**Ammonia Promoted Fragmentation of
2-Alkyl- and 2,4-Dialkyl-3-iodo-1-oxocyclohexan-2,4-carbolactones**

Mingshi Dai, Xuqing Zhang, Seock-Kyu Khim,* and Arthur G. Schultz

Department of Chemistry, Rensselaer Polytechnic Institute, Troy, New York 12180

Supporting Information

Table of Contents

General Procedure for Fragmentation of 1 with NH ₃	(S1)
Cyclization of 5f	(S5)
Hoffmann Rearrangement of 5g	(S5)
Cyclization of 16 in the Presence of TFA	(S6)
Figure 1. ORTEP drawing of 15	(S8)
Table 1. Crystal data and structure refinement for 15	(S9)
Figure 2. Energy-minimized structures of 14 and 15 .	(S10)
Figure 3. Energy-minimized structures of 18 and 19 .	(S11)
¹ H and ¹³ C NMR spectra of 5b , 14+15 , 18 , and 19	(S12)

General Procedure for Fragmentation of **1 with NH₃.** To a solution of **1a** (280 mg, 1.0 mmol) in dry THF (5 mL) was introduced NH₃ (ca. 3 mL by condensing with cold-finger condenser) at -78 °C. The resulting solution was stirred for 0.5 h and slowly allowed to warm to room temperature under a stream of nitrogen until NH₃ and THF were completely evaporated. ¹H NMR spectrum analysis of the crude mixture showed the ratio of **5a** and **6a** to be 76:24. The crude

residue was partitioned between water and CH₂Cl₂. The organic layers were separated, dried over anhydrous Na₂SO₄, and concentrated under reduced pressure which was purified by flash column chromatography (hexanes/EtOAc, 4:1 to 1:1) to give **5a** (99 mg, 59%) and **6a** (30 mg, 18%).

(5R)-[3-Methyl-5-(2'-aminocarbonyl)ethyl]furan-2(5H)-one (5a): white solid; $[\alpha]_D^{25} -121.4$ (*c* 2.52, MeOH); ¹H NMR (500 MHz, CDCl₃) δ 7.05 (s, 1 H), 5.85 (br s, 1H), 5.69 (br s, 1H), 4.97 (m, 1H), 2.43-2.32 (m, 2H), 2.26-2.20 (m, 1H), 1.90 (d, *J* = 1.5 Hz, 3H), 1.82-1.74 (m, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 173.9, 164.4, 148.7, 130.1, 80.1, 30.4, 28.6, 10.6; IR 3422, 3207, 1748 1669 cm⁻¹; CIMS 170 (*M*⁺ + 1, 100). Anal. Calcd for C₈H₁₁NO₃: C, 56.80; H, 6.55; N, 8.28. Found: C, 56.72; H, 6.40; N, 8.17. **(2R,2E)-2-Methyl-3-[tetrahydro-5-oxofuranyl]-2-propenamide (6a):** white solid; $[\alpha]_D^{25} -72.6$ (*c* 1.15, MeOH); ¹H NMR (500 MHz, CD₃OD) δ 6.36 (d, *J* = 8.0 Hz, 1H), 5.26 (q, *J* = 7.6 Hz, 1H), 2.62-2.58 (m, 2H), 2.51-2.45 (m, 1H), 2.07-1.99 (m, 1H), 1.94 (s, 3H); ¹³C NMR (125 MHz, CD₃OD) δ 177.1, 173.0, 137.9, 131.4, 67.3, 32.0, 31.1, 12.9; IR 3689, 3373, 1734, 1668 cm⁻¹; CIMS 170 (*M*⁺ + 1, 100). Anal. Calcd for C₈H₁₁NO₃: C, 56.80; H, 6.55; N, 8.28. Found: C, 56.77; H, 6.49; N, 8.16.

