.487
16(1)	521.555	513.706
17(1)	347.716	335.520
18(1)	326.727	326.562
19(1)	232.690	229.463
20(1)	127.598	122.418
21(1)	58.017	55.904

Quartic Centrifugal Distortion Constants (MHz)

(Asymmetrically reduced)	(Symmetrically reduced)
DELTA N = 0.002804302	D N = 0.002722762
DELTA K = 0.342138440	D K = 0.341730739
DELTA NK = -0.054267725	D NK = -0.053778484
delta N = 0.000890498	d 1 = -0.000890498
delta K = 0.011100715	d 2 = -0.000040770

Sextic Centrifugal Distortion Constants (MHz)

(Asymmetrically reduced)	(Symmetrically reduced)
PHI N = -0.1202538338D-07	H N = -0.1178967745D-07
PHI K = 0.7461090626D-04	H K = 0.7447449196D-04
PHI NK = 0.7332072904D-06	H NK = 0.6733297863D-06
PHI KN = -0.1342370271D-04	H KN = -0.1322764661D-04
phi N = -0.4151098385D-08	h 1 = -0.4204778530D-08
phi K = 0.2556203861D-05	h 2 = -0.1178529632D-09
phi NK = -0.2699292505D-06	h 3 = 0.5368014477D-10

Nuclear quadrupole coupling constants [Chi] (MHz):

7 N(14)			
aa=	-0.7294	ba=	3.1034
ab=	3.1034	bb=	-1.1614
ac=	0.5860	bc=	-0.4169
		cc=	1.8908

Zero-point correction=	0.060374 (Hartree/Particle)
Thermal correction to Energy=	0.066493
Thermal correction to Enthalpy=	0.067438
Thermal correction to Gibbs Free Energy=	0.029866
Sum of electronic and zero-point Energies=	-320.678872
Sum of electronic and thermal Energies=	-320.672753
Sum of electronic and thermal Enthalpies=	-320.671809
Sum of electronic and thermal Free Energies=	-320.709380

Table S5. CCSD/cc-pVQZ Results for Conformer I of Cyanomethyl Formate

CCSD/CC-PVQZ ENERGY=-320.84751156

Atomic coordinates in a,b,c system

	a	b	c
O	-2.270669	0.568730	0.000000
C	-1.734525	-0.496650	0.000000
H	-2.239893	-1.463429	0.000000
O	-0.407711	-0.687201	0.000000
C	0.342705	0.522608	0.000000
C	1.762995	0.163366	0.000000
N	2.886556	-0.082159	0.000000
H	0.110699	1.115469	0.881700
H	0.110699	1.115469	-0.881700

Rotational constants (GHZ): 19.7317024 1.7841393 1.6529660

Electric Dipole Moments mu_a, mu_b, mu_c, mu

-2.2625 -0.0935 0.0000 2.2644

! Optimized Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	!
! R1	R(1,2)	1.1927	estimate D2E/DX2	!
! R2	R(2,3)	1.0909	estimate D2E/DX2	!
! R3	R(2,4)	1.3404	estimate D2E/DX2	!
! R4	R(4,5)	1.4236	estimate D2E/DX2	!
! R5	R(5,6)	1.465	estimate D2E/DX2	!
! R6	R(5,8)	1.0875	estimate D2E/DX2	!
! R7	R(5,9)	1.0875	estimate D2E/DX2	!
! R8	R(6,7)	1.1501	estimate D2E/DX2	!
! A1	A(1,2,3)	125.6886	estimate D2E/DX2	!
! A2	A(1,2,4)	124.8865	estimate D2E/DX2	!
! A3	A(3,2,4)	109.4248	estimate D2E/DX2	!
! A4	A(2,4,5)	113.6377	estimate D2E/DX2	!
! A5	A(4,5,6)	107.6163	estimate D2E/DX2	!
! A6	A(4,5,8)	110.5371	estimate D2E/DX2	!
! A7	A(4,5,9)	110.5371	estimate D2E/DX2	!
! A8	A(6,5,8)	109.9075	estimate D2E/DX2	!
! A9	A(6,5,9)	109.9075	estimate D2E/DX2	!
! A10	A(8,5,9)	108.3362	estimate D2E/DX2	!
! A11	L(5,6,7,3,-1)	181.8676	estimate D2E/DX2	!
! A12	L(5,6,7,3,-2)	180.0	estimate D2E/DX2	!
! D1	D(1,2,3,4)	180.0	estimate D2E/DX2	!
! D2	D(1,2,4,5)	0.0	estimate D2E/DX2	!
! D3	D(3,2,4,5)	180.0	estimate D2E/DX2	!
! D4	D(2,4,5,6)	180.0	estimate D2E/DX2	!
! D5	D(2,4,5,8)	59.9697	estimate D2E/DX2	!
! D6	D(2,4,5,9)	-59.9697	estimate D2E/DX2	!

Distance matrix (angstroms):

		1	2	3	4	5
1	O	0.000000				
2	C	1.192677	0.000000			
3	H	2.032386	1.090898	0.000000		
4	O	2.246765	1.340420	1.989822	0.000000	
5	C	2.613781	2.313817	3.257932	1.423644	0.000000
6	C	4.053978	3.559245	4.320826	2.331403	1.465014
7	N	5.198137	4.639631	5.309273	3.349375	2.614750
8	H	2.597539	2.604062	3.599076	2.072624	1.087525
9	H	2.597539	2.604062	3.599076	2.072624	1.087525
		6	7	8	9	
6	C	0.000000				
7	N	1.150078	0.000000			
8	H	2.100948	3.149146	0.000000		
9	H	2.100948	3.149146	1.763395	0.000000	

Table S6. CCSD/cc-pVQZ Results for Conformer II of Cyanomethyl Formate

CCSD/CC-PVQZ ENERGY=-320.84731259

Atomic coordinates in a,b,c system

	a	b	c
O	-1.452575	-1.064362	0.338215
C	-1.538702	-0.110287	-0.369274
H	-2.310084	0.056763	-1.122240
O	-0.696276	0.938620	-0.358457
C	0.364478	0.843523	0.581832
C	1.455289	-0.006013	0.080104
N	2.326473	-0.648920	-0.308626
H	0.007808	0.442727	1.526621
H	0.734691	1.853521	0.720361

Electric Dipole Moments mu_a, mu_b, mu_c, mu

2.5970 3.4880 0.6596 4.3983

Rotational constants (GHZ): 7.7049192 2.6081105 2.2059994

----- ! Optimized Parameters ! ! (Angstroms and Degrees) ! -----			
! Name	Definition	Value	Derivative Info. !
! R1	R(1,2)	1.1909	estimate D2E/DX2 !
! R2	R(2,3)	1.0908	estimate D2E/DX2 !
! R3	R(2,4)	1.3454	estimate D2E/DX2 !
! R4	R(4,5)	1.4207	estimate D2E/DX2 !
! R5	R(5,6)	1.4708	estimate D2E/DX2 !
! R6	R(5,8)	1.0865	estimate D2E/DX2 !
! R7	R(5,9)	1.0846	estimate D2E/DX2 !
! R8	R(6,7)	1.1504	estimate D2E/DX2 !
! A1	A(1,2,3)	125.7256	estimate D2E/DX2 !
! A2	A(1,2,4)	125.0682	estimate D2E/DX2 !
! A3	A(3,2,4)	109.2055	estimate D2E/DX2 !
! A4	A(2,4,5)	114.876	estimate D2E/DX2 !
! A5	A(4,5,6)	111.5076	estimate D2E/DX2 !
! A6	A(4,5,8)	110.8005	estimate D2E/DX2 !
! A7	A(4,5,9)	106.0848	estimate D2E/DX2 !
! A8	A(6,5,8)	109.0883	estimate D2E/DX2 !
! A9	A(6,5,9)	109.1648	estimate D2E/DX2 !
! A10	A(8,5,9)	110.1516	estimate D2E/DX2 !
! A11	L(5,6,7,1,-1)	181.4103	estimate D2E/DX2 !
! A12	L(5,6,7,1,-2)	180.0236	estimate D2E/DX2 !
! D1	D(1,2,3,4)	179.7186	estimate D2E/DX2 !
! D2	D(1,2,4,5)	0.4746	estimate D2E/DX2 !
! D3	D(3,2,4,5)	-179.8046	estimate D2E/DX2 !
! D4	D(2,4,5,6)	80.2537	estimate D2E/DX2 !
! D5	D(2,4,5,8)	-41.4619	estimate D2E/DX2 !
! D6	D(2,4,5,9)	-161.0048	estimate D2E/DX2 !

Distance matrix (angstroms):

		1	2	3	4	5
1	O	0.000000				
2	C	1.190888	0.000000			
3	H	2.031048	1.090825	0.000000		
4	O	2.251505	1.345362	1.991337	0.000000	
5	C	2.645949	2.331615	3.267436	1.420699	0.000000
6	C	3.105225	3.029323	3.953181	2.390374	1.470820
7	N	3.856450	3.902997	4.760005	3.414641	2.621019
8	H	2.411705	2.508365	3.540908	2.072477	1.086497
9	H	3.666633	3.195642	3.986751	2.012103	1.084594
		6	7	8	9	
6	C	0.000000				
7	N	1.150395	0.000000			
8	H	2.094990	3.152149	0.000000		
9	H	2.094528	3.139238	1.780099	0.000000	

Table S7. CCSD/cc-pVQZ Results for Conformer III of Cyanomethyl Formate

CCSD/CC-PVQZ ENERGY=-320.83852151

Atomic coordinates in a,b,c system

	a	b	c
O	-2.386527	-0.594483	-0.086777
C	-1.335855	-0.222647	0.312261
H	-0.885385	-0.532952	1.264930
O	-0.572288	0.652483	-0.383345
C	0.662326	1.000579	0.209725
C	1.678939	-0.049833	0.027299
N	2.470431	-0.875824	-0.096347
H	0.552604	1.202619	1.275075
H	0.995028	1.909483	-0.280382

Electric Dipole Moments mu_a, mu_b, mu_c, mu

0.7785 3.1189 2.2990 3.9521

Rotational constants (GHZ): 10.3351974 2.0051785 1.7691656

! Initial Parameters !				
! (Angstroms and Degrees) !				

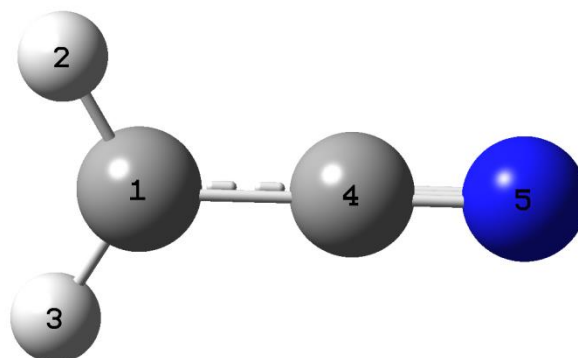
! Name	Definition	Value	Derivative Info.	!

! R1	R(1,2)	1.1838	estimate D2E/DX2	!
! R2	R(2,3)	1.0985	estimate D2E/DX2	!
! R3	R(2,4)	1.3538	estimate D2E/DX2	!
! R4	R(4,5)	1.4132	estimate D2E/DX2	!
! R5	R(5,6)	1.4731	estimate D2E/DX2	!
! R6	R(5,8)	1.0899	estimate D2E/DX2	!
! R7	R(5,9)	1.0849	estimate D2E/DX2	!
! R8	R(6,7)	1.1507	estimate D2E/DX2	!
! A1	A(1,2,3)	124.5789	estimate D2E/DX2	!
! A2	A(1,2,4)	122.0348	estimate D2E/DX2	!
! A3	A(3,2,4)	113.3848	estimate D2E/DX2	!
! A4	A(2,4,5)	115.8704	estimate D2E/DX2	!
! A5	A(4,5,6)	112.0418	estimate D2E/DX2	!
! A6	A(4,5,8)	111.5879	estimate D2E/DX2	!
! A7	A(4,5,9)	106.54	estimate D2E/DX2	!
! A8	A(6,5,8)	108.8266	estimate D2E/DX2	!
! A9	A(6,5,9)	109.2565	estimate D2E/DX2	!
! A10	A(8,5,9)	108.491	estimate D2E/DX2	!
! A11	L(5,6,7,3,-1)	179.3315	estimate D2E/DX2	!
! A12	L(5,6,7,3,-2)	180.8626	estimate D2E/DX2	!
! D1	D(1,2,3,4)	-179.5559	estimate D2E/DX2	!
! D2	D(1,2,4,5)	-179.5663	estimate D2E/DX2	!
! D3	D(3,2,4,5)	0.865	estimate D2E/DX2	!
! D4	D(2,4,5,6)	78.111	estimate D2E/DX2	!
! D5	D(2,4,5,8)	-44.2069	estimate D2E/DX2	!
! D6	D(2,4,5,9)	-162.4564	estimate D2E/DX2	!

Distance matrix (angstroms):

		1	2	3	4	5
1	O	0.000000				
2	C	1.183809	0.000000			
3	H	2.020971	1.098540	0.000000		
4	O	2.221337	1.353792	2.054287	0.000000	
5	C	3.453641	2.345106	2.420865	1.413214	0.000000
6	C	4.103373	3.033159	2.888061	2.393721	1.473142
7	N	4.865109	3.883480	3.637601	3.417049	2.623702
8	H	3.704417	2.554343	2.253913	2.078073	1.089876
9	H	4.212153	3.214065	3.448105	2.011747	1.084897
		6	7	8	9	
6	C	0.000000				
7	N	1.150656	0.000000			
8	H	2.096237	3.143053	0.000000		
9	H	2.097933	3.157312	1.764891	0.000000	

Table S8. UMP2/cc-pVTZ Results for H₂CC≡N



! Initial Parameters !				
! (Angstroms and Degrees) !				

! Name	Definition	Value	Derivative Info.	!

! R1	R(1,2)	1.0744	calculate D2E/DX2 analytically	!
! R2	R(1,3)	1.0744	calculate D2E/DX2 analytically	!
! R3	R(1,4)	1.4095	calculate D2E/DX2 analytically	!
! R4	R(4,5)	1.1406	calculate D2E/DX2 analytically	!
! A1	A(2,1,3)	121.0167	calculate D2E/DX2 analytically	!
! A2	A(2,1,4)	119.4916	calculate D2E/DX2 analytically	!
! A3	A(3,1,4)	119.4916	calculate D2E/DX2 analytically	!
! A4	L(1,4,5,2,-1)	179.9999	calculate D2E/DX2 analytically	!
! A5	L(1,4,5,2,-2)	180.1258	calculate D2E/DX2 analytically	!
! D1	D(2,1,4,3)	-179.8948	calculate D2E/DX2 analytically	!

Distance matrix (angstroms):						
		1	2	3	4	5
1	C	0.000000				
2	H	1.074432	0.000000			
3	H	1.074432	1.870431	0.000000		
4	C	1.409527	2.152273	2.152273	0.000000	
5	N	2.550081	3.217918	3.217918	1.140555	0.000000

Standard orientation:					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	-0.003024	1.202370	0.000000
2	1	0	-0.003300	1.731310	0.935215
3	1	0	-0.003300	1.731310	-0.935215

4	6	0	0.000000	-0.207154	0.000000
5	7	0	0.003534	-1.347703	0.000000

Rotational constants (GHZ): 286.6667804 10.3047002 9.9471366

Harmonic frequencies (cm**⁻¹), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

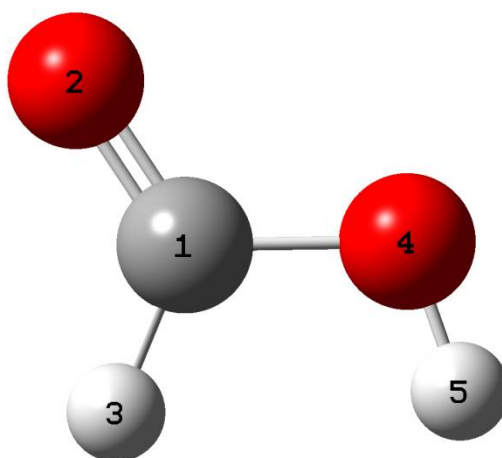
			1			2			3	
			A''			A'			A'	
Frequencies --			417.6739			468.6871			602.1199	
Red. masses --			3.1277			2.0486			2.4042	
Frc consts --			0.3215			0.2651			0.5135	
IR Inten --			1.1685			5.5817			48.8132	
Atom	AN		X	Y	Z	X	Y	Z	X	Y
1	6		0.00	0.00	0.06	-0.02	0.00	0.00	0.24	0.00
2	1		0.00	-0.53	0.36	0.67	0.00	0.00	-0.66	0.00
3	1		0.00	0.53	0.36	0.67	0.00	0.00	-0.66	0.00
4	6		0.00	0.00	-0.37	-0.26	0.00	0.00	-0.24	0.00
5	7		0.00	0.00	0.21	0.14	0.00	0.00	0.09	0.00

			4			5			6	
			A'			A''			A'	
Frequencies --			1017.8058			1073.8443			1473.4674	
Red. masses --			5.0047			1.5196			1.1552	
Frc consts --			3.0546			1.0324			1.4777	
IR Inten --			14.4399			0.1231			1.7432	
Atom	AN		X	Y	Z	X	Y	Z	X	Y
1	6		0.00	0.46	0.00	0.00	0.00	0.15	0.00	-0.11
2	1		0.00	0.57	-0.04	0.00	0.65	-0.22	0.00	0.58
3	1		0.00	0.57	0.04	0.00	-0.65	-0.22	0.00	0.58
4	6		0.00	-0.23	0.00	0.00	0.00	-0.15	0.00	0.00
5	7		0.00	-0.28	0.00	0.00	0.00	0.03	0.00	0.01

			7			8			9	
			A'			A'			A''	
Frequencies --			2734.3092			3247.7156			3373.9129	
Red. masses --			12.6837			1.0490			1.1222	
Frc consts --			55.8716			6.5189			7.5266	
IR Inten --			86.1502			1.8014			5.2805	
Atom	AN		X	Y	Z	X	Y	Z	X	Y
1	6		0.00	-0.05	0.00	0.00	-0.06	0.00	0.00	0.00
2	1		0.00	-0.03	-0.06	0.00	0.34	0.62	0.00	-0.35
3	1		0.00	-0.03	0.06	0.00	0.34	-0.62	0.00	0.35
4	6		0.00	0.78	0.00	0.00	0.00	0.00	0.00	0.00
5	7		0.00	-0.62	0.00	0.00	0.00	0.00	0.00	0.00

Zero-point correction=	0.032827 (Hartree/Particle)
Thermal correction to Energy=	0.036427
Thermal correction to Enthalpy=	0.037371
Thermal correction to Gibbs Free Energy=	0.008600
Sum of electronic and zero-point Energies=	-131.778965
Sum of electronic and thermal Energies=	-131.775366
Sum of electronic and thermal Enthalpies=	-131.774422
Sum of electronic and thermal Free Energies=	-131.803192

Table S9. UMP2/cc-pVTZ Results for HCOOH



! Optimized Parameters ! ! (Angstroms and Degrees) !				
! Name	Definition	Value	Derivative Info.	
! R1	R(1,2)	1.197	-DE/DX =	-0.0001
! R2	R(1,3)	1.0993	-DE/DX =	-0.0002
! R3	R(1,4)	1.3515	-DE/DX =	0.0002
! R4	R(4,5)	0.9637	-DE/DX =	0.0001
! A1	A(2,1,3)	124.0491	-DE/DX =	0.0001
! A2	A(2,1,4)	122.6112	-DE/DX =	0.0
! A3	A(3,1,4)	113.3397	-DE/DX =	0.0
! A4	A(1,4,5)	108.4323	-DE/DX =	-0.0001
! D1	D(2,1,3,4)	-179.9728	-DE/DX =	0.0
! D2	D(2,1,4,5)	179.985	-DE/DX =	0.0
! D3	D(3,1,4,5)	0.0118	-DE/DX =	0.0

Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1 A					2 A			3 A		
Frequencies	--	527.4641			661.0639			1047.0168		
Red. masses	--	1.1198			6.3873			1.6785		
Frc consts	--	0.1836			1.6446			1.0841		
IR Inten	--	85.2069			10.8423			0.0030		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	-0.05	0.02	0.34	0.00	0.00	0.00	0.23
2	8	0.00	0.00	0.05	0.34	-0.17	0.00	0.00	0.00	-0.06
3	1	0.00	0.00	-0.16	-0.08	0.34	0.00	0.00	0.00	-0.97
4	8	0.00	0.00	-0.06	-0.36	-0.06	0.00	0.00	0.00	-0.05

5	1	0.00	0.00	0.98	0.21	-0.67	0.00	0.00	0.00	-0.01
		4			5			6		
		A			A			A		
Frequencies	--	1131.0882			1285.8004			1436.0895		
Red. masses	--	2.4844			1.6915			1.1498		
Frc consts	--	1.8727			1.6476			1.3972		
IR Inten	--	43.2995			309.4736			0.0352		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.16	-0.20	0.00	-0.10	0.13	0.00	0.04	-0.05	0.00
2	8	0.09	0.05	0.00	0.05	-0.01	0.00	0.05	0.06	0.00
3	1	0.37	-0.20	0.00	0.04	0.14	0.00	-0.99	0.03	0.00
4	8	-0.19	0.07	0.00	0.07	-0.14	0.00	-0.01	-0.03	0.00
5	1	-0.64	0.55	0.00	-0.67	0.69	0.00	-0.08	0.05	0.00
		7			8			9		
		A			A			A		
Frequencies	--	1855.7508			3031.9057			3838.3672		
Red. masses	--	8.1659			1.0907			1.0660		
Frc consts	--	16.5690			5.9074			9.2536		
IR Inten	--	244.1525			75.5496			77.6906		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.58	0.26	0.00	-0.01	-0.09	0.00	0.00	0.00	0.00
2	8	-0.36	-0.21	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	1	-0.29	0.41	0.00	0.07	0.99	0.00	0.00	0.00	0.00
4	8	-0.04	-0.03	0.00	0.00	0.00	0.00	0.05	0.04	0.00
5	1	-0.29	0.28	0.00	0.01	-0.02	0.00	-0.74	-0.67	0.00

Zero-point correction= 0.033750 (Hartree/Particle)
 Thermal correction to Energy= 0.036989
 Thermal correction to Enthalpy= 0.037933
 Thermal correction to Gibbs Free Energy= 0.009667
 Sum of electronic and zero-point Energies= -189.430140
 Sum of electronic and thermal Energies= -189.426901
 Sum of electronic and thermal Enthalpies= -189.425957
 Sum of electronic and thermal Free Energies= -189.454223

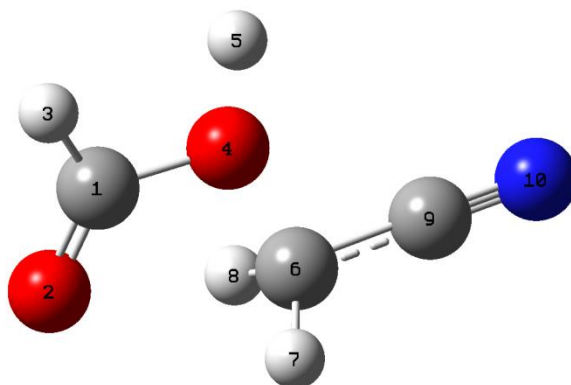
Table S10. UMP2/cc-pVTZ Results for H

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	0.000000	0.000000	0.000000

1\1\GINC-COMPUTE-17-8\FOpt\UMP2-FC\CC-pVTZ\H1(2)\ROOT\20-Nov-2014\0\#\ump2/cc-pvtz opt geom=connectivity\\Hydrogen atom\\0,2\H,-0.04115226,-0.3292181,0.\\Version=EM64L-G09RevC.01\State=2-A1G\HF=-0.4998098\MP2=-0.4998098\PUHF=-0.4998098\PMF2-0=-0.4998098\S2=0.75\S2-1=0.75\S2A=0.75\RMSD=7.121e-10\RMSF=0.000e+00\Dipole=0.,0.,0.\PG=OH [O(H1)]\\@

Table S11. UMP2/cc-pVTZ Results for the Transition State



! Optimized Parameters ! ! (Angstroms and Degrees) !				
! Name	Definition	Value	Derivative Info.	!
! R1	R(1,2)	1.198	-DE/DX = 0.0	!
! R2	R(1,3)	1.0887	-DE/DX = 0.0	!
! R3	R(1,4)	1.3915	-DE/DX = 0.0	!
! R4	R(4,5)	1.2181	-DE/DX = 0.0	!
! R5	R(4,6)	1.6765	-DE/DX = 0.0	!
! R6	R(6,7)	1.0805	-DE/DX = 0.0	!
! R7	R(6,8)	1.0805	-DE/DX = 0.0	!
! R8	R(6,9)	1.4468	-DE/DX = 0.0	!
! R9	R(9,10)	1.1456	-DE/DX = 0.0	!
! A1	A(2,1,3)	125.9715	-DE/DX = 0.0	!
! A2	A(2,1,4)	123.6045	-DE/DX = 0.0	!
! A3	A(3,1,4)	110.424	-DE/DX = 0.0	!
! A4	A(1,4,5)	102.9053	-DE/DX = 0.0	!
! A5	A(1,4,6)	107.4073	-DE/DX = 0.0	!
! A6	A(5,4,6)	149.6874	-DE/DX = 0.0	!
! A7	A(4,6,7)	105.8907	-DE/DX = 0.0	!
! A8	A(4,6,8)	105.8896	-DE/DX = 0.0	!
! A9	A(4,6,9)	103.2016	-DE/DX = 0.0	!
! A10	A(7,6,8)	113.1217	-DE/DX = 0.0	!
! A11	A(7,6,9)	113.7693	-DE/DX = 0.0	!
! A12	A(8,6,9)	113.7691	-DE/DX = 0.0	!
! A13	L(6,9,10,5,-1)	180.6958	-DE/DX = 0.0	!
! A14	L(6,9,10,5,-2)	180.0	-DE/DX = 0.0	!
! D1	D(2,1,4,5)	-180.0059	-DE/DX = 0.0	!
! D2	D(2,1,4,6)	0.0013	-DE/DX = 0.0	!
! D3	D(3,1,4,5)	-0.006	-DE/DX = 0.0	!
! D4	D(3,1,4,6)	-179.9989	-DE/DX = 0.0	!
! D5	D(1,4,6,7)	-60.1609	-DE/DX = 0.0	!
! D6	D(1,4,6,8)	60.2067	-DE/DX = 0.0	!
! D7	D(1,4,6,9)	180.0225	-DE/DX = 0.0	!

! D8	D(5,4,6,7)	119.8529	-DE/DX =	0.0	!
! D9	D(5,4,6,8)	-119.7795	-DE/DX =	0.0	!
! D10	D(5,4,6,9)	0.0364	-DE/DX =	0.0	!

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	O	1.197969	0.000000			
3	H	1.088653	2.037742	0.000000		
4	O	1.391479	2.283969	2.044170	0.000000	
5	H	2.043783	3.191774	2.050250	1.218087	0.000000
6	C	2.478429	2.625970	3.468459	1.676491	2.796463
7	H	2.678663	2.553313	3.694166	2.229354	3.352288
8	H	2.679002	2.553952	3.694407	2.229338	3.352059
9	C	3.655053	4.029597	4.486296	2.451902	3.159802
10	N	4.700114	5.159990	5.439135	3.400202	3.839952
		6	7	8	9	10
6	C	0.000000				
7	H	1.080485	0.000000			
8	H	1.080485	1.803268	0.000000		
9	C	1.446823	2.126243	2.126241	0.000000	
10	N	2.592350	3.183442	3.183441	1.145574	0.000000

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.779429	0.423344	0.000093
2	8	0	-2.173393	-0.707993	0.000194
3	1	0	-2.401190	1.316977	0.000177
4	8	0	-0.431696	0.769507	-0.000149
5	1	0	-0.463574	1.987177	-0.000301
6	6	0	0.452045	-0.655142	-0.000294
7	1	0	0.168760	-1.179100	0.901185
8	1	0	0.169038	-1.178718	-0.902083
9	6	0	1.823213	-0.193410	0.000012
10	7	0	2.913244	0.158972	0.000256

Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

			1			2			3		
			A			A			A		
Frequencies	--	-3231.3654				52.6250			163.1949		
Red. masses	--	1.4083				4.6471			6.6724		
Frc consts	--	8.6641				0.0076			0.1047		
IR Inten	--	32168.1188				8.2008			8.9175		
Atom	AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6		0.01	0.00	0.00	0.00	0.00	0.10	0.12	0.08	0.00
2	8		0.00	0.00	0.00	0.00	0.00	0.22	-0.15	0.17	0.00
3	1		0.06	0.03	0.00	0.00	0.00	0.22	0.32	0.22	0.00
4	8		0.03	-0.13	0.00	0.00	0.00	-0.20	0.18	-0.22	0.00
5	1		-0.01	0.98	0.00	0.00	0.00	-0.28	0.43	-0.21	0.00
6	6		-0.07	0.09	0.00	0.00	0.00	-0.34	0.03	-0.31	0.00
7	1		-0.01	-0.01	-0.01	-0.14	-0.19	-0.49	0.04	-0.30	0.01
8	1		-0.01	-0.01	0.01	0.14	0.19	-0.49	0.04	-0.30	-0.01
9	6		0.00	0.01	0.00	0.00	0.00	-0.01	-0.04	-0.08	0.00
10	7		0.00	0.00	0.00	0.00	0.00	0.27	-0.19	0.37	0.00

			4			5			6		
			A			A			A		
Frequencies	--	219.6147				254.5856			392.9763		
Red. masses	--	2.2399				9.6805			3.1870		
Frc consts	--	0.0636				0.3697			0.2900		
IR Inten	--	32.4714				1.1121			0.5403		
Atom	AN		X	Y	Z	X	Y	Z	X	Y	Z
1	6		0.00	0.00	0.22	0.21	0.02	0.00	0.00	0.00	0.00

2	8	0.00	0.00	-0.14	0.50	-0.09	0.00	0.00	0.00	0.00
3	1	0.00	0.00	0.86	0.00	-0.13	0.00	0.00	0.00	-0.01
4	8	0.00	0.00	-0.16	0.11	0.20	0.00	0.00	0.00	0.01
5	1	0.00	0.00	-0.23	-0.07	0.21	0.00	0.00	0.00	0.21
6	6	0.00	0.00	0.08	-0.27	-0.06	0.00	0.00	0.00	0.04
7	1	-0.02	0.16	0.16	-0.37	0.00	0.00	0.37	0.34	0.36
8	1	0.02	-0.16	0.16	-0.37	0.00	0.00	-0.37	-0.34	0.36
9	6	0.00	0.00	0.03	-0.28	-0.16	0.00	0.00	0.00	-0.38
10	7	0.00	0.00	-0.01	-0.35	0.04	0.00	0.00	0.00	0.21

7					8			9		
A					A			A		
Frequencies	--	439.8830			560.2747			703.5511		
Red. masses	--	1.1947			7.1881			8.2503		
Frc consts	--	0.1362			1.3294			2.4061		
IR Inten	--	0.3659			7.9200			5.6879		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.02	-0.08	-0.03	0.00	-0.28	0.31	0.00
2	8	0.00	0.00	-0.03	-0.07	-0.04	0.00	0.37	0.12	0.00
3	1	0.00	0.00	-0.03	-0.12	-0.06	0.00	-0.42	0.22	0.00
4	8	0.00	0.00	0.10	-0.04	0.15	0.00	-0.33	-0.24	0.00
5	1	0.00	0.00	-0.98	-0.38	0.27	0.00	0.36	-0.08	0.00
6	6	0.00	0.00	-0.01	-0.01	0.13	0.00	0.00	-0.12	0.00
7	1	0.06	-0.07	-0.03	-0.27	0.20	-0.04	0.09	-0.20	-0.01
8	1	-0.06	0.07	-0.03	-0.27	0.20	0.04	0.09	-0.20	0.01
9	6	0.00	0.00	-0.04	0.30	-0.58	0.00	0.12	-0.07	0.00
10	7	0.00	0.00	0.02	0.03	0.25	0.00	0.09	0.06	0.00

10					11			12		
A					A			A		
Frequencies	--	860.5931			865.2570			995.7922		
Red. masses	--	1.3997			1.3673			3.5024		
Frc consts	--	0.6108			0.6031			2.0462		
IR Inten	--	176.1413			0.7029			47.3844		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.06	-0.02	0.00	0.00	0.00	0.01	0.12	0.01	0.00
2	8	0.00	-0.04	0.00	0.00	0.00	0.00	0.03	0.08	0.00
3	1	0.02	0.03	0.00	0.00	0.00	-0.06	0.20	0.06	0.00
4	8	0.04	-0.05	0.00	0.00	0.00	0.06	-0.09	-0.14	0.00
5	1	0.90	-0.25	0.00	0.00	0.00	-0.05	-0.64	-0.27	0.00
6	6	0.00	0.15	0.00	0.00	0.00	-0.15	0.25	0.21	0.00
7	1	-0.07	0.20	0.00	-0.17	0.65	0.16	0.30	0.20	0.00
8	1	-0.07	0.20	0.00	0.17	-0.65	0.16	0.30	0.20	0.00
9	6	-0.02	-0.03	0.00	0.00	0.00	0.07	-0.10	-0.10	0.00
10	7	-0.04	0.00	0.00	0.00	0.00	-0.02	-0.18	-0.04	0.00

13					14			15		
A					A			A		
Frequencies	--	1028.8456			1030.9617			1125.1515		
Red. masses	--	1.6775			2.2146			2.1768		
Frc consts	--	1.0462			1.3868			1.6236		
IR Inten	--	0.2944			52.9948			242.9061		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.23	0.21	-0.04	0.00	-0.19	0.04	0.00
2	8	0.00	0.00	-0.06	-0.01	0.04	0.00	0.04	0.00	0.00
3	1	0.00	0.00	-0.97	0.29	0.01	0.00	-0.09	0.11	0.00
4	8	0.00	0.00	-0.05	-0.12	-0.09	0.00	0.19	-0.10	0.00
5	1	0.00	0.00	0.02	-0.06	-0.32	0.00	-0.64	-0.32	0.00
6	6	0.00	0.00	0.01	-0.13	0.01	0.00	-0.02	0.03	0.00
7	1	0.01	-0.02	0.00	-0.52	0.29	0.03	-0.34	0.28	0.03
8	1	-0.01	0.02	0.00	-0.52	0.29	-0.03	-0.33	0.28	-0.04
9	6	0.00	0.00	0.00	0.05	0.04	0.00	0.00	0.03	0.00
10	7	0.00	0.00	0.00	0.09	0.02	0.00	0.02	0.00	0.00

16					17			18		
A					A			A		
Frequencies	--	1125.8706			1221.3981			1387.7138		
Red. masses	--	1.2183			1.8374			1.1476		
Frc consts	--	0.9099			1.6150			1.3021		
IR Inten	--	0.2115			258.0029			15.7880		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	0.00	-0.03	0.00	-0.06	0.00	0.00
2	8	0.00	0.00	0.00	0.01	0.02	0.00	0.01	-0.06	0.00
3	1	0.00	0.00	-0.01	0.21	0.11	0.00	0.78	0.61	0.00

4	8	0.00	0.00	0.01	0.04	-0.03	0.00	-0.03	0.03	0.00
5	1	0.00	0.00	-0.01	-0.17	-0.43	0.00	-0.01	0.08	0.00
6	6	0.00	0.00	0.09	-0.21	0.14	0.00	0.02	-0.03	0.00
7	1	-0.69	0.03	-0.13	0.39	-0.40	-0.10	-0.02	0.02	0.01
8	1	0.69	-0.03	-0.13	0.39	-0.40	0.10	-0.02	0.02	-0.01
9	6	0.00	0.00	-0.11	0.02	-0.03	0.00	0.00	0.00	0.00
10	7	0.00	0.00	0.02	0.05	0.02	0.00	0.00	0.00	0.00

19					20			21		
A					A			A		
Frequencies	--	1466.7016			1810.2955			3154.6277		
Red. masses	--	1.1252			9.0021			1.0966		
Frc consts	--	1.4261			17.3818			6.4300		
IR Inten	--	1.3877			226.8960			1.4633		

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	0.23	0.61	0.00	0.05	-0.08	0.00
2	8	0.00	0.00	0.00	-0.15	-0.44	0.00	0.00	0.01	0.00
3	1	0.00	-0.01	0.00	-0.43	0.26	0.00	-0.58	0.81	0.00
4	8	0.00	0.00	0.00	0.02	-0.05	0.00	0.00	0.00	0.00
5	1	0.00	0.01	0.00	-0.17	-0.23	0.00	0.00	0.00	0.00
6	6	-0.08	-0.06	0.00	-0.03	0.05	0.00	0.00	0.00	0.00
7	1	0.38	0.42	0.41	0.08	-0.02	-0.01	0.00	0.00	-0.01
8	1	0.38	0.42	-0.41	0.08	-0.02	0.01	0.00	0.00	0.01
9	6	0.00	-0.02	0.00	0.00	-0.01	0.00	-0.01	0.00	0.00
10	7	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00

22					23			24		
A					A			A		
Frequencies	--	3178.9639			3227.4912			3286.2503		
Red. masses	--	1.3086			3.7689			1.1157		
Frc consts	--	7.7917			23.1308			7.0992		
IR Inten	--	160.9001			490.1416			1.3529		

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	1	-0.01	0.02	0.00	-0.01	0.03	0.00	0.00	0.00	0.00
4	8	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
5	1	0.00	-0.04	0.00	-0.01	-0.03	0.00	0.00	0.00	0.00
6	6	0.02	0.05	0.00	-0.08	-0.05	0.00	0.00	0.00	0.10
7	1	-0.19	-0.32	0.59	0.18	0.26	-0.53	0.20	0.34	-0.59
8	1	-0.19	-0.32	-0.59	0.18	0.26	0.53	-0.20	-0.34	-0.59
9	6	0.11	0.04	0.00	0.36	0.12	0.00	0.00	0.00	0.00
10	7	-0.09	-0.03	0.00	-0.27	-0.09	0.00	0.00	0.00	0.00

Zero-point correction=	0.065048 (Hartree/Particle)
Thermal correction to Energy=	0.071527
Thermal correction to Enthalpy=	0.072471
Thermal correction to Gibbs Free Energy=	0.033777
Sum of electronic and zero-point Energies=	-321.117389
Sum of electronic and thermal Energies=	-321.110910
Sum of electronic and thermal Enthalpies=	-321.109966
Sum of electronic and thermal Free Energies=	-321.148660

Comments for the Spectroscopy Tables:

Hamiltonian: Watson's A-reduction I^r representation¹

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

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-test²

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 fit²

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

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

Uncertainties: The uncertainties represent one standard deviation

Significant digits: the number of significant digits of each fitted constant is 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 (if applied) are in Hz, and the principal axis inertial constants and the inertial defect are in $\text{u } \text{\AA}^2$

Table S12. Microwave Spectrum of the Ground Vibrational State of Conformer I of HC(O)OCH₂C≡N

Watson A-reduction

Total number of transitions: 330

Transition						obs. frequency	obs.- calc.	weight	t	distortion total	corrections higher	fixed
4	0	4	5	0	5	17081.680	0.120	0.20	0.5	-0.099	-7.3E-8	
4	1	4	5	1	5	16765.400	0.259	0.10	2.2	-0.067	-5.9E-6	
4	1	3	5	1	4	17421.240	0.317	0.15	1.8	-0.092	-5.9E-6	
5	1	4	6	1	5	20903.300	0.308	0.15	1.7	-0.170	-7.1E-6	
6	1	5	7	1	6	24384.220	0.337	0.15	1.9	-0.280	-8.4E-6	
7	1	7	8	1	8	26814.960	0.207	0.10	1.9	-0.324	-9.8E-6	
7	1	6	8	1	7	27863.420	0.039	0.15	0.2	-0.427	-9.8E-6	
7	2	6	8	2	7	27345.110	0.240	0.10	2.0	-0.280	-1.5E-4	
7	2	5	8	2	6	27406.140	-0.134	0.10	-1.1	-0.290	-1.5E-4	
7	3	5	8	3	6	27362.500	0.029	0.15	0.2	-0.123	-7.5E-4	
7	3	4	8	3	5	27363.100	-0.017	0.15	-0.1	-0.123	-7.5E-4	
8	1	8	9	1	9	30162.010	-0.032	0.10	-0.3	-0.469	-1.1E-5	
8	2	7	9	2	8	30759.890	0.148	0.10	1.2	-0.436	-1.7E-4	
8	2	6	9	2	7	30847.180	-0.113	0.10	-0.9	-0.454	-1.7E-4	
8	3	6	9	3	7	30784.560	-0.209	0.20	-0.9	-0.261	-8.5E-4	
8	3	5	9	3	6	30785.760	-0.192	0.20	-0.8	-0.262	-8.5E-4	
9	4	6	10	4	7	34201.890	0.044	0.20	0.2	-0.163	-3.0E-3	
9	4	5	10	4	6	34201.890	0.032	0.20	0.1	-0.163	-3.0E-3	
9	5	5	10	5	6	34199.340	0.187	0.20	0.8	0.195	-7.3E-3	
9	5	4	10	5	5	34199.340	0.187	0.20	0.8	0.195	-7.3E-3	
10	1	10	11	1	11	36852.080	0.200	0.15	1.2	-0.875	-1.5E-5	
10	2	8	11	2	9	37745.450	0.004	0.10	0.0	-0.929	-2.0E-4	
10	3	8	11	3	9	37630.960	-0.326	0.15	-1.8	-0.675	-1.0E-3	
10	3	7	11	3	8	37634.640	0.062	0.10	0.5	-0.676	-1.0E-3	
10	4	7	11	4	8	37623.640	-0.082	0.15	-0.5	-0.365	-3.3E-3	
10	4	6	11	4	7	37623.640	-0.107	0.15	-0.6	-0.365	-3.3E-3	
10	5	6	11	5	7	37620.080	0.020	0.10	0.2	0.029	-8.0E-3	
10	5	5	11	5	6	37620.080	0.020	0.10	0.2	0.029	-8.0E-3	
11	1	11	12	1	12	40194.200	0.023	0.15	0.1	-1.143	-1.7E-5	
11	2	10	12	2	11	40997.160	0.153	0.10	1.3	-1.179	-2.3E-4	
11	2	9	12	2	10	41203.310	-0.100	0.10	-0.9	-1.252	-2.2E-4	
11	3	9	12	3	10	41055.790	0.232	0.10	2.0	-0.959	-1.1E-3	
11	3	8	12	3	9	41060.710	0.035	0.10	0.3	-0.962	-1.1E-3	
11	4	8	12	4	9	41046.090	0.012	0.10	0.1	-0.621	-3.6E-3	
11	4	7	12	4	8	41046.090	-0.036	0.10	-0.3	-0.621	-3.6E-3	
12	1	11	13	1	12	45231.870	0.167	0.15	1.0	-1.900	-2.1E-5	
12	2	11	13	2	12	44406.690	0.129	0.10	1.1	-1.533	-2.5E-4	
12	2	10	13	2	11	44667.690	-0.027	0.10	-0.2	-1.641	-2.4E-4	
12	3	10	13	3	11	44480.840	0.322	0.15	1.8	-1.303	-1.2E-3	
12	3	9	13	3	10	44488.180	-0.006	0.15	-0.0	-1.307	-1.2E-3	
12	4	9	13	4	10	44468.980	0.023	0.10	0.2	-0.935	-3.9E-3	
12	4	8	13	4	9	44468.960	-0.082	0.10	-0.7	-0.935	-3.9E-3	
12	5	8	13	5	9	44462.660	-0.087	0.10	-0.7	-0.467	-9.5E-3	
12	5	7	13	5	8	44462.600	-0.148	0.10	-1.2	-0.467	-9.5E-3	
13	1	13	14	1	14	46872.820	-0.168	0.10	-1.7	-1.826	-2.3E-5	
13	2	12	14	2	13	47814.390	-0.086	0.10	-0.7	-1.946	-2.7E-4	
13	2	11	14	2	12	48138.560	0.012	0.10	0.1	-2.101	-2.6E-4	
13	3	11	14	3	12	47906.260	0.099	0.10	0.8	-1.710	-1.3E-3	
13	3	10	14	3	11	47917.160	-0.140	0.10	-1.2	-1.717	-1.3E-3	
13	4	10	14	4	11	47892.390	-0.008	0.10	-0.1	-1.312	-4.2E-3	
13	4	9	14	4	10	47892.390	-0.152	0.10	-1.3	-1.313	-4.2E-3	
13	5	9	14	5	10	47884.480	-0.100	0.10	-0.8	-0.808	-0.010	
13	5	8	14	5	9	47884.480	-0.101	0.10	-0.9	-0.808	-0.010	
14	2	13	15	2	14	51220.450	-0.178	0.10	-1.5	-2.425	-2.9E-4	
14	2	12	15	2	13	51615.640	-0.321	0.15	-1.8	-2.640	-2.8E-4	
14	3	12	15	3	13	51332.600	0.133	0.10	1.1	-2.185	-1.4E-3	
14	3	11	15	3	12	51347.970	-0.254	0.10	-2.1	-2.197	-1.4E-3	
14	4	11	15	4	12	51316.560	0.118	0.10	1.0	-1.758	-4.5E-3	

14	4	10	15	4	11	51316.630	-0.048	0.10	-0.4	-1.758	-4.5E-3
14	5	10	15	5	11	51306.730	-0.043	0.10	-0.4	-1.216	-0.011
14	5	9	15	5	10	51306.730	-0.045	0.10	-0.4	-1.216	-0.011
14	6	9	15	6	10	51301.950	-0.073	0.10	-0.6	-0.562	-0.023
14	6	8	15	6	9	51301.950	-0.073	0.10	-0.6	-0.562	-0.023
15	2	14	16	2	15	54624.960	0.063	0.15	0.4	-2.972	-3.2E-4
15	3	13	16	3	14	54759.170	-0.233	0.10	-2.0	-2.734	-1.5E-3
15	3	12	16	3	13	54781.020	-0.161	0.10	-1.4	-2.753	-1.5E-3
15	4	12	16	4	13	54741.000	-0.127	0.15	-0.7	-2.278	-4.8E-3
15	4	11	16	4	12	54741.400	-0.100	0.15	-0.6	-2.278	-4.8E-3
15	5	11	16	5	12	54729.350	-0.002	0.10	-0.0	-1.698	-0.012
15	5	10	16	5	11	54729.350	-0.005	0.10	-0.0	-1.698	-0.012
15	6	10	16	6	11	54723.430	-0.062	0.10	-0.5	-0.999	-0.024
15	6	9	16	6	10	54723.430	-0.062	0.10	-0.5	-0.999	-0.024
16	2	15	17	2	16	58027.240	0.076	0.15	0.4	-3.591	-3.4E-4
16	3	14	17	3	15	58186.840	-0.081	0.10	-0.7	-3.362	-1.6E-3
16	3	13	17	3	14	58216.330	-0.083	0.10	-0.7	-3.391	-1.6E-3
16	4	13	17	4	14	58166.660	0.172	0.10	1.4	-2.875	-5.1E-3
16	5	12	17	5	13	58152.380	0.038	0.10	0.3	-2.257	-0.012
16	5	11	17	5	12	58152.380	0.032	0.10	0.3	-2.257	-0.012
16	6	11	17	6	12	58145.320	0.102	0.10	0.9	-1.513	-0.026
16	6	10	17	6	11	58145.320	0.102	0.10	0.9	-1.513	-0.026
16	7	10	17	7	11	58141.440	0.001	0.10	0.0	-0.643	-0.048
16	7	9	17	7	10	58141.440	0.001	0.10	0.0	-0.643	-0.048
17	2	16	18	2	17	61427.080	-0.231	0.10	-2.0	-4.288	-3.7E-4
17	3	15	18	3	16	61615.080	0.121	0.10	1.0	-4.073	-1.7E-3
17	3	14	18	3	15	61653.950	-0.229	0.10	-1.9	-4.116	-1.7E-3
17	4	14	18	4	15	61592.770	0.209	0.10	1.8	-3.557	-5.4E-3
17	5	13	18	5	14	61575.770	0.001	0.10	0.0	-2.899	-0.013
17	5	12	18	5	13	61575.770	-0.009	0.10	-0.1	-2.899	-0.013
17	6	12	18	6	13	61567.270	0.052	0.10	0.4	-2.110	-0.027
17	6	11	18	6	12	61567.270	0.051	0.10	0.4	-2.110	-0.027
18	2	17	19	2	18	64825.410	0.185	0.15	1.0	-5.065	-4.0E-4
18	2	16	19	2	17	65587.540	-0.031	0.10	-0.3	-5.709	-3.5E-4
18	3	16	19	3	17	65043.180	-0.261	0.15	-1.5	-4.873	-1.8E-3
18	4	15	19	4	16	65019.520	0.142	0.20	0.6	-4.327	-5.7E-3
18	4	14	19	4	15	65020.720	0.083	0.20	0.3	-4.329	-5.7E-3
18	5	14	19	5	15	64999.640	-0.020	0.10	-0.2	-3.630	-0.014
18	5	13	19	5	14	64999.640	-0.035	0.10	-0.3	-3.630	-0.014
18	6	13	19	6	14	64989.380	-0.129	0.10	-1.1	-2.794	-0.029
18	6	12	19	6	13	64989.380	-0.129	0.10	-1.1	-2.794	-0.029
19	2	17	20	2	18	69093.730	0.025	0.10	0.2	-6.734	-3.7E-4
19	3	17	20	3	18	68472.230	-0.045	0.15	-0.3	-5.765	-1.9E-3
19	3	16	20	3	17	68538.200	-0.245	0.15	-1.4	-5.854	-1.9E-3
19	4	16	20	4	17	68447.190	0.224	0.20	0.9	-5.191	-6.0E-3
19	4	15	20	4	16	68448.990	0.215	0.20	0.9	-5.194	-6.0E-3
19	5	15	20	5	16	68424.090	0.052	0.10	0.4	-4.453	-0.015
19	5	14	20	5	15	68424.090	0.027	0.10	0.2	-4.453	-0.015
19	6	14	20	6	15	68412.120	0.014	0.10	0.1	-3.571	-0.030
19	6	13	20	6	14	68412.120	0.014	0.10	0.1	-3.571	-0.030
19	7	13	20	7	14	68405.520	-0.041	0.10	-0.3	-2.544	-0.056
19	7	12	20	7	13	68405.520	-0.041	0.10	-0.3	-2.544	-0.056
20	2	18	21	2	19	72603.950	0.193	0.20	0.8	-7.874	-4.0E-4
20	3	18	21	3	19	71901.440	0.080	0.10	0.7	-6.756	-2.0E-3
20	3	17	21	3	18	71985.560	0.007	0.10	0.1	-6.881	-2.0E-3
20	4	17	21	4	18	71875.090	-0.262	0.10	-2.2	-6.154	-6.3E-3
20	4	16	21	4	17	71878.160	0.258	0.10	2.2	-6.159	-6.3E-3
20	5	16	21	5	17	71848.970	0.040	0.10	0.3	-5.374	-0.015
20	5	15	21	5	16	71848.910	-0.060	0.10	-0.5	-5.374	-0.015
20	6	15	21	6	16	71835.040	0.015	0.10	0.1	-4.446	-0.032
20	6	14	21	6	15	71834.910	-0.116	0.10	-1.0	-4.446	-0.032
20	7	14	21	7	15	71827.040	-0.298	0.30	-0.8	-3.366	-0.059
20	7	13	21	7	14	71827.040	-0.298	0.30	-0.8	-3.366	-0.059
20	8	13	21	8	14	71822.890	-0.061	0.10	-0.5	-2.135	-0.100
20	8	12	21	8	13	71822.890	-0.061	0.10	-0.5	-2.135	-0.100
21	2	20	22	2	21	75004.690	0.221	0.20	0.9	-7.919	-5.1E-4
21	3	19	22	3	20	75330.610	0.033	0.15	0.2	-7.849	-2.1E-3
21	3	18	22	3	19	75436.270	-0.137	0.10	-1.2	-8.021	-2.1E-3
21	4	18	22	4	19	75304.430	-0.128	0.10	-1.1	-7.222	-6.6E-3
21	4	17	22	4	18	75307.960	-0.134	0.10	-1.1	-7.229	-6.6E-3

21	5	17	22	5	18	75274.520	0.158	0.10	1.3	-6.399	-0.016
21	5	16	22	5	17	75274.520	0.097	0.10	0.8	-6.399	-0.016
21	6	16	22	6	17	75258.340	0.057	0.10	0.5	-5.423	-0.033
21	6	15	22	6	16	75258.340	0.056	0.10	0.5	-5.423	-0.033
21	7	15	22	7	16	75249.400	0.065	0.10	0.5	-4.289	-0.062
21	7	14	22	7	15	75249.400	0.065	0.10	0.5	-4.289	-0.062
21	8	14	22	8	15	75244.120	-0.046	0.10	-0.4	-2.998	-0.105
21	8	13	22	8	14	75244.120	-0.046	0.10	-0.4	-2.998	-0.105
22	2	21	23	2	22	78392.410	0.039	0.10	0.3	-9.057	-5.5E-4
22	3	20	23	3	21	78759.640	-0.159	0.15	-0.9	-9.050	-2.3E-3
22	3	19	23	3	20	78891.350	0.009	0.10	0.1	-9.282	-2.2E-3
22	4	19	23	4	20	78734.360	-0.240	0.10	-2.0	-8.399	-6.9E-3
22	4	18	23	4	19	78739.640	0.210	0.10	1.8	-8.410	-6.9E-3
22	5	18	23	5	19	78700.560	0.202	0.10	1.7	-7.532	-0.017
22	5	17	23	5	18	78700.560	0.111	0.10	0.9	-7.533	-0.017
22	6	17	23	6	18	78682.000	0.104	0.10	0.9	-6.508	-0.035
22	6	16	23	6	17	78682.000	0.103	0.10	0.9	-6.508	-0.035
22	7	16	23	7	17	78671.440	-0.121	0.10	-1.0	-5.320	-0.064
22	7	15	23	7	16	78671.440	-0.121	0.10	-1.0	-5.320	-0.064
22	8	15	23	8	16	78665.410	-0.120	0.10	-1.0	-3.969	-0.110
22	8	14	23	8	15	78665.410	-0.120	0.10	-1.0	-3.969	-0.110
23	3	21	24	3	22	82188.870	-0.017	0.15	-0.1	-10.363	-2.4E-3
23	3	20	24	3	21	82350.720	0.025	0.10	0.2	-10.673	-2.3E-3
23	4	19	24	4	20	82172.050	0.052	0.10	0.4	-9.707	-7.2E-3
23	5	19	24	5	20	82126.990	0.047	0.10	0.4	-8.779	-0.018
23	5	18	24	5	19	82126.990	-0.087	0.10	-0.7	-8.779	-0.018
23	6	18	24	6	19	82105.970	0.090	0.10	0.8	-7.705	-0.036
23	6	17	24	6	18	82105.970	0.088	0.10	0.7	-7.705	-0.036
23	7	17	24	7	18	82094.040	0.012	0.10	0.1	-6.463	-0.067
23	7	16	24	7	17	82094.040	0.012	0.10	0.1	-6.463	-0.067
23	8	16	24	8	17	82087.160	0.109	0.10	0.9	-5.051	-0.114
23	8	15	24	8	16	82087.160	0.109	0.10	0.9	-5.051	-0.114
23	9	15	24	9	16	82082.800	-0.128	0.10	-1.1	-3.471	-0.183
23	9	14	24	9	15	82082.800	-0.128	0.10	-1.1	-3.471	-0.183
24	3	22	25	3	23	85618.030	0.338	0.15	1.9	-11.792	-2.5E-3
24	4	21	25	4	22	85597.130	-0.108	0.20	-0.5	-11.103	-7.6E-3
24	4	20	25	4	21	85605.750	-0.144	0.10	-1.2	-11.126	-7.5E-3
24	5	20	25	5	21	85554.450	0.308	0.15	1.7	-10.145	-0.018
24	5	19	25	5	20	85554.450	0.114	0.15	0.6	-10.145	-0.018
24	6	19	25	6	20	85530.320	0.068	0.10	0.6	-9.020	-0.038
24	6	18	25	6	19	85530.320	0.066	0.10	0.6	-9.020	-0.038
24	7	18	25	7	19	85516.720	-0.025	0.10	-0.2	-7.723	-0.070
24	7	17	25	7	18	85516.720	-0.025	0.10	-0.2	-7.723	-0.070
24	8	17	25	8	18	85508.840	0.105	0.10	0.9	-6.250	-0.119
24	8	16	25	8	17	85508.840	0.105	0.10	0.9	-6.250	-0.119
24	9	16	25	9	17	85504.030	0.094	0.10	0.8	-4.603	-0.191
24	9	15	25	9	16	85504.030	0.094	0.10	0.8	-4.603	-0.191
25	2	23	26	2	24	90181.120	0.091	0.10	0.9	-15.425	-5.6E-4
25	3	23	26	3	24	89046.140	0.085	0.15	0.5	-13.341	-2.6E-3
25	3	22	26	3	23	89284.070	0.066	0.15	0.4	-13.871	-2.5E-3
25	4	22	26	4	23	89029.700	-0.141	0.10	-1.2	-12.641	-7.9E-3
25	4	21	26	4	22	89041.170	-0.052	0.10	-0.4	-12.673	-7.9E-3
25	5	21	26	5	22	88982.050	0.070	0.10	0.6	-11.634	-0.019
25	5	20	26	5	21	88982.050	-0.206	0.10	-1.7	-11.635	-0.019
25	6	20	26	6	21	88954.910	-0.117	0.10	-1.0	-10.458	-0.039
25	6	19	26	6	20	88954.910	-0.121	0.10	-1.0	-10.458	-0.039
25	7	19	26	7	20	88939.780	0.058	0.10	0.5	-9.104	-0.073
25	7	18	26	7	19	88939.780	0.057	0.10	0.5	-9.104	-0.073
25	8	18	26	8	19	88930.800	0.212	0.10	1.8	-7.570	-0.124
25	8	17	26	8	18	88930.800	0.212	0.10	1.8	-7.570	-0.124
25	9	17	26	9	18	88924.800	-0.252	0.10	-2.1	-5.856	-0.199
25	9	16	26	9	17	88924.800	-0.252	0.10	-2.1	-5.856	-0.199
26	3	24	27	3	25	92473.880	0.067	0.10	0.6	-15.015	-2.8E-3
26	4	23	27	4	24	92463.230	-0.064	0.20	-0.3	-14.309	-8.2E-3
26	4	22	27	4	23	92478.120	0.024	0.10	0.2	-14.355	-8.2E-3
26	5	22	27	5	23	92410.560	0.081	0.15	0.5	-13.254	-0.020
26	5	21	27	5	22	92410.960	0.093	0.15	0.5	-13.255	-0.020
26	6	21	27	6	22	92380.300	0.078	0.10	0.7	-12.024	-0.041
26	6	20	27	6	21	92380.300	0.072	0.10	0.6	-12.024	-0.041
26	7	20	27	7	21	92363.030	0.058	0.10	0.5	-10.614	-0.076

26	7	19	27	7	20	92363.030	0.058	0.10	0.5	-10.614	-0.076
26	8	19	27	8	20	92352.840	0.221	0.10	1.9	-9.017	-0.129
26	8	18	27	8	19	92352.840	0.221	0.10	1.9	-9.017	-0.129
26	9	18	27	9	19	92346.690	0.410	0.20	1.7	-7.235	-0.206
26	9	17	27	9	18	92346.690	0.410	0.20	1.7	-7.235	-0.206
26	10	17	27	10	18	92342.560	0.090	0.10	0.8	-5.270	-0.314
26	10	16	27	10	17	92342.560	0.090	0.10	0.8	-5.270	-0.314
27	2	26	28	2	27	95288.530	-0.388	0.20	-1.7	-16.291	-8.5E-4
27	3	25	28	3	26	95900.850	0.056	0.15	0.3	-16.818	-2.9E-3
27	3	24	28	3	25	96238.730	-0.129	0.10	-1.2	-17.681	-2.7E-3
27	4	23	28	4	24	95916.570	-0.071	0.10	-0.6	-16.176	-8.5E-3
27	5	23	28	5	24	95839.740	0.076	0.15	0.4	-15.007	-0.021
27	5	22	28	5	23	95840.240	0.036	0.15	0.2	-15.010	-0.021
27	6	22	28	6	23	95805.870	0.017	0.10	0.1	-13.723	-0.042
27	6	21	28	6	22	95805.870	0.008	0.10	0.1	-13.723	-0.042
27	7	21	28	7	22	95786.440	-0.063	0.10	-0.5	-12.255	-0.078
27	7	20	28	7	21	95786.440	-0.063	0.10	-0.5	-12.255	-0.078
27	8	20	28	8	21	95774.810	-0.022	0.10	-0.2	-10.596	-0.134
27	8	19	28	8	20	95774.810	-0.022	0.10	-0.2	-10.596	-0.134
27	9	19	28	9	20	95767.550	-0.074	0.10	-0.6	-8.745	-0.214
27	9	18	28	9	19	95767.550	-0.074	0.10	-0.6	-8.745	-0.214
27	10	18	28	10	19	95763.450	0.227	0.10	1.9	-6.706	-0.326
27	10	17	28	10	18	95763.450	0.227	0.10	1.9	-6.706	-0.326
28	3	25	29	3	26	99724.920	-0.108	0.15	-0.6	-19.836	-2.8E-3
28	4	25	29	4	26	99332.750	0.062	0.15	0.3	-18.058	-8.9E-3
28	4	24	29	4	25	99357.090	0.095	0.10	0.8	-18.145	-8.8E-3
28	5	24	29	5	25	99269.610	0.052	0.20	0.2	-16.901	-0.021
28	5	23	29	5	24	99270.210	-0.088	0.20	-0.4	-16.905	-0.021
28	6	23	29	6	24	99231.990	0.053	0.10	0.4	-15.560	-0.044
28	6	22	29	6	23	99231.990	0.039	0.10	0.3	-15.561	-0.044
28	7	22	29	7	23	99210.580	0.254	0.15	1.4	-14.034	-0.081
28	7	21	29	7	22	99210.580	0.254	0.15	1.4	-14.034	-0.081
28	8	21	29	8	22	99197.190	-0.046	0.10	-0.4	-12.311	-0.138
28	8	20	29	8	21	99197.190	-0.046	0.10	-0.4	-12.311	-0.138
28	9	20	29	9	21	99189.210	0.120	0.10	1.0	-10.391	-0.222
28	9	19	29	9	20	99189.210	0.120	0.10	1.0	-10.391	-0.222
28	10	19	29	10	20	99183.930	-0.118	0.10	-1.0	-8.278	-0.338
28	10	18	29	10	19	99183.930	-0.118	0.10	-1.0	-8.278	-0.338
29	2	27	30	2	28	104220.950	0.200	0.30	0.6	-23.882	-8.0E-4
29	3	27	30	3	28	102751.500	-0.220	0.10	-1.9	-20.825	-3.2E-3
29	3	26	30	3	27	103217.350	0.070	0.10	0.7	-22.169	-2.9E-3
29	4	26	30	4	27	102768.800	0.221	0.20	0.9	-20.149	-9.2E-3
29	4	25	30	4	26	102799.010	-0.298	0.15	-1.7	-20.267	-9.2E-3
29	5	25	30	5	26	102700.420	0.240	0.20	1.0	-18.941	-0.022
29	5	24	30	5	25	102701.120	-0.065	0.20	-0.3	-18.945	-0.022
29	6	24	30	6	25	102658.310	-0.180	0.10	-1.5	-17.542	-0.045
29	6	23	30	6	24	102658.310	-0.200	0.10	-1.7	-17.542	-0.045
29	7	23	30	7	24	102634.740	0.288	0.15	1.6	-15.955	-0.084
29	7	22	30	7	23	102634.740	0.288	0.15	1.6	-15.955	-0.084
29	8	22	30	8	23	102619.950	0.114	0.10	1.0	-14.168	-0.143
29	8	21	30	8	22	102619.950	0.114	0.10	1.0	-14.168	-0.143
29	9	21	30	9	22	102610.550	-0.130	0.10	-1.1	-12.179	-0.229
29	9	20	30	9	21	102610.550	-0.130	0.10	-1.1	-12.179	-0.229
29	10	20	30	10	21	102604.880	-0.066	0.10	-0.6	-9.990	-0.349
29	10	19	30	10	20	102604.880	-0.066	0.10	-0.6	-9.990	-0.349
30	4	27	31	4	28	106205.200	-0.016	0.10	-0.1	-22.392	-9.6E-3
30	4	26	31	4	27	106243.760	0.017	0.10	0.1	-22.549	-9.5E-3
30	5	26	31	5	27	106131.670	0.117	0.20	0.5	-21.131	-0.023
30	5	25	31	5	26	106132.970	0.067	0.20	0.3	-21.138	-0.023
30	6	25	31	6	26	106085.480	-0.049	0.10	-0.4	-19.672	-0.047
30	6	24	31	6	25	106085.480	-0.078	0.10	-0.7	-19.672	-0.047
30	7	24	31	7	25	106058.950	0.058	0.10	0.5	-18.024	-0.087
30	7	23	31	7	24	106058.950	0.058	0.10	0.5	-18.024	-0.087
30	8	23	31	8	24	106042.730	0.090	0.10	0.8	-16.172	-0.148
30	8	22	31	8	23	106042.730	0.090	0.10	0.8	-16.172	-0.148
30	9	22	31	9	23	106032.160	-0.240	0.10	-2.0	-14.113	-0.237
30	9	21	31	9	22	106032.160	-0.240	0.10	-2.0	-14.113	-0.237
31	2	30	32	2	31	108750.640	0.240	0.20	1.1	-24.123	-1.2E-3
31	2	29	32	2	30	111216.060	-0.297	0.15	-3.6	-28.967	-9.9E-4
31	3	29	32	3	30	109597.320	-0.080	0.20	-0.3	-25.392	-3.6E-3