(5R)-[3-(3'-Chloro)propyl-5-(2'-aminocarbonyl)ethyl]furan-2(5H)-one (5b): white solid; mp 101–102 °C; $[\alpha]_D^{26} -21.7$ (*c* 0.23, MeOH); ¹H NMR (500 MHz, CDCl₃) δ 7.10 (s, 1H), 5.69 (br d, *J* = 60.5 Hz, 2H), 5.03 (m, 1H), 3.55 (t, *J* = 6.4 Hz, 2H), 2.46 (t, *J* = 7.4 Hz, 2H), 2.43-2.33 (m, 2H), 2.28-2.22 (m, 1H), 2.07-2.00 (m, 2H), 1.85-1.77 (m, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 173.8, 173.4, 148.9, 133.0, 80.2, 43.9, 30.2, 29.9, 28.5, 22.6; IR 3386, 3180, 1738, 1653 cm⁻¹; CIMS 234 (*M*⁺ + 1, 32), 232 (*M*⁺ + 1, 100); HRMS calcd for C₁₀H₁₄³⁵ClNO₃ (*M*⁺ + 1) 232.0740, found 232.0744.

(5R)-[3-(3'-Benzyloxy)propyl-5-(2'-aminocarbonyl)ethyl]furan-2(5H)-one (5c): white solid; mp 75–77 °C; $[\alpha]_D^{25} -17.5$ (*c* 1.2, MeOH); ^1H NMR (500 MHz, CDCl_3) δ 7.27 (m, 2H), 7.24 (m, 2H), 7.20 (m, 1H), 6.89 (s, 1H), 6.04 (s, 1H), 5.88 (s, 1H), 4.86 (m, 1H), 4.40 (s, 2H), 3.41 (t, *J* = 5.4 Hz, 2H), 2.28 (t, *J* = 7.1 Hz, 2H), 2.23 (m, 2H), 2.09 (m, 1H), 1.76 (t, *J* = 6.9 Hz, 2H), 1.67 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 174.2, 173.6, 148.1, 138.1, 133.8, 128.2, 127.8, 127.5, 127.4, 80.1, 72.7, 68.9, 30.0, 27.2, 21.9; IR 3348, 1754, 1666 cm^{-1} ; CIMS 304 ($\text{M}^+ + 1$, 100). Anal. Calcd for $\text{C}_{17}\text{H}_{21}\text{NO}_4$: C, 67.33; H, 6.93. Found: C, 67.05; H, 6.93.

(5R)-[3-[(2'-Trimethylsilyl)ethyloxy]methyl-5-(2'-aminocarbonyl)ethyl]furan-2(5H)-one (5d): white solid; mp 83–85 °C; $[\alpha]_D^{25} -15.3$ (*c* 5.10, MeOH); ^1H NMR (500 MHz, CDCl_3) δ 7.28 (s, 1H), 6.35 (s, 1H), 6.16 (s, 1H), 5.02 (s, 1H), 4.11 (s, 2H), 3.54 (t, *J* = 7.8 Hz, 2H), 2.34 (d, *J* = 4.9 Hz, 2H), 2.18 (d, *J* = 7.8 Hz, 1H), 1.75 (m, 1H), 0.91 (t, *J* = 7.8 Hz, 2H), -0.04 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) δ 174.3, 172.1, 149.8, 131.8, 80.9, 68.5, 63.5, 30.3, 28.4, 17.8, -1.7; IR 3350, 1756, 1668 cm^{-1} ; CIMS 287 ($\text{M}^+ + 1$, 100). Anal. Calcd for $\text{C}_{13}\text{H}_{23}\text{NO}_4\text{Si}$: C, 54.74; H, 8.07. Found: C, 54.41; H, 8.11.

(5R)-[3-Methyl-5-methyl-5-(2'-aminocarbonyl)ethyl]furan-2(5H)-one (5e): white solid; mp 86–88 °C; $[\alpha]_D^{25} -37.5$ (*c* 0.8, CHCl_3); ^1H NMR (500 MHz, CDCl_3) δ 6.94 (s, 1H), 5.93 (br s, 1H), 5.65 (br s, 1H), 2.23–2.01 (m, 4H), 1.86 (s, 3H), 1.43 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 174.6, 174.1, 153.1, 129.3, 86.1, 33.2, 29.6, 24.6, 10.6; IR 1746, 1667 cm^{-1} ; CIMS 184 ($\text{M}^+ + 1$, 100). Anal. Calcd for $\text{C}_9\text{H}_{13}\text{NO}_3$: C, 59.00; H, 7.15; N, 7.65. Found: C, 59.02; H, 7.07; N, 7.65.