31	3	28	32	3	29	110220.390	0.026	0.10	0.3	-27.399	-3.1E-3
31	4	28	32	4	29	109642.400	-0.152	0.10	-1.3	-24.792	-9.9E-3
31	4	27	32	4	28	109690.660	0.181	0.10	1.6	-24.999	-9.8E-3
31	6	26	32	6	27	109513.010	-0.061	0.10	-0.5	-21.956	-0.049
31	6	25	32	6	26	109513.010	-0.101	0.10	-0.9	-21.956	-0.049
31	7	25	32	7	26	109483.670	0.015	0.10	0.1	-20.245	-0.090
31	7	24	32	7	25	109483.670	0.014	0.10	0.1	-20.245	-0.090
31	8	24	32	8	25	109465.630	-0.024	0.10	-0.2	-18.328	-0.153
31	8	23	32	8	24	109465.630	-0.024	0.10	-0.2	-18.328	-0.153
31	9	23	32	9	24	109454.230	-0.024	0.10	-0.2	-16.199	-0.245
31	9	22	32	9	23	109454.230	-0.024	0.10	-0.2	-16.199	-0.245
31	10	22	32	10	23	109446.960	-0.017	0.10	-0.1	-13.858	-0.373
31	10	21	32	10	22	109446.960	-0.017	0.10	-0.1	-13.858	-0.373
31	11	21	32	11	22	109442.280	-0.159	0.10	-1.4	-11.311	-0.546
31	11	20	32	11	21	109442.280	-0.159	0.10	-1.4	-11.311	-0.546
32	4	29	33	4	30	113080.340	-0.189	0.10	-1.6	-27.353	-0.010
32	4	28	33	4	29	113139.650	-0.059	0.10	-0.5	-27.624	-0.010
32	5	28	33	5	29	112996.840	0.213	0.15	1.2	-25.986	-0.024
32	6	27	33	6	28	112941.400	0.269	0.10	2.3	-24.400	-0.050
32	6	26	33	6	27	112941.400	0.212	0.10	1.8	-24.400	-0.050
32	7	26	33	7	27	112908.770	0.017	0.10	0.1	-22.625	-0.093
32	7	25	33	7	26	112908.770	0.016	0.10	0.1	-22.625	-0.093
32	8	25	33	8	26	112888.930	0.044	0.10	0.4	-20.641	-0.158
32	8	24	33	8	25	112888.930	0.044	0.10	0.4	-20.641	-0.158
32	9	24	33	9	25	112876.240	-0.005	0.10	-0.0	-18.440	-0.252
32	9	23	33	9	24	112876.240	-0.005	0.10	-0.0	-18.440	-0.252
32	10	23	33	10	24	112868.150	0.037	0.10	0.3	-16.023	-0.384
32	10	22	33	10	23	112868.150	0.037	0.10	0.3	-16.023	-0.384
32	11	22	33	11	23	112862.630	-0.342	0.20	-1.4	-13.394	-0.563
32	11	21	33	11	22	112862.630	-0.342	0.20	-1.4	-13.394	-0.563
33	2	32	34	2	33	115461.370	-0.189	0.20	-0.9	-28.785	-1.5E-3
33	4	30	34	4	31	116519.100	0.020	0.15	0.1	-30.080	-0.011
33	4	29	34	4	30	116591.880	0.239	0.10	2.1	-30.433	-0.010
33	5	28	34	5	29	116433.530	0.075	0.10	0.6	-28.680	-0.025
33	6	28	34	6	29	116369.870	0.143	0.10	1.2	-27.009	-0.052
33	6	27	34	6	28	116369.870	0.064	0.10	0.5	-27.009	-0.052
33	7	27	34	7	28	116334.300	0.103	0.10	0.9	-25.168	-0.095
33	7	26	34	7	27	116334.300	0.102	0.10	0.9	-25.168	-0.095
33	8	26	34	8	27	116312.200	-0.141	0.10	-1.2	-23.116	-0.163
33	8	25	34	8	26	116312.200	-0.141	0.10	-1.2	-23.116	-0.163
33	9	25	34	9	26	116298.270	-0.108	0.10	-0.9	-20.843	-0.260
33	9	24	34	9	25	116298.270	-0.108	0.10	-0.9	-20.843	-0.260
33	10	24	34	10	25	116289.090	-0.244	0.10	-2.1	-18.349	-0.396
33	10	23	34	10	24	116289.090	-0.244	0.10	-2.1	-18.349	-0.396
33	11	23	34	11	24	116283.630	0.084	0.15	0.5	-15.638	-0.580
33	11	22	34	11	23	116283.630	0.084	0.15	0.5	-15.638	-0.580
33	12	22	34	12	23	116280.180	0.156	0.10	1.5	-12.717	-0.821
33	12	21	34	12	22	116280.180	0.156	0.10	1.5	-12.717	-0.821
34	4	31	35	4	32	119957.970	-0.156	0.10	-1.4	-32.978	-0.011
34	5	30	35	5	31	119864.990	0.076	0.15	0.4	-31.511	-0.026
34	7	28	35	7	29	119759.890	-0.106	0.10	-0.9	-27.879	-0.098
34	7	27	35	7	28	119759.890	-0.108	0.10	-0.9	-27.879	-0.098
34	8	27	35	8	28	119735.820	-0.207	0.15	-1.2	-25.758	-0.167
34	8	26	35	8	27	119735.820	-0.207	0.15	-1.2	-25.758	-0.167
34	9	26	35	9	27	119720.670	0.012	0.10	0.1	-23.412	-0.268
34	9	25	35	9	26	119720.670	0.012	0.10	0.1	-23.412	-0.268
34	10	25	35	10	26	119710.760	0.119	0.10	1.0	-20.841	-0.408
34	10	24	35	10	25	119710.760	0.119	0.10	1.0	-20.841	-0.408
34	11	24	35	11	25	119704.200	0.037	0.10	0.3	-18.047	-0.597
34	11	23	35	11	24	119704.200	0.037	0.10	0.3	-18.047	-0.597
34	12	23	35	12	24	119700.280	0.137	0.20	0.6	-15.038	-0.845
34	12	22	35	12	23	119700.280	0.137	0.20	0.6	-15.038	-0.845

rms deviation: 1.1906

Rotational constants (MHz) and kappa:

19304.2	1775.2182	1644.0460	-0.9851449
+-	2.3	0.0043	0.0044
			0.0000016

Inertial constants and defect (uÅ^2):

	26.1797	284.68561	307.39959	-3.466
+-	0.0032	0.00070	0.00083	0.004

Quartic distortion constants:

	0.200139	-2.0098	0	0.02535	0
+-	0.00032	0.016	fixed	0.0016	fixed

Sextic and higher distortion constants:

	0	0	-0.5820	0	0
+-	fixed	fixed	0.12	fixed	fixed
	0	0			
+-	fixed	fixed			

Significant Digits and Correlation Matrix:

6	0.585	-0.513	0.036	0.128	-0.253	0.094
	8	-0.970	-0.148	0.116	0.535	0.082
		8	0.270	0.019	-0.574	0.054
			6	-0.315	-0.458	-0.128
				5	0.140	0.938
					4	0.063
						4

Table S13. Microwave Spectrum of the First Excited State of the Torsional Vibration (ν_{21}) of Conformer I of HC(O)OCH₂C≡N

Watson A-reduction

Total number of transitions: 238

Transition						obs. frequency	obs.- calc.	weight	t	distortion	corrections
										total	fixed
4	1	3	5	1	4	17458.930	0.145	0.20	0.6	-0.086	
5	1	4	6	1	5	20948.850	0.368	0.20	1.5	-0.167	
7	1	7	8	1	8	26908.830	0.059	0.10	0.6	-0.338	
7	1	6	8	1	7	27924.290	0.063	0.15	0.4	-0.437	
7	2	6	8	2	7	27422.520	0.319	0.10	2.5	-0.226	
7	2	5	8	2	6	27481.870	0.062	0.10	0.5	-0.235	
7	3	5	8	3	6	27439.540	0.137	0.15	0.7	0.043	
7	3	4	8	3	5	27440.140	0.109	0.15	0.6	0.043	
7	4	4	8	4	5	27436.340	-0.210	0.15	-1.1	0.424	
7	4	3	8	4	4	27436.340	-0.213	0.15	-1.1	0.424	
8	1	8	9	1	9	30268.160	0.228	0.15	1.3	-0.497	
8	2	6	9	2	7	30931.750	-0.057	0.10	-0.5	-0.403	
9	2	8	10	2	9	34270.420	0.094	0.10	0.7	-0.592	
9	2	7	10	2	8	34387.040	0.170	0.10	1.4	-0.621	
10	2	8	11	2	9	37847.300	-0.131	0.10	-1.1	-0.897	
10	3	8	11	3	9	37736.680	-0.097	0.10	-0.8	-0.489	
10	3	7	11	3	8	37739.980	-0.000	0.10	-0.0	-0.490	
10	4	7	11	4	8	37729.630	-0.031	0.10	-0.2	0.036	
10	4	6	11	4	7	37729.630	-0.056	0.10	-0.4	0.036	
11	2	9	12	2	10	41313.640	-0.218	0.10	-1.8	-1.235	
11	3	9	12	3	10	41170.210	-0.306	0.15	-1.6	-0.775	
11	4	8	12	4	9	41161.570	0.006	0.15	0.0	-0.202	
11	4	7	12	4	8	41161.570	-0.041	0.15	-0.2	-0.202	
12	2	11	13	2	12	44533.040	0.094	0.10	0.8	-1.535	
12	2	10	13	2	11	44786.220	-0.211	0.10	-1.7	-1.644	
12	3	10	13	3	11	44604.980	0.063	0.10	0.5	-1.125	
12	3	9	13	3	10	44612.740	0.361	0.15	1.9	-1.129	
12	4	9	13	4	10	44593.690	-0.278	0.10	-2.2	-0.503	
12	4	8	13	4	9	44593.790	-0.261	0.10	-2.1	-0.503	
13	2	12	14	2	13	47950.980	0.198	0.10	1.6	-1.975	
13	2	11	14	2	12	48265.280	-0.045	0.10	-0.4	-2.130	
13	3	11	14	3	12	48040.240	0.267	0.10	2.1	-1.543	
13	4	10	14	4	11	48026.910	-0.001	0.10	-0.0	-0.872	
13	4	9	14	4	10	48027.010	-0.042	0.10	-0.3	-0.873	
13	5	9	14	5	10	48019.410	-0.281	0.10	-2.2	-0.013	
13	5	8	14	5	9	48019.410	-0.282	0.10	-2.2	-0.013	
14	3	12	15	3	13	51475.560	-0.104	0.10	-0.8	-2.036	
14	3	11	15	3	12	51490.900	-0.097	0.10	-0.8	-2.048	
14	4	11	15	4	12	51460.500	0.069	0.15	0.4	-1.316	
14	4	10	15	4	11	51460.700	0.039	0.15	0.2	-1.316	
14	5	10	15	5	11	51451.440	-0.001	0.15	-0.0	-0.394	
14	5	9	15	5	10	51451.440	-0.002	0.15	-0.0	-0.394	
15	2	14	16	2	15	54781.020	-0.161	0.20	-0.6	-3.068	
15	2	13	16	2	14	55242.170	0.019	0.10	0.2	-3.362	
15	3	13	16	3	14	54912.070	0.114	0.10	0.9	-2.609	
15	3	12	16	3	13	54933.460	0.312	0.15	1.6	-2.628	
15	4	12	16	4	13	54894.300	-0.264	0.15	-1.4	-1.839	
15	4	11	16	4	12	54894.700	-0.228	0.15	-1.2	-1.839	
15	5	11	16	5	12	54883.600	0.043	0.10	0.3	-0.854	
15	5	10	16	5	11	54883.600	0.040	0.10	0.3	-0.854	
16	2	15	17	2	16	58193.320	-0.190	0.10	-1.5	-3.731	
16	2	14	17	2	15	58739.860	0.085	0.10	0.7	-4.121	
16	3	14	17	3	15	58348.750	-0.054	0.10	-0.4	-3.266	
16	3	13	17	3	14	58377.470	-0.030	0.10	-0.2	-3.295	
16	4	13	17	4	14	58329.410	0.064	0.15	0.3	-2.447	
16	4	12	17	4	13	58330.010	0.104	0.15	0.5	-2.448	
16	5	12	17	5	13	58316.150	0.086	0.10	0.7	-1.398	
16	5	11	17	5	12	58316.150	0.081	0.10	0.6	-1.398	

16	6	11	17	6	12	58309.680	-0.020	0.10	-0.2	-0.124
16	6	10	17	6	11	58309.680	-0.020	0.10	-0.2	-0.124
17	3	15	18	3	16	61786.320	0.176	0.10	1.4	-4.014
17	4	14	18	4	15	61764.540	-0.270	0.20	-1.1	-3.145
17	4	13	18	4	14	61765.340	-0.308	0.20	-1.2	-3.147
17	5	13	18	5	14	61748.930	-0.056	0.10	-0.4	-2.032
17	5	12	18	5	13	61748.930	-0.065	0.10	-0.5	-2.032
17	6	12	18	6	13	61741.250	-0.020	0.15	-0.1	-0.681
17	6	11	18	6	12	61741.250	-0.020	0.15	-0.1	-0.681
18	2	16	19	2	17	65751.490	-0.091	0.15	-0.5	-5.958
18	3	16	19	3	17	65223.950	0.047	0.10	0.4	-4.857
18	4	15	19	4	16	65201.080	0.096	0.20	0.4	-3.940
18	4	14	19	4	15	65202.280	0.067	0.20	0.3	-3.942
18	5	14	19	5	15	65182.320	-0.027	0.10	-0.2	-2.761
18	5	13	19	5	14	65182.320	-0.043	0.10	-0.3	-2.761
18	6	13	19	6	14	65172.900	-0.211	0.10	-1.7	-1.333
18	6	12	19	6	13	65172.900	-0.211	0.10	-1.7	-1.333
19	2	17	20	2	18	69264.800	0.201	0.10	1.8	-7.048
19	3	17	20	3	18	68661.920	-0.072	0.10	-0.6	-5.801
19	3	16	20	3	17	68725.960	-0.413	0.15	-2.2	-5.892
19	4	16	20	4	17	68638.120	0.222	0.15	1.2	-4.836
19	4	15	20	4	16	68639.460	-0.202	0.15	-1.1	-4.839
19	5	15	20	5	16	68616.170	-0.002	0.10	-0.0	-3.591
19	5	14	20	5	15	68616.170	-0.027	0.10	-0.2	-3.591
19	6	14	20	6	15	68605.170	-0.069	0.10	-0.5	-2.086
19	6	13	20	6	14	68605.170	-0.069	0.10	-0.6	-2.086
19	7	13	20	7	14	68599.430	-0.230	0.10	-1.8	-0.314
19	7	12	20	7	13	68599.430	-0.230	0.10	-1.8	-0.314
20	2	18	21	2	19	72781.250	-0.136	0.10	-1.2	-8.259
20	3	18	21	3	19	72100.430	0.121	0.10	1.0	-6.851
20	3	17	21	3	18	72182.270	0.045	0.10	0.4	-6.978
20	4	17	21	4	18	72075.310	-0.264	0.20	-1.0	-5.839
20	4	16	21	4	17	72078.290	0.229	0.10	1.8	-5.844
20	5	16	21	5	17	72050.600	0.115	0.10	0.9	-4.527
20	5	15	21	5	16	72050.600	0.076	0.10	0.6	-4.527
20	6	15	21	6	16	72037.840	0.171	0.10	1.4	-2.943
20	6	14	21	6	15	72037.840	0.170	0.10	1.4	-2.943
21	2	20	22	2	21	75222.170	0.187	0.15	1.0	-8.387
21	3	19	22	3	20	75538.840	0.099	0.10	0.8	-8.012
21	3	18	22	3	19	75641.730	0.025	0.10	0.2	-8.187
21	4	18	22	4	19	75514.240	0.206	0.10	1.6	-6.955
21	4	17	22	4	18	75517.280	-0.203	0.10	-1.6	-6.962
21	5	17	22	5	18	75485.280	-0.030	0.10	-0.2	-5.575
21	5	16	22	5	17	75485.280	-0.089	0.10	-0.7	-5.575
21	6	16	22	6	17	75470.370	-0.047	0.10	-0.4	-3.912
21	6	15	22	6	16	75470.370	-0.048	0.10	-0.4	-3.912
21	7	15	22	7	16	75462.500	-0.083	0.15	-0.4	-1.959
21	7	14	22	7	15	75462.500	-0.083	0.15	-0.4	-1.959
22	3	20	23	3	21	78977.190	0.027	0.10	0.2	-9.289
22	3	19	23	3	20	79105.300	0.163	0.10	1.3	-9.526
22	4	19	23	4	20	78953.070	-0.224	0.10	-1.8	-8.189
22	4	18	23	4	19	78958.230	0.225	0.10	1.8	-8.200
22	5	18	23	5	19	78920.630	-0.041	0.10	-0.3	-6.740
22	5	17	23	5	18	78920.730	-0.030	0.10	-0.2	-6.740
22	6	17	23	6	18	78903.520	0.023	0.10	0.2	-4.998
22	6	16	23	6	17	78903.520	0.022	0.10	0.2	-4.998
22	7	16	23	7	17	78894.430	0.074	0.15	0.4	-2.953
22	7	15	23	7	16	78894.430	0.074	0.15	0.4	-2.953
22	8	15	23	8	16	78889.270	-0.271	0.20	-1.1	-0.603
22	8	14	23	8	15	78889.270	-0.271	0.20	-1.1	-0.603
23	2	21	24	2	22	83345.630	-0.046	0.20	-0.2	-12.670
23	3	21	24	3	22	82415.470	0.033	0.10	0.3	-10.687
23	3	20	24	3	21	82573.020	0.169	0.20	0.7	-11.004
23	4	20	24	4	21	82393.400	0.036	0.10	0.3	-9.548
23	4	19	24	4	20	82399.750	0.040	0.10	0.3	-9.564
23	5	19	24	5	20	82356.580	-0.011	0.10	-0.1	-8.028
23	5	18	24	5	19	82356.680	-0.042	0.10	-0.3	-8.028
23	6	18	24	6	19	82336.990	0.065	0.10	0.5	-6.205
23	6	17	24	6	18	82336.990	0.063	0.10	0.5	-6.205
23	7	17	24	7	18	82326.120	-0.229	0.15	-1.2	-4.069

23	7	16	24	7	17	82326.120	-0.229	0.15	-1.2	-4.069
23	8	16	24	8	17	82320.650	-0.011	0.20	-0.0	-1.614
23	8	15	24	8	16	82320.650	-0.011	0.20	-0.0	-1.614
24	2	23	25	2	24	85408.960	0.136	0.20	0.5	-12.397
24	2	22	25	2	23	86868.560	-0.123	0.20	-0.5	-14.412
24	4	21	25	4	22	85834.360	0.109	0.15	0.6	-11.036
24	4	20	25	4	21	85842.880	0.187	0.10	1.5	-11.060
24	5	20	25	5	21	85793.120	0.026	0.10	0.2	-9.444
24	5	19	25	5	20	85793.120	-0.163	0.10	-1.3	-9.445
24	6	19	25	6	20	85770.810	0.094	0.10	0.7	-7.539
24	6	18	25	6	19	85770.810	0.092	0.10	0.7	-7.539
24	7	18	25	7	19	85758.550	-0.023	0.10	-0.2	-5.311
24	7	17	25	7	18	85758.550	-0.023	0.10	-0.2	-5.311
24	8	17	25	8	18	85751.840	-0.087	0.15	-0.5	-2.751
24	8	16	25	8	17	85751.840	-0.087	0.15	-0.5	-2.751
24	14	11	25	14	12	85754.600	0.176	0.10	1.5	19.673
24	14	10	25	14	11	85754.600	0.176	0.10	1.5	19.673
25	2	23	26	2	24	90391.010	0.052	0.20	0.2	-16.296
25	3	23	26	3	24	89290.840	-0.117	0.10	-0.9	-13.865
25	4	22	26	4	23	89275.870	-0.084	0.10	-0.7	-12.659
25	4	21	26	4	22	89287.490	0.437	0.15	2.3	-12.693
25	5	21	26	5	22	89230.320	0.117	0.15	0.6	-10.995
25	5	20	26	5	21	89230.320	-0.153	0.15	-0.8	-10.996
25	6	20	26	6	21	89204.890	0.005	0.10	0.0	-9.007
25	6	19	26	6	20	89204.890	0.001	0.10	0.0	-9.007
25	7	19	26	7	20	89191.200	0.164	0.10	1.3	-6.685
25	7	18	26	7	19	89191.200	0.164	0.10	1.3	-6.685
25	8	18	26	8	19	89183.400	0.056	0.15	0.3	-4.021
25	8	17	26	8	18	89183.400	0.056	0.15	0.3	-4.021
26	2	24	27	2	25	93911.750	0.107	0.15	0.9	-18.325
26	4	23	27	4	24	92718.620	0.153	0.10	1.2	-14.424
26	4	22	27	4	23	92732.880	-0.022	0.10	-0.2	-14.472
26	5	22	27	5	23	92667.960	0.019	0.15	0.1	-12.685
26	5	21	27	5	22	92668.360	0.040	0.15	0.2	-12.687
26	6	21	27	6	22	92639.810	0.363	0.15	1.9	-10.613
26	6	20	27	6	21	92639.810	0.357	0.15	1.9	-10.613
26	8	19	27	8	20	92615.310	0.391	0.15	2.1	-5.427
26	8	18	27	8	19	92615.310	0.391	0.15	2.1	-5.427
27	4	23	28	4	24	96180.320	-0.041	0.10	-0.3	-16.401
27	5	23	28	5	24	96106.270	-0.059	0.15	-0.3	-14.521
27	5	22	28	5	23	96106.770	-0.086	0.15	-0.5	-14.524
27	6	22	28	6	23	96074.470	0.051	0.10	0.4	-12.363
27	6	21	28	6	22	96074.470	0.042	0.10	0.3	-12.363
27	7	21	28	7	22	96056.670	-0.050	0.10	-0.4	-9.852
27	7	20	28	7	21	96056.670	-0.050	0.10	-0.4	-9.852
27	8	20	28	8	21	96046.700	0.044	0.10	0.3	-6.976
27	8	19	28	8	20	96046.700	0.044	0.10	0.3	-6.976
28	4	25	29	4	26	99605.870	0.012	0.15	0.1	-18.399
28	5	24	29	5	25	99545.600	0.212	0.15	1.1	-16.509
28	5	23	29	5	24	99546.300	0.188	0.15	1.0	-16.512
28	6	23	29	6	24	99509.750	-0.064	0.10	-0.5	-14.263
28	6	22	29	6	23	99509.750	-0.077	0.10	-0.6	-14.263
28	7	22	29	7	23	99490.220	0.260	0.10	2.1	-11.656
28	7	21	29	7	22	99490.220	0.260	0.10	2.1	-11.656
28	8	21	29	8	22	99478.230	-0.333	0.15	-1.8	-8.673
28	8	20	29	8	21	99478.230	-0.333	0.15	-1.8	-8.673
28	16	13	29	16	14	99481.660	-0.155	0.20	-0.6	29.185
28	16	12	29	16	13	99481.660	-0.155	0.20	-0.6	29.185
29	3	26	30	3	27	103486.310	0.208	0.15	1.2	-23.246
29	4	26	30	4	27	103050.710	0.025	0.10	0.2	-20.621
29	4	25	30	4	26	103080.640	-0.012	0.10	-0.1	-20.742
29	5	25	30	5	26	102985.290	0.149	0.15	0.8	-18.653
29	5	24	30	5	25	102986.290	0.167	0.15	0.9	-18.658
29	6	24	30	6	25	102945.720	0.071	0.10	0.6	-16.318
29	6	23	30	6	24	102945.720	0.051	0.10	0.4	-16.318
29	7	23	30	7	24	102923.440	-0.038	0.10	-0.3	-13.613
29	7	22	30	7	23	102923.440	-0.038	0.10	-0.3	-13.613
29	8	22	30	8	23	102910.590	-0.056	0.10	-0.4	-10.523
29	8	21	30	8	22	102910.590	-0.056	0.10	-0.4	-10.523
29	9	21	30	9	22	102903.090	-0.223	0.10	-1.8	-7.037

29	9	20	30	9	21	102903.090	-0.223	0.10	-1.8	-7.037
30	3	27	31	3	28	106991.780	0.129	0.15	0.8	-25.930
30	4	27	31	4	28	106496.270	0.051	0.10	0.4	-23.006
30	4	26	31	4	27	106533.740	-0.048	0.10	-0.4	-23.168
30	5	26	31	5	27	106425.600	-0.004	0.15	-0.0	-20.961
30	5	25	31	5	26	106427.000	0.076	0.15	0.4	-20.968
30	6	25	31	6	26	106382.030	0.090	0.10	0.7	-18.534
30	6	24	31	6	25	106382.030	0.062	0.10	0.5	-18.534
30	7	24	31	7	25	106357.090	-0.194	0.10	-1.6	-15.731
30	7	23	31	7	24	106357.090	-0.194	0.10	-1.6	-15.731
30	8	23	31	8	24	106342.700	-0.209	0.15	-1.1	-12.532
30	8	22	31	8	23	106342.700	-0.209	0.15	-1.1	-12.532
30	9	22	31	9	23	106334.280	-0.296	0.15	-1.6	-8.926
30	9	21	31	9	22	106334.280	-0.296	0.15	-1.6	-8.926
30	11	20	31	11	21	106328.320	0.033	0.15	0.2	-0.476
30	11	19	31	11	20	106328.320	0.033	0.15	0.2	-0.476
30	12	19	31	12	20	106328.420	0.022	0.15	0.1	4.374
30	12	18	31	12	19	106328.420	0.022	0.15	0.1	4.374
31	3	28	32	3	29	110503.000	-0.196	0.10	-3.2	-28.819
31	4	28	32	4	29	109942.220	-0.191	0.15	-1.0	-25.560
31	4	27	32	4	28	109989.130	-0.014	0.10	-0.1	-25.775
31	5	26	32	5	27	109868.680	0.126	0.15	0.7	-23.447
31	6	26	32	6	27	109818.800	0.099	0.10	0.8	-20.916
31	6	25	32	6	26	109818.800	0.060	0.10	0.5	-20.917
31	7	25	32	7	26	109791.200	-0.187	0.10	-1.5	-18.014
31	7	24	32	7	25	109791.200	-0.188	0.10	-1.5	-18.014
31	8	24	32	8	25	109775.270	-0.090	0.10	-0.7	-14.705
31	8	23	32	8	24	109775.270	-0.090	0.10	-0.7	-14.705
31	9	23	32	9	24	109765.890	-0.062	0.15	-0.3	-10.979
31	9	22	32	9	23	109765.890	-0.062	0.15	-0.3	-10.979
31	10	22	32	10	23	109760.970	0.204	0.20	0.8	-6.829
31	10	21	32	10	22	109760.970	0.204	0.20	0.8	-6.829
31	11	21	32	11	22	109758.770	0.303	0.20	1.2	-2.251
31	11	20	32	11	21	109758.770	0.303	0.20	1.2	-2.251
31	12	20	32	12	21	109758.570	0.309	0.20	1.2	2.757
31	12	19	32	12	20	109758.570	0.309	0.20	1.2	2.757
31	13	19	32	13	20	109759.770	0.117	0.20	0.5	8.196
31	13	18	32	13	19	109759.770	0.117	0.20	0.5	8.196
31	16	16	32	16	17	109770.650	-0.017	0.10	-0.2	27.108
31	16	15	32	16	16	109770.650	-0.017	0.10	-0.2	27.108

rms deviation: 1.2708

Rotational constants (MHz) and kappa:

	18710.7	1777.9569	1650.9341	-0.985109
+-	4.7	0.0074	0.0077	0.000003

Inertial constants and defect (uA**2):

	27.0101	284.24709	306.11705	-5.1402
+-	0.0068	0.0012	0.0014	0.0088

Quartic distortion constants:

	0.216872	-3.3927	0	0.02414	0
+-	0.00054	0.0052	fixed	0.0029	fixed

Significant Digits and Correlation Matrix:

6	0.732	-0.667	0.133	0.043	-0.430
8		-0.983	-0.144	0.082	0.239
		8	0.296	-0.095	-0.321
			6	-0.470	-0.555
				5	0.205
					4

Table S14. Microwave Spectrum of the Second Excited State of the Torsional Vibration ($2\nu_{21}$) of Conformer I of $\text{HC(O)OCH}_2\text{C}\equiv\text{N}$

Watson A-reduction

Total number of transitions: 214

Transition						obs. frequency	obs.- calc.	weight	t	distortion	corrections
										total	fixed
7	2	6	8	2	7	27519.880	0.086	0.10	0.6	-0.126	
7	2	5	8	2	6	27577.240	0.235	0.15	1.1	-0.128	
8	2	7	9	2	8	30956.770	0.060	0.20	0.2	-0.297	
8	2	6	9	2	7	31038.320	0.035	0.10	0.3	-0.300	
9	2	8	10	2	9	34392.560	0.011	0.10	0.1	-0.522	
9	2	7	10	2	8	34504.560	0.141	0.10	1.0	-0.528	
10	2	9	11	2	10	37827.450	0.260	0.10	1.9	-0.808	
10	2	8	11	2	9	37975.750	-0.074	0.10	-0.5	-0.818	
10	3	8	11	3	9	37869.840	-0.079	0.10	-0.6	-0.135	
10	3	7	11	3	8	37872.680	-0.306	0.10	-2.2	-0.136	
11	2	10	12	2	11	41260.720	0.204	0.10	1.5	-1.161	
11	2	9	12	2	10	41452.580	-0.274	0.10	-2.0	-1.176	
11	3	9	12	3	10	41315.610	0.020	0.10	0.1	-0.428	
11	3	8	12	3	9	41320.110	-0.248	0.10	-1.8	-0.429	
11	4	8	12	4	9	41307.560	0.084	0.15	0.4	0.604	
11	4	7	12	4	8	41307.560	0.040	0.15	0.2	0.604	
12	2	11	13	2	12	44692.420	0.012	0.10	0.1	-1.586	
12	2	10	13	2	11	44935.910	0.131	0.10	1.0	-1.608	
12	3	10	13	3	11	44762.290	0.406	0.15	2.0	-0.794	
12	3	9	13	3	10	44768.940	-0.089	0.10	-0.7	-0.795	
12	4	9	13	4	10	44751.850	-0.039	0.10	-0.3	0.324	
12	4	8	13	4	9	44751.850	-0.118	0.10	-0.9	0.324	
13	2	11	14	2	12	48424.610	-0.159	0.10	-1.2	-2.122	
13	3	11	14	3	12	48208.940	0.146	0.10	1.1	-1.239	
13	3	10	14	3	11	48219.300	0.124	0.10	0.9	-1.241	
13	4	10	14	4	11	48196.850	0.043	0.10	0.3	-0.035	
13	4	9	14	4	10	48196.950	0.008	0.10	0.1	-0.035	
14	2	12	15	2	13	51919.830	-0.046	0.10	-0.3	-2.723	
14	3	12	15	3	13	51656.450	0.149	0.10	1.1	-1.770	
14	3	11	15	3	12	51670.960	-0.027	0.10	-0.2	-1.773	
14	4	11	15	4	12	51642.340	0.075	0.10	0.6	-0.479	
14	4	10	15	4	11	51642.540	0.056	0.10	0.4	-0.479	
14	5	10	15	5	11	51634.360	-0.051	0.20	-0.2	1.180	
14	5	9	15	5	10	51634.360	-0.053	0.20	-0.2	1.180	
15	2	13	16	2	14	55421.080	0.054	0.10	0.4	-3.417	
15	3	13	16	3	14	55104.470	0.099	0.10	0.7	-2.392	
15	3	12	16	3	13	55124.840	0.170	0.10	1.2	-2.397	
15	4	12	16	4	13	55088.030	-0.266	0.15	-1.3	-1.015	
15	4	11	16	4	12	55088.430	-0.213	0.15	-1.0	-1.015	
15	5	11	16	5	12	55078.440	-0.116	0.20	-0.4	0.755	
15	5	10	16	5	11	55078.440	-0.119	0.20	-0.4	0.755	
16	2	15	17	2	16	58403.270	-0.050	0.15	-0.2	-4.134	
16	2	14	17	2	15	58928.180	0.176	0.10	1.3	-4.211	
16	3	14	17	3	15	58552.860	-0.099	0.10	-0.7	-3.112	
16	4	13	17	4	14	58535.170	0.237	0.20	0.9	-1.649	
16	4	12	17	4	13	58535.670	0.202	0.20	0.7	-1.649	
16	5	12	17	5	13	58523.040	-0.019	0.20	-0.1	0.232	
16	5	11	17	5	12	58523.040	-0.025	0.20	-0.1	0.232	
17	2	15	18	2	16	62440.300	-0.153	0.10	-1.2	-5.112	
17	3	15	18	3	16	62002.280	0.274	0.10	2.0	-3.936	
17	3	14	18	3	15	62038.600	0.032	0.10	0.2	-3.947	
17	4	14	18	4	15	61982.000	-0.207	0.20	-0.7	-2.387	
17	4	13	18	4	14	61982.800	-0.208	0.20	-0.8	-2.387	
17	5	13	18	5	14	61967.660	-0.283	0.15	-1.4	-0.394	
17	5	12	18	5	13	61967.660	-0.292	0.15	-1.4	-0.394	
18	2	17	19	2	18	65247.420	0.223	0.10	1.7	-5.998	
18	2	16	19	2	17	65957.930	0.048	0.10	0.4	-6.124	
18	3	16	19	3	17	65451.560	0.122	0.10	0.9	-4.869	