(2R,3S,4R)-2-Aminocarbonyl-2,4-dimethyl-3,4-epoxycyclohexan-1-one (7e): colorless oil; $[\alpha]_D^{25} -190.9$ (*c* 1.1, CHCl_3); ^1H NMR (500 MHz, CDCl_3) δ 6.93 (br s, 1H), 5.61 (br s, 1H), 3.34 (s, 1H), 2.61–2.10 (m, 4H), 1.50 (s, 3H), 1.43 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 208.2,

171.9, 62.6, 58.0, 54.8, 34.8, 26.7, 22.1, 20.3; IR 1711, 1660 cm^{-1} ; CIMS 184 ($\text{M}^+ + 1$, 100).

Anal. Calcd for $\text{C}_9\text{H}_{13}\text{NO}_3$: C, 59.00; H, 7.15; N, 7.65. Found: C, 59.03; H, 7.18; N, 7.64.

(5R)-[3-Ethyl-5-methyl-5-(2'-aminocarbonyl)ethyl]furan-2(5H)-one (5f): white solid; mp 75–78 °C; $[\alpha]_D^{25} -21.0$ (c 1.0, CHCl_3); ^1H NMR (500 MHz, CDCl_3) δ 6.89 (s, 1H), 6.15 (br s, 1H), 5.87 (br s, 1H), 2.20 (m, 3H), 2.04 (m, 3H), 1.40 (s, 3H), 1.09 (t, $J = 7.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 174.8, 173.6, 151.5, 135.3, 86.2, 33.2, 29.5, 24.6, 18.6, 11.8; IR 3350, 1746, 1667 cm^{-1} ; CIMS 198 ($\text{M}^+ + 1$, 100). Anal. Calcd for $\text{C}_{10}\text{H}_{15}\text{NO}_3$: C, 60.90; H, 7.67; N, 7.10. Found: C, 61.07; H, 7.64; N, 7.19.

(2R,3S,4R)-2-Aminocarbonyl-2-ethyl-3,4-epoxy-4-methylcyclohexan-1-one (7f): white solid; $[\alpha]_D^{25} -165.5$ (c 0.9, CHCl_3); ^1H NMR (500 MHz, CDCl_3) δ 6.83 (br s, 1H), 6.05 (br s, 1H), 3.36 (s, 1H), 2.54 (m, 1H), 2.29–2.03 (m, 4H), 1.80 (m, 1H), 1.51 (s, 3H), 0.86 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 209.4, 171.2, 62.1, 59.6, 58.1, 35.6, 29.6, 26.9, 22.1, 9.6; IR 3346, 3349, 1682 cm^{-1} ; CIMS 198 ($\text{M}^+ + 1$, 100). Anal. Calcd for $\text{C}_{10}\text{H}_{15}\text{NO}_3$: C, 60.90; H, 7.67; N, 7.10. Found: C, 60.99; H, 7.51; N, 7.12.

(5R)-[3-Ethyl-5-benzyl-5-(2'-aminocarbonyl)ethyl]furan-2(5H)-one (5g): white solid; mp 112–115 °C; $[\alpha]_D^{25} +1.70$ (c 1.2, CHCl_3); ^1H NMR (500 MHz, CDCl_3) δ 7.22–7.03 (m, 5H), 6.80 (s, 1H), 6.00 (br s, 1H), 5.83 (br s, 1H), 3.00 (AB q, $J = 13.7$ Hz, 2H), 2.23–1.96 (m, 6H), 0.89 (t, $J = 7.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 174.7, 173.3, 149.9, 136.5, 134.5, 130.4, 128.3, 127.1, 88.1, 44.5, 31.5, 29.1, 18.4, 11.8; IR 3346, 1747, 1669 cm^{-1} ; CIMS 274 ($\text{M}^+ + 1$, 100). Anal. Calcd for $\text{C}_{16}\text{H}_{19}\text{NO}_3$: C, 70.31; H, 7.01; N, 5.12. Found: C, 70.48; H, 7.03; N, 5.07.

(2R,3S,4R)-2-Aminocarbonyl-2-ethyl-4-benzyl-3,4-epoxycyclohexan-1-one (7g): white solid; mp 109–111 °C; $[\alpha]_D^{25} -46.4$ (c 1.2, CHCl_3); ^1H NMR (500 MHz, CDCl_3) δ 7.32–7.23 (m, 5H),

6.87 (br s, 1H), 5.89 (br s, 1H), 3.51 (s, 1H), 3.00 (AB q, $J = 14.2$ Hz, 2H), 2.48 (m, 1H), 2.20 (m, 2H), 2.05 (m, 2H), 1.75 (m, 2H), 0.80 (t, $J = 7.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 209.3, 171.1, 136.1, 129.8, 128.8, 127.3, 61.0, 60.9, 59.5, 42.6, 35.6, 29.5, 24.4, 9.4; IR 3345, 1682, 1462 cm^{-1} ; CIMS 274 ($\text{M}^+ + 1$, 100). Anal. Calcd for $\text{C}_{16}\text{H}_{19}\text{NO}_3$: C, 70.31; H, 7.01; N, 5.12. Found: C, 70.19; H, 6.96; N, 5.08.

Cyclization of 5f. To a solution of butenolide amide **5f** (200 mg, 1.01 mmol) and $\text{Si}(\text{OEt})_4$ (0.49 mL, 2.20 mmol) in CH_2Cl_2 (2 mL) was added CsF (334 mg, 2.20 mmol) at room temperature. The reaction mixture was stirred overnight and diluted with water. The reaction mixture was then extracted with 10% MeOH in CH_2Cl_2 . The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. Flash column chromatography (EtOAc) of the crude residue gave an inseparable mixture of **14** and **15** in a ratio of 1:1 (152 mg, 76%) as a white solid. **(3R,3aR,7aR)-3-Ethyltertahydro-7a-methyl-furo[3,2-*b*]pyridine-2,5(3H,4H)-dione (14)**; white solid; ^1H NMR (500 MHz, CDCl_3) δ 7.53 (br s, 1H), 3.60 (dd, $J = 6.8, 3.4$ Hz, 1H), 2.60 (m, 1H), 2.47-1.70 (m, 6H), 1.57 (s, 3H), 1.09 (t, $J = 7.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 175.7, 172.1, 79.4, 61.2, 51.6, 30.9, 27.9, 26.3, 23.1, 11.4; IR 1769, 1662 cm^{-1} ; CIMS 198 ($\text{M}^+ + 1$, 100). **(3S,3aR,7aR)-3-Ethyltertahydro-7a-methyl-furo[3,2-*b*]pyridine-2,5(3H,4H)-dione (15)**. The same reaction described above was performed for 72 h. Flash column chromatography (EtOAc) of the crude residue provided **15** (122 mg, 62%) as a white solid. The compound was crystallized from hexanes/EtOAc (3:1). $[\alpha]_{\text{D}}^{25} -116.7$ (c 1.2, CHCl_3); ^1H NMR (500 MHz, CDCl_3) δ 6.94 (br s, 1H), 3.93 (d, $J = 6.1$ Hz, 1H), 2.76 (m, 1H), 2.48-1.52 (m, 6H), 1.50 (s, 3H), 1.06 (t, $J = 7.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 176.1, 172.0, 79.4, 58.7, 47.3, 31.1, 26.4, 25.5, 17.9, 12.4; IR 1769, 1662 cm^{-1} ; CIMS 198 ($\text{M}^+ + 1$, 100). Anal. Calcd for $\text{C}_{10}\text{H}_{15}\text{NO}_3$: C, 60.90; H, 7.67; N, 7.10. Found: C, 60.68; H, 7.63; N, 6.93.