18	3	15	19	3	16	65499.340	0.058	0.10	0.4	-4.886
18	4	15	19	4	16	65430.370	0.224	0.20	0.8	-3.234
18	4	14	19	4	15	65431.570	0.249	0.20	0.9	-3.235
18	5	14	19	5	15	65413.360	0.129	0.20	0.5	-1.130
18	5	13	19	5	14	65413.360	0.114	0.20	0.4	-1.130
19	3	17	20	3	18	68901.360	0.189	0.10	1.4	-5.918
19	3	16	20	3	17	68962.970	0.102	0.10	0.8	-5.943
19	4	16	20	4	17	68878.860	0.084	0.20	0.3	-4.198
19	4	15	20	4	16	68880.560	0.098	0.20	0.4	-4.199
19	5	15	20	5	16	68858.570	-0.374	0.20	-1.4	-1.983
19	5	14	20	5	15	68858.570	-0.397	0.20	-1.4	-1.983
19	6	14	20	6	15	68849.590	-0.121	0.20	-0.4	0.722
19	6	13	20	6	14	68849.590	-0.122	0.20	-0.4	0.722
20	2	19	21	2	20	72082.030	-0.167	0.15	-0.8	-8.320
20	2	18	21	2	19	73005.080	-0.015	0.10	-0.1	-8.508
20	3	17	21	3	18	72429.310	-0.306	0.15	-1.5	-7.123
20	4	17	21	4	18	72327.880	-0.239	0.10	-1.7	-5.284
20	4	16	21	4	17	72330.720	0.223	0.10	1.6	-5.286
20	5	16	21	5	17	72305.090	-0.015	0.10	-0.1	-2.957
20	5	15	21	5	16	72305.090	-0.052	0.10	-0.4	-2.957
20	6	15	21	6	16	72294.160	0.034	0.20	0.1	-0.116
20	6	14	21	6	15	72294.160	0.033	0.20	0.1	-0.116
21	2	20	22	2	21	75496.470	0.357	0.15	1.8	-9.667
21	2	19	22	2	20	76533.280	-0.066	0.10	-0.6	-9.892
21	3	19	22	3	20	75801.090	-0.042	0.10	-0.3	-8.388
21	3	18	22	3	19	75899.850	0.022	0.10	0.2	-8.435
21	4	18	22	4	19	75778.070	-0.124	0.15	-0.6	-6.499
21	4	17	22	4	18	75781.560	0.068	0.15	0.3	-6.501
21	5	17	22	5	18	75751.770	0.034	0.10	0.2	-4.060
21	5	16	22	5	17	75751.770	-0.022	0.10	-0.2	-4.060
21	6	16	22	6	17	75738.410	-0.414	0.20	-1.5	-1.083
21	6	15	22	6	16	75738.410	-0.415	0.20	-1.5	-1.083
21	11	11	22	11	12	75737.120	-0.123	0.15	-0.6	21.891
21	11	10	22	11	11	75737.120	-0.123	0.15	-0.6	21.891
21	12	10	22	12	11	75741.730	-0.103	0.20	-0.4	28.106
21	12	9	22	12	10	75741.730	-0.103	0.20	-0.4	28.106
22	2	20	23	2	21	80063.430	-0.128	0.10	-1.3	-11.410
22	3	20	23	3	21	79251.120	-0.009	0.10	-0.1	-9.821
22	3	19	23	3	20	79374.130	0.313	0.20	1.1	-9.884
22	4	19	23	4	20	79228.880	-0.136	0.10	-1.0	-7.848
22	4	18	23	4	19	79233.370	-0.151	0.10	-1.1	-7.851
22	5	18	23	5	19	79198.750	-0.109	0.10	-0.8	-5.297
22	5	17	23	5	18	79198.850	-0.094	0.10	-0.7	-5.297
22	6	17	23	6	18	79183.750	-0.069	0.20	-0.2	-2.184
22	6	16	23	6	17	79183.750	-0.070	0.20	-0.3	-2.184
22	12	11	23	12	12	79184.250	-0.168	0.20	-0.6	28.333
22	12	10	23	12	11	79184.250	-0.168	0.20	-0.6	28.333
23	3	21	24	3	22	82701.020	0.054	0.10	0.4	-11.394
23	3	20	24	3	21	82852.200	0.301	0.20	1.1	-11.478
23	4	20	24	4	21	82680.680	0.085	0.10	0.6	-9.338
23	4	19	24	4	20	82686.880	0.214	0.20	0.8	-9.343
23	5	19	24	5	20	82646.460	-0.037	0.10	-0.3	-6.675
23	5	18	24	5	19	82646.560	-0.062	0.10	-0.4	-6.675
23	6	18	24	6	19	82629.000	-0.123	0.10	-0.9	-3.426
23	6	17	24	6	18	82629.000	-0.125	0.10	-0.9	-3.426
23	7	17	24	7	18	82620.590	-0.170	0.15	-0.8	0.410
23	7	16	24	7	17	82620.590	-0.170	0.15	-0.8	0.410
23	8	16	24	8	17	82617.080	-0.290	0.15	-1.4	4.834
23	8	15	24	8	16	82617.080	-0.290	0.15	-1.4	4.834
23	9	15	24	9	16	82616.780	-0.290	0.15	-1.4	9.847
23	9	14	24	9	15	82616.780	-0.290	0.15	-1.4	9.847
23	12	12	24	12	13	82627.120	0.148	0.15	0.7	28.420
23	12	11	24	12	12	82627.120	0.148	0.15	0.7	28.420
23	13	11	24	13	12	82632.880	0.177	0.10	1.3	35.790
23	13	10	24	13	11	82632.880	0.177	0.10	1.3	35.790
24	2	22	25	2	23	87126.470	0.169	0.15	1.1	-14.871
24	3	22	25	3	23	86150.770	0.269	0.10	2.0	-13.112
24	3	21	25	3	22	86334.480	0.092	0.10	0.7	-13.223
24	4	21	25	4	22	86133.290	0.354	0.15	1.7	-10.975
24	4	20	25	4	21	86141.130	0.117	0.20	0.4	-10.982

24	5	20	25	5	21	86094.810	0.139	0.10	1.0	-8.199
24	5	19	25	5	20	86095.010	0.159	0.10	1.2	-8.200
24	6	19	25	6	20	86074.610	-0.142	0.20	-0.5	-4.814
24	6	18	25	6	19	86074.610	-0.144	0.20	-0.5	-4.814
24	7	18	25	7	19	86064.840	-0.117	0.15	-0.6	-0.817
24	7	17	25	7	18	86064.840	-0.117	0.15	-0.6	-0.817
24	11	14	25	11	15	86064.840	0.023	0.15	0.1	21.298
24	11	13	25	11	14	86064.840	0.023	0.15	0.1	21.298
24	12	13	25	12	14	86069.710	0.215	0.10	1.6	28.361
24	12	12	25	12	13	86069.710	0.215	0.10	1.6	28.361
24	13	12	25	13	13	86075.210	-0.110	0.20	-0.4	36.038
24	13	11	25	13	12	86075.210	-0.110	0.20	-0.4	36.038
25	3	23	26	3	24	89599.740	0.153	0.10	1.1	-14.982
25	3	22	26	3	23	89821.620	0.027	0.10	0.2	-15.125
25	4	22	26	4	23	89586.220	0.182	0.10	1.3	-12.766
25	4	21	26	4	22	89596.690	0.031	0.10	0.2	-12.776
25	5	21	26	5	22	89543.330	-0.071	0.20	-0.3	-9.877
25	5	20	26	5	21	89543.530	-0.129	0.20	-0.5	-9.877
25	6	20	26	6	21	89520.680	-0.038	0.10	-0.3	-6.354
25	6	19	26	6	20	89520.680	-0.042	0.10	-0.3	-6.354
25	12	14	26	12	15	89511.950	-0.035	0.15	-0.2	28.150
25	12	13	26	12	14	89511.950	-0.035	0.15	-0.2	28.150
26	3	24	27	3	25	93048.060	-0.006	0.10	-0.0	-17.010
26	4	22	27	4	23	93053.670	-0.040	0.10	-0.3	-14.729
26	5	22	27	5	23	92992.540	-0.170	0.20	-0.6	-11.714
26	5	21	27	5	22	92992.940	-0.133	0.20	-0.5	-11.714
27	3	24	28	3	25	96811.160	-0.110	0.10	-1.1	-19.432
27	4	23	28	4	24	96512.090	-0.193	0.10	-1.4	-16.850
27	5	23	28	5	24	96442.750	0.132	0.20	0.5	-13.716
27	5	22	28	5	23	96443.250	0.128	0.20	0.5	-13.717
27	6	22	28	6	23	96413.440	-0.280	0.20	-1.0	-9.919
27	6	21	28	6	22	96413.440	-0.288	0.20	-1.0	-9.919
27	8	20	28	8	21	96391.430	-0.121	0.20	-0.4	-0.276
27	8	19	28	8	20	96391.430	-0.121	0.20	-0.4	-0.276
27	13	15	28	13	16	96403.220	0.362	0.15	1.8	35.844
27	13	14	28	13	15	96403.220	0.362	0.15	1.8	35.844
28	3	25	29	3	26	100314.470	0.249	0.15	1.4	-21.849
28	4	25	29	4	26	99949.690	-0.118	0.10	-0.9	-19.117
28	4	24	29	4	25	99972.190	-0.314	0.20	-1.1	-19.144
28	5	24	29	5	25	99893.200	0.056	0.15	0.3	-15.890
28	5	23	29	5	24	99893.900	0.064	0.15	0.3	-15.891
28	6	23	29	6	24	99860.650	-0.133	0.10	-1.0	-11.955
28	6	22	29	6	23	99860.650	-0.146	0.10	-1.1	-11.955
28	7	22	29	7	23	99843.630	-0.238	0.10	-1.8	-7.314
28	7	21	29	7	22	99843.630	-0.238	0.10	-1.8	-7.314
28	12	17	29	12	18	99839.310	0.065	0.15	0.3	26.541
28	12	16	29	12	17	99839.310	0.065	0.15	0.3	26.541
28	17	12	29	17	13	99880.860	-0.255	0.10	-2.2	78.191
28	17	11	29	17	12	99880.860	-0.255	0.10	-2.2	78.191
29	4	25	30	4	26	103434.670	0.158	0.10	1.2	-21.617
29	5	25	30	5	26	103344.640	0.332	0.20	1.2	-18.241
29	5	24	30	5	25	103345.540	0.293	0.20	1.1	-18.243
29	6	24	30	6	25	103307.920	-0.319	0.15	-1.6	-14.168
29	6	23	30	6	24	103307.920	-0.338	0.15	-1.6	-14.168
29	7	23	30	7	24	103289.580	0.411	0.20	1.5	-9.366
29	7	22	30	7	23	103289.580	0.410	0.20	1.5	-9.366
29	8	22	30	8	23	103279.230	-0.193	0.15	-0.9	-3.831
29	8	21	30	8	22	103279.230	-0.193	0.15	-0.9	-3.831
30	4	27	31	4	28	106862.490	0.014	0.15	0.1	-24.230
30	4	26	31	4	27	106898.730	0.269	0.10	2.1	-24.277
30	5	26	31	5	27	106795.830	-0.298	0.20	-1.1	-20.777
30	5	25	31	5	26	106797.130	-0.259	0.20	-0.9	-20.779
30	6	25	31	6	26	106755.940	-0.164	0.15	-0.8	-16.565
30	6	25	31	6	26	106755.940	-0.164	0.15	-0.8	-16.565
30	6	24	31	6	25	106755.940	-0.190	0.15	-0.9	-16.565
30	6	24	31	6	25	106755.940	-0.190	0.15	-0.9	-16.565
30	7	24	31	7	25	106735.080	0.363	0.15	1.8	-11.601
30	7	23	31	7	24	106735.080	0.363	0.15	1.8	-11.601
30	8	23	31	8	24	106723.350	-0.222	0.15	-1.1	-5.881
30	8	22	31	8	23	106723.350	-0.222	0.15	-1.1	-5.881

30	12	19	31	12	20	106723.750	-0.147	0.15	-0.7	24.594
30	12	18	31	12	19	106723.750	-0.147	0.15	-0.7	24.594
30	17	14	31	17	15	106767.180	0.016	0.10	0.1	79.808
30	17	13	31	17	14	106767.180	0.016	0.10	0.1	79.808
31	4	28	32	4	29	110320.040	0.296	0.10	2.3	-27.067
31	5	26	32	5	27	110250.230	-0.068	0.10	-0.5	-23.505
31	6	26	32	6	27	110204.260	-0.130	0.10	-1.0	-19.152
31	6	25	32	6	26	110204.260	-0.168	0.10	-1.3	-19.152
31	7	25	32	7	26	110180.720	0.201	0.20	0.7	-14.026
31	7	24	32	7	25	110180.720	0.201	0.20	0.7	-14.026
31	9	23	32	9	24	110162.230	0.277	0.20	1.0	-1.431
31	9	22	32	9	23	110162.230	0.277	0.20	1.0	-1.431
31	10	22	32	10	23	110160.730	0.264	0.20	1.0	6.042
31	10	21	32	10	22	110160.730	0.264	0.20	1.0	6.042
31	13	19	32	13	20	110172.390	0.284	0.10	2.2	33.169
31	13	18	32	13	19	110172.390	0.284	0.10	2.2	33.169

rms deviation: 1.3884

Rotational constants (MHz) and kappa:

	18114.4	1781.6220	1659.4118	-0.985146
+-	7.8	0.013	0.013	0.000004

Inertial constants and defect (uA**2):

	27.8993	283.66235	304.55315	-7.008
+-	0.012	0.0021	0.0024	0.017

Quartic distortion constants:

	0.25357	-6.1409	0	0	0
+-	0.00056	0.0042	fixed	fixed	fixed

Significant Digits and Correlation Matrix:

6	0.983	-0.975	-0.130	0.138
8		-0.993	-0.079	0.073
8			0.179	-0.067
5				-0.354
5				

Table S15. Microwave Spectrum of the Third Excited State of the Torsional Vibration ($3\nu_{21}$) of Conformer I of $\text{HC(O)OCH}_2\text{C}\equiv\text{N}$

Watson A-reduction

Total number of transitions: 70

Transition						obs. frequency	obs.- calc.	weight	t	distortion	corrections
										total	fixed
7	2	6	8	2	7	27646.960	-0.127	0.10	-0.7	0.061	
7	2	5	8	2	6	27700.960	-0.257	0.10	-1.5	0.057	
8	2	7	9	2	8	31100.230	0.197	0.15	0.8	-0.125	
8	2	6	9	2	7	31177.270	0.055	0.10	0.3	-0.131	
9	2	8	10	2	9	34552.310	0.367	0.15	1.4	-0.379	
10	2	8	11	2	9	38143.320	-0.015	0.10	-0.1	-0.726	
10	3	8	11	3	9	38043.900	0.188	0.10	1.1	0.505	
10	3	7	11	3	8	38046.930	0.327	0.15	1.3	0.504	
11	2	10	12	2	11	41452.580	0.385	0.20	1.1	-1.121	
11	2	9	12	2	10	41634.100	-0.085	0.10	-0.5	-1.148	
11	3	9	12	3	10	41505.110	0.170	0.10	1.0	0.201	
11	3	8	12	3	9	41509.560	0.126	0.10	0.8	0.199	
12	2	10	13	2	11	45130.530	-0.064	0.10	-0.4	-1.664	
12	3	10	13	3	11	44966.430	-0.307	0.15	-1.2	-0.195	
12	3	9	13	3	10	44973.260	-0.212	0.10	-1.3	-0.197	
13	3	11	14	3	12	48429.140	0.045	0.10	0.3	-0.690	
13	3	10	14	3	11	48438.640	-0.239	0.10	-1.4	-0.694	
14	2	13	15	2	14	51791.850	-0.110	0.10	-0.7	-2.931	
14	3	12	15	3	13	51891.620	-0.372	0.15	-1.4	-1.292	
14	3	11	15	3	12	51905.660	-0.174	0.20	-0.5	-1.298	
15	3	13	16	3	14	55355.320	-0.077	0.10	-0.5	-2.009	
16	3	14	17	3	15	58819.520	0.255	0.10	1.5	-2.847	
16	3	13	17	3	14	58845.540	0.366	0.15	1.4	-2.861	
17	2	16	18	2	17	62116.120	-0.204	0.10	-1.4	-5.756	
17	2	15	18	2	16	62697.960	0.357	0.15	1.5	-5.935	
17	3	15	18	3	16	62283.870	0.333	0.15	1.3	-3.815	
17	3	14	18	3	15	62317.840	-0.156	0.10	-0.9	-3.836	
18	3	16	19	3	17	65748.030	-0.115	0.10	-0.7	-4.920	
18	3	15	19	3	16	65793.540	0.304	0.15	1.2	-4.950	
19	3	16	20	3	17	69271.400	0.248	0.10	1.5	-6.213	
20	2	18	21	2	19	73296.350	0.159	0.10	1.3	-10.130	
20	3	17	21	3	18	72752.020	0.005	0.10	0.0	-7.633	
20	4	17	21	4	18	72657.470	-0.237	0.10	-1.4	-4.317	
20	4	16	21	4	17	72659.640	-0.299	0.15	-1.2	-4.319	
21	3	19	22	3	20	76143.020	-0.073	0.10	-0.4	-9.134	
21	3	18	22	3	19	76235.730	-0.380	0.15	-1.5	-9.217	
21	4	18	22	4	19	76123.050	0.181	0.15	0.7	-5.727	
21	4	17	22	4	18	76126.270	0.305	0.20	0.9	-5.731	
22	2	20	23	2	21	80376.200	-0.232	0.15	-1.1	-13.726	
22	3	20	23	3	21	79608.370	0.270	0.10	1.7	-10.863	
22	4	19	23	4	20	79588.480	-0.218	0.10	-1.3	-7.305	
22	4	18	23	4	19	79593.270	0.343	0.20	1.0	-7.311	
23	2	21	24	2	22	83918.840	0.353	0.15	1.7	-15.784	
24	3	22	25	3	23	86537.840	0.426	0.15	1.7	-14.852	
24	3	21	25	3	22	86710.550	-0.177	0.10	-1.2	-15.049	
24	4	21	25	4	22	86522.410	0.029	0.10	0.2	-10.998	
24	4	20	25	4	21	86530.050	0.088	0.20	0.3	-11.011	
25	2	24	26	2	25	89551.400	-0.096	0.10	9.9	-19.737	
25	3	22	26	3	23	90210.440	-0.249	0.15	-1.0	-17.381	
25	4	21	26	4	22	90000.470	0.266	0.10	1.6	-13.146	
26	2	24	27	2	25	94542.170	-0.195	0.10	9.9	-23.067	
26	4	23	27	4	24	93459.070	0.312	0.15	1.2	-15.458	
26	4	22	27	4	23	93471.450	-0.274	0.10	-1.7	-15.483	
27	4	23	28	4	24	96944.970	0.342	0.20	1.0	-18.030	
27	5	23	28	5	24	96881.270	-0.201	0.20	-0.6	-12.379	
27	5	22	28	5	23	96881.770	-0.172	0.20	-0.5	-12.380	
28	3	25	29	3	26	100739.840	0.266	0.15	1.3	-25.670	
28	4	25	29	4	26	100397.630	-0.107	0.15	-0.4	-20.747	

28	4	24	29	4	25	100419.270	0.236	0.15	0.9	-20.794
28	5	24	29	5	25	100346.820	-0.007	0.15	-0.0	-14.927
28	5	23	29	5	24	100347.420	-0.053	0.15	-0.2	-14.929
29	4	26	30	4	27	103868.340	0.197	0.20	0.6	-23.722
29	4	25	30	4	26	103894.920	-0.151	0.10	-1.0	-23.785
30	3	27	31	3	28	107784.770	-0.129	0.10	9.9	-32.360
30	4	27	31	4	28	107339.300	0.185	0.10	1.4	-26.926
30	4	26	31	4	27	107372.920	0.040	0.10	0.3	-27.011
30	6	25	31	6	26	107244.920	-0.019	0.10	-0.2	-13.105
30	6	24	31	6	25	107244.920	-0.044	0.10	-0.5	-13.105
31	7	25	32	7	26	110689.990	0.056	0.20	0.2	-6.851
31	7	24	32	7	25	110689.990	0.056	0.20	0.2	-6.851

rms deviation: 1.7623

Rotational constants (MHz) and kappa:

	17354.5	1786.4613	1670.4045	-0.985201
+-	7.9	0.013	0.013	0.000005

Inertial constants and defect (uA**2):

	29.1210	282.89394	302.54891	-9.466
+-	0.013	0.0020	0.0024	0.017

Quartic distortion constants:

	0.31657	-11.074	0	0	0
+-	0.0015	0.083	fixed	fixed	fixed

Significant Digits and Correlation Matrix:

6	0.944	-0.927	-0.175	0.068
8		-0.971	0.042	-0.091
8			0.094	0.116
5				-0.672
5				

Table S16. Microwave Spectrum of the First Excited State of the Lowest Bending Vibration (ν_{20}) of Conformer I of $\text{HC(O)OCH}_2\text{C}\equiv\text{N}$

Watson A-reduction

Total number of transitions: 158

Transition						obs. frequency		obs.- weight		t	distortion	corrections
								calc.			total	fixed
7	1	7	8	1	8	26831.960	0.173	0.15		1.2	-0.377	
8	1	8	9	1	9	30181.390	0.234	0.20		1.0	-0.550	
8	2	7	9	2	8	30788.490	0.251	0.10		1.7	-0.393	
8	2	6	9	2	7	30876.430	0.100	0.10		0.7	-0.395	
9	1	9	10	1	10	33529.040	0.070	0.20		0.3	-0.769	
10	2	8	11	2	9	37781.440	0.216	0.10		1.4	-0.849	
10	3	7	11	3	8	37669.450	-0.273	0.10		-1.8	-0.525	
11	3	9	12	3	10	41093.670	-0.261	0.10		-1.8	-0.801	
11	3	8	12	3	9	41099.230	0.198	0.10		1.3	-0.802	
11	4	8	12	4	9	41084.410	-0.112	0.10		-0.8	-0.311	
11	4	7	12	4	8	41084.410	-0.159	0.10		-1.1	-0.311	
12	2	11	13	2	12	44447.320	-0.223	0.10		-1.5	-1.513	
12	2	10	13	2	11	44710.750	0.308	0.15		1.4	-1.524	
12	3	10	13	3	11	44521.800	-0.316	0.15		-1.4	-1.137	
12	3	9	13	3	10	44529.700	-0.060	0.10		-0.4	-1.138	
12	4	9	13	4	10	44510.530	-0.083	0.10		-0.6	-0.607	
12	4	8	13	4	9	44510.630	-0.067	0.10		-0.5	-0.607	
13	2	12	14	2	13	47858.730	0.182	0.10		1.2	-1.942	
13	3	11	14	3	12	47950.980	-0.011	0.20		-0.0	-1.538	
13	4	10	14	4	11	47937.400	0.130	0.15		0.6	-0.966	
13	4	9	14	4	10	47937.500	0.088	0.15		0.4	-0.966	
13	5	9	14	5	10	47929.440	-0.192	0.10		-1.3	-0.231	
13	5	8	14	5	9	47929.440	-0.193	0.10		-1.3	-0.231	
14	2	12	15	2	13	51666.120	0.210	0.10		1.5	-2.460	
14	3	12	15	3	13	51380.660	0.122	0.10		0.8	-2.008	
14	4	11	15	4	12	51364.550	0.018	0.10		0.1	-1.396	
14	4	10	15	4	11	51364.750	-0.015	0.10		-0.1	-1.396	
14	5	10	15	5	11	51354.780	-0.266	0.15		-1.2	-0.608	
14	5	9	15	5	10	51354.780	-0.268	0.15		-1.2	-0.608	
15	2	13	16	2	14	55153.520	-0.047	0.20		-0.2	-3.039	
15	3	13	16	3	14	54811.020	0.296	0.15		1.3	-2.553	
15	3	12	16	3	13	54832.600	0.160	0.10		1.1	-2.556	
15	5	11	16	5	12	54781.020	0.172	0.30		0.4	-1.060	
15	5	10	16	5	11	54781.020	0.169	0.30		0.4	-1.060	
15	6	10	16	6	11	54775.340	0.064	0.15		0.3	-0.033	
15	6	9	16	6	10	54775.340	0.064	0.15		0.3	-0.033	
16	2	14	17	2	15	58647.710	0.114	0.10		0.8	-3.699	
16	3	14	17	3	15	58241.560	0.059	0.10		0.4	-3.178	
16	3	13	17	3	14	58271.020	0.107	0.10		0.7	-3.181	
16	4	13	17	4	14	58220.970	-0.055	0.15		-0.2	-2.483	
16	4	12	17	4	13	58221.570	-0.022	0.15		-0.1	-2.483	
16	5	12	17	5	13	58207.180	0.118	0.10		0.8	-1.590	
16	5	11	17	5	12	58207.180	0.113	0.10		0.8	-1.590	
16	6	11	17	6	12	58199.910	-0.328	0.15		-1.5	-0.500	
16	6	10	17	6	11	58199.910	-0.328	0.10		-2.2	-0.500	
17	3	14	18	3	15	61711.650	-0.279	0.15		-1.2	-3.892	
17	5	13	18	5	14	61633.780	0.065	0.10		0.4	-2.206	
17	5	12	18	5	13	61633.780	0.056	0.10		0.4	-2.206	
17	6	12	18	6	13	61625.060	-0.414	0.20		-1.4	-1.051	
17	6	11	18	6	12	61625.060	-0.414	0.20		-1.4	-1.051	
18	2	17	19	2	18	64884.840	0.347	0.15		1.6	-5.222	
18	2	16	19	2	17	65653.000	-0.143	0.10		-1.2	-5.281	
18	3	16	19	3	17	65104.670	0.098	0.10		0.7	-4.685	
18	3	15	19	3	16	65155.810	0.043	0.10		0.3	-4.693	
18	4	15	19	4	16	65080.480	0.101	0.20		0.3	-3.909	
18	4	14	19	4	15	65081.680	0.056	0.20		0.2	-3.910	
18	5	14	19	5	15	65060.710	-0.122	0.10		-0.8	-2.911	
18	5	13	19	5	14	65060.710	-0.137	0.10		-0.9	-2.911	

18	6	13	19	6	14	65050.680	-0.321	0.15	-1.4	-1.691
18	6	12	19	6	13	65050.680	-0.321	0.10	-2.2	-1.691
19	5	15	20	5	16	68488.440	0.001	0.10	0.0	-3.710
19	5	14	20	5	15	68488.440	-0.024	0.10	-0.2	-3.710
19	6	14	20	6	15	68476.620	-0.214	0.15	-1.0	-2.427
19	6	13	20	6	14	68476.620	-0.214	0.15	-1.0	-2.427
20	2	18	21	2	19	72677.990	0.104	0.10	1.1	-7.244
20	3	18	21	3	19	71968.730	-0.360	0.20	-1.2	-6.571
20	3	17	21	3	18	72053.090	-0.025	0.20	-0.1	-6.586
20	4	17	21	4	18	71942.810	-0.031	0.10	-0.2	-5.714
20	4	16	21	4	17	71945.640	0.278	0.10	1.9	-5.715
20	5	16	21	5	17	71916.490	-0.073	0.10	-0.5	-4.609
20	5	15	21	5	16	71916.490	-0.112	0.10	-0.7	-4.609
20	6	15	21	6	16	71902.720	-0.270	0.20	-0.9	-3.261
20	6	14	21	6	15	71902.720	-0.271	0.20	-0.9	-3.261
21	2	20	22	2	21	75072.340	-0.244	0.15	-1.1	-8.275
21	3	19	22	3	20	75401.410	-0.215	0.15	-1.0	-7.668
21	3	18	22	3	19	75507.520	0.253	0.10	1.7	-7.689
21	4	18	22	4	19	75375.330	0.029	0.10	0.2	-6.771
21	5	17	22	5	18	75345.300	0.072	0.10	0.5	-5.613
21	5	16	22	5	17	75345.300	0.012	0.10	0.1	-5.613
21	6	16	22	6	17	75329.470	-0.016	0.10	-0.1	-4.200
21	6	15	22	6	16	75329.470	-0.016	0.10	-0.1	-4.200
22	4	18	23	4	19	78813.490	0.109	0.10	0.7	-7.938
22	5	18	23	5	19	78774.180	-0.281	0.20	-0.9	-6.726
22	5	17	23	5	18	78774.280	-0.270	0.20	-0.9	-6.726
22	6	17	23	6	18	78756.430	0.093	0.10	0.6	-5.249
22	6	16	23	6	17	78756.430	0.092	0.10	0.6	-5.249
23	3	21	24	3	22	82266.750	0.138	0.10	1.0	-10.194
23	3	20	24	3	21	82428.440	0.228	0.10	1.6	-10.232
23	4	20	24	4	21	82243.130	0.363	0.15	1.6	-9.218
23	4	19	24	4	20	82249.430	0.228	0.10	1.5	-9.220
23	5	19	24	5	20	82204.190	-0.096	0.10	-0.6	-7.953
23	5	18	24	5	19	82204.290	-0.127	0.10	-0.8	-7.954
23	6	18	24	6	19	82183.300	-0.260	0.10	-1.7	-6.411
23	6	17	24	6	18	82183.300	-0.262	0.10	-1.8	-6.411
23	7	17	24	7	18	82172.050	-0.160	0.20	-0.5	-4.591
23	7	16	24	7	17	82172.050	-0.160	0.20	-0.5	-4.591
24	4	21	25	4	22	85677.800	0.006	0.10	0.0	-10.618
24	4	20	25	4	21	85686.630	0.273	0.10	1.8	-10.621
24	5	20	25	5	21	85634.800	0.071	0.15	0.3	-9.301
24	5	19	25	5	20	85635.000	0.081	0.15	0.4	-9.301
24	6	19	25	6	20	85611.040	-0.132	0.10	-0.9	-7.694
24	6	18	25	6	19	85611.040	-0.135	0.10	-0.9	-7.694
24	8	17	25	8	18	85590.940	0.113	0.15	0.5	-3.609
24	8	16	25	8	17	85590.940	0.113	0.15	0.5	-3.609
25	2	24	26	2	25	88618.440	-0.249	0.20	-0.9	-13.884
25	4	22	26	4	23	89113.590	-0.098	0.10	-0.7	-12.143
25	4	21	26	4	22	89124.790	-0.160	0.10	-1.1	-12.148
25	5	21	26	5	22	89065.850	0.035	0.15	0.2	-10.772
25	5	20	26	5	21	89066.150	0.065	0.15	0.3	-10.772
25	6	20	26	6	21	89039.190	0.000	0.15	0.0	-9.100
25	6	19	26	6	20	89039.190	-0.004	0.15	-0.0	-9.100
26	3	24	27	3	25	92561.810	0.165	0.10	1.2	-14.887
26	6	21	27	6	22	92467.530	-0.099	0.10	-0.7	-10.636
26	6	20	27	6	21	92467.530	-0.104	0.10	-0.7	-10.636
26	7	20	27	7	21	92451.320	0.411	0.20	1.4	-8.587
26	7	19	27	7	20	92451.320	0.411	0.20	1.4	-8.587
26	8	19	27	8	20	92441.540	0.288	0.15	1.3	-6.224
26	8	18	27	8	19	92441.540	0.288	0.15	1.3	-6.224
27	3	25	28	3	26	95991.750	-0.266	0.20	-0.9	-16.713
27	5	23	28	5	24	95929.990	-0.020	0.15	-0.1	-14.109
27	5	22	28	5	23	95930.490	-0.049	0.15	-0.2	-14.109
27	6	22	28	6	23	95896.720	0.214	0.10	1.4	-12.307
27	6	21	28	6	22	95896.720	0.205	0.10	1.4	-12.307
27	7	21	28	7	22	95877.990	0.298	0.10	2.0	-10.181
27	7	20	28	7	21	95877.990	0.298	0.10	2.0	-10.181
27	8	20	28	8	21	95866.820	0.085	0.10	0.6	-7.730
27	8	19	28	8	20	95866.820	0.085	0.10	0.6	-7.730
28	3	26	29	3	27	99421.520	0.075	0.10	0.6	-18.677