Hoffmann Rearrangement of 5f. To a solution of butenolide amide **5f** (160 mg, 0.80 mmol) in pyridine (8 mL) was added Pb(OAc)₄ (1.06 g, 2.40 mmol) at room temperature. The reaction mixture was stirred at 60 °C for 2 h. The resulting mixture was then treated with anhydrous *t*-BuOH (600 µL) via syringe and stirred at 60 °C overnight. The reaction mixture was cooled to room temperature and diluted with diethyl ether and washed with water and brine. The combined organic layers were dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. Flash column chromatography (hexanes/EtOAc, 2:1) of the crude residue gave **16** (192 mg, 88%) as a pale yellow oil. **(5R)-[3-Ethyl-5-methyl-5-[[2'-(*t*-butoxy)carbonylamino]ethyl]furan-2(5H)-one (16):** $[\alpha]_D^{25} -25.7$ (c 1.4, CHCl₃); ¹H NMR (500 MHz, CDCl₃) δ 6.91 (s, 1 H), 4.76 (br s, 1 H), 3.04 (m, 2 H), 2.22 (AB q, *J* = 7.4 Hz, 2 H), 1.90 (m, 2 H), 1.38 (s, 3 H), 1.36 (s, 6 H), 1.09 (t, *J* = 7.4 Hz, 3 H); ¹³C NMR (125 MHz, CDCl₃) δ 173.0, 155.9, 151.3, 135.1, 85.7, 79.3, 38.3, 36.0, 28.4, 24.4, 18.5, 11.8; IR 3855, 1756, 1704 cm⁻¹; CIMS 270 (M⁺ + 1, 2), 214 (100). Anal. Calcd for C₁₄H₂₃NO₄: C, 62.43; H, 8.61; N, 5.20. Found: C, 62.22; H, 8.61; N, 5.14.

Cyclization of 16 in the Presence of TFA. To a solution of **16** (168 mg, 0.62 mmol) in CH₂Cl₂ (10 mL) was added TFA (0.5 mL) at room temperature. The reaction mixture was stirred overnight and neutralized with saturated aqueous NaHCO₃ solution and extracted with CH₂Cl₂. The combined organic layers were dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. Flash column chromatography (MeOH/EtOAc, 1:10) of the crude residue gave a mixture of **18** and **19** (63 mg, 95%) in a ratio of 1:7 as a yellow oil. **(3R,3aR,6aR)-3-Ethylhexahydro-6a-methyl-2H-furo[3,2-*b*]pyrrol-2-one (18):** yellow oil; $[\alpha]_D^{25} +37.5$ (c 0.4, CHCl₃); ¹H NMR (500 MHz, CDCl₃) δ 3.54 (d, *J* = 6.6 Hz, 1H), 3.00 (m, 2H), 2.54 (m, 1H), 2.19 (m, 1H), 1.85 (m, 3H), 1.60 (m, 1H), 1.50 (s, 3H), 1.03 (t, *J* = 7.3 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 178.0, 92.0, 65.0, 46.3, 45.7, 40.0, 23.1, 18.7, 12.6; IR 3853, 1759 cm⁻¹; CIMS 170 (M⁺

+ 1, 100); HRMS calcd for C₉H₁₅NO₂ (M⁺ + 1) 170.1182, found 170.1179. . **(3*S*,3*aR*,6*aR*)-3-Ethylhexahydro-6*a*-methyl-2*H*-furo[3,2-*b*]pyrrol-2-one (19)**: yellow oil; [α]_D²⁵ +39.1 (*c* 1.1, CHCl₃); ¹H NMR (500 MHz, CDCl₃) δ 3.34 (d, *J* = 2.5 Hz, 1H), 3.00 (m, 2H), 2.40-1.62 (m, 6H), 1.56 (s, 3H), 1.06 (t, *J* = 7.5 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 178.8, 92.5, 68.6, 51.4, 45.5, 40.8, 25.7, 24.6, 11.9; IR 1755 cm⁻¹; CIMS 170 (M⁺ + 1, 100); HRMS calcd for C₉H₁₅NO₂ (M⁺ + 1) 170.1182, found 170.1178.

Figure 1. ORTEP drawing of **15**.

Table 1. Crystal data and structure refinement for 15.