28	4	25	29	4	26	99426.620	0.133	0.10	0.9	-17.516
28	5	24	29	5	25	99362.880	-0.287	0.20	-1.0	-15.984
28	5	23	29	5	24	99363.580	-0.313	0.20	-1.0	-15.985
29	3	26	30	3	27	103315.440	-0.255	0.10	-3.6	-20.949
29	4	26	30	4	27	102865.720	-0.005	0.10	-0.0	-19.590
29	5	25	30	5	26	102797.220	0.160	0.20	0.5	-18.004
29	5	24	30	5	25	102798.220	0.174	0.20	0.6	-18.005
29	6	24	30	6	25	102755.690	0.047	0.10	0.3	-16.071
29	6	23	30	6	24	102755.690	0.028	0.10	0.2	-16.071
29	7	23	30	7	24	102732.280	0.132	0.10	0.9	-13.792
29	7	22	30	7	23	102732.280	0.132	0.10	0.9	-13.792
29	8	22	30	8	23	102718.320	0.044	0.15	0.2	-11.165
29	8	21	30	8	22	102718.320	0.044	0.15	0.2	-11.165
30	3	28	31	3	29	106276.680	-0.067	0.15	-0.3	-23.039
30	4	27	31	4	28	106305.680	-0.046	0.10	-0.3	-21.813
30	6	25	31	6	26	106185.730	-0.206	0.15	-0.9	-18.175
30	6	24	31	6	25	106185.730	-0.234	0.15	-1.1	-18.175
30	7	24	31	7	25	106159.660	-0.182	0.30	-0.4	-15.819
30	7	23	31	7	24	106159.660	-0.182	0.30	-0.4	-15.819
30	8	23	31	8	24	106144.340	-0.007	0.10	-0.1	-13.104
30	8	22	31	8	23	106144.340	-0.007	0.10	-0.1	-13.104
31	3	28	32	3	29	110325.990	-0.339	0.15	-2.2	-25.691
31	5	27	32	5	28	109667.500	0.361	0.20	1.2	-22.498
31	5	26	32	5	27	109669.300	0.398	0.20	1.3	-22.499
31	6	26	32	6	27	109616.480	-0.256	0.10	-1.8	-20.433
31	6	25	32	6	26	109616.480	-0.295	0.10	-2.1	-20.433
31	7	25	32	7	26	109587.450	-0.411	0.20	-1.4	-18.000
31	7	24	32	7	25	109587.450	-0.412	0.20	-1.4	-18.000
31	8	24	32	8	25	109570.640	0.011	0.10	0.1	-15.197
31	8	23	32	8	24	109570.640	0.011	0.10	0.1	-15.197

rms deviation: 1.5109

Rotational constants (MHz) and kappa:

	19752.9	1777.8267	1644.6077	-0.985286
+-	7.6	0.014	0.014	0.000003

Inertial constants and defect (uÅ**2):

	25.5851	284.26791	307.29461	-2.56
+-	0.0098	0.0022	0.0026	0.01

Quartic distortion constants:

	0.20690	-2.915	0	0	0
+-	0.00074	0.023	fixed	fixed	fixed

Significant Digits and Correlation Matrix:

6	0.962	-0.950	-0.013	0.035
8		-0.991	0.109	-0.081
8			-0.032	0.117
5				-0.552
4				

Table S17. Microwave Spectrum of the Ground Vibrational State of Conformer II of HC(O)OCH₂C≡N

Watson A-reduction

Total number of transitions: 641

Transition						obs. frequency	obs.- calc.	weight	t	distortion total	corrections higher	fixed
5	1	5	6	1	6	27439.840	0.157	0.10	1.1	-2.411	4.0E-4	
5	1	4	6	1	5	29849.730	0.122	0.10	0.8	-6.273	-4.4E-3	
5	2	4	6	2	5	28732.150	0.174	0.10	1.2	-3.230	-3.3E-4	
5	2	3	6	2	4	29498.060	0.226	0.10	1.6	-5.534	-3.5E-3	
5	4	2	6	4	3	28927.170	-0.198	0.20	-0.7	1.098	-6.8E-3	
5	4	1	6	4	2	28928.170	-0.179	0.20	-0.6	1.090	-6.8E-3	
6	1	6	7	1	7	31944.810	0.359	0.15	1.7	-3.898	1.5E-4	
6	2	5	7	2	6	33458.530	0.236	0.20	0.8	-5.614	-1.3E-3	
6	2	4	7	2	5	34597.810	0.051	0.20	0.2	-9.856	-8.7E-3	
6	3	4	7	3	5	33796.550	0.378	0.15	1.7	-4.540	-2.0E-3	
6	3	3	7	3	4	33905.240	0.064	0.20	0.2	-5.234	-3.3E-3	
6	4	3	7	4	4	33769.940	0.115	0.20	0.4	-1.138	-6.0E-3	
6	4	2	7	4	3	33773.140	0.067	0.20	0.2	-1.169	-6.0E-3	
7	1	7	7	2	6	21584.210	0.060	0.15	0.3	-3.330	-2.9E-3	
7	2	6	7	3	5	26788.750	0.347	0.15	1.6	0.795	4.6E-4	
7	0	7	8	0	8	36880.840	-0.155	0.10	-1.1	-6.175	-2.4E-3	
7	1	7	8	1	8	36427.270	0.139	0.10	1.0	-5.795	-5.3E-4	
7	2	6	8	2	7	38157.020	0.026	0.10	0.2	-8.702	-3.5E-3	
7	3	5	8	3	6	38639.710	-0.107	0.10	-0.7	-8.298	-4.3E-3	
7	4	4	8	4	5	38621.140	0.129	0.30	0.3	-4.543	-6.0E-3	
7	5	3	8	5	4	38578.100	-0.157	0.10	-1.1	0.667	-0.019	
7	5	2	8	5	3	38578.300	-0.122	0.10	-0.8	0.664	-0.019	
8	1	8	8	2	7	23314.060	0.047	0.15	0.2	-6.237	-5.8E-3	
8	0	8	9	0	9	41238.720	-0.159	0.15	-0.7	-8.186	-3.5E-3	
8	1	8	9	1	9	40889.940	0.221	0.15	1.0	-8.135	-1.9E-3	
8	1	7	9	1	8	44195.120	-0.055	0.10	-0.4	-17.758	-0.024	
8	2	7	9	2	8	42825.540	0.180	0.10	1.2	-12.504	-7.2E-3	
8	2	6	9	2	7	44812.830	0.020	0.10	0.1	-22.853	-0.035	
8	3	6	9	3	7	43477.790	0.112	0.10	0.8	-13.219	-9.4E-3	
8	4	5	9	4	6	43481.250	0.249	0.10	1.7	-9.307	-8.1E-3	
8	4	4	9	4	5	43501.760	-0.239	0.10	-1.7	-9.589	-9.0E-3	
8	5	4	9	5	5	43422.150	-0.082	0.15	-0.4	-3.343	-0.018	
8	5	3	9	5	4	43422.650	-0.113	0.15	-0.5	-3.353	-0.018	
8	7	2	9	7	3	43376.000	-0.065	0.10	-0.4	11.961	-0.121	
8	7	1	9	7	2	43376.000	-0.065	0.10	-0.4	11.961	-0.121	
9	7	3	9	8	2	77868.680	-0.089	0.15	-0.4	-118.446	1.206	
9	7	2	9	8	1	77868.680	-0.089	0.15	-0.4	-118.446	1.206	
9	0	9	10	0	10	45590.980	-0.013	0.10	-0.1	-10.731	-5.2E-3	
9	1	9	10	1	10	45334.960	0.033	0.10	0.2	-10.955	-4.1E-3	
9	1	8	10	1	9	48809.690	-0.087	0.10	-0.6	-22.169	-0.035	
9	2	8	10	2	9	47461.480	0.007	0.10	0.0	-17.006	-0.013	
9	3	7	10	3	8	48304.140	0.151	0.10	1.0	-19.358	-0.019	
9	3	6	10	3	7	48915.240	-0.048	0.10	-0.3	-25.950	-0.040	
9	4	6	10	4	7	48349.200	0.108	0.10	0.7	-15.614	-0.014	
9	5	5	10	5	6	48273.760	0.084	0.15	0.4	-8.881	-0.018	
9	5	4	10	5	5	48275.160	0.009	0.15	0.0	-8.913	-0.018	
10	1	10	10	2	9	27376.460	0.259	0.10	1.8	-16.656	-0.020	
10	2	9	10	3	8	28766.100	0.040	0.10	0.3	-1.869	-8.2E-3	
10	2	8	10	3	7	21470.650	0.100	0.10	0.7	25.213	0.057	
10	3	8	10	4	7	36341.020	0.049	0.10	0.3	7.932	0.017	
10	3	7	10	4	6	35037.200	0.060	0.10	0.4	19.570	0.049	
10	7	4	10	8	3	77859.120	-0.001	0.10	-0.0	-107.978	1.082	
10	7	3	10	8	2	77859.120	-0.001	0.10	-0.0	-107.978	1.082	
10	1	10	11	1	11	49765.970	0.218	0.10	1.5	-14.304	-7.7E-3	
10	1	9	11	1	10	53330.050	-0.081	0.10	-0.6	-26.498	-0.046	
10	3	8	11	3	9	53112.780	-0.053	0.20	-0.2	-26.726	-0.033	
10	3	7	11	3	8	54037.260	0.039	0.10	0.3	-38.036	-0.076	

10	4	7	11	4	8	53223.820	0.187	0.10	1.3	-23.630	-0.027
10	4	6	11	4	7	53311.220	0.019	0.15	0.1	-25.237	-0.034
10	6	5	11	6	6	53072.860	0.362	0.15	1.7	-7.147	-0.043
10	6	4	11	6	5	53072.860	0.279	0.15	1.3	-7.150	-0.043
10	7	4	11	7	5	53040.760	-0.124	0.10	-0.9	3.122	-0.106
10	7	3	11	7	4	53040.760	-0.125	0.10	-0.9	3.121	-0.106
10	8	3	11	8	4	53025.700	0.010	0.10	0.1	14.726	-0.228
10	8	2	11	8	3	53025.700	0.010	0.10	0.1	14.726	-0.228
11	0	11	11	1	10	25066.540	0.272	0.15	1.3	-51.437	-0.113
11	1	11	11	2	10	29675.000	0.169	0.15	0.8	-24.539	-0.034
11	2	10	11	3	9	29814.770	0.259	0.10	1.8	-6.408	-0.020
11	3	9	11	4	8	36451.760	-0.010	0.10	-0.1	11.028	0.023
11	3	8	11	4	7	34311.220	0.100	0.15	0.5	32.368	0.092
11	4	8	11	5	7	46453.370	-0.140	0.15	-0.6	6.899	0.047
11	7	5	11	8	7	77844.080	0.152	0.10	1.1	-96.374	0.960
11	7	4	11	8	3	77844.080	0.154	0.10	1.1	-96.374	0.960
11	8	4	11	9	3	88209.750	-0.310	0.15	-1.4	-162.033	2.094
11	8	3	11	9	2	88209.750	-0.310	0.15	-1.4	-162.033	2.094
11	0	11	12	0	12	54309.260	-0.227	0.10	-1.6	-17.731	-0.013
11	1	10	12	1	11	57764.500	0.139	0.20	0.5	-30.766	-0.057
11	2	10	12	2	11	56634.150	-0.080	0.10	-0.6	-28.020	-0.032
11	3	8	12	3	9	59207.210	0.026	0.10	0.2	-53.019	-0.133
11	4	8	12	4	9	58101.920	0.016	0.10	0.1	-33.485	-0.049
11	5	6	12	5	7	58009.400	-0.030	0.10	-0.2	-25.632	-0.036
11	6	6	12	6	7	57921.880	-0.021	0.10	-0.1	-15.312	-0.044
11	6	5	12	6	6	57922.080	-0.055	0.10	-0.4	-15.320	-0.044
12	0	12	12	1	11	28521.360	0.218	0.15	1.0	-64.472	-0.157
12	2	11	12	3	10	31078.770	-0.094	0.10	-0.7	-13.677	-0.043
12	2	10	12	3	9	20030.090	0.134	0.10	0.9	26.815	0.081
12	3	10	12	4	9	36655.010	-0.081	0.10	-0.6	12.833	0.029
12	3	9	12	4	8	33365.310	-0.031	0.10	-0.2	48.544	0.160
12	4	9	12	5	8	46352.760	-0.056	0.15	-0.3	14.982	0.061
12	4	8	12	5	7	46040.920	0.167	0.15	0.8	20.714	0.084
12	7	6	12	8	5	77821.730	-0.148	0.10	-1.0	-83.590	0.843
12	7	5	12	8	4	77821.730	-0.143	0.10	-1.0	-83.589	0.843
12	0	12	13	0	13	58679.120	-0.141	0.10	-1.0	-22.284	-0.020
12	1	11	13	1	12	62131.750	0.111	0.10	0.8	-35.270	-0.067
12	3	10	13	3	11	62656.480	0.225	0.10	1.6	-44.983	-0.085
12	4	9	13	4	10	62979.940	-0.172	0.10	-1.2	-45.261	-0.084
12	6	7	13	6	8	62777.750	0.089	0.15	0.4	-25.578	-0.053
12	6	6	13	6	7	62778.350	0.094	0.15	0.4	-25.601	-0.053
12	7	6	13	7	7	62720.910	0.006	0.10	0.0	-12.986	-0.092
12	7	5	13	7	6	62720.910	-0.007	0.10	-0.0	-12.987	-0.092
12	8	5	13	8	6	62690.650	0.086	0.10	0.6	1.036	-0.199
12	8	4	13	8	5	62690.650	0.086	0.10	0.6	1.036	-0.199
13	2	12	13	3	11	32562.840	-0.010	0.15	-0.0	-24.165	-0.082
13	2	11	13	3	10	19773.250	-0.098	0.15	-0.4	18.705	0.059
13	3	11	13	4	10	36978.980	0.032	0.10	0.2	12.555	0.029
13	3	10	13	4	9	32216.750	-0.155	0.10	-1.1	67.385	0.259
13	4	10	13	5	9	46250.470	-0.052	0.10	-0.4	23.419	0.086
13	5	9	13	6	8	56797.470	0.124	0.10	0.9	7.457	0.120
13	7	7	13	8	6	77791.520	-0.018	0.10	-0.1	-69.567	0.736
13	7	6	13	8	5	77791.520	-0.000	0.10	-0.0	-69.566	0.736
13	0	13	14	0	14	63054.710	-0.042	0.10	-0.3	-27.590	-0.031
13	1	13	14	1	14	62999.400	-0.076	0.10	-0.5	-28.087	-0.031
13	1	12	14	1	13	66457.270	0.077	0.15	0.4	-40.466	-0.077
13	2	12	14	2	13	65681.020	0.261	0.20	0.9	-41.620	-0.063
13	2	11	14	2	12	69414.950	0.182	0.10	1.3	-73.231	-0.255
13	3	10	14	3	11	69590.160	0.243	0.10	1.7	-90.251	-0.327
13	4	9	14	4	10	68295.310	0.060	0.10	0.4	-70.718	-0.202
13	5	9	14	5	10	67762.800	0.105	0.10	0.7	-50.638	-0.099
13	5	8	14	5	9	67796.250	-0.059	0.10	-0.4	-51.842	-0.106
13	6	8	14	6	9	67640.120	-0.132	0.15	-0.6	-38.178	-0.074
13	6	7	14	6	8	67641.420	-0.225	0.15	-1.0	-38.241	-0.074
13	7	7	14	7	8	67567.430	-0.018	0.10	-0.1	-24.278	-0.095
13	7	6	14	7	7	67567.430	-0.053	0.10	-0.4	-24.280	-0.095
13	8	6	14	8	7	67527.310	0.057	0.10	0.4	-8.947	-0.186
13	8	5	14	8	6	67527.310	0.057	0.10	0.4	-8.947	-0.186
14	0	14	14	1	13	35376.080	0.119	0.15	0.6	-90.334	-0.249
14	1	13	14	2	12	23990.320	0.366	0.15	1.7	-109.061	-0.472

14	2	13	14	3	12	34263.980	0.123	0.10	0.9	-38.254	-0.142
14	2	12	14	3	11	19948.540	0.043	0.10	0.3	1.685	-0.013
14	3	11	14	4	10	30922.260	0.022	0.10	0.2	86.918	0.384
14	4	11	14	5	10	46159.850	0.138	0.10	1.0	31.760	0.122
14	4	10	14	5	9	45183.850	0.158	0.10	1.1	53.987	0.236
14	7	8	14	8	7	77751.510	0.167	0.15	0.8	-54.236	0.645
14	7	7	14	8	6	77751.510	0.220	0.15	1.0	-54.233	0.645
14	8	7	14	9	6	88165.410	-0.016	0.10	-0.1	-115.294	1.505
14	8	6	14	9	5	88165.410	-0.016	0.10	-0.1	-115.294	1.505
14	0	14	15	0	15	67434.220	-0.145	0.10	-1.0	-33.690	-0.045
14	2	13	15	2	14	70162.710	-0.040	0.10	-0.3	-49.431	-0.084
14	2	12	15	2	13	74069.850	-0.075	0.10	-0.5	-83.193	-0.320
14	3	12	15	3	13	72071.850	-0.259	0.15	-1.2	-67.361	-0.172
14	3	11	15	3	12	74742.230	-0.001	0.10	-0.0	-111.315	-0.470
14	4	11	15	4	12	72716.760	0.139	0.10	1.0	-74.591	-0.204
14	5	9	15	5	10	72717.430	0.284	0.20	1.0	-69.528	-0.177
14	7	8	15	7	9	72418.830	0.037	0.10	0.3	-38.025	-0.109
14	7	7	15	7	8	72418.930	0.045	0.10	0.3	-38.031	-0.109
14	8	7	15	8	8	72367.090	0.040	0.10	0.3	-21.294	-0.179
14	8	6	15	8	7	72367.090	0.038	0.10	0.3	-21.295	-0.179
14	9	6	15	9	7	72339.130	0.087	0.10	0.6	-2.945	-0.349
14	9	5	15	9	6	72339.130	0.087	0.10	0.6	-2.945	-0.349
15	1	15	15	2	14	40146.340	0.057	0.15	0.3	-74.843	-0.148
15	1	14	15	2	13	27295.140	0.247	0.10	1.8	-145.495	-0.702
15	2	14	15	3	13	36173.280	0.065	0.10	0.5	-56.184	-0.229
15	3	13	15	4	12	38095.220	0.021	0.10	0.1	2.055	-0.014
15	3	12	15	4	11	29574.940	0.031	0.10	0.2	103.864	0.521
15	4	12	15	5	11	46097.950	-0.064	0.10	-0.4	39.319	0.166
15	4	11	15	5	10	44506.140	0.204	0.10	1.4	78.827	0.392
15	8	8	15	9	7	88137.170	-0.249	0.10	-1.7	-96.945	1.335
15	8	7	15	9	6	88137.170	-0.247	0.10	-1.7	-96.945	1.335
15	1	14	16	1	15	75072.340	-0.055	0.10	-0.4	-54.378	-0.107
15	2	14	16	2	15	74621.550	-0.235	0.20	-0.8	-57.989	-0.109
15	3	13	16	3	14	76725.440	-0.023	0.10	-0.2	-79.831	-0.230
15	3	12	16	3	13	79833.850	0.045	0.10	0.3	-133.168	-0.643
15	4	12	16	4	13	77563.760	0.132	0.10	0.9	-91.985	-0.296
15	5	10	16	5	11	77662.370	-0.078	0.10	-0.5	-91.034	-0.287
15	6	9	16	6	10	77393.690	-0.077	0.10	-0.5	-71.714	-0.178
15	7	9	16	7	10	77275.110	-0.165	0.10	-1.1	-54.463	-0.142
15	7	8	16	7	9	77275.310	-0.188	0.10	-1.3	-54.479	-0.142
15	8	8	16	8	9	77209.970	-0.190	0.10	-1.3	-36.222	-0.184
15	8	7	16	8	8	77209.970	-0.195	0.10	-1.4	-36.223	-0.184
15	9	7	16	9	8	77173.610	-0.029	0.10	-0.2	-16.372	-0.330
15	9	6	16	9	7	77173.610	-0.029	0.10	-0.2	-16.372	-0.330
15	11	5	16	11	6	77149.370	-0.022	0.10	-0.2	28.750	-1.077
15	11	4	16	11	5	77149.370	-0.022	0.10	-0.2	28.750	-1.077
16	1	15	16	2	14	30842.510	-0.016	0.10	-0.1	-183.122	-0.975
16	2	15	16	3	14	38277.160	0.267	0.15	1.2	-78.026	-0.350
16	3	14	16	4	13	38933.460	0.096	0.15	0.4	-10.099	-0.080
16	3	13	16	4	12	28295.180	0.170	0.10	1.2	113.922	0.641
16	4	13	16	5	12	46087.500	0.259	0.10	1.8	45.147	0.211
16	4	12	16	5	11	43614.680	0.202	0.10	1.4	110.903	0.628
16	5	12	16	6	11	56364.750	0.049	0.10	0.3	48.389	0.269
16	5	11	16	6	10	56139.900	0.221	0.15	1.0	57.270	0.330
16	8	9	16	9	8	88100.600	-0.299	0.10	-2.1	-77.095	1.188
16	8	8	16	9	7	88100.600	-0.291	0.10	-2.0	-77.094	1.188
16	0	16	17	0	17	76200.330	-0.230	0.10	-1.6	-48.448	-0.092
16	1	16	17	1	17	76185.660	-0.037	0.10	-0.3	-48.752	-0.093
16	1	15	17	1	16	79388.890	-0.044	0.10	-0.3	-63.378	-0.131
16	2	15	17	2	16	79061.840	0.267	0.15	1.2	-67.375	-0.139
16	2	14	17	2	15	83069.750	-0.058	0.15	-0.3	-99.768	-0.433
16	3	14	17	3	15	81341.070	-0.168	0.10	-1.2	-93.033	-0.298
16	4	13	17	4	14	82388.460	-0.251	0.10	-1.7	-110.990	-0.412
16	4	12	17	4	13	83765.450	0.258	0.10	1.8	-156.760	-0.787
16	5	12	17	5	13	82453.730	-0.273	0.15	-1.3	-108.096	-0.375
16	5	11	17	5	12	82638.720	0.207	0.15	1.0	-117.132	-0.449
16	6	10	17	6	11	82285.010	0.121	0.15	0.6	-93.213	-0.276
16	7	10	17	7	11	82137.160	-0.065	0.15	-0.3	-73.841	-0.199
16	7	9	17	7	10	82137.660	-0.071	0.15	-0.3	-73.879	-0.200
16	8	9	17	8	10	82056.720	-0.067	0.10	-0.5	-53.957	-0.206

16	8	8	17	8	9	82056.720	-0.080	0.10	-0.6	-53.958	-0.206
16	9	8	17	9	9	82010.520	0.070	0.10	0.5	-32.513	-0.322
16	9	7	17	9	8	82010.520	0.069	0.10	0.5	-32.513	-0.322
16	10	7	17	10	8	81985.720	0.028	0.20	0.1	-9.266	-0.580
16	10	6	17	10	7	81985.720	0.028	0.20	0.1	-9.266	-0.580
17	0	17	17	1	16	45150.810	0.134	0.15	0.6	-132.086	-0.375
17	1	16	17	2	15	34523.550	0.150	0.10	1.1	-219.511	-1.278
17	2	16	17	3	15	40556.610	0.053	0.10	0.4	-103.684	-0.509
17	2	15	17	3	14	23611.060	-0.171	0.15	-0.8	-122.974	-0.836
17	3	15	17	4	14	39980.730	-0.108	0.10	-0.7	-28.056	-0.194
17	3	14	17	4	13	27213.810	0.066	0.10	0.5	112.305	0.698
17	4	14	17	5	13	46152.480	-0.053	0.10	-0.4	48.041	0.248
17	4	13	17	5	12	42487.860	0.060	0.10	0.4	150.531	0.965
17	5	13	17	6	12	56183.040	-0.259	0.10	-1.8	64.034	0.374
17	5	12	17	6	11	55786.330	0.275	0.15	1.3	81.188	0.503
17	8	10	17	9	9	88054.440	-0.122	0.10	-0.9	-55.651	1.073
17	8	9	17	9	8	88054.440	-0.101	0.10	-0.7	-55.649	1.073
17	10	8	17	11	7	108844.720	-0.311	0.15	-1.5	-226.137	4.472
17	10	7	17	11	6	108844.720	-0.311	0.15	-1.5	-226.137	4.472
17	0	17	18	0	18	80585.120	-0.060	0.10	-0.4	-57.205	-0.126
17	1	16	18	1	17	83717.930	-0.001	0.10	-0.0	-73.725	-0.162
17	2	16	18	2	17	83485.810	0.108	0.10	0.8	-77.680	-0.174
17	2	15	18	2	16	87434.310	0.038	0.10	0.3	-107.205	-0.477
17	4	14	18	4	15	87186.250	-0.197	0.10	-1.4	-131.392	-0.554
17	4	13	18	4	14	89010.990	0.295	0.15	1.4	-194.403	-1.131
17	5	13	18	5	14	87354.880	-0.101	0.10	-0.7	-132.856	-0.541
17	6	12	18	6	13	87165.590	0.253	0.20	0.9	-116.868	-0.407
17	7	11	18	7	12	87005.110	0.145	0.15	0.7	-96.422	-0.291
17	7	10	18	7	11	87006.210	0.161	0.15	0.7	-96.512	-0.292
17	8	10	18	8	11	86907.340	0.204	0.15	0.9	-74.735	-0.255
17	8	9	18	8	10	86907.340	0.170	0.15	0.8	-74.738	-0.255
17	9	9	18	9	10	86849.520	-0.069	0.10	-0.5	-51.585	-0.330
17	9	8	18	9	9	86849.520	-0.070	0.10	-0.5	-51.585	-0.330
17	10	8	18	10	9	86817.520	0.075	0.10	0.5	-26.644	-0.554
17	10	7	18	10	8	86817.520	0.075	0.10	0.5	-26.644	-0.554
18	1	17	18	2	16	38239.760	0.020	0.10	0.1	-252.991	-1.593
18	2	16	18	3	15	25943.790	-0.105	0.10	-0.7	-192.210	-1.425
18	3	16	18	4	15	41247.330	0.104	0.10	0.7	-52.531	-0.372
18	3	15	18	4	14	26457.550	0.047	0.10	0.3	94.342	0.633
18	4	15	18	5	14	46321.060	-0.006	0.10	-0.0	46.577	0.261
18	5	14	18	6	13	55993.600	-0.055	0.10	-0.4	80.022	0.508
18	5	13	18	6	12	55321.570	0.087	0.10	0.6	111.516	0.766
18	10	9	18	11	8	108830.150	0.161	0.10	1.2	-199.237	4.057
18	10	8	18	11	7	108830.150	0.161	0.10	1.2	-199.237	4.057
18	1	17	19	1	18	88058.900	-0.127	0.10	-0.9	-85.361	-0.202
18	2	17	19	2	18	87897.170	-0.245	0.10	-1.7	-88.999	-0.217
18	2	16	19	2	17	91737.070	0.065	0.10	0.5	-115.474	-0.518
18	3	15	19	3	16	94585.030	0.031	0.10	0.2	-196.116	-1.298
18	5	14	19	5	15	92251.450	-0.096	0.10	-0.7	-160.351	-0.755
18	5	13	19	5	14	92713.630	-0.023	0.10	-0.2	-186.979	-1.020
18	6	13	19	6	14	92065.100	-0.153	0.10	-1.1	-144.837	-0.595
18	8	11	19	8	12	91761.360	-0.057	0.15	-0.3	-98.807	-0.338
18	8	10	19	8	11	91761.410	-0.087	0.15	-0.4	-98.815	-0.338
18	9	10	19	9	11	91691.290	0.122	0.10	0.8	-73.817	-0.365
18	9	9	19	9	10	91691.290	0.120	0.10	0.8	-73.818	-0.365
18	10	9	19	10	10	91650.530	-0.087	0.10	-0.6	-47.087	-0.544
18	10	8	19	10	9	91650.530	-0.087	0.10	-0.6	-47.087	-0.544
18	12	7	19	12	8	91623.520	0.169	0.10	1.2	12.419	-1.545
18	12	6	19	12	7	91623.520	0.169	0.10	1.2	12.419	-1.545
18	14	5	19	14	6	91639.790	0.395	0.15	1.8	80.427	-3.762
18	14	4	19	14	5	91639.790	0.395	0.15	1.8	80.427	-3.762
19	1	18	19	2	17	41917.770	0.052	0.10	0.4	-283.104	-1.909
19	2	17	19	3	16	28791.850	-0.040	0.10	-0.3	-272.852	-2.205
19	3	16	19	4	15	26135.450	0.014	0.10	0.1	55.911	0.374
19	4	16	19	5	15	46620.560	0.072	0.10	0.5	39.184	0.228
19	4	15	19	5	14	39580.840	0.145	0.10	1.0	243.741	1.949
19	5	15	19	6	14	55807.120	-0.242	0.10	-1.7	95.536	0.667
19	10	10	19	11	9	108809.380	0.075	0.10	0.5	-170.528	3.680
19	10	9	19	11	8	108809.380	0.075	0.10	0.5	-170.528	3.680
19	1	18	20	1	19	92410.390	0.176	0.20	0.6	-98.247	-0.253

19	2	18	20	2	19	92299.520	0.035	0.10	0.2	-101.425	-0.269
19	3	16	20	3	17	99292.900	0.098	0.10	0.7	-213.210	-1.524
19	4	15	20	4	16	99490.220	0.013	0.10	0.1	-275.535	-2.060
19	5	14	20	5	15	97828.370	0.217	0.10	1.5	-232.755	-1.484
19	6	14	20	6	15	96971.560	0.120	0.10	0.8	-176.540	-0.848
19	6	13	20	6	14	97042.130	-0.307	0.15	-1.4	-182.302	-0.912
19	8	12	20	8	13	96619.720	-0.120	0.15	-0.6	-126.435	-0.467
19	8	11	20	8	12	96619.920	-0.097	0.15	-0.4	-126.455	-0.468
19	9	11	20	9	12	96535.080	-0.217	0.10	-1.5	-99.447	-0.434
19	9	10	20	9	11	96535.080	-0.222	0.10	-1.5	-99.448	-0.434
19	10	10	20	10	11	96485.340	0.085	0.10	0.6	-70.814	-0.559
19	10	9	20	10	10	96485.340	0.085	0.10	0.6	-70.814	-0.559
19	11	9	20	11	10	96458.040	-0.115	0.20	-0.4	-40.215	-0.887
19	11	8	20	11	9	96458.040	-0.115	0.20	-0.4	-40.215	-0.887
19	12	8	20	12	9	96447.200	-0.042	0.20	-0.1	-7.489	-1.470
19	12	7	20	12	8	96447.200	-0.042	0.20	-0.1	-7.489	-1.470
19	13	7	20	13	8	96448.300	-0.027	0.20	-0.1	27.435	-2.367
19	13	6	20	13	7	96448.300	-0.027	0.20	-0.1	27.435	-2.367
19	15	5	20	15	6	96476.550	0.106	0.10	0.8	103.936	-5.361
19	15	4	20	15	5	96476.550	0.106	0.10	0.8	103.936	-5.361
20	1	19	20	2	18	45512.560	0.229	0.10	1.6	-310.567	-2.220
20	2	19	20	3	18	48232.340	-0.103	0.10	-0.7	-200.769	-1.243
20	3	18	20	4	17	44442.940	0.025	0.10	0.2	-122.672	-0.991
20	3	17	20	4	16	26333.040	0.199	0.10	1.4	-6.415	-0.162
20	4	17	20	5	16	47077.290	0.062	0.10	0.4	24.246	0.122
20	4	16	20	5	15	37918.720	0.080	0.10	0.6	286.521	2.524
20	5	16	20	6	15	55640.140	0.072	0.10	0.5	109.388	0.842
20	5	15	20	6	14	53928.760	0.243	0.15	1.1	201.041	1.731
20	6	15	20	7	14	66368.770	0.006	0.10	0.0	108.018	0.878
20	10	11	20	11	10	108782.130	-0.075	0.10	-0.5	-139.929	3.352
20	10	10	20	11	9	108782.130	-0.075	0.10	-0.5	-139.929	3.352
20	11	10	20	12	9	119150.530	0.238	0.10	1.8	-252.471	6.244
20	11	9	20	12	8	119150.530	0.238	0.10	1.8	-252.471	6.244
20	1	20	21	1	21	93735.660	-0.254	0.30	-0.6	-89.730	-0.295
20	1	19	21	1	20	96768.750	-0.313	0.15	-1.4	-112.372	-0.315
20	2	18	21	2	19	100261.600	0.140	0.10	1.0	-138.623	-0.624
20	4	16	21	4	17	104662.980	0.203	0.10	1.4	-315.901	-2.627
20	5	15	21	5	16	103000.270	-0.059	0.10	-0.4	-286.638	-2.109
20	11	10	21	11	11	101286.690	-0.381	0.15	-1.8	-65.469	-0.877
20	11	9	21	11	10	101286.690	-0.381	0.15	-1.8	-65.469	-0.877
21	1	20	21	2	19	49004.960	0.233	0.10	1.7	-336.817	-2.529
21	2	19	21	3	18	35704.450	-0.028	0.10	-0.2	-448.804	-4.265
21	3	19	21	4	18	46359.780	0.145	0.10	1.0	-168.418	-1.462
21	3	18	21	4	17	27109.600	0.054	0.10	0.4	-95.240	-1.064
21	4	18	21	5	17	47714.900	0.016	0.10	0.1	0.217	-0.092
21	4	17	21	5	16	36256.160	-0.032	0.10	-0.2	315.784	3.042
21	5	17	21	6	16	55511.430	0.056	0.10	0.4	119.997	1.012
21	5	16	21	6	15	52928.960	0.122	0.10	0.9	265.204	2.539
21	10	12	21	11	11	108747.930	0.056	0.10	0.4	-107.342	3.085
21	10	11	21	11	10	108747.930	0.056	0.10	0.4	-107.342	3.085
21	11	11	21	12	10	119134.510	0.065	0.10	0.5	-217.742	5.713
21	11	10	21	12	9	119134.510	0.065	0.10	0.5	-217.742	5.713
21	1	21	22	1	22	98119.730	-0.092	0.10	-0.6	-102.742	-0.380
21	1	20	22	1	21	101133.070	-0.261	0.10	-1.8	-127.751	-0.391
21	2	20	22	2	21	101083.000	-0.207	0.10	-1.4	-129.926	-0.405
21	2	19	22	2	20	104523.670	0.190	0.10	1.3	-154.384	-0.705
21	5	16	22	5	17	108227.340	-0.242	0.10	-1.7	-348.275	-2.922
21	6	15	22	6	16	106986.360	-0.098	0.10	-0.7	-269.507	-1.827
21	9	13	22	9	14	106231.800	0.148	0.10	1.0	-161.908	-0.726
21	9	12	22	9	13	106231.800	0.121	0.10	0.8	-161.913	-0.726
21	11	11	22	11	12	106116.680	0.002	0.10	0.0	-94.363	-0.901
21	11	10	22	11	11	106116.680	0.002	0.10	0.0	-94.363	-0.901
21	12	10	22	12	11	106095.030	-0.236	0.20	-0.8	-57.544	-1.365
21	12	9	22	12	10	106095.030	-0.236	0.20	-0.8	-57.544	-1.365
21	13	9	22	13	10	106089.300	0.044	0.10	0.3	-18.443	-2.163
21	13	8	22	13	9	106089.300	0.044	0.10	0.3	-18.443	-2.163
21	15	7	22	15	8	106110.270	0.182	0.10	1.3	66.821	-5.040
21	15	6	22	15	7	106110.270	0.182	0.10	1.3	66.821	-5.040
22	2	20	22	3	19	39547.790	0.117	0.10	0.8	-532.251	-5.445
22	3	20	22	4	19	48471.340	-0.003	0.10	-0.0	-220.829	-2.056

22	3	19	22	4	18	28499.910	0.254	0.10	1.8	-211.841	-2.422
22	4	19	22	5	18	48552.680	-0.140	0.10	-1.0	-34.253	-0.448
22	4	18	22	5	17	34727.180	0.191	0.10	1.3	321.941	3.362
22	5	18	22	6	17	55444.410	0.079	0.10	0.6	125.399	1.151
22	5	17	22	6	16	51687.820	0.106	0.10	0.7	343.972	3.634
22	6	16	22	7	15	65438.240	-0.024	0.10	-0.2	197.859	1.972
22	10	13	22	11	12	108705.570	0.118	0.10	0.8	-72.653	2.890
22	10	12	22	11	11	108705.570	0.119	0.10	0.8	-72.653	2.890
22	11	12	22	12	11	119113.170	0.138	0.15	0.6	-180.923	5.249
22	11	11	22	12	10	119113.170	0.138	0.15	0.6	-180.923	5.249
22	1	22	23	1	23	102502.450	0.039	0.30	0.1	-116.972	-0.483
22	2	20	23	2	21	108799.620	-0.082	0.10	-0.6	-172.799	-0.812
22	3	20	23	3	21	108348.340	-0.242	0.10	-1.7	-188.308	-0.908
22	3	19	23	3	20	112745.140	-0.004	0.10	-0.0	-246.691	-2.006
22	5	18	23	5	19	111688.860	-0.099	0.10	-0.7	-292.667	-2.174
22	6	17	23	6	18	111709.450	0.300	0.15	1.4	-294.750	-2.107
22	6	16	23	6	17	112006.610	0.176	0.10	1.2	-324.714	-2.529
22	7	16	23	7	17	111438.130	-0.124	0.10	-0.9	-267.188	-1.682
22	9	14	23	9	15	111083.890	-0.214	0.10	-1.5	-199.276	-0.977
22	9	13	23	9	14	111083.890	-0.273	0.10	-1.9	-199.286	-0.977
22	10	13	23	10	14	110998.470	0.080	0.10	0.6	-164.050	-0.864
22	10	12	23	10	13	110998.470	0.078	0.10	0.5	-164.051	-0.864
22	12	11	23	12	12	110919.280	-0.052	0.10	-0.4	-88.120	-1.357
22	12	10	23	12	11	110919.280	-0.052	0.10	-0.4	-88.120	-1.357
22	13	10	23	13	11	110909.130	0.094	0.10	0.7	-46.817	-2.083
22	13	9	23	13	10	110909.130	0.094	0.10	0.7	-46.817	-2.083
23	3	21	23	4	20	50759.380	-0.082	0.10	-0.6	-279.243	-2.783
23	3	20	23	4	19	30509.250	-0.153	0.10	-1.1	-355.138	-4.302
23	4	20	23	5	19	49605.040	-0.038	0.10	-0.3	-80.198	-0.987
23	4	19	23	5	18	33470.060	0.088	0.10	0.6	295.876	3.316
23	5	19	23	6	18	55464.540	0.018	0.10	0.1	123.316	1.218
23	6	18	23	7	17	65603.730	-0.108	0.10	-0.7	188.655	1.957
23	7	17	23	8	16	76631.710	-0.088	0.15	-0.4	164.699	1.766
23	10	14	23	11	13	108653.910	-0.122	0.10	-0.9	-35.732	2.782
23	10	13	23	11	12	108653.910	-0.119	0.10	-0.8	-35.731	2.782
23	0	23	24	0	24	106884.140	-0.090	0.10	-0.6	-132.435	-0.608
23	1	23	24	1	24	106883.540	-0.136	0.20	-0.5	-132.475	-0.608
23	1	22	24	1	23	109871.240	0.107	0.10	0.7	-162.421	-0.591
23	2	22	24	2	23	109849.240	-0.015	0.20	-0.1	-163.767	-0.603
23	3	20	24	3	21	117041.340	0.060	0.10	0.4	-255.858	-2.100
23	4	19	24	4	20	119644.810	-0.076	0.15	-0.4	-421.330	-4.529
23	6	18	24	6	19	116618.310	0.033	0.10	0.2	-341.546	-2.730
23	7	17	24	7	18	116343.840	0.179	0.10	1.2	-314.838	-2.254
23	7	16	24	7	17	116387.590	0.034	0.10	0.2	-320.732	-2.346
23	9	15	24	9	16	115939.340	-0.219	0.15	-1.0	-241.114	-1.319
23	9	14	24	9	15	115939.340	-0.343	0.15	-1.6	-241.137	-1.319
23	10	14	24	10	15	115839.200	-0.109	0.10	-0.8	-203.311	-1.098
23	10	13	24	10	14	115839.200	-0.113	0.10	-0.8	-203.312	-1.098
23	13	11	24	13	12	115728.260	-0.020	0.20	-0.1	-79.099	-2.034
23	13	10	24	13	11	115728.260	-0.020	0.20	-0.1	-79.099	-2.034
24	2	23	24	3	22	59622.570	-0.164	0.10	-1.2	-365.048	-2.811
24	2	22	24	3	21	47441.340	-0.142	0.10	-1.0	-668.465	-7.794
24	3	22	24	4	21	53202.520	-0.136	0.15	-0.6	-342.834	-3.644
24	4	21	24	5	20	50879.580	-0.097	0.15	-0.4	-138.234	-1.748
24	4	20	24	5	19	32614.150	0.078	0.10	0.5	230.026	2.711
24	5	20	24	6	19	55598.680	-0.144	0.10	-1.0	111.272	1.161
24	5	19	24	6	18	48475.300	0.050	0.10	0.3	532.915	6.711
24	6	19	24	7	18	65329.140	-0.082	0.10	-0.6	215.363	2.433
24	7	18	24	8	17	76386.840	-0.391	0.15	-1.8	201.273	2.299
24	0	24	25	0	25	111264.160	0.226	0.15	1.0	-149.279	-0.757
24	1	24	25	1	25	111263.860	0.267	0.15	1.2	-149.307	-0.757
24	1	23	25	1	24	114242.200	0.037	0.10	0.3	-181.816	-0.721
24	2	23	25	2	24	114227.890	0.030	0.15	0.1	-182.846	-0.730
24	2	22	25	2	23	117402.310	0.061	0.10	0.4	-216.291	-1.106
24	3	22	25	3	23	117169.550	-0.047	0.10	-0.3	-228.907	-1.215
24	6	18	25	6	19	122178.160	-0.154	0.10	-1.1	-465.514	-4.680
24	7	18	25	7	19	121253.980	-0.162	0.10	-1.1	-367.500	-2.968
24	12	13	25	12	14	120567.620	0.250	0.10	1.8	-161.500	-1.492
24	12	12	25	12	13	120567.620	0.250	0.10	1.8	-161.500	-1.492
25	2	24	25	3	23	62564.110	-0.361	0.15	-1.7	-411.108	-3.295

25	2	23	25	3	22	51320.700	0.068	0.10	0.5	-720.017	-8.884
25	3	23	25	4	22	55778.140	-0.083	0.15	-0.4	-410.708	-4.639
25	3	22	25	4	21	36249.700	-0.115	0.10	-0.8	-699.932	-9.665
25	4	22	25	5	21	52378.250	-0.066	0.10	-0.5	-208.491	-2.766
25	4	21	25	5	20	32267.110	0.088	0.10	0.6	118.883	1.350
25	5	21	25	6	20	55873.940	-0.010	0.10	-0.1	86.749	0.918
25	5	20	25	6	19	46582.530	0.120	0.10	0.8	625.709	8.522
25	6	19	25	7	18	63364.010	0.186	0.10	1.3	408.603	5.425
25	7	18	25	8	17	75951.650	0.157	0.10	1.1	261.852	3.285
25	10	16	25	11	15	108520.300	-0.036	0.10	-0.3	45.432	2.888
25	10	15	25	11	14	108520.300	-0.020	0.10	-0.1	45.435	2.888
25	0	25	26	0	26	115642.370	0.038	0.15	0.2	-167.505	-0.934
25	1	25	26	1	26	115642.150	0.028	0.15	0.1	-167.525	-0.934
25	1	24	26	1	25	118613.550	0.080	0.10	0.6	-202.666	-0.874
26	2	24	26	3	23	55088.230	-0.187	0.10	-1.3	-763.749	-9.915
26	3	24	26	4	23	58463.520	0.102	0.10	0.7	-482.011	-5.763
26	3	23	26	4	22	39826.390	-0.135	0.10	-1.0	-881.853	-12.985
26	4	23	26	5	22	54096.430	-0.061	0.10	-0.4	-290.585	-4.070
26	4	22	26	5	21	32509.700	-0.036	0.10	-0.2	-40.983	-0.968
26	5	22	26	6	21	56315.040	0.114	0.10	0.8	47.366	0.416
26	5	21	26	6	20	44613.070	0.082	0.10	0.6	698.629	10.235
26	6	20	26	7	19	62305.860	0.068	0.10	0.5	518.984	7.515
26	8	19	26	9	18	86933.920	-0.401	0.15	-1.9	235.883	3.215
26	8	18	26	9	17	86915.850	0.296	0.15	1.4	239.045	3.270
26	11	16	26	12	15	118957.900	-0.141	0.15	-0.7	-10.525	4.345
26	11	15	26	12	14	118957.900	-0.140	0.15	-0.7	-10.525	4.345
27	2	25	27	3	24	58728.940	0.149	0.10	1.1	-803.552	-10.917
27	3	25	27	4	24	61236.520	-0.062	0.10	-0.4	-556.010	-7.011
27	3	24	27	4	23	43726.000	-0.162	0.10	-1.2	-1054.232	-16.512
27	4	24	27	5	23	56023.940	-0.062	0.10	-0.4	-383.642	-5.682
27	4	23	27	5	22	33395.010	0.182	0.10	1.3	-250.755	-4.425
27	5	23	27	6	22	56943.700	0.044	0.10	0.3	-8.928	-0.424
27	5	22	27	6	21	42692.190	0.011	0.10	0.1	734.521	11.515
27	6	22	27	7	21	64636.430	-0.148	0.10	-1.0	269.653	3.831
27	6	21	27	7	20	61009.790	0.001	0.10	0.0	654.516	10.277
27	7	21	27	8	20	75490.490	-0.108	0.10	-0.8	326.361	4.683
27	7	20	27	8	19	75053.270	-0.141	0.10	-1.0	390.233	5.797
28	2	27	28	3	26	71459.800	-0.120	0.10	-0.9	-562.145	-4.941
28	2	26	28	3	25	62244.100	-0.081	0.10	-0.6	-843.141	-11.932
28	3	26	28	4	25	64077.740	-0.248	0.10	-1.7	-632.155	-8.377
28	3	25	28	4	24	47821.980	-0.311	0.15	-1.5	-1206.624	-20.041
28	4	25	28	5	24	58145.710	-0.082	0.10	-0.6	-486.373	-7.614
28	4	24	28	5	23	34946.120	0.071	0.10	0.5	-508.462	-9.166
28	5	24	28	6	23	57777.690	0.005	0.10	0.0	-83.684	-1.682
28	5	23	28	6	22	40961.660	0.014	0.10	0.1	716.606	11.950
28	6	22	28	7	21	59456.220	0.203	0.10	1.4	813.816	13.778
28	7	22	28	8	21	75148.690	0.171	0.15	0.8	370.858	5.740
29	0	29	29	1	28	81285.330	-0.169	0.15	-0.9	-482.583	-0.010
29	1	29	29	2	28	81289.920	0.136	0.10	1.3	-481.835	2.3E-3
29	3	27	29	4	26	66970.060	-0.316	0.15	-1.5	-710.109	-9.854
29	3	26	29	4	25	51994.860	-0.212	0.10	-1.5	-1332.636	-23.390
29	4	26	29	5	25	60443.060	0.006	0.10	0.0	-597.202	-9.867
29	5	25	29	6	24	58829.300	0.024	0.10	0.2	-177.801	-3.437
29	5	24	29	6	23	39563.700	0.029	0.10	0.2	630.760	11.096
29	6	23	29	7	22	57646.810	0.089	0.10	0.6	989.446	17.972
29	7	23	29	8	22	74796.300	-0.063	0.10	-0.4	414.344	6.896
29	7	22	29	8	21	73736.530	0.265	0.10	1.9	585.000	10.241
29	11	19	29	12	18	118747.770	0.005	0.10	0.0	145.725	5.168
29	11	18	29	12	17	118747.770	0.016	0.10	0.1	145.729	5.168
30	2	28	30	3	27	68955.640	-0.128	0.15	-0.6	-932.366	-14.161
30	3	27	30	4	26	56145.040	-0.119	0.10	-0.8	-1431.198	-26.448
30	4	27	30	5	26	62894.700	0.211	0.10	1.5	-714.420	-12.432
30	4	26	30	5	25	39984.530	-0.364	0.15	-1.7	-1135.250	-22.577
30	5	26	30	6	25	60104.950	0.115	0.10	0.8	-291.430	-5.757
30	5	25	30	6	24	38626.750	-0.009	0.10	-0.1	466.973	8.509
30	6	25	30	7	24	64594.590	-0.137	0.10	-1.0	221.003	3.671
30	6	24	30	7	23	55615.540	-0.144	0.10	-1.0	1166.422	22.629
30	7	24	30	8	23	74445.300	-0.183	0.10	-1.3	454.383	8.102
31	1	30	31	2	29	80322.580	0.035	0.15	0.2	-745.472	-7.036
31	2	29	31	3	28	72186.130	-0.187	0.15	-0.9	-985.078	-15.436

31	3	28	31	4	27	60202.240	0.161	0.10	1.1	-1506.220	-29.194
31	4	28	31	5	27	65477.540	-0.065	0.15	-0.3	-836.348	-15.295
31	4	27	31	5	26	43356.580	-0.060	0.10	-0.4	-1473.868	-30.904
31	5	26	31	6	25	38255.600	0.020	0.10	0.1	219.691	3.778
31	6	25	31	7	24	53433.540	0.062	0.10	0.4	1322.467	27.294
31	7	25	31	8	24	74110.660	0.138	0.10	1.0	487.782	9.281
31	7	24	31	8	23	71780.520	-0.289	0.15	-1.3	890.712	18.109
31	8	24	31	9	23	85464.220	-0.190	0.10	-1.3	515.317	9.733
31	8	23	31	9	22	85205.550	-0.064	0.10	-0.4	573.060	11.045
31	11	21	31	12	20	118549.990	-0.096	0.15	-0.5	266.491	6.762
31	11	20	31	12	19	118549.990	-0.048	0.15	-0.2	266.508	6.762
31	12	20	32	11	21	35897.640	-0.180	0.10	-1.3	-905.777	-13.546
31	12	19	32	11	22	35897.640	-0.080	0.10	-0.6	-905.739	-13.545
32	2	30	32	3	29	75354.530	-0.035	0.10	-0.3	-1044.095	-16.845
32	3	29	32	4	28	64125.600	-0.041	0.10	-0.3	-1564.829	-31.694
32	4	29	32	5	28	68169.850	-0.078	0.10	-0.6	-961.488	-18.435
32	4	28	32	5	27	47166.090	-0.210	0.10	-1.5	-1802.186	-39.811
32	5	28	32	6	27	63323.560	0.109	0.10	0.8	-573.894	-12.298
32	5	27	32	6	26	38526.060	-0.018	0.10	-0.1	-112.457	-3.456
32	6	27	32	7	26	65261.120	-0.162	0.10	-1.1	84.178	1.140
32	6	26	32	7	25	51205.770	-0.072	0.10	-0.5	1430.314	31.286
32	7	26	32	8	25	73809.120	-0.243	0.10	-1.7	510.604	10.323
32	7	25	32	8	24	70481.890	-0.044	0.10	-0.3	1099.608	23.940
32	8	25	32	9	24	85085.410	-0.159	0.10	-1.1	582.044	11.761
33	2	31	33	3	30	78473.230	-0.128	0.15	-0.6	-1109.579	-18.403
33	4	30	33	5	29	70949.990	-0.047	0.10	-0.3	-1088.634	-21.833
33	4	29	33	5	28	51288.520	-0.121	0.10	-0.9	-2099.728	-48.792
33	5	29	33	6	28	65250.270	0.067	0.10	0.5	-739.254	-16.573
33	5	28	33	6	27	39484.050	-0.062	0.10	-0.4	-526.507	-13.470
33	6	27	33	7	26	49064.820	-0.151	0.10	-1.1	1461.439	33.751
33	7	27	33	8	26	73562.390	-0.406	0.15	-1.9	518.259	11.080
33	7	26	33	8	25	68930.490	-0.107	0.10	-0.8	1348.603	31.310
33	8	25	33	9	24	84054.180	-0.207	0.10	-1.5	804.211	17.893
33	13	21	34	12	22	34983.110	-0.093	0.15	-0.4	-1032.537	-17.908
33	13	20	34	12	23	34983.110	-0.078	0.15	-0.4	-1032.530	-17.908
34	3	32	34	4	31	81776.990	-0.103	0.15	-0.5	-1127.925	-18.833
34	3	31	34	4	30	71533.290	0.156	0.10	1.1	-1664.164	-36.432
34	4	31	34	5	30	73798.350	0.015	0.10	0.1	-1216.943	-25.468
34	4	30	34	5	29	55592.900	0.155	0.10	1.1	-2350.801	-57.347
34	5	30	34	6	29	67369.720	0.033	0.10	0.2	-917.445	-21.519
34	5	29	34	6	28	41145.070	0.179	0.10	1.3	-1013.877	-26.399
34	6	29	34	7	28	66689.370	0.155	0.10	1.1	-162.542	-4.704
34	6	28	34	7	27	47155.690	-0.141	0.10	-1.0	1390.158	33.742
34	7	28	34	8	27	73394.050	0.152	0.10	1.1	505.690	11.366
34	7	27	34	8	26	67113.470	-0.152	0.10	-1.1	1631.616	40.238
34	8	27	34	9	26	84267.550	-0.317	0.15	-1.5	717.848	16.475
34	8	26	34	9	25	83315.090	0.143	0.15	0.7	959.990	22.870
35	3	32	35	4	31	75035.300	0.353	0.15	1.7	-1717.437	-38.922
35	4	32	35	5	31	76697.550	-0.009	0.10	-0.1	-1345.942	-29.327
35	4	31	35	5	30	59957.570	0.346	0.15	1.6	-2547.678	-65.094
35	5	30	35	6	29	43491.920	0.404	0.15	1.9	-1558.488	-42.140
35	6	29	35	7	28	45620.560	-0.353	0.15	-1.6	1196.931	30.322
35	7	29	35	8	28	73327.240	0.100	0.10	0.7	467.641	10.964
35	8	28	35	9	27	83844.650	0.006	0.10	0.0	781.756	19.037
36	4	32	36	5	31	64282.900	0.115	0.10	0.8	-2691.728	-71.852
36	5	32	36	6	31	72109.710	0.028	0.10	0.2	-1300.878	-33.307
36	5	31	36	6	30	46473.220	-0.153	0.10	-1.1	-2135.817	-60.275
36	6	31	36	7	30	68983.840	0.278	0.10	2.0	-526.706	-14.935
36	6	30	36	7	29	44586.740	-0.086	0.10	-0.6	870.065	22.645
36	7	30	36	8	29	73387.340	0.043	0.10	0.3	398.987	9.625
36	7	29	36	8	28	62755.650	-0.204	0.10	-1.5	2223.258	61.245
36	9	27	36	10	26	94897.170	0.014	0.15	0.1	932.897	24.106
36	13	24	37	12	25	49767.840	-0.043	0.10	-0.3	-1581.303	-30.479
36	13	24	37	12	25	49767.840	-0.043	0.15	-0.2	-1581.303	-30.479
36	13	23	37	12	26	49767.840	0.068	0.10	0.5	-1581.242	-30.477
36	13	23	37	12	26	49767.840	0.068	0.15	0.3	-1581.242	-30.477
36	14	23	37	13	24	38954.320	-0.048	0.10	-0.3	-1357.940	-27.489
36	14	22	37	13	25	38954.320	-0.043	0.10	-0.3	-1357.937	-27.489
37	5	33	37	6	32	74687.550	0.407	0.15	1.9	-1500.530	-40.059
37	6	32	37	7	31	70464.960	0.009	0.10	0.1	-750.374	-21.928

37	6	31	37	7	30	44155.160	0.032	0.10	0.2	405.685	10.006
37	7	31	37	8	30	73598.590	0.341	0.15	1.6	295.086	7.085
37	7	30	37	8	29	60334.080	-0.227	0.10	-1.6	2466.487	71.493
37	14	24	38	13	25	43843.450	0.071	0.15	0.3	-1560.461	-32.338
37	14	23	38	13	26	43843.450	0.080	0.15	0.4	-1560.456	-32.338
38	3	35	38	4	34	84945.190	-0.066	0.15	-0.3	-1929.743	-47.948
38	4	34	38	5	33	72567.240	0.357	0.15	1.7	-2862.241	-82.742
38	5	34	38	6	33	77373.540	0.009	0.10	0.1	-1702.259	-47.311
38	5	33	38	6	32	53980.420	-0.195	0.10	-1.5	-3259.834	-100.426
38	6	32	38	7	31	44397.860	0.014	0.10	0.1	-193.040	-8.130
38	7	32	38	8	31	73981.920	0.152	0.10	1.1	152.139	3.076
38	7	31	38	8	30	57886.720	0.063	0.10	0.5	2618.732	79.650
38	14	25	39	13	26	48741.070	0.169	0.10	1.2	-1775.983	-38.147
38	14	24	39	13	27	48741.070	0.186	0.10	1.3	-1775.971	-38.147
38	15	24	39	14	25	38011.800	-0.143	0.10	-1.0	-1522.222	-35.232
38	15	23	39	14	26	38011.800	-0.143	0.10	-1.0	-1522.222	-35.232
39	3	36	39	4	35	88106.740	0.394	0.15	2.0	-2021.092	-51.637
39	4	35	39	5	34	76470.630	-0.011	0.10	-0.1	-2916.681	-87.410
39	5	34	39	6	33	58265.900	-0.055	0.10	-0.4	-3741.043	-120.284
39	6	34	39	7	33	74066.770	-0.037	0.10	-0.3	-1266.809	-39.813
39	7	33	39	8	32	74556.650	0.232	0.10	1.7	-32.505	-2.662
39	7	32	39	8	31	55546.420	-0.135	0.10	-1.0	2636.958	83.916
39	8	31	39	9	30	76875.130	-0.016	0.10	-0.1	2455.257	78.632
39	14	26	40	13	27	53647.820	0.364	0.15	1.7	-2005.233	-45.020
39	14	25	40	13	28	53647.820	0.396	0.15	1.8	-2005.210	-45.019
39	15	25	40	14	26	42863.940	-0.259	0.15	-1.2	-1745.848	-40.837
39	15	24	40	14	27	42863.940	-0.258	0.15	-1.2	-1745.847	-40.837
40	5	35	40	6	34	62730.230	-0.167	0.10	-1.4	-4135.742	-138.596
40	6	34	40	7	33	47040.060	-0.237	0.10	-1.8	-1744.417	-61.780
40	7	34	40	8	33	75336.950	0.324	0.15	1.5	-260.107	-10.357
40	7	33	40	8	32	53458.320	0.066	0.10	0.5	2484.454	82.426
40	8	32	40	9	31	74855.650	0.044	0.10	0.3	2915.052	98.160
40	15	26	41	14	27	47722.160	0.101	0.10	0.7	-1982.934	-47.535
40	15	25	41	14	28	47722.160	0.104	0.10	0.7	-1982.932	-47.535
41	4	37	41	5	36	83811.550	0.033	0.10	0.3	-3024.880	-96.790
41	8	33	41	9	32	72583.180	0.230	0.10	1.8	3393.318	119.837
42	4	38	42	5	37	87281.940	0.104	0.15	0.5	-3093.772	-102.014
42	5	38	42	6	37	88815.060	-0.074	0.10	-0.7	-2502.950	-80.430
42	7	36	42	8	35	77547.130	0.078	0.15	0.4	-841.502	-32.324
42	7	35	42	8	34	50583.270	0.132	0.10	1.0	1576.296	55.537
42	9	33	42	10	32	89934.750	-0.019	0.15	-0.1	2415.531	88.135
42	15	28	43	14	29	57456.090	0.174	0.10	1.2	-2500.277	-64.667
42	15	27	43	14	30	57456.090	0.183	0.10	1.3	-2500.269	-64.667
42	16	27	43	15	28	46706.390	-0.053	0.10	-0.4	-2202.170	-58.984
42	16	26	43	15	29	46706.390	-0.053	0.10	-0.4	-2202.170	-58.984
42	17	26	43	16	27	36124.840	-0.209	0.15	-1.0	-1880.287	-56.860
42	17	25	43	16	28	36124.840	-0.209	0.15	-1.0	-1880.287	-56.860
43	4	39	43	5	38	90644.800	-0.053	0.10	-0.7	-3177.719	-107.826
43	10	34	43	11	33	103924.560	-0.084	0.10	-0.7	1598.733	58.247
44	9	36	44	10	35	91488.880	0.229	0.10	1.7	1502.539	57.259
44	11	34	44	12	33	115507.970	-0.231	0.10	-2.1	1603.681	60.045
44	17	28	45	16	29	45690.600	0.073	0.10	0.5	-2433.819	-72.889
44	17	27	45	16	30	45690.600	0.074	0.10	0.5	-2433.819	-72.889
44	18	27	45	17	28	35176.270	-0.304	0.15	-1.4	-2074.497	-71.592
44	18	26	45	17	29	35176.270	-0.304	0.15	-1.4	-2074.497	-71.592
45	17	29	46	16	30	50475.020	0.270	0.10	1.9	-2732.965	-83.136
45	17	28	46	16	31	50475.020	0.270	0.10	1.9	-2732.965	-83.136
45	18	28	46	17	29	39924.640	0.026	0.10	0.2	-2368.770	-79.861
45	18	27	46	17	30	39924.640	0.026	0.10	0.2	-2368.770	-79.861
46	8	39	46	9	38	83758.530	-0.083	0.10	-1.1	-336.090	-18.054
46	10	37	46	11	36	102375.320	0.009	0.10	0.1	2023.767	84.598
46	11	36	46	12	35	114668.300	0.003	0.10	0.0	1939.548	79.925
46	15	32	47	14	33	77006.020	0.111	0.15	0.5	-3729.844	-117.594
46	15	31	47	14	34	77006.020	0.207	0.15	1.0	-3729.744	-117.589
47	16	32	48	15	33	70859.750	0.125	0.10	0.9	-3735.534	-120.439
47	16	31	48	15	34	70859.750	0.133	0.10	1.0	-3735.524	-120.439
47	19	29	48	18	30	38936.270	-0.340	0.15	-1.6	-2599.476	-98.902
47	19	28	48	18	31	38936.270	-0.340	0.15	-1.6	-2599.476	-98.902
48	18	31	49	17	32	54162.710	0.071	0.15	0.3	-3344.462	-114.699
48	18	30	49	17	33	54162.710	0.071	0.15	0.3	-3344.462	-114.699

48	19	30	49	18	31	43647.690	-0.026	0.15	-0.1	-2935.360-109.965
48	19	30	49	18	31	43647.690	-0.026	0.15	-0.1	-2935.360-109.965
48	19	29	49	18	32	43647.690	-0.026	0.15	-0.1	-2935.360-109.965
48	19	29	49	18	32	43647.690	-0.026	0.15	-0.1	-2935.360-109.965
49	17	33	50	16	34	69622.940	-0.141	0.10	-1.1	-4094.658-142.313
49	17	32	50	16	35	69622.940	-0.140	0.10	-1.1	-4094.656-142.313
49	19	31	50	18	32	48355.640	-0.323	0.15	-1.5	-3287.502-122.945
49	19	30	50	18	33	48355.640	-0.323	0.15	-1.5	-3287.502-122.945
50	17	34	51	16	35	74413.190	-0.108	0.10	-0.9	-4480.124-162.456
50	17	33	51	16	36	74413.190	-0.106	0.10	-0.9	-4480.121-162.456
50	18	33	51	17	34	63649.150	-0.171	0.10	-1.3	-4078.813-147.768
50	18	32	51	17	35	63649.150	-0.171	0.10	-1.3	-4078.813-147.768
50	19	32	51	18	33	53061.080	-0.172	0.15	-0.8	-3656.525-137.998
50	19	31	51	18	34	53061.080	-0.172	0.15	-0.8	-3656.525-137.998
51	19	33	52	18	34	57763.680	0.204	0.15	1.0	-4043.080-155.288
51	19	32	52	18	35	57763.680	0.204	0.15	1.0	-4043.080-155.288
51	20	32	52	19	33	47287.620	0.026	0.10	0.2	-3586.510-148.750
51	20	31	52	19	34	47287.620	0.026	0.10	0.2	-3586.510-148.750
51	21	31	52	20	32	36939.200	0.180	0.15	0.9	-3097.910-149.489
51	21	30	52	20	33	36939.200	0.180	0.15	0.9	-3097.910-149.489
52	19	34	53	18	35	62462.520	0.003	0.15	0.0	-4447.844-174.990
52	19	33	53	18	36	62462.520	0.003	0.15	0.0	-4447.844-174.990
55	22	34	56	21	35	45124.210	0.098	0.10	1.1	-4230.616-215.548
55	22	33	56	21	36	45124.210	0.098	0.10	1.1	-4230.616-215.548

rms deviation: 1.3228

Rotational constants (MHz) and kappa:

	7608.5723	2608.94813	2198.40201	-0.8482317
+-	0.0026	0.00071	0.00072	0.0000002

Inertial constants and defect (uA**2):

	66.422327	193.709898	229.884741	-30.24748
+-	0.000023	0.000053	0.000076	0.00006

Quartic distortion constants:

	6.442424	-36.44317	99.9412	2.136463	17.3434
+-	0.00073	0.0042	0.011	0.00033	0.013

Sextic and higher distortion constants:

	-0.0900085	1.06019	-5.41637	13.1693	-0.0362933
+-	0.00029	0.0025	0.020	0.049	0.00016

	-1.01578	0
+-	0.0098	fixed

Significant Digits and Correlation Matrix:

8	0.638	0.559	0.682	0.675	0.645
	9	0.579	0.716	0.506	0.358
		9	0.774	0.381	0.351
			7	0.346	0.629
				7	0.021
					6