Identification code	15 (rpi21m)		
Empirical formula	C10 H15 N O3		
Formula weight	197.23		
Temperature	198(2) K		
Wavelength	0.71073 Å		
Crystal system	Orthorhombic		
Space group	C222(1)		
Unit cell dimensions	a = 10.6675(4) Å	α= 90°.	
	b = 11.0586(5) Å	β= 90°.	
	c = 16.5092(7) Å	γ= 90°.	
Volume	1947.55(14) Å ³		
Z	8		
Density (calculated)	1.345 Mg/m ³		
Absorption coefficient	0.099 mm ⁻¹		
F(000)	848		
Crystal size	0.56 x 0.40 x 0.39 mm ³		
Theta range for data collection	2.47 to 28.27°.		
Index ranges	-14<= <i>h</i> <=10, -14<= <i>k</i> <=14, -22<= <i>l</i> <=21		
Reflections collected	7904		
Independent reflections	2420 [R(int) = 0.0189]		
Completeness to theta = 28.27°	99.9 %		
Absorption correction	SADABS		
Max. and min. transmission	0.9623 and 0.9465		
Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	2420 / 0 / 147		
Goodness-of-fit on F ²	1.034		
Final R indices [I>2σ(I)]	R1 = 0.0303, wR2 = 0.0810		
R indices (all data)	R1 = 0.0312, wR2 = 0.0822		
Absolute structure parameter	0.3(7)		
Largest diff. peak and hole	0.269 and -0.151 e.Å ⁻³		

14 (E = 17.0689 kcal/mol)

15 (E = 16.7884 kcal/mol)

Figure 2. Energy-minimized structures of **14** and **15**.

18 ($E = 18.5587$ kcal/mol)

19 ($E = 17.6032$ kcal/mol)

Figure 3. Energy-minimized structures of **18** and **19**.

SPECTRAL LINES FOR γ b= 9.2
 τ 1= 13267.6, τ 2= 9679.0

INDEX	FREQ. (Hz)	PPM	HEIGHT
1	21848.9	173.82	17.9
2	21800.8	173.43	11.8
3	19714.8	148.98	48.7
4	16719.8	133.01	31.1
5	10082.7	80.21	64.9
6	9711.6	77.26	129.7
7	9679.6	77.00	134.3
8	9647.5	76.75	133.1
9	5522.9	43.94	47.6
10	3736.0	30.20	47.5
11	3754.3	29.87	56.2
12	3578.6	28.47	59.2
13	2843.3	22.62	59.4

SPECTRAL LINES FOR THE 5.6

FT= 10262.4, $\tau^*_{p_0}$ = 9707.9

INDEX	FREQ. (Hz)	PPM	HEIGHT
1	22144.3	176.17	6.9
2	22083.3	175.68	10.3
3	21642.3	172.17	6.0
4	21631.6	172.09	8.3
5	10008.6	79.62	19.5
6	9981.1	79.40	12.6
7	9738.5	77.47	21.4
8	9706.5	77.22	21.5
9	9674.4	76.96	20.4
10	7686.5	61.23	17.9
11	7391.4	58.58	9.4
12	6488.3	51.62	17.5
13	5941.3	47.26	16.9
14	3923.2	31.21	15.5
15	3891.2	30.96	13.5
16	3512.0	27.94	9.9
17	3314.4	26.37	9.1
18	3302.9	26.38	16.8
19	3189.3	25.37	17.8
20	3303.1	23.20	15.3
21	2248.5	17.89	12.1
22	1552.7	12.35	12.7
23	1438.3	11.44	13.2

SPECTRAL LINES FOR TH= 5.3
 $\tau(T) = 10270.2$, $\tau(T)_{\text{ref}} = 9707.9$

INDEX	FREQ. (Mc)	PPM	HEIGHT
1	22375.4	178.00	11.2
2	11563.5	91.99	18.6
3	9740.0	72.46	51.4
4	9708.7	72.64	51.2
5	9676.7	76.38	52.3
6	8172.1	65.01	32.8
7	5534.5	46.75	21.8
8	5749.7	45.74	14.6
9	5015.7	39.90	12.5
10	2857.0	23.05	16.4
11	2851.2	23.02	13.3
12	2149.9	16.69	13.2
13	1589.3	12.64	13.0

SPECTRAL LINES FOR T1= 10.6
 $r(1) = 10284.0$, $r(0) = 9707.9$

INDEX	FREQ. (Hz)	PPM	HEIGHT
1	22479.2	178.83	11.7
2	11821.4	92.45	20.7
3	9740.0	~~77.40~~	21.8
4	9707.9	~~76.83~~	23.1
5	9675.9	~~76.26~~	22.3
6	8827.6	68.64	51.6
7	6463.1	51.42	48.1
8	5719.9	45.50	49.5
9	5127.9	40.79	48.2
10	3227.3	25.67	57.5
11	3093.8	24.62	44.8
12	1493.9	11.88	39.9