0.065	0.009	0.466	0.255	0.368	-0.163	0.045	0.009
0.428	-0.081	0.297	0.393	0.047	0.097	0.383	-0.083
-0.410	-0.071	0.362	0.335	-0.014	0.166	-0.316	-0.094
-0.147	0.237	0.719	0.134	0.224	0.021	-0.170	0.207
0.254	-0.390	0.085	0.698	0.238	-0.202	0.314	-0.390
-0.065	0.176	0.521	-0.203	0.320	-0.033	-0.113	0.190
7	-0.296	-0.264	0.244	0.021	-0.062	0.946	-0.264
	6	0.600	-0.565	0.133	-0.049	-0.465	0.953
		6	-0.431	0.642	-0.434	-0.408	0.624
			6	-0.450	0.431	0.401	-0.617
				6	-0.944	-0.044	0.143
					6	-0.019	-0.051
						6	-0.483
							6

Table S18. Microwave Spectrum of the First Excited State of the Torsional Vibration (ν_{21}) of Conformer II of HC(O)OCH₂C≡N

Watson A-reduction

Total number: 655

Transition						obs. frequency	obs.- calc.	weight	t	distortion total	corrections higher	fixed
2	1	1	3	2	2	30068.290	-0.290	0.15	-1.3	-0.874	2.5E-4	
3	1	3	4	2	2	36777.980	-0.339	0.15	-1.5	-2.003	-1.0E-3	
3	1	2	4	2	3	34218.500	-0.407	0.15	-1.8	-0.188	4.1E-4	
4	2	2	5	2	3	23931.960	0.315	0.20	1.0	-2.507	-1.7E-3	
5	0	5	6	1	6	30236.660	-0.056	0.10	-0.4	0.328	4.7E-3	
5	0	5	6	0	6	27684.120	0.029	0.20	0.1	-3.940	-1.9E-3	
5	1	5	6	1	6	27043.030	-0.360	0.20	-1.2	-2.691	1.2E-3	
5	2	4	6	2	5	28230.520	0.017	0.10	0.1	-3.300	4.4E-5	
5	3	3	6	3	4	28411.280	0.004	0.10	0.0	-1.066	-2.6E-3	
5	3	2	6	4	3	66750.050	0.325	0.15	1.4	-14.633	0.014	
5	4	2	6	5	1	77722.510	0.134	0.15	0.6	-37.704	0.106	
5	4	1	6	5	2	77722.310	0.089	0.15	0.4	-37.703	0.106	
6	0	6	7	1	7	34045.590	0.217	0.15	1.0	-0.159	7.8E-3	
6	1	6	7	0	7	29526.500	0.154	0.10	1.0	-9.812	-9.5E-3	
6	1	5	7	2	6	45568.080	-0.099	0.10	-0.7	2.720	0.011	
6	1	5	7	1	6	34058.760	0.097	0.10	0.6	-11.136	-0.015	
6	2	5	7	2	6	32884.650	0.173	0.10	1.2	-6.022	-1.1E-3	
6	2	4	7	3	5	59674.730	-0.307	0.15	-1.4	-1.179	3.0E-3	
6	3	4	7	4	3	71498.490	0.294	0.15	1.3	-12.781	3.0E-3	
6	3	3	7	4	4	71442.770	-0.350	0.15	-1.6	-12.437	3.7E-3	
6	3	3	7	3	4	33240.300	-0.147	0.10	-1.0	-4.615	-4.3E-3	
6	4	3	7	5	2	82449.830	-0.142	0.20	-0.5	-33.593	0.070	
6	4	2	7	5	3	82449.030	-0.161	0.20	-0.5	-33.585	0.070	
7	1	7	7	2	6	21964.190	0.013	0.20	0.0	-3.032	-5.2E-3	
7	2	6	7	3	5	28085.660	0.037	0.20	0.1	0.673	-3.6E-3	
7	0	7	8	1	8	37888.710	-0.160	0.10	-1.1	-1.267	0.011	
7	0	7	8	0	8	36423.500	0.005	0.10	0.0	-7.439	-4.0E-3	
7	1	7	8	1	8	35922.590	0.121	0.10	0.8	-6.652	5.4E-4	
7	2	5	8	3	6	63755.440	-0.215	0.10	-1.4	1.294	0.012	
7	2	5	8	2	6	38833.730	0.012	0.10	0.1	-17.263	-0.029	
7	3	5	8	3	6	37915.840	-0.054	0.10	-0.4	-8.149	-4.8E-3	
7	3	4	8	3	5	38067.340	-0.069	0.10	-0.5	-9.663	-0.010	
7	4	4	8	4	5	37894.640	-0.048	0.15	-0.2	-2.664	-0.011	
7	5	3	8	5	4	37862.810	0.156	0.15	0.7	4.682	-0.046	
7	5	2	8	5	3	37862.910	0.168	0.15	0.7	4.681	-0.046	
7	6	2	8	7	1	109051.770	-0.069	0.10	-0.5	-118.240	0.752	
7	6	1	8	7	2	109051.770	-0.069	0.10	-0.5	-118.240	0.752	
8	2	7	8	3	6	28485.940	0.064	0.15	0.3	2.118	-4.4E-3	
8	0	8	9	1	9	41799.070	-0.056	0.10	-0.4	-3.230	0.014	
8	0	8	9	0	9	40737.640	-0.054	0.15	-0.2	-9.753	-5.3E-3	
8	1	8	9	0	9	39272.300	-0.019	0.10	-0.1	-15.925	-0.021	
8	1	8	9	1	9	40333.520	-0.231	0.10	-1.5	-9.402	-9.3E-4	
8	1	7	9	2	8	52357.200	-0.225	0.10	-1.5	6.105	0.040	
8	2	7	9	1	8	33220.280	-0.020	0.15	-0.1	-41.416	-0.093	
8	2	7	9	2	8	42121.480	-0.072	0.10	-0.5	-14.043	-9.4E-3	
8	2	6	9	3	7	67587.450	-0.032	0.10	-0.2	4.866	0.030	
8	2	6	9	2	7	43831.930	0.176	0.10	1.2	-25.699	-0.057	
8	3	6	9	4	5	80989.330	0.051	0.10	0.3	-11.394	-0.013	
8	3	6	9	3	7	42665.780	0.235	0.10	1.6	-13.691	-0.011	
8	3	5	9	4	6	80687.030	-0.002	0.10	-0.0	-8.603	-4.1E-3	
8	3	5	9	3	6	42935.520	-0.030	0.10	-0.2	-16.921	-0.025	
8	4	4	9	4	5	42670.100	0.061	0.20	0.2	-8.003	-0.012	
8	5	4	9	5	5	42611.720	0.090	0.15	0.4	0.609	-0.039	
8	5	3	9	5	4	42612.020	0.104	0.15	0.5	0.602	-0.039	
9	2	8	9	3	7	29030.110	0.241	0.15	1.1	2.470	-6.3E-3	
9	2	7	9	3	6	24306.970	0.159	0.20	0.5	24.877	0.065	
9	0	9	10	1	10	45789.600	-0.325	0.15	-1.4	-6.191	0.016	
9	0	9	10	0	10	45038.860	-0.072	0.10	-0.5	-12.642	-7.2E-3	

9	1	9	10	0	10	43977.100	-0.399	0.15	-1.8	-19.166	-0.027
9	1	9	10	1	10	44728.420	-0.073	0.10	-0.5	-12.714	-3.6E-3
9	1	8	10	2	9	55601.300	-0.248	0.10	-1.7	8.008	0.065
9	2	8	10	1	9	39147.750	-0.004	0.15	-0.0	-54.358	-0.147
9	2	8	10	3	7	77433.070	-0.228	0.10	-1.5	-30.150	-0.082
9	2	8	10	2	9	46700.380	0.085	0.10	0.6	-19.364	-0.018
9	2	7	10	3	8	71163.710	0.265	0.15	1.2	9.864	0.062
9	2	7	10	2	8	48806.880	0.152	0.10	1.0	-35.853	-0.099
9	3	7	10	3	8	47407.820	0.103	0.10	0.7	-20.701	-0.024
9	3	6	10	3	7	47852.440	0.093	0.10	0.6	-26.932	-0.055
9	4	6	10	4	7	47426.620	0.273	0.10	1.8	-14.666	-0.017
9	4	5	10	4	6	47453.970	-0.077	0.10	-0.5	-15.227	-0.020
9	5	5	10	6	4	107576.320	-0.239	0.15	-1.1	-52.901	0.085
9	5	5	10	5	6	47366.100	-0.070	0.20	-0.2	-5.197	-0.033
9	5	4	10	6	5	107575.920	-0.223	0.15	-1.0	-52.891	0.086
9	5	4	10	5	5	47366.900	-0.062	0.20	-0.2	-5.219	-0.033
9	6	4	10	7	3	118518.200	0.274	0.10	2.0	-101.058	0.443
9	6	4	10	6	5	47335.130	0.327	0.15	1.4	6.060	-0.108
9	6	3	10	7	4	118518.200	0.278	0.10	2.0	-101.058	0.443
9	6	3	10	6	4	47335.130	0.315	0.15	1.4	6.059	-0.108
10	2	9	10	3	8	29737.410	0.119	0.10	0.8	1.133	-0.012
10	4	7	10	5	6	49172.940	0.099	0.10	0.7	-9.291	4.7E-3
10	0	10	11	0	11	49338.460	-0.205	0.10	-1.4	-16.231	-0.010
10	1	10	11	0	11	48587.600	-0.072	0.10	-0.5	-22.683	-0.034
10	1	10	11	1	11	49109.120	0.131	0.10	0.9	-16.640	-8.0E-3
10	1	9	11	2	10	58803.440	0.282	0.10	1.9	9.455	0.098
10	2	9	11	1	10	45008.810	0.118	0.10	0.8	-67.725	-0.216
10	3	8	11	3	9	52137.560	-0.101	0.10	-0.7	-29.221	-0.046
10	3	7	11	3	8	52821.440	0.013	0.10	0.1	-40.202	-0.109
10	4	7	11	4	8	52201.760	0.182	0.10	1.2	-23.529	-0.032
11	2	10	11	3	9	30624.560	0.225	0.10	1.5	-2.549	-0.027
11	2	9	11	3	8	22432.950	0.088	0.10	0.6	41.166	0.159
11	3	8	11	4	7	36808.940	0.019	0.10	0.1	35.082	0.123
11	0	11	12	1	12	53999.210	0.246	0.15	1.1	-15.192	0.011
11	0	11	12	0	12	53642.500	-0.107	0.10	-0.7	-20.609	-0.016
11	1	11	12	0	12	53121.160	-0.129	0.10	-0.9	-26.653	-0.041
11	1	11	12	1	12	53477.680	0.033	0.10	0.2	-21.236	-0.015
11	1	10	12	1	11	56993.070	-0.056	0.10	-0.4	-38.336	-0.110
11	2	10	12	1	11	50751.120	-0.081	0.10	-0.5	-80.522	-0.294
11	2	10	12	2	11	55771.890	-0.150	0.10	-1.0	-32.539	-0.049
11	2	9	12	3	10	77604.070	0.036	0.10	0.2	24.815	0.193
11	3	9	12	3	10	56850.520	-0.130	0.10	-0.9	-39.251	-0.080
11	3	8	12	4	9	93686.400	-0.345	0.15	-1.5	2.708	0.074
11	3	8	12	3	9	57839.510	0.071	0.10	0.5	-57.047	-0.198
11	4	8	12	5	7	105999.580	0.228	0.15	1.0	-21.962	-0.040
11	4	8	12	4	9	56981.280	0.168	0.10	1.1	-34.549	-0.061
11	4	7	12	4	8	57080.980	0.164	0.20	0.5	-37.250	-0.080
11	5	7	12	6	6	117001.920	0.257	0.10	1.8	-44.062	-0.024
11	5	7	12	5	8	56893.930	0.175	0.20	0.6	-22.975	-0.042
11	6	6	12	6	7	56835.080	0.063	0.10	0.4	-8.947	-0.082
11	6	5	12	6	6	56835.080	-0.046	0.10	-0.3	-8.952	-0.082
11	7	5	12	7	6	56807.480	0.365	0.15	1.6	7.007	-0.223
11	7	4	12	7	5	56807.480	0.364	0.15	1.6	7.007	-0.223
12	1	11	12	2	10	17741.490	0.174	0.10	1.2	-46.692	-0.246
12	2	11	12	3	10	31703.230	0.285	0.15	1.3	-9.261	-0.059
12	2	10	12	3	9	21650.620	-0.116	0.10	-0.8	44.718	0.201
12	3	10	12	4	9	38515.590	0.016	0.10	0.1	19.059	0.040
12	3	9	12	4	8	36050.220	-0.078	0.10	-0.5	54.880	0.241
12	0	12	13	1	13	58193.320	0.213	0.20	0.7	-21.151	2.2E-3
12	0	12	13	0	13	57952.480	-0.051	0.10	-0.3	-25.835	-0.024
12	1	12	13	0	13	57596.060	-0.113	0.10	-0.7	-31.252	-0.051
12	1	12	13	1	13	57836.650	-0.100	0.10	-0.7	-26.568	-0.025
12	1	11	13	2	12	65285.820	0.062	0.10	0.4	7.645	0.174
12	1	11	13	1	12	61353.650	-0.051	0.10	-0.3	-43.906	-0.130
12	2	11	13	1	12	56332.620	-0.243	0.10	-1.6	-91.889	-0.376
12	2	11	13	2	12	60264.920	0.000	0.10	0.0	-40.338	-0.072
12	2	10	13	3	11	80524.610	-0.136	0.10	-0.9	34.672	0.304
12	2	10	13	2	11	63438.480	0.210	0.15	0.9	-74.560	-0.342
12	3	10	13	4	9	100653.130	0.006	0.10	0.0	-38.983	-0.142
12	3	10	13	3	11	61542.110	-0.167	0.10	-1.1	-50.742	-0.128

12	3	9	13	4	10	97609.590	-0.204	0.10	-1.4	11.888	0.160
12	4	9	13	5	8	110695.030	0.159	0.10	1.1	-23.242	-0.049
12	4	9	13	4	10	61762.640	0.152	0.20	0.5	-47.867	-0.111
12	4	8	13	5	9	110474.770	-0.267	0.10	-1.8	-17.740	-0.013
12	4	8	13	4	9	61934.840	0.282	0.15	1.2	-53.166	-0.152
12	5	7	13	6	8	121691.740	-0.029	0.10	-0.2	-40.718	-0.059
12	5	7	13	5	8	61676.600	-0.032	0.10	-0.2	-35.829	-0.070
12	7	6	13	7	7	61553.230	-0.090	0.15	-0.4	-2.330	-0.196
12	7	5	13	7	6	61553.230	-0.095	0.15	-0.4	-2.331	-0.196
13	1	12	13	2	11	19825.950	0.066	0.10	0.5	-77.346	-0.457
13	2	12	13	3	11	32980.450	0.147	0.10	1.0	-19.666	-0.115
13	3	11	13	4	10	38735.520	-0.265	0.10	-1.8	21.934	0.057
13	3	10	13	4	9	35090.810	-0.004	0.10	-0.0	79.152	0.421
13	4	10	13	5	9	48915.240	-0.300	0.20	-1.0	25.252	0.067
13	4	9	13	5	8	48557.220	-0.101	0.10	-0.7	34.799	0.134
13	0	13	14	1	14	62428.950	0.061	0.10	0.4	-28.023	-0.012
13	0	13	14	0	14	62268.160	0.037	0.10	0.2	-31.954	-0.037
13	1	13	14	0	14	62027.440	-0.106	0.10	-0.7	-36.638	-0.064
13	1	13	14	1	14	62188.120	-0.192	0.10	-1.3	-32.707	-0.038
13	1	12	14	1	13	65659.560	-0.189	0.10	-1.3	-49.840	-0.149
13	2	12	14	1	13	61727.710	0.017	0.10	0.1	-101.392	-0.453
13	2	12	14	2	13	64730.450	0.013	0.10	0.1	-48.927	-0.100
13	2	11	14	2	12	68182.360	0.192	0.10	1.3	-88.906	-0.463
13	3	11	14	2	12	51095.840	0.148	0.10	1.0	-198.138	-1.109
13	3	10	14	4	11	101258.170	-0.041	0.10	-0.3	25.757	0.306
13	4	10	14	4	11	66542.860	0.401	0.15	1.8	-63.569	-0.187
13	4	9	14	4	10	66823.900	-0.216	0.10	-1.4	-73.310	-0.271
13	5	8	14	5	9	66465.570	-0.163	0.10	-1.1	-51.497	-0.124
13	6	8	14	6	9	66353.110	0.161	0.20	0.5	-33.463	-0.091
13	6	7	14	6	8	66353.710	0.109	0.20	0.4	-33.501	-0.092
13	7	7	14	7	8	66302.340	-0.041	0.15	-0.2	-14.190	-0.175
13	7	6	14	7	7	66302.340	-0.055	0.15	-0.2	-14.191	-0.175
14	2	12	14	3	11	20889.300	0.208	0.10	1.4	29.777	0.154
14	3	12	14	4	11	39069.700	0.138	0.10	0.9	21.978	0.063
14	3	11	14	4	10	33950.070	-0.109	0.10	-0.7	106.811	0.669
14	4	11	14	5	10	48820.300	-0.321	0.15	-1.4	38.160	0.137
14	0	14	15	1	15	66694.940	0.171	0.10	1.1	-35.794	-0.032
14	0	14	15	0	15	66588.240	0.002	0.10	0.0	-39.012	-0.056
14	1	14	15	0	15	66427.230	-0.242	0.10	-1.6	-42.943	-0.081
14	1	14	15	1	15	66533.950	-0.054	0.10	-0.4	-39.725	-0.058
14	1	13	15	2	14	72173.160	-0.085	0.10	-0.6	-5.858	0.220
14	2	13	15	1	14	66928.680	-0.324	0.15	-1.4	-109.139	-0.520
14	2	12	15	2	13	72845.300	0.190	0.10	1.3	-102.967	-0.598
14	3	12	15	2	13	57731.990	-0.131	0.10	-0.9	-237.493	-1.514
14	3	11	15	4	12	104610.890	0.327	0.15	1.5	45.055	0.531
14	3	11	15	3	12	73026.950	0.076	0.10	0.5	-126.983	-0.769
14	4	11	15	5	10	120123.200	-0.148	0.15	-0.7	-33.892	-0.093
14	4	11	15	4	12	71317.160	0.057	0.10	0.4	-81.671	-0.295
14	5	10	15	5	11	71233.700	-0.173	0.10	-1.1	-68.847	-0.199
14	5	9	15	5	10	71267.710	0.019	0.10	0.1	-70.589	-0.217
14	7	8	15	7	9	71054.390	-0.100	0.10	-0.7	-28.820	-0.168
14	7	7	15	7	8	71054.390	-0.138	0.10	-0.9	-28.823	-0.168
15	2	14	15	3	13	36134.950	0.190	0.10	1.3	-53.780	-0.349
15	2	13	15	3	12	21071.030	0.173	0.10	1.1	5.761	-0.018
15	3	13	15	4	12	39540.200	0.248	0.10	1.7	18.058	0.043
15	3	12	15	4	11	32679.790	0.095	0.10	0.6	135.281	0.979
15	4	12	15	5	11	48737.240	-0.151	0.10	-1.0	50.985	0.232
15	4	11	15	5	10	47710.320	0.081	0.10	0.5	84.536	0.523
15	0	15	16	0	16	70911.410	-0.165	0.10	-1.1	-47.055	-0.082
15	1	15	16	1	16	70874.930	-0.212	0.15	-0.9	-47.694	-0.084
15	1	14	16	2	15	75828.830	-0.258	0.10	-1.7	-17.751	0.214
15	2	14	16	1	15	71946.960	-0.241	0.10	-1.6	-115.691	-0.576
15	2	14	16	2	15	73587.370	-0.221	0.10	-1.5	-68.567	-0.173
15	2	13	16	3	14	88568.630	-0.015	0.10	-0.1	66.707	0.864
15	3	13	16	4	12	117372.610	-0.037	0.10	-0.3	-148.250	-1.020
15	3	12	16	3	13	78056.730	0.228	0.10	1.5	-154.748	-1.081
15	4	12	16	4	13	76082.190	0.182	0.10	1.2	-102.121	-0.442
15	4	11	16	4	12	76736.840	0.152	0.10	1.0	-129.551	-0.742
15	5	11	16	5	12	76025.340	-0.182	0.10	-1.2	-90.230	-0.326
15	5	10	16	5	11	76085.520	0.098	0.10	0.6	-93.666	-0.365

15	6	9	16	6	10	75893.830	-0.146	0.15	-0.6	-69.826	-0.203
15	7	9	16	7	10	75809.710	-0.126	0.15	-0.6	-46.483	-0.183
15	7	8	16	7	9	75809.810	-0.117	0.15	-0.5	-46.491	-0.184
15	8	8	16	8	9	75768.360	0.240	0.10	1.6	-21.199	-0.340
15	8	7	16	8	8	75768.360	0.238	0.10	1.6	-21.199	-0.340
16	2	15	16	3	14	38001.320	0.098	0.10	0.7	-78.247	-0.552
16	2	14	16	3	13	21706.820	0.084	0.10	0.6	-32.923	-0.363
16	3	14	16	4	13	40167.700	-0.208	0.15	-0.9	8.971	-0.023
16	3	13	16	4	12	31359.960	0.079	0.10	0.5	160.478	1.319
16	4	13	16	5	12	48680.690	-0.214	0.10	-1.4	62.876	0.348
16	4	12	16	5	11	47059.090	0.117	0.10	0.8	120.421	0.899
16	0	16	17	1	17	75283.160	0.339	0.15	1.5	-54.107	-0.098
16	0	16	17	0	17	75236.950	-0.016	0.20	-0.1	-56.135	-0.116
16	1	16	17	0	17	75166.720	-0.147	0.10	-1.0	-58.713	-0.138
16	1	16	17	1	17	75212.860	0.138	0.10	0.9	-56.685	-0.119
16	1	15	17	2	16	79624.590	-0.337	0.15	-1.5	-32.610	0.184
16	1	15	17	1	16	78444.400	-0.137	0.10	-0.9	-74.710	-0.218
16	2	15	17	1	16	76804.120	-0.027	0.10	-0.2	-121.834	-0.621
16	2	15	17	2	16	77984.400	-0.137	0.10	-0.9	-79.734	-0.219
16	2	14	17	3	15	91177.350	0.058	0.10	0.4	73.429	1.104
16	3	14	17	3	15	80029.050	-0.220	0.15	-1.0	-109.342	-0.495
16	3	13	17	4	14	110441.780	0.073	0.10	0.5	99.873	1.307
16	3	13	17	3	14	83034.000	0.066	0.10	0.4	-183.544	-1.457
16	4	13	17	4	14	80832.570	0.057	0.10	0.4	-124.792	-0.633
16	4	12	17	4	13	81766.320	-0.054	0.10	-0.4	-166.897	-1.146
16	5	12	17	5	13	80821.340	0.238	0.10	1.6	-114.986	-0.509
16	5	11	17	5	12	80922.590	-0.118	0.10	-0.8	-121.428	-0.589
16	6	11	17	6	12	80668.400	0.231	0.10	1.5	-92.767	-0.320
16	6	10	17	6	11	80673.800	-0.149	0.10	-1.0	-93.227	-0.327
16	7	10	17	7	11	80568.650	0.045	0.15	0.2	-67.455	-0.233
16	7	9	17	7	10	80568.850	0.039	0.15	0.2	-67.475	-0.234
16	8	9	17	8	10	80515.410	-0.007	0.10	-0.0	-40.051	-0.326
16	8	8	17	8	9	80515.410	-0.012	0.10	-0.1	-40.052	-0.326
16	10	7	17	10	8	80484.810	0.243	0.10	1.6	22.252	-1.341
16	10	6	17	10	7	80484.810	0.243	0.10	1.6	22.252	-1.341
16	11	6	17	11	7	80491.400	0.109	0.30	0.2	57.414	-2.439
16	11	5	17	11	6	80491.400	0.109	0.30	0.2	57.414	-2.439
16	13	4	17	13	5	80531.630	0.318	0.15	1.4	135.740	-6.332
16	13	3	17	13	4	80531.630	0.318	0.15	1.4	135.740	-6.332
17	2	16	17	3	15	40046.030	0.075	0.10	0.5	-107.855	-0.828
17	2	15	17	3	14	22834.680	-0.072	0.10	-0.5	-88.720	-0.954
17	3	14	17	4	13	30092.610	0.289	0.10	1.9	177.126	1.629
17	4	14	17	5	13	48669.240	-0.253	0.10	-1.7	72.682	0.472
17	4	13	17	5	12	46215.380	0.073	0.10	0.5	165.890	1.456
17	5	13	17	6	12	59535.150	-0.286	0.20	-0.9	73.419	0.418
17	0	17	18	1	18	79593.270	-0.047	0.15	-0.2	-64.737	-0.146
17	0	17	18	0	18	79563.620	0.150	0.15	0.7	-66.308	-0.162
17	1	17	18	0	18	79517.590	-0.026	0.10	-0.2	-68.337	-0.181
17	1	16	18	2	17	83544.770	0.082	0.10	0.5	-49.815	0.128
17	2	16	18	1	17	81526.720	-0.165	0.10	-1.1	-128.363	-0.659
17	2	16	18	2	17	82364.320	0.022	0.10	0.1	-91.915	-0.274
17	2	15	18	3	16	93843.200	-0.035	0.10	-0.2	74.601	1.337
17	3	15	18	3	16	84571.980	0.120	0.10	0.8	-126.575	-0.634
17	3	14	18	3	15	87944.520	0.077	0.10	0.5	-212.619	-1.890
17	3	14	18	4	15	112971.660	-0.094	0.10	-0.7	133.918	1.891
17	4	13	18	4	14	86840.550	0.228	0.10	1.5	-210.423	-1.699
17	5	13	18	5	14	85618.320	-0.292	0.10	-1.9	-143.228	-0.761
17	5	12	18	5	13	85784.600	0.308	0.15	1.4	-154.750	-0.918
17	6	12	18	6	13	85451.070	0.267	0.10	1.8	-119.701	-0.503
17	7	11	18	7	12	85330.950	-0.023	0.15	-0.1	-92.026	-0.331
17	7	10	18	7	11	85331.350	-0.064	0.10	-0.4	-92.073	-0.332
17	8	10	18	8	11	85264.640	-0.056	0.10	-0.4	-62.335	-0.343
17	8	9	18	8	10	85264.640	-0.068	0.10	-0.4	-62.337	-0.343
17	9	9	18	9	10	85231.960	0.032	0.10	0.2	-30.257	-0.613
17	9	8	18	9	9	85231.960	0.032	0.10	0.2	-30.257	-0.613
17	10	8	18	10	9	85221.040	0.293	0.10	1.9	4.497	-1.225
17	10	7	18	10	8	85221.040	0.293	0.10	1.9	4.497	-1.225
18	2	17	18	3	16	42253.620	0.103	0.10	0.7	-142.515	-1.188
18	2	16	18	3	15	24475.090	0.182	0.10	1.2	-163.265	-1.866
18	3	16	18	4	15	41963.130	-0.141	0.10	-0.9	-29.403	-0.399

18	3	15	18	4	14	28988.160	-0.039	0.10	-0.3	179.322	1.820
18	4	15	18	5	14	48724.100	-0.025	0.10	-0.2	78.953	0.583
18	4	14	18	5	13	45159.190	-0.087	0.10	-0.6	221.563	2.237
18	0	18	19	1	19	83909.850	0.139	0.10	0.9	-76.434	-0.208
18	0	18	19	0	19	83890.280	-0.086	0.10	-0.6	-77.634	-0.221
18	1	18	19	0	19	83860.520	0.001	0.10	0.0	-79.205	-0.237
18	1	18	19	1	19	83879.720	-0.144	0.10	-1.0	-78.005	-0.224
18	1	17	19	1	18	86979.920	-0.181	0.10	-1.2	-99.501	-0.310
18	2	17	19	2	18	86729.960	0.205	0.10	1.4	-105.219	-0.337
18	3	16	19	3	17	89082.440	0.215	0.10	1.4	-144.673	-0.789
18	5	14	19	5	15	90415.160	-0.246	0.10	-1.6	-174.986	-1.095
18	6	13	19	6	14	90238.790	0.001	0.10	0.0	-150.707	-0.766
18	6	12	19	6	13	90258.250	-0.025	0.10	-0.2	-152.580	-0.796
18	7	12	19	7	13	90097.140	0.035	0.15	0.2	-120.501	-0.494
18	7	11	19	7	12	90098.040	0.035	0.15	0.2	-120.606	-0.495
18	8	11	19	8	12	90016.090	0.053	0.10	0.4	-88.327	-0.407
18	8	10	19	8	11	90016.090	0.025	0.10	0.2	-88.331	-0.407
18	9	10	19	9	11	89974.020	-0.010	0.10	-0.1	-53.866	-0.587
18	9	9	19	9	10	89974.020	-0.010	0.10	-0.1	-53.866	-0.587
18	10	9	19	10	10	89957.190	0.125	0.15	0.6	-16.723	-1.120
18	10	8	19	10	9	89957.190	0.125	0.15	0.6	-16.723	-1.120
18	11	8	19	11	9	89957.290	-0.011	0.15	-0.0	23.276	-2.108
18	11	7	19	11	8	89957.290	-0.011	0.15	-0.0	23.276	-2.108
18	12	7	19	12	8	89970.250	0.161	0.10	1.1	66.181	-3.667
18	12	6	19	12	7	89970.250	0.161	0.10	1.1	66.181	-3.667
19	1	19	19	2	18	50510.700	-0.055	0.20	-0.2	-182.341	-0.685
19	2	18	19	3	17	44606.000	0.014	0.15	0.1	-181.970	-1.641
19	2	17	19	3	16	26625.640	0.089	0.10	0.6	-256.587	-3.167
19	3	17	19	4	16	43153.290	0.184	0.10	1.2	-60.739	-0.774
19	3	16	19	4	15	28156.390	0.064	0.10	0.4	161.196	1.771
19	4	16	19	5	15	48867.420	-0.051	0.10	-0.3	79.977	0.653
19	4	15	19	5	14	43889.840	0.097	0.10	0.6	286.085	3.267
19	5	15	19	6	14	59190.840	-0.169	0.10	-1.1	121.225	1.003
19	0	19	20	1	20	88229.770	0.164	0.10	1.1	-89.268	-0.285
19	0	19	20	0	20	88216.970	-0.143	0.10	-1.0	-90.174	-0.296
19	1	19	20	0	20	88197.350	-0.417	0.15	-1.8	-91.374	-0.310
19	1	19	20	1	20	88210.280	0.019	0.10	0.1	-90.468	-0.299
19	1	18	20	2	19	91670.710	0.092	0.10	0.6	-89.025	-0.054
19	1	18	20	1	19	91263.130	-0.019	0.20	-0.1	-114.364	-0.378
19	2	18	20	1	19	90676.020	-0.061	0.10	-0.4	-145.094	-0.736
19	2	18	20	2	19	91083.600	0.049	0.10	0.3	-119.756	-0.412
19	2	17	20	3	18	99556.370	0.167	0.10	1.1	52.148	1.630
19	2	17	20	2	18	94890.600	0.172	0.10	1.1	-158.103	-1.144
19	4	15	20	4	16	97061.280	0.373	0.20	1.2	-311.687	-3.309
19	5	15	20	5	16	95208.490	0.282	0.10	1.9	-210.192	-1.523
19	5	14	20	5	15	95603.450	0.009	0.10	0.1	-242.467	-2.049
19	6	14	20	6	15	95031.850	0.104	0.10	0.7	-186.056	-1.130
19	6	13	20	6	14	95065.720	0.187	0.10	1.2	-189.601	-1.189
19	7	13	20	7	14	94867.070	-0.071	0.20	-0.2	-153.200	-0.739
19	7	12	20	7	13	94868.870	-0.033	0.20	-0.1	-153.424	-0.743
19	8	12	20	8	13	94769.600	0.084	0.10	0.6	-118.317	-0.535
19	8	11	20	8	12	94769.600	0.022	0.10	0.1	-118.326	-0.535
19	9	11	20	9	12	94716.970	-0.088	0.10	-0.6	-81.308	-0.605
19	9	10	20	9	11	94716.970	-0.089	0.10	-0.6	-81.309	-0.605
19	10	10	20	10	11	94693.160	-0.323	0.15	-1.4	-41.656	-1.038
19	10	9	20	10	10	94693.160	-0.323	0.15	-1.4	-41.656	-1.038
19	11	9	20	11	10	94689.450	-0.156	0.10	-1.0	0.896	-1.941
19	11	8	20	11	9	94689.450	-0.156	0.10	-1.0	0.896	-1.941
19	12	8	20	12	9	94699.970	-0.032	0.20	-0.1	46.439	-3.434
19	12	7	20	12	8	94699.970	-0.032	0.20	-0.1	46.439	-3.434
19	13	7	20	13	8	94721.550	0.290	0.20	1.0	94.972	-5.648
19	13	6	20	13	7	94721.550	0.290	0.20	1.0	94.972	-5.648
19	14	6	20	14	7	94751.130	0.020	0.10	0.1	146.437	-8.731
19	14	5	20	14	6	94751.130	0.020	0.10	0.1	146.437	-8.731
20	2	18	20	3	17	29259.110	0.030	0.10	0.2	-366.399	-4.898
20	3	18	20	4	17	44544.260	-0.146	0.10	-1.0	-101.178	-1.320
20	3	17	20	4	16	27693.330	0.054	0.10	0.4	117.424	1.336
20	4	17	20	5	16	49122.660	-0.111	0.10	-0.7	73.847	0.638
20	4	16	20	5	15	42432.210	-0.068	0.10	-0.5	355.304	4.526
20	5	15	20	6	14	58038.420	0.202	0.10	1.4	214.761	2.412

20	0	20	21	1	21	92551.570	0.213	0.10	1.4	-103.316	-0.381
20	1	20	21	0	21	92530.440	-0.379	0.15	-1.7	-104.898	-0.401
20	1	19	21	2	20	95835.660	0.203	0.10	1.3	-110.298	-0.177
20	1	19	21	1	20	95555.060	0.039	0.10	0.3	-130.798	-0.463
20	2	19	21	1	20	95147.550	-0.001	0.10	-0.0	-156.136	-0.787
20	2	19	21	2	20	95427.890	-0.098	0.10	-0.6	-135.637	-0.500
20	2	18	21	3	19	102677.770	0.008	0.10	0.1	26.775	1.623
20	2	18	21	2	19	99116.780	-0.188	0.10	-1.3	-170.456	-1.221
20	3	18	21	3	19	98011.950	-0.036	0.10	-0.2	-183.476	-1.151
20	4	16	21	4	17	102162.340	0.037	0.10	0.2	-365.934	-4.362
20	5	16	21	5	17	99993.280	0.076	0.10	0.5	-248.676	-2.056
20	5	15	21	5	16	100572.780	-0.249	0.10	-1.7	-299.260	-2.955
20	6	15	21	6	16	99828.570	-0.397	0.15	-1.7	-225.984	-1.614
20	6	14	21	6	15	99885.920	0.315	0.15	1.4	-232.436	-1.732
20	7	14	21	7	15	99641.390	0.204	0.10	1.4	-190.454	-1.089
20	8	13	21	8	14	99524.890	-0.316	0.15	-1.4	-152.609	-0.746
20	8	12	21	8	13	99524.990	-0.348	0.15	-1.5	-152.631	-0.746
20	10	11	21	10	12	99429.830	-0.130	0.20	-0.4	-70.558	-0.996
20	10	10	21	10	11	99429.830	-0.130	0.20	-0.4	-70.558	-0.996
20	11	10	21	11	11	99421.520	0.168	0.10	1.1	-25.347	-1.791
20	11	9	21	11	10	99421.520	0.168	0.10	1.1	-25.347	-1.791
20	12	9	21	12	10	99428.630	-0.273	0.20	-0.9	22.921	-3.193
20	12	8	21	12	9	99428.630	-0.273	0.20	-0.9	22.921	-3.193
20	13	8	21	13	9	99448.950	0.278	0.20	0.9	74.275	-5.341
20	13	7	21	13	8	99448.950	0.278	0.20	0.9	74.275	-5.341
20	14	7	21	14	8	99478.230	0.181	0.20	0.6	128.673	-8.388
20	14	6	21	14	7	99478.230	0.181	0.20	0.6	128.673	-8.388
20	15	6	21	15	7	99514.900	-0.324	0.15	-1.5	186.026	-12.498
20	15	5	21	15	6	99514.900	-0.324	0.15	-1.5	186.026	-12.498
21	1	20	21	2	19	46387.830	0.144	0.10	1.0	-450.409	-5.400
21	2	20	21	3	19	49668.200	0.158	0.10	1.1	-273.678	-2.842
21	3	18	21	4	17	27677.460	0.022	0.10	0.1	43.454	0.351
21	4	18	21	5	17	49512.540	-0.057	0.10	-0.4	58.565	0.485
21	5	17	21	6	16	58850.640	0.331	0.15	1.5	168.053	1.838
21	5	16	21	6	15	57350.950	0.156	0.10	1.0	281.585	3.635
21	0	21	22	1	22	96874.140	0.304	0.15	1.3	-118.655	-0.499
21	1	21	22	0	22	96860.450	-0.176	0.10	-1.2	-119.832	-0.516
21	1	20	22	2	21	100045.520	0.100	0.10	0.7	-132.466	-0.320
21	2	20	22	1	21	99573.160	-0.197	0.10	-1.3	-169.282	-0.854
21	2	20	22	2	21	99764.710	-0.274	0.20	-0.9	-152.965	-0.606
21	2	19	22	2	20	103326.410	0.043	0.20	0.1	-185.864	-1.318
21	3	19	22	2	20	99765.300	-0.274	0.10	-1.8	-383.095	-4.162
21	3	18	22	3	19	106735.080	-0.410	0.15	-1.8	-312.311	-3.839
21	4	18	22	4	19	104220.950	-0.183	0.20	-0.6	-263.760	-2.349
21	4	17	22	4	18	107225.280	0.229	0.10	1.5	-420.180	-5.559
21	5	17	22	5	18	104765.990	-0.197	0.10	-1.3	-290.166	-2.704
21	5	16	22	5	17	105588.770	0.129	0.10	0.9	-365.964	-4.170
21	6	16	22	6	17	104629.090	-0.259	0.10	-1.7	-270.667	-2.244
21	6	15	22	6	16	104721.430	0.075	0.10	0.5	-281.993	-2.466
21	8	14	22	8	15	104283.290	0.113	0.15	0.5	-191.525	-1.063
21	8	13	22	8	14	104283.590	0.148	0.15	0.7	-191.572	-1.064
21	9	13	22	9	14	104205.800	-0.098	0.20	-0.3	-148.810	-0.846
21	9	12	22	9	13	104205.800	-0.106	0.20	-0.3	-148.811	-0.846
21	10	12	22	10	13	104166.400	-0.045	0.10	-0.3	-103.697	-1.012
21	10	11	22	10	12	104166.400	-0.046	0.10	-0.3	-103.697	-1.012
21	11	11	22	11	12	104152.280	-0.182	0.10	-1.2	-55.704	-1.674
21	11	10	22	11	11	104152.280	-0.182	0.10	-1.2	-55.704	-1.674
21	13	9	22	13	10	104174.550	-0.070	0.10	-0.5	49.645	-5.016
21	13	8	22	13	9	104174.550	-0.070	0.10	-0.5	49.645	-5.016
21	14	8	22	14	9	104203.520	0.267	0.20	0.9	107.048	-7.998
21	14	7	22	14	8	104203.520	0.267	0.20	0.9	107.048	-7.998
22	2	21	22	3	20	52338.840	-0.121	0.10	-0.8	-325.043	-3.592
22	2	20	22	3	19	35729.210	-0.166	0.10	-1.1	-614.354	-9.575
22	3	20	22	4	19	47921.160	0.131	0.10	0.9	-210.525	-3.064
22	3	19	22	4	18	28166.840	-0.159	0.10	-1.1	-64.414	-1.369
22	4	18	22	5	17	39206.610	0.018	0.10	0.1	476.194	7.323
22	5	18	22	6	17	58713.410	-0.061	0.10	-0.4	187.552	2.299
22	5	17	22	6	16	56483.560	0.052	0.10	0.3	365.555	5.338
22	6	17	22	7	16	69977.450	-0.049	0.10	-0.3	194.006	2.150
22	6	16	22	7	15	69766.550	0.247	0.15	1.1	217.207	2.569

22	7	16	22	8	15	81427.500	-0.325	0.15	-1.5	136.038	1.158
22	0	22	23	1	23	101196.410	0.137	0.10	0.9	-135.362	-0.643
22	1	22	23	0	23	101187.720	-0.075	0.10	-0.5	-136.229	-0.657
22	1	21	23	2	22	104287.900	0.200	0.10	1.3	-155.521	-0.484
22	2	21	23	1	22	103965.940	0.007	0.10	0.0	-184.643	-0.943
22	2	21	23	2	22	104095.810	-0.263	0.10	-1.8	-171.837	-0.732
22	2	20	23	3	21	109506.920	0.318	0.15	1.4	-47.573	1.226
22	2	20	23	2	21	107534.650	0.346	0.15	1.5	-204.789	-1.449
22	3	20	23	2	21	104863.980	0.004	0.10	0.0	-383.553	-4.255
22	3	20	23	3	21	106835.880	-0.394	0.15	-1.7	-226.337	-1.580
22	4	19	23	4	20	108804.620	-0.111	0.10	-0.7	-294.957	-2.840
22	5	18	23	5	19	109522.410	-0.346	0.15	-1.5	-334.303	-3.472
22	5	17	23	5	18	110650.840	0.327	0.15	1.4	-442.721	-5.750
22	6	17	23	6	18	109431.630	0.312	0.15	1.4	-320.197	-3.042
22	6	16	23	6	17	109576.020	-0.404	0.15	-1.8	-339.401	-3.448
22	7	16	23	7	17	109201.220	-0.179	0.10	-1.2	-279.987	-2.210
22	7	15	23	7	16	109212.170	0.173	0.10	1.2	-281.702	-2.248
22	9	14	23	9	15	108951.400	-0.300	0.15	-1.3	-189.460	-1.113
22	9	13	23	9	14	108951.400	-0.318	0.15	-1.4	-189.464	-1.113
22	10	13	23	10	14	108902.880	-0.006	0.10	-0.0	-141.350	-1.108
22	10	12	23	10	13	108902.880	-0.007	0.10	-0.0	-141.350	-1.108
22	11	12	23	11	13	108882.910	0.058	0.20	0.2	-90.435	-1.611
22	11	11	23	11	12	108882.910	0.058	0.20	0.2	-90.435	-1.611
22	12	11	23	12	12	108883.310	0.035	0.20	0.1	-36.409	-2.754
22	12	10	23	12	11	108883.310	0.035	0.20	0.1	-36.409	-2.754
22	13	10	23	13	11	108898.830	-0.158	0.10	-1.1	20.844	-4.687
22	13	9	23	13	10	108898.830	-0.158	0.10	-1.1	20.844	-4.687
22	14	9	23	14	10	108926.590	-0.005	0.10	-0.0	81.333	-7.574
22	14	8	23	14	9	108926.590	-0.005	0.10	-0.0	81.333	-7.574
22	15	8	23	15	9	108963.910	0.153	0.10	1.1	144.995	-11.595
22	15	7	23	15	8	108963.910	0.153	0.10	1.1	144.995	-11.595
22	16	7	23	16	8	109008.720	-0.068	0.10	-0.5	211.719	-16.944
22	16	6	23	16	7	109008.720	-0.068	0.10	-0.5	211.719	-16.944
23	1	22	23	2	21	53236.960	-0.043	0.10	-0.3	-523.953	-6.904
23	3	20	23	4	19	29199.910	-0.002	0.10	-0.0	-208.718	-4.014
23	4	20	23	5	19	50775.420	-0.256	0.10	-1.7	-7.187	-0.502
23	5	19	23	6	18	58621.820	-0.213	0.10	-1.4	201.659	2.729
23	5	18	23	6	17	55409.530	0.111	0.10	0.7	468.875	7.641
23	6	17	23	7	16	69401.890	0.015	0.20	0.0	274.906	3.769
23	7	17	23	8	16	81270.240	0.326	0.15	1.5	180.626	1.856
23	1	23	24	0	24	105512.460	-0.244	0.15	-1.1	-154.146	-0.828
23	1	22	24	1	23	108464.610	-0.052	0.10	-0.3	-189.461	-0.848
23	2	22	24	1	23	108334.570	0.048	0.10	0.3	-202.267	-1.058
23	2	22	24	2	23	108422.810	0.370	0.15	1.6	-192.340	-0.882
23	2	21	24	3	22	113188.340	-0.149	0.10	-1.0	-92.461	0.851
23	3	21	24	3	22	111216.060	-0.131	0.10	-0.9	-249.676	-1.824
23	3	20	24	3	21	115563.210	0.412	0.15	1.8	-341.667	-4.530
23	4	20	24	4	21	113353.880	0.239	0.10	1.6	-326.853	-3.373
23	6	18	24	6	19	114232.990	0.210	0.15	0.9	-374.557	-4.031
23	6	17	24	6	18	114455.520	0.247	0.10	1.7	-406.043	-4.746
23	7	17	24	7	18	113987.230	-0.126	0.10	-0.8	-332.940	-3.040
23	7	16	24	7	17	114005.770	0.319	0.15	1.4	-336.092	-3.114
23	8	16	24	8	17	113806.090	-0.100	0.20	-0.3	-284.585	-2.124
23	8	15	24	8	16	113807.090	-0.077	0.20	-0.3	-284.786	-2.128
23	9	15	24	9	16	113698.450	0.040	0.10	0.3	-235.128	-1.512
23	9	14	24	9	15	113698.450	0.002	0.10	0.0	-235.137	-1.513
23	10	14	24	10	15	113639.210	-0.012	0.10	-0.1	-183.807	-1.308
23	10	13	24	10	14	113639.210	-0.013	0.10	-0.1	-183.807	-1.308
23	11	13	24	11	14	113612.200	-0.231	0.10	-1.5	-129.810	-1.623
23	11	12	24	11	13	113612.200	-0.231	0.10	-1.5	-129.810	-1.623
23	12	12	24	12	13	113608.320	-0.214	0.10	-1.4	-72.724	-2.594
23	12	11	24	12	12	113608.320	-0.214	0.10	-1.4	-72.724	-2.594
23	13	11	24	13	12	113621.550	-0.104	0.10	-0.7	-12.371	-4.374
23	13	10	24	13	11	113621.550	-0.104	0.10	-0.7	-12.371	-4.374
23	15	9	24	15	10	113684.930	0.161	0.10	1.1	118.224	-11.061
23	15	8	24	15	9	113684.930	0.161	0.10	1.1	118.224	-11.061
23	16	8	24	16	9	113730.280	0.051	0.10	0.4	188.323	-16.358
23	16	7	24	16	8	113730.280	0.051	0.10	0.4	188.323	-16.358
24	1	23	24	2	22	56522.560	-0.396	0.15	-1.8	-561.683	-7.682
24	2	23	24	3	22	57872.840	-0.072	0.10	-0.5	-436.879	-5.382

24	2	22	24	3	21	43202.260	-0.397	0.15	-1.8	-852.679	-15.260
24	3	22	24	4	21	52026.680	-0.256	0.10	-1.7	-356.321	-5.873
24	3	21	24	4	20	30793.200	-0.142	0.10	-1.0	-389.982	-7.760
24	4	21	24	5	20	51680.620	0.045	0.10	0.3	-61.000	-1.491
24	4	20	24	5	19	36225.700	0.229	0.10	1.5	500.860	8.987
24	5	19	24	6	18	54111.680	-0.104	0.10	-0.7	591.317	10.631
24	6	19	24	7	18	69501.930	-0.226	0.10	-1.5	275.833	3.972
24	6	18	24	7	17	68952.410	0.357	0.15	1.6	344.858	5.400
24	7	18	24	8	17	81088.700	-0.048	0.10	-0.3	228.981	2.773
24	0	24	25	0	25	109837.430	-0.261	0.20	-0.9	-173.376	-1.030
24	1	24	25	1	25	109836.730	-0.196	0.20	-0.6	-173.450	-1.031
24	1	23	25	2	24	112833.110	0.228	0.10	1.6	-204.628	-0.883
24	2	23	25	1	24	112685.800	-0.038	0.10	-0.3	-222.166	-1.206
24	2	22	25	3	23	117016.720	0.126	0.10	0.9	-139.812	0.384
24	2	22	25	2	23	115980.280	0.396	0.15	1.8	-252.759	-1.851
24	3	22	25	2	23	114542.320	0.310	0.10	2.1	-387.490	-4.327
24	3	22	25	3	23	115578.360	-0.359	0.15	-1.6	-274.542	-2.092
24	3	21	25	3	22	119849.750	0.417	0.15	1.9	-353.308	-4.746
24	6	18	25	6	19	119363.360	0.293	0.10	2.0	-483.532	-6.449
24	7	18	25	7	19	118776.800	-0.017	0.20	-0.1	-391.767	-4.096
24	7	17	25	7	18	118806.870	0.007	0.15	0.0	-397.382	-4.236
24	9	16	25	9	17	118446.150	0.138	0.10	0.9	-286.146	-2.075
24	9	15	25	9	16	118446.150	0.062	0.10	0.4	-286.165	-2.075
24	11	14	25	11	15	118340.940	-0.163	0.20	-0.5	-174.108	-1.736
24	11	13	25	11	14	118340.940	-0.163	0.20	-0.5	-174.108	-1.736
24	13	12	25	13	13	118342.340	-0.149	0.20	-0.5	-50.252	-4.098
24	13	11	25	13	12	118342.340	-0.149	0.20	-0.5	-50.252	-4.098
24	15	10	25	15	11	118403.370	-0.050	0.10	-0.4	86.972	-10.496
24	15	9	25	15	10	118403.370	-0.050	0.10	-0.4	86.972	-10.496
25	2	24	25	3	23	60706.820	0.153	0.10	1.1	-496.867	-6.414
25	2	23	25	3	22	47072.030	-0.075	0.10	-0.5	-953.228	-18.155
25	3	22	25	4	21	32941.510	0.060	0.10	0.4	-605.502	-12.724
25	4	22	25	5	21	52781.650	-0.124	0.10	-0.8	-130.401	-2.920
25	4	21	25	5	20	35111.000	0.192	0.10	1.3	448.854	8.563
25	5	21	25	6	20	58657.700	-0.249	0.10	-1.7	202.956	3.199
25	7	19	25	8	18	80883.200	-0.047	0.10	-0.3	281.299	3.938
25	2	24	26	1	25	117024.420	-0.249	0.10	-1.8	-244.336	-1.391
25	3	23	26	2	24	119186.300	0.020	0.10	0.1	-394.061	-4.364
25	4	22	26	3	23	115791.550	-0.218	0.10	-1.6	-991.319	-17.585
26	1	25	26	2	24	62868.450	0.171	0.10	1.2	-646.591	-9.388
26	2	25	26	3	24	63568.820	-0.314	0.15	-1.4	-559.440	-7.532
26	2	24	26	3	23	50921.880	-0.048	0.10	-0.3	-1038.432	-20.946
26	3	23	26	4	22	35612.270	-0.284	0.10	-1.9	-848.380	-18.924
26	4	23	26	5	22	54083.570	-0.294	0.10	-2.0	-216.011	-4.869
26	4	22	26	5	21	34387.040	-0.098	0.10	-0.7	341.765	6.769
26	5	22	26	6	21	58829.300	-0.015	0.30	-0.0	184.133	3.032
26	5	21	26	6	20	50877.240	0.107	0.10	0.7	871.310	18.569
26	6	21	26	7	20	68994.050	0.082	0.10	0.6	358.002	6.359
26	6	20	26	7	19	67708.680	0.322	0.15	1.4	538.156	10.602
26	7	20	26	8	19	80652.770	-0.136	0.10	-0.9	337.656	5.380
26	7	20	26	8	19	80652.770	-0.136	0.15	-0.6	337.656	5.380
26	7	19	26	8	18	80540.120	0.398	0.15	1.8	358.090	5.884
26	2	25	27	1	26	121354.550	0.178	0.10	1.4	-268.768	-1.617
27	2	25	27	3	24	54697.850	0.044	0.10	0.3	-1109.981	-23.595
27	3	25	27	4	24	59276.570	0.211	0.10	1.4	-629.748	-12.348
27	4	24	27	5	23	55586.600	0.080	0.10	0.5	-317.889	-7.411
27	4	23	27	5	22	34138.030	-0.191	0.10	-1.3	173.326	3.188
27	5	23	27	6	22	59132.040	-0.012	0.10	-0.1	148.201	2.423
27	5	22	27	6	21	49023.020	0.078	0.10	0.5	1004.574	23.068
27	6	22	27	7	21	68752.230	-0.167	0.10	-1.1	394.478	7.663
27	6	21	27	7	20	66861.840	0.136	0.10	0.9	671.577	14.609
27	7	21	27	8	20	80397.950	-0.096	0.10	-0.7	397.933	7.123
28	2	27	28	3	26	69345.370	-0.224	0.10	-1.7	-692.606	-10.014
28	2	26	28	3	25	58368.850	0.280	0.10	1.9	-1171.769	-26.124
28	3	26	28	4	25	61908.620	0.282	0.10	1.9	-731.391	-15.110
28	3	25	28	4	24	42265.640	-0.151	0.10	-1.1	-1368.777	-34.402
28	4	25	28	5	24	57284.710	0.019	0.10	0.1	-435.520	-10.610
28	4	24	28	5	23	34426.230	-0.029	0.10	-0.2	-60.403	-2.595
28	5	24	28	6	23	59586.190	0.007	0.10	0.0	92.256	1.217
28	5	23	28	6	22	47113.190	-0.137	0.10	-0.9	1109.382	27.295

28	6	22	28	7	21	65827.410	0.067	0.10	0.5	836.102	19.903
29	1	28	29	2	27	72000.130	-0.154	0.10	-1.2	-808.559	-12.543
29	2	27	29	3	26	61922.570	-0.060	0.10	-0.4	-1228.590	-28.600
29	3	27	29	4	26	64616.880	-0.320	0.15	-1.4	-836.746	-18.160
29	3	26	29	4	25	46066.320	-0.138	0.10	-1.0	-1617.407	-43.039
29	4	26	29	5	25	59169.430	0.387	0.15	1.7	-567.844	-14.509
29	4	25	29	5	24	35291.070	-0.282	0.10	-1.9	-360.797	-10.964
29	5	25	29	6	24	60209.500	0.408	0.15	1.8	13.778	-0.751
29	5	24	29	6	23	45253.540	0.011	0.10	0.1	1164.623	30.540
29	6	24	29	7	23	68367.050	-0.354	0.15	-1.6	443.329	10.036
29	6	23	29	7	22	64580.530	0.346	0.15	1.5	1034.504	26.736
29	7	22	29	8	21	79365.910	0.259	0.10	1.8	626.023	14.438
30	3	28	30	4	27	67386.190	-0.235	0.10	-1.6	-945.163	-21.486
30	4	27	30	5	26	61226.770	0.157	0.10	1.1	-713.345	-19.137
30	4	26	30	5	25	36751.340	0.020	0.10	0.1	-725.669	-22.226
30	5	26	30	6	25	61014.640	-0.048	0.10	-0.3	-89.187	-3.650
30	5	25	30	6	24	43560.280	0.072	0.10	0.5	1149.687	31.953
30	6	25	30	7	24	68260.550	0.314	0.15	1.4	448.015	10.806
30	6	24	30	7	23	63104.670	0.137	0.10	0.9	1265.254	35.257
30	7	24	30	8	23	79508.290	0.205	0.10	1.4	595.959	14.253
30	7	23	30	8	22	78813.750	-0.180	0.10	-1.2	752.420	19.102
31	1	30	31	2	29	77934.670	-0.385	0.15	-1.8	-942.669	-15.140
31	3	28	31	4	27	54100.980	-0.068	0.10	-0.5	-2030.031	-60.086
31	4	28	31	5	27	63441.810	0.191	0.10	1.3	-870.181	-24.500
31	4	27	31	5	26	38800.360	-0.212	0.10	-1.5	-1147.681	-36.525
31	5	26	31	6	25	42150.000	-0.157	0.10	-1.1	1046.843	30.613
31	6	25	31	7	24	61401.080	-0.057	0.10	-0.4	1520.145	45.401
31	7	24	31	8	23	78151.670	0.150	0.10	1.0	906.830	25.163
32	1	31	32	2	30	80873.060	0.026	0.15	0.1	-1017.758	-16.597
32	3	30	32	4	29	73049.650	-0.122	0.10	-0.8	-1169.784	-28.930
32	3	29	32	4	28	58150.260	0.414	0.15	1.9	-2183.257	-67.854
32	4	29	32	5	28	65796.550	0.186	0.10	1.2	-1036.338	-30.589
32	4	28	32	5	27	41408.370	0.001	0.10	0.0	-1613.050	-53.750
32	5	28	32	6	27	63208.840	0.077	0.10	0.5	-372.726	-12.887
32	5	27	32	6	26	41130.040	-0.017	0.20	-0.1	842.826	25.593
32	6	27	32	7	26	68317.910	-0.026	0.10	-0.2	395.884	10.461
32	6	26	32	7	25	59493.520	-0.231	0.10	-1.6	1782.628	56.776
32	7	26	32	8	25	78862.150	-0.150	0.10	-1.0	726.573	20.290
32	7	25	32	8	24	77354.930	-0.059	0.10	-0.4	1096.664	33.043
33	2	31	33	3	30	75113.890	0.013	0.10	0.1	-1483.186	-39.670
33	3	31	33	4	30	75921.020	-0.040	0.10	-0.3	-1285.854	-33.039
33	3	30	33	4	29	62127.920	0.239	0.10	1.7	-2303.651	-74.944
33	4	30	33	5	29	68272.120	-0.040	0.10	-0.3	-1209.804	-37.381
33	4	30	33	5	29	68272.120	-0.040	0.20	-0.1	-1209.804	-37.381
33	4	29	33	5	28	44518.330	0.141	0.10	1.0	-2101.586	-73.474
33	5	29	33	6	28	64603.600	0.230	0.10	1.5	-553.274	-19.503
33	5	28	33	6	27	40588.970	-0.066	0.10	-0.4	529.341	16.019
33	6	28	33	7	27	68524.390	0.165	0.10	1.1	330.037	8.812
33	6	27	33	7	26	57432.920	-0.192	0.10	-1.3	2027.736	68.573
33	7	27	33	8	26	78550.300	-0.178	0.10	-1.2	782.974	23.411
34	2	32	34	3	31	78221.840	-0.078	0.10	-0.6	-1564.534	-43.075
34	3	31	34	4	30	65994.610	0.366	0.15	1.6	-2398.856	-81.439
34	4	31	34	5	30	70850.410	0.212	0.10	1.4	-1388.727	-44.842
34	5	30	34	6	29	66193.120	0.201	0.10	1.4	-758.217	-27.589
34	5	29	34	6	28	40594.590	-0.103	0.10	-0.7	102.805	1.099
34	6	29	34	7	28	68874.700	-0.053	0.10	-0.4	232.125	5.778
34	7	28	34	8	27	78263.170	-0.213	0.10	-1.4	827.747	26.351
34	7	27	34	8	26	75254.690	-0.239	0.10	-1.6	1613.312	56.302
34	8	26	34	9	25	89851.550	0.012	0.10	0.1	1025.742	32.518
35	2	33	35	3	32	81279.310	0.080	0.10	0.6	-1654.637	-46.825
35	3	33	35	4	32	81700.550	-0.155	0.10	-1.1	-1526.544	-42.044
35	4	31	35	5	30	51906.230	-0.100	0.10	-0.7	-3048.461	-117.223
35	5	31	35	6	30	67969.570	-0.031	0.10	-0.2	-985.474	-37.206
35	5	30	35	6	29	41192.000	0.114	0.10	0.8	-435.820	-19.835
35	6	30	35	7	29	69386.370	-0.008	0.10	-0.1	98.751	1.041
35	7	29	35	8	28	78016.670	-0.076	0.10	-0.5	855.641	28.841
35	7	28	35	8	27	73900.810	-0.070	0.10	-0.5	1951.082	72.697
35	8	28	35	9	27	89851.550	-0.150	0.15	-0.7	1008.559	33.294
35	8	27	35	9	26	89321.130	0.116	0.10	0.9	1197.579	41.090
36	4	33	36	5	32	76241.650	0.124	0.10	0.8	-1757.047	-61.625

36	4	32	36	5	31	55981.140	0.031	0.10	0.2	-3458.693	-139.224
36	5	31	36	6	30	42402.630	-0.062	0.10	-0.4	-1080.249	-47.247
36	6	31	36	7	30	70072.960	0.022	0.10	0.1	-72.598	-5.711
36	6	30	36	7	29	51207.460	-0.214	0.10	-1.5	2332.618	92.306
36	8	29	36	9	28	89481.970	-0.220	0.10	-1.7	1113.266	39.340
36	8	28	36	9	27	88700.220	-0.310	0.15	-1.4	1403.301	51.865
37	2	35	37	3	34	87277.320	0.049	0.10	0.5	-1861.345	-55.462
37	4	34	37	5	33	79022.550	-0.031	0.10	-0.2	-1944.469	-70.881
37	4	33	37	5	32	60170.020	-0.197	0.10	-1.5	-3803.930	-160.015
37	5	32	37	6	31	44225.840	-0.279	0.15	-1.3	-1817.148	-81.267
37	6	31	37	7	30	49484.060	0.217	0.10	1.6	2182.981	90.268
37	7	31	37	8	30	77715.770	-0.252	0.10	-1.7	836.899	31.049
37	7	30	37	8	29	70509.340	-0.050	0.10	-0.4	2771.066	116.134
37	8	29	37	9	28	87972.150	0.217	0.10	1.7	1651.923	65.474
38	3	35	38	4	34	80173.440	-0.002	0.10	-0.0	-2709.645	-106.138
38	4	35	38	5	34	81842.150	0.086	0.10	0.6	-2133.434	-80.686
38	4	34	38	5	33	64380.970	-0.118	0.10	-1.0	-4078.298	-178.939
38	4	34	38	5	33	64380.970	-0.118	0.10	-1.0	-4078.298	-178.939
38	5	34	38	6	33	74295.290	0.250	0.10	1.7	-1772.002	-75.262
38	6	33	38	7	32	72007.880	0.089	0.10	0.6	-533.771	-26.395
38	6	32	38	7	31	48121.980	0.381	0.15	1.7	1866.937	80.087
38	7	32	38	8	31	77699.730	-0.140	0.10	-1.0	777.622	29.892
39	3	36	39	4	35	83440.090	-0.053	0.10	-0.5	-2803.360	-113.205
39	5	35	39	6	34	76681.770	0.136	0.10	1.0	-2058.137	-90.852
39	6	34	39	7	33	73264.640	0.242	0.15	1.1	-822.853	-40.790
39	6	34	39	7	33	73264.640	0.242	0.10	1.7	-822.853	-40.790
39	6	33	39	7	32	47215.470	0.251	0.10	1.8	1372.262	60.081
39	7	33	39	8	32	77798.690	0.092	0.10	0.6	676.816	26.555
39	8	32	39	9	31	88349.660	0.056	0.10	0.4	1400.431	59.121
40	6	35	40	7	34	74712.240	-0.204	0.10	-1.5	-1148.421	-58.098
40	6	34	40	7	33	46838.890	-0.191	0.10	-1.4	695.025	28.834
40	7	34	40	8	33	78030.170	0.007	0.10	0.1	528.935	20.493
40	8	33	40	9	32	87997.690	0.231	0.10	1.8	1470.444	65.347
41	7	35	41	8	34	78410.740	0.021	0.10	0.2	329.354	11.155
41	8	34	41	9	33	87679.850	0.331	0.15	1.6	1516.695	70.685
42	7	36	42	8	35	78953.870	-0.067	0.10	-0.5	74.661	-1.994
43	7	37	43	8	36	79670.300	-0.152	0.10	-1.4	-237.115	-19.446

rms deviation: 1.5231

Rotational constants (MHz) and kappa:

	7852.3358	2549.46137	2170.81547	-0.8667097
+-	0.0051	0.0015	0.0015	0.0000003

Inertial constants and defect (uA**2):

	64.360349	198.229744	232.806096	-29.7840
+-	0.000041	0.00012	0.00016	0.0001

Quartic distortion constants:

	7.40033	-51.5050	163.912	2.443708	22.0791
+-	0.0039	0.0099	0.15	0.00050	0.020

Sextic and higher distortion constants:

	-0.150355	2.1423	-12.290	24.20	-0.0623764
+-	0.0033	0.0060	0.031	1.2	0.00027

	-1.9455	0
+-	0.017	fixed

Significant Digits and Correlation Matrix:

8	0.210	0.069	0.133	0.135	0.759		
	9	0.800	0.881	-0.216	0.118		
		9	0.897	-0.223	0.022		
			6	-0.348	0.125		
				6	-0.407		
					6		
0.225	-0.091	0.131	-0.013	0.152	0.649	0.227	-0.123
0.323	0.017	0.802	-0.169	-0.102	0.115	0.287	0.013
-0.261	0.002	0.828	-0.139	-0.138	0.038	-0.225	0.011
-0.014	0.109	0.978	-0.285	-0.173	0.134	-0.023	0.113
0.077	-0.340	-0.347	0.878	0.615	-0.456	0.117	-0.361
0.149	-0.019	0.133	-0.442	-0.260	0.965	0.159	-0.046
7	-0.237	-0.034	0.072	0.029	0.115	0.966	-0.256
	6	0.115	-0.489	0.054	0.006	-0.377	0.970
		6	-0.292	-0.198	0.149	-0.044	0.124
			5	0.271	-0.512	0.155	-0.528
				5	-0.331	0.001	0.050
					4	0.124	-0.022
						6	-0.418
							5

References

- (1) Watson, J. K. G.: *Vibrational Spectra and Structure*; Elsevier: Amsterdam, 1977; Vol. 6.
- (2) Hamilton, W. C.: *Statistics in Physical Science*; The Ronald Press Company: New York, 1964